



Full wwPDB EM Validation Report ⓘ

Oct 20, 2024 – 08:54 PM EDT

PDB ID : 8SES
EMDB ID : EMD-40427
Title : Cryo-EM Structure of RyR1 + Adenine
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.98 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

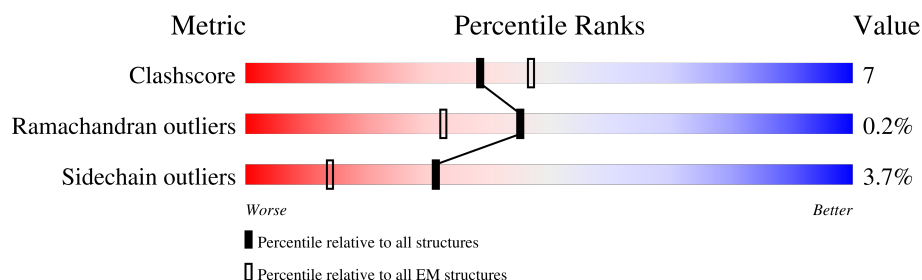
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.98 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	
1	B	5037	
1	C	5037	
1	D	5037	
2	E	350	
2	F	350	
2	G	350	
2	H	350	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 142940 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		
1	B	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		
1	C	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		
1	D	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

Continued on next page...

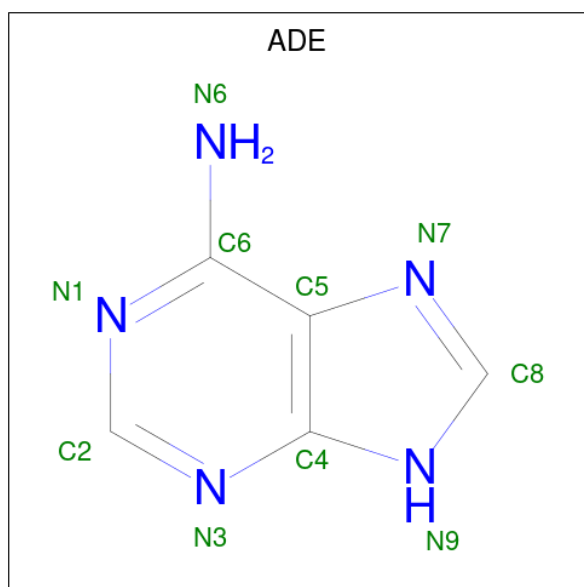
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0

- Molecule 4 is ADENINE (three-letter code: ADE) (formula: C₅H₅N₅) (labeled as "Ligand of Interest" by depositor).

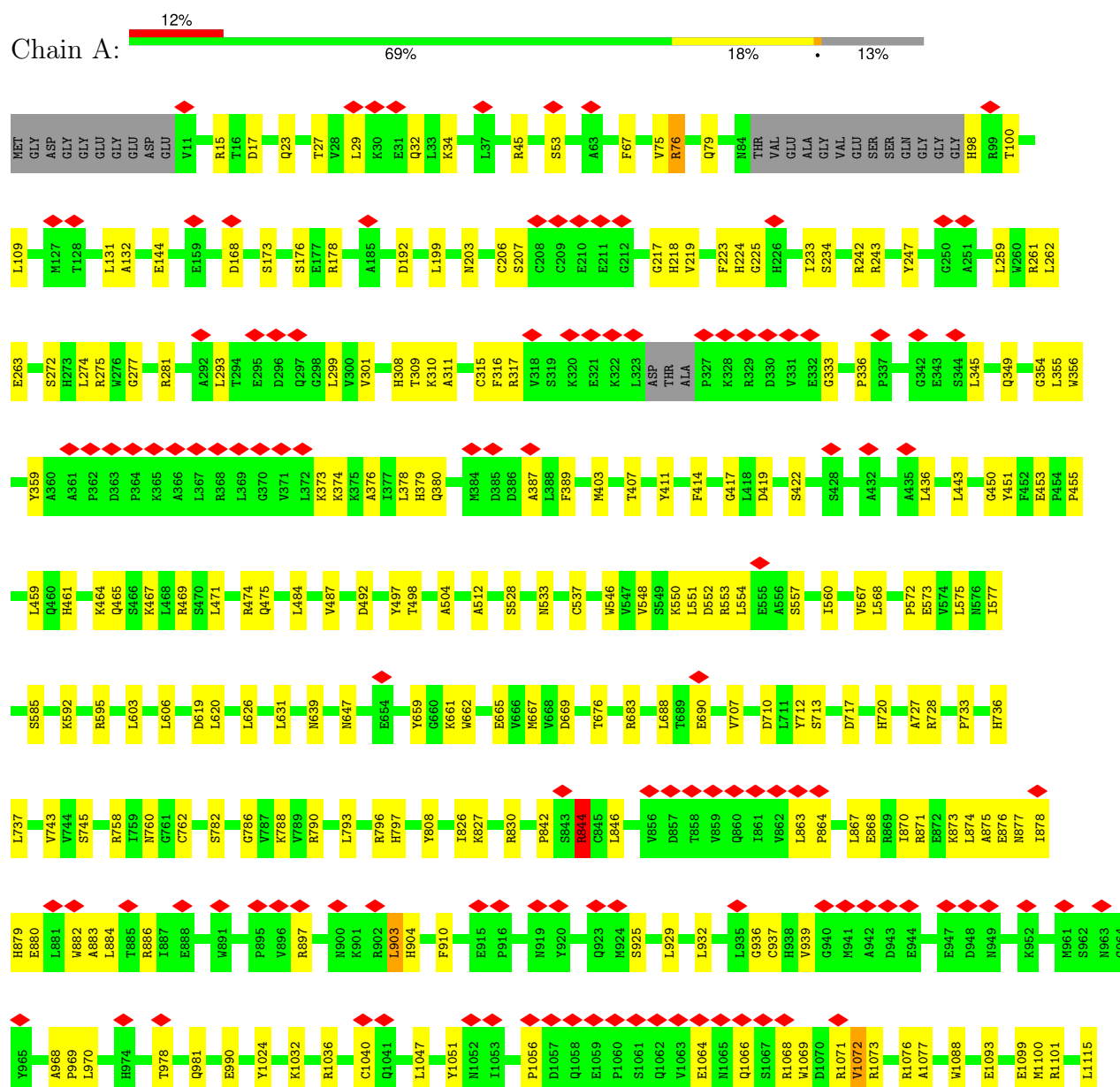


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total 10	C 5	N 5	0
4	B	1	Total 10	C 5	N 5	0
4	C	1	Total 10	C 5	N 5	0
4	D	1	Total 10	C 5	N 5	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Ryanodine receptor 1



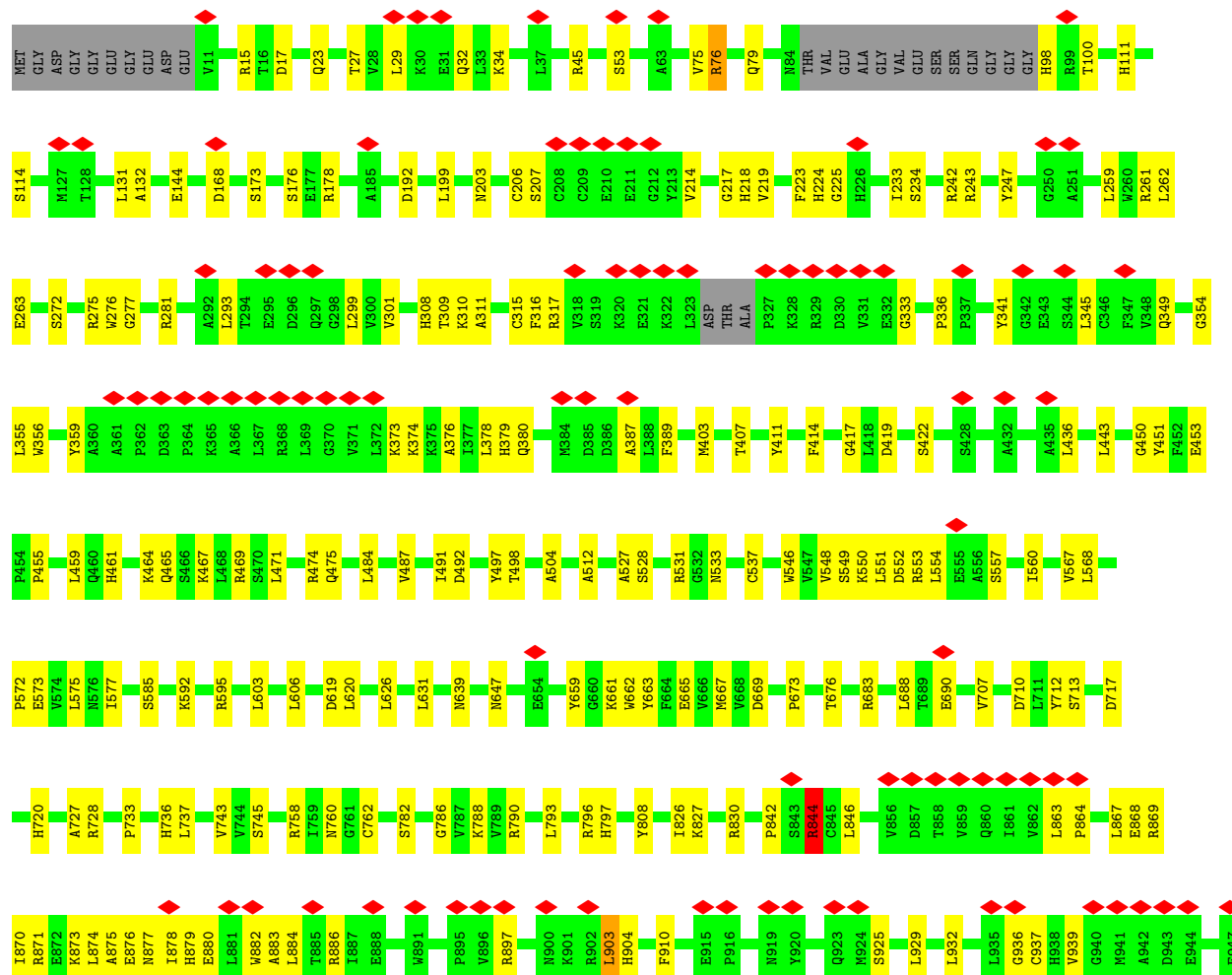


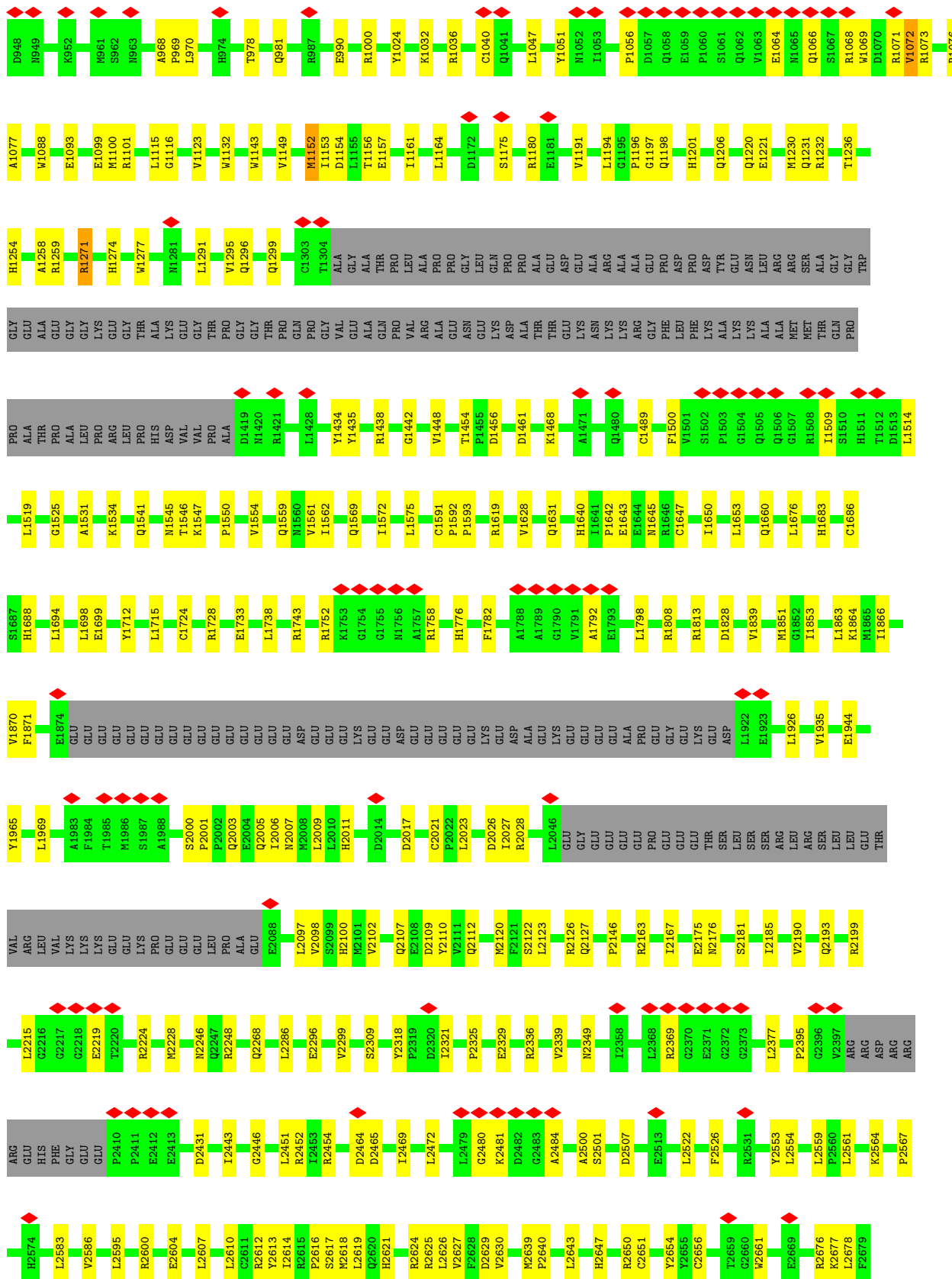
E3825	L3826	G3827	F3828	F3829	Q3830	L3835	L3842	R3849	Q3850	G3857	M3858	V3859	N3860	E3861	D3862	G3863	T3864	V3865	I3866	N3867	R3868	Q3869	N3870	G3871	E3872	M3875	D3878	R3886	F3887	L3888	Q3889	S3784	C3785	C3786	K3787	G3788	T3789	L3800	L3805	N3809	E3810	V3812	K3823	K3824	E3944	E3945	Q3946	G3947	K3948	R3949	P4106								
E3718	D3719		I3728	M3729	L3735	E3736	GLU	GLY	GLY	ASN	GLY	GLU	ALA	GLU	GLU	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	S3768	R3769	L3770	H3771	T3772	R3773	V3779	L3780	I3783	S3784	C3785	C3786	K3787	G3788	T3789	L3800	L3805	N3809	E3810	V3812	K3823	K3824	E3944	E3945	Q3946	G3947	K3948	R3949	P4106							
L3603	Y3604	H3605	L3606	T3609	E3610	H3611	P3612	Y3613	K3614	S3615	K3616	K3617	A3618	V3619	W3620	H3621	K3622	L3623	L3624	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	M3638	L3641	L3644	E3670	I3674	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	V3690	E3691	E3692	K3693	K3694	P3695								
ASP	GLN	GLU	ARG	THR	LYS	LYS	R3498	R3499	G3500	D3501	Q3506	K3515	K3516	P3519	M3524	L3535	T3538	A3541	L3542	K3543	N3555	N3556	L3557	H3558	L3559	Q3560	G3561	K3562	V3563	E3564	G3565	S3566	L3569	M3573	Y3576	L3579	P3580	G3581	R3582	E3583	E3584	D3585	A3586	D3587	R3595														
L3392	L3393	V3394	R3395	R3403	Y3406	R3419	R3420	W3423	L3424	P3427	L3434	M3437	I3441	N3450	R3453	E3454	N3457	N3465	N3466	M3467	S3468	F3469	L3470	T3471	A3472	D3473	S3474	K3475	S3476	K3477	M3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	SER																		
P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	A3304	P3208	N3211	N3214	A3215	C3216	S3217	V3218	T3221	K3222	S3223	P3224	R3225	T3229	L3230	A3135	L3136	L3140	L3143	F3144	Q3145	H3146	I3147	A3148	Q3149	F3152	G3153	D3154	I3157	L3158	D3159	V3160	P3161	Q3162	S3171	S3174														
R3187	F3188	G3191	L3194	A3195	R3196	M3201	P3202	V3203	A3204	P3208	N3211	N3214	A3215	C3216	S3217	V3218	T3221	K3222	S3223	P3224	R3225	T3229	L3230	A3135	L3136	L3140	L3143	F3144	Q3145	H3146	I3147	A3148	Q3149	F3152	G3153	D3154	I3157	L3158	D3159	V3160	P3161	Q3162	S3171	S3174															
P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	A3304	P3208	N3211	N3214	A3215	C3216	S3217	V3218	T3221	K3222	S3223	P3224	R3225	T3229	L3230	A3135	L3136	L3140	L3143	F3144	Q3145	H3146	I3147	A3148	Q3149	F3152	G3153	D3154	I3157	L3158	D3159	V3160	P3161	Q3162	S3171	S3174														
L3075	G3084	P3085	E3086	E3104	V3107	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	N3128	L3129	T3130	T3131	T3132	T3133	Q3007	Q3008	Y3009	F3010	T3011	Y3016	T3020	F3021	A3022	K3023	V3024	L3025	V2937	T2938	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	R3051	T2948	S2949	R2954	F2955	L2960	L2963	M2967	S2970			
Q2971	E2972	L2973	E2974	E2978	A2979	S2982	S2983	G2984	V2985	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	K2996	F2997	F2998	T3001	L3002	E2925	L2926	L2927	K2928	L2929	L2930	Q2931	M2932	N2933	G2934	V2935	A2936	V2937	T2938	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	R3051	T2948	S2949	R2954	F2955	L2960	L2963	M2967	S2970							
L2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	D2790	L2791	R2792	F2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	K2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	N2816	L2817	A2818	V2819	E2820	V2821	T2822	E2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG		
LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	E2875	E2876	Q2877	L2878	A2879	E2880	Y2881	Y2882	H2883	E2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900





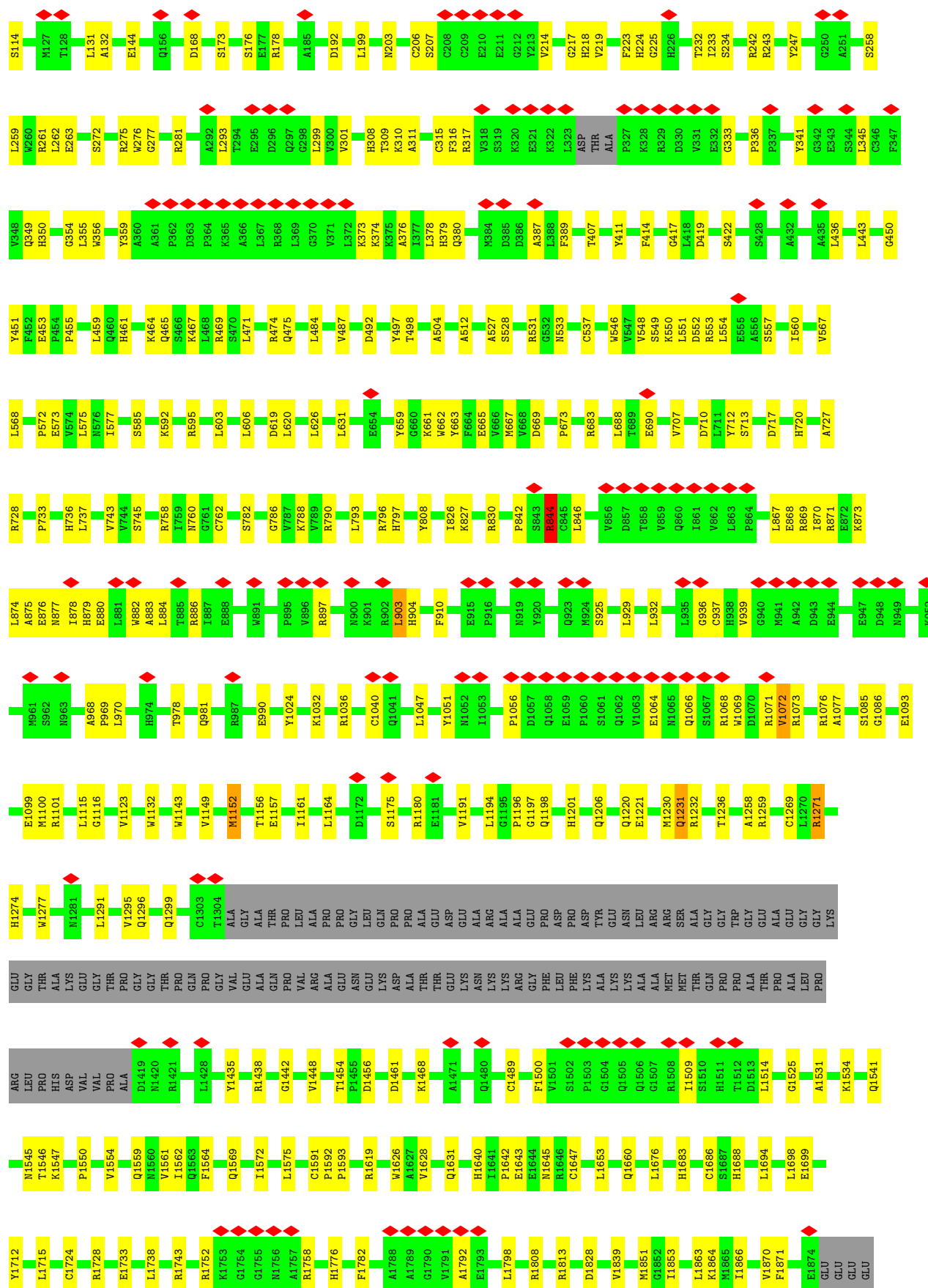


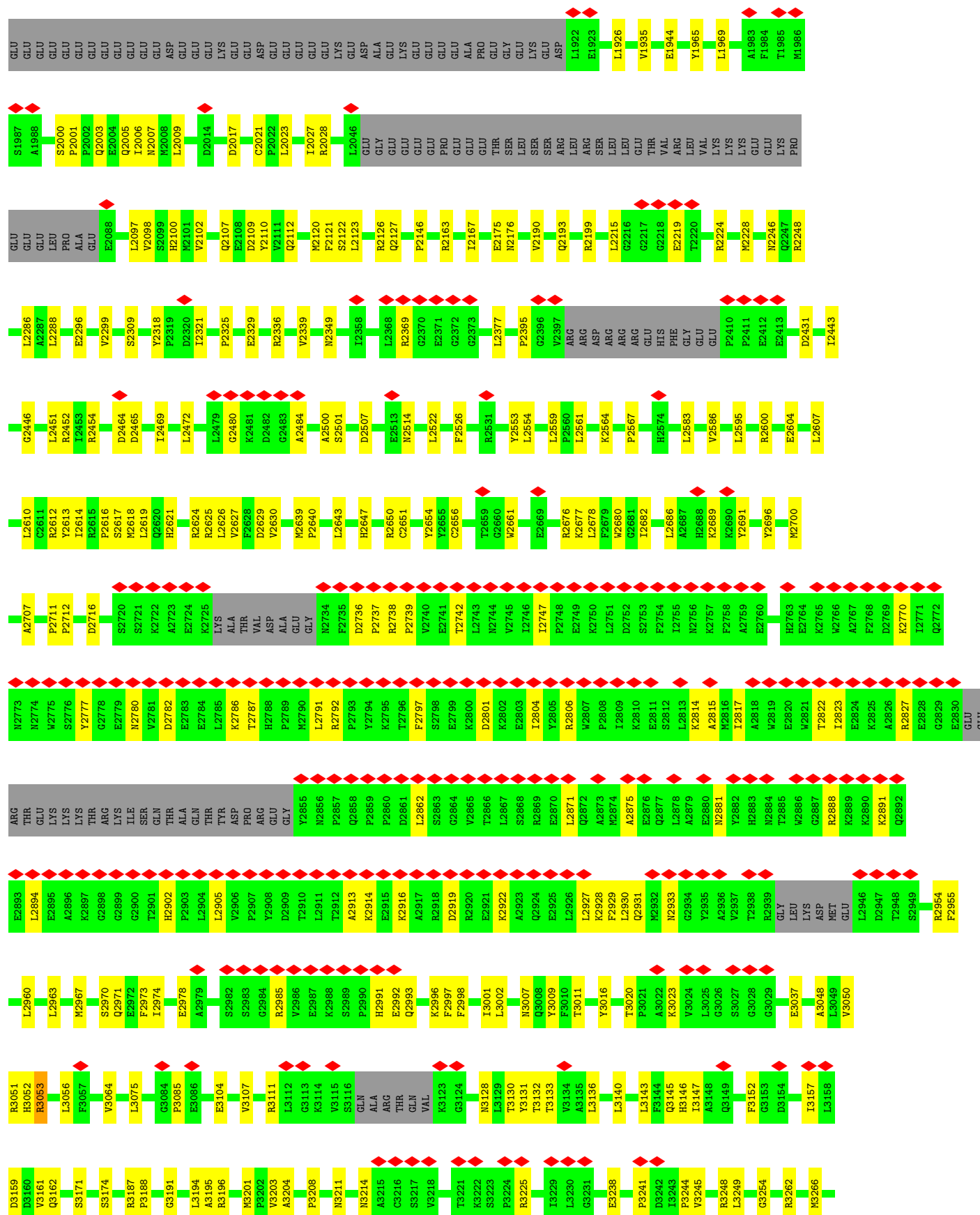




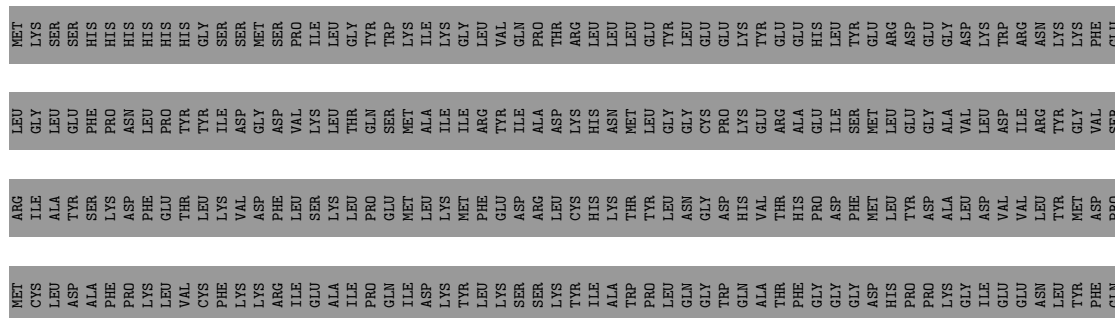
R3769	M3638	V3563	R3350	I3943	L3143	A3022	R2939	K2879	W2819	F2768	K2680
L3770	I3641	E3564	L3354	P3244	F3144	K3023	GLY	E2880	E2820	A2769	G2681
H3771	I3644	G3565	F3358	V3245	Q3145	V3024	LEU	L2881	W2821	E2760	I2682
R3773	L3644	S3566	T3361	R3248	A3148	G3026	ASP	Y2882	T2822	H2763	L2686
V3779	E3670	L3569	T3361	L3249	Q3149	S3027	MET	Y2883	I2823	E2764	K2687
L3780	I3674	M3573	R3366	G3254	F3152	G3028	GLU	Y2884	E2824	K2765	H2688
I3783	G3681	V3576	E3377	R3262	G3153	G3029	L2946	T2885	K2825	W2766	K2689
S3784	E3682	L3579	E3377	M3266	D3154	E3037	T2947	Y2886	E2826	A2767	V2690
A3785	Q3683	P3580	R3380	E3271	I3157	A3048	T2948	Y2887	R2827	Y2696	Y2691
C3786	E3684	G3581	L3381	P3275	L3158	L3049	S2949	K2888	E2828	F2768	
K3787	E3685	R3582	E3382	M3276	Q3161	V3050	R2954	K2889	G2829	D2769	W2700
G3788	E3686	E3583	A3383	N3276	H3162	R3051	F2955	K2890	E2830	I2770	W2700
T3797	E3687	A3384	A3383	E3290	V3161	R3052	L2960	Q2892	GLU	A2707	
L3800	E3688	A3385	A3384	P3291	Q3162	R3053	L2963	E2893	GLU	P2711	
L3805	E3689	D3585	A3385	P3292	S3171	L3056	M2967	E2895	LYS	N2774	
N3809	V3690	A3586	A3387	P3293	S3174	F3057	S2970	A2896	LYS	W2776	D2716
A3810	E3691	A3587	E3388	P3294	R3187	V3064	Q2971	K2897	LYS	Y2777	
E3811	E3692	A3588	E3389	A3295	P3188	L3076	E2972	G2898	ARG	G2778	
V3812	K3693	A3589	E3390	L3296	R3196	E3085	I2974	G2899	LYS	E2779	
E3825	K3694	P3590	R3403	P3297	G3191	P3085	E2978	G2900	ILE	N2780	
V3826	P3695	V3600	L3392	P3297	L3194	F3085	E2978	T2901	SER	V2781	
G3827	K3713	L3603	L3393	A3298	A3195	E3086	A2979	H2902	GLN	D2782	
F3828	S3714	V3604	V3394	A3299	R3196	E3086	A2979	T2903	THR	Y2782	
F3829	K3715	L3606	R3403	A3300	M3201	E3104	S2982	L2904	ALA	G2783	
Q3830	K3715	L3606	L3406	P3301	P3202	V3107	S2983	L2905	THR	E2784	
L3835	E3718	T3609	V3406	P3302	V3203	R3111	G2984	V2906	THR	L2785	
L3842	D3719	E3610	R3414	P3303	A3204	R3111	G2985	P2907	TVR	K2786	
Q3850	I3728	H3611	V3415	P3303	P3208	L3112	V2986	Y2908	ASP	Y2787	
G3857	M3729	P3612	V3416	C3304	N3211	G3113	E2987	D2909	PRO	G2788	
N3859	L3735	V3613	N3419	S3309	N3214	V3115	V2988	T2911	GLU	P2789	
V3859	E3736	K3614	R3420	N3318	A3215	GLN	K2996	L2912	GLY	M2790	
N3860	GLY	S3615	V3423	I3319	C3216	ALA	K2997	L2911	N2856	D2796	
E3861	GLY	K3516	L3424	R3320	S3217	ARG	F2998	T2912	P2857	D2796	
D3862	ASN	P3519	F3427	I3321	V3218	THR	K2999	A2913	Q2858	R2792	
G3863	GLY	M3524	L3434	N3325	E3218	VAL	Q2993	K2914	P2859	Y2794	
T3864	ALA	L3535	M3437	N3326	T3221	K3123	K2996	E2915	P2860	K2795	
V3865	GLU	L3535	K3437	I3329	K3222	G3124	F2997	K2916	D2861	T2796	
N3867	GLU	T3538	T3441	D3330	S3223	G3124	F2998	A2917	L2862	F2797	
R3868	GLU	T3538	T3441	F3331	P3224	N3128	R2918	R2917	S2863	S2798	
R3869	GLU	A3541	N3450	A3332	R3225	T3130	D2919	D2919	Q2864	E2799	
Q3870	V3749	L3542	R3453	K3336	E3225	T3131	R2920	R2920	V2865	K2800	
N3871	E3750	K3543	E3454	R3337	I3229	T3132	R2921	E2921	T2866	D2801	
G3871	V3751	N3555	N3457	L3338	L3230	T3133	E2922	A2923	L2867	K2802	
E3872	S3752	R3557	N3457	A3339	G3231	A3135	E2925	Q2924	S2868	P2748	
N3875	F3753	R3629	N3465	V3340	E3238	L3136	Y3010	Q2925	E2803	E2749	
D3878	E3754	R3630	N3466	Q3343	P3241	L3140	T3011	L2926	I2804	K2750	
	K3756	A3631	N3467	P3344	Y3015		Y3015	L2927	Q2871	L2751	
	S3768	V3632	K3467	I3345	T3020		T3020	K2928	Q2873	D2752	
		V3633			P3021		P3021	F2929	W2874	S2753	
		C3635			D3242			L2930	A2875	F2754	
		F3636						Q2931	E2876	I2755	
		R3637						M2932	Q2877	K2810	
								N2933	L2878	S2812	
								G2934		L2813	
								Y2935		K2814	
								A2936		A2815	
								V2937		M2816	
								T2938		I2817	
										A2818	

R3866	R3867	L3888	Q3889	L3890	L3891	Q3900	Q3927	S3928	S3929	L3930	S3931	D3932	V3935	G3939	E3945	K3948	R3949	N3963	S3964	L3965	T3966	E3967	Y3968	G3991	F3992	V3995	M3999	Q4009	Q4020	M4023	L4030	I4040	V4049	M4057	L4058	L4059	K4060	L4066	K4069																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G4073	S4074	A4075	A4076	D4079	Y4080	T4082	D4083	K4090	K4091	D4092	F4093	Q4094	K4095	A4096	M4097	D4098	Q4100	K4101	Q4102	F4103	T4104	G4105	P4106	L4111	L4112	S4115	E4116	A4117	D4118	E4119	N4120	E4121	M4122	I4123	A4129	Q4133	D4138	I4139	N4142	S4151	E4152	H4156	P4157	N4158	R4159	L4160																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
E4165	E4168	S4169	L4170	L4171	R4175	L4178	G4179	R4180	T4181	E4182	I4183	R4188	R4189	E4191	R4192	T4193	Y4194	S4198	E4199	T4200	M4201	R4202	A4203	Q4204	M4207	P4208	Q4209	V4210	K4211	E4212	S4213	R4214	R4215	Q4216	F4217	F4219	E4224	G4225	G4226	A4228	S4229	K4230	M4231	S4236	P4254	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
GLY	GLU	PRO	GLU	VAL	ARG	ARG	LEU	ALA	ASP	GLY	ASP	THR	GLU	ALA	GLY	GLU	ALA	GLY	GLU	ALA	GLY	GLU	GLY	VAL	ALA	ALA	GLY	GLY	ALA	THR	VAL	GLY	GLY	ALA	GLY	LEU	ARG	GLY	LEU	VAL	GLY	THR	ARG	ARG	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
VAL	ARG	ARG	VAL	LEU	ARG	ARG	GLY	ASP	LEU	THR	ASP	ALA	ALA	GLY	THR	GLY	GLY	ALA	ALA	ALA	ALA	ALA	ALA	GLY	GLY	ALA	ALA	GLY	ALA	THR	GLY	TRP	GLY	ASP	GLY	GLY	LEU	VAL	GLY	GLY	GLY	VAL	VAL	VAL	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
THR	GLU	LEU	VAL	ALA	ALA	ASP	GLY	GLY	PRO	ASP	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
PRO	GLU	PRO	GLU	LYS	ALA	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
L4567	F4568	L4569	L4576	L4577	L4578	F4579	F4580	K4581	Y4582	S4583	S4585	P4586	P4587	GLY	GLY	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
L4632	E4633	E4634	M4639	L4646	S4647	L4648	T4651	I4658	Y4661	N4662	K4675	E4676	R4679	K4680	L4686	Q4691	D4694	D4695	D4696	V4697	K4698	G4699	Q4700	L4704	V4720	K4721	R4722	L4725	D4730	I4731	F4732	G4733	R4734	I4737	M4743	D4744	L4745	L4748	GLU	ILE	THR	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
HIS	ASN	GLU	ARG	LYS	PRO	ASP	PRO	PRO	PRO	GLY	LEU	LEU	THR	TRP	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
R4860	K4861	F4862	Y4863	K4864	M4865	S4866	E4867	D4868	E4869	D4870	E4871	D4872	D4873	M4874	D4878	M4879	M4880	T4881	C4882	Y4883	L4884	F4885	H4886	M4887	Y4888	Y4889	R4892	D4899	E4900	I4901	E4902	E4908	Y4909	E4910	L4911	Y4912	R4913	V4914	D4917	I4918	Q4933	I4936	E4942	L4943	R4944	D4945	Q4946	Q4949	V4950	K4951																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
E4952	C4958	C4961	S4965	D4966	Y4967	F4968	T4971	P4972	H4973	G4974	H4978	T4979	L4980	S4981	E4982	H4983	M4984	L4985	M4989	K4998	E5002	K5012	R5029	K5030	Q5031	D5034	Q5035	L5036	S5037	D5038	Q5039	L5040	Q5041	Q5042	Q5043	Q5044	Q5045	Q5046	Q5047	Q5048	Q5049	Q5050	Q5051	Q5052	Q5053	Q5054	Q5055	Q5056	Q5057	Q5058	Q5059	Q5060	Q5061	Q5062	Q5063	Q5064	Q5065	Q5066	Q5067	Q5068	Q5069	Q5070	Q5071	Q5072	Q5073	Q5074	Q5075	Q5076	Q5077	Q5078	Q5079	Q5080	Q5081	Q5082	Q5083	Q5084	Q5085	Q5086	Q5087	Q5088	Q5089	Q5090	Q5091	Q5092	Q5093	Q5094	Q5095	Q5096	Q5097	Q5098	Q5099	Q5100	Q5101	Q5102	Q5103	Q5104	Q5105	Q5106	Q5107	Q5108	Q5109	Q5110	Q5111	Q5112	Q5113	Q5114	Q5115	Q5116	Q5117	Q5118	Q5119	Q5120	Q5121	Q5122	Q5123	Q5124	Q5125	Q5126	Q5127	Q5128	Q5129	Q5130	Q5131	Q5132	Q5133	Q5134	Q5135	Q5136	Q5137	Q5138	Q5139	Q5140	Q5141	Q5142	Q5143	Q5144	Q5145	Q5146	Q5147	Q5148	Q5149	Q5150	Q5151	Q5152	Q5153	Q5154	Q5155	Q5156	Q5157	Q5158	Q5159	Q5160	Q5161	Q5162	Q5163	Q5164	Q5165	Q5166	Q5167	Q5168	Q5169	Q5170	Q5171	Q5172	Q5173	Q5174	Q5175	Q5176	Q5177	Q5178	Q5179	Q5180	Q5181	Q5182	Q5183	Q5184	Q5185	Q5186	Q5187	Q5188	Q5189	Q5190	Q5191	Q5192	Q5193	Q5194	Q5195	Q5196	Q5197	Q5198	Q5199	Q5200	Q5201	Q5202	Q5203	Q5204	Q5205	Q5206	Q5207	Q5208	Q5209	Q5210	Q5211	Q5212	Q5213	Q5214	Q5215	Q5216	Q5217	Q5218	Q5219	Q5220	Q5221	Q5222	Q5223	Q5224	Q5225	Q5226	Q5227	Q5228	Q5229	Q5230	Q5231	Q5232	Q5233	Q5234	Q5235	Q5236	Q5237	Q5238	Q5239	Q5240	Q5241	Q5242	Q5243	Q5244	Q5245	Q5246	Q5247	Q5248	Q5249	Q5250	Q5251	Q5252	Q5253	Q5254	Q5255	Q5256	Q5257	Q5258	Q5259	Q5260	Q5261	Q5262	Q5263	Q5264	Q5265	Q5266	Q5267	Q5268	Q5269	Q5270	Q5271	Q5272	Q5273	Q5274	Q5275	Q5276	Q5277	Q5278	Q5279	Q5280	Q5281	Q5282	Q5283	Q5284	Q5285	Q5286	Q5287	Q5288	Q5289	Q5290	Q5291	Q5292	Q5293	Q5294	Q5295	Q5296	Q5297	Q5298	Q5299	Q5300	Q5301	Q5302	Q5303	Q5304	Q5305	Q5306	Q5307	Q5308	Q5309	Q5310	Q5311	Q5312	Q5313	Q5314	Q5315	Q5316	Q5317	Q5318	Q5319	Q5320	Q5321	Q5322	Q5323	Q5324	Q5325	Q5326	Q5327	Q5328	Q5329	Q5330	Q5331	Q5332	Q5333	Q5334	Q5335	Q5336	Q5337	Q5338	Q5339	Q5340	Q5341	Q5342	Q5343	Q5344	Q5345	Q5346	Q5347	Q5348	Q5349	Q5350	Q5351	Q5352	Q5353	Q5354	Q5355	Q5356	Q5357	Q5358	Q5359	Q5360	Q5361	Q5362	Q5363	Q5364	Q5365	Q5366	Q5367	Q5368	Q5369	Q5370	Q5371	Q5372	Q5373	Q5374	Q5375	Q5376	Q5377	Q5378	Q5379	Q5380	Q5381	Q5382	Q5383	Q5384	Q5385	Q5386	Q5387	Q5388	Q5389	Q5390	Q5391	Q5392	Q5393	Q5394	Q5395	Q5396	Q5397	Q5398	Q5399	Q5400	Q5401	Q5402	Q5403	Q5404	Q5405	Q5406	Q5407	Q5408	Q5409	Q5410	Q5411	Q5412	Q5413	Q5414	Q5415	Q5416	Q5417	Q5418	Q5419	Q5420	Q5421	Q5422	Q5423	Q5424	Q5425	Q5426	Q5427	Q5428	Q5429	Q5430	Q5431	Q5432	Q5433	Q5434	Q5435	Q5436	Q5437	Q5438	Q5439	Q5440	Q5441	Q5442	Q5443	Q5444	Q5445	Q5446	Q5447	Q5448	Q5449	Q5450	Q5451	Q5452	Q5453	Q5454	Q5455	Q5456	Q5457	Q5458	Q5459	Q5460	Q5461	Q5462	Q5463	Q5464	Q5465	Q5466	Q5467	Q5468	Q5469	Q5470	Q5471	Q5472	Q5473	Q5474	Q5475	Q5476	Q5477	Q5478	Q5479	Q5480	Q5481	Q5482	Q5483	Q5484	Q5485	Q5486	Q5487	Q5488	Q5489	Q5490	Q5491	Q5492	Q5493	Q5494	Q5495	Q5496	Q5497	Q5498	Q5499	Q5500	Q5501	Q5502	Q5503	Q5504	Q5505	Q5506	Q5507	Q5508	Q5509	Q5510	Q5511	Q5512	Q5513	Q5514	Q5515	Q5516	Q5517	Q5518	Q5519	Q5520	Q5521	Q5522	Q5523	Q5524	Q5525	Q5526	Q5527	Q5528	Q5529	Q5530	Q5531	Q5532	Q5533	Q5534	Q5535	Q5536	Q5537	Q5538	Q5539	Q5540	Q5541	Q5542	Q5543	Q5544	Q5545	Q5546	Q5547	Q5548	Q5549	Q5550	Q5551	Q5552	Q5553	Q5554	Q5555	Q5556	Q5557	Q5558	Q5559	Q5560	Q5561	Q5562	Q5563	Q5564	Q5565	Q5566	Q5567	Q5568	Q5569	Q5570	Q5571	Q5572	Q5573	Q5574	Q5575	Q5576	Q5577	Q5578	Q5579	Q5580	Q5581	Q5582	Q5583	Q5584	Q5585	Q5586	Q5587	Q5588	Q5589	Q5590	Q5591	Q5592	Q5593	Q5594	Q5595	Q5596	Q5597	Q5598	Q5599	Q5600	Q5601	Q5602	Q5603	Q5604	Q5605	Q5606	Q5607	Q5608	Q5609	Q5610	Q5611	Q5612	Q5613	Q5614	Q5615	Q5616	Q5617	Q5618	Q5619	Q5620	Q5621	Q5622	Q5623	Q5624	Q5625	Q5626	Q5627	Q5628	Q5629	Q5630	Q5631	Q5632	Q5633	Q5634	Q5635	Q5636	Q5637	Q5638	Q5639	Q5640	Q5641	Q5642	Q5643	Q5644	Q5645	Q5646	Q5647	Q5648	Q5649	Q5650	Q5651	Q5652	Q5653	Q5654	Q5655	Q5656	Q5657	Q5658	Q5659	Q5660	Q5661	Q5662	Q5663	Q5664	Q5665	Q5666	Q5667	Q5668	Q5669	Q5670	Q5671	Q5672	Q5673	Q5674	Q5675	Q5676	Q5677	Q5678	Q5679	Q5680	Q5681	Q5682	Q5683	Q5684	Q5685	Q5686	Q5687	Q5688	Q5689	Q5690	Q5691	Q5692	Q5693	Q5694	Q5695	Q5696	Q5697	Q5698	Q5699	Q5700	Q5701	Q5702	Q5703	Q5704	Q5705	Q5706	Q5707	Q5708	Q5709	Q5710	Q5711	Q5712	Q5713	Q5714	Q5715	Q5716	Q5717	Q5718	Q5719	Q5720	Q5721	Q5722	Q5723	Q5724	Q5725	Q5726	Q5727	Q5728	Q5729	Q5730	Q5731	Q5732	Q5733	Q5734	Q5735	Q5736	Q5737	Q5738	Q5739	Q5740	Q5741	Q5742	Q5743	Q5744	Q5745	Q5746	Q5747	Q5748	Q5749	Q5750	Q5751	Q5752	Q5753	Q5754	Q5755	Q5756	Q5757	Q5758	Q5759	Q5760	Q5761	Q5762	Q5763	Q5764	Q5765	Q5766	Q5767	Q5768	Q5769	Q5770	Q5771	Q5772	Q5773	Q5774	Q5775	Q5776	Q5777	Q5778	Q5779	Q5780	Q5781	Q5782	Q5783	Q5784	Q5785	Q5786	Q5787	Q5788	Q5789	Q5790	Q5791	Q5792	Q5793	Q5794	Q5795	Q5796	Q5797	Q5798	Q5799	Q5800	Q5801	Q5802	Q5803	Q5804	Q5805	Q5806	Q5807	Q5808	Q5809	Q5810	Q5811	Q5812









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21706	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.200	Depositor
Minimum map value	-0.744	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.305	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADE

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	0.35	0/35720	0.68	15/48374 (0.0%)
1	B	0.35	0/35720	0.68	16/48374 (0.0%)
1	C	0.35	0/35720	0.68	16/48374 (0.0%)
1	D	0.35	0/35720	0.68	15/48374 (0.0%)
2	E	0.33	0/834	0.67	0/1123
2	F	0.33	0/834	0.67	0/1123
2	G	0.33	0/834	0.67	0/1123
2	H	0.33	0/834	0.67	0/1123
All	All	0.35	0/146216	0.68	62/197988 (0.0%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ARG	CG-CD-NE	7.00	126.51	111.80
1	C	844	ARG	CA-CB-CG	6.99	128.78	113.40
1	D	844	ARG	CA-CB-CG	6.99	128.78	113.40
1	A	844	ARG	CA-CB-CG	6.99	128.77	113.40
1	B	76	ARG	CG-CD-NE	6.98	126.46	111.80
1	C	76	ARG	CG-CD-NE	6.98	126.46	111.80
1	D	76	ARG	CG-CD-NE	6.98	126.46	111.80
1	B	844	ARG	CA-CB-CG	6.98	128.75	113.40
1	B	903	LEU	CA-CB-CG	6.46	130.15	115.30
1	C	903	LEU	CA-CB-CG	6.45	130.13	115.30
1	A	903	LEU	CA-CB-CG	6.45	130.13	115.30
1	D	903	LEU	CA-CB-CG	6.45	130.13	115.30
1	B	1072	VAL	CG1-CB-CG2	-6.33	100.78	110.90
1	D	1072	VAL	CG1-CB-CG2	-6.31	100.80	110.90
1	C	1072	VAL	CG1-CB-CG2	-6.31	100.81	110.90
1	A	1072	VAL	CG1-CB-CG2	-6.29	100.84	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4578	LEU	CA-CB-CG	6.05	129.22	115.30
1	C	4578	LEU	CA-CB-CG	6.03	129.18	115.30
1	D	4578	LEU	CA-CB-CG	6.03	129.18	115.30
1	B	4578	LEU	CA-CB-CG	6.03	129.17	115.30
1	A	3296	LEU	CA-CB-CG	6.01	129.12	115.30
1	D	3296	LEU	CA-CB-CG	6.00	129.10	115.30
1	B	3296	LEU	CA-CB-CG	5.99	129.07	115.30
1	C	3296	LEU	CA-CB-CG	5.99	129.07	115.30
1	B	3276	MET	CA-CB-CG	5.90	123.33	113.30
1	C	3276	MET	CA-CB-CG	5.90	123.33	113.30
1	A	3276	MET	CA-CB-CG	5.88	123.30	113.30
1	D	3276	MET	CA-CB-CG	5.86	123.27	113.30
1	C	1152	MET	CA-CB-CG	5.83	123.21	113.30
1	D	1152	MET	CA-CB-CG	5.83	123.21	113.30
1	B	1152	MET	CA-CB-CG	5.81	123.18	113.30
1	A	1152	MET	CA-CB-CG	5.79	123.15	113.30
1	B	131	LEU	CA-CB-CG	5.69	128.40	115.30
1	C	131	LEU	CA-CB-CG	5.69	128.39	115.30
1	D	131	LEU	CA-CB-CG	5.69	128.38	115.30
1	A	131	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	3194	LEU	CA-CB-CG	5.49	127.92	115.30
1	B	3932	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	3932	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	3194	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	3194	LEU	CA-CB-CG	5.47	127.88	115.30
1	D	3194	LEU	CA-CB-CG	5.46	127.87	115.30
1	C	3932	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	3932	ASP	CB-CG-OD1	5.44	123.19	118.30
1	D	2700	MET	CA-CB-CG	5.37	122.43	113.30
1	A	2700	MET	CA-CB-CG	5.36	122.42	113.30
1	B	2700	MET	CA-CB-CG	5.36	122.41	113.30
1	C	2700	MET	CA-CB-CG	5.36	122.41	113.30
1	C	471	LEU	CA-CB-CG	5.06	126.93	115.30
1	B	471	LEU	CA-CB-CG	5.05	126.92	115.30
1	D	29	LEU	CA-CB-CG	5.05	126.93	115.30
1	D	471	LEU	CA-CB-CG	5.05	126.92	115.30
1	C	29	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	29	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	471	LEU	CA-CB-CG	5.04	126.89	115.30
1	B	29	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	844	ARG	N-CA-CB	5.01	119.63	110.60
1	B	4985	LEU	CA-CB-CG	5.01	126.83	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	844	ARG	N-CA-CB	5.01	119.62	110.60
1	C	844	ARG	N-CA-CB	5.01	119.62	110.60
1	D	844	ARG	N-CA-CB	5.01	119.62	110.60
1	C	4985	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

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	34906	0	34529	480	0
1	B	34906	0	34529	492	0
1	C	34906	0	34529	496	0
1	D	34906	0	34529	491	0
2	E	818	0	824	20	0
2	F	818	0	824	20	0
2	G	818	0	824	18	0
2	H	818	0	824	19	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	10	0	4	1	0
4	B	10	0	4	1	0
4	C	10	0	4	1	0
4	D	10	0	4	1	0
All	All	142940	0	141428	2006	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 7.

All (2006) 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:C:844:ARG:HH12	1:C:1197:GLY:HA3	1.45	0.80
1:B:844:ARG:HH12	1:B:1197:GLY:HA3	1.45	0.80
1:A:844:ARG:HH12	1:A:1197:GLY:HA3	1.45	0.79
1:D:844:ARG:HH12	1:D:1197:GLY:HA3	1.45	0.79
1:B:34:LYS:H	1:B:53:SER:HB3	1.49	0.78
1:C:34:LYS:H	1:C:53:SER:HB3	1.49	0.78
1:D:34:LYS:H	1:D:53:SER:HB3	1.49	0.77
1:A:34:LYS:H	1:A:53:SER:HB3	1.49	0.76
1:C:3377:GLU:HA	1:C:3380:ARG:HG2	1.72	0.72
1:D:3377:GLU:HA	1:D:3380:ARG:HG2	1.72	0.72
1:A:2927:LEU:HG	1:A:2931:GLN:HE22	1.55	0.72
1:B:3377:GLU:HA	1:B:3380:ARG:HG2	1.72	0.71
1:D:2927:LEU:HG	1:D:2931:GLN:HE22	1.55	0.71
1:A:3377:GLU:HA	1:A:3380:ARG:HG2	1.72	0.71
1:C:2927:LEU:HG	1:C:2931:GLN:HE22	1.55	0.70
1:B:2927:LEU:HG	1:B:2931:GLN:HE22	1.55	0.70
1:B:4211:LYS:HB3	1:B:4215:ARG:HH21	1.57	0.70
1:A:4211:LYS:HB3	1:A:4215:ARG:HH21	1.57	0.69
1:A:4892:ARG:NH2	1:B:4899:ASP:OD1	2.25	0.69
1:D:4211:LYS:HB3	1:D:4215:ARG:HH21	1.57	0.69
1:A:2215:LEU:O	1:A:2219:GLU:HB2	1.93	0.69
1:C:3420:ARG:HH12	1:C:3519:PRO:HD2	1.57	0.69
1:D:2215:LEU:O	1:D:2219:GLU:HB2	1.93	0.69
1:C:4211:LYS:HB3	1:C:4215:ARG:HH21	1.57	0.68
1:B:3420:ARG:HH12	1:B:3519:PRO:HD2	1.57	0.68
1:A:168:ASP:HB3	1:A:199:LEU:HD11	1.76	0.68
1:A:533:ASN:O	1:A:537:CYS:HB2	1.94	0.68
1:A:3420:ARG:HH12	1:A:3519:PRO:HD2	1.57	0.67
1:C:533:ASN:O	1:C:537:CYS:HB2	1.94	0.67
1:D:3420:ARG:HH12	1:D:3519:PRO:HD2	1.57	0.67
1:B:168:ASP:HB3	1:B:199:LEU:HD11	1.76	0.67
1:D:533:ASN:O	1:D:537:CYS:HB2	1.94	0.67
1:B:533:ASN:O	1:B:537:CYS:HB2	1.94	0.67
1:C:2215:LEU:O	1:C:2219:GLU:HB2	1.93	0.67
1:D:168:ASP:HB3	1:D:199:LEU:HD11	1.76	0.67
1:C:168:ASP:HB3	1:C:199:LEU:HD11	1.76	0.67
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.69	0.66
1:B:842:PRO:HG3	1:B:1073:ARG:HE	1.60	0.66
2:G:90:VAL:HG12	2:G:91:ILE:HG13	1.78	0.66
1:C:842:PRO:HG3	1:C:1073:ARG:HE	1.61	0.66
1:C:1258:ALA:HB3	1:C:1271:ARG:HB3	1.77	0.66
1:A:842:PRO:HG3	1:A:1073:ARG:HE	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2215:LEU:O	1:B:2219:GLU:HB2	1.93	0.66
1:A:1258:ALA:HB3	1:A:1271:ARG:HB3	1.77	0.66
1:B:1258:ALA:HB3	1:B:1271:ARG:HB3	1.77	0.66
1:D:842:PRO:HG3	1:D:1073:ARG:HE	1.61	0.66
1:D:3948:LYS:HD3	1:D:4009:GLN:HE21	1.61	0.66
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.69	0.66
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.69	0.65
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.69	0.65
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.78	0.65
1:B:2248:ARG:HH22	1:B:3870:ASN:HB2	1.61	0.65
2:F:90:VAL:HG12	2:F:91:ILE:HG13	1.78	0.65
2:H:90:VAL:HG12	2:H:91:ILE:HG13	1.78	0.65
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.78	0.65
1:C:2248:ARG:HH22	1:C:3870:ASN:HB2	1.61	0.65
1:A:475:GLN:NE2	1:A:528:SER:O	2.30	0.65
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.78	0.65
1:D:475:GLN:NE2	1:D:528:SER:O	2.30	0.65
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	1.78	0.65
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.78	0.65
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.78	0.65
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.78	0.65
1:C:475:GLN:NE2	1:C:528:SER:O	2.30	0.65
1:B:173:SER:HB3	1:B:178:ARG:H	1.62	0.64
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	1.79	0.64
1:D:1258:ALA:HB3	1:D:1271:ARG:HB3	1.77	0.64
1:A:3948:LYS:HD3	1:A:4009:GLN:HE21	1.61	0.64
1:A:4978:HIS:HA	1:A:4982:GLU:HG3	1.78	0.64
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.78	0.64
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	1.79	0.64
1:B:3948:LYS:HD3	1:B:4009:GLN:HE21	1.61	0.64
1:D:2248:ARG:HH22	1:D:3870:ASN:HB2	1.61	0.64
2:E:90:VAL:HG12	2:E:91:ILE:HG13	1.78	0.64
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.79	0.64
1:D:4978:HIS:HA	1:D:4982:GLU:HG3	1.78	0.64
1:A:2248:ARG:HH22	1:A:3870:ASN:HB2	1.61	0.64
1:B:475:GLN:NE2	1:B:528:SER:O	2.30	0.64
1:C:173:SER:HB3	1:C:178:ARG:H	1.62	0.64
1:C:3948:LYS:HD3	1:C:4009:GLN:HE21	1.61	0.64
1:B:3927:GLN:HE21	1:B:3991:GLY:HA3	1.63	0.64
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.79	0.64
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.78	0.63
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.81	0.63
1:D:173:SER:HB3	1:D:178:ARG:H	1.62	0.63
1:A:173:SER:HB3	1:A:178:ARG:H	1.62	0.63
1:D:293:LEU:HD12	1:D:378:LEU:HD23	1.81	0.63
1:C:3927:GLN:HE21	1:C:3991:GLY:HA3	1.63	0.63
1:D:3927:GLN:HE21	1:D:3991:GLY:HA3	1.63	0.63
1:A:293:LEU:HD12	1:A:378:LEU:HD23	1.81	0.63
1:A:3927:GLN:HE21	1:A:3991:GLY:HA3	1.63	0.63
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.81	0.62
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.81	0.62
1:A:451:TYR:O	1:A:474:ARG:NH1	2.33	0.62
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.82	0.62
1:B:293:LEU:HD12	1:B:378:LEU:HD23	1.81	0.62
1:B:451:TYR:O	1:B:474:ARG:NH1	2.33	0.62
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.82	0.62
1:D:451:TYR:O	1:D:474:ARG:NH1	2.33	0.62
1:D:667:MET:HB3	1:D:790:ARG:HB2	1.82	0.62
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.18	0.62
1:B:234:SER:HB2	1:B:242:ARG:HA	1.82	0.62
1:C:234:SER:HB2	1:C:242:ARG:HA	1.82	0.62
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.81	0.62
2:F:49:ARG:HH21	2:F:50:ILE:HG12	1.65	0.62
1:A:3050:VAL:HG11	1:A:3064:VAL:HG11	1.82	0.61
2:H:49:ARG:HH21	2:H:50:ILE:HG12	1.65	0.61
1:C:293:LEU:HD12	1:C:378:LEU:HD23	1.81	0.61
1:D:3050:VAL:HG11	1:D:3064:VAL:HG11	1.82	0.61
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.34	0.61
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.18	0.61
2:E:49:ARG:HH21	2:E:50:ILE:HG12	1.65	0.61
1:C:451:TYR:O	1:C:474:ARG:NH1	2.33	0.61
1:A:234:SER:HB2	1:A:242:ARG:HA	1.82	0.61
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.83	0.61
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.18	0.61
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.33	0.61
1:C:2630:VAL:HG12	1:C:2682:ILE:HD11	1.83	0.61
1:D:3420:ARG:HH22	1:D:3519:PRO:HB2	1.66	0.61
1:C:3420:ARG:HH22	1:C:3519:PRO:HB2	1.66	0.61
1:A:3420:ARG:HH22	1:A:3519:PRO:HB2	1.66	0.61
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.82	0.61
1:B:4892:ARG:NH2	1:C:4899:ASP:OD1	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3050:VAL:HG11	1:C:3064:VAL:HG11	1.82	0.61
1:D:234:SER:HB2	1:D:242:ARG:HA	1.82	0.61
2:G:49:ARG:HH21	2:G:50:ILE:HG12	1.65	0.61
1:A:2630:VAL:HG12	1:A:2682:ILE:HD11	1.83	0.60
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.34	0.60
1:B:3050:VAL:HG11	1:B:3064:VAL:HG11	1.82	0.60
1:B:3420:ARG:HH22	1:B:3519:PRO:HB2	1.66	0.60
1:D:2630:VAL:HG12	1:D:2682:ILE:HD11	1.83	0.60
1:A:1569:GLN:HB2	1:A:1572:ILE:HD12	1.84	0.60
1:C:667:MET:HB3	1:C:790:ARG:HB2	1.82	0.60
1:A:667:MET:HB3	1:A:790:ARG:HB2	1.82	0.60
1:A:4680:LYS:HE3	1:A:4686:LEU:HD22	1.83	0.60
1:B:317:ARG:NH1	1:B:349:GLN:OE1	2.34	0.60
1:B:4680:LYS:HE3	1:B:4686:LEU:HD22	1.83	0.60
1:B:667:MET:HB3	1:B:790:ARG:HB2	1.82	0.60
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.82	0.60
1:C:1569:GLN:HB2	1:C:1572:ILE:HD12	1.84	0.60
1:C:4892:ARG:NH2	1:D:4899:ASP:OD1	2.34	0.60
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.18	0.60
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.35	0.60
1:D:1569:GLN:HB2	1:D:1572:ILE:HD12	1.84	0.60
1:C:317:ARG:NH1	1:C:349:GLN:OE1	2.34	0.60
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.83	0.60
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.84	0.60
1:D:317:ARG:NH1	1:D:349:GLN:OE1	2.34	0.60
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.83	0.59
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.33	0.59
1:A:317:ARG:NH1	1:A:349:GLN:OE1	2.34	0.59
1:D:359:TYR:HA	1:D:376:ALA:HA	1.85	0.59
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.83	0.59
1:A:359:TYR:HA	1:A:376:ALA:HA	1.85	0.59
1:A:1808:ARG:NH1	1:A:1853:ILE:O	2.36	0.59
1:C:359:TYR:HA	1:C:376:ALA:HA	1.85	0.59
1:C:1196:PRO:O	1:C:1198:GLN:NE2	2.36	0.59
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.34	0.59
1:D:4680:LYS:HE3	1:D:4686:LEU:HD22	1.83	0.59
1:D:2001:PRO:HG2	1:D:3864:THR:HB	1.85	0.59
1:B:359:TYR:HA	1:B:376:ALA:HA	1.85	0.59
1:D:683:ARG:HG2	1:D:717:ASP:HB3	1.85	0.59
1:A:2929:PHE:O	1:A:2933:ASN:ND2	2.36	0.58
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.83	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2929:PHE:O	1:B:2933:ASN:ND2	2.36	0.58
1:C:1808:ARG:NH1	1:C:1853:ILE:O	2.36	0.58
1:C:4680:LYS:HE3	1:C:4686:LEU:HD22	1.83	0.58
1:C:1969:LEU:HD12	1:C:2009:LEU:HD13	1.85	0.58
1:D:3053:ARG:HA	1:D:3056:LEU:HD13	1.86	0.58
1:B:3053:ARG:HA	1:B:3056:LEU:HD13	1.86	0.58
1:C:683:ARG:HG2	1:C:717:ASP:HB3	1.85	0.58
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.85	0.58
1:A:882:TRP:O	1:A:886:ARG:NH1	2.36	0.58
1:A:1196:PRO:O	1:A:1198:GLN:NE2	2.36	0.58
1:A:3007:ASN:O	1:A:3011:THR:OG1	2.21	0.58
1:C:1808:ARG:HD3	1:C:1853:ILE:HG22	1.85	0.58
1:C:3007:ASN:O	1:C:3011:THR:OG1	2.21	0.58
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.85	0.58
1:A:1969:LEU:HD12	1:A:2009:LEU:HD13	1.85	0.58
1:A:2001:PRO:HG2	1:A:3864:THR:HB	1.85	0.58
1:B:1808:ARG:HD3	1:B:1853:ILE:HG22	1.85	0.58
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.85	0.58
1:D:1808:ARG:NH1	1:D:1853:ILE:O	2.36	0.58
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.85	0.58
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.36	0.58
1:B:882:TRP:O	1:B:886:ARG:NH1	2.37	0.58
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.85	0.58
1:C:3053:ARG:HA	1:C:3056:LEU:HD13	1.86	0.58
1:D:3007:ASN:O	1:D:3011:THR:OG1	2.21	0.58
1:A:3053:ARG:HA	1:A:3056:LEU:HD13	1.86	0.58
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.85	0.58
1:C:882:TRP:O	1:C:886:ARG:NH1	2.37	0.58
1:C:3309:SER:OG	1:C:3350:ARG:NH2	2.37	0.58
1:D:459:LEU:O	1:D:464:LYS:NZ	2.37	0.58
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.85	0.58
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.36	0.58
1:D:882:TRP:O	1:D:886:ARG:NH1	2.37	0.58
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.85	0.58
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.34	0.57
1:B:3007:ASN:O	1:B:3011:THR:OG1	2.21	0.57
1:C:2747:ILE:HB	1:C:2814:LYS:HG2	1.86	0.57
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.33	0.57
1:D:1969:LEU:HD12	1:D:2009:LEU:HD13	1.85	0.57
1:D:2929:PHE:O	1:D:2933:ASN:ND2	2.36	0.57
1:A:1808:ARG:HD3	1:A:1853:ILE:HG22	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.37	0.57
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.85	0.57
1:B:1969:LEU:HD12	1:B:2009:LEU:HD13	1.85	0.57
1:B:3309:SER:OG	1:B:3350:ARG:NH2	2.37	0.57
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	1.85	0.57
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.36	0.57
1:A:659:TYR:O	1:A:662:TRP:NE1	2.37	0.57
1:B:2001:PRO:HG2	1:B:3864:THR:HB	1.85	0.57
1:C:277:GLY:HA2	1:C:315:CYS:HB3	1.87	0.57
1:C:659:TYR:O	1:C:662:TRP:NE1	2.37	0.57
1:D:1808:ARG:HD3	1:D:1853:ILE:HG22	1.85	0.57
1:A:4899:ASP:OD1	1:D:4892:ARG:NH2	2.38	0.57
1:B:277:GLY:HA2	1:B:315:CYS:HB3	1.87	0.57
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.85	0.57
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.85	0.57
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.33	0.57
1:A:1683:HIS:NE2	1:A:1798:LEU:O	2.36	0.57
1:B:2747:ILE:HB	1:B:2814:LYS:HG2	1.86	0.57
1:B:4864:ASN:ND2	1:B:4874:MET:SD	2.78	0.57
1:A:459:LEU:O	1:A:464:LYS:NZ	2.37	0.57
1:A:3850:GLN:NE2	1:A:3872:GLU:OE1	2.38	0.57
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.85	0.57
1:B:659:TYR:O	1:B:662:TRP:NE1	2.37	0.57
1:B:1196:PRO:O	1:B:1198:GLN:NE2	2.36	0.57
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.85	0.57
1:D:659:TYR:O	1:D:662:TRP:NE1	2.37	0.57
1:A:3107:VAL:HG11	1:A:3171:SER:HB2	1.87	0.57
1:C:277:GLY:N	1:C:316:PHE:O	2.38	0.57
1:C:2446:GLY:HA2	1:C:2451:LEU:HD21	1.86	0.57
1:C:4864:ASN:ND2	1:C:4874:MET:SD	2.78	0.57
1:D:1870:VAL:HG11	1:D:2097:LEU:HD22	1.86	0.57
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.38	0.57
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.36	0.57
1:A:277:GLY:N	1:A:316:PHE:O	2.38	0.57
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.70	0.57
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.37	0.57
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.35	0.57
1:D:2446:GLY:HA2	1:D:2451:LEU:HD21	1.86	0.57
1:D:3850:GLN:NE2	1:D:3872:GLU:OE1	2.38	0.57
1:C:2929:PHE:O	1:C:2933:ASN:ND2	2.36	0.56
1:C:3107:VAL:HG11	1:C:3171:SER:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1299:GLN:NE2	1:D:1545:ASN:OD1	2.38	0.56
1:D:2747:ILE:HB	1:D:2814:LYS:HG2	1.86	0.56
1:A:2747:ILE:HB	1:A:2814:LYS:HG2	1.86	0.56
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.70	0.56
1:D:4864:ASN:ND2	1:D:4874:MET:SD	2.78	0.56
1:A:1870:VAL:HG11	1:A:2097:LEU:HD22	1.86	0.56
1:B:277:GLY:N	1:B:316:PHE:O	2.38	0.56
1:B:1870:VAL:HG11	1:B:2097:LEU:HD22	1.86	0.56
1:B:2110:TYR:O	1:B:2112:GLN:NE2	2.39	0.56
1:B:2891:LYS:HA	1:B:2894:LEU:HB3	1.87	0.56
1:B:3107:VAL:HG11	1:B:3171:SER:HB2	1.87	0.56
1:B:3850:GLN:NE2	1:B:3872:GLU:OE1	2.38	0.56
1:C:1277:TRP:HD1	1:C:1559:GLN:HG3	1.71	0.56
1:C:2001:PRO:HG2	1:C:3864:THR:HB	1.85	0.56
1:D:277:GLY:HA2	1:D:315:CYS:HB3	1.87	0.56
1:D:1196:PRO:O	1:D:1198:GLN:NE2	2.36	0.56
1:D:1277:TRP:HD1	1:D:1559:GLN:HG3	1.71	0.56
1:D:2110:TYR:O	1:D:2112:GLN:NE2	2.39	0.56
1:D:2656:CYS:HA	1:D:2711:PRO:HG3	1.87	0.56
1:D:2770:LYS:HD3	1:D:2787:THR:HB	1.88	0.56
1:D:2891:LYS:HA	1:D:2894:LEU:HB3	1.87	0.56
1:A:277:GLY:HA2	1:A:315:CYS:HB3	1.87	0.56
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.38	0.56
1:A:3628:ARG:NH1	1:A:3857:GLY:O	2.38	0.56
1:A:4864:ASN:ND2	1:A:4874:MET:SD	2.78	0.56
1:C:1299:GLN:NE2	1:C:1545:ASN:OD1	2.38	0.56
1:D:3628:ARG:NH1	1:D:3857:GLY:O	2.38	0.56
1:A:1299:GLN:NE2	1:A:1545:ASN:OD1	2.38	0.56
1:A:3309:SER:OG	1:A:3350:ARG:NH2	2.37	0.56
1:B:2446:GLY:HA2	1:B:2451:LEU:HD21	1.86	0.56
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.38	0.56
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.33	0.56
1:C:3628:ARG:NH1	1:C:3857:GLY:O	2.38	0.56
1:C:3850:GLN:NE2	1:C:3872:GLU:OE1	2.38	0.56
1:D:3107:VAL:HG11	1:D:3171:SER:HB2	1.87	0.56
1:B:2656:CYS:HA	1:B:2711:PRO:HG3	1.87	0.56
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.38	0.56
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.33	0.56
1:A:2110:TYR:O	1:A:2112:GLN:NE2	2.39	0.56
1:C:1870:VAL:HG11	1:C:2097:LEU:HD22	1.86	0.56
1:C:2656:CYS:HA	1:C:2711:PRO:HG3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:GLY:N	1:D:316:PHE:O	2.38	0.56
1:A:595:ARG:NH2	1:A:631:LEU:O	2.39	0.56
1:B:1299:GLN:NE2	1:B:1545:ASN:OD1	2.38	0.56
1:C:223:PHE:HB2	1:C:389:PHE:HB2	1.88	0.56
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.37	0.56
1:B:4030:LEU:HG	1:B:4040:ILE:HD11	1.88	0.56
1:C:2770:LYS:HD3	1:C:2787:THR:HB	1.87	0.56
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.70	0.56
1:D:3420:ARG:NH1	1:D:3516:LYS:O	2.39	0.56
1:A:2927:LEU:O	1:A:2931:GLN:NE2	2.39	0.56
1:B:595:ARG:NH2	1:B:631:LEU:O	2.39	0.56
1:B:1277:TRP:HD1	1:B:1559:GLN:HG3	1.71	0.56
1:B:3420:ARG:NH1	1:B:3516:LYS:O	2.39	0.56
1:C:2110:TYR:O	1:C:2112:GLN:NE2	2.39	0.56
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.39	0.56
1:C:4030:LEU:HG	1:C:4040:ILE:HD11	1.88	0.56
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.24	0.56
1:D:4983:HIS:O	4:D:5102:ADE:N6	2.39	0.56
1:A:1277:TRP:HD1	1:A:1559:GLN:HG3	1.71	0.55
1:A:2770:LYS:HD3	1:A:2787:THR:HB	1.87	0.55
1:A:3420:ARG:NH1	1:A:3516:LYS:O	2.39	0.55
1:B:2971:GLN:HA	1:B:2974:ILE:HG12	1.88	0.55
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.36	0.55
1:B:3693:LYS:NZ	1:B:3695:PRO:O	2.39	0.55
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.70	0.55
1:C:1206:GLN:NE2	1:C:1230:MET:O	2.39	0.55
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.39	0.55
1:D:3900:GLN:NE2	1:D:3967:GLU:O	2.40	0.55
1:A:2656:CYS:HA	1:A:2711:PRO:HG3	1.87	0.55
1:A:2971:GLN:HA	1:A:2974:ILE:HG12	1.89	0.55
1:B:1206:GLN:NE2	1:B:1230:MET:O	2.39	0.55
1:C:1792:ALA:O	1:C:2176:ASN:ND2	2.38	0.55
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	2.24	0.55
1:A:2891:LYS:HA	1:A:2894:LEU:HB3	1.87	0.55
1:C:595:ARG:NH2	1:C:631:LEU:O	2.39	0.55
1:C:2927:LEU:O	1:C:2931:GLN:NE2	2.39	0.55
1:D:595:ARG:NH2	1:D:631:LEU:O	2.39	0.55
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.40	0.55
1:A:3693:LYS:NZ	1:A:3695:PRO:O	2.39	0.55
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.40	0.55
1:D:2927:LEU:O	1:D:2931:GLN:NE2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3309:SER:OG	1:D:3350:ARG:NH2	2.37	0.55
1:D:3693:LYS:NZ	1:D:3695:PRO:O	2.39	0.55
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.39	0.55
1:B:3628:ARG:NH1	1:B:3857:GLY:O	2.38	0.55
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.24	0.55
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.40	0.55
1:D:417:GLY:HA3	1:D:436:LEU:HD21	1.88	0.55
1:A:144:GLU:OE1	1:D:2452:ARG:NH1	2.40	0.55
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.89	0.55
1:A:3900:GLN:NE2	1:A:3967:GLU:O	2.40	0.55
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.40	0.55
1:B:2770:LYS:HD3	1:B:2787:THR:HB	1.87	0.55
1:C:3693:LYS:NZ	1:C:3695:PRO:O	2.39	0.55
1:D:223:PHE:HB2	1:D:389:PHE:HB2	1.88	0.55
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.89	0.55
1:A:3132:THR:HG23	1:A:3136:LEU:HD23	1.88	0.55
1:B:1792:ALA:O	1:B:2176:ASN:ND2	2.38	0.55
1:B:2927:LEU:O	1:B:2931:GLN:NE2	2.39	0.55
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.39	0.55
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.37	0.55
1:C:2891:LYS:HA	1:C:2894:LEU:HB3	1.87	0.55
1:C:4983:HIS:O	4:C:5102:ADE:N6	2.39	0.55
1:D:1792:ALA:O	1:D:2176:ASN:ND2	2.38	0.55
1:A:223:PHE:HB2	1:A:389:PHE:HB2	1.88	0.55
1:A:1206:GLN:NE2	1:A:1230:MET:O	2.39	0.55
1:A:2446:GLY:HA2	1:A:2451:LEU:HD21	1.86	0.55
1:A:4983:HIS:O	4:A:5102:ADE:N6	2.39	0.55
1:B:459:LEU:O	1:B:464:LYS:NZ	2.37	0.55
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	1.89	0.55
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	1.89	0.55
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.39	0.55
1:B:1152:MET:HB2	1:B:1161:ILE:HB	1.89	0.55
1:B:3132:THR:HG23	1:B:3136:LEU:HD23	1.88	0.55
1:C:2452:ARG:NH1	1:D:144:GLU:OE1	2.40	0.55
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.39	0.55
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.89	0.54
1:A:4030:LEU:HG	1:A:4040:ILE:HD11	1.88	0.54
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.39	0.54
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.89	0.54
1:C:3420:ARG:NH1	1:C:3516:LYS:O	2.39	0.54
1:A:3825:GLU:OE1	1:A:3828:PHE:N	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PHE:HB2	1:B:389:PHE:HB2	1.88	0.54
1:B:417:GLY:HA3	1:B:436:LEU:HD21	1.88	0.54
1:C:417:GLY:HA3	1:C:436:LEU:HD21	1.88	0.54
1:C:3900:GLN:NE2	1:C:3967:GLU:O	2.40	0.54
1:D:2971:GLN:HA	1:D:2974:ILE:HG12	1.89	0.54
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.39	0.54
2:F:74:LEU:HB2	2:F:99:PHE:HB2	1.90	0.54
1:A:1152:MET:HB2	1:A:1161:ILE:HB	1.89	0.54
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.39	0.54
1:C:2626:LEU:HD22	1:C:2640:PRO:HB3	1.89	0.54
1:C:3132:THR:HG23	1:C:3136:LEU:HD23	1.88	0.54
1:A:417:GLY:HA3	1:A:436:LEU:HD21	1.88	0.54
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.90	0.54
1:D:497:TYR:O	1:D:553:ARG:NH2	2.37	0.54
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.89	0.54
1:D:1733:GLU:OE2	1:D:2163:ARG:NH2	2.41	0.54
1:D:4030:LEU:HG	1:D:4040:ILE:HD11	1.88	0.54
1:B:3208:PRO:HA	1:B:3211:ASN:HB2	1.89	0.54
1:B:4581:LYS:NZ	1:B:4582:VAL:O	2.38	0.54
1:C:3053:ARG:HG3	1:C:3056:LEU:HD22	1.90	0.54
1:C:3208:PRO:HA	1:C:3211:ASN:HB2	1.89	0.54
2:H:74:LEU:HB2	2:H:99:PHE:HB2	1.90	0.54
1:C:459:LEU:O	1:C:464:LYS:NZ	2.37	0.54
1:C:2971:GLN:HA	1:C:2974:ILE:HG12	1.89	0.54
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.89	0.54
1:B:355:LEU:HD22	1:B:380:GLN:HA	1.90	0.54
1:B:2452:ARG:NH1	1:C:144:GLU:OE1	2.40	0.54
1:D:2992:GLU:OE2	1:D:2996:LYS:NZ	2.41	0.54
1:D:3208:PRO:HA	1:D:3211:ASN:HB2	1.89	0.54
1:C:1152:MET:HB2	1:C:1161:ILE:HB	1.89	0.54
1:B:1733:GLU:OE2	1:B:2163:ARG:NH2	2.41	0.54
1:D:2650:ARG:NH1	1:D:2651:CYS:SG	2.81	0.54
1:D:3053:ARG:HG3	1:D:3056:LEU:HD22	1.90	0.54
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.90	0.54
1:B:2650:ARG:NH1	1:B:2651:CYS:SG	2.81	0.54
1:A:3329:ILE:O	1:A:3403:ARG:NH2	2.40	0.53
1:B:551:LEU:HD11	1:B:585:SER:HB3	1.90	0.53
1:B:3900:GLN:NE2	1:B:3967:GLU:O	2.40	0.53
1:C:2480:GLY:O	1:C:2484:ALA:N	2.42	0.53
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.89	0.53
1:C:3111:ARG:HH12	1:C:3174:SER:HB2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:LEU:HD11	1:D:585:SER:HB3	1.90	0.53
1:D:1206:GLN:NE2	1:D:1230:MET:O	2.39	0.53
1:D:3132:THR:HG23	1:D:3136:LEU:HD23	1.88	0.53
2:G:74:LEU:HB2	2:G:99:PHE:HB2	1.90	0.53
1:A:1733:GLU:OE2	1:A:2163:ARG:NH2	2.41	0.53
1:A:2480:GLY:O	1:A:2484:ALA:N	2.41	0.53
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.90	0.53
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.89	0.53
1:C:2919:ASP:HA	1:C:2922:LYS:HD2	1.89	0.53
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.39	0.53
1:D:2919:ASP:HA	1:D:2922:LYS:HD2	1.89	0.53
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.89	0.53
1:B:1259:ARG:NH2	1:B:1591:CYS:SG	2.82	0.53
1:B:2919:ASP:HA	1:B:2922:LYS:HD2	1.89	0.53
1:D:1259:ARG:NH2	1:D:1591:CYS:SG	2.82	0.53
1:A:355:LEU:HD22	1:A:380:GLN:HA	1.90	0.53
1:A:455:PRO:HB3	1:A:467:LYS:HD2	1.91	0.53
1:A:2650:ARG:NH1	1:A:2651:CYS:SG	2.81	0.53
1:A:3053:ARG:HG3	1:A:3056:LEU:HD22	1.90	0.53
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.33	0.53
1:C:2003:GLN:O	1:C:2007:ASN:ND2	2.42	0.53
1:C:2650:ARG:NH1	1:C:2651:CYS:SG	2.81	0.53
1:D:455:PRO:HB3	1:D:467:LYS:HD2	1.91	0.53
1:D:707:VAL:HG13	1:D:713:SER:HB2	1.90	0.53
1:D:1683:HIS:NE2	1:D:1798:LEU:O	2.36	0.53
1:A:2003:GLN:O	1:A:2007:ASN:ND2	2.41	0.53
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.33	0.53
1:B:2003:GLN:O	1:B:2007:ASN:ND2	2.42	0.53
1:B:2654:TYR:HB2	1:B:2661:TRP:HB2	1.91	0.53
1:B:3329:ILE:O	1:B:3403:ARG:NH2	2.40	0.53
1:B:3827:GLY:HA2	1:B:3830:GLN:HB2	1.91	0.53
1:C:2654:TYR:HB2	1:C:2661:TRP:HB2	1.91	0.53
1:D:206:CYS:SG	1:D:207:SER:N	2.82	0.53
1:D:1152:MET:HB2	1:D:1161:ILE:HB	1.89	0.53
1:D:2003:GLN:O	1:D:2007:ASN:ND2	2.42	0.53
1:D:3366:ARG:NH1	1:D:3437:MET:SD	2.82	0.53
2:F:38:SER:O	2:F:42:ARG:NH2	2.42	0.53
1:A:1259:ARG:NH2	1:A:1591:CYS:SG	2.82	0.53
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.90	0.53
1:D:1461:ASP:OD2	1:D:1468:LYS:NZ	2.40	0.53
1:B:2023:LEU:O	1:B:2028:ARG:NE	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3366:ARG:NH1	1:B:3437:MET:SD	2.82	0.53
1:C:356:TRP:O	1:C:379:HIS:N	2.42	0.53
2:E:38:SER:O	2:E:42:ARG:NH2	2.42	0.53
2:G:38:SER:O	2:G:42:ARG:NH2	2.42	0.53
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.90	0.53
1:A:3208:PRO:HA	1:A:3211:ASN:HB2	1.89	0.53
1:A:3875:MET:HB3	1:A:3878:ASP:HB3	1.91	0.53
1:B:2480:GLY:O	1:B:2484:ALA:N	2.41	0.53
1:B:3053:ARG:HG3	1:B:3056:LEU:HD22	1.90	0.53
1:B:4983:HIS:O	4:B:5102:ADE:N6	2.39	0.53
1:C:355:LEU:HD22	1:C:380:GLN:HA	1.90	0.53
1:C:1259:ARG:NH2	1:C:1591:CYS:SG	2.82	0.53
1:D:3825:GLU:OE1	1:D:3828:PHE:N	2.36	0.53
1:A:3827:GLY:HA2	1:A:3830:GLN:HB2	1.91	0.53
1:B:455:PRO:HB3	1:B:467:LYS:HD2	1.91	0.53
1:B:3111:ARG:HH12	1:B:3174:SER:HB2	1.74	0.53
1:B:3145:GLN:OE1	1:B:3196:ARG:NE	2.42	0.53
1:B:3875:MET:HB3	1:B:3878:ASP:HB3	1.91	0.53
1:C:497:TYR:O	1:C:553:ARG:NH2	2.37	0.53
1:C:4958:CYS:SG	1:C:4978:HIS:CD2	3.02	0.53
1:B:206:CYS:SG	1:B:207:SER:N	2.82	0.53
1:B:3825:GLU:OE1	1:B:3828:PHE:N	2.36	0.53
1:C:206:CYS:SG	1:C:207:SER:N	2.82	0.53
1:C:455:PRO:HB3	1:C:467:LYS:HD2	1.91	0.53
1:C:707:VAL:HG13	1:C:713:SER:HB2	1.90	0.53
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.90	0.53
1:D:2480:GLY:O	1:D:2484:ALA:N	2.42	0.53
1:D:3111:ARG:HH12	1:D:3174:SER:HB2	1.73	0.53
1:A:497:TYR:O	1:A:553:ARG:NH2	2.37	0.52
1:A:2919:ASP:HA	1:A:2922:LYS:HD2	1.89	0.52
1:B:2927:LEU:HD12	1:B:2930:LEU:HD12	1.92	0.52
1:C:1291:LEU:HD12	1:C:1550:PRO:HG2	1.92	0.52
1:C:3875:MET:HB3	1:C:3878:ASP:HB3	1.91	0.52
1:D:4581:LYS:NZ	1:D:4582:VAL:O	2.38	0.52
1:A:2927:LEU:HD12	1:A:2930:LEU:HD12	1.91	0.52
1:A:3111:ARG:HH12	1:A:3174:SER:HB2	1.74	0.52
1:B:497:TYR:O	1:B:553:ARG:NH2	2.37	0.52
1:B:2507:ASP:OD2	1:B:2564:LYS:NZ	2.41	0.52
1:C:688:LEU:HD23	1:C:690:GLU:H	1.75	0.52
1:C:1461:ASP:OD2	1:C:1468:LYS:NZ	2.40	0.52
1:D:2654:TYR:HB2	1:D:2661:TRP:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4958:CYS:SG	1:D:4978:HIS:CD2	3.02	0.52
2:E:74:LEU:HB2	2:E:99:PHE:HB2	1.90	0.52
1:A:2707:ALA:HB1	1:A:3009:TYR:HD1	1.75	0.52
1:A:3366:ARG:NH1	1:A:3437:MET:SD	2.82	0.52
1:A:3579:LEU:HD12	1:A:3582:ARG:HE	1.75	0.52
1:B:1291:LEU:HD12	1:B:1550:PRO:HG2	1.92	0.52
1:B:3415:TYR:O	1:B:3419:ASN:ND2	2.37	0.52
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.41	0.52
1:C:1733:GLU:OE2	1:C:2163:ARG:NH2	2.41	0.52
1:C:3415:TYR:O	1:C:3419:ASN:ND2	2.37	0.52
1:D:3875:MET:HB3	1:D:3878:ASP:HB3	1.91	0.52
1:A:551:LEU:HD11	1:A:585:SER:HB3	1.90	0.52
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.41	0.52
1:B:2707:ALA:HB1	1:B:3009:TYR:HD1	1.75	0.52
1:B:4958:CYS:SG	1:B:4978:HIS:CD2	3.02	0.52
1:C:551:LEU:HD11	1:C:585:SER:HB3	1.90	0.52
1:C:2707:ALA:HB1	1:C:3009:TYR:HD1	1.75	0.52
1:C:2927:LEU:HD12	1:C:2930:LEU:HD12	1.92	0.52
1:A:4958:CYS:SG	1:A:4978:HIS:CD2	3.02	0.52
1:B:3579:LEU:HD12	1:B:3582:ARG:HE	1.75	0.52
1:B:3603:LEU:HD13	1:B:3606:LEU:HD13	1.92	0.52
1:C:3603:LEU:HD13	1:C:3606:LEU:HD13	1.92	0.52
1:D:355:LEU:HD22	1:D:380:GLN:HA	1.90	0.52
1:D:1291:LEU:HD12	1:D:1550:PRO:HG2	1.91	0.52
1:D:2927:LEU:HD12	1:D:2930:LEU:HD12	1.91	0.52
1:A:3145:GLN:OE1	1:A:3196:ARG:NE	2.42	0.52
1:A:4581:LYS:NZ	1:A:4582:VAL:O	2.38	0.52
1:B:1683:HIS:NE2	1:B:1798:LEU:O	2.36	0.52
1:C:1683:HIS:NE2	1:C:1798:LEU:O	2.36	0.52
1:C:3145:GLN:OE1	1:C:3196:ARG:NE	2.42	0.52
1:C:3366:ARG:NH1	1:C:3437:MET:SD	2.82	0.52
2:H:38:SER:O	2:H:42:ARG:NH2	2.42	0.52
1:A:688:LEU:HD23	1:A:690:GLU:H	1.75	0.52
1:A:1291:LEU:HD12	1:A:1550:PRO:HG2	1.92	0.52
1:B:4057:MET:HA	1:B:4060:LYS:HB3	1.91	0.52
1:D:2707:ALA:HB1	1:D:3009:TYR:HD1	1.75	0.52
1:D:3145:GLN:OE1	1:D:3196:ARG:NE	2.42	0.52
1:D:3579:LEU:HD12	1:D:3582:ARG:HE	1.75	0.52
1:D:3827:GLY:HA2	1:D:3830:GLN:HB2	1.91	0.52
1:A:2452:ARG:NH1	1:B:144:GLU:OE1	2.42	0.52
1:A:2561:LEU:HA	1:A:2564:LYS:HZ3	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2801:ASP:HA	1:A:2804:ILE:HG12	1.92	0.52
1:A:2902:HIS:HB3	1:A:2905:LEU:HG	1.92	0.52
1:B:2777:TYR:HB3	1:B:2791:LEU:HD23	1.92	0.52
1:B:2902:HIS:HB3	1:B:2905:LEU:HG	1.92	0.52
1:C:2902:HIS:HB3	1:C:2905:LEU:HG	1.92	0.52
1:D:356:TRP:O	1:D:379:HIS:N	2.42	0.52
1:D:688:LEU:HD23	1:D:690:GLU:H	1.75	0.52
1:D:2902:HIS:HB3	1:D:2905:LEU:HG	1.92	0.52
1:A:595:ARG:NH1	1:A:1643:GLU:OE2	2.43	0.52
1:A:3641:LEU:HA	1:A:3644:LEU:HD23	1.92	0.52
1:B:356:TRP:O	1:B:379:HIS:N	2.42	0.52
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	2.24	0.52
1:C:2777:TYR:HB3	1:C:2791:LEU:HD23	1.92	0.52
1:C:3825:GLU:OE1	1:C:3828:PHE:N	2.36	0.52
1:D:595:ARG:NH1	1:D:1643:GLU:OE2	2.43	0.52
1:A:15:ARG:HA	1:A:100:THR:HA	1.91	0.52
1:A:2654:TYR:HB2	1:A:2661:TRP:HB2	1.91	0.52
1:A:2967:MET:SD	1:A:2970:SER:OG	2.67	0.52
1:A:2967:MET:O	1:A:2970:SER:OG	2.28	0.52
1:B:2967:MET:O	1:B:2970:SER:OG	2.28	0.52
1:C:355:LEU:HB2	1:C:378:LEU:HG	1.92	0.52
1:D:355:LEU:HB2	1:D:378:LEU:HG	1.92	0.52
1:D:554:LEU:HD11	1:D:1593:PRO:HD3	1.93	0.52
1:D:3603:LEU:HD13	1:D:3606:LEU:HD13	1.92	0.52
1:A:355:LEU:HB2	1:A:378:LEU:HG	1.92	0.51
1:A:554:LEU:HD11	1:A:1593:PRO:HD3	1.92	0.51
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.91	0.51
1:A:2296:GLU:HA	1:A:2299:VAL:HG12	1.93	0.51
1:B:595:ARG:NH1	1:B:1643:GLU:OE2	2.43	0.51
1:B:3751:VAL:HG13	1:B:3756:LYS:HD3	1.93	0.51
1:C:15:ARG:HA	1:C:100:THR:HA	1.92	0.51
1:C:2967:MET:O	1:C:2970:SER:OG	2.28	0.51
1:A:1438:ARG:HA	1:A:1514:LEU:O	2.10	0.51
1:A:3751:VAL:HG13	1:A:3756:LYS:HD3	1.92	0.51
1:B:355:LEU:HB2	1:B:378:LEU:HG	1.92	0.51
1:B:688:LEU:HD23	1:B:690:GLU:H	1.75	0.51
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.93	0.51
1:D:1438:ARG:HA	1:D:1514:LEU:O	2.10	0.51
2:H:21:THR:HG22	2:H:49:ARG:HD2	1.93	0.51
1:B:554:LEU:HD11	1:B:1593:PRO:HD3	1.93	0.51
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3827:GLY:HA2	1:C:3830:GLN:HB2	1.91	0.51
1:D:247:TYR:HB2	1:D:374:LYS:HB2	1.92	0.51
1:D:2296:GLU:HA	1:D:2299:VAL:HG12	1.93	0.51
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.93	0.51
2:F:21:THR:HG22	2:F:49:ARG:HD2	1.93	0.51
1:A:206:CYS:SG	1:A:207:SER:N	2.82	0.51
1:B:2954:ARG:NH1	1:B:3016:TYR:OH	2.44	0.51
1:C:2023:LEU:O	1:C:2028:ARG:NE	2.41	0.51
1:C:3751:VAL:HG13	1:C:3756:LYS:HD3	1.92	0.51
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.91	0.51
1:D:2801:ASP:HA	1:D:2804:ILE:HG12	1.92	0.51
1:D:3204:ALA:HB3	1:D:3214:ASN:HD21	1.74	0.51
1:A:1792:ALA:O	1:A:2176:ASN:ND2	2.38	0.51
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.24	0.51
1:B:1461:ASP:OD2	1:B:1468:LYS:NZ	2.40	0.51
1:B:2992:GLU:OE2	1:B:2996:LYS:NZ	2.41	0.51
1:C:247:TYR:HB2	1:C:374:LYS:HB2	1.92	0.51
1:D:2954:ARG:NH1	1:D:3016:TYR:OH	2.44	0.51
1:A:3603:LEU:HD13	1:A:3606:LEU:HD13	1.92	0.51
1:B:247:TYR:HB2	1:B:374:LYS:HB2	1.92	0.51
1:B:2801:ASP:HA	1:B:2804:ILE:HG12	1.92	0.51
1:C:554:LEU:HD11	1:C:1593:PRO:HD3	1.93	0.51
1:C:3579:LEU:HD12	1:C:3582:ARG:HE	1.75	0.51
1:D:4057:MET:HA	1:D:4060:LYS:HB3	1.91	0.51
2:E:21:THR:HG22	2:E:49:ARG:HD2	1.93	0.51
2:G:21:THR:HG22	2:G:49:ARG:HD2	1.93	0.51
1:A:4219:PHE:HE1	1:A:4946:GLN:HB3	1.76	0.51
1:B:1438:ARG:HA	1:B:1514:LEU:O	2.10	0.51
1:B:3204:ALA:HB3	1:B:3214:ASN:HD21	1.74	0.51
1:C:595:ARG:NH1	1:C:1643:GLU:OE2	2.43	0.51
1:C:844:ARG:NH1	1:C:1197:GLY:HA3	2.21	0.51
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.91	0.51
1:C:1438:ARG:HA	1:C:1514:LEU:O	2.10	0.51
1:D:15:ARG:HA	1:D:100:THR:HA	1.92	0.51
1:D:3329:ILE:O	1:D:3403:ARG:NH2	2.40	0.51
1:A:2954:ARG:NH1	1:A:3016:TYR:OH	2.44	0.51
1:A:4057:MET:HA	1:A:4060:LYS:HB3	1.91	0.51
1:B:788:LYS:HA	1:B:1628:VAL:O	2.11	0.51
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.29	0.51
1:D:2967:MET:O	1:D:2970:SER:OG	2.28	0.51
1:A:356:TRP:O	1:A:379:HIS:N	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:MET:O	1:A:407:THR:OG1	2.19	0.51
1:A:450:GLY:HA2	1:A:453:GLU:HG2	1.93	0.51
1:A:2777:TYR:HB3	1:A:2791:LEU:HD23	1.92	0.51
1:A:2913:ALA:HA	1:A:2916:LYS:HB3	1.93	0.51
1:A:3204:ALA:HB3	1:A:3214:ASN:HD21	1.74	0.51
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.39	0.51
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.33	0.51
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.29	0.51
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.24	0.51
1:D:2777:TYR:HB3	1:D:2791:LEU:HD23	1.92	0.51
1:D:3037:GLU:HG2	1:D:3085:PRO:HD2	1.93	0.51
1:D:3366:ARG:HA	1:D:3441:ILE:HD11	1.93	0.51
1:A:247:TYR:HB2	1:A:374:LYS:HB2	1.92	0.51
1:B:15:ARG:HA	1:B:100:THR:HA	1.92	0.51
1:C:2296:GLU:HA	1:C:2299:VAL:HG12	1.92	0.51
1:C:2507:ASP:OD2	1:C:2564:LYS:NZ	2.41	0.51
1:C:2967:MET:SD	1:C:2970:SER:OG	2.67	0.51
1:C:2992:GLU:OE2	1:C:2996:LYS:NZ	2.41	0.51
1:C:3329:ILE:O	1:C:3403:ARG:NH2	2.40	0.51
1:D:450:GLY:HA2	1:D:453:GLU:HG2	1.93	0.51
2:E:27:THR:HA	2:E:38:SER:HA	1.93	0.51
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.93	0.50
1:B:2296:GLU:HA	1:B:2299:VAL:HG12	1.93	0.50
1:B:3245:VAL:O	1:B:3249:LEU:HB2	2.12	0.50
1:C:2954:ARG:NH1	1:C:3016:TYR:OH	2.44	0.50
1:C:3204:ALA:HB3	1:C:3214:ASN:HD21	1.74	0.50
1:D:2464:ASP:OD1	1:D:2464:ASP:N	2.44	0.50
1:D:3751:VAL:HG13	1:D:3756:LYS:HD3	1.92	0.50
1:D:4219:PHE:HE1	1:D:4946:GLN:HB3	1.76	0.50
2:G:27:THR:HA	2:G:38:SER:HA	1.93	0.50
1:A:2023:LEU:O	1:A:2028:ARG:NE	2.41	0.50
1:A:3037:GLU:HG2	1:A:3085:PRO:HD2	1.93	0.50
1:A:4563:ARG:NH2	1:A:4815:ASP:OD1	2.45	0.50
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.93	0.50
1:B:3641:LEU:HA	1:B:3644:LEU:HD23	1.92	0.50
1:C:2801:ASP:HA	1:C:2804:ILE:HG12	1.92	0.50
1:C:2913:ALA:HA	1:C:2916:LYS:HB3	1.93	0.50
1:D:1944:GLU:HB3	1:D:2123:LEU:HD21	1.93	0.50
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.33	0.50
1:C:4069:LYS:HD3	1:C:4133:GLN:HG3	1.94	0.50
1:C:4853:VAL:O	1:C:4857:ASN:ND2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3641:LEU:HA	1:D:3644:LEU:HD23	1.92	0.50
2:H:78:PRO:HA	2:H:81:ALA:HB3	1.93	0.50
1:A:2992:GLU:OE2	1:A:2996:LYS:NZ	2.41	0.50
1:A:3245:VAL:O	1:A:3249:LEU:HB2	2.11	0.50
1:A:3771:HIS:NE2	1:A:3811:GLU:OE2	2.45	0.50
1:B:2913:ALA:HA	1:B:2916:LYS:HB3	1.93	0.50
1:C:450:GLY:HA2	1:C:453:GLU:HG2	1.93	0.50
1:C:4057:MET:HA	1:C:4060:LYS:HB3	1.91	0.50
1:D:2967:MET:SD	1:D:2970:SER:OG	2.67	0.50
1:D:4069:LYS:HD3	1:D:4133:GLN:HG3	1.94	0.50
1:A:788:LYS:HA	1:A:1628:VAL:O	2.11	0.50
1:B:450:GLY:HA2	1:B:453:GLU:HG2	1.93	0.50
1:B:3052:HIS:NE2	1:B:3128:ASN:OD1	2.45	0.50
1:C:3366:ARG:HA	1:C:3441:ILE:HD11	1.93	0.50
1:D:939:VAL:HB	1:D:1051:TYR:HB3	1.94	0.50
2:F:78:PRO:HA	2:F:81:ALA:HB3	1.93	0.50
2:H:27:THR:HA	2:H:38:SER:HA	1.93	0.50
1:A:939:VAL:HB	1:A:1051:TYR:HB3	1.94	0.50
1:B:3037:GLU:HG2	1:B:3085:PRO:HD2	1.93	0.50
1:B:3104:GLU:HA	1:B:3107:VAL:HG22	1.94	0.50
1:D:3771:HIS:NE2	1:D:3811:GLU:OE2	2.45	0.50
1:B:272:SER:OG	1:B:333:GLY:O	2.29	0.50
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.94	0.50
1:B:4563:ARG:NH2	1:B:4815:ASP:OD1	2.45	0.50
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.45	0.50
1:A:3688:GLU:HG3	1:A:3690:VAL:HG12	1.94	0.50
1:A:4069:LYS:HD3	1:A:4133:GLN:HG3	1.93	0.50
1:A:4938:ASP:OD1	1:D:4944:ARG:NH2	2.45	0.50
1:B:1944:GLU:HB3	1:B:2123:LEU:HD21	1.93	0.50
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.45	0.50
1:D:2913:ALA:HA	1:D:2916:LYS:HB3	1.93	0.50
2:F:27:THR:HA	2:F:38:SER:HA	1.93	0.50
1:A:2464:ASP:OD1	1:A:2464:ASP:N	2.44	0.50
1:A:4853:VAL:O	1:A:4857:ASN:ND2	2.44	0.50
1:B:1724:CYS:SG	1:B:1728:ARG:NH1	2.83	0.50
1:B:2967:MET:SD	1:B:2970:SER:OG	2.67	0.50
1:B:4725:LEU:HA	1:B:4737:ILE:HG21	1.94	0.50
1:C:842:PRO:O	1:C:1197:GLY:N	2.45	0.50
1:C:1640:HIS:HA	1:C:1647:CYS:HA	1.94	0.50
1:C:3354:LEU:HA	1:C:3358:PHE:HB2	1.93	0.50
1:C:4563:ARG:NH2	1:C:4815:ASP:OD1	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLN:NE2	1:A:354:GLY:O	2.45	0.49
1:A:842:PRO:O	1:A:1197:GLY:N	2.45	0.49
1:B:1640:HIS:HA	1:B:1647:CYS:HA	1.94	0.49
1:C:3052:HIS:NE2	1:C:3128:ASN:OD1	2.45	0.49
1:C:3641:LEU:HA	1:C:3644:LEU:HD23	1.92	0.49
1:D:710:ASP:N	1:D:710:ASP:OD1	2.45	0.49
2:G:78:PRO:HA	2:G:81:ALA:HB3	1.93	0.49
1:A:1944:GLU:HB3	1:A:2123:LEU:HD21	1.93	0.49
1:A:3188:PRO:O	1:A:3191:GLY:N	2.45	0.49
1:B:939:VAL:HB	1:B:1051:TYR:HB3	1.94	0.49
1:C:272:SER:OG	1:C:333:GLY:O	2.29	0.49
1:C:3771:HIS:NE2	1:C:3811:GLU:OE2	2.45	0.49
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.95	0.49
1:D:3104:GLU:HA	1:D:3107:VAL:HG22	1.94	0.49
1:D:3524:MET:O	1:D:3595:ARG:NH1	2.45	0.49
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.41	0.49
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.95	0.49
1:A:3965:LEU:HA	1:A:3968:TYR:HD2	1.78	0.49
1:B:2464:ASP:OD1	1:B:2464:ASP:N	2.44	0.49
1:B:3188:PRO:O	1:B:3191:GLY:N	2.45	0.49
1:B:3771:HIS:NE2	1:B:3811:GLU:OE2	2.45	0.49
1:C:1944:GLU:HB3	1:C:2123:LEU:HD21	1.93	0.49
1:C:3037:GLU:HG2	1:C:3085:PRO:HD2	1.93	0.49
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.41	0.49
1:D:3245:VAL:O	1:D:3249:LEU:HB2	2.11	0.49
1:A:3159:ASP:OD1	1:A:3159:ASP:N	2.46	0.49
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.45	0.49
1:B:4069:LYS:HD3	1:B:4133:GLN:HG3	1.94	0.49
1:C:1698:LEU:O	1:C:1712:TYR:OH	2.28	0.49
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.45	0.49
1:D:272:SER:OG	1:D:333:GLY:O	2.29	0.49
1:D:1640:HIS:HA	1:D:1647:CYS:HA	1.94	0.49
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.94	0.49
1:A:1640:HIS:HA	1:A:1647:CYS:HA	1.94	0.49
1:A:3524:MET:O	1:A:3595:ARG:NH1	2.45	0.49
1:C:788:LYS:HA	1:C:1628:VAL:O	2.11	0.49
1:C:3187:ARG:HD3	1:C:3271:GLU:HG3	1.94	0.49
1:C:3188:PRO:O	1:C:3191:GLY:N	2.45	0.49
1:D:743:VAL:HB	1:D:760:ASN:HA	1.95	0.49
1:D:4563:ARG:NH2	1:D:4815:ASP:OD1	2.45	0.49
1:A:1699:GLU:OE2	1:A:1813:ARG:NH2	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1724:CYS:SG	1:A:1728:ARG:NH1	2.83	0.49
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.45	0.49
1:A:3052:HIS:NE2	1:A:3128:ASN:OD1	2.45	0.49
1:B:842:PRO:O	1:B:1197:GLY:N	2.45	0.49
1:B:3354:LEU:HA	1:B:3358:PHE:HB2	1.93	0.49
1:B:3366:ARG:HA	1:B:3441:ILE:HD11	1.93	0.49
1:B:3965:LEU:HA	1:B:3968:TYR:HD2	1.78	0.49
1:B:4179:GLY:O	1:B:4194:TYR:HA	2.12	0.49
1:C:939:VAL:HB	1:C:1051:TYR:HB3	1.94	0.49
1:C:4090:LYS:HG2	1:C:4123:ILE:HD11	1.95	0.49
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.36	0.49
1:D:1724:CYS:SG	1:D:1728:ARG:NH1	2.83	0.49
1:D:3188:PRO:O	1:D:3191:GLY:N	2.45	0.49
1:D:3354:LEU:HA	1:D:3358:PHE:HB2	1.93	0.49
1:B:3688:GLU:HG3	1:B:3690:VAL:HG12	1.94	0.49
1:B:4219:PHE:HE1	1:B:4946:GLN:HB3	1.76	0.49
1:B:4848:VAL:HG11	1:B:4887:MET:HG3	1.95	0.49
1:C:877:ASN:HA	1:C:970:LEU:H	1.78	0.49
1:C:2464:ASP:N	1:C:2464:ASP:OD1	2.44	0.49
1:C:3524:MET:O	1:C:3595:ARG:NH1	2.45	0.49
1:D:4848:VAL:HG11	1:D:4887:MET:HG3	1.95	0.49
1:B:3752:SER:OG	1:B:3755:GLU:OE1	2.25	0.49
1:C:710:ASP:OD1	1:C:710:ASP:N	2.45	0.49
1:C:1642:PRO:O	1:C:1645:ASN:ND2	2.46	0.49
1:C:3245:VAL:O	1:C:3249:LEU:HB2	2.11	0.49
1:C:3886:ARG:NH1	1:C:3889:GLN:OE1	2.46	0.49
1:D:3688:GLU:HG3	1:D:3690:VAL:HG12	1.94	0.49
1:D:4090:LYS:HG2	1:D:4123:ILE:HD11	1.95	0.49
1:D:4179:GLY:O	1:D:4194:TYR:HA	2.12	0.49
2:G:68:LEU:HA	2:G:103:LEU:HD22	1.95	0.49
1:A:27:THR:OG1	1:A:32:GLN:OE1	2.28	0.49
1:A:2102:VAL:HG13	1:A:2120:MET:HG2	1.95	0.49
1:A:2640:PRO:HA	1:A:2643:LEU:HB3	1.95	0.49
1:A:3104:GLU:HA	1:A:3107:VAL:HG22	1.94	0.49
1:B:796:ARG:O	1:B:1619:ARG:NH2	2.45	0.49
1:C:743:VAL:HB	1:C:760:ASN:HA	1.95	0.49
1:C:1724:CYS:SG	1:C:1728:ARG:NH1	2.83	0.49
1:C:3414:ARG:HE	1:C:3472:ALA:HB3	1.78	0.49
1:C:3965:LEU:HA	1:C:3968:TYR:HD2	1.78	0.49
1:C:4179:GLY:O	1:C:4194:TYR:HA	2.12	0.49
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.24	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2640:PRO:HA	1:D:2643:LEU:HB3	1.95	0.49
1:D:3052:HIS:NE2	1:D:3128:ASN:OD1	2.45	0.49
1:D:3414:ARG:HE	1:D:3472:ALA:HB3	1.78	0.49
1:D:4152:GLU:OE2	1:D:4192:ARG:NH1	2.46	0.49
1:D:4725:LEU:HA	1:D:4737:ILE:HG21	1.94	0.49
2:F:68:LEU:HA	2:F:103:LEU:HD22	1.95	0.49
1:A:877:ASN:HA	1:A:970:LEU:H	1.78	0.49
1:A:2862:LEU:O	1:A:2928:LYS:NZ	2.41	0.49
1:A:4848:VAL:HG11	1:A:4887:MET:HG3	1.95	0.49
1:C:4725:LEU:HA	1:C:4737:ILE:HG21	1.94	0.49
1:C:4848:VAL:HG11	1:C:4887:MET:HG3	1.95	0.49
1:D:796:ARG:O	1:D:1619:ARG:NH2	2.45	0.49
1:D:3187:ARG:HD3	1:D:3271:GLU:HG3	1.94	0.49
2:E:78:PRO:HA	2:E:81:ALA:HB3	1.93	0.49
2:H:68:LEU:HA	2:H:103:LEU:HD22	1.95	0.49
1:A:4090:LYS:HG2	1:A:4123:ILE:HD11	1.95	0.48
1:A:4548:ARG:HE	1:A:4548:ARG:HB3	1.43	0.48
1:B:1642:PRO:O	1:B:1645:ASN:ND2	2.46	0.48
1:B:2309:SER:OG	1:B:2321:ILE:O	2.26	0.48
1:B:3187:ARG:HD3	1:B:3271:GLU:HG3	1.94	0.48
1:C:4214:LYS:HB3	1:C:4214:LYS:HE2	1.61	0.48
1:D:875:ALA:O	1:D:879:HIS:ND1	2.46	0.48
1:D:877:ASN:HA	1:D:970:LEU:H	1.78	0.48
1:D:2023:LEU:O	1:D:2028:ARG:NE	2.41	0.48
1:D:3415:TYR:O	1:D:3419:ASN:ND2	2.37	0.48
1:D:3965:LEU:HA	1:D:3968:TYR:HD2	1.78	0.48
1:A:4725:LEU:HA	1:A:4737:ILE:HG21	1.94	0.48
1:B:3566:SER:HB3	1:B:3569:LEU:HG	1.95	0.48
1:B:4704:LEU:O	1:B:4774:LYS:NZ	2.36	0.48
1:C:4152:GLU:OE2	1:C:4192:ARG:NH1	2.46	0.48
1:C:4219:PHE:HE1	1:C:4946:GLN:HB3	1.76	0.48
1:D:842:PRO:O	1:D:1197:GLY:N	2.45	0.48
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.94	0.48
1:D:2431:ASP:HB2	1:D:2501:SER:HB3	1.96	0.48
2:G:24:VAL:HG12	2:G:103:LEU:HA	1.95	0.48
1:B:1525:GLY:O	1:B:1541:GLN:HA	2.13	0.48
1:C:796:ARG:O	1:C:1619:ARG:NH2	2.45	0.48
1:C:2431:ASP:HB2	1:C:2501:SER:HB3	1.95	0.48
1:C:4888:TYR:HD2	1:C:4889:VAL:HG22	1.78	0.48
1:D:349:GLN:NE2	1:D:354:GLY:O	2.44	0.48
1:D:788:LYS:HA	1:D:1628:VAL:O	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2102:VAL:HG13	1:D:2120:MET:HG2	1.95	0.48
1:D:2309:SER:OG	1:D:2321:ILE:O	2.26	0.48
1:D:3524:MET:HA	1:D:3582:ARG:HH22	1.78	0.48
2:F:24:VAL:HG12	2:F:103:LEU:HA	1.95	0.48
1:A:3354:LEU:HA	1:A:3358:PHE:HB2	1.93	0.48
1:A:4918:ILE:HD11	1:D:4888:TYR:HA	1.94	0.48
1:B:877:ASN:HA	1:B:970:LEU:H	1.78	0.48
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.95	0.48
1:B:1863:LEU:HD13	1:B:1866:ILE:HD11	1.95	0.48
1:B:2640:PRO:HA	1:B:2643:LEU:HB3	1.95	0.48
1:B:4152:GLU:OE2	1:B:4192:ARG:NH1	2.46	0.48
1:C:4581:LYS:NZ	1:C:4582:VAL:O	2.38	0.48
1:D:1699:GLU:OE2	1:D:1813:ARG:NH2	2.38	0.48
1:A:1175:SER:OG	1:A:1180:ARG:NH2	2.47	0.48
1:A:4152:GLU:OE2	1:A:4192:ARG:NH1	2.46	0.48
1:A:4179:GLY:O	1:A:4194:TYR:HA	2.12	0.48
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.94	0.48
1:B:2514:ASN:OD1	1:B:2514:ASN:N	2.45	0.48
1:B:2627:VAL:HG22	1:B:2678:LEU:HG	1.95	0.48
1:B:3414:ARG:HE	1:B:3472:ALA:HB3	1.78	0.48
1:B:3524:MET:HA	1:B:3582:ARG:HH22	1.78	0.48
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.94	0.48
1:C:1525:GLY:O	1:C:1541:GLN:HA	2.13	0.48
1:C:1863:LEU:HD13	1:C:1866:ILE:HD11	1.95	0.48
1:C:2640:PRO:HA	1:C:2643:LEU:HB3	1.95	0.48
1:C:3104:GLU:HA	1:C:3107:VAL:HG22	1.94	0.48
1:D:1525:GLY:O	1:D:1541:GLN:HA	2.13	0.48
1:D:2507:ASP:OD2	1:D:2564:LYS:NZ	2.41	0.48
1:A:345:LEU:HB3	1:A:387:ALA:HB1	1.96	0.48
1:A:2616:PRO:HA	1:A:2619:LEU:HB2	1.96	0.48
1:A:3171:SER:O	1:A:3174:SER:OG	2.28	0.48
1:B:111:HIS:ND1	1:B:114:SER:OG	2.35	0.48
1:B:2107:GLN:O	1:B:3683:GLN:NE2	2.47	0.48
1:B:4853:VAL:O	1:B:4857:ASN:ND2	2.44	0.48
1:C:2742:THR:HG22	1:C:2815:ALA:HB2	1.96	0.48
1:C:3566:SER:HB3	1:C:3569:LEU:HG	1.95	0.48
1:D:2616:PRO:HA	1:D:2619:LEU:HB2	1.96	0.48
1:D:4888:TYR:HD2	1:D:4889:VAL:HG22	1.78	0.48
2:H:24:VAL:HG12	2:H:103:LEU:HA	1.95	0.48
1:A:743:VAL:HB	1:A:760:ASN:HA	1.95	0.48
1:A:796:ARG:O	1:A:1619:ARG:NH2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:ILE:HG12	1:D:3424:LEU:HD11	1.96	0.48
1:A:3414:ARG:HE	1:A:3472:ALA:HB3	1.78	0.48
1:B:875:ALA:O	1:B:879:HIS:ND1	2.46	0.48
1:B:2102:VAL:HG13	1:B:2120:MET:HG2	1.95	0.48
1:B:4090:LYS:HG2	1:B:4123:ILE:HD11	1.95	0.48
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.94	0.48
1:C:1296:GLN:HA	1:C:1546:THR:O	2.14	0.48
1:C:3688:GLU:HG3	1:C:3690:VAL:HG12	1.94	0.48
1:C:4892:ARG:HD3	1:D:4918:ILE:HD13	1.96	0.48
1:D:345:LEU:HB3	1:D:387:ALA:HB1	1.96	0.48
1:D:1295:VAL:O	1:D:1547:LYS:HA	2.14	0.48
1:D:2561:LEU:HA	1:D:2564:LYS:HZ3	1.78	0.48
2:F:99:PHE:HB3	2:F:101:VAL:HG23	1.96	0.48
1:A:1525:GLY:O	1:A:1541:GLN:HA	2.13	0.48
1:A:3886:ARG:NH1	1:A:3889:GLN:OE1	2.46	0.48
1:B:349:GLN:NE2	1:B:354:GLY:O	2.44	0.48
1:B:710:ASP:OD1	1:B:710:ASP:N	2.45	0.48
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	1.96	0.48
1:B:1175:SER:OG	1:B:1180:ARG:NH2	2.47	0.48
1:B:1296:GLN:HA	1:B:1546:THR:O	2.14	0.48
1:B:2522:LEU:HD12	1:B:2526:PHE:HB2	1.95	0.48
1:B:4157:ASP:OD1	1:B:4159:ARG:NH1	2.47	0.48
1:C:345:LEU:HB3	1:C:387:ALA:HB1	1.96	0.48
1:C:875:ALA:O	1:C:879:HIS:ND1	2.46	0.48
1:C:2107:GLN:O	1:C:3683:GLN:NE2	2.47	0.48
1:D:844:ARG:NH1	1:D:1197:GLY:HA3	2.21	0.48
1:D:1698:LEU:O	1:D:1712:TYR:OH	2.28	0.48
1:D:1863:LEU:HD13	1:D:1866:ILE:HD11	1.95	0.48
1:D:2742:THR:HG22	1:D:2815:ALA:HB2	1.96	0.48
1:A:875:ALA:O	1:A:879:HIS:ND1	2.46	0.48
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	1.96	0.48
1:A:1295:VAL:O	1:A:1547:LYS:HA	2.14	0.48
1:A:2017:ASP:OD1	1:A:2017:ASP:N	2.47	0.48
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.39	0.48
1:A:3366:ARG:HA	1:A:3441:ILE:HD11	1.93	0.48
1:B:2616:PRO:HA	1:B:2619:LEU:HB2	1.96	0.48
1:B:4892:ARG:HD3	1:C:4918:ILE:HD13	1.96	0.48
1:C:2102:VAL:HG13	1:C:2120:MET:HG2	1.95	0.48
1:C:2522:LEU:HD12	1:C:2526:PHE:HB2	1.95	0.48
1:C:3524:MET:HA	1:C:3582:ARG:HH22	1.79	0.48
1:A:710:ASP:N	1:A:710:ASP:OD1	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.95	0.48
1:A:1642:PRO:O	1:A:1645:ASN:ND2	2.46	0.48
1:A:2469:ILE:HA	1:A:2472:LEU:HG	1.96	0.48
1:A:2522:LEU:HD12	1:A:2526:PHE:HB2	1.95	0.48
1:A:4627:MET:H	1:A:4627:MET:HG3	1.42	0.48
1:B:3130:THR:HA	1:B:3133:THR:HG22	1.96	0.48
1:C:2736:ASP:HA	1:C:2891:LYS:HE2	1.96	0.48
1:D:2522:LEU:HD12	1:D:2526:PHE:HB2	1.95	0.48
1:A:3187:ARG:HD3	1:A:3271:GLU:HG3	1.95	0.47
1:B:3927:GLN:HA	1:B:3992:PHE:HE1	1.79	0.47
1:B:4888:TYR:HD2	1:B:4889:VAL:HG22	1.78	0.47
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.95	0.47
1:C:4704:LEU:O	1:C:4774:LYS:NZ	2.36	0.47
1:C:4722:ARG:H	1:C:4722:ARG:HG2	1.45	0.47
1:D:1864:LYS:NZ	1:D:1871:PHE:O	2.45	0.47
2:E:68:LEU:HA	2:E:103:LEU:HD22	1.95	0.47
1:A:1296:GLN:HA	1:A:1546:THR:O	2.14	0.47
1:A:2736:ASP:HA	1:A:2891:LYS:HE2	1.96	0.47
1:B:1295:VAL:O	1:B:1547:LYS:HA	2.14	0.47
1:B:2742:THR:HG22	1:B:2815:ALA:HB2	1.96	0.47
1:C:2616:PRO:HA	1:C:2619:LEU:HB2	1.96	0.47
1:D:1175:SER:OG	1:D:1180:ARG:NH2	2.47	0.47
1:D:1642:PRO:O	1:D:1645:ASN:ND2	2.46	0.47
1:D:2469:ILE:HA	1:D:2472:LEU:HG	1.96	0.47
2:G:99:PHE:HB3	2:G:101:VAL:HG23	1.96	0.47
1:A:3519:PRO:HB3	1:B:1220:GLN:HB2	1.96	0.47
1:A:3566:SER:HB3	1:A:3569:LEU:HG	1.95	0.47
1:A:4157:ASP:OD1	1:A:4159:ARG:NH1	2.47	0.47
1:B:345:LEU:HB3	1:B:387:ALA:HB1	1.96	0.47
1:B:2736:ASP:HA	1:B:2891:LYS:HE2	1.96	0.47
1:C:1776:HIS:HB3	1:C:1798:LEU:HD13	1.97	0.47
1:C:3130:THR:HA	1:C:3133:THR:HG22	1.96	0.47
1:D:1296:GLN:HA	1:D:1546:THR:O	2.14	0.47
1:D:2736:ASP:HA	1:D:2891:LYS:HE2	1.96	0.47
1:D:3195:ALA:HB2	1:D:3275:PRO:HB3	1.97	0.47
1:D:4627:MET:H	1:D:4627:MET:HG3	1.42	0.47
2:E:24:VAL:HG12	2:E:103:LEU:HA	1.95	0.47
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.36	0.47
1:C:4138:ASP:OD1	1:C:4139:ILE:N	2.48	0.47
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.95	0.47
1:A:4888:TYR:HD2	1:A:4889:VAL:HG22	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:VAL:HB	1:B:760:ASN:HA	1.95	0.47
1:B:1776:HIS:HB3	1:B:1798:LEU:HD13	1.97	0.47
1:C:592:LYS:HB3	1:C:1592:PRO:HB3	1.97	0.47
1:C:1175:SER:OG	1:C:1180:ARG:NH2	2.47	0.47
1:D:2107:GLN:O	1:D:3683:GLN:NE2	2.47	0.47
1:D:3842:LEU:HB2	1:D:3929:SER:HB2	1.97	0.47
1:A:1863:LEU:HD13	1:A:1866:ILE:HD11	1.95	0.47
1:A:3524:MET:HA	1:A:3582:ARG:HH22	1.79	0.47
1:B:688:LEU:HD22	1:B:712:TYR:HD1	1.80	0.47
1:B:733:PRO:HG2	1:B:762:CYS:HB3	1.97	0.47
1:B:2689:LYS:O	1:B:2993:GLN:NE2	2.47	0.47
1:B:4138:ASP:OD1	1:B:4139:ILE:N	2.48	0.47
1:C:3195:ALA:HB2	1:C:3275:PRO:HB3	1.97	0.47
1:C:4157:ASP:OD1	1:C:4159:ARG:NH1	2.47	0.47
1:D:688:LEU:HD22	1:D:712:TYR:HD1	1.80	0.47
1:D:3130:THR:HA	1:D:3133:THR:HG22	1.96	0.47
2:E:99:PHE:HB3	2:E:101:VAL:HG23	1.96	0.47
1:A:592:LYS:HB3	1:A:1592:PRO:HB3	1.97	0.47
1:A:688:LEU:HD22	1:A:712:TYR:HD1	1.80	0.47
1:A:733:PRO:HG2	1:A:762:CYS:HB3	1.97	0.47
1:A:2617:SER:OG	1:A:2618:MET:SD	2.72	0.47
1:B:567:VAL:HG13	1:B:568:LEU:HD12	1.97	0.47
1:B:592:LYS:HB3	1:B:1592:PRO:HB3	1.97	0.47
1:B:2431:ASP:HB2	1:B:2501:SER:HB3	1.95	0.47
1:B:5030:LYS:HB2	1:B:5030:LYS:HE2	1.59	0.47
1:C:1699:GLU:OE2	1:C:1813:ARG:NH2	2.38	0.47
1:C:2689:LYS:O	1:C:2993:GLN:NE2	2.47	0.47
1:D:27:THR:OG1	1:D:32:GLN:OE1	2.28	0.47
1:D:592:LYS:HB3	1:D:1592:PRO:HB3	1.97	0.47
1:D:884:LEU:HD13	1:D:968:ALA:H	1.80	0.47
1:D:3886:ARG:NH1	1:D:3889:GLN:OE1	2.46	0.47
1:D:3927:GLN:HA	1:D:3992:PHE:HE1	1.79	0.47
1:D:4157:ASP:OD1	1:D:4159:ARG:NH1	2.47	0.47
1:A:1776:HIS:HB3	1:A:1798:LEU:HD13	1.97	0.47
1:A:2742:THR:HG22	1:A:2815:ALA:HB2	1.96	0.47
1:A:2817:ILE:HG13	1:A:2822:THR:HA	1.96	0.47
1:A:3130:THR:HA	1:A:3133:THR:HG22	1.96	0.47
1:A:4823:LEU:HD23	1:A:4823:LEU:HA	1.80	0.47
1:C:673:PRO:HB3	2:G:71:ARG:HH22	1.80	0.47
1:C:884:LEU:HD13	1:C:968:ALA:H	1.80	0.47
1:C:1077:ALA:HA	1:C:1236:THR:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2627:VAL:HG22	1:C:2678:LEU:HG	1.95	0.47
1:D:567:VAL:HG13	1:D:568:LEU:HD12	1.97	0.47
1:D:4138:ASP:OD1	1:D:4139:ILE:N	2.48	0.47
1:A:272:SER:OG	1:A:333:GLY:O	2.29	0.47
1:A:2107:GLN:O	1:A:3683:GLN:NE2	2.47	0.47
1:A:2431:ASP:HB2	1:A:2501:SER:HB3	1.96	0.47
1:B:844:ARG:NH1	1:B:1197:GLY:HA3	2.21	0.47
1:B:3886:ARG:NH1	1:B:3889:GLN:OE1	2.46	0.47
1:B:4772:ASP:HB3	1:B:4775:TYR:HB3	1.97	0.47
1:C:349:GLN:NE2	1:C:354:GLY:O	2.44	0.47
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	1.96	0.47
1:C:4548:ARG:HE	1:C:4548:ARG:HB3	1.43	0.47
1:D:673:PRO:HB3	2:H:71:ARG:HH22	1.80	0.47
1:D:733:PRO:HG2	1:D:762:CYS:HB3	1.97	0.47
1:D:1077:ALA:HA	1:D:1236:THR:HG22	1.96	0.47
1:D:2627:VAL:HG22	1:D:2678:LEU:HG	1.95	0.47
2:H:99:PHE:HB3	2:H:101:VAL:HG23	1.96	0.47
1:A:572:PRO:HA	1:A:575:LEU:HD13	1.97	0.47
1:A:1232:ARG:NH2	1:A:1828:ASP:O	2.36	0.47
1:A:2627:VAL:HG22	1:A:2678:LEU:HG	1.96	0.47
1:A:4902:GLU:O	1:A:4913:ARG:NH2	2.32	0.47
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.36	0.47
1:C:1295:VAL:O	1:C:1547:LYS:HA	2.14	0.47
1:C:4190:ILE:H	1:C:4190:ILE:HG12	1.43	0.47
1:D:2689:LYS:O	1:D:2993:GLN:NE2	2.47	0.47
2:G:23:VAL:HG22	2:G:47:LYS:HB3	1.97	0.47
1:A:567:VAL:HG13	1:A:568:LEU:HD12	1.97	0.46
1:A:603:LEU:HA	1:A:606:LEU:HD12	1.98	0.46
1:A:2689:LYS:O	1:A:2993:GLN:NE2	2.47	0.46
1:B:1077:ALA:HA	1:B:1236:THR:HG22	1.96	0.46
1:B:2469:ILE:HA	1:B:2472:LEU:HG	1.96	0.46
1:B:2817:ILE:HG13	1:B:2822:THR:HA	1.96	0.46
1:C:567:VAL:HG13	1:C:568:LEU:HD12	1.97	0.46
1:C:688:LEU:HD22	1:C:712:TYR:HD1	1.80	0.46
1:C:2469:ILE:HA	1:C:2472:LEU:HG	1.96	0.46
1:C:3337:ARG:HA	1:C:3340:VAL:HG12	1.97	0.46
1:C:4772:ASP:HB3	1:C:4775:TYR:HB3	1.97	0.46
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	1.96	0.46
1:D:4677:LEU:HD12	1:D:4677:LEU:HA	1.83	0.46
1:D:4853:VAL:O	1:D:4857:ASN:ND2	2.44	0.46
1:A:3195:ALA:HB2	1:A:3275:PRO:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3927:GLN:HA	1:A:3992:PHE:HE1	1.79	0.46
1:A:4168:GLU:O	1:A:4171:LEU:N	2.48	0.46
1:A:4576:ILE:HD13	1:A:4639:MET:HB3	1.97	0.46
1:B:2625:ARG:NE	1:B:2629:ASP:OD2	2.47	0.46
1:B:3343:GLN:NE2	1:B:3469:PHE:O	2.47	0.46
1:C:2817:ILE:HG13	1:C:2822:THR:HA	1.96	0.46
1:D:3566:SER:HB3	1:D:3569:LEU:HG	1.95	0.46
2:E:62:GLY:O	2:E:66:MET:HG3	2.16	0.46
2:G:62:GLY:O	2:G:66:MET:HG3	2.16	0.46
1:A:1461:ASP:OD2	1:A:1468:LYS:NZ	2.40	0.46
1:A:3805:LEU:HB3	1:A:3890:LEU:HB3	1.98	0.46
1:A:4138:ASP:OD1	1:A:4139:ILE:N	2.48	0.46
1:A:4772:ASP:HB3	1:A:4775:TYR:HB3	1.97	0.46
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.15	0.46
1:B:2815:ALA:HB1	1:B:2881:ASN:HD21	1.80	0.46
1:B:3454:GLU:HA	1:B:3457:ASN:HB2	1.98	0.46
1:B:4151:SER:HA	1:B:4160:LEU:HD21	1.97	0.46
1:C:3157:ILE:HG23	1:C:3161:VAL:HG12	1.98	0.46
1:C:3752:SER:OG	1:C:3755:GLU:OE1	2.25	0.46
1:C:3842:LEU:HB2	1:C:3929:SER:HB2	1.97	0.46
1:D:3343:GLN:NE2	1:D:3469:PHE:O	2.47	0.46
1:D:4958:CYS:HB3	1:D:4961:CYS:SG	2.56	0.46
2:F:62:GLY:O	2:F:66:MET:HG3	2.16	0.46
1:B:884:LEU:HD13	1:B:968:ALA:H	1.80	0.46
1:B:1851:MET:HB3	1:B:1853:ILE:HG12	1.98	0.46
1:B:2017:ASP:N	1:B:2017:ASP:OD1	2.47	0.46
1:B:4214:LYS:HB3	1:B:4214:LYS:HE2	1.61	0.46
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.15	0.46
1:C:4861:LYS:H	1:C:4861:LYS:HG3	1.46	0.46
1:D:2815:ALA:HB1	1:D:2881:ASN:HD21	1.80	0.46
1:D:4151:SER:HA	1:D:4160:LEU:HD21	1.97	0.46
2:H:62:GLY:O	2:H:66:MET:HG3	2.16	0.46
1:A:5030:LYS:HB2	1:A:5030:LYS:HE2	1.59	0.46
1:B:1698:LEU:O	1:B:1712:TYR:OH	2.28	0.46
1:B:3157:ILE:HG23	1:B:3161:VAL:HG12	1.97	0.46
1:B:4576:ILE:HD13	1:B:4639:MET:HB3	1.97	0.46
1:C:2561:LEU:HA	1:C:2564:LYS:HZ3	1.81	0.46
1:C:3454:GLU:HA	1:C:3457:ASN:HB2	1.98	0.46
1:D:4772:ASP:HB3	1:D:4775:TYR:HB3	1.97	0.46
2:E:23:VAL:HG22	2:E:47:LYS:HB3	1.97	0.46
2:F:23:VAL:HG22	2:F:47:LYS:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASP:HA	1:A:422:SER:HB3	1.98	0.46
1:A:573:GLU:O	1:A:577:ILE:HG12	2.16	0.46
1:A:826:ILE:HG22	1:A:827:LYS:HD2	1.98	0.46
1:A:884:LEU:HD13	1:A:968:ALA:H	1.80	0.46
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.24	0.46
1:A:2815:ALA:HB1	1:A:2881:ASN:HD21	1.80	0.46
1:B:3195:ALA:HB2	1:B:3275:PRO:HB3	1.97	0.46
1:B:3421:ALA:O	1:B:3425:THR:OG1	2.28	0.46
1:B:3713:LYS:NZ	1:B:3715:LYS:O	2.42	0.46
1:B:3932:ASP:HA	1:B:3935:TRP:HB2	1.98	0.46
1:C:826:ILE:HG22	1:C:827:LYS:HD2	1.98	0.46
1:C:1099:GLU:OE2	1:C:1101:ARG:NE	2.46	0.46
1:C:3927:GLN:HA	1:C:3992:PHE:HE1	1.79	0.46
1:C:4958:CYS:HB3	1:C:4961:CYS:SG	2.55	0.46
1:D:3157:ILE:HG23	1:D:3161:VAL:HG12	1.98	0.46
1:D:3337:ARG:HA	1:D:3340:VAL:HG12	1.97	0.46
1:D:4190:ILE:N	1:D:5031:GLN:HE22	2.14	0.46
1:D:4214:LYS:HE2	1:D:4214:LYS:HB3	1.61	0.46
1:D:5030:LYS:HE2	1:D:5030:LYS:HB2	1.59	0.46
1:A:1077:ALA:HA	1:A:1236:THR:HG22	1.96	0.46
1:A:4958:CYS:HB3	1:A:4961:CYS:SG	2.55	0.46
1:B:403:MET:O	1:B:407:THR:OG1	2.19	0.46
1:B:3842:LEU:HB2	1:B:3929:SER:HB2	1.97	0.46
1:C:733:PRO:HG2	1:C:762:CYS:HB3	1.97	0.46
1:C:1851:MET:HB3	1:C:1853:ILE:HG12	1.98	0.46
1:C:1864:LYS:NZ	1:C:1871:PHE:O	2.45	0.46
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.15	0.46
1:A:844:ARG:NH1	1:A:1197:GLY:HA3	2.21	0.46
1:A:1965:TYR:OH	1:A:2027:ILE:O	2.31	0.46
1:B:603:LEU:HA	1:B:606:LEU:HD12	1.98	0.46
1:B:4580:TYR:HE2	1:B:4630:TYR:HB3	1.81	0.46
1:B:4958:CYS:HB3	1:B:4961:CYS:SG	2.55	0.46
1:C:224:HIS:CD2	1:C:225:GLY:H	2.34	0.46
1:D:546:TRP:O	1:D:549:SER:OG	2.28	0.46
1:D:573:GLU:O	1:D:577:ILE:HG12	2.16	0.46
1:D:826:ILE:HG22	1:D:827:LYS:HD2	1.98	0.46
1:D:2973:PHE:HB2	1:D:2991:HIS:CD2	2.51	0.46
1:D:3254:GLY:HA2	1:D:3318:ASN:ND2	2.31	0.46
1:D:4867:GLU:H	1:D:4867:GLU:HG2	1.35	0.46
1:A:3254:GLY:HA2	1:A:3318:ASN:ND2	2.31	0.46
1:A:3752:SER:OG	1:A:3755:GLU:OE1	2.25	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:PRO:HA	1:B:575:LEU:HD13	1.97	0.46
1:C:572:PRO:HA	1:C:575:LEU:HD13	1.97	0.46
1:C:2616:PRO:HG3	1:C:2647:HIS:HE1	1.81	0.46
1:C:2625:ARG:NE	1:C:2629:ASP:OD2	2.47	0.46
1:C:2973:PHE:HB2	1:C:2991:HIS:CD2	2.51	0.46
1:C:4151:SER:HA	1:C:4160:LEU:HD21	1.97	0.46
1:D:414:PHE:HA	1:D:436:LEU:HD22	1.98	0.46
1:D:419:ASP:HA	1:D:422:SER:HB3	1.98	0.46
1:D:572:PRO:HA	1:D:575:LEU:HD13	1.97	0.46
1:D:1776:HIS:HB3	1:D:1798:LEU:HD13	1.97	0.46
1:D:1851:MET:HB3	1:D:1853:ILE:HG12	1.98	0.46
1:D:2286:LEU:HD12	1:D:2286:LEU:HA	1.82	0.46
1:D:3454:GLU:HA	1:D:3457:ASN:HB2	1.97	0.46
1:A:224:HIS:CD2	1:A:225:GLY:H	2.34	0.46
1:A:2443:ILE:HD12	1:A:2454:ARG:HE	1.81	0.46
1:A:3454:GLU:HA	1:A:3457:ASN:HB2	1.98	0.46
1:A:4183:ILE:HG12	1:A:4193:ILE:HD11	1.98	0.46
1:A:4190:ILE:N	1:A:5031:GLN:HE22	2.14	0.46
1:A:4677:LEU:HD12	1:A:4677:LEU:HA	1.82	0.46
1:B:27:THR:OG1	1:B:32:GLN:OE1	2.28	0.46
1:B:3805:LEU:HB3	1:B:3890:LEU:HB3	1.98	0.46
1:C:2443:ILE:HD12	1:C:2454:ARG:HE	1.81	0.46
1:D:2817:ILE:HG13	1:D:2822:THR:HA	1.96	0.46
1:D:3674:ILE:HD13	1:D:3770:LEU:HD21	1.98	0.46
1:D:4902:GLU:O	1:D:4913:ARG:NH2	2.32	0.46
1:A:1851:MET:HB3	1:A:1853:ILE:HG12	1.98	0.45
1:B:3392:LEU:HA	1:B:3395:ARG:HD2	1.98	0.45
1:C:2815:ALA:HB1	1:C:2881:ASN:HD21	1.80	0.45
1:C:3890:LEU:HD23	1:C:3890:LEU:HA	1.85	0.45
1:D:4183:ILE:HG12	1:D:4193:ILE:HD11	1.98	0.45
1:A:2175:GLU:HG3	1:A:2228:MET:HB3	1.98	0.45
1:A:3729:MET:HG3	1:A:3800:LEU:HD13	1.99	0.45
1:A:3842:LEU:HB2	1:A:3929:SER:HB2	1.97	0.45
1:A:3932:ASP:HA	1:A:3935:TRP:HB2	1.98	0.45
1:B:224:HIS:CD2	1:B:225:GLY:H	2.34	0.45
1:B:2973:PHE:HB2	1:B:2991:HIS:CD2	2.51	0.45
1:B:3337:ARG:HA	1:B:3340:VAL:HG12	1.97	0.45
1:B:3995:VAL:O	1:B:3999:MET:HB2	2.16	0.45
1:C:4190:ILE:N	1:C:5031:GLN:HE22	2.14	0.45
1:D:603:LEU:HA	1:D:606:LEU:HD12	1.97	0.45
2:H:23:VAL:HG22	2:H:47:LYS:HB3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.15	0.45
1:A:2817:ILE:HD12	1:A:2823:ILE:HG22	1.99	0.45
1:A:3157:ILE:HG23	1:A:3161:VAL:HG12	1.98	0.45
1:A:4580:TYR:HE2	1:A:4630:TYR:HB3	1.81	0.45
1:B:826:ILE:HG22	1:B:827:LYS:HD2	1.98	0.45
1:B:2686:LEU:HB3	1:B:2997:PHE:HE1	1.82	0.45
1:C:3254:GLY:HA2	1:C:3318:ASN:ND2	2.31	0.45
1:C:4183:ILE:HG12	1:C:4193:ILE:HD11	1.98	0.45
1:D:217:GLY:N	1:D:262:LEU:O	2.45	0.45
1:D:224:HIS:CD2	1:D:225:GLY:H	2.34	0.45
1:D:4576:ILE:HD13	1:D:4639:MET:HB3	1.97	0.45
1:A:548:VAL:HA	1:A:551:LEU:HD23	1.99	0.45
1:A:3535:LEU:O	1:A:3538:THR:OG1	2.29	0.45
1:B:2121:PHE:O	1:B:3725:TYR:OH	2.28	0.45
1:B:4190:ILE:N	1:B:5031:GLN:HE22	2.14	0.45
1:C:3713:LYS:NZ	1:C:3715:LYS:O	2.42	0.45
1:C:3785:ALA:HA	1:C:3787:LYS:HE3	1.99	0.45
1:D:407:THR:HG22	1:D:411:TYR:CE2	2.52	0.45
1:D:3729:MET:HG3	1:D:3800:LEU:HD13	1.98	0.45
1:D:3805:LEU:HB3	1:D:3890:LEU:HB3	1.98	0.45
1:D:4704:LEU:O	1:D:4774:LYS:NZ	2.36	0.45
1:A:484:LEU:HA	1:A:487:VAL:HG22	1.99	0.45
1:A:1220:GLN:HB2	1:D:3519:PRO:HB3	1.99	0.45
1:A:2616:PRO:HG3	1:A:2647:HIS:HE1	1.81	0.45
1:A:2973:PHE:HB2	1:A:2991:HIS:CD2	2.51	0.45
1:A:4861:LYS:H	1:A:4861:LYS:HG3	1.46	0.45
1:B:1866:ILE:HA	1:B:1926:LEU:HD23	1.98	0.45
1:B:2443:ILE:HD12	1:B:2454:ARG:HE	1.81	0.45
1:B:3519:PRO:HB3	1:C:1220:GLN:HB2	1.99	0.45
1:B:4059:LEU:HD12	1:B:4170:ILE:HG21	1.99	0.45
1:C:484:LEU:HA	1:C:487:VAL:HG22	1.99	0.45
1:C:4580:TYR:HE2	1:C:4630:TYR:HB3	1.81	0.45
1:D:484:LEU:HA	1:D:487:VAL:HG22	1.99	0.45
1:D:2686:LEU:HB3	1:D:2997:PHE:HE1	1.82	0.45
1:D:4168:GLU:O	1:D:4171:LEU:N	2.48	0.45
1:D:4821:LYS:HE3	1:D:4821:LYS:HB3	1.76	0.45
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.99	0.45
1:A:3634:ALA:O	1:A:3638:MET:HB3	2.16	0.45
1:A:3674:ILE:HD13	1:A:3770:LEU:HD21	1.98	0.45
1:B:3785:ALA:HA	1:B:3787:LYS:HE3	1.99	0.45
1:B:4168:GLU:O	1:B:4171:LEU:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4183:ILE:HG12	1:B:4193:ILE:HD11	1.98	0.45
1:C:414:PHE:HA	1:C:436:LEU:HD22	1.98	0.45
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	1.99	0.45
1:D:2175:GLU:HG3	1:D:2228:MET:HB3	1.99	0.45
1:A:76:ARG:O	1:A:79:GLN:N	2.49	0.45
1:A:243:ARG:HA	1:A:301:VAL:HG22	1.99	0.45
1:A:4151:SER:HA	1:A:4160:LEU:HD21	1.97	0.45
1:A:4704:LEU:O	1:A:4774:LYS:NZ	2.36	0.45
1:B:419:ASP:HA	1:B:422:SER:HB3	1.98	0.45
1:B:484:LEU:HA	1:B:487:VAL:HG22	1.99	0.45
1:B:863:LEU:HA	1:B:864:PRO:HD3	1.85	0.45
1:B:1965:TYR:OH	1:B:2027:ILE:O	2.31	0.45
1:B:3634:ALA:O	1:B:3638:MET:HB3	2.16	0.45
1:B:3729:MET:HG3	1:B:3800:LEU:HD13	1.99	0.45
1:C:243:ARG:HA	1:C:301:VAL:HG22	1.99	0.45
1:C:419:ASP:HA	1:C:422:SER:HB3	1.98	0.45
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.99	0.45
1:C:2175:GLU:HG3	1:C:2228:MET:HB3	1.98	0.45
1:C:3779:VAL:HG13	1:C:3797:THR:HG22	1.99	0.45
1:C:3805:LEU:HB3	1:C:3890:LEU:HB3	1.98	0.45
1:D:3416:VAL:HG13	1:D:3423:TRP:HZ3	1.82	0.45
1:D:3932:ASP:HA	1:D:3935:TRP:HB2	1.98	0.45
1:D:4059:LEU:HD12	1:D:4170:ILE:HG21	1.99	0.45
1:A:1698:LEU:O	1:A:1712:TYR:OH	2.28	0.45
1:A:2677:LYS:HE2	1:A:2677:LYS:HB3	1.77	0.45
1:A:3337:ARG:HA	1:A:3340:VAL:HG12	1.97	0.45
1:B:407:THR:HG22	1:B:411:TYR:CE2	2.52	0.45
1:B:548:VAL:HA	1:B:551:LEU:HD23	1.99	0.45
1:B:573:GLU:O	1:B:577:ILE:HG12	2.16	0.45
1:C:647:ASN:OD1	1:C:647:ASN:N	2.50	0.45
1:C:2686:LEU:HB3	1:C:2997:PHE:HE1	1.82	0.45
1:C:3519:PRO:HB3	1:D:1220:GLN:HB2	1.99	0.45
1:C:3634:ALA:O	1:C:3638:MET:HB3	2.16	0.45
2:F:105:ASN:ND2	2:F:107:GLU:O	2.50	0.45
1:A:1866:ILE:HA	1:A:1926:LEU:HD23	1.98	0.45
1:A:3392:LEU:HA	1:A:3395:ARG:HD2	1.98	0.45
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.99	0.45
1:B:1864:LYS:NZ	1:B:1871:PHE:O	2.45	0.45
1:B:2616:PRO:HG3	1:B:2647:HIS:HE1	1.81	0.45
1:B:3254:GLY:HA2	1:B:3318:ASN:ND2	2.31	0.45
1:B:3524:MET:HG2	1:B:3595:ARG:HD2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4097:MET:HE3	1:B:4111:LEU:HD23	1.99	0.45
1:C:3932:ASP:HA	1:C:3935:TRP:HB2	1.98	0.45
1:C:3995:VAL:O	1:C:3999:MET:HB2	2.16	0.45
1:B:243:ARG:HA	1:B:301:VAL:HG22	1.99	0.45
1:B:673:PRO:HB3	2:F:71:ARG:HH22	1.80	0.45
1:B:2817:ILE:HD12	1:B:2823:ILE:HG22	1.99	0.45
1:C:1866:ILE:HA	1:C:1926:LEU:HD23	1.98	0.45
1:C:3809:ASN:HB3	1:C:3812:VAL:HB	1.99	0.45
1:D:76:ARG:O	1:D:79:GLN:N	2.49	0.45
1:D:243:ARG:HA	1:D:301:VAL:HG22	1.99	0.45
1:D:299:LEU:HD13	1:D:378:LEU:HD22	1.98	0.45
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.99	0.45
1:D:1866:ILE:HA	1:D:1926:LEU:HD23	1.98	0.45
1:D:2443:ILE:HD12	1:D:2454:ARG:HE	1.81	0.45
1:D:2616:PRO:HG3	1:D:2647:HIS:HE1	1.81	0.45
1:D:4580:TYR:HE2	1:D:4630:TYR:HB3	1.81	0.45
1:D:4911:LEU:HD22	1:D:4911:LEU:HA	1.87	0.45
1:A:299:LEU:HD13	1:A:378:LEU:HD22	1.98	0.44
1:A:414:PHE:HA	1:A:436:LEU:HD22	1.98	0.44
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.99	0.44
1:A:3995:VAL:O	1:A:3999:MET:HB2	2.16	0.44
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.50	0.44
1:B:4722:ARG:H	1:B:4722:ARG:HG2	1.45	0.44
1:B:4861:LYS:H	1:B:4861:LYS:HG3	1.46	0.44
1:C:603:LEU:HA	1:C:606:LEU:HD12	1.98	0.44
1:C:661:LYS:HB3	1:C:808:TYR:HA	1.99	0.44
1:C:4049:VAL:HG21	1:C:4159:ARG:HE	1.82	0.44
1:C:4576:ILE:HD13	1:C:4639:MET:HB3	1.97	0.44
1:D:548:VAL:HA	1:D:551:LEU:HD23	1.99	0.44
1:D:2190:VAL:HA	1:D:2193:GLN:HB2	2.00	0.44
1:D:3301:PRO:HA	1:D:3302:PRO:HD3	1.88	0.44
1:D:3785:ALA:HA	1:D:3787:LYS:HE3	1.99	0.44
1:D:4861:LYS:H	1:D:4861:LYS:HG3	1.46	0.44
1:A:407:THR:HG22	1:A:411:TYR:CE2	2.52	0.44
1:A:793:LEU:HB2	1:A:797:HIS:HB2	1.99	0.44
1:A:1149:VAL:HG12	1:A:1164:LEU:HA	1.99	0.44
1:A:1839:VAL:HG23	1:A:1935:VAL:HG22	1.99	0.44
1:A:4059:LEU:HD12	1:A:4170:ILE:HG21	1.99	0.44
1:B:661:LYS:HB3	1:B:808:TYR:HA	1.99	0.44
1:C:2017:ASP:N	1:C:2017:ASP:OD1	2.47	0.44
1:C:2190:VAL:HA	1:C:2193:GLN:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2586:VAL:HG13	1:C:2607:LEU:HD21	2.00	0.44
1:C:3392:LEU:HA	1:C:3395:ARG:HD2	1.98	0.44
1:C:3524:MET:HG2	1:C:3595:ARG:HD2	1.99	0.44
1:C:4732:PHE:HD2	1:C:4737:ILE:HG12	1.82	0.44
1:D:2017:ASP:OD1	1:D:2017:ASP:N	2.47	0.44
1:D:2712:PRO:HA	1:D:2955:PHE:HD2	1.83	0.44
1:D:3634:ALA:O	1:D:3638:MET:HB3	2.16	0.44
1:D:3995:VAL:O	1:D:3999:MET:HB2	2.16	0.44
1:D:4548:ARG:HE	1:D:4548:ARG:HB3	1.43	0.44
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.33	0.44
1:D:4584:ASP:HA	1:D:4628:VAL:HG12	2.00	0.44
2:E:105:ASN:ND2	2:E:107:GLU:O	2.50	0.44
1:A:1442:GLY:HA2	1:A:1509:ILE:HG23	2.00	0.44
1:A:3107:VAL:O	1:A:3111:ARG:HB2	2.18	0.44
1:A:3785:ALA:HA	1:A:3787:LYS:HE3	1.99	0.44
1:B:2199:ARG:NE	1:B:2246:ASN:OD1	2.50	0.44
1:B:3674:ILE:HD13	1:B:3770:LEU:HD21	1.98	0.44
1:C:34:LYS:HD3	1:C:34:LYS:HA	1.82	0.44
1:C:461:HIS:O	1:C:465:GLN:HG2	2.18	0.44
1:C:573:GLU:O	1:C:577:ILE:HG12	2.16	0.44
1:C:1149:VAL:HG12	1:C:1164:LEU:HA	1.99	0.44
1:C:2817:ILE:HD12	1:C:2823:ILE:HG22	1.99	0.44
1:C:3674:ILE:HD13	1:C:3770:LEU:HD21	1.98	0.44
1:D:2325:PRO:O	1:D:2329:GLU:HB2	2.18	0.44
1:D:3579:LEU:HB2	1:D:3582:ARG:HG2	1.99	0.44
1:D:4865:LYS:HD2	1:D:4865:LYS:HA	1.63	0.44
1:A:45:ARG:HG2	1:A:443:LEU:HD21	2.00	0.44
1:A:2686:LEU:HB3	1:A:2997:PHE:HE1	1.82	0.44
1:A:3779:VAL:HG13	1:A:3797:THR:HG22	1.99	0.44
1:A:4732:PHE:HD2	1:A:4737:ILE:HG12	1.83	0.44
1:B:465:GLN:O	1:B:469:ARG:HG2	2.18	0.44
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.99	0.44
1:B:2561:LEU:HA	1:B:2564:LYS:HZ3	1.82	0.44
1:B:3416:VAL:HG13	1:B:3423:TRP:HZ3	1.82	0.44
1:B:4190:ILE:H	1:B:4190:ILE:HG12	1.43	0.44
1:C:2286:LEU:HD12	1:C:2286:LEU:HA	1.82	0.44
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.50	0.44
1:C:4888:TYR:HA	1:D:4918:ILE:HD11	1.99	0.44
1:D:3670:GLU:HG3	1:D:3728:ILE:HG23	2.00	0.44
1:D:4049:VAL:HG21	1:D:4159:ARG:HE	1.82	0.44
1:A:1864:LYS:NZ	1:A:1871:PHE:O	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2586:VAL:HG13	1:A:2607:LEU:HD21	2.00	0.44
1:B:76:ARG:O	1:B:79:GLN:N	2.49	0.44
1:B:1442:GLY:HA2	1:B:1509:ILE:HG23	2.00	0.44
1:B:2780:ASN:ND2	1:B:2782:ASP:OD2	2.51	0.44
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.83	0.44
1:C:76:ARG:O	1:C:79:GLN:N	2.49	0.44
1:C:3670:GLU:HG3	1:C:3728:ILE:HG23	2.00	0.44
1:C:4059:LEU:HD12	1:C:4170:ILE:HG21	1.99	0.44
1:D:465:GLN:O	1:D:469:ARG:HG2	2.18	0.44
1:D:3779:VAL:HG13	1:D:3797:THR:HG22	1.99	0.44
1:D:4097:MET:HE3	1:D:4111:LEU:HD23	1.98	0.44
2:E:17:LYS:HG2	2:E:20:GLN:HE22	1.83	0.44
2:H:105:ASN:ND2	2:H:107:GLU:O	2.50	0.44
1:B:2175:GLU:HG3	1:B:2228:MET:HB3	1.98	0.44
1:B:3107:VAL:O	1:B:3111:ARG:HB2	2.18	0.44
1:B:3779:VAL:HG13	1:B:3797:THR:HG22	1.99	0.44
1:C:407:THR:HG22	1:C:411:TYR:CE2	2.52	0.44
1:C:1839:VAL:HG23	1:C:1935:VAL:HG22	1.99	0.44
1:C:3051:ARG:HA	1:C:3131:TYR:CZ	2.53	0.44
1:C:3729:MET:HG3	1:C:3800:LEU:HD13	1.98	0.44
1:D:461:HIS:O	1:D:465:GLN:HG2	2.18	0.44
1:D:786:GLY:HA2	1:D:1631:GLN:HA	1.99	0.44
1:D:2199:ARG:NE	1:D:2246:ASN:OD1	2.50	0.44
1:D:3140:LEU:HA	1:D:3143:LEU:HD12	2.00	0.44
1:A:661:LYS:HB3	1:A:808:TYR:HA	2.00	0.44
1:A:873:LYS:HG2	1:A:970:LEU:HD13	1.99	0.44
1:A:2625:ARG:NE	1:A:2629:ASP:OD2	2.47	0.44
1:A:2676:ARG:HE	1:A:2680:TRP:HE1	1.66	0.44
1:B:1099:GLU:OE2	1:B:1101:ARG:NE	2.46	0.44
1:B:2586:VAL:HG13	1:B:2607:LEU:HD21	2.00	0.44
1:B:3809:ASN:HB3	1:B:3812:VAL:HB	1.99	0.44
1:B:4865:LYS:HD2	1:B:4865:LYS:HA	1.63	0.44
1:C:548:VAL:HA	1:C:551:LEU:HD23	1.99	0.44
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.53	0.44
1:C:1072:VAL:HG23	1:C:1194:LEU:C	2.38	0.44
1:C:1965:TYR:OH	1:C:2027:ILE:O	2.31	0.44
1:C:2780:ASN:ND2	1:C:2782:ASP:OD2	2.51	0.44
1:C:3107:VAL:O	1:C:3111:ARG:HB2	2.18	0.44
1:C:3140:LEU:HA	1:C:3143:LEU:HD12	2.00	0.44
1:C:4168:GLU:O	1:C:4171:LEU:N	2.48	0.44
1:C:4902:GLU:O	1:C:4913:ARG:NH2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1099:GLU:OE2	1:D:1101:ARG:NE	2.46	0.44
1:D:2586:VAL:HG13	1:D:2607:LEU:HD21	2.00	0.44
1:D:2817:ILE:HD12	1:D:2823:ILE:HG22	1.99	0.44
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.83	0.44
1:D:3107:VAL:O	1:D:3111:ARG:HB2	2.18	0.44
1:D:3332:ALA:O	1:D:3336:LYS:NZ	2.51	0.44
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.25	0.44
2:G:105:ASN:ND2	2:G:107:GLU:O	2.50	0.44
1:A:281:ARG:NH2	1:A:309:THR:OG1	2.51	0.44
1:A:626:LEU:HB3	1:A:1688:HIS:CE1	2.53	0.44
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.83	0.44
1:A:3332:ALA:O	1:A:3336:LYS:NZ	2.51	0.44
1:A:3779:VAL:O	1:A:3783:ILE:HG12	2.18	0.44
1:B:414:PHE:HA	1:B:436:LEU:HD22	1.98	0.44
1:B:626:LEU:HB3	1:B:1688:HIS:CE1	2.53	0.44
1:B:786:GLY:HA2	1:B:1631:GLN:HA	1.99	0.44
1:C:45:ARG:HG2	1:C:443:LEU:HD21	2.00	0.44
1:C:299:LEU:HD13	1:C:378:LEU:HD22	1.98	0.44
1:C:546:TRP:O	1:C:549:SER:OG	2.28	0.44
1:C:2098:VAL:HG13	1:C:2127:GLN:HG3	2.00	0.44
1:C:2325:PRO:O	1:C:2329:GLU:HB2	2.18	0.44
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.83	0.44
1:C:4584:ASP:HA	1:C:4628:VAL:HG12	2.00	0.44
1:D:45:ARG:HG2	1:D:443:LEU:HD21	2.00	0.44
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.53	0.44
1:D:2621:HIS:HA	1:D:2624:ARG:HG2	2.00	0.44
2:F:17:LYS:HG2	2:F:20:GLN:HE22	1.83	0.44
1:A:2712:PRO:HA	1:A:2955:PHE:HD2	1.83	0.44
1:A:3524:MET:HG2	1:A:3595:ARG:HD2	1.99	0.44
1:A:4918:ILE:HD13	1:D:4892:ARG:HD3	2.00	0.44
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.53	0.44
1:B:1686:CYS:HB2	1:B:1782:PHE:HZ	1.83	0.44
1:B:2676:ARG:HE	1:B:2680:TRP:HE1	1.66	0.44
1:C:2737:PRO:HG2	1:C:2888:ARG:HB2	1.99	0.44
1:C:3332:ALA:O	1:C:3336:LYS:NZ	2.51	0.44
1:C:5030:LYS:HE2	1:C:5030:LYS:HB2	1.59	0.44
1:D:626:LEU:HB3	1:D:1688:HIS:CE1	2.53	0.44
1:D:1686:CYS:HB2	1:D:1782:PHE:HZ	1.83	0.44
1:D:1839:VAL:HG23	1:D:1935:VAL:HG22	1.99	0.44
1:D:2098:VAL:HG13	1:D:2127:GLN:HG3	2.00	0.44
1:D:2121:PHE:O	1:D:3725:TYR:OH	2.28	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:7:ILE:HD11	2:E:73:LYS:HB2	2.00	0.44
2:H:17:LYS:HG2	2:H:20:GLN:HE22	1.83	0.44
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.53	0.43
1:A:2621:HIS:HA	1:A:2624:ARG:HG2	2.00	0.43
1:A:2737:PRO:HG2	1:A:2888:ARG:HB2	1.99	0.43
1:A:3354:LEU:N	1:A:3415:TYR:OH	2.51	0.43
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.33	0.43
1:B:17:ASP:N	1:B:69:LEU:O	2.44	0.43
1:B:663:TYR:OH	1:B:665:GLU:OE2	2.35	0.43
1:B:1072:VAL:HG23	1:B:1194:LEU:C	2.38	0.43
1:B:3354:LEU:N	1:B:3415:TYR:OH	2.51	0.43
1:B:4049:VAL:HG21	1:B:4159:ARG:HE	1.83	0.43
1:C:403:MET:O	1:C:407:THR:OG1	2.19	0.43
1:C:793:LEU:HB2	1:C:797:HIS:HB2	1.99	0.43
1:C:2199:ARG:NE	1:C:2246:ASN:OD1	2.50	0.43
1:C:2712:PRO:HA	1:C:2955:PHE:HD2	1.83	0.43
1:C:3147:ILE:HA	1:C:3152:PHE:HB2	2.01	0.43
1:D:661:LYS:HB3	1:D:808:TYR:HA	1.99	0.43
1:D:1149:VAL:HG12	1:D:1164:LEU:HA	1.99	0.43
1:D:2625:ARG:NE	1:D:2629:ASP:OD2	2.47	0.43
1:D:3809:ASN:HB3	1:D:3812:VAL:HB	1.99	0.43
2:H:7:ILE:HD11	2:H:73:LYS:HB2	2.00	0.43
1:A:293:LEU:H	1:A:311:ALA:HB1	1.84	0.43
1:A:2325:PRO:O	1:A:2329:GLU:HB2	2.18	0.43
1:A:3579:LEU:HB2	1:A:3582:ARG:HG2	1.99	0.43
1:B:2621:HIS:HA	1:B:2624:ARG:HG2	2.00	0.43
1:B:3596:VAL:O	1:B:3600:SER:OG	2.27	0.43
1:C:465:GLN:O	1:C:469:ARG:HG2	2.18	0.43
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.99	0.43
1:C:3416:VAL:HG13	1:C:3423:TRP:HZ3	1.82	0.43
1:D:552:ASP:OD1	1:D:552:ASP:N	2.50	0.43
1:D:2676:ARG:HE	1:D:2680:TRP:HE1	1.66	0.43
1:D:2716:ASP:OD1	1:D:2716:ASP:N	2.51	0.43
1:D:2780:ASN:ND2	1:D:2782:ASP:OD2	2.51	0.43
1:A:786:GLY:HA2	1:A:1631:GLN:HA	1.99	0.43
1:A:2567:PRO:HG3	1:A:2613:TYR:CZ	2.53	0.43
1:A:2765:LYS:HD3	1:A:2765:LYS:HA	1.85	0.43
1:A:2998:PHE:HA	1:A:3002:LEU:HD13	2.00	0.43
1:A:3140:LEU:HA	1:A:3143:LEU:HD12	2.00	0.43
1:A:3416:VAL:HG13	1:A:3423:TRP:HZ3	1.82	0.43
1:B:299:LEU:HD13	1:B:378:LEU:HD22	1.98	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.33	0.43
1:C:1100:MET:HB2	1:C:1143:TRP:CZ2	2.53	0.43
1:C:1686:CYS:HB2	1:C:1782:PHE:HZ	1.83	0.43
1:C:2621:HIS:HA	1:C:2624:ARG:HG2	2.00	0.43
1:C:2998:PHE:HA	1:C:3002:LEU:HD13	2.00	0.43
1:C:3579:LEU:HB2	1:C:3582:ARG:HG2	1.99	0.43
1:D:281:ARG:NH2	1:D:309:THR:OG1	2.51	0.43
1:D:720:HIS:CG	1:D:727:ALA:HB1	2.54	0.43
1:D:873:LYS:HG2	1:D:970:LEU:HD13	1.99	0.43
1:D:1072:VAL:HG23	1:D:1194:LEU:C	2.38	0.43
1:D:1100:MET:HB2	1:D:1143:TRP:CZ2	2.53	0.43
1:D:2737:PRO:HG2	1:D:2888:ARG:HB2	1.99	0.43
1:D:3392:LEU:HA	1:D:3395:ARG:HD2	1.98	0.43
1:A:465:GLN:O	1:A:469:ARG:HG2	2.18	0.43
1:A:647:ASN:OD1	1:A:647:ASN:N	2.50	0.43
1:A:1686:CYS:HB2	1:A:1782:PHE:HZ	1.83	0.43
1:A:2286:LEU:HD12	1:A:2286:LEU:HA	1.82	0.43
1:B:2190:VAL:HA	1:B:2193:GLN:HB2	2.00	0.43
1:B:2739:PRO:HG3	1:B:2888:ARG:HG2	2.00	0.43
1:B:3201:MET:HG3	1:B:3203:VAL:H	1.83	0.43
1:B:4888:TYR:HA	1:C:4918:ILE:HD11	1.99	0.43
1:C:863:LEU:HA	1:C:864:PRO:HD3	1.85	0.43
1:C:936:GLY:HA3	1:C:1056:PRO:HB3	2.00	0.43
1:C:1115:LEU:HB3	1:C:1123:VAL:HG11	2.01	0.43
1:C:2677:LYS:HB3	1:C:2677:LYS:HE2	1.77	0.43
1:C:2739:PRO:HG3	1:C:2888:ARG:HG2	2.00	0.43
1:C:4097:MET:HE3	1:C:4111:LEU:HD23	1.99	0.43
1:D:1442:GLY:HA2	1:D:1509:ILE:HG23	2.00	0.43
1:D:2677:LYS:HE2	1:D:2677:LYS:HB3	1.77	0.43
1:D:3147:ILE:HA	1:D:3152:PHE:HB2	2.01	0.43
1:D:3262:ARG:O	1:D:3266:MET:HG2	2.18	0.43
2:G:7:ILE:HD11	2:G:73:LYS:HB2	2.00	0.43
1:A:3415:TYR:O	1:A:3419:ASN:ND2	2.37	0.43
1:A:3890:LEU:HD23	1:A:3890:LEU:HA	1.85	0.43
1:A:3945:GLU:OE1	1:A:3949:ARG:NH1	2.52	0.43
1:A:4584:ASP:HA	1:A:4628:VAL:HG12	2.00	0.43
1:B:873:LYS:HG2	1:B:970:LEU:HD13	1.99	0.43
1:B:936:GLY:HA3	1:B:1056:PRO:HB3	2.00	0.43
1:B:1100:MET:HB2	1:B:1143:TRP:CZ2	2.53	0.43
1:B:2677:LYS:HB3	1:B:2677:LYS:HE2	1.77	0.43
1:B:2712:PRO:HA	1:B:2955:PHE:HD2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4902:GLU:O	1:B:4913:ARG:NH2	2.32	0.43
1:C:17:ASP:HB2	1:C:98:HIS:HE1	1.84	0.43
1:C:111:HIS:ND1	1:C:114:SER:OG	2.35	0.43
1:C:504:ALA:HB2	1:C:512:ALA:HB2	2.00	0.43
1:C:626:LEU:HB3	1:C:1688:HIS:CE1	2.53	0.43
1:C:786:GLY:HA2	1:C:1631:GLN:HA	1.99	0.43
1:C:1435:TYR:HB3	1:C:1575:LEU:HD21	2.00	0.43
1:C:2567:PRO:HG3	1:C:2613:TYR:CZ	2.53	0.43
1:C:2676:ARG:HE	1:C:2680:TRP:HE1	1.66	0.43
1:C:3779:VAL:O	1:C:3783:ILE:HG12	2.18	0.43
1:C:3945:GLU:OE1	1:C:3949:ARG:NH1	2.52	0.43
1:D:17:ASP:HB2	1:D:98:HIS:HE1	1.84	0.43
1:D:2567:PRO:HG3	1:D:2613:TYR:CZ	2.53	0.43
1:D:3573:MET:HA	1:D:3576:TYR:HB3	2.00	0.43
1:D:3945:GLU:OE1	1:D:3949:ARG:NH1	2.52	0.43
1:D:4888:TYR:CD2	1:D:4889:VAL:HG22	2.54	0.43
2:G:56:ILE:HG12	2:G:81:ALA:HA	2.01	0.43
2:H:56:ILE:HG12	2:H:81:ALA:HA	2.00	0.43
1:A:1072:VAL:HG23	1:A:1194:LEU:C	2.38	0.43
1:A:1100:MET:HB2	1:A:1143:TRP:CZ2	2.53	0.43
1:A:2190:VAL:HA	1:A:2193:GLN:HB2	2.00	0.43
1:A:2716:ASP:OD1	1:A:2716:ASP:N	2.52	0.43
1:A:3262:ARG:O	1:A:3266:MET:HG2	2.18	0.43
1:A:4171:LEU:O	1:A:4175:ARG:HB2	2.19	0.43
1:B:504:ALA:HB2	1:B:512:ALA:HB2	2.00	0.43
1:B:793:LEU:HB2	1:B:797:HIS:HB2	1.99	0.43
1:B:1149:VAL:HG12	1:B:1164:LEU:HA	1.99	0.43
1:B:3579:LEU:HB2	1:B:3582:ARG:HG2	1.99	0.43
1:C:878:ILE:HD11	1:C:925:SER:HB2	2.01	0.43
1:C:3343:GLN:NE2	1:C:3469:PHE:O	2.47	0.43
1:C:3354:LEU:N	1:C:3415:TYR:OH	2.51	0.43
1:D:878:ILE:HD11	1:D:925:SER:HB2	2.01	0.43
1:D:2617:SER:OG	1:D:2618:MET:SD	2.72	0.43
1:D:3944:GLU:OE1	1:D:3946:GLN:N	2.47	0.43
2:F:56:ILE:HG12	2:F:81:ALA:HA	2.00	0.43
1:A:878:ILE:HD11	1:A:925:SER:HB2	2.01	0.43
1:A:2507:ASP:OD2	1:A:2564:LYS:NZ	2.41	0.43
1:A:2739:PRO:HG3	1:A:2888:ARG:HG2	2.00	0.43
1:A:3147:ILE:HA	1:A:3152:PHE:HB2	2.01	0.43
1:A:3809:ASN:HB3	1:A:3812:VAL:HB	1.99	0.43
1:A:4968:PHE:O	1:A:4974:GLY:HA3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3140:LEU:HA	1:B:3143:LEU:HD12	2.00	0.43
1:B:3262:ARG:O	1:B:3266:MET:HG2	2.18	0.43
1:B:3670:GLU:HG3	1:B:3728:ILE:HG23	2.00	0.43
1:B:3945:GLU:OE1	1:B:3949:ARG:NH1	2.52	0.43
1:C:3201:MET:HG3	1:C:3203:VAL:H	1.83	0.43
1:C:3262:ARG:O	1:C:3266:MET:HG2	2.18	0.43
1:C:4888:TYR:CD2	1:C:4889:VAL:HG22	2.54	0.43
1:D:936:GLY:HA3	1:D:1056:PRO:HB3	2.00	0.43
1:D:1115:LEU:HB3	1:D:1123:VAL:HG11	2.01	0.43
1:D:2006:ILE:HG23	1:D:3641:LEU:HD11	2.01	0.43
1:D:3201:MET:HG3	1:D:3203:VAL:H	1.83	0.43
1:D:4732:PHE:HD2	1:D:4737:ILE:HG12	1.83	0.43
1:A:2006:ILE:HG23	1:A:3641:LEU:HD11	2.01	0.43
1:B:45:ARG:HG2	1:B:443:LEU:HD21	2.00	0.43
1:B:461:HIS:O	1:B:465:GLN:HG2	2.18	0.43
1:B:720:HIS:CG	1:B:727:ALA:HB1	2.54	0.43
1:B:2098:VAL:HG13	1:B:2127:GLN:HG3	2.00	0.43
1:B:2325:PRO:O	1:B:2329:GLU:HB2	2.18	0.43
1:B:4732:PHE:HD2	1:B:4737:ILE:HG12	1.82	0.43
1:B:4823:LEU:HD23	1:B:4823:LEU:HA	1.80	0.43
1:C:27:THR:OG1	1:C:32:GLN:OE1	2.28	0.43
1:C:2339:VAL:HG12	1:C:2349:ASN:HB3	2.01	0.43
1:C:3249:LEU:HD12	1:C:3249:LEU:HA	1.86	0.43
1:C:3450:ASN:HA	1:C:3453:ARG:HG2	2.01	0.43
1:C:3596:VAL:O	1:C:3600:SER:OG	2.27	0.43
1:D:3524:MET:HG2	1:D:3595:ARG:HD2	1.99	0.43
1:D:3779:VAL:O	1:D:3783:ILE:HG12	2.18	0.43
1:D:4171:LEU:O	1:D:4175:ARG:HB2	2.19	0.43
1:A:461:HIS:O	1:A:465:GLN:HG2	2.18	0.43
1:A:720:HIS:CG	1:A:727:ALA:HB1	2.54	0.43
1:A:2309:SER:OG	1:A:2321:ILE:O	2.26	0.43
1:A:3573:MET:HA	1:A:3576:TYR:HB3	2.00	0.43
1:A:4049:VAL:HG21	1:A:4159:ARG:HE	1.82	0.43
1:B:217:GLY:N	1:B:262:LEU:O	2.45	0.43
1:B:2567:PRO:HG3	1:B:2613:TYR:CZ	2.53	0.43
1:B:3147:ILE:HA	1:B:3152:PHE:HB2	2.01	0.43
1:B:3779:VAL:O	1:B:3783:ILE:HG12	2.18	0.43
1:B:3944:GLU:OE1	1:B:3946:GLN:N	2.47	0.43
1:C:293:LEU:H	1:C:311:ALA:HB1	1.83	0.43
1:C:873:LYS:HG2	1:C:970:LEU:HD13	1.99	0.43
1:C:1442:GLY:HA2	1:C:1509:ILE:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2006:ILE:HG23	1:C:3641:LEU:HD11	2.01	0.43
1:C:4646:LEU:HD23	1:C:4646:LEU:HA	1.89	0.43
1:C:4968:PHE:O	1:C:4974:GLY:HA3	2.19	0.43
1:D:293:LEU:H	1:D:311:ALA:HB1	1.84	0.43
1:D:4968:PHE:O	1:D:4974:GLY:HA3	2.19	0.43
1:A:2780:ASN:ND2	1:A:2782:ASP:OD2	2.51	0.43
1:A:3343:GLN:NE2	1:A:3469:PHE:O	2.47	0.43
1:A:3670:GLU:HG3	1:A:3728:ILE:HG23	2.00	0.43
1:B:261:ARG:HH11	1:B:263:GLU:HG2	1.84	0.43
1:B:293:LEU:H	1:B:311:ALA:HB1	1.83	0.43
1:B:878:ILE:HD11	1:B:925:SER:HB2	2.01	0.43
1:B:1839:VAL:HG23	1:B:1935:VAL:HG22	1.99	0.43
1:B:2862:LEU:O	1:B:2928:LYS:NZ	2.41	0.43
1:B:3320:LEU:HD21	1:B:3361:THR:HG21	2.01	0.43
1:B:3332:ALA:O	1:B:3336:LYS:NZ	2.51	0.43
1:B:4968:PHE:O	1:B:4974:GLY:HA3	2.19	0.43
1:C:720:HIS:CG	1:C:727:ALA:HB1	2.54	0.43
1:C:3238:GLU:HA	1:C:3241:PRO:HG3	2.01	0.43
1:D:2288:LEU:O	1:D:3849:ARG:NH1	2.42	0.43
1:D:2339:VAL:HG12	1:D:2349:ASN:HB3	2.01	0.43
1:D:4864:ASN:HD21	1:D:4872:PRO:HB2	1.84	0.43
1:A:3051:ARG:HA	1:A:3131:TYR:CZ	2.53	0.42
1:A:3245:VAL:H	1:A:3248:ARG:HE	1.67	0.42
1:A:4821:LYS:HE3	1:A:4821:LYS:HB3	1.76	0.42
1:A:4944:ARG:NH2	1:B:4938:ASP:OD1	2.50	0.42
1:B:736:HIS:ND1	1:B:737:LEU:O	2.38	0.42
1:B:1435:TYR:HB3	1:B:1575:LEU:HD21	2.00	0.42
1:B:2006:ILE:HG23	1:B:3641:LEU:HD11	2.01	0.42
1:B:2737:PRO:HG2	1:B:2888:ARG:HB2	1.99	0.42
1:B:3051:ARG:HA	1:B:3131:TYR:CZ	2.53	0.42
1:C:2716:ASP:OD1	1:C:2716:ASP:N	2.51	0.42
1:D:218:HIS:O	1:D:261:ARG:HA	2.19	0.42
1:D:504:ALA:HB2	1:D:512:ALA:HB2	2.00	0.42
1:D:1435:TYR:HB3	1:D:1575:LEU:HD21	2.00	0.42
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.50	0.42
1:D:3535:LEU:O	1:D:3538:THR:OG1	2.29	0.42
2:H:18:LYS:HA	2:H:50:ILE:HD11	2.01	0.42
1:A:261:ARG:HH11	1:A:263:GLU:HG2	1.85	0.42
1:A:504:ALA:HB2	1:A:512:ALA:HB2	2.00	0.42
1:A:1064:GLU:O	1:A:1071:ARG:NH2	2.53	0.42
1:A:2604:GLU:HG2	1:A:2639:MET:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1115:LEU:HB3	1:B:1123:VAL:HG11	2.01	0.42
1:B:2998:PHE:HA	1:B:3002:LEU:HD13	2.00	0.42
1:B:3450:ASN:HA	1:B:3453:ARG:HG2	2.01	0.42
1:B:4584:ASP:HA	1:B:4628:VAL:HG12	2.00	0.42
1:C:261:ARG:HH11	1:C:263:GLU:HG2	1.84	0.42
1:D:793:LEU:HB2	1:D:797:HIS:HB2	1.99	0.42
1:D:2998:PHE:HA	1:D:3002:LEU:HD13	2.00	0.42
1:D:3051:ARG:HA	1:D:3131:TYR:CZ	2.53	0.42
2:G:17:LYS:HG2	2:G:20:GLN:HE22	1.83	0.42
1:A:217:GLY:N	1:A:262:LEU:O	2.45	0.42
1:A:1115:LEU:HB3	1:A:1123:VAL:HG11	2.01	0.42
1:A:1435:TYR:HB3	1:A:1575:LEU:HD21	2.00	0.42
1:A:3201:MET:HG3	1:A:3203:VAL:H	1.84	0.42
1:A:3424:LEU:HD11	1:B:1216:ILE:HG12	2.00	0.42
1:A:4097:MET:HE3	1:A:4111:LEU:HD23	2.01	0.42
1:B:17:ASP:HB2	1:B:98:HIS:HE1	1.84	0.42
1:B:281:ARG:NH2	1:B:309:THR:OG1	2.51	0.42
1:B:2716:ASP:N	1:B:2716:ASP:OD1	2.51	0.42
1:B:4112:LEU:O	1:B:4115:SER:OG	2.38	0.42
1:C:4171:LEU:O	1:C:4175:ARG:HB2	2.19	0.42
1:D:34:LYS:HD3	1:D:34:LYS:HA	1.82	0.42
1:D:736:HIS:ND1	1:D:737:LEU:O	2.38	0.42
1:D:3354:LEU:N	1:D:3415:TYR:OH	2.51	0.42
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.42	0.42
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	2.02	0.42
1:A:4869:GLU:H	1:A:4869:GLU:HG2	1.69	0.42
1:B:1066:GLN:NE2	1:B:1461:ASP:OD1	2.53	0.42
1:B:2607:LEU:HD23	1:B:2607:LEU:HA	1.91	0.42
1:B:2765:LYS:HA	1:B:2765:LYS:HD3	1.85	0.42
1:B:3354:LEU:HD11	1:B:3434:LEU:HD12	2.00	0.42
1:B:3573:MET:HA	1:B:3576:TYR:HB3	2.00	0.42
1:B:4171:LEU:O	1:B:4175:ARG:HB2	2.19	0.42
1:B:4867:GLU:H	1:B:4867:GLU:HG2	1.34	0.42
1:B:4888:TYR:CD2	1:B:4889:VAL:HG22	2.54	0.42
1:D:3238:GLU:HA	1:D:3241:PRO:HG3	2.01	0.42
1:D:3320:LEU:HD21	1:D:3361:THR:HG21	2.01	0.42
1:D:3354:LEU:HD11	1:D:3434:LEU:HD12	2.00	0.42
1:A:936:GLY:HA3	1:A:1056:PRO:HB3	2.01	0.42
1:A:2098:VAL:HG13	1:A:2127:GLN:HG3	2.00	0.42
1:A:2736:ASP:OD1	1:A:2736:ASP:N	2.50	0.42
1:B:1064:GLU:O	1:B:1071:ARG:NH2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2122:SER:O	1:B:2126:ARG:HG3	2.20	0.42
1:B:2604:GLU:HG2	1:B:2639:MET:HG3	2.00	0.42
1:B:3821:LYS:O	1:B:3824:LYS:NZ	2.47	0.42
1:C:1277:TRP:CD1	1:C:1559:GLN:HG3	2.52	0.42
1:C:3244:PRO:HB2	1:C:3249:LEU:HD13	2.02	0.42
1:C:4675:LYS:O	1:C:4679:ARG:HG2	2.20	0.42
1:C:4944:ARG:NH2	1:D:4938:ASP:OD1	2.52	0.42
1:D:275:ARG:HE	1:D:336:PRO:HD2	1.85	0.42
1:D:3788:GLY:HA2	1:D:3835:LEU:HG	2.02	0.42
1:D:4675:LYS:O	1:D:4679:ARG:HG2	2.20	0.42
2:F:7:ILE:HD11	2:F:73:LYS:HB2	2.00	0.42
1:A:552:ASP:N	1:A:552:ASP:OD1	2.50	0.42
1:A:3244:PRO:HB2	1:A:3249:LEU:HD13	2.02	0.42
1:A:4850:LEU:HD23	1:A:4850:LEU:HA	1.86	0.42
1:B:34:LYS:HD3	1:B:34:LYS:HA	1.82	0.42
1:C:1000:ARG:HA	1:C:1000:ARG:HD3	1.82	0.42
1:C:2604:GLU:HG2	1:C:2639:MET:HG3	2.00	0.42
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	2.02	0.42
1:C:3573:MET:HA	1:C:3576:TYR:HB3	2.00	0.42
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	2.02	0.42
1:A:17:ASP:HB2	1:A:98:HIS:HE1	1.84	0.42
1:A:3320:LEU:HD21	1:A:3361:THR:HG21	2.01	0.42
1:A:4675:LYS:O	1:A:4679:ARG:HG2	2.20	0.42
1:A:4867:GLU:H	1:A:4867:GLU:HG2	1.34	0.42
1:B:1277:TRP:CD1	1:B:1559:GLN:HG3	2.52	0.42
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.42	0.42
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.55	0.42
1:C:218:HIS:O	1:C:261:ARG:HA	2.19	0.42
1:C:552:ASP:N	1:C:552:ASP:OD1	2.50	0.42
1:C:3535:LEU:O	1:C:3538:THR:OG1	2.29	0.42
1:D:261:ARG:HH11	1:D:263:GLU:HG2	1.84	0.42
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.49	0.42
1:D:1066:GLN:NE2	1:D:1461:ASP:OD1	2.53	0.42
1:D:3244:PRO:HB2	1:D:3249:LEU:HD13	2.02	0.42
2:E:56:ILE:HG12	2:E:81:ALA:HA	2.01	0.42
1:A:3301:PRO:HA	1:A:3302:PRO:HD3	1.88	0.42
1:B:1968:LYS:HB3	1:B:1968:LYS:HE2	1.90	0.42
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	2.02	0.42
1:B:3244:PRO:HA	1:B:3248:ARG:HH21	1.84	0.42
1:B:3245:VAL:H	1:B:3248:ARG:HE	1.67	0.42
1:C:1066:GLN:NE2	1:C:1461:ASP:OD1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2122:SER:O	1:C:2126:ARG:HG3	2.20	0.42
1:C:2862:LEU:O	1:C:2928:LYS:NZ	2.41	0.42
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.55	0.42
1:C:4864:ASN:HD21	1:C:4872:PRO:HB2	1.84	0.42
1:D:2514:ASN:OD1	1:D:2514:ASN:N	2.45	0.42
1:D:2604:GLU:HG2	1:D:2639:MET:HG3	2.00	0.42
1:D:3245:VAL:H	1:D:3248:ARG:HE	1.67	0.42
2:G:18:LYS:HA	2:G:50:ILE:HD11	2.01	0.42
1:A:1066:GLN:NE2	1:A:1461:ASP:OD1	2.52	0.42
1:A:1269:CYS:HA	1:A:1564:PHE:O	2.20	0.42
1:A:3823:LYS:HA	1:A:3823:LYS:HD3	1.83	0.42
1:B:3238:GLU:HA	1:B:3241:PRO:HG3	2.01	0.42
1:B:4850:LEU:HD23	1:B:4850:LEU:HA	1.86	0.42
1:C:3354:LEU:HD11	1:C:3434:LEU:HD12	2.00	0.42
1:C:4813:LEU:HD23	1:C:4813:LEU:HA	1.95	0.42
1:D:132:ALA:HB1	1:D:192:ASP:HB3	2.01	0.42
1:D:308:HIS:HD2	1:D:310:LYS:HB2	1.85	0.42
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.85	0.42
1:D:3244:PRO:HA	1:D:3248:ARG:HH21	1.84	0.42
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.55	0.42
1:A:2339:VAL:HG12	1:A:2349:ASN:HB3	2.01	0.42
1:A:2502:MET:HB3	1:A:2502:MET:HE2	1.95	0.42
1:A:2583:LEU:HA	1:A:2586:VAL:HG12	2.02	0.42
1:B:546:TRP:CE2	1:B:550:LYS:HE2	2.55	0.42
1:B:557:SER:HA	1:B:560:ILE:HG22	2.01	0.42
1:B:2339:VAL:HG12	1:B:2349:ASN:HB3	2.01	0.42
1:B:4864:ASN:HD21	1:B:4872:PRO:HB2	1.84	0.42
1:C:217:GLY:N	1:C:262:LEU:O	2.45	0.42
1:C:276:TRP:HD1	1:C:316:PHE:HB3	1.85	0.42
1:C:2765:LYS:HD3	1:C:2765:LYS:HA	1.85	0.42
1:C:3320:LEU:HD21	1:C:3361:THR:HG21	2.01	0.42
1:D:1064:GLU:O	1:D:1071:ARG:NH2	2.53	0.42
1:D:4581:LYS:HB3	1:D:4581:LYS:HE3	1.78	0.42
1:D:4661:TYR:OH	1:D:4786:ASP:OD2	2.34	0.42
2:E:18:LYS:HA	2:E:50:ILE:HD11	2.01	0.42
1:A:863:LEU:HA	1:A:864:PRO:HD3	1.85	0.41
1:A:3249:LEU:HD12	1:A:3249:LEU:HA	1.86	0.41
1:A:3788:GLY:HA2	1:A:3835:LEU:HG	2.02	0.41
1:A:4743:MET:H	1:A:4743:MET:HG3	1.63	0.41
1:B:276:TRP:HD1	1:B:316:PHE:HB3	1.85	0.41
1:B:2583:LEU:HA	1:B:2586:VAL:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:TRP:CE2	1:C:550:LYS:HE2	2.55	0.41
1:D:2318:TYR:CZ	1:D:2395:PRO:HD3	2.55	0.41
1:D:2739:PRO:HG3	1:D:2888:ARG:HG2	2.00	0.41
1:A:308:HIS:HD2	1:A:310:LYS:HB2	1.85	0.41
1:A:1968:LYS:HB3	1:A:1968:LYS:HE2	1.90	0.41
1:A:2691:TYR:HA	1:A:2696:TYR:HE2	1.85	0.41
1:A:3354:LEU:HD11	1:A:3434:LEU:HD12	2.00	0.41
1:A:3450:ASN:HA	1:A:3453:ARG:HG2	2.01	0.41
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.55	0.41
1:A:4569:LEU:HD12	1:A:4569:LEU:HA	1.95	0.41
1:A:4888:TYR:CD2	1:A:4889:VAL:HG22	2.54	0.41
1:B:308:HIS:HD2	1:B:310:LYS:HB2	1.85	0.41
1:B:1269:CYS:HA	1:B:1564:PHE:O	2.20	0.41
1:B:2682:ILE:O	1:B:2686:LEU:HB2	2.21	0.41
1:B:3244:PRO:HB2	1:B:3249:LEU:HD13	2.02	0.41
1:C:132:ALA:HB1	1:C:192:ASP:HB3	2.02	0.41
1:C:2481:LYS:HE2	1:C:2481:LYS:HB2	1.92	0.41
1:C:2617:SER:OG	1:C:2618:MET:SD	2.72	0.41
1:C:3718:GLU:OE2	1:C:3719:ASP:N	2.54	0.41
1:D:276:TRP:HD1	1:D:316:PHE:HB3	1.85	0.41
1:D:880:GLU:HB3	1:D:883:ALA:HB3	2.02	0.41
1:D:2682:ILE:O	1:D:2686:LEU:HB2	2.21	0.41
1:A:3238:GLU:HA	1:A:3241:PRO:HG3	2.01	0.41
1:A:3718:GLU:OE2	1:A:3719:ASP:N	2.54	0.41
1:A:3780:LEU:HD23	1:A:3780:LEU:HA	1.88	0.41
1:A:4864:ASN:HD21	1:A:4872:PRO:HB2	1.84	0.41
1:B:219:VAL:HG12	1:B:259:LEU:HD12	2.02	0.41
1:B:880:GLU:HB3	1:B:883:ALA:HB3	2.02	0.41
1:B:1699:GLU:OE2	1:B:1813:ARG:NH2	2.38	0.41
1:C:2318:TYR:CZ	1:C:2395:PRO:HD3	2.55	0.41
1:C:2691:TYR:HA	1:C:2696:TYR:HE2	1.85	0.41
1:C:3780:LEU:HD23	1:C:3780:LEU:HA	1.88	0.41
1:D:546:TRP:CE2	1:D:550:LYS:HE2	2.55	0.41
1:D:669:ASP:HB2	1:D:788:LYS:O	2.20	0.41
1:D:1269:CYS:HA	1:D:1564:PHE:O	2.20	0.41
1:D:2377:LEU:N	1:D:2465:ASP:OD2	2.54	0.41
1:D:3159:ASP:OD1	1:D:3159:ASP:N	2.46	0.41
1:A:546:TRP:CE2	1:A:550:LYS:HE2	2.55	0.41
1:A:3944:GLU:OE1	1:A:3946:GLN:N	2.47	0.41
1:A:4188:ARG:HA	1:A:4188:ARG:HD2	1.78	0.41
1:A:4795:TYR:CZ	1:A:4812:HIS:HB3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4914:VAL:HG12	1:D:4888:TYR:CD1	2.56	0.41
1:B:1088:TRP:HB2	1:B:1153:ILE:HG22	2.03	0.41
1:C:2500:ALA:HB2	1:C:2553:TYR:HD1	1.85	0.41
1:C:2696:TYR:HD1	1:C:3001:ILE:HD11	1.86	0.41
1:C:4188:ARG:HD2	1:C:4188:ARG:HA	1.78	0.41
1:D:1231[B]:GLN:H	1:D:1231[B]:GLN:HG3	1.51	0.41
1:D:2696:TYR:HD1	1:D:3001:ILE:HD11	1.86	0.41
1:D:3718:GLU:OE2	1:D:3719:ASP:N	2.54	0.41
1:A:132:ALA:HB1	1:A:192:ASP:HB3	2.02	0.41
1:A:176:SER:O	1:A:178:ARG:NH1	2.54	0.41
1:A:218:HIS:O	1:A:261:ARG:HA	2.19	0.41
1:A:1277:TRP:CD1	1:A:1559:GLN:HG3	2.52	0.41
1:A:2500:ALA:HB2	1:A:2553:TYR:HD1	1.85	0.41
1:A:2682:ILE:O	1:A:2686:LEU:HB2	2.21	0.41
1:A:4930:ALA:HB2	1:D:4933:GLN:HE21	1.86	0.41
1:B:464:LYS:HE2	1:B:464:LYS:HB2	1.89	0.41
1:B:990:GLU:HG3	1:B:1024:TYR:HB3	2.03	0.41
1:B:1231[B]:GLN:H	1:B:1231[B]:GLN:HG3	1.51	0.41
1:B:1694:LEU:HD12	1:B:1715:LEU:HB2	2.02	0.41
1:B:2377:LEU:N	1:B:2465:ASP:OD2	2.54	0.41
1:B:2500:ALA:HB2	1:B:2553:TYR:HD1	1.85	0.41
1:B:2696:TYR:HD1	1:B:3001:ILE:HD11	1.86	0.41
1:B:4795:TYR:CZ	1:B:4812:HIS:HB3	2.56	0.41
1:B:4827:LEU:HD23	1:B:4827:LEU:HA	1.87	0.41
1:C:176:SER:O	1:C:178:ARG:NH1	2.54	0.41
1:C:275:ARG:HE	1:C:336:PRO:HD2	1.85	0.41
1:C:669:ASP:HB2	1:C:788:LYS:O	2.20	0.41
1:C:990:GLU:HG3	1:C:1024:TYR:HB3	2.03	0.41
1:C:2377:LEU:N	1:C:2465:ASP:OD2	2.54	0.41
1:C:4865:LYS:HD2	1:C:4865:LYS:HA	1.63	0.41
1:D:219:VAL:HG12	1:D:259:LEU:HD12	2.02	0.41
1:D:869:ARG:CZ	1:D:870:ILE:HB	2.51	0.41
1:D:2122:SER:O	1:D:2126:ARG:HG3	2.20	0.41
1:D:2583:LEU:HA	1:D:2586:VAL:HG12	2.02	0.41
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.45	0.41
1:A:275:ARG:HE	1:A:336:PRO:HD2	1.85	0.41
1:A:557:SER:HA	1:A:560:ILE:HG22	2.01	0.41
1:A:669:ASP:HB2	1:A:788:LYS:O	2.20	0.41
1:A:990:GLU:HG3	1:A:1024:TYR:HB3	2.03	0.41
1:A:1694:LEU:HD12	1:A:1715:LEU:HB2	2.02	0.41
1:A:2122:SER:O	1:A:2126:ARG:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2696:TYR:HD1	1:A:3001:ILE:HD11	1.86	0.41
1:A:2927:LEU:HD12	1:A:2927:LEU:HA	1.92	0.41
1:A:3244:PRO:HA	1:A:3248:ARG:HH21	1.84	0.41
1:A:4581:LYS:HE3	1:A:4581:LYS:HB3	1.77	0.41
1:B:67:PHE:HB3	1:B:109:LEU:HD11	2.03	0.41
1:B:75:VAL:O	1:B:79:GLN:HG2	2.21	0.41
1:B:3890:LEU:HD23	1:B:3890:LEU:HA	1.85	0.41
1:B:4675:LYS:O	1:B:4679:ARG:HG2	2.20	0.41
1:C:2309:SER:OG	1:C:2321:ILE:O	2.26	0.41
1:C:3245:VAL:H	1:C:3248:ARG:HE	1.67	0.41
1:C:3788:GLY:HA2	1:C:3835:LEU:HG	2.02	0.41
1:C:4112:LEU:O	1:C:4115:SER:OG	2.37	0.41
1:D:3890:LEU:HD23	1:D:3890:LEU:HA	1.85	0.41
1:D:4066:LEU:HD23	1:D:4133:GLN:HE22	1.86	0.41
1:A:67:PHE:HB3	1:A:109:LEU:HD11	2.03	0.41
1:A:2199:ARG:NE	1:A:2246:ASN:OD1	2.50	0.41
1:B:487:VAL:O	1:B:491:ILE:HD12	2.21	0.41
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.86	0.41
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.46	0.41
1:C:475:GLN:OE1	1:C:533:ASN:ND2	2.53	0.41
1:C:557:SER:HA	1:C:560:ILE:HG22	2.01	0.41
1:C:736:HIS:ND1	1:C:737:LEU:O	2.38	0.41
1:C:1064:GLU:O	1:C:1071:ARG:NH2	2.53	0.41
1:C:3244:PRO:HA	1:C:3248:ARG:HH21	1.84	0.41
1:C:3888:LEU:HD23	1:C:3891:LEU:HD21	2.03	0.41
1:C:4020:GLN:HA	1:C:4023:MET:HB3	2.02	0.41
1:C:4911:LEU:HD22	1:C:4911:LEU:HA	1.87	0.41
1:D:557:SER:HA	1:D:560:ILE:HG22	2.01	0.41
1:D:3888:LEU:HD23	1:D:3891:LEU:HD21	2.03	0.41
1:D:4850:LEU:HD23	1:D:4850:LEU:HA	1.86	0.41
1:A:1088:TRP:HB2	1:A:1153:ILE:HG22	2.03	0.41
1:A:1221:GLU:OE1	1:A:1221:GLU:N	2.54	0.41
1:B:176:SER:O	1:B:178:ARG:NH1	2.54	0.41
1:B:869:ARG:CZ	1:B:870:ILE:HB	2.51	0.41
1:B:2318:TYR:CZ	1:B:2395:PRO:HD3	2.55	0.41
1:C:281:ARG:NH2	1:C:309:THR:OG1	2.51	0.41
1:C:1068:ARG:O	1:C:1071:ARG:HG2	2.21	0.41
1:C:2001:PRO:O	1:C:2005:GLN:HG3	2.21	0.41
1:C:2583:LEU:HA	1:C:2586:VAL:HG12	2.02	0.41
1:C:2682:ILE:O	1:C:2686:LEU:HB2	2.21	0.41
1:C:3842:LEU:HD12	1:C:3930:ILE:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4795:TYR:CZ	1:C:4812:HIS:HB3	2.55	0.41
1:C:4869:GLU:H	1:C:4869:GLU:HG2	1.69	0.41
1:C:4878:ASP:HB3	1:C:4881:THR:OG1	2.21	0.41
1:D:23:GLN:OE1	1:D:203:ASN:ND2	2.54	0.41
1:D:1277:TRP:CD1	1:D:1559:GLN:HG3	2.52	0.41
1:D:4878:ASP:HB3	1:D:4881:THR:OG1	2.21	0.41
2:F:18:LYS:HA	2:F:50:ILE:HD11	2.01	0.41
1:A:75:VAL:O	1:A:79:GLN:HG2	2.21	0.41
1:A:498:THR:HA	1:A:553:ARG:HH12	1.86	0.41
1:A:619:ASP:OD1	1:A:620:LEU:N	2.54	0.41
1:A:1099:GLU:OE2	1:A:1101:ARG:NE	2.46	0.41
1:A:2318:TYR:CZ	1:A:2395:PRO:HD3	2.55	0.41
1:A:2494:PHE:HE2	1:A:2499:LYS:HE3	1.86	0.41
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.54	0.41
1:B:218:HIS:O	1:B:261:ARG:HA	2.19	0.41
1:B:436:LEU:HD23	1:B:436:LEU:HA	1.87	0.41
1:B:1068:ARG:O	1:B:1071:ARG:HG2	2.21	0.41
1:B:1085:SER:OG	1:B:1086:GLY:N	2.54	0.41
1:B:1274:HIS:HB3	1:B:1277:TRP:HB2	2.03	0.41
1:B:1782:PHE:O	2:F:82:TYR:OH	2.30	0.41
1:B:2691:TYR:HA	1:B:2696:TYR:HE2	1.85	0.41
1:B:3788:GLY:HA2	1:B:3835:LEU:HG	2.02	0.41
1:C:487:VAL:O	1:C:491:ILE:HD12	2.21	0.41
1:C:663:TYR:OH	1:C:665:GLU:OE2	2.35	0.41
1:C:880:GLU:HB3	1:C:883:ALA:HB3	2.02	0.41
1:C:1434:TYR:HD1	1:C:1519:LEU:HG	1.86	0.41
1:C:2927:LEU:HD12	1:C:2927:LEU:HA	1.91	0.41
1:C:4627:MET:H	1:C:4627:MET:HG3	1.42	0.41
1:D:1500:PHE:HB3	1:D:1531:ALA:HB1	2.03	0.41
1:D:2691:TYR:HA	1:D:2696:TYR:HE2	1.85	0.41
1:D:2862:LEU:O	1:D:2928:LYS:NZ	2.41	0.41
1:D:3420:ARG:HE	1:D:3420:ARG:HB3	1.50	0.41
1:D:3713:LYS:NZ	1:D:3715:LYS:O	2.42	0.41
1:D:4646:LEU:HD23	1:D:4646:LEU:HA	1.89	0.41
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.54	0.41
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.49	0.41
1:A:1068:ARG:O	1:A:1071:ARG:HG2	2.21	0.41
1:A:2181:SER:O	1:A:2185:ILE:HG12	2.21	0.41
1:A:3420:ARG:HE	1:A:3420:ARG:HB3	1.50	0.41
1:B:498:THR:HA	1:B:553:ARG:HH12	1.86	0.41
1:B:1434:TYR:HD1	1:B:1519:LEU:HG	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4085:ARG:O	1:B:4085:ARG:NH1	2.50	0.41
1:B:4582:VAL:HG11	1:C:4860:ARG:HD3	2.03	0.41
1:B:4627:MET:H	1:B:4627:MET:HG3	1.42	0.41
1:C:436:LEU:HD23	1:C:436:LEU:HA	1.87	0.41
1:C:464:LYS:HB2	1:C:464:LYS:HE2	1.90	0.41
1:C:527:ALA:O	1:C:531:ARG:HB2	2.21	0.41
1:C:1500:PHE:HB3	1:C:1531:ALA:HB1	2.03	0.41
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.86	0.41
1:C:4801:LEU:HD23	1:C:4801:LEU:HA	1.93	0.41
1:C:4823:LEU:HD23	1:C:4823:LEU:HA	1.80	0.41
1:D:498:THR:HA	1:D:553:ARG:HH12	1.86	0.41
1:D:990:GLU:HG3	1:D:1024:TYR:HB3	2.03	0.41
1:D:1274:HIS:HB3	1:D:1277:TRP:HB2	2.03	0.41
1:D:2607:LEU:HD23	1:D:2607:LEU:HA	1.91	0.41
1:A:219:VAL:HG12	1:A:259:LEU:HD12	2.02	0.40
1:A:665:GLU:HG2	1:A:745:SER:HA	2.04	0.40
1:A:880:GLU:HB3	1:A:883:ALA:HB3	2.02	0.40
1:A:2377:LEU:N	1:A:2465:ASP:OD2	2.54	0.40
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.86	0.40
1:A:3888:LEU:HD23	1:A:3891:LEU:HD21	2.03	0.40
1:B:132:ALA:HB1	1:B:192:ASP:HB3	2.02	0.40
1:B:1849:LEU:HD23	1:B:1849:LEU:HA	1.91	0.40
1:B:1990:GLU:OE2	1:B:1994:ARG:NH1	2.48	0.40
1:B:2181:SER:O	1:B:2185:ILE:HG12	2.21	0.40
1:B:3718:GLU:OE2	1:B:3719:ASP:N	2.54	0.40
1:B:3842:LEU:HD12	1:B:3930:ILE:HA	2.03	0.40
1:B:4020:GLN:HA	1:B:4023:MET:HB3	2.02	0.40
1:B:4743:MET:H	1:B:4743:MET:HG3	1.63	0.40
1:C:23:GLN:OE1	1:C:203:ASN:ND2	2.54	0.40
1:C:219:VAL:HG12	1:C:259:LEU:HD12	2.02	0.40
1:C:639:ASN:ND2	1:C:676:THR:OG1	2.55	0.40
1:C:4661:TYR:OH	1:C:4786:ASP:OD2	2.34	0.40
1:D:111:HIS:ND1	1:D:114:SER:OG	2.35	0.40
1:D:214:VAL:HG22	1:D:341:TYR:CZ	2.57	0.40
1:D:663:TYR:OH	1:D:665:GLU:OE2	2.35	0.40
1:D:3195:ALA:O	1:D:3279:SER:OG	2.32	0.40
1:D:4112:LEU:O	1:D:4115:SER:OG	2.38	0.40
1:D:4869:GLU:H	1:D:4869:GLU:HG2	1.69	0.40
2:E:28:GLY:N	2:E:37:ASP:O	2.54	0.40
1:A:1254:HIS:HB3	1:A:1274:HIS:CE1	2.57	0.40
1:A:1274:HIS:HB3	1:A:1277:TRP:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2001:PRO:O	1:A:2005:GLN:HG3	2.21	0.40
1:A:4020:GLN:HA	1:A:4023:MET:HB3	2.02	0.40
1:B:275:ARG:HE	1:B:336:PRO:HD2	1.85	0.40
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.49	0.40
1:B:790:ARG:HA	1:B:1626:TRP:O	2.21	0.40
1:B:2007:ASN:O	1:B:2011:HIS:HB2	2.21	0.40
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.55	0.40
1:B:2927:LEU:HD12	1:B:2927:LEU:HA	1.92	0.40
1:B:4059:LEU:HD13	1:B:4059:LEU:HA	1.88	0.40
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.49	0.40
1:C:869:ARG:CZ	1:C:870:ILE:HB	2.51	0.40
1:C:1088:TRP:HB2	1:C:1153:ILE:HG22	2.03	0.40
1:C:1221:GLU:N	1:C:1221:GLU:OE1	2.54	0.40
1:C:1694:LEU:HD12	1:C:1715:LEU:HB2	2.02	0.40
1:C:2026:ASP:N	1:C:2026:ASP:OD1	2.54	0.40
1:C:2268[A]:GLN:H	1:C:2268[A]:GLN:HG3	1.68	0.40
1:D:232:THR:HG22	1:D:258:SER:HB3	2.03	0.40
1:D:527:ALA:O	1:D:531:ARG:HB2	2.21	0.40
1:D:1068:ARG:O	1:D:1071:ARG:HG2	2.21	0.40
1:D:1085:SER:OG	1:D:1086:GLY:N	2.54	0.40
1:D:2001:PRO:O	1:D:2005:GLN:HG3	2.21	0.40
1:D:2109:ASP:OD1	1:D:2109:ASP:N	2.55	0.40
1:D:2554:LEU:HB3	1:D:2559:LEU:HD13	2.04	0.40
1:D:2610:LEU:O	1:D:2614:ILE:HG12	2.22	0.40
1:D:3582:ARG:HD3	1:D:3582:ARG:HA	1.77	0.40
1:D:4020:GLN:HA	1:D:4023:MET:HB3	2.02	0.40
2:E:38:SER:OG	2:E:39:SER:N	2.54	0.40
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.89	0.40
1:A:2007:ASN:O	1:A:2011:HIS:HB2	2.21	0.40
1:A:2159:LEU:HD11	1:A:2163:ARG:HE	1.87	0.40
1:A:4808:PHE:HD1	1:A:4808:PHE:HA	1.80	0.40
1:B:214:VAL:HG22	1:B:341:TYR:CZ	2.57	0.40
1:B:619:ASP:OD1	1:B:620:LEU:N	2.54	0.40
1:B:1221:GLU:OE1	1:B:1221:GLU:N	2.54	0.40
1:B:1254:HIS:HB3	1:B:1274:HIS:CE1	2.57	0.40
1:B:2494:PHE:HE2	1:B:2499:LYS:HE3	1.86	0.40
1:B:4677:LEU:HD12	1:B:4677:LEU:HA	1.83	0.40
1:C:75:VAL:O	1:C:79:GLN:HG2	2.21	0.40
1:C:619:ASP:OD1	1:C:620:LEU:N	2.54	0.40
1:C:1254:HIS:HB3	1:C:1274:HIS:CE1	2.57	0.40
1:C:2109:ASP:OD1	1:C:2109:ASP:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2181:SER:O	1:C:2185:ILE:HG12	2.21	0.40
1:C:2268[B]:GLN:H	1:C:2268[B]:GLN:HG3	1.68	0.40
1:C:3963:ASN:O	1:C:3966:THR:OG1	2.34	0.40
1:C:4066:LEU:HD23	1:C:4133:GLN:HE22	1.86	0.40
1:D:350:HIS:O	1:D:354:GLY:N	2.54	0.40
1:D:2792:ARG:HB2	1:D:2797:PHE:HD1	1.86	0.40
1:D:3450:ASN:HA	1:D:3453:ARG:HG2	2.01	0.40
2:H:38:SER:OG	2:H:39:SER:N	2.54	0.40
1:B:665:GLU:HG2	1:B:745:SER:HA	2.04	0.40
1:B:4066:LEU:HD23	1:B:4133:GLN:HE22	1.86	0.40
1:C:214:VAL:HG22	1:C:341:TYR:CZ	2.57	0.40
1:C:1274:HIS:HB3	1:C:1277:TRP:HB2	2.03	0.40
1:C:2610:LEU:O	1:C:2614:ILE:HG12	2.22	0.40
1:D:75:VAL:O	1:D:79:GLN:HG2	2.21	0.40
1:D:475:GLN:OE1	1:D:533:ASN:ND2	2.53	0.40
1:D:1221:GLU:OE1	1:D:1221:GLU:N	2.54	0.40
1:D:1694:LEU:HD12	1:D:1715:LEU:HB2	2.02	0.40
1:D:4722:ARG:H	1:D:4722:ARG:HG2	1.45	0.40
2:F:77:THR:HG22	2:F:80:VAL:HG22	2.03	0.40
1:A:639:ASN:ND2	1:A:676:THR:OG1	2.54	0.40
1:A:736:HIS:ND1	1:A:737:LEU:O	2.38	0.40
1:B:2001:PRO:O	1:B:2005:GLN:HG3	2.21	0.40
1:B:2355:ARG:HA	1:B:2358:ILE:HG12	2.04	0.40
1:B:3888:LEU:HD23	1:B:3891:LEU:HD21	2.03	0.40
1:C:308:HIS:HD2	1:C:310:LYS:HB2	1.85	0.40
1:C:498:THR:HA	1:C:553:ARG:HH12	1.86	0.40
1:C:1650:ILE:HA	1:C:1653:LEU:HD23	2.03	0.40
1:C:2007:ASN:O	1:C:2011:HIS:HB2	2.21	0.40
1:C:2554:LEU:HB3	1:C:2559:LEU:HD13	2.04	0.40
1:C:3296:LEU:HG	1:C:3297:PRO:HD3	2.04	0.40
1:D:176:SER:O	1:D:178:ARG:NH1	2.54	0.40
1:D:619:ASP:OD1	1:D:620:LEU:N	2.54	0.40
1:D:665:GLU:HG2	1:D:745:SER:HA	2.04	0.40
1:D:790:ARG:HA	1:D:1626:TRP:O	2.21	0.40
1:D:1965:TYR:OH	1:D:2027:ILE:O	2.31	0.40
1:D:3842:LEU:HD12	1:D:3930:ILE:HA	2.03	0.40
2:E:77:THR:HG22	2:E:80:VAL:HG22	2.03	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 PDB entries followed by that with respect to all EM entries.

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	4353/5037 (86%)	4129 (95%)	217 (5%)	7 (0%)	44	76
1	B	4353/5037 (86%)	4128 (95%)	218 (5%)	7 (0%)	44	76
1	C	4353/5037 (86%)	4131 (95%)	215 (5%)	7 (0%)	44	76
1	D	4353/5037 (86%)	4129 (95%)	217 (5%)	7 (0%)	44	76
2	E	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
2	F	105/350 (30%)	96 (91%)	9 (9%)	0	100	100
2	G	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
2	H	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
All	All	17832/21548 (83%)	16898 (95%)	906 (5%)	28 (0%)	45	76

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1069	TRP
1	A	3615	SER
1	A	4910	GLU
1	B	1069	TRP
1	B	3615	SER
1	B	4910	GLU
1	C	1069	TRP
1	C	3615	SER
1	C	4910	GLU
1	D	1069	TRP
1	D	3615	SER
1	D	4910	GLU
1	A	3692	GLU
1	A	3693	LYS
1	A	4691	GLN
1	A	4694	ASP
1	B	3692	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3693	LYS
1	B	4691	GLN
1	B	4694	ASP
1	C	3692	GLU
1	C	3693	LYS
1	C	4691	GLN
1	C	4694	ASP
1	D	3692	GLU
1	D	3693	LYS
1	D	4691	GLN
1	D	4694	ASP

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 PDB entries followed by that with respect to all EM entries.

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	3805/4276 (89%)	3656 (96%)	149 (4%)	27	50
1	B	3805/4276 (89%)	3655 (96%)	150 (4%)	27	50
1	C	3805/4276 (89%)	3655 (96%)	150 (4%)	27	50
1	D	3805/4276 (89%)	3656 (96%)	149 (4%)	27	50
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100
All	All	15572/18320 (85%)	14974 (96%)	598 (4%)	31	51

All (598) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	LYS
1	A	830	ARG
1	A	844	ARG
1	A	846	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1231[A]	GLN
1	A	1231[B]	GLN
1	A	1271	ARG
1	A	1534	LYS
1	A	1743[A]	ARG
1	A	1743[B]	ARG
1	A	1752	ARG
1	A	1758	ARG
1	A	2100[A]	HIS
1	A	2100[B]	HIS
1	A	2224	ARG
1	A	2336	ARG
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2612[A]	ARG
1	A	2612[B]	ARG
1	A	2738	ARG
1	A	2786	LYS
1	A	2806	ARG
1	A	2827	ARG
1	A	2914	LYS
1	A	2985	ARG
1	A	3053	ARG
1	A	3225	ARG
1	A	3614	LYS
1	A	3622	LYS
1	A	4178	LEU
1	A	4181	ILE
1	A	4182	GLU
1	A	4183	ILE
1	A	4190	ILE
1	A	4198	SER
1	A	4199	GLU
1	A	4200	THR
1	A	4202	ARG
1	A	4204	GLN
1	A	4207	MET
1	A	4209	GLN
1	A	4211	LYS
1	A	4213	SER
1	A	4214	LYS
1	A	4217	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4224	GLU
1	A	4227	GLU
1	A	4230	LYS
1	A	4231	MET
1	A	4236	SER
1	A	4544	LEU
1	A	4545	GLU
1	A	4548	ARG
1	A	4550	LYS
1	A	4552	LEU
1	A	4555	LEU
1	A	4564	PHE
1	A	4567	LEU
1	A	4569	LEU
1	A	4576	ILE
1	A	4577	LEU
1	A	4578	LEU
1	A	4580	TYR
1	A	4581	LYS
1	A	4582	VAL
1	A	4583	SER
1	A	4584	ASP
1	A	4585	SER
1	A	4627	MET
1	A	4628	VAL
1	A	4632	LEU
1	A	4634	GLU
1	A	4648	LEU
1	A	4651	THR
1	A	4658	ILE
1	A	4662	ASN
1	A	4676	GLU
1	A	4686	LEU
1	A	4697	VAL
1	A	4698	LYS
1	A	4700	GLN
1	A	4720	VAL
1	A	4722	ARG
1	A	4730	ASP
1	A	4731	ILE
1	A	4734	ARG
1	A	4745	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4748	LEU
1	A	4772	ASP
1	A	4773	VAL
1	A	4780	PHE
1	A	4785	THR
1	A	4788	SER
1	A	4792	LEU
1	A	4795	TYR
1	A	4796	MET
1	A	4797	VAL
1	A	4800	LEU
1	A	4808	PHE
1	A	4813	LEU
1	A	4814	LEU
1	A	4821	LYS
1	A	4822	THR
1	A	4823	LEU
1	A	4843	LEU
1	A	4844	LEU
1	A	4861	LYS
1	A	4863	TYR
1	A	4865	LYS
1	A	4867	GLU
1	A	4870	ASP
1	A	4871	GLU
1	A	4873	ASP
1	A	4880	MET
1	A	4881	THR
1	A	4882	CYS
1	A	4884	LEU
1	A	4886	HIS
1	A	4887	MET
1	A	4889	VAL
1	A	4908	GLU
1	A	4911	LEU
1	A	4914	VAL
1	A	4917	ASP
1	A	4933	GLN
1	A	4936	ILE
1	A	4942	GLU
1	A	4945	ASP
1	A	4949	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4950	VAL
1	A	4951	LYS
1	A	4952	GLU
1	A	4965	SER
1	A	4966	ASP
1	A	4967	TYR
1	A	4971	THR
1	A	4973	HIS
1	A	4980	LEU
1	A	4982	GLU
1	A	4985	LEU
1	A	4989	MET
1	A	4998	LYS
1	A	5002	GLU
1	A	5012	LYS
1	A	5029	ARG
1	A	5030	LYS
1	A	5034	ASP
1	A	5036	LEU
1	B	373	LYS
1	B	830	ARG
1	B	844	ARG
1	B	846	LEU
1	B	1231[A]	GLN
1	B	1231[B]	GLN
1	B	1271	ARG
1	B	1534	LYS
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	1752	ARG
1	B	1758	ARG
1	B	2100[A]	HIS
1	B	2100[B]	HIS
1	B	2224	ARG
1	B	2336	ARG
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2612[A]	ARG
1	B	2612[B]	ARG
1	B	2738	ARG
1	B	2786	LYS
1	B	2806	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2827	ARG
1	B	2914	LYS
1	B	2985	ARG
1	B	3053	ARG
1	B	3225	ARG
1	B	3614	LYS
1	B	3622	LYS
1	B	4178	LEU
1	B	4181	ILE
1	B	4182	GLU
1	B	4183	ILE
1	B	4190	ILE
1	B	4198	SER
1	B	4199	GLU
1	B	4200	THR
1	B	4202	ARG
1	B	4204	GLN
1	B	4207	MET
1	B	4209	GLN
1	B	4211	LYS
1	B	4213	SER
1	B	4214	LYS
1	B	4217	PHE
1	B	4224	GLU
1	B	4227	GLU
1	B	4230	LYS
1	B	4231	MET
1	B	4236	SER
1	B	4544	LEU
1	B	4545	GLU
1	B	4548	ARG
1	B	4550	LYS
1	B	4552	LEU
1	B	4555	LEU
1	B	4564	PHE
1	B	4567	LEU
1	B	4569	LEU
1	B	4576	ILE
1	B	4577	LEU
1	B	4578	LEU
1	B	4580	TYR
1	B	4581	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4582	VAL
1	B	4583	SER
1	B	4584	ASP
1	B	4585	SER
1	B	4627	MET
1	B	4628	VAL
1	B	4632	LEU
1	B	4634	GLU
1	B	4648	LEU
1	B	4651	THR
1	B	4658	ILE
1	B	4662	ASN
1	B	4676	GLU
1	B	4686	LEU
1	B	4697	VAL
1	B	4698	LYS
1	B	4700	GLN
1	B	4720	VAL
1	B	4722	ARG
1	B	4730	ASP
1	B	4731	ILE
1	B	4734	ARG
1	B	4743	MET
1	B	4745	LEU
1	B	4748	LEU
1	B	4772	ASP
1	B	4773	VAL
1	B	4780	PHE
1	B	4785	THR
1	B	4788	SER
1	B	4792	LEU
1	B	4795	TYR
1	B	4796	MET
1	B	4797	VAL
1	B	4800	LEU
1	B	4808	PHE
1	B	4813	LEU
1	B	4814	LEU
1	B	4821	LYS
1	B	4822	THR
1	B	4823	LEU
1	B	4843	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4844	LEU
1	B	4861	LYS
1	B	4863	TYR
1	B	4865	LYS
1	B	4867	GLU
1	B	4870	ASP
1	B	4871	GLU
1	B	4873	ASP
1	B	4880	MET
1	B	4881	THR
1	B	4882	CYS
1	B	4884	LEU
1	B	4886	HIS
1	B	4887	MET
1	B	4889	VAL
1	B	4908	GLU
1	B	4911	LEU
1	B	4914	VAL
1	B	4917	ASP
1	B	4933	GLN
1	B	4936	ILE
1	B	4942	GLU
1	B	4945	ASP
1	B	4949	GLN
1	B	4950	VAL
1	B	4951	LYS
1	B	4952	GLU
1	B	4965	SER
1	B	4966	ASP
1	B	4967	TYR
1	B	4971	THR
1	B	4973	HIS
1	B	4980	LEU
1	B	4982	GLU
1	B	4985	LEU
1	B	4989	MET
1	B	4998	LYS
1	B	5002	GLU
1	B	5012	LYS
1	B	5029	ARG
1	B	5030	LYS
1	B	5034	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	5036	LEU
1	C	373	LYS
1	C	830	ARG
1	C	844	ARG
1	C	846	LEU
1	C	1231[A]	GLN
1	C	1231[B]	GLN
1	C	1271	ARG
1	C	1534	LYS
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	1752	ARG
1	C	1758	ARG
1	C	2100[A]	HIS
1	C	2100[B]	HIS
1	C	2224	ARG
1	C	2336	ARG
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2612[A]	ARG
1	C	2612[B]	ARG
1	C	2738	ARG
1	C	2786	LYS
1	C	2806	ARG
1	C	2827	ARG
1	C	2914	LYS
1	C	2985	ARG
1	C	3053	ARG
1	C	3225	ARG
1	C	3614	LYS
1	C	3622	LYS
1	C	4178	LEU
1	C	4181	ILE
1	C	4182	GLU
1	C	4183	ILE
1	C	4190	ILE
1	C	4198	SER
1	C	4199	GLU
1	C	4200	THR
1	C	4202	ARG
1	C	4204	GLN
1	C	4207	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4209	GLN
1	C	4211	LYS
1	C	4213	SER
1	C	4214	LYS
1	C	4217	PHE
1	C	4224	GLU
1	C	4227	GLU
1	C	4230	LYS
1	C	4231	MET
1	C	4236	SER
1	C	4544	LEU
1	C	4545	GLU
1	C	4548	ARG
1	C	4550	LYS
1	C	4552	LEU
1	C	4555	LEU
1	C	4564	PHE
1	C	4567	LEU
1	C	4569	LEU
1	C	4576	ILE
1	C	4577	LEU
1	C	4578	LEU
1	C	4580	TYR
1	C	4581	LYS
1	C	4582	VAL
1	C	4583	SER
1	C	4584	ASP
1	C	4585	SER
1	C	4627	MET
1	C	4628	VAL
1	C	4632	LEU
1	C	4634	GLU
1	C	4648	LEU
1	C	4651	THR
1	C	4658	ILE
1	C	4662	ASN
1	C	4676	GLU
1	C	4686	LEU
1	C	4697	VAL
1	C	4698	LYS
1	C	4700	GLN
1	C	4720	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4722	ARG
1	C	4730	ASP
1	C	4731	ILE
1	C	4734	ARG
1	C	4743	MET
1	C	4745	LEU
1	C	4748	LEU
1	C	4772	ASP
1	C	4773	VAL
1	C	4780	PHE
1	C	4785	THR
1	C	4788	SER
1	C	4792	LEU
1	C	4795	TYR
1	C	4796	MET
1	C	4797	VAL
1	C	4800	LEU
1	C	4808	PHE
1	C	4813	LEU
1	C	4814	LEU
1	C	4821	LYS
1	C	4822	THR
1	C	4823	LEU
1	C	4843	LEU
1	C	4844	LEU
1	C	4861	LYS
1	C	4863	TYR
1	C	4865	LYS
1	C	4867	GLU
1	C	4870	ASP
1	C	4871	GLU
1	C	4873	ASP
1	C	4880	MET
1	C	4881	THR
1	C	4882	CYS
1	C	4884	LEU
1	C	4886	HIS
1	C	4887	MET
1	C	4889	VAL
1	C	4908	GLU
1	C	4911	LEU
1	C	4914	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4917	ASP
1	C	4933	GLN
1	C	4936	ILE
1	C	4942	GLU
1	C	4945	ASP
1	C	4949	GLN
1	C	4950	VAL
1	C	4951	LYS
1	C	4952	GLU
1	C	4965	SER
1	C	4966	ASP
1	C	4967	TYR
1	C	4971	THR
1	C	4973	HIS
1	C	4980	LEU
1	C	4982	GLU
1	C	4985	LEU
1	C	4989	MET
1	C	4998	LYS
1	C	5002	GLU
1	C	5012	LYS
1	C	5029	ARG
1	C	5030	LYS
1	C	5034	ASP
1	C	5036	LEU
1	D	373	LYS
1	D	830	ARG
1	D	844	ARG
1	D	846	LEU
1	D	1231[A]	GLN
1	D	1231[B]	GLN
1	D	1271	ARG
1	D	1534	LYS
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	1752	ARG
1	D	1758	ARG
1	D	2100[A]	HIS
1	D	2100[B]	HIS
1	D	2224	ARG
1	D	2336	ARG
1	D	2369[A]	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2369[B]	ARG
1	D	2612[A]	ARG
1	D	2612[B]	ARG
1	D	2738	ARG
1	D	2786	LYS
1	D	2806	ARG
1	D	2827	ARG
1	D	2914	LYS
1	D	2985	ARG
1	D	3053	ARG
1	D	3225	ARG
1	D	3614	LYS
1	D	3622	LYS
1	D	4178	LEU
1	D	4181	ILE
1	D	4182	GLU
1	D	4183	ILE
1	D	4190	ILE
1	D	4198	SER
1	D	4199	GLU
1	D	4200	THR
1	D	4202	ARG
1	D	4204	GLN
1	D	4207	MET
1	D	4209	GLN
1	D	4211	LYS
1	D	4213	SER
1	D	4214	LYS
1	D	4217	PHE
1	D	4224	GLU
1	D	4227	GLU
1	D	4230	LYS
1	D	4231	MET
1	D	4236	SER
1	D	4544	LEU
1	D	4545	GLU
1	D	4548	ARG
1	D	4550	LYS
1	D	4552	LEU
1	D	4555	LEU
1	D	4564	PHE
1	D	4567	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4569	LEU
1	D	4576	ILE
1	D	4577	LEU
1	D	4578	LEU
1	D	4580	TYR
1	D	4581	LYS
1	D	4582	VAL
1	D	4583	SER
1	D	4584	ASP
1	D	4585	SER
1	D	4627	MET
1	D	4628	VAL
1	D	4632	LEU
1	D	4634	GLU
1	D	4648	LEU
1	D	4651	THR
1	D	4658	ILE
1	D	4662	ASN
1	D	4676	GLU
1	D	4686	LEU
1	D	4697	VAL
1	D	4698	LYS
1	D	4700	GLN
1	D	4720	VAL
1	D	4722	ARG
1	D	4730	ASP
1	D	4731	ILE
1	D	4734	ARG
1	D	4745	LEU
1	D	4748	LEU
1	D	4772	ASP
1	D	4773	VAL
1	D	4780	PHE
1	D	4785	THR
1	D	4788	SER
1	D	4792	LEU
1	D	4795	TYR
1	D	4796	MET
1	D	4797	VAL
1	D	4800	LEU
1	D	4808	PHE
1	D	4813	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4814	LEU
1	D	4821	LYS
1	D	4822	THR
1	D	4823	LEU
1	D	4843	LEU
1	D	4844	LEU
1	D	4861	LYS
1	D	4863	TYR
1	D	4865	LYS
1	D	4867	GLU
1	D	4870	ASP
1	D	4871	GLU
1	D	4873	ASP
1	D	4880	MET
1	D	4881	THR
1	D	4882	CYS
1	D	4884	LEU
1	D	4886	HIS
1	D	4887	MET
1	D	4889	VAL
1	D	4908	GLU
1	D	4911	LEU
1	D	4914	VAL
1	D	4917	ASP
1	D	4933	GLN
1	D	4936	ILE
1	D	4942	GLU
1	D	4945	ASP
1	D	4949	GLN
1	D	4950	VAL
1	D	4951	LYS
1	D	4952	GLU
1	D	4965	SER
1	D	4966	ASP
1	D	4967	TYR
1	D	4971	THR
1	D	4973	HIS
1	D	4980	LEU
1	D	4982	GLU
1	D	4985	LEU
1	D	4989	MET
1	D	4998	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	5002	GLU
1	D	5012	LYS
1	D	5029	ARG
1	D	5030	LYS
1	D	5034	ASP
1	D	5036	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	226	HIS
1	A	475	GLN
1	A	489	ASN
1	A	533	ASN
1	A	838	HIS
1	A	877	ASN
1	A	1066	GLN
1	A	1299	GLN
1	A	1300	HIS
1	A	1463	ASN
1	A	1545	ASN
1	A	1610	ASN
1	A	2931	GLN
1	A	2933	ASN
1	A	3214	ASN
1	A	3318	ASN
1	A	3457	ASN
1	A	4728	HIS
1	A	4886	HIS
1	A	5031	GLN
1	B	98	HIS
1	B	226	HIS
1	B	475	GLN
1	B	489	ASN
1	B	533	ASN
1	B	838	HIS
1	B	877	ASN
1	B	1066	GLN
1	B	1299	GLN
1	B	1463	ASN
1	B	1545	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1610	ASN
1	B	2931	GLN
1	B	3214	ASN
1	B	3318	ASN
1	B	3325	ASN
1	B	3457	ASN
1	B	4133	GLN
1	B	4728	HIS
1	B	4886	HIS
1	B	4933	GLN
1	B	5031	GLN
1	C	98	HIS
1	C	226	HIS
1	C	475	GLN
1	C	489	ASN
1	C	533	ASN
1	C	838	HIS
1	C	877	ASN
1	C	1066	GLN
1	C	1299	GLN
1	C	1463	ASN
1	C	1545	ASN
1	C	1610	ASN
1	C	2931	GLN
1	C	2933	ASN
1	C	3214	ASN
1	C	3318	ASN
1	C	3457	ASN
1	C	4728	HIS
1	C	4864	ASN
1	C	4886	HIS
1	C	4933	GLN
1	C	5031	GLN
1	D	98	HIS
1	D	226	HIS
1	D	475	GLN
1	D	489	ASN
1	D	533	ASN
1	D	838	HIS
1	D	877	ASN
1	D	1066	GLN
1	D	1299	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1463	ASN
1	D	1545	ASN
1	D	1610	ASN
1	D	2931	GLN
1	D	3214	ASN
1	D	3318	ASN
1	D	3325	ASN
1	D	3457	ASN
1	D	4133	GLN
1	D	4728	HIS
1	D	4864	ASN
1	D	4886	HIS
1	D	4933	GLN
1	D	5031	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADE	D	5102	-	8,11,11	0.95	0	6,15,15	1.10	0
4	ADE	C	5102	-	8,11,11	0.95	0	6,15,15	1.10	0
4	ADE	B	5102	-	8,11,11	0.95	0	6,15,15	1.10	0
4	ADE	A	5102	-	8,11,11	0.95	0	6,15,15	1.10	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
4	ADE	D	5102	-	-	-	0/2/2/2
4	ADE	C	5102	-	-	-	0/2/2/2
4	ADE	B	5102	-	-	-	0/2/2/2
4	ADE	A	5102	-	-	-	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

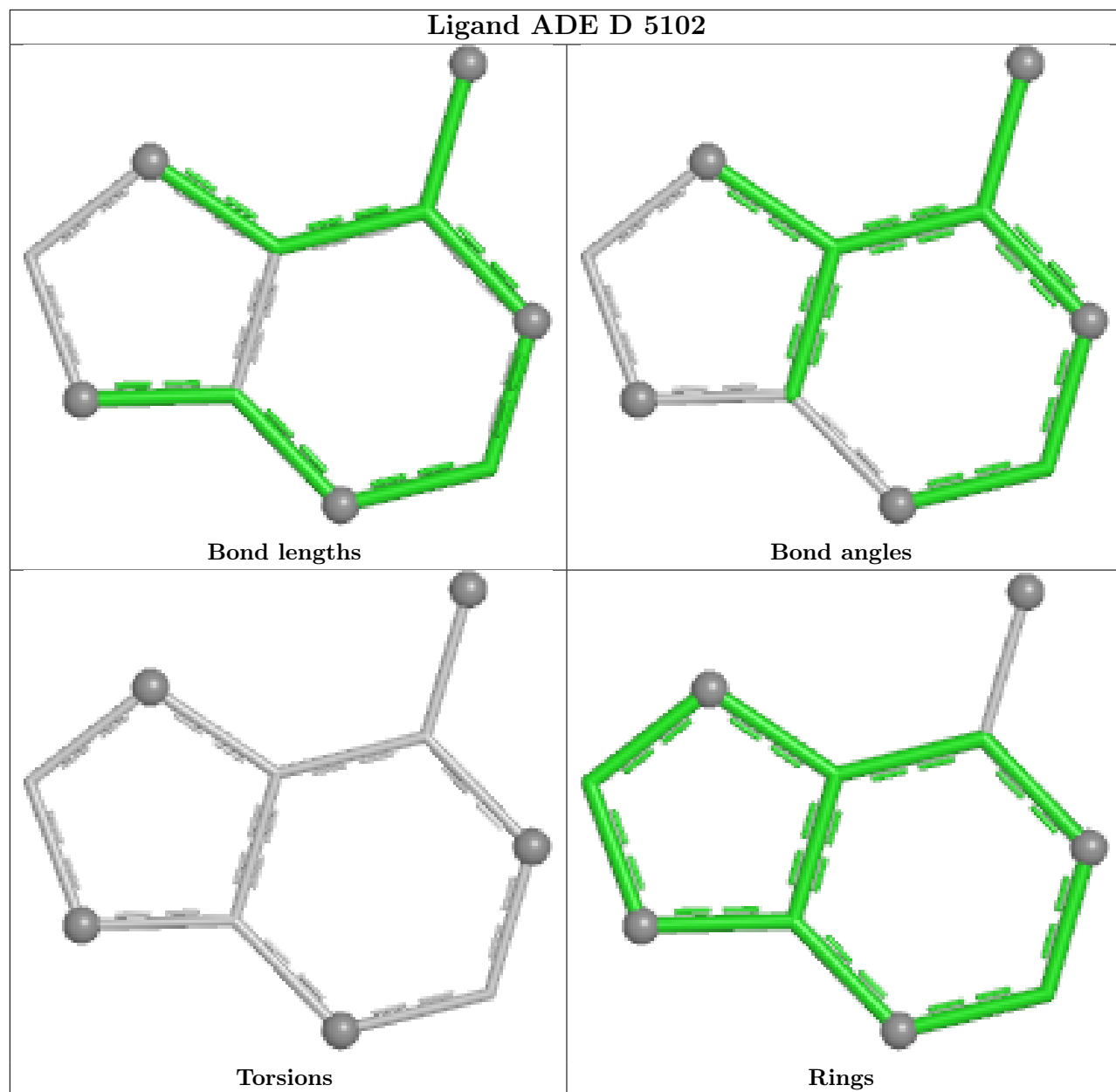
There are no torsion outliers.

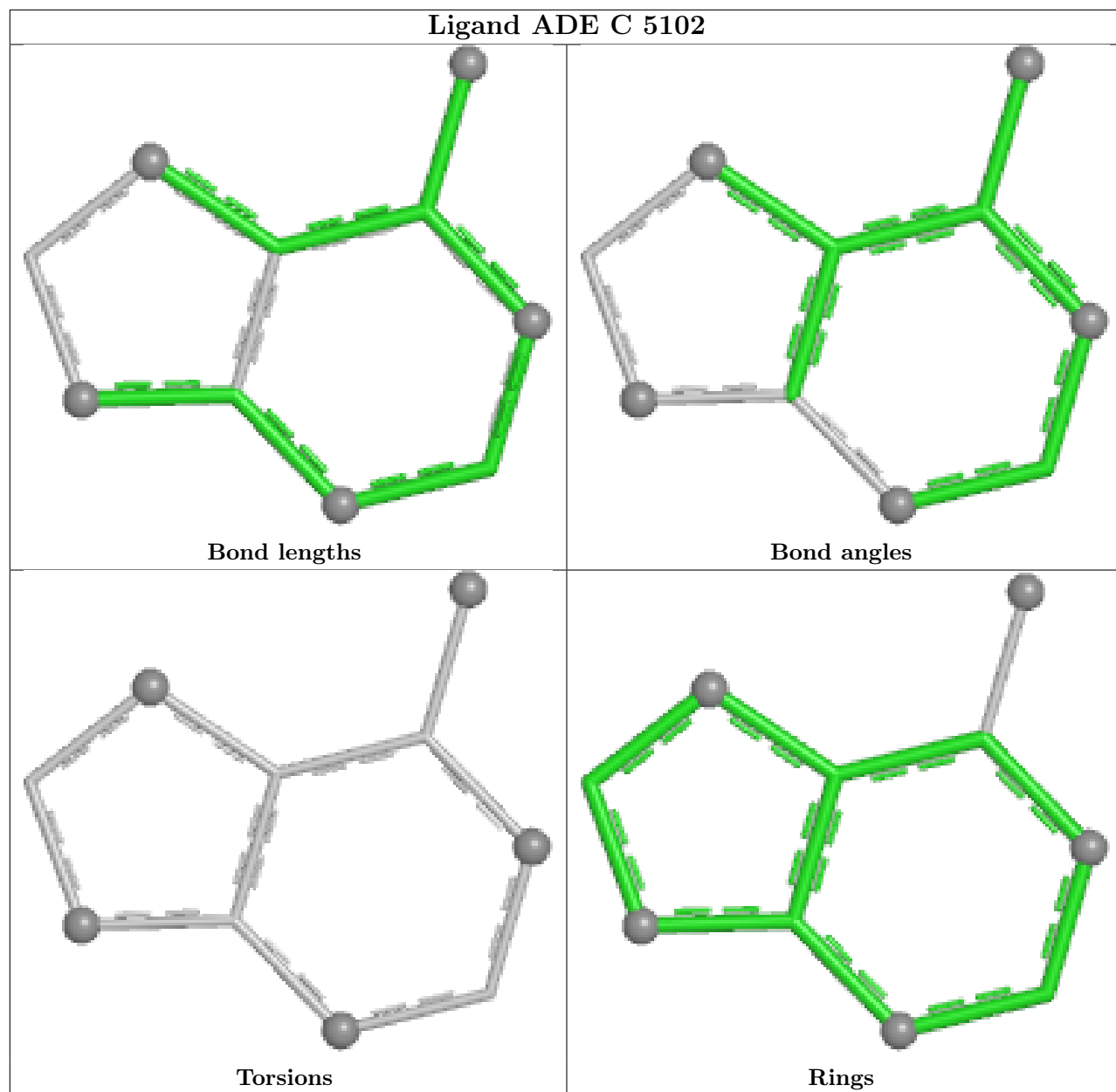
There are no ring outliers.

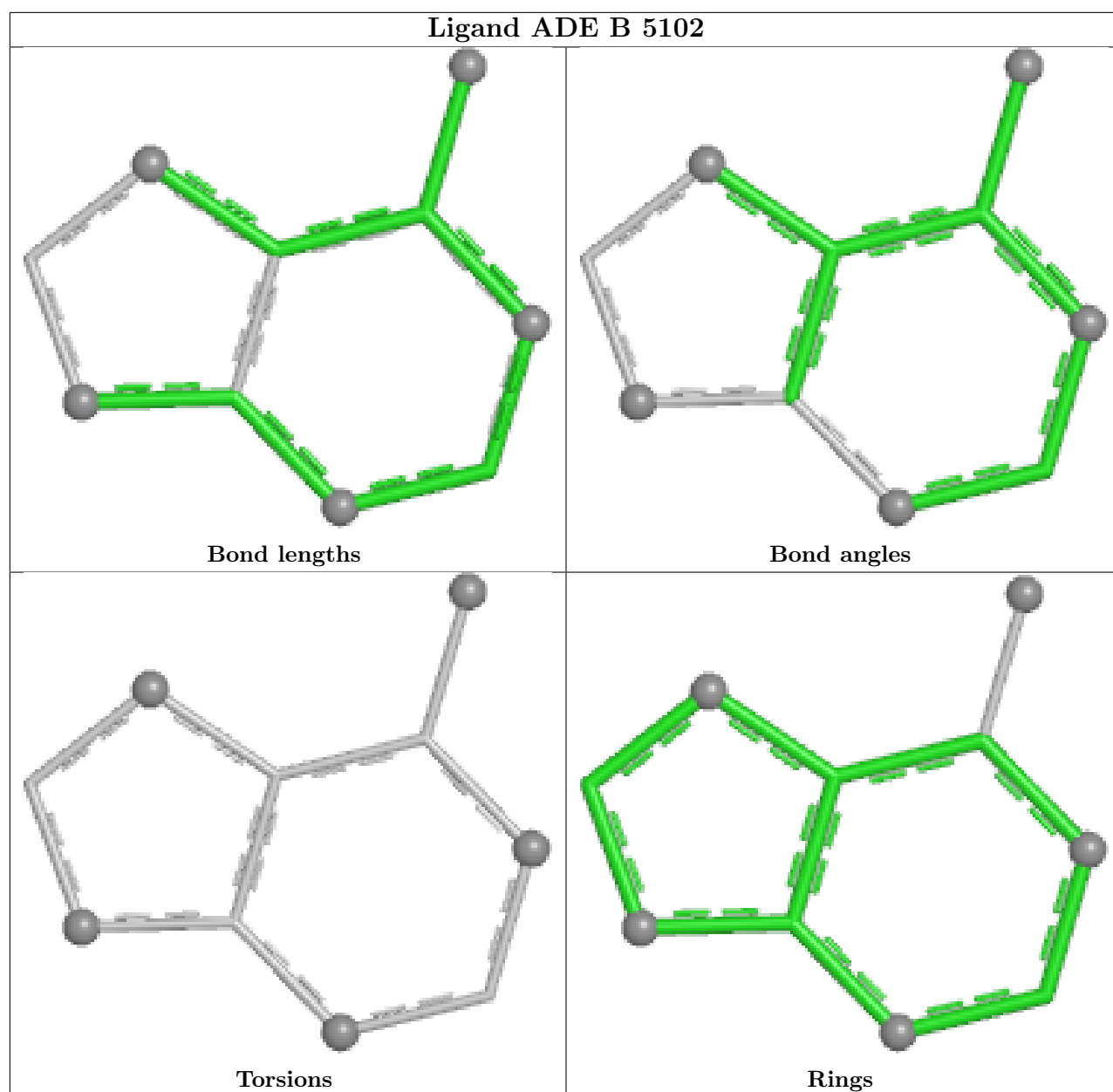
4 monomers are involved in 4 short contacts:

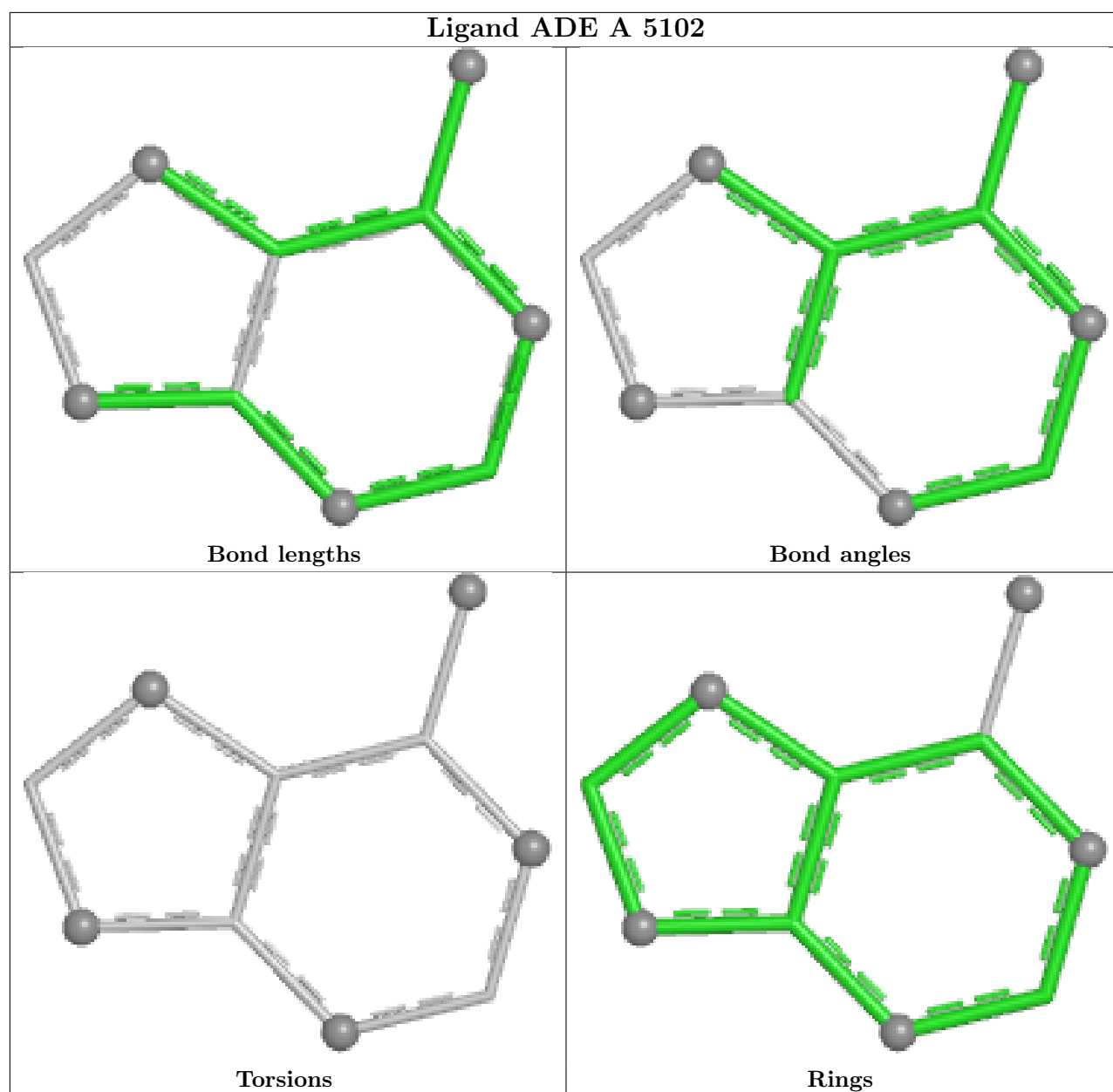
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5102	ADE	1	0
4	C	5102	ADE	1	0
4	B	5102	ADE	1	0
4	A	5102	ADE	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

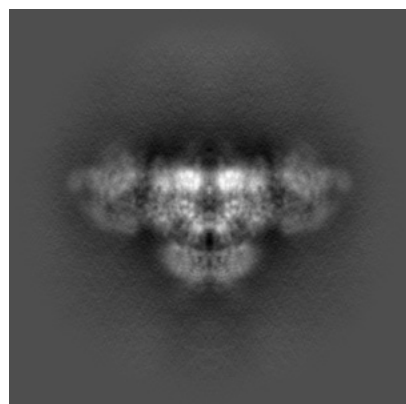
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40427. These allow visual inspection of the internal detail of the map and identification of artifacts.

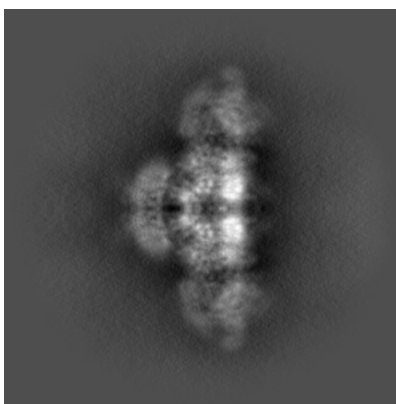
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

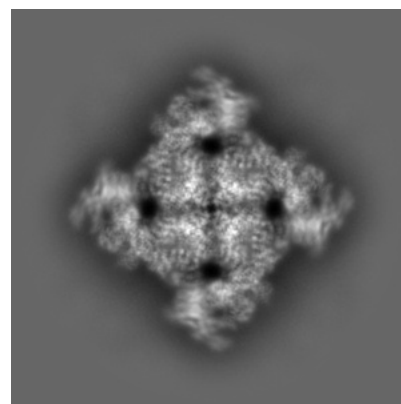
6.1.1 Primary map



X

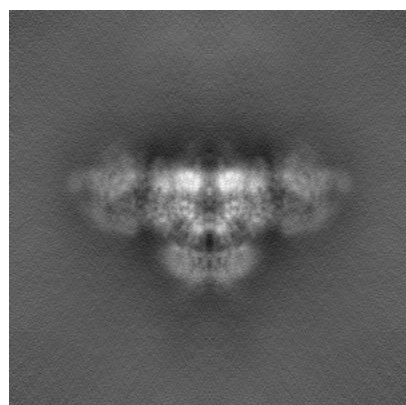


Y

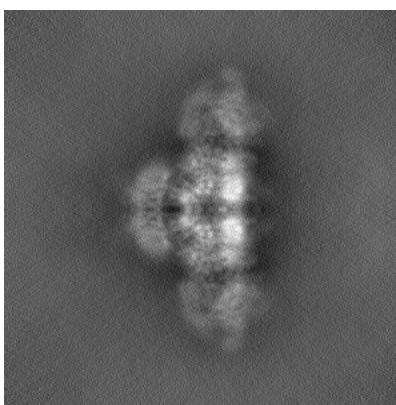


Z

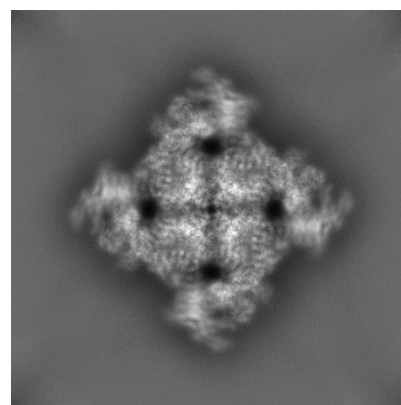
6.1.2 Raw map



X



Y

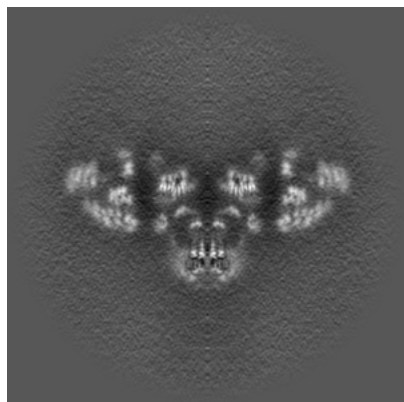


Z

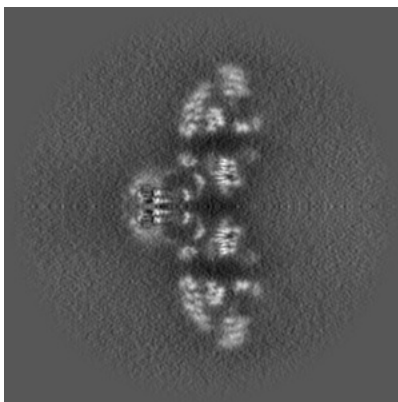
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

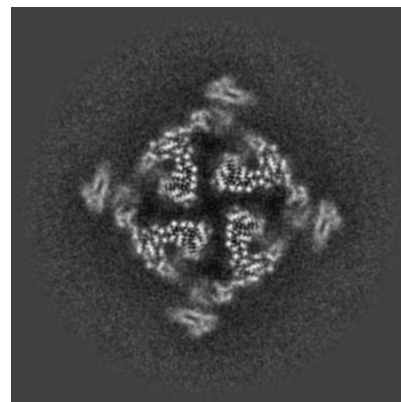
6.2.1 Primary map



X Index: 200

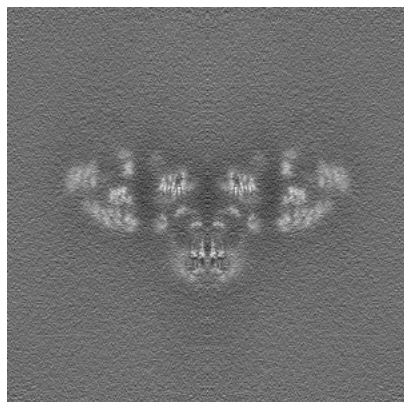


Y Index: 200

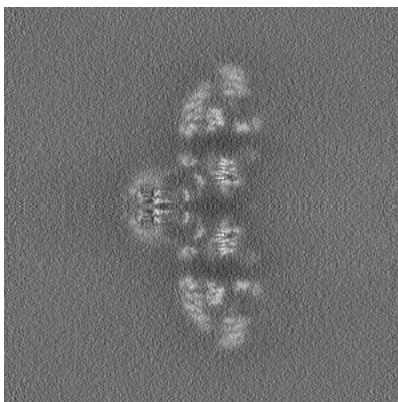


Z Index: 200

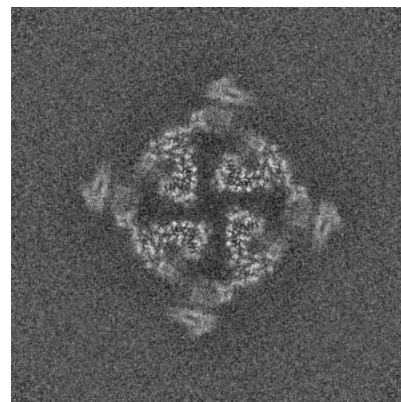
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

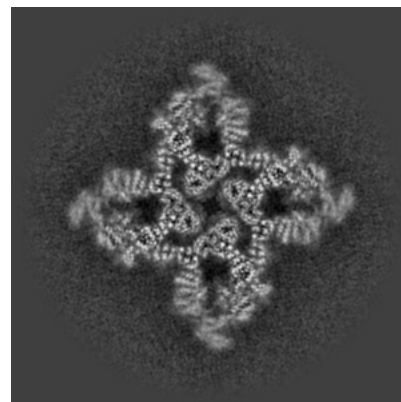
6.3.1 Primary map



X Index: 182

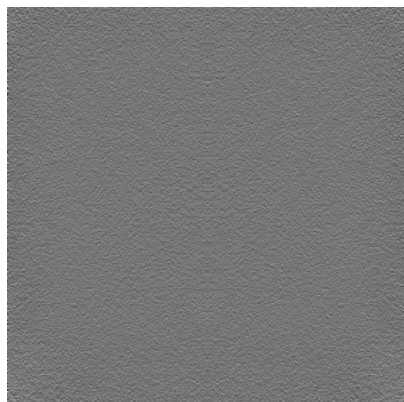


Y Index: 182

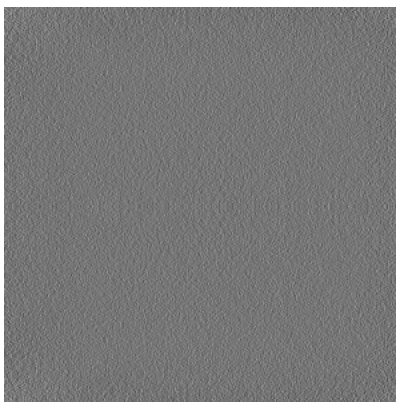


Z Index: 225

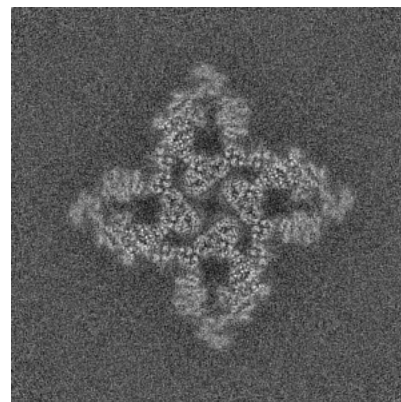
6.3.2 Raw map



X Index: 0



Y Index: 0

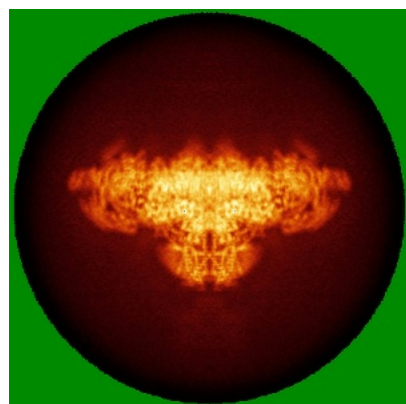


Z Index: 224

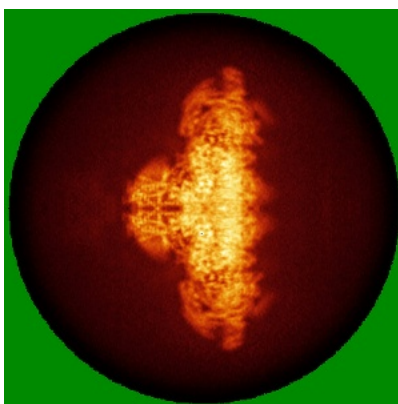
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

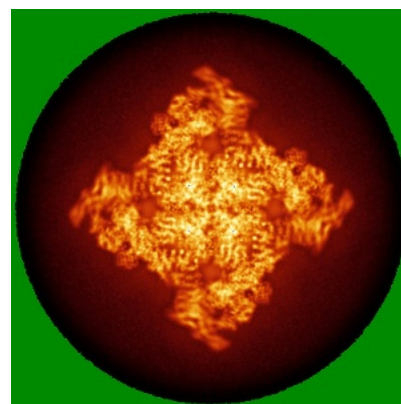
6.4.1 Primary map



X

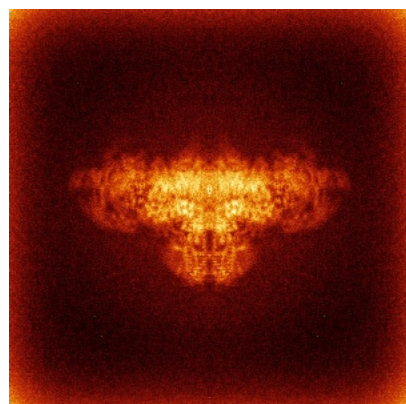


Y

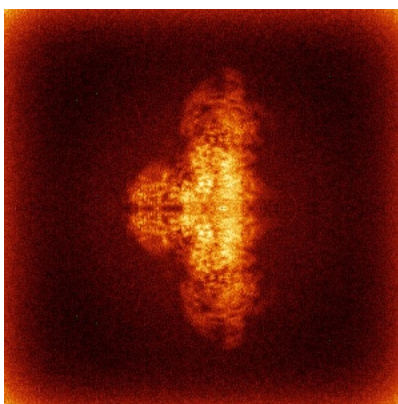


Z

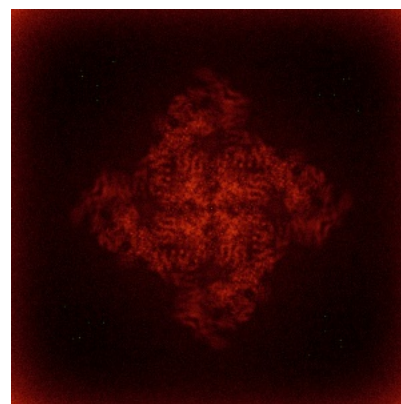
6.4.2 Raw map



X



Y

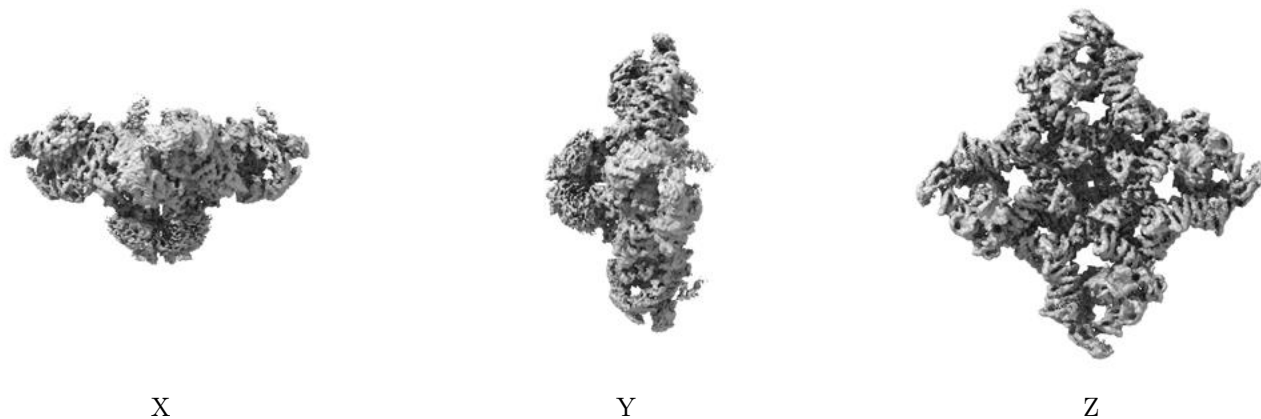


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

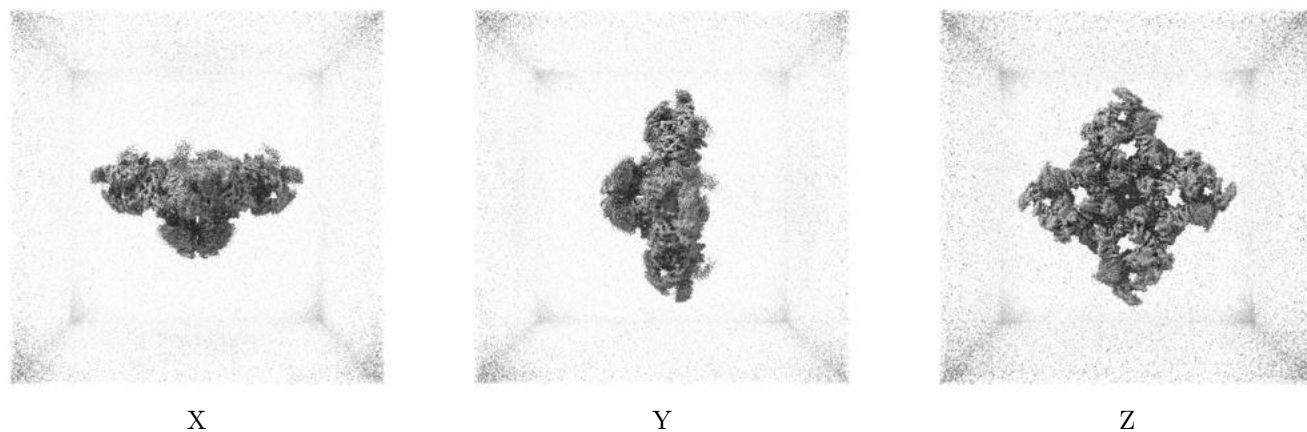
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.305. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

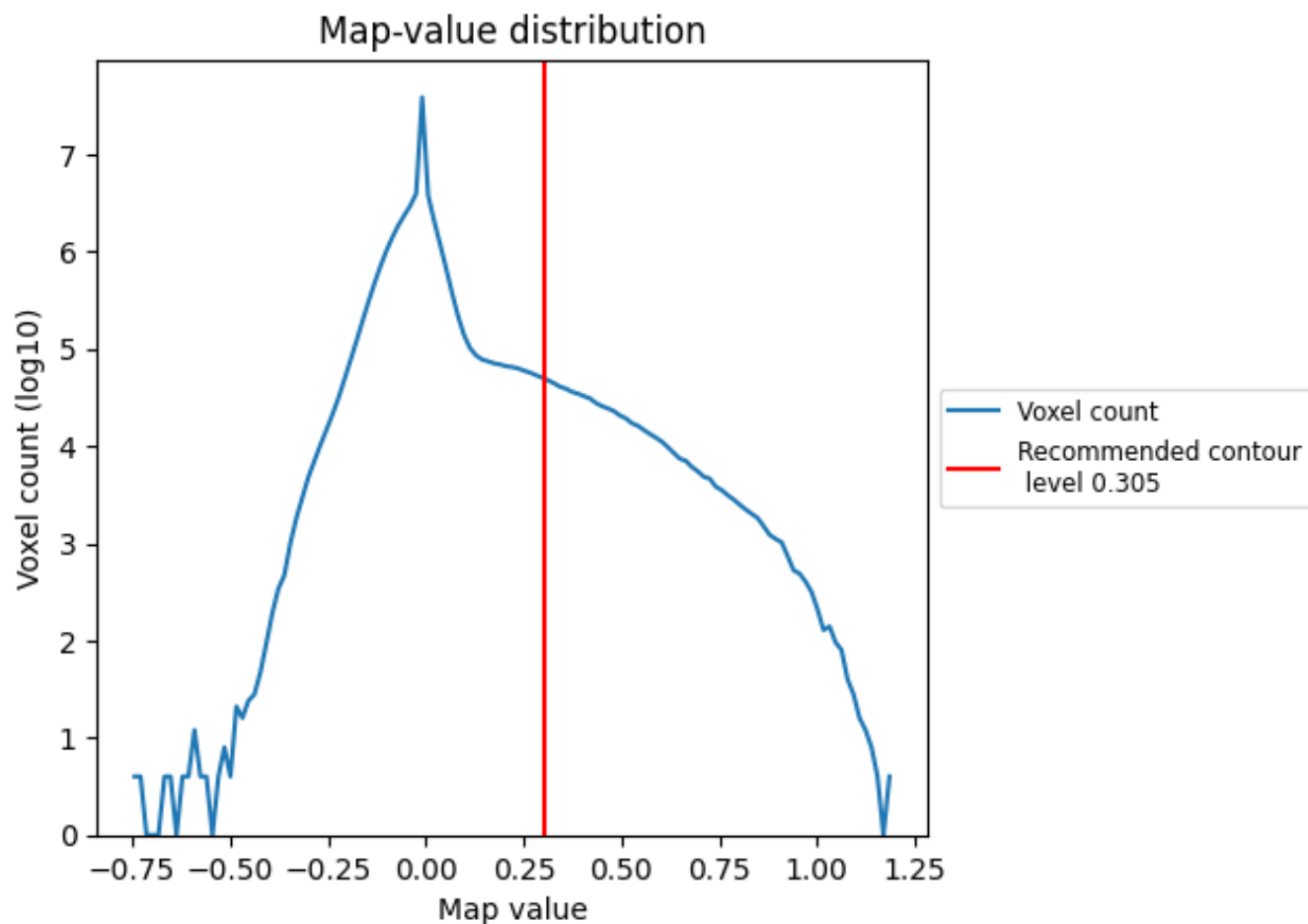
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

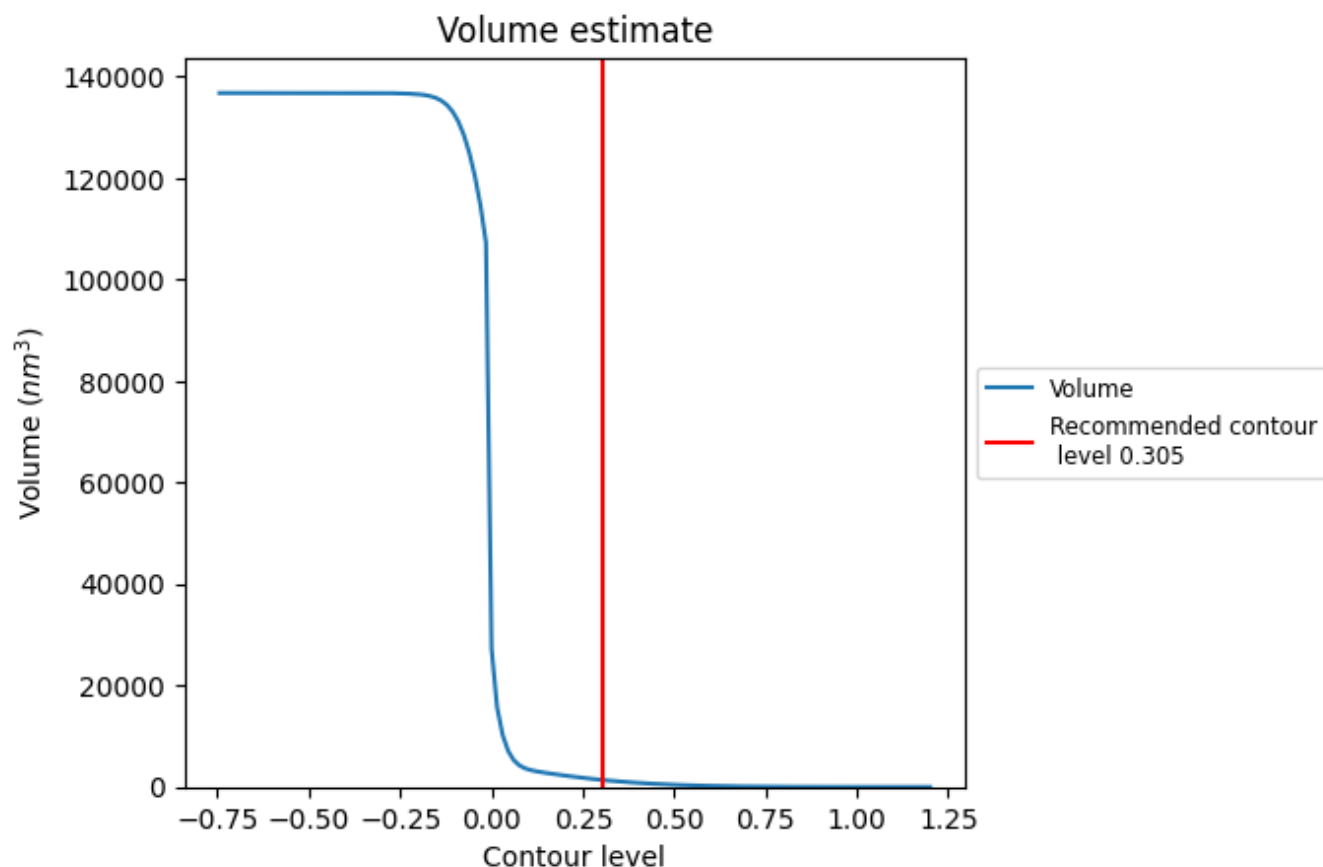
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

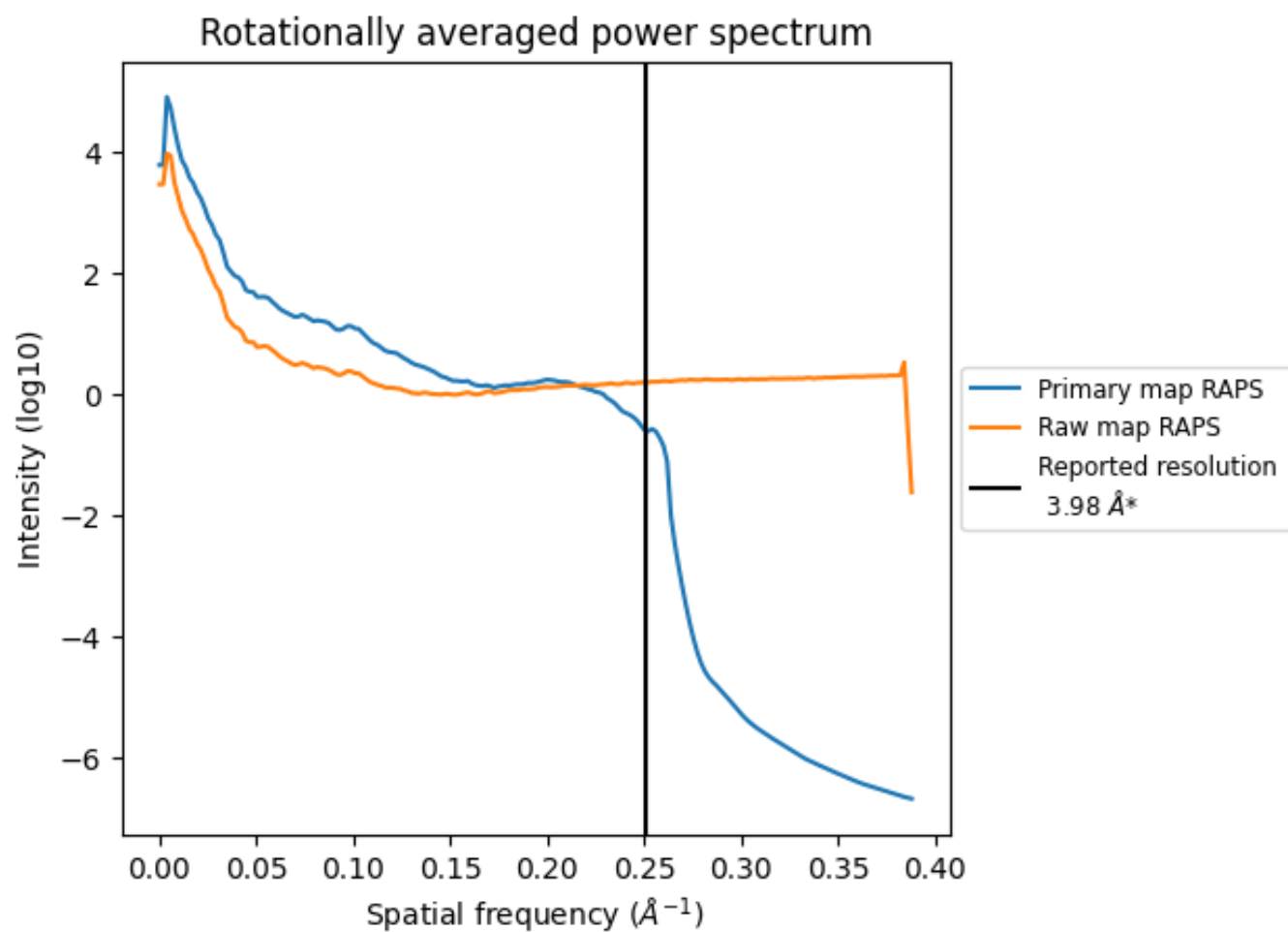
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1365 nm^3 ; this corresponds to an approximate mass of 1233 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

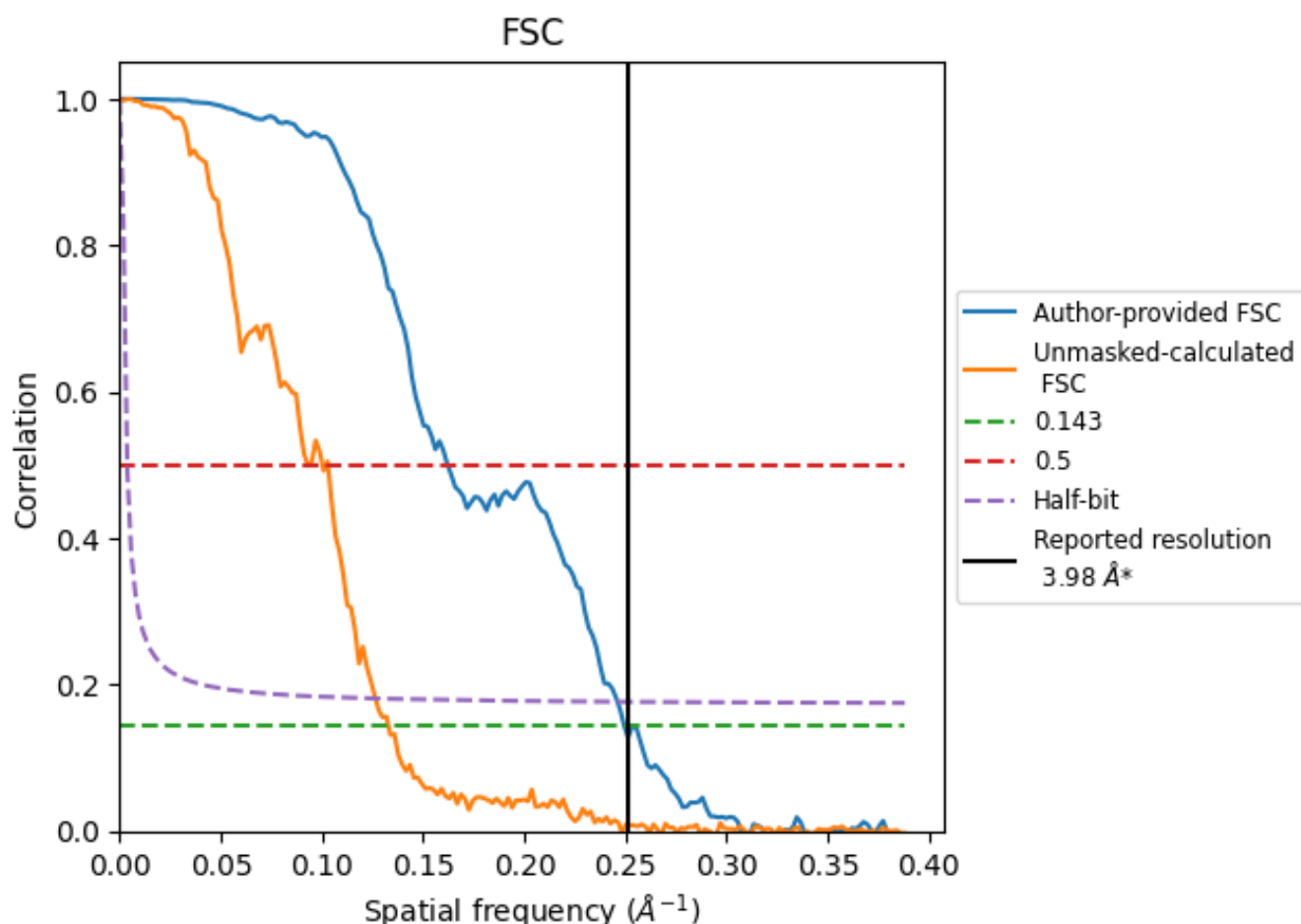


*Reported resolution corresponds to spatial frequency of 0.251 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

8.2 Resolution estimates [i](#)

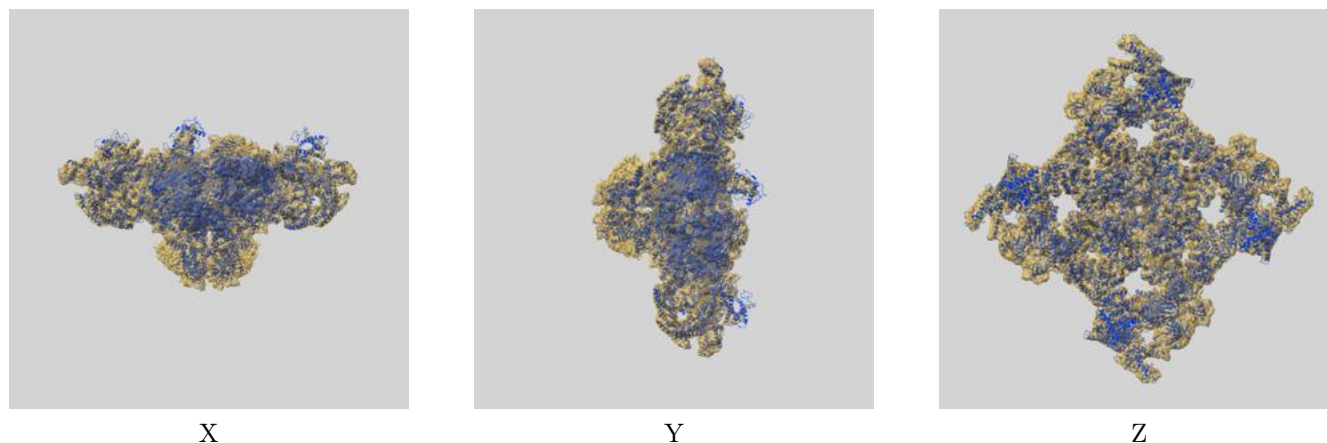
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.98	-	-
Author-provided FSC curve	4.01	6.17	4.06
Unmasked-calculated*	7.52	10.75	7.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.52 differs from the reported value 3.98 by more than 10 %

9 Map-model fit [i](#)

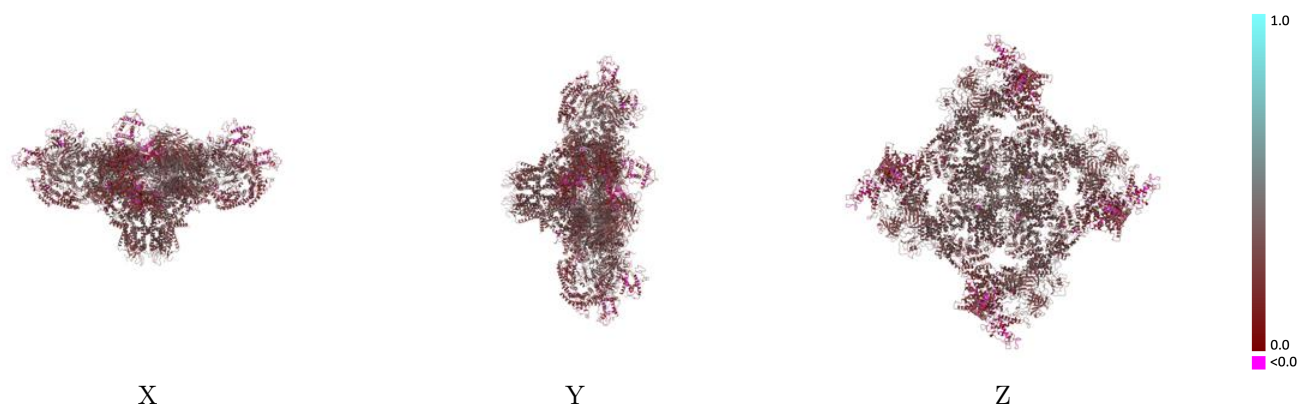
This section contains information regarding the fit between EMDB map EMD-40427 and PDB model 8SES. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



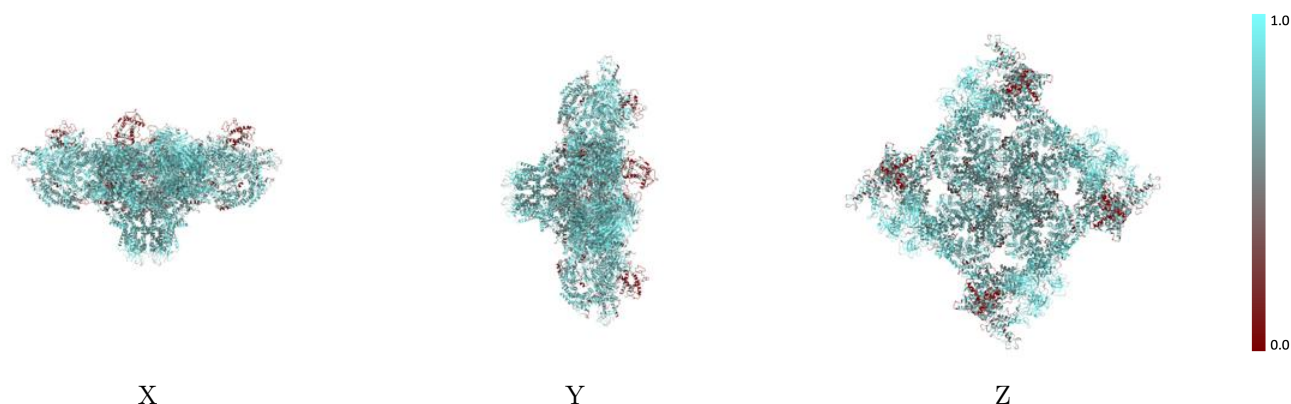
The images above show the 3D surface view of the map at the recommended contour level 0.305 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



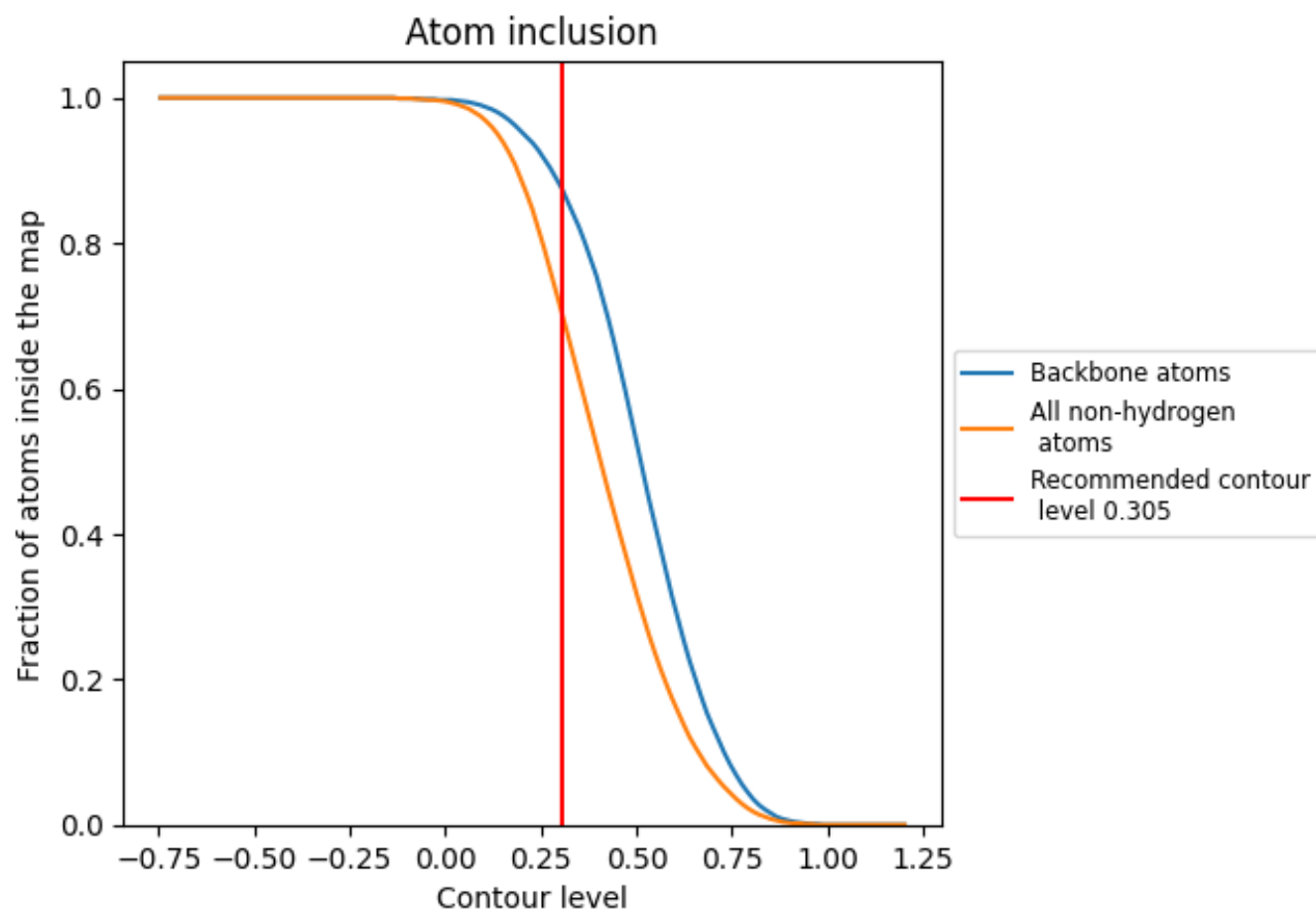
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.305).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.305) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7040	<div></div> 0.2840
A	<div></div> 0.7000	<div></div> 0.2820
B	<div></div> 0.7010	<div></div> 0.2820
C	<div></div> 0.7010	<div></div> 0.2820
D	<div></div> 0.7010	<div></div> 0.2830
E	<div></div> 0.8610	<div></div> 0.3440
F	<div></div> 0.8610	<div></div> 0.3430
G	<div></div> 0.8610	<div></div> 0.3420
H	<div></div> 0.8610	<div></div> 0.3450

1.0

0.0

<0.0