



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 07:13 PM EST

PDB ID : 7JMH  
EMDB ID : EMD-22394  
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots  
- Frame 35 - State 4 (S4)  
Authors : Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.  
Deposited on : 2020-07-31  
Resolution : 4.50 Å(reported)  
Based on initial model : 5TB4

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

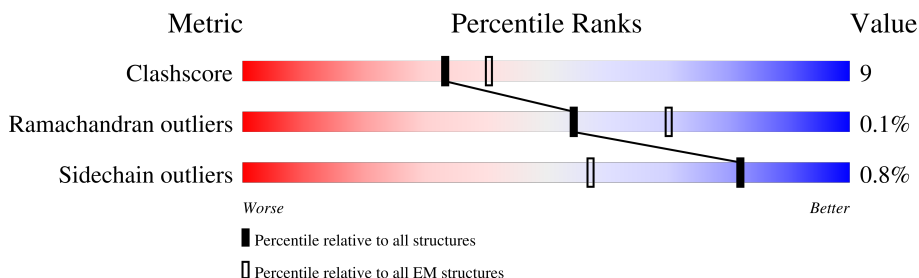
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	107	<div> <div>30%</div> <div>69%</div> <div>31%</div> </div>
1	F	107	<div> <div>44%</div> <div>68%</div> <div>32%</div> </div>
1	H	107	<div> <div>46%</div> <div>70%</div> <div>30%</div> </div>
1	J	107	<div> <div>43%</div> <div>67%</div> <div>33%</div> </div>
2	B	4687	<div> <div>34%</div> <div>71%</div> <div>18%</div> <div>11%</div> </div>
2	E	4687	<div> <div>38%</div> <div>71%</div> <div>18%</div> <div>11%</div> </div>
2	G	4687	<div> <div>44%</div> <div>70%</div> <div>18%</div> <div>11%</div> </div>
2	I	4687	<div> <div>43%</div> <div>71%</div> <div>18%</div> <div>11%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called ryanodine receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

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

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of

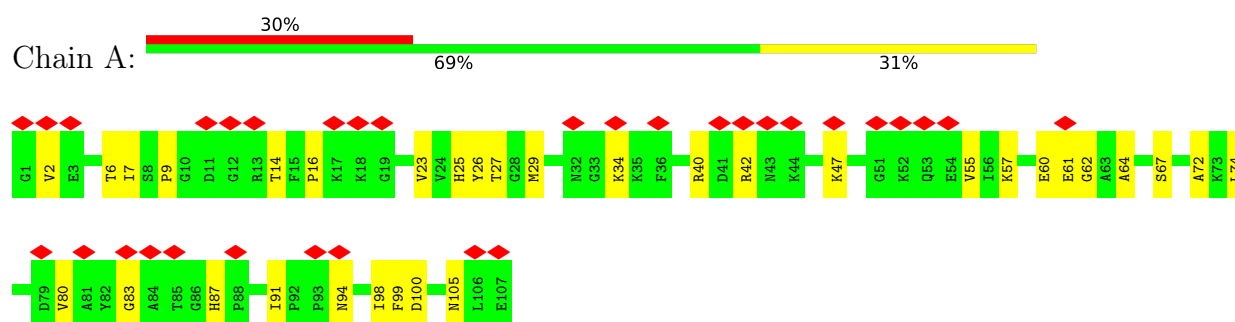
Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0

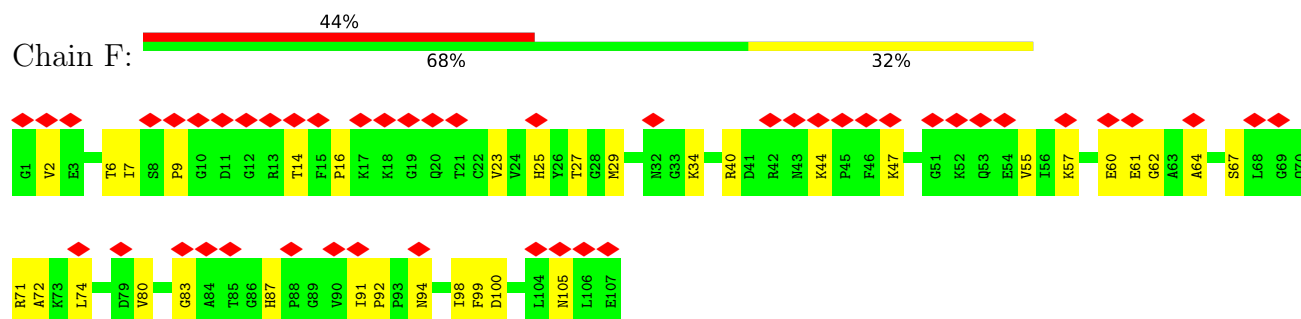
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

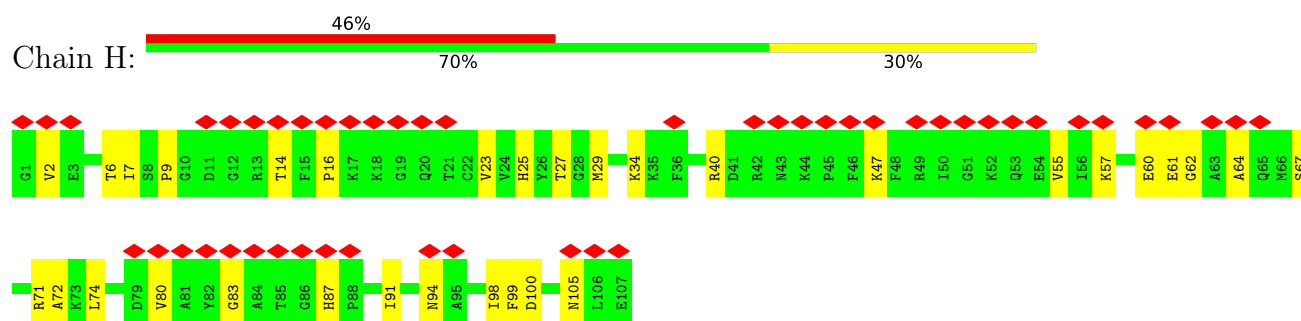
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



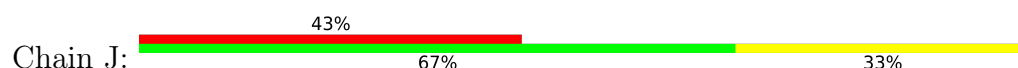
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

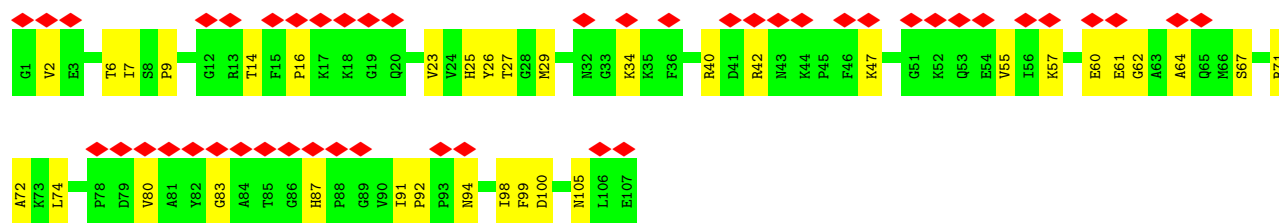


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

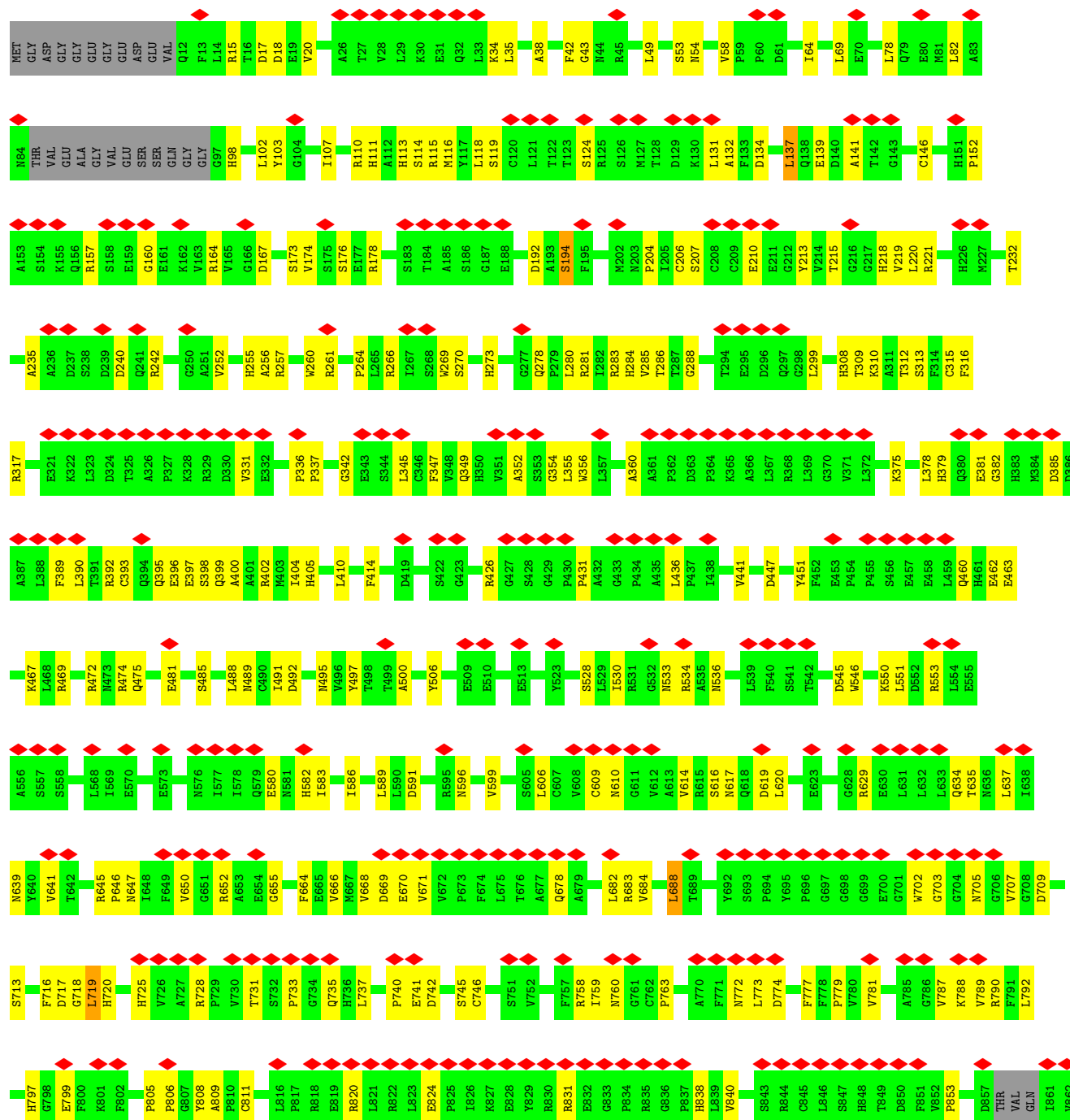


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 2: ryanodine receptor type 1

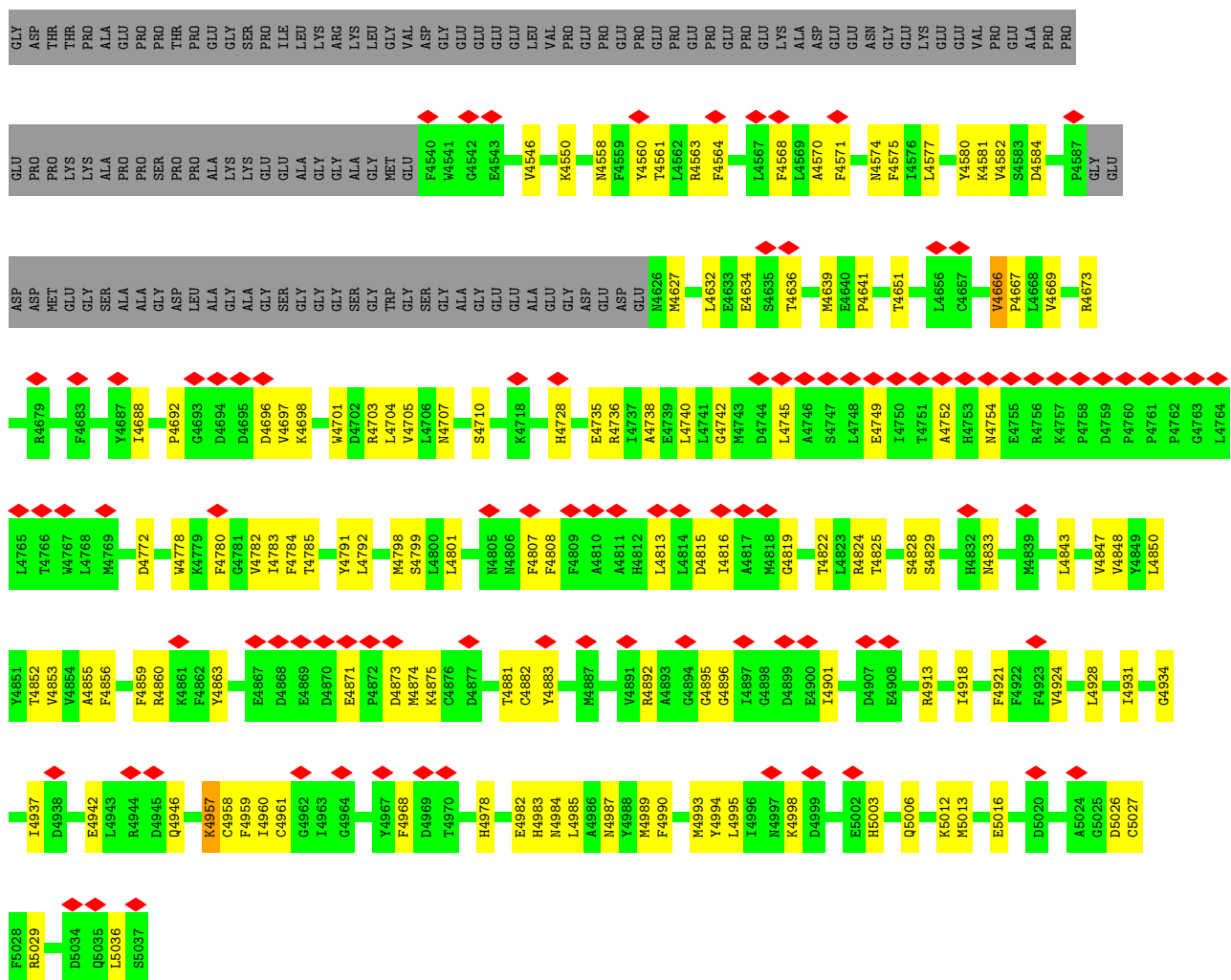




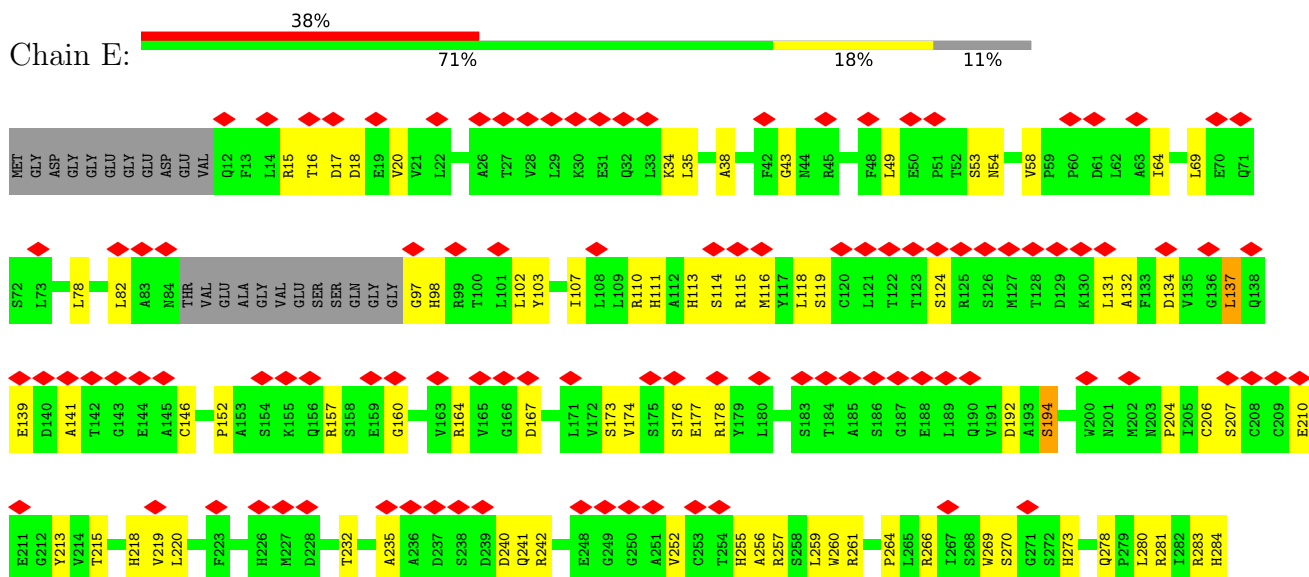
X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3030	X3031	X3034	X3038	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3146	X3149	X3153	X3157	X3172	X3173	X3176	X3183												
T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2959	X2995	X2996	X2997	X3010	X3013	X3014	X3015	X3016	X3017	X3018			
ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	T2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	E2875	Q2877	L2878	E2880	M2881	T2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909
M2790	L2791	R2792	P2793	T2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	V2805	R2806	V2807	F2808	L2809	K2810	E2811	S2812	K2813	K2814	A2815	M2816	L2817	A2818	V2819	E2820	T2821	T2822	L2823	E2824	K2825	A2826	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLY	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	
X2585	X2586	X2597	X2603	X2604	X2605	X2606	X2610	X2611	X2614	X2617	X2618	X2619	X2620	X2623	X2624	X2625	X2626	X2627	X2641	X2645	X2646	X2649	X2650	X2651	X2652	X2653	X2656	X2657	X2658	X2659	X2663	X2664	X2665	X2671	X2672	X2673	X2674	X2675	X2676	X2683	X2687	X2688	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699						
D2465	L2466	T2469	T2470	S2471	L2472	T2473	L2474	Q2475	Q2476	T2477	T2478	L2479	X2487	X2488	X2502	X2510	X2511	X2512	X2513	X2514	X2515	X2516	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2526	X2529	X2530	X2533	X2536	X2537	X2551	X2554	X2555	X2556	X2557	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568									
E2381	E2382	A2391	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	PRO	GLU	N2414	A2428	L2429	I2430	L2433	Q2434	R2435	C2436	A2437	E2438	M2440	H2441	Q2444	A2445	G2446	K2447	G2448	A2449	A2450	L2451	R2452	A2455	L2456	L2457	R2459	L2460	V2461	P2462	L2463	D2464								
E2292	Q2293	D2294	L2295	E2296	S2300	A2303	G2304	L2307	Q2308	S2309	C2310	P2311	M2312	L2313	L2314	A2315	Y2318	P2319	D2320	L2321	R2330	L2335	R2336	V2341	N2342	G2343	E2344	S2345	V2346	E2347	E2348	R2355	L2358	R2359	K2360	P2361	E2362	C2363	L2368	R2369	G2370	E2371	G2372	G2373	L2376	A2378											
L2215	G2216	G2217	G2218	E2219	T2220	K2221	E2222	T2223	S2231	R2234	F2235	Y2238	S2243	N2246	Q2247	R2248	F2251	D2252	H2253	L2254	S2255	Y2256	L2257	E2258	E2259	M2260	L2261	L2262	L2263	G2264	L2265	G2266	M2267	Q2268	G2269	S2270	L2273	A2276	V2280	L2281	D2282	N2283	N2284	E2285	L2286	A2287	L2288	A2289	L2290	Q2291							
M2120	F2121	L2124	Q2127	G2132	L2135	A2137	L2138	P2139	R2140	A2141	Y2142	T2143	I2144	S2145	P2146	S2147	S2148	V2149	S2154	L2155	C2158	L2159	I2162	R2163	S2164	L2165	L2166	L2167	M2170	N2184	I2185	N2188	K2189	V2190	F2191	Y2192	Q2193	N2196	L2197	M2198	R2199	H2204	E2205	V2212													
GLU	GLU	GLU	PRO	GLU	GLU	THR	SER	LEU	SER	SER	ARG	LEU	ARG	SER	LEU	LEU	GLU	THR	VAL	LYS	LYS	GLU	GLU	LEU	PRO	ALA	GLU	K2089	K2090	P2091	Q2092	S2093	L2094	Q2095	V2102	V2103	R2104	Q2107	V2110	L2116	V2117	R2118	A2119														

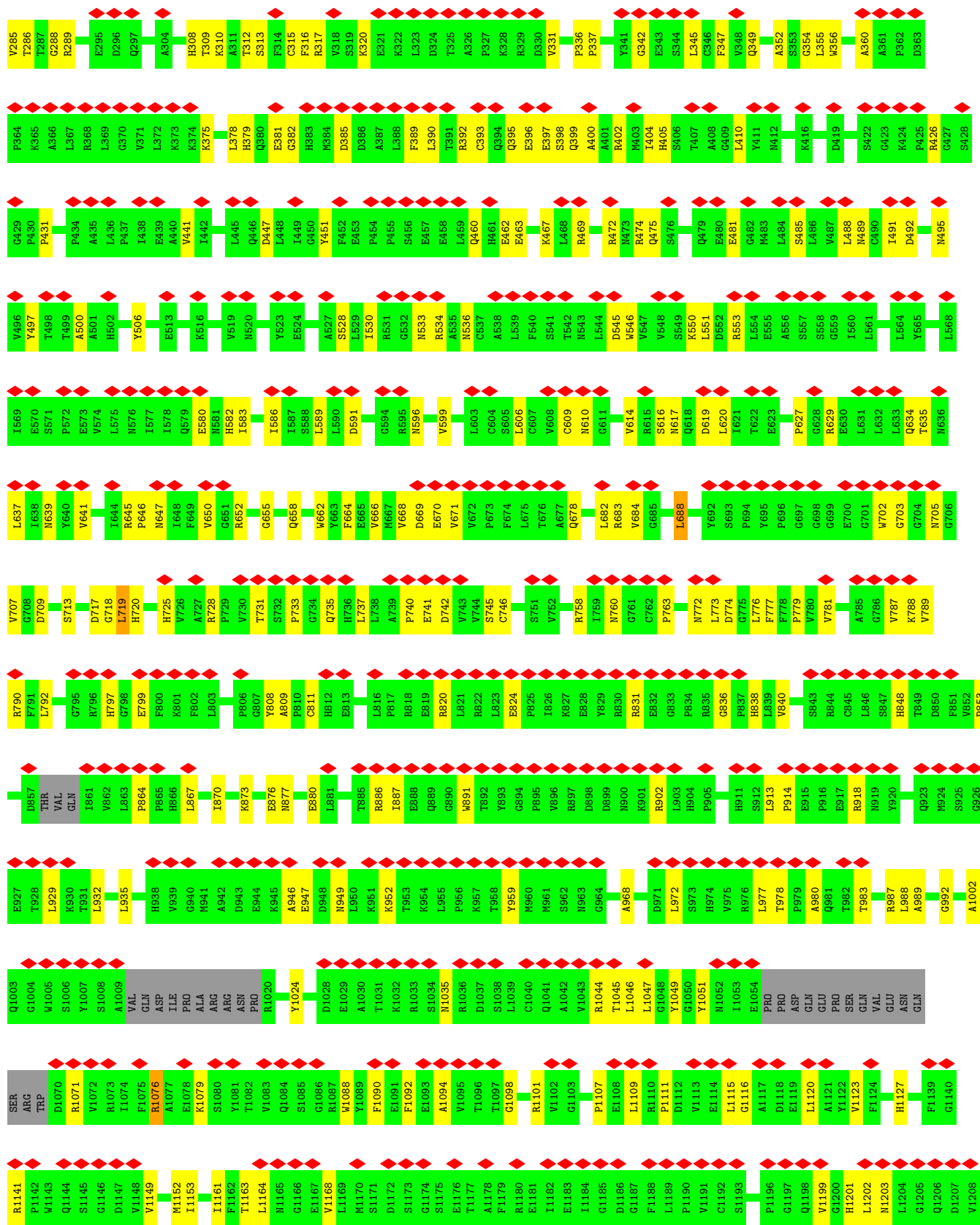




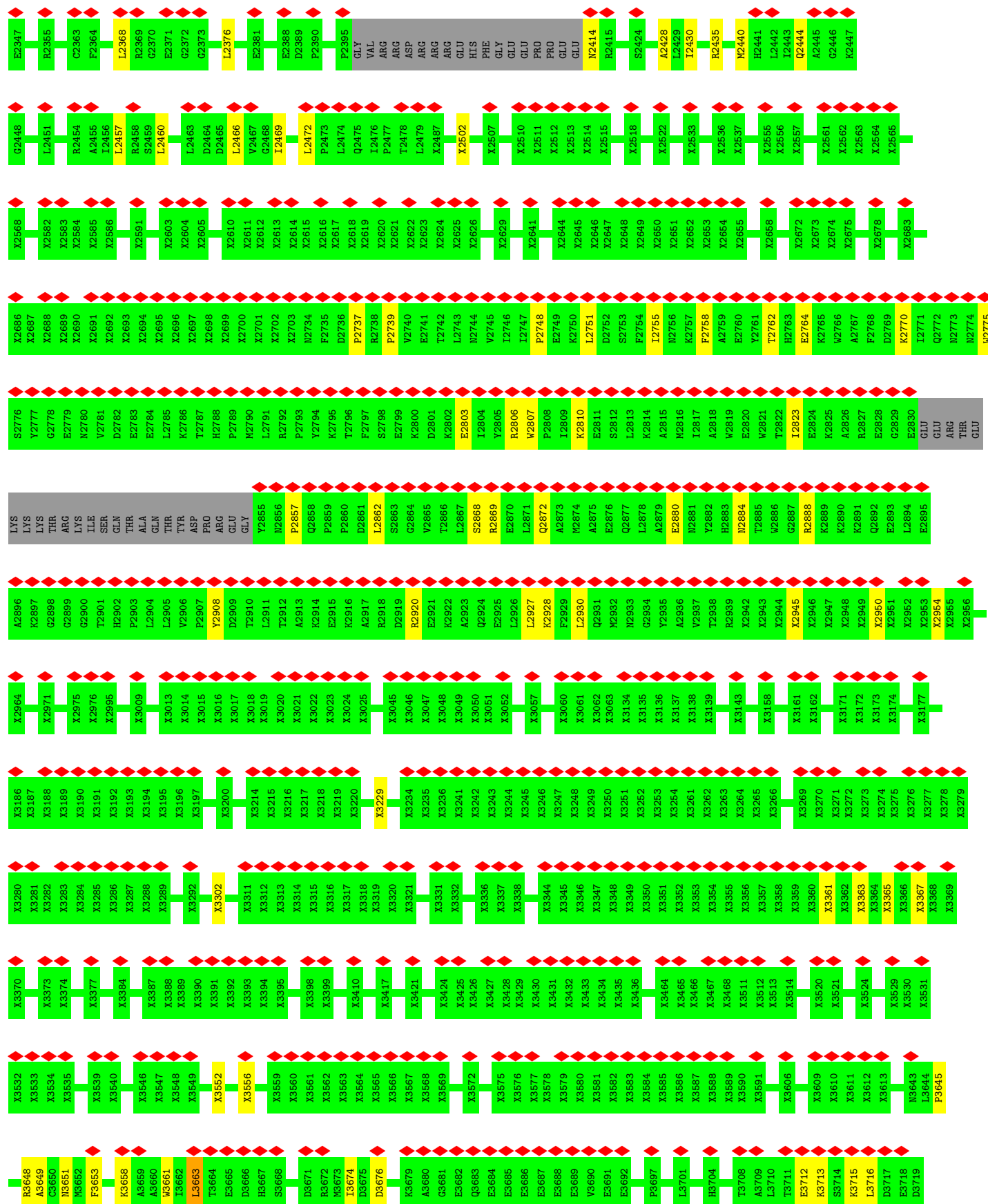


- Molecule 2: ryanodine receptor type 1

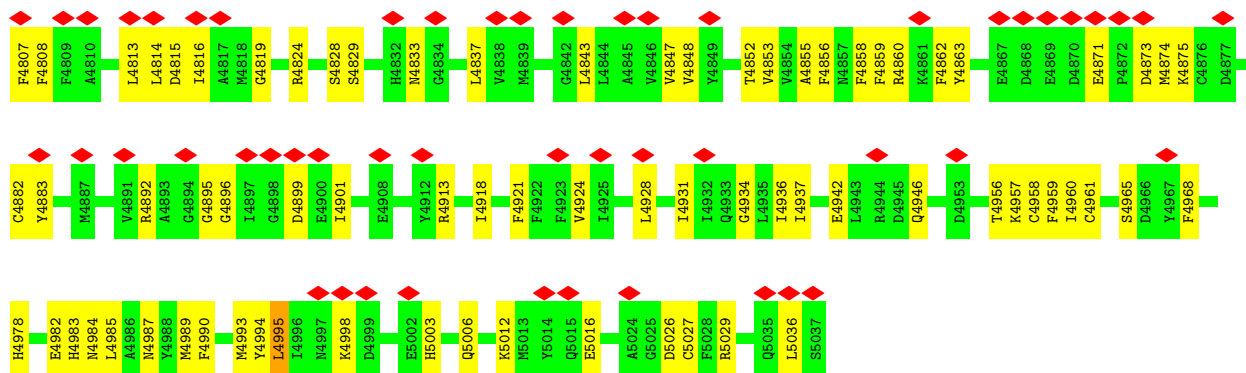




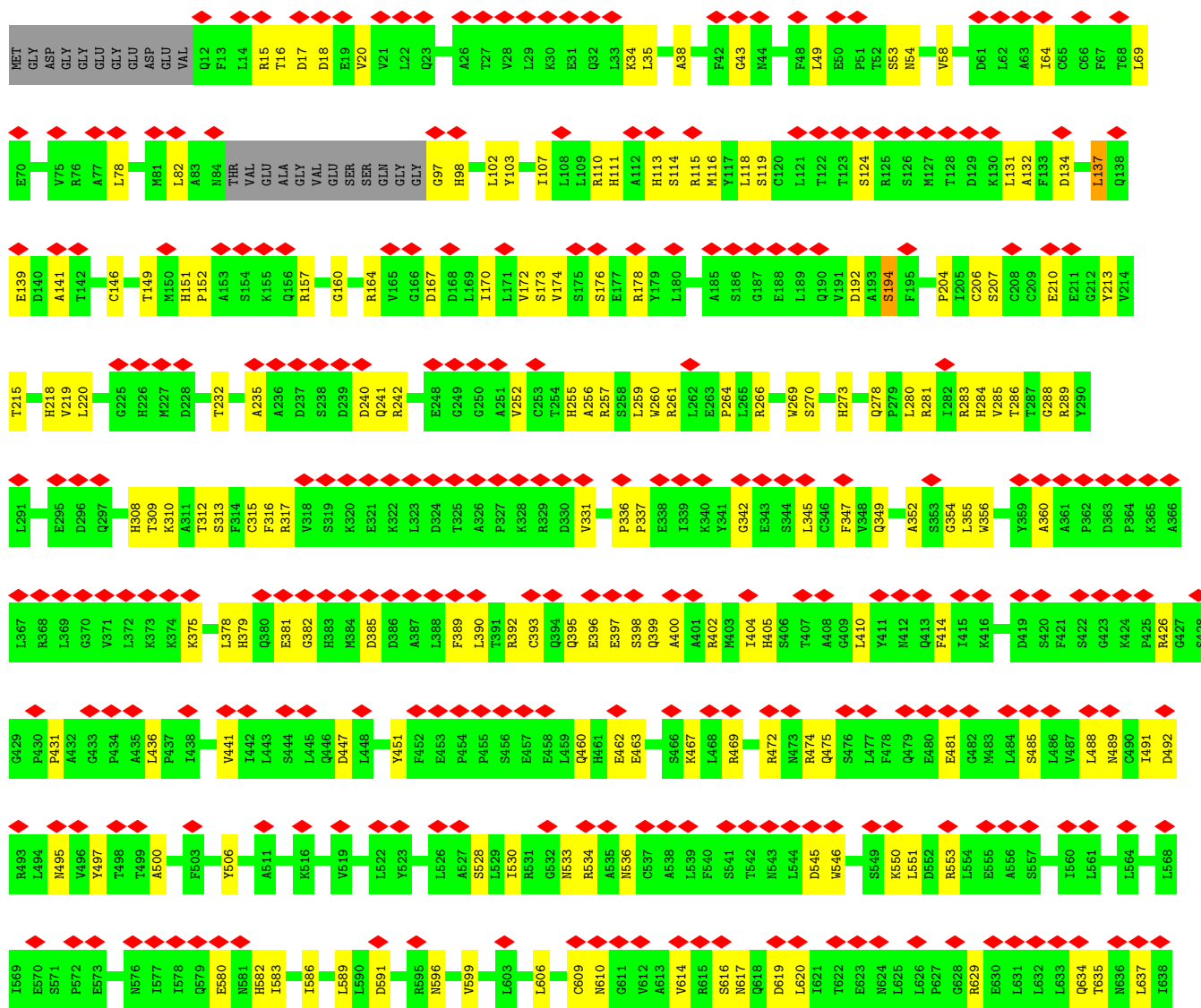
S2261	M2170	K2090	E2018	V1859	GLY	G1724	L1653	K1585	X1507	L1270	S1209
L2265	N2184	P2091	E2019	K1860	VAL	R1725	E1652	M1586	X1508	R1271	S1210
G2266	I2185	Q2092	D2020	M1865	ALA	S1726	L1653	P1587	X1509	L1272	L1211
G2267	M2186	S2093	C2021	P1868	E1793	R1727	S1654	Q1590	X1510	A1273	R1212
Q2268	N2187	L2094	P2022	E1869	A1794	M1730	R1656	C1591	X1511	H1274	F1213
G2269	N2188	Q2095	P2023	V1870	P1795	E1733	L1659	R1594	X1512	X1279	F1214
	K2189	E2096	P2024	F1871	A1796	I1735	Q1660	L1595	X1516	A1215	A1215
	V2102	V2102	E2025	E1873	R1797	P1736	H1663	E1596	X1517	I1216	I1216
	R2103	R2103	I2027	E1874	L1798	L1738	H1665	V1597	X1518	X1280	X1280
	Q2107	Q2107	R2028	GLU	P1800	T1739	L1667	Q1598	X1519	X1282	G1217
	V2111	V2111	C2043	E1874	A1801	P1740	L1669	M1599	X1520	X1283	G1218
	E2115	E2115	Q2044	GLU	I1802	R1743	R1668	L1600	X1521	X1286	L1219
L2116	L2116	L2116	Q2045	GLU	A1805	A1744	R1669	S1603	X1522	X1289	Q1220
A2119	Q2047	Q1952	E2047	GLU	A1806	I1745	Y1670	S1604	X1523	X1290	F1223
M2120	G2048	V1955	G2048	GLU	L1807	T1746	R1671	V1605	X1524	X1291	E1224
F2121	GLU	V1960	GLU	D1809	R1808	L1747	L1676	S1606	X1525	X1292	P1225
S2122	GLU	A1960	GLU	GLU	D1809	F1748	G1677	M1608	X1526	X1293	F1226
L2123	GLU	R1964	GLU	GLU	L1812	P1749	M1678	P1609	X1527	X1294	A1227
L2124	PRO	Y1965	GLU	GLU	R1813	P1750	N1679	X1529	X1528	I1228	I1228
H2125	GLU	Q1973	GLU	GLU	R1816	G1751	V1681	X1530	X1530	M1229	M1229
Q2126	GLU	R1974	GLU	GLU	E1817	A1752	A1682	X1531	X1531	M1230	Q1231
Q2127	THR	R1974	GLU	ASP	E1817	K1753	H1683	X1532	X1532	R1232	R1232
L2131	THR	S1975	GLU	GLU	R1820	G1754	A1684	X1533	X1533	P1233	P1233
G2132	SER	R1976	GLU	GLU	D1821	G1755	S1687	X1534	X1534	V1234	V1234
E2133	SER	Y1977	GLU	GLU	G1822	M1756	GLU	X1535	X1535	T1235	T1235
L2135	ARG	M1981	GLU	GLU	G1823	A1757	D1690	X1536	X1536	T1236	T1236
R2136	ARG	R1982	GLU	ASP	Q1824	R1758	Q1691	X1537	X1537	W1237	W1237
A2137	SER	A1983	GLU	GLU	H1825	L1762	A1692	X1538	X1538	F1238	F1238
L2138	LEU	F1984	GLU	GLU	A1826	P1763	L1694	X1539	X1539	S1239	S1239
P2139	LEU	T1985	GLU	GLU	R1827	G1764	L1695	X1540	X1540	K1240	K1240
R2140	GLU	M1986	GLU	GLU	D1828	V1765	H1696	X1541	X1541	S1241	S1241
A2141	THR	S1987	GLU	GLU	P1829	G1766	E1699	X1542	X1542	L1242	L1242
Y2142	VAL	A1988	GLU	ALA	V1830	V1767	D1700	X1543	X1543	P1243	P1243
T2143	VAL	E1990	GLU	ALA	Q1837	T1768	A1701	X1544	X1544	Q1244	Q1244
L2144	LYS	T1991	GLU	GLU	F1838	L1771	H1702	X1545	X1545	F1245	F1245
S2145	LYS	A1992	GLU	GLU	V1839	R1772	L1703	X1546	X1546	E1246	E1246
P2146	GLU	T1995	GLU	GLU	V1841	P1773	Q1631	X1547	X1547	P1247	P1247
S2148	GLU	R1996	GLU	GLU	L1842	P1774	D1632	X1548	X1548	V1248	V1248
V2149	PRO	E1997	GLU	ALA	K1843	H1775	P1633	X1549	X1549	P1249	P1249
S2154	GLU	F1998	GLU	GLU	L1844	H1776	L1634	X1550	X1550	P1250	P1250
L2155	GLU	Q2003	GLU	GLU	V1845	F1777	Y1711	X1551	X1551	E1251	E1251
C2158	LEU	E2004	GLU	GLU	L1848	S1778	Y1712	X1552	X1552	H1252	H1252
L2159	PRO	N2007	GLU	GLU	L1849	P1779	D1713	X1561	X1561	X1470	X1470
R2163	ALA	K2013	GLU	ASP	V1850	G1781	M1637	X1562	X1562	X1471	X1471
L2166	GLU	A2016	GLU	GLU	M1851	F1782	L1639	X1563	X1563	E1256	E1256
L2167	GLU	D2017	GLU	GLU	G1852	V1783	H1718	M1573	X1487	A1258	A1258
						A1784	I1720	P1574	X1487	X1487	X1487
						L1786	E1721	X1489	X1489	X1499	X1499
						P1787	A1723	X1500	X1500	D1261	D1261
						A1788		X1501	X1501	T1263	T1263
						ALA		X1502	X1502	V1264	V1264
								X1503	X1503	D1265	D1265
								X1505	X1505	P1268	P1268
								X1506	X1506	C1269	C1269

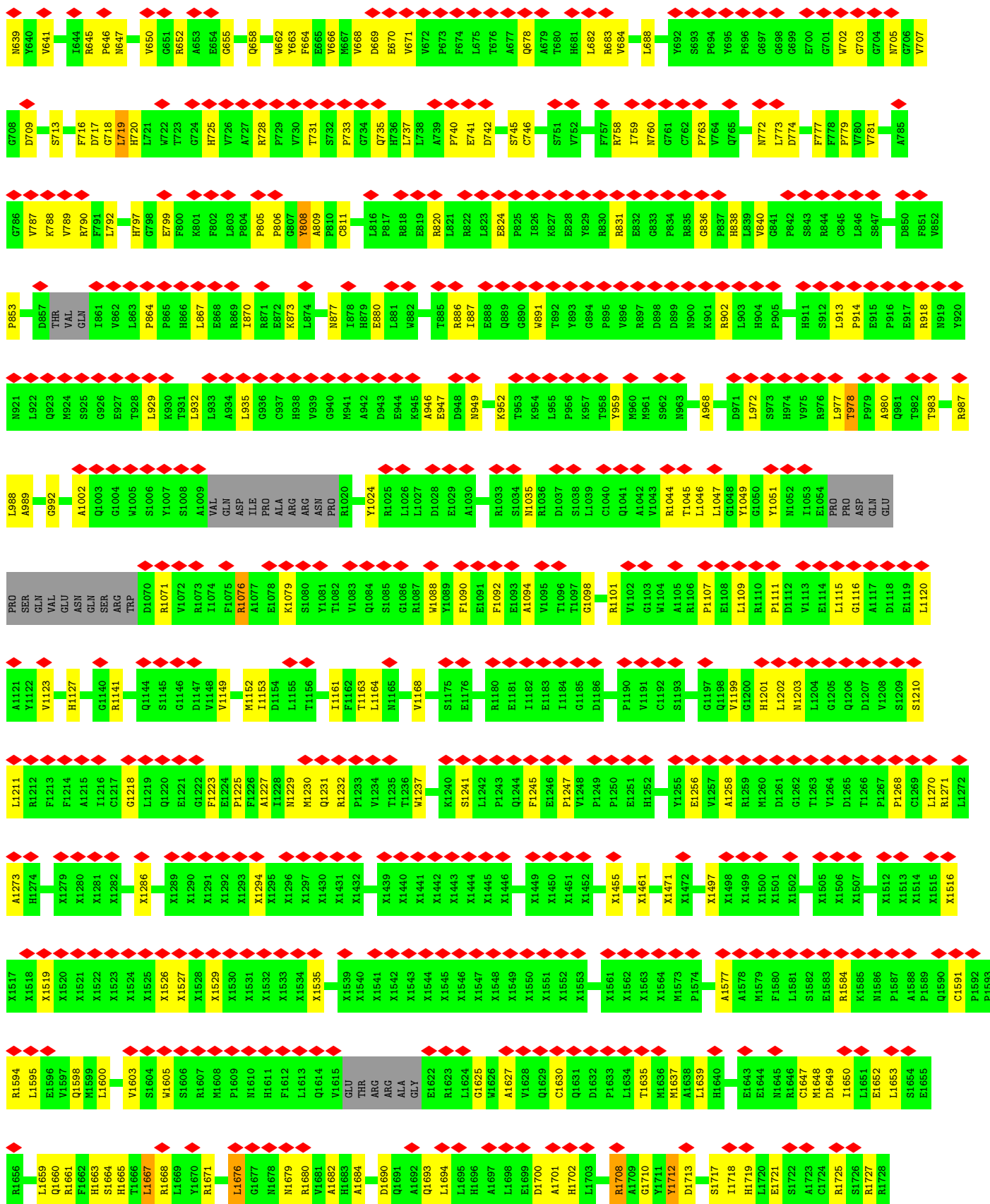






• Molecule 2: ryanodine receptor type 1



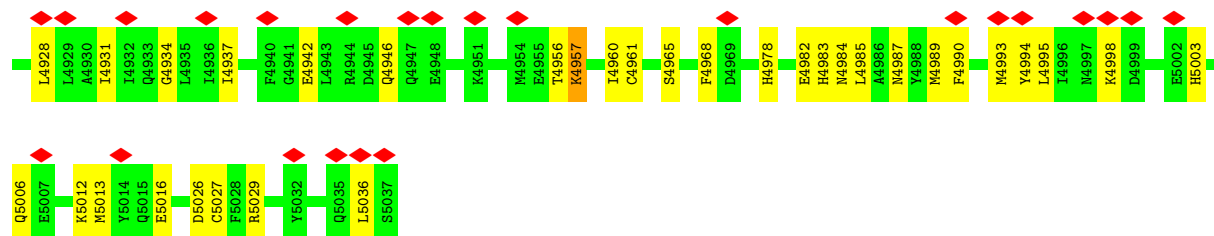




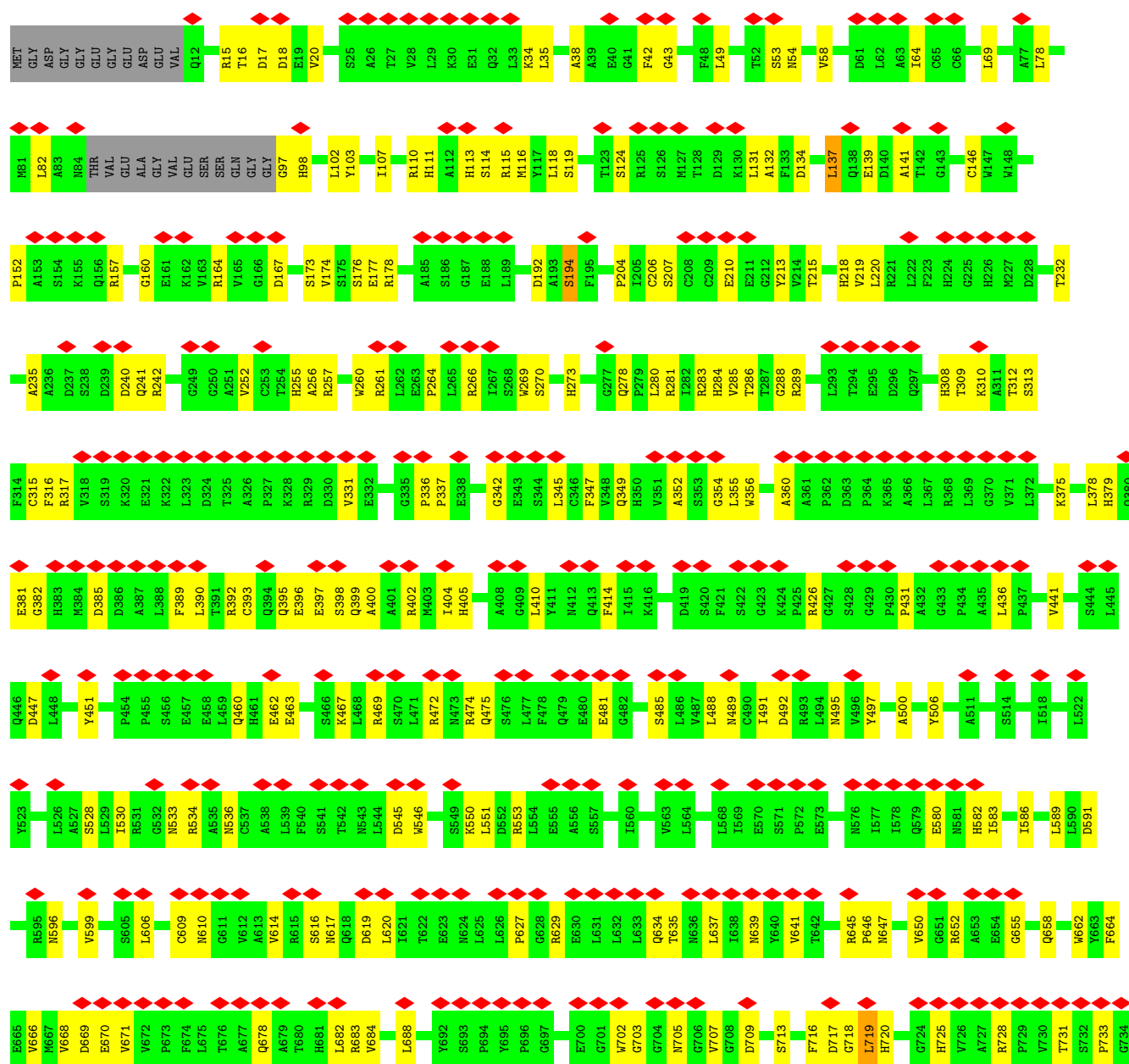
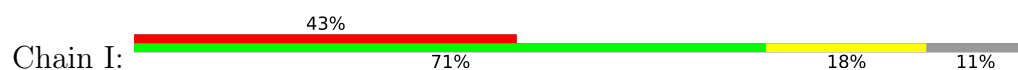


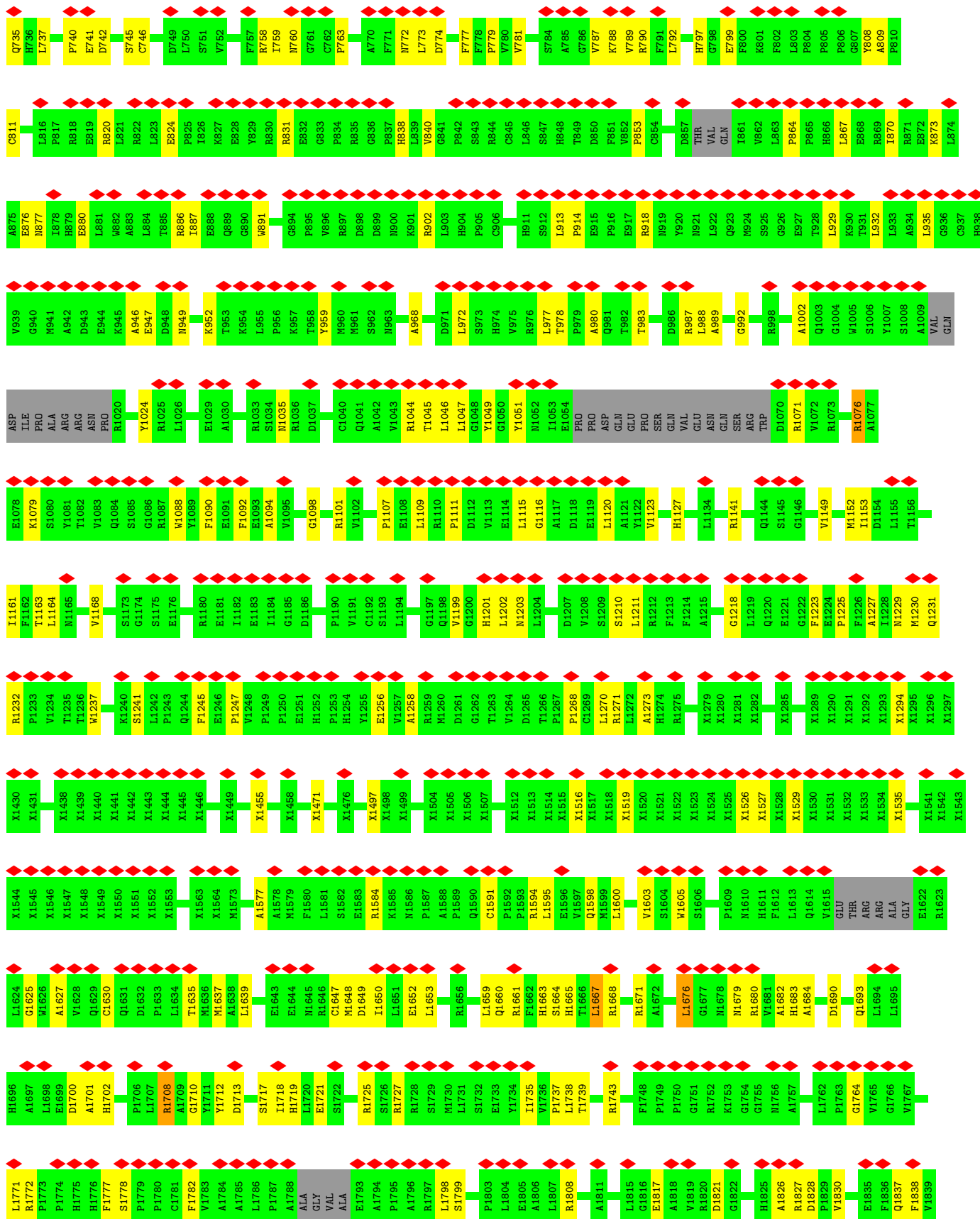
L3844	L3845	L3846	F3847	F3848	F3849	Q3850	L3851	L3852	L3853	E3854	L3855	L3856	G3857	L3858	S3784	A3785	G3786	K3787	G3788	E3789	T3790	G3791	A3792	S3795	S3796	T3797	L3798	L3799	L3800	G3801	L3802	S3803	L3804	L3805	L3806	G3807	T3881	L3882	L3883	L3884	F3885	L3886	Q3889	E3893	N3896	F3899	L3903	R3904	Q3905	M3836	L3842	D3843	T3910	T3911	T3912	L3913	N3914		
S3768	R3769	L3770	H3771	T3772	R3773	G3774	A3775	A3776	V3779	L3780	Q3781	M3782	L3783	S3784	A3785	G3786	K3787	G3788	E3789	T3790	G3791	A3792	S3795	S3796	T3797	L3798	L3799	L3800	G3801	L3802	S3803	L3804	L3805	L3806	G3807	T3881	L3882	L3883	L3884	F3885	L3886	Q3889	E3893	N3896	F3899	L3903	R3904	Q3905	M3836	L3842	D3843	T3910	T3911	T3912	L3913	N3914			
T3708	A3709	L3710	T3711	E3712	K3713	S3714	K3715	L3716	D3717	E3718	D3719	Y3720	L3721	Y3722	K3723	A3724	A3725	A3726	D3727	L3728	M3729	A3730	K3731	S3732	G3733	H3734	L3735	E3736	G3737	G3738	G3739	E3740	N3741	GLY	ALA	GLY	GLY	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3759	K3760	Q3761	R3762	L3763	L3764	V3765	Q3766	Q3767			
X3609	X3610	X3611	X3612	X3613	H3643	T3646	H3647	H3648	A3649	C3650	N3651	K3652	F3653	L3654	E3655	K3658	A3659	L3663	T3664	E3665	D3666	H3667	S3668	F3669	E3670	D3671	R3672	M3673	L3674	D3675	D3676	K3679	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	V3690	E3691	E3692	K3693	P3697	L3698	L3701	V3702	L3703	H3704								
X3518	X3521	X3522	X3525	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3540	X3548	X3552	X3556	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3572	X3573	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3606										
X3377	X3380	X3381	X3384	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3398	X3399	X3409	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515										
X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3324	X3325	X3328	X3332	X3333	X3337	X3338	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3373	X3374								
X3218	X3219	X3229	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3291	X3292	X3295	X3296	X3299	X3302	X3303							
G2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2961	X2964	X2965	X2968	X2971	X2975	X2976	X2995	X2996	X2997	X2998	X3001	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3028	X3029	X3030	X3031	X3032	X3035	X3036									
X3045	X3046	X3047	X3048	X3049	X3053	X3056	X3057	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3158	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3177	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3214	X3215	X3216	X3217									
M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	R2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	K2897	G2898	Q2899	T2901	R2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	R2914	E2915	K2916	A2917	S2863	G2864	V2865	T2866	L2867	S2868	R2869	Q2924	E2925	L2926	L2927	K2928	P2929	L2930	M2932	N2933		
K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	Y2822	H2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	D2782	ALA	GLN	E2783	E2784	T2785	ASP	P2786	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873





• Molecule 2: ryanodine receptor type 1





S2776	X2686	X2563	T2478	PRO	G2343	M2267	P2195	A2119	PRO	L1980	GLU	P1840
V2777	X2687	X2564	L2479	PRO	E2344	Q2268	N2196	M2120	GLU	M1981	ASP	V1841
G2778	X2688	X2565	X2487	GLU	S2345	G2269	L2197	F2121	GLU	R1982	ALA	L1842
E2779	X2689	X2566	X2488	N2414	V2346	S2270	H2204	S2122	THR	A1983	LYS	K1843
N2780	X2690	X2567	X2489	H2420	E2347	T2271	E2205	L2123	SER	F1984	GLU	L1844
V2781	X2691	X2585	X2490	H2420	E2348	T2272	T2206	L2124	LEU	T1985	GLU	V1845
D2782	X2692	X2586	X2493	H2420	N2349	D2274	V2207	R2126	SER	S1986	GLU	S1846
E2783	X2693	X2586	X2493	H2420	A2350	D2275	N2208	Q2127	ARG	T1847	GLU	T1847
E2784	X2694	X2598	X2499	A2427	N2351	A2276	V2275	L2131	LEU	M1848	ALA	L1848
K2785	X2695	X2598	X2499	A2427	V2354	V2280	N2211	G2132	ARG	S1987	PRO	G1852
K2786	X2696	X2603	X2500	A2428	R2355	D2281	V2212	L2135	GLY	A1988	GLY	G1852
T2787	X2697	X2604	X2501	L2429	L2356	D2282	V2214	R2136	LEU	A1989	GLU	T1853
H2788	X2698	X2605	X2502	T2430	L2357	N2283	L2215	A2137	GLU	T1991	LYS	F1854
P2789	X2699	X2606	X2503	L2433	L2358	N2284	G2216	R2137	THR	A1992	ASP	G1855
M2790	X2700	X2607	X2510	G2434	R2359	N2285	G2217	L2138	ARG	E1997	LYS	D1856
L2791	X2701	X2608	X2511	E2435	K2360	L2286	G2218	R2139	LEU	F1998	LYS	E1857
D2792	X2702	X2609	X2512	C2436	P2361	A2287	E2219	R2140	VAL	R1999	GLU	E1857
P2793	X2703	X2610	X2513	A2437	E2362	L2288	T2220	A2141	VAL	S2000	ASP	D1856
V2794	N2734	X2611	X2514	P2438	E2363	L2289	K2221	T2142	ARG	P2001	LYS	E1857
K2795	F2735	X2612	X2515	E2439	F2364	Q2291	E2222	T2143	LEU	P2002	LYS	E1857
T2796	D2736	X2613	X2516	H2440	F2364	E2292	T2223	S2145	PRO	Q2003	GLU	E1874
T2797	P2737	X2614	X2517	L2442	L2368	L2295	K2227	P2146	GLU	E2004	GLU	E1874
T2798	R2738	X2615	X2518	L2443	R2369	E2296	S2231	S2147	GLU	N2007	GLU	E1874
E2799	P2739	X2616	X2519	Q2444	E2370	K2297	F2235	S2148	LEU	M2008	GLU	E1874
K2800	V2740	X2617	X2520	A2445	E2371	V2298	R2234	T2152	ALA	H2011	GLU	E1874
D2801	E2741	X2618	X2521	G2446	G2370	V2299	F2235	M2153	GLU	K2012	GLU	E1874
K2802	T2742	X2619	X2522	G2447	G2372	S2300	T2236	S2154	PRO	P2013	GLU	E1874
E2803	L2743	X2620	X2523	K2448	G2373	Y2301	Y2238	L2155	GLU	A2016	GLU	E1874
T2804	N2744	X2624	X2524	E2449	S2374	L2302	F2239	C2158	GLU	D2017	GLU	E1874
T2805	V2745	X2625	X2525	A2450	G2375	L2303	C2240	L2159	GLU	E2018	GLU	E1874
K2806	L2746	X2626	X2526	L2451	L2376	L2307	R2244	R2162	GLU	E2019	GLU	E1874
N2807	T2747	X2627	X2527	L2457	L2377	M2312	Q2247	L2166	GLU	C2021	GLU	E1874
P2808	P2748	X2629	X2529	T2461	A2378	L2313	R2248	T2167	GLU	P2022	GLU	E1874
T2809	E2749	X2644	X2530	P2462	E2381	L2314	F2251	Q2104	GLU	L2023	GLU	E1874
K2810	K2750	X2645	X2531	L2463	E2382	L2314	H2253	V2103	GLU	H1952	GLU	E1874
E2811	L2751	X2646	X2532	A2455	E2383	L2314	Q2245	R2105	GLU	Q1952	GLU	E1874
S2812	D2752	X2647	X2533	T2456	L2384	L2314	R2246	A2106	GLU	R1954	GLU	E1874
L2813	S2753	X2648	X2534	S2459	R2385	L2314	Q2247	Q2107	GLU	V1955	GLU	E1874
K2814	F2754	X2649	X2535	L2460	E2388	A2315	R2248	Y2110	GLU	L1951	GLU	E1874
A2815	L2755	X2650	X2537	V2461	E2388	A2315	R2248	V2111	GLU	H1953	GLU	E1874
H2816	N2756	X2651	X2544	P2462	A2391	Y2318	F2251	V2111	GLU	R1954	GLU	E1874
L2817	K2757	X2652	X2545	L2463	R2392	P2319	H2253	Q2112	GLU	A1959	GLU	E1874
A2818	F2758	X2653	X2548	D2464	P2395	I2321	L2254	S2113	GLU	A1960	GLU	E1874
N2819	A2759	X2654	X2548	D2465	GLY	T2320	S2255	E2115	GLU	C2042	GLU	E1874
E2820	E2760	X2655	X2551	V2467	VAL	I2321	Y2256	E2116	GLU	G2043	GLU	E1874
N2821	Y2761	X2655	X2552	G2468	ARG	Q2322	L2257	L2117	GLU	Y1965	GLU	E1874
T2822	T2762	X2656	X2553	T2469	ARG	R2330	L2258	V2117	GLU	Q1973	GLU	E1874
L2823	H2763	X2657	X2553	T2470	ASP	Y2331	L2258	R2118	GLU	R1976	GLU	E1874
E2824	T2764	X2658	X2554	S2471	ARG	L2332	E2259	N2188	GLU	Y1977	GLU	E1874
K2825	K2765	X2659	X2555	T2472	ARG	L2335	N2260	K2189	GLU			E1874
A2826	N2766	X2673	X2557	L2473	ARG	R2336	S2261	V2190	GLU			E1874
D2827	A2767	X2674	X2557	P2473	GLU	R2336	Q2261	F2191	GLU			E1874
E2828	T2768	X2675	X2558	L2474	HIS		T2263	Y2192	GLU			E1874
G2829	F2768	X2676	X2559	Q2475	PHE		L2264	Q2193	GLU			E1874
D2769	D2769	X2677	X2560	L2476	GLY		L2265	H2194	GLU			E1874
K2770	N2770	X2683	X2561	T2477	GLU		Q2266		GLU			E1874
L2771	L2771		X2562	P2477	GLU				GLU			E1874
Q2772	Q2772				GLU				GLU			E1874
N2773	N2773				ARG				THR			E1874
N2774	N2774				GLU				GLU			E1874
W2775	W2775				GLU				GLU			E1874

LYS	LYS	THR	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													</
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	----





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.486	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	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, CA

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	0.33	0/834	0.59	0/1123
1	F	0.33	0/834	0.59	0/1123
1	H	0.33	0/834	0.59	0/1123
1	J	0.33	0/834	0.59	0/1123
2	B	0.34	0/25428	0.58	6/34534 (0.0%)
2	E	0.34	0/25428	0.58	6/34534 (0.0%)
2	G	0.34	0/25428	0.58	6/34534 (0.0%)
2	I	0.34	0/25428	0.58	6/34534 (0.0%)
All	All	0.34	0/105048	0.58	24/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	23
2	E	0	23
2	G	0	23
2	I	0	23
All	All	0	92

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1667	LEU	CA-CB-CG	6.02	129.15	115.30
2	G	1667	LEU	CA-CB-CG	6.02	129.14	115.30
2	B	1667	LEU	CA-CB-CG	5.99	129.08	115.30
2	B	719	LEU	CA-CB-CG	5.98	129.06	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	719	LEU	CA-CB-CG	5.98	129.06	115.30
2	I	1667	LEU	CA-CB-CG	5.98	129.05	115.30
2	I	719	LEU	CA-CB-CG	5.97	129.03	115.30
2	G	719	LEU	CA-CB-CG	5.96	129.01	115.30
2	I	4985	LEU	CA-CB-CG	5.66	128.31	115.30
2	E	4985	LEU	CA-CB-CG	5.66	128.31	115.30
2	G	4985	LEU	CA-CB-CG	5.64	128.28	115.30
2	B	4985	LEU	CA-CB-CG	5.63	128.25	115.30
2	G	977	LEU	CA-CB-CG	5.61	128.19	115.30
2	B	977	LEU	CA-CB-CG	5.60	128.18	115.30
2	E	977	LEU	CA-CB-CG	5.59	128.16	115.30
2	I	977	LEU	CA-CB-CG	5.59	128.15	115.30
2	E	4639	MET	C-N-CA	5.25	134.82	121.70
2	I	4639	MET	C-N-CA	5.25	134.81	121.70
2	B	4639	MET	C-N-CA	5.23	134.77	121.70
2	G	4639	MET	C-N-CA	5.22	134.75	121.70
2	G	2290	LEU	CA-CB-CG	5.19	127.23	115.30
2	B	2290	LEU	CA-CB-CG	5.17	127.20	115.30
2	I	2290	LEU	CA-CB-CG	5.16	127.16	115.30
2	E	2290	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (92) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	137	LEU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	194	SER	Peptide
2	B	2188	ASN	Peptide
2	B	2291	GLN	Peptide
2	B	2292	GLU	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	240	ASP	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3786	CYS	Peptide
2	B	3971	GLY	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	B	4666	VAL	Peptide
2	B	4696	ASP	Peptide
2	B	4807	PHE	Peptide
2	B	4873	ASP	Peptide
2	B	4901	ILE	Peptide
2	B	808	TYR	Peptide
2	E	137	LEU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	194	SER	Peptide
2	E	2188	ASN	Peptide
2	E	2291	GLN	Peptide
2	E	2292	GLU	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	240	ASP	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3786	CYS	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4696	ASP	Peptide
2	E	4807	PHE	Peptide
2	E	4873	ASP	Peptide
2	E	4901	ILE	Peptide
2	E	808	TYR	Peptide
2	G	137	LEU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	194	SER	Peptide
2	G	2188	ASN	Peptide
2	G	2291	GLN	Peptide
2	G	2292	GLU	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	240	ASP	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3786	CYS	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4696	ASP	Peptide
2	G	4807	PHE	Peptide
2	G	4873	ASP	Peptide
2	G	4901	ILE	Peptide
2	G	808	TYR	Peptide
2	I	137	LEU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	194	SER	Peptide
2	I	2188	ASN	Peptide
2	I	2291	GLN	Peptide
2	I	2292	GLU	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	240	ASP	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3786	CYS	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4696	ASP	Peptide
2	I	4807	PHE	Peptide
2	I	4873	ASP	Peptide
2	I	4901	ILE	Peptide
2	I	808	TYR	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	18	0
1	F	818	0	824	20	0
1	H	818	0	824	18	0
1	J	818	0	824	20	0
2	B	29369	0	24713	491	0
2	E	29369	0	24712	503	0
2	G	29369	0	24716	502	0
2	I	29369	0	24713	489	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102150	2033	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 9.

All (2033) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4859:PHE:HA	2:G:4862:PHE:CD2	1.88	1.08
2:G:4859:PHE:HA	2:G:4862:PHE:HD2	1.28	0.97
2:E:4859:PHE:HA	2:E:4862:PHE:CD2	2.05	0.92
2:E:4859:PHE:HA	2:E:4862:PHE:HD2	1.43	0.83
2:G:4859:PHE:CA	2:G:4862:PHE:HD2	1.99	0.73
2:E:4855:ALA:HA	2:E:4859:PHE:HB2	1.71	0.72
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.56	0.71
2:B:853:PRO:HB3	2:B:1024:TYR:H	1.56	0.71
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.90	0.70
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.90	0.70
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.56	0.69
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.58	0.69
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.58	0.69
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.91	0.69
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.58	0.69
2:G:853:PRO:HB3	2:G:1024:TYR:H	1.56	0.69
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.91	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.76	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.58	0.68
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.26	0.68
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.26	0.68
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.26	0.68
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.26	0.68
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.76	0.68
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.76	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.68
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.67
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.76	0.67
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.76	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.76	0.67
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.66
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.76	0.66
2:B:132:ALA:HA	2:B:194:SER:HB2	1.77	0.66
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.77	0.66
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.78	0.66
2:I:132:ALA:HA	2:I:194:SER:HB2	1.77	0.66
2:E:132:ALA:HA	2:E:194:SER:HB2	1.77	0.66
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.61	0.66
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.78	0.66
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.78	0.65
2:E:4934:GLY:HA3	2:G:4937:ILE:HD12	1.78	0.65
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.30	0.65
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.78	0.65
2:G:4177:TYR:HA	2:G:4202:ARG:HH22	1.61	0.65
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.61	0.65
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.76	0.65
2:G:132:ALA:HA	2:G:194:SER:HB2	1.77	0.65
2:I:4177:TYR:HA	2:I:4202:ARG:HH22	1.61	0.65
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.78	0.65
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.79	0.65
2:B:3990:VAL:HG13	2:B:4051:SER:HB2	1.78	0.65
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.78	0.65
2:B:3903:LEU:HG	2:B:3915:ILE:HD12	1.79	0.65
2:E:4177:TYR:HA	2:E:4202:ARG:HH22	1.61	0.65
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.79	0.64
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.79	0.64
2:B:4177:TYR:HA	2:B:4202:ARG:HH22	1.61	0.64
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.61	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.77	0.64
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.61	0.64
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.61	0.64
2:G:3990:VAL:HG13	2:G:4051:SER:HB2	1.78	0.64
2:E:3903:LEU:HG	2:E:3915:ILE:HD12	1.79	0.64
2:G:3903:LEU:HG	2:G:3915:ILE:HD12	1.79	0.64
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.30	0.64
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.61	0.64
2:G:1232:ARG:HH21	2:G:1701:ALA:HB1	1.63	0.64
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.80	0.64
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.30	0.64
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.30	0.64
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.80	0.64
2:I:3903:LEU:HG	2:I:3915:ILE:HD12	1.79	0.64
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.61	0.64
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.80	0.64
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.61	0.64
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.79	0.64
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.80	0.63
2:G:606:LEU:O	2:G:617:ASN:ND2	2.31	0.63
2:E:1232:ARG:HH21	2:E:1701:ALA:HB1	1.63	0.63
2:E:3990:VAL:HG13	2:E:4051:SER:HB2	1.79	0.63
2:B:606:LEU:O	2:B:617:ASN:ND2	2.31	0.63
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.81	0.63
2:I:1232:ARG:HH21	2:I:1701:ALA:HB1	1.63	0.63
2:E:606:LEU:O	2:E:617:ASN:ND2	2.31	0.63
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.79	0.63
2:B:111:HIS:HD2	2:B:114:SER:H	1.47	0.63
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.79	0.63
2:I:3990:VAL:HG13	2:I:4051:SER:HB2	1.78	0.63
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.79	0.63
2:I:111:HIS:HD2	2:I:114:SER:H	1.47	0.63
2:I:606:LEU:O	2:I:617:ASN:ND2	2.31	0.63
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.79	0.63
2:B:1232:ARG:HH21	2:B:1701:ALA:HB1	1.63	0.63
2:G:111:HIS:HD2	2:G:114:SER:H	1.47	0.63
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.81	0.63
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.32	0.62
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.32	0.62
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.81	0.62
2:B:3767:GLN:HB3	2:B:3772:THR:HG22	1.82	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:261:ARG:HB3	2:E:283:ARG:HB3	1.82	0.62
2:G:1101:ARG:HE	2:G:1115:LEU:HB3	1.64	0.62
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.33	0.62
2:I:3767:GLN:HB3	2:I:3772:THR:HG22	1.82	0.62
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.33	0.61
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.61
2:E:1973:GLN:O	2:E:1977:TYR:N	2.33	0.61
2:E:1101:ARG:HE	2:E:1115:LEU:HB3	1.64	0.61
2:G:261:ARG:HB3	2:G:283:ARG:HB3	1.82	0.61
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.81	0.61
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.32	0.61
2:E:4581:LYS:HB2	2:E:4632:LEU:HB2	1.82	0.61
2:B:1973:GLN:O	2:B:1977:TYR:N	2.33	0.61
2:E:111:HIS:HD2	2:E:114:SER:H	1.47	0.61
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.32	0.61
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.32	0.61
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.32	0.61
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.33	0.61
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.33	0.61
2:G:18:ASP:HB2	2:G:69:LEU:HD12	1.83	0.61
2:G:4581:LYS:HB2	2:G:4632:LEU:HB2	1.82	0.61
2:B:1101:ARG:HE	2:B:1115:LEU:HB3	1.64	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.83	0.60
2:B:261:ARG:HB3	2:B:283:ARG:HB3	1.82	0.60
2:B:1211:LEU:HD11	2:B:1225:PRO:HB3	1.84	0.60
2:E:18:ASP:HB2	2:E:69:LEU:HD12	1.83	0.60
2:G:3882:GLN:HB2	2:G:3957:VAL:HG22	1.82	0.60
2:I:261:ARG:HB3	2:I:283:ARG:HB3	1.82	0.60
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.82	0.60
2:B:4581:LYS:HB2	2:B:4632:LEU:HB2	1.82	0.60
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.83	0.60
2:G:4704:LEU:HD22	2:G:4778:TRP:HB2	1.83	0.60
2:B:4829:SER:O	2:B:4833:ASN:ND2	2.35	0.60
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.82	0.60
2:E:3767:GLN:HB3	2:E:3772:THR:HG22	1.82	0.60
2:G:4961:CYS:SG	2:G:4978:HIS:NE2	2.75	0.60
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.33	0.60
2:I:1101:ARG:HE	2:I:1115:LEU:HB3	1.64	0.60
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.83	0.60
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.84	0.60
2:G:3767:GLN:HB3	2:G:3772:THR:HG22	1.82	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1973:GLN:O	2:I:1977:TYR:N	2.33	0.60
2:I:4581:LYS:HB2	2:I:4632:LEU:HB2	1.82	0.60
2:I:4961:CYS:SG	2:I:4978:HIS:NE2	2.75	0.60
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.67	0.60
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.84	0.60
2:E:4961:CYS:SG	2:E:4978:HIS:NE2	2.75	0.60
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.84	0.60
2:G:4829:SER:O	2:G:4833:ASN:ND2	2.35	0.60
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.67	0.60
2:E:1211:LEU:HD11	2:E:1225:PRO:HB3	1.84	0.60
2:I:1211:LEU:HD11	2:I:1225:PRO:HB3	1.84	0.60
2:E:4829:SER:O	2:E:4833:ASN:ND2	2.35	0.60
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.82	0.60
2:B:3882:GLN:HB2	2:B:3957:VAL:HG22	1.82	0.59
2:B:4704:LEU:HD22	2:B:4778:TRP:HB2	1.83	0.59
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.83	0.59
2:I:18:ASP:HB2	2:I:69:LEU:HD12	1.83	0.59
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.84	0.59
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.67	0.59
2:E:4704:LEU:HD22	2:E:4778:TRP:HB2	1.83	0.59
2:I:4829:SER:O	2:I:4833:ASN:ND2	2.35	0.59
2:E:3882:GLN:HB2	2:E:3957:VAL:HG22	1.83	0.59
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.83	0.59
2:E:1271:ARG:HA	2:E:1471:UNK:HA	1.85	0.59
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.84	0.59
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.36	0.59
2:I:3882:GLN:HB2	2:I:3957:VAL:HG22	1.82	0.59
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.36	0.59
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.82	0.59
2:G:1211:LEU:HD11	2:G:1225:PRO:HB3	1.83	0.59
2:I:1777:PHE:HA	2:I:1799:SER:HB2	1.85	0.59
2:B:18:ASP:HB2	2:B:69:LEU:HD12	1.83	0.59
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.67	0.59
2:G:1777:PHE:HA	2:G:1799:SER:HB2	1.85	0.59
2:G:2205:GLU:HG2	2:G:2253:HIS:HE1	1.67	0.59
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.36	0.59
2:G:1218:GLY:HA2	2:G:1223:PHE:HB2	1.85	0.59
2:E:4895:GLY:O	2:G:4892:ARG:NH2	2.34	0.59
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.83	0.59
2:I:4704:LEU:HD22	2:I:4778:TRP:HB2	1.83	0.59
2:B:1218:GLY:HA2	2:B:1223:PHE:HB2	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.83	0.59
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.36	0.59
2:G:1973:GLN:O	2:G:1977:TYR:N	2.33	0.59
2:B:1777:PHE:HA	2:B:1799:SER:HB2	1.85	0.59
2:I:1218:GLY:HA2	2:I:1223:PHE:HB2	1.85	0.59
2:E:2205:GLU:HG2	2:E:2253:HIS:HE1	1.67	0.58
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.85	0.58
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.85	0.58
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.85	0.58
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.83	0.58
2:B:2205:GLU:HG2	2:B:2253:HIS:HE1	1.67	0.58
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.85	0.58
2:E:1777:PHE:HA	2:E:1799:SER:HB2	1.85	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.85	0.58
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.36	0.58
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.33	0.58
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.85	0.58
2:I:2205:GLU:HG2	2:I:2253:HIS:HE1	1.67	0.58
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.86	0.58
2:B:4241:THR:HB	2:B:4989:MET:HE1	1.85	0.58
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.85	0.58
1:A:6:THR:HA	1:A:72:ALA:HA	1.85	0.58
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.76	0.58
2:B:3846:ALA:HB1	2:B:3873:LYS:HG2	1.86	0.58
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.36	0.58
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.36	0.58
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.85	0.58
2:I:627:PRO:HB2	1:J:92:PRO:HD3	1.85	0.58
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.85	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.58
1:F:6:THR:HA	1:F:72:ALA:HA	1.85	0.58
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.58
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.85	0.58
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.86	0.58
2:E:3846:ALA:HB1	2:E:3873:LYS:HG2	1.86	0.58
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.37	0.58
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.37	0.58
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.86	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.85	0.58
1:J:27:THR:HB	1:J:100:ASP:HB3	1.86	0.58
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.36	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.85	0.57
2:E:1218:GLY:HA2	2:E:1223:PHE:HB2	1.85	0.57
1:A:27:THR:HB	1:A:100:ASP:HB3	1.86	0.57
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.37	0.57
2:E:2440:MET:O	2:E:2444:GLN:N	2.36	0.57
1:H:27:THR:HB	1:H:100:ASP:HB3	1.86	0.57
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.37	0.57
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.85	0.57
2:B:546:TRP:O	2:B:550:LYS:NZ	2.31	0.57
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.85	0.57
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.86	0.57
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.85	0.57
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.87	0.57
2:G:1830:VAL:HB	2:G:1837:GLN:HA	1.87	0.57
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.87	0.57
1:F:27:THR:HB	1:F:100:ASP:HB3	1.86	0.57
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.86	0.57
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.85	0.57
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.86	0.57
2:I:2440:MET:O	2:I:2444:GLN:N	2.36	0.57
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.86	0.57
1:J:6:THR:HA	1:J:72:ALA:HA	1.85	0.57
2:B:1271:ARG:HA	2:B:1471:UNK:HA	1.86	0.57
2:B:4937:ILE:HD12	2:I:4934:GLY:HA3	1.86	0.57
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.86	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.57
2:I:1271:ARG:HA	2:I:1471:UNK:HA	1.86	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.76	0.57
2:I:3846:ALA:HB1	2:I:3873:LYS:HG2	1.86	0.57
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.86	0.57
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.87	0.57
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.85	0.57
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.38	0.57
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.85	0.57
2:G:645:ARG:N	2:G:824:GLU:O	2.38	0.57
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.86	0.57
2:I:1830:VAL:HB	2:I:1837:GLN:HA	1.87	0.57
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.86	0.57
2:B:4177:TYR:HE1	2:B:4199:GLU:HB2	1.70	0.57
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3846:ALA:HB1	2:G:3873:LYS:HG2	1.86	0.57
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.38	0.57
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.87	0.57
2:B:4151:SER:HA	2:B:4160:LEU:HD21	1.87	0.57
2:E:1830:VAL:HB	2:E:1837:GLN:HA	1.87	0.57
2:E:3843:ASP:H	2:E:3874:VAL:HG13	1.70	0.57
2:E:4201:ASN:O	2:E:4205:TRP:N	2.38	0.57
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.57
2:B:645:ARG:N	2:B:824:GLU:O	2.38	0.56
2:E:4859:PHE:CA	2:E:4862:PHE:HD2	2.18	0.56
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.38	0.56
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.76	0.56
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.38	0.56
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.86	0.56
2:G:4151:SER:HA	2:G:4160:LEU:HD21	1.87	0.56
2:G:4177:TYR:HE1	2:G:4199:GLU:HB2	1.70	0.56
2:G:4815:ASP:O	2:G:4819:GLY:N	2.37	0.56
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.56
2:I:4151:SER:HA	2:I:4160:LEU:HD21	1.87	0.56
2:E:315:CYS:SG	2:E:316:PHE:N	2.79	0.56
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.56
2:G:451:TYR:O	2:G:474:ARG:NH1	2.38	0.56
2:G:2281:ILE:HG23	2:G:2341:VAL:HG11	1.88	0.56
2:I:645:ARG:N	2:I:824:GLU:O	2.38	0.56
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.85	0.56
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.56
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.38	0.56
1:H:6:THR:HA	1:H:72:ALA:HA	1.85	0.56
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.38	0.56
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.87	0.56
2:B:1830:VAL:HB	2:B:1837:GLN:HA	1.86	0.56
2:E:4012:LEU:O	2:E:4016:LEU:N	2.39	0.56
2:E:4151:SER:HA	2:E:4160:LEU:HD21	1.87	0.56
2:E:4177:TYR:HE1	2:E:4199:GLU:HB2	1.70	0.56
2:I:683:ARG:NH1	2:I:707:VAL:O	2.37	0.56
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.38	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.87	0.56
2:G:315:CYS:SG	2:G:316:PHE:N	2.79	0.56
2:G:682:LEU:HD13	2:G:787:VAL:HG11	1.88	0.56
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:CYS:SG	2:B:316:PHE:N	2.79	0.56
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.87	0.56
2:I:4201:ASN:O	2:I:4205:TRP:N	2.38	0.56
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.56
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.87	0.56
2:E:451:TYR:O	2:E:474:ARG:NH1	2.38	0.56
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.38	0.56
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.87	0.56
2:G:3765:TYR:O	2:G:3769:ARG:N	2.36	0.56
2:I:682:LEU:HD13	2:I:787:VAL:HG11	1.88	0.56
2:E:4241:THR:HB	2:E:4989:MET:HE1	1.86	0.55
2:G:17:ASP:HB2	2:G:98:HIS:HE1	1.71	0.55
2:G:4241:THR:HB	2:G:4989:MET:HE1	1.86	0.55
2:I:2281:ILE:HG23	2:I:2341:VAL:HG11	1.88	0.55
2:B:451:TYR:O	2:B:474:ARG:NH1	2.39	0.55
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.76	0.55
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.87	0.55
2:B:17:ASP:HB2	2:B:98:HIS:HE1	1.71	0.55
2:B:682:LEU:HD13	2:B:787:VAL:HG11	1.88	0.55
2:B:3843:ASP:H	2:B:3874:VAL:HG13	1.71	0.55
2:I:635:THR:O	1:J:34:LYS:NZ	2.34	0.55
2:E:2281:ILE:HG23	2:E:2341:VAL:HG11	1.88	0.55
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.40	0.55
2:I:315:CYS:SG	2:I:316:PHE:N	2.79	0.55
2:I:4815:ASP:O	2:I:4819:GLY:N	2.37	0.55
2:B:4563:ARG:NH1	2:B:4815:ASP:OD2	2.36	0.55
2:E:682:LEU:HD13	2:E:787:VAL:HG11	1.88	0.55
2:E:4924:VAL:O	2:E:4928:LEU:N	2.35	0.55
2:G:157:ARG:NH2	2:G:167:ASP:OD1	2.38	0.55
2:G:3843:ASP:H	2:G:3874:VAL:HG13	1.70	0.55
2:G:4114:CYS:O	2:G:4131:ARG:NH2	2.40	0.55
2:G:4184:MET:HB3	2:G:4190:ILE:HD13	1.89	0.55
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.87	0.55
2:B:1090:PHE:HD2	2:B:1202:LEU:HD11	1.72	0.55
2:B:2440:MET:O	2:B:2444:GLN:N	2.36	0.55
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.40	0.55
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.88	0.55
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.88	0.55
2:B:4697:VAL:O	2:B:4701:TRP:N	2.39	0.55
2:I:451:TYR:O	2:I:474:ARG:NH1	2.38	0.55
2:B:1667:LEU:O	2:B:1671:ARG:NH1	2.40	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.88	0.55
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.80	0.55
2:G:4201:ASN:O	2:G:4205:TRP:N	2.38	0.55
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.72	0.55
2:I:4114:CYS:O	2:I:4131:ARG:NH2	2.40	0.55
2:I:4563:ARG:NH1	2:I:4815:ASP:OD2	2.36	0.55
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.40	0.55
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.40	0.55
2:B:4815:ASP:O	2:B:4819:GLY:N	2.37	0.55
2:E:331:VAL:HG11	2:E:336:PRO:HD2	1.89	0.55
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.40	0.55
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.88	0.55
2:G:1667:LEU:O	2:G:1671:ARG:NH1	2.40	0.55
2:I:1090:PHE:HD2	2:I:1202:LEU:HD11	1.72	0.55
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.40	0.55
2:I:4177:TYR:HE1	2:I:4199:GLU:HB2	1.70	0.55
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	1.89	0.55
2:B:2281:ILE:HG23	2:B:2341:VAL:HG11	1.88	0.55
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.89	0.55
2:B:4114:CYS:O	2:B:4131:ARG:NH2	2.40	0.55
2:E:4114:CYS:O	2:E:4131:ARG:NH2	2.40	0.55
2:I:17:ASP:HB2	2:I:98:HIS:HE1	1.71	0.55
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.89	0.55
2:I:1258:ALA:HB3	2:I:1271:ARG:HB3	1.89	0.55
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.89	0.54
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.72	0.54
2:E:3767:GLN:NE2	2:E:3804:ILE:O	2.40	0.54
2:G:331:VAL:HG11	2:G:336:PRO:HD2	1.89	0.54
2:G:635:THR:O	1:H:34:LYS:NZ	2.40	0.54
2:G:1258:ALA:HB3	2:G:1271:ARG:HB3	1.89	0.54
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.80	0.54
2:I:488:LEU:O	2:I:492:ASP:N	2.39	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.54
2:E:1667:LEU:O	2:E:1671:ARG:NH1	2.40	0.54
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.40	0.54
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.38	0.54
2:I:4184:MET:HB3	2:I:4190:ILE:HD13	1.89	0.54
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.80	0.54
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.88	0.54
2:E:1090:PHE:HD2	2:E:1202:LEU:HD11	1.72	0.54
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.40	0.54
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	1.89	0.54
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.40	0.54
2:E:4184:MET:HB3	2:E:4190:ILE:HD13	1.89	0.54
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.88	0.54
2:I:331:VAL:HG11	2:I:336:PRO:HD2	1.89	0.54
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.40	0.54
2:B:3992:PHE:O	2:B:3996:PHE:N	2.38	0.54
2:E:645:ARG:N	2:E:824:GLU:O	2.38	0.54
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.40	0.54
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.72	0.54
2:E:4697:VAL:O	2:E:4701:TRP:N	2.39	0.54
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.89	0.54
2:B:1258:ALA:HB3	2:B:1271:ARG:HB3	1.89	0.54
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.40	0.54
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.40	0.54
2:G:731:THR:OG1	2:G:1519:UNK:O	2.25	0.54
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.54
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.72	0.54
2:I:3767:GLN:NE2	2:I:3804:ILE:O	2.40	0.54
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.80	0.54
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.89	0.54
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.89	0.54
2:I:1667:LEU:O	2:I:1671:ARG:NH1	2.40	0.54
2:I:3843:ASP:H	2:I:3874:VAL:HG13	1.71	0.54
2:B:3767:GLN:NE2	2:B:3804:ILE:O	2.40	0.54
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.89	0.54
2:E:1258:ALA:HB3	2:E:1271:ARG:HB3	1.89	0.54
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.89	0.54
2:E:4815:ASP:O	2:E:4819:GLY:N	2.37	0.54
2:I:4012:LEU:O	2:I:4016:LEU:N	2.39	0.54
2:B:647:ASN:ND2	2:B:820:ARG:O	2.41	0.54
2:B:731:THR:OG1	2:B:1519:UNK:O	2.27	0.54
2:B:4012:LEU:O	2:B:4016:LEU:N	2.39	0.54
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.89	0.54
2:I:157:ARG:NH2	2:I:167:ASP:OD1	2.38	0.54
2:I:1713:ASP:O	2:I:1717:SER:N	2.41	0.54
2:I:4848:VAL:HG23	2:I:4883:TYR:HE1	1.73	0.54
1:J:62:GLY:HA3	1:J:74:LEU:HD21	1.90	0.54
2:E:17:ASP:HB2	2:E:98:HIS:HE1	1.71	0.53
2:G:1090:PHE:HD2	2:G:1202:LEU:HD11	1.72	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1271:ARG:HA	2:G:1471:UNK:HA	1.89	0.53
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.90	0.53
2:G:3767:GLN:NE2	2:G:3804:ILE:O	2.41	0.53
2:G:4012:LEU:O	2:G:4016:LEU:N	2.39	0.53
2:B:157:ARG:NH2	2:B:167:ASP:OD1	2.38	0.53
2:B:331:VAL:HG11	2:B:336:PRO:HD2	1.89	0.53
2:B:3932:ASP:HA	2:B:3935:TRP:HD1	1.73	0.53
2:B:4184:MET:HB3	2:B:4190:ILE:HD13	1.89	0.53
2:E:4848:VAL:HG23	2:E:4883:TYR:HE1	1.73	0.53
2:G:2336:ARG:HD3	2:G:2435:ARG:HD2	1.89	0.53
2:G:4848:VAL:HG23	2:G:4883:TYR:HE1	1.73	0.53
2:I:4024:VAL:HG23	2:I:4027:LEU:HD12	1.90	0.53
2:B:111:HIS:N	2:B:116:MET:O	2.36	0.53
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.91	0.53
2:E:4824:ARG:O	2:E:4828:SER:N	2.38	0.53
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.41	0.53
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.89	0.53
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.40	0.53
2:B:891:TRP:HA	2:B:902:ARG:HB3	1.90	0.53
2:E:3992:PHE:O	2:E:3996:PHE:N	2.38	0.53
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.41	0.53
2:G:2440:MET:O	2:G:2444:GLN:N	2.36	0.53
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.91	0.53
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.42	0.53
2:B:1721:GLU:HG2	2:B:1725:ARG:HH12	1.73	0.53
2:B:4924:VAL:O	2:B:4928:LEU:N	2.35	0.53
2:E:1231:GLN:NE2	2:E:1821:ASP:O	2.42	0.53
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.38	0.53
2:I:3932:ASP:HA	2:I:3935:TRP:HD1	1.73	0.53
2:I:4088:ILE:HG23	2:I:4123:ILE:HB	1.90	0.53
2:B:2336:ARG:HD3	2:B:2435:ARG:HD2	1.89	0.53
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.91	0.53
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	1.89	0.53
1:F:62:GLY:HA3	1:F:74:LEU:HD21	1.90	0.53
2:G:4088:ILE:HG23	2:G:4123:ILE:HB	1.90	0.53
2:I:1231:GLN:NE2	2:I:1821:ASP:O	2.42	0.53
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.89	0.53
1:A:62:GLY:HA3	1:A:74:LEU:HD21	1.90	0.53
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.90	0.53
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.42	0.53
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.42	0.53
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.42	0.53
2:E:731:THR:OG1	2:E:1519:UNK:O	2.27	0.53
2:E:891:TRP:HA	2:E:902:ARG:HB3	1.90	0.53
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.39	0.53
2:E:2336:ARG:HD3	2:E:2435:ARG:HD2	1.89	0.53
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	1.89	0.53
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.91	0.53
2:I:647:ASN:ND2	2:I:820:ARG:O	2.41	0.53
2:I:2336:ARG:HD3	2:I:2435:ARG:HD2	1.89	0.53
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.38	0.53
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.90	0.53
2:E:488:LEU:O	2:E:492:ASP:N	2.39	0.53
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.90	0.53
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.42	0.53
2:E:157:ARG:NH2	2:E:167:ASP:OD1	2.38	0.53
2:E:1721:GLU:HG2	2:E:1725:ARG:HH12	1.73	0.53
2:G:15:ARG:HD3	2:G:98:HIS:HB3	1.91	0.53
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.40	0.53
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.42	0.53
2:G:891:TRP:HA	2:G:902:ARG:HB3	1.90	0.53
2:G:3932:ASP:HA	2:G:3935:TRP:HD1	1.73	0.53
2:G:4024:VAL:HG23	2:G:4027:LEU:HD12	1.90	0.53
2:I:15:ARG:HD3	2:I:98:HIS:HB3	1.91	0.53
2:I:891:TRP:HA	2:I:902:ARG:HB3	1.90	0.53
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.91	0.53
2:I:4697:VAL:O	2:I:4701:TRP:N	2.39	0.53
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.91	0.52
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.74	0.52
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.91	0.52
2:B:4201:ASN:O	2:B:4205:TRP:N	2.38	0.52
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.40	0.52
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.91	0.52
2:G:488:LEU:O	2:G:492:ASP:N	2.39	0.52
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.42	0.52
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.41	0.52
2:B:4780:PHE:O	2:B:4784:PHE:N	2.42	0.52
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.74	0.52
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.91	0.52
2:G:395:GLN:HG3	2:G:397:GLU:H	1.75	0.52
2:G:1231:GLN:NE2	2:G:1821:ASP:O	2.42	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4782:VAL:O	2:G:4785:THR:OG1	2.26	0.52
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.91	0.52
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.92	0.52
2:E:206:CYS:SG	2:E:207:SER:N	2.83	0.52
2:I:1865:MET:N	2:I:1865:MET:SD	2.83	0.52
2:B:1865:MET:N	2:B:1865:MET:SD	2.83	0.52
2:B:4024:VAL:HG23	2:B:4027:LEU:HD12	1.90	0.52
2:B:4782:VAL:O	2:B:4785:THR:OG1	2.26	0.52
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.91	0.52
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.41	0.52
2:E:2265:LEU:HB3	2:E:2330:ARG:HG2	1.92	0.52
1:H:62:GLY:HA3	1:H:74:LEU:HD21	1.90	0.52
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.90	0.52
1:A:57:LYS:HB2	1:A:80:VAL:HB	1.92	0.52
2:B:206:CYS:SG	2:B:207:SER:N	2.83	0.52
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.91	0.52
2:B:1713:ASP:O	2:B:1717:SER:N	2.41	0.52
2:B:4892:ARG:NH2	2:I:4895:GLY:O	2.43	0.52
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.42	0.52
2:E:3932:ASP:HA	2:E:3935:TRP:HD1	1.73	0.52
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.91	0.52
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.43	0.52
2:B:1231:GLN:NE2	2:B:1821:ASP:O	2.42	0.52
2:B:4848:VAL:HG23	2:B:4883:TYR:HE1	1.73	0.52
2:E:647:ASN:ND2	2:E:820:ARG:O	2.41	0.52
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.43	0.52
2:E:4024:VAL:HG23	2:E:4027:LEU:HD12	1.90	0.52
1:F:57:LYS:HB2	1:F:80:VAL:HB	1.92	0.52
2:G:1721:GLU:HG2	2:G:1725:ARG:HH12	1.74	0.52
2:G:4697:VAL:O	2:G:4701:TRP:N	2.39	0.52
2:B:395:GLN:HG3	2:B:397:GLU:H	1.74	0.52
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.43	0.52
2:E:4782:VAL:O	2:E:4785:THR:OG1	2.26	0.52
2:G:206:CYS:SG	2:G:207:SER:N	2.83	0.52
2:G:2265:LEU:HB3	2:G:2330:ARG:HG2	1.92	0.52
2:G:4824:ARG:O	2:G:4828:SER:N	2.38	0.52
2:G:4924:VAL:O	2:G:4928:LEU:N	2.35	0.52
2:I:317:ARG:HB2	2:I:347:PHE:HB2	1.92	0.52
2:I:4782:VAL:O	2:I:4785:THR:OG1	2.26	0.52
2:B:4040:ILE:O	2:B:4044:MET:N	2.41	0.52
2:E:395:GLN:HG3	2:E:397:GLU:H	1.75	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.92	0.52
2:E:4088:ILE:HG23	2:E:4123:ILE:HB	1.90	0.52
2:E:4563:ARG:NH1	2:E:4815:ASP:OD2	2.36	0.52
2:G:317:ARG:HB2	2:G:347:PHE:HB2	1.92	0.52
2:G:647:ASN:ND2	2:G:820:ARG:O	2.41	0.52
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.74	0.52
2:I:880:GLU:OE1	2:I:968:ALA:N	2.43	0.52
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.92	0.52
2:I:2457:LEU:HD23	2:I:2460:LEU:HD12	1.92	0.52
2:B:880:GLU:OE1	2:B:968:ALA:N	2.43	0.52
2:E:15:ARG:HD3	2:E:98:HIS:HB3	1.91	0.52
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.91	0.52
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.74	0.52
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.92	0.52
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.92	0.52
2:G:1865:MET:N	2:G:1865:MET:SD	2.83	0.52
2:G:3992:PHE:O	2:G:3996:PHE:N	2.38	0.52
2:I:1721:GLU:HG2	2:I:1725:ARG:HH12	1.73	0.52
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.91	0.52
2:E:728:ARG:NH2	2:E:1527:UNK:O	2.43	0.52
2:E:2368:LEU:HD13	2:E:2376:LEU:HB2	1.91	0.52
2:G:111:HIS:CD2	2:G:114:SER:H	2.28	0.52
2:G:2457:LEU:HD23	2:G:2460:LEU:HD12	1.92	0.52
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.42	0.52
1:J:25:HIS:HB3	1:J:40:ARG:HD3	1.92	0.52
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.92	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.42	0.51
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.91	0.51
2:B:2368:LEU:HD13	2:B:2376:LEU:HB2	1.91	0.51
2:B:4088:ILE:HG23	2:B:4123:ILE:HB	1.90	0.51
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.92	0.51
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.91	0.51
2:G:792:LEU:HD22	2:G:799:GLU:H	1.75	0.51
2:G:2368:LEU:HD13	2:G:2376:LEU:HB2	1.91	0.51
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.40	0.51
2:I:1684:ALA:HA	2:I:1782:PHE:HZ	1.75	0.51
2:I:4780:PHE:O	2:I:4784:PHE:N	2.42	0.51
2:I:4855:ALA:HA	2:I:4859:PHE:HB2	1.92	0.51
2:B:15:ARG:HD3	2:B:98:HIS:HB3	1.91	0.51
2:B:2457:LEU:HD23	2:B:2460:LEU:HD12	1.92	0.51
2:E:1865:MET:N	2:E:1865:MET:SD	2.83	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.43	0.51
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.90	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.92	0.51
2:I:206:CYS:SG	2:I:207:SER:N	2.83	0.51
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.91	0.51
2:I:1727:ARG:HH12	2:I:1772:ARG:HB3	1.76	0.51
2:I:4571:PHE:O	2:I:4575:PHE:N	2.43	0.51
2:B:43:GLY:N	2:B:447:ASP:OD2	2.43	0.51
2:B:1659:LEU:O	2:B:1663:HIS:N	2.41	0.51
2:E:111:HIS:CD2	2:E:114:SER:H	2.28	0.51
2:G:1684:ALA:HA	2:G:1782:PHE:HZ	1.76	0.51
2:G:1713:ASP:O	2:G:1717:SER:N	2.41	0.51
2:I:111:HIS:N	2:I:116:MET:O	2.36	0.51
2:I:4824:ARG:O	2:I:4828:SER:N	2.38	0.51
2:B:111:HIS:CD2	2:B:114:SER:H	2.28	0.51
1:F:87:HIS:N	1:F:91:ILE:O	2.44	0.51
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.91	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.93	0.51
2:G:4040:ILE:O	2:G:4044:MET:N	2.41	0.51
1:H:57:LYS:HB2	1:H:80:VAL:HB	1.92	0.51
1:H:87:HIS:N	1:H:91:ILE:O	2.44	0.51
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.91	0.51
2:I:4040:ILE:O	2:I:4044:MET:N	2.41	0.51
1:A:87:HIS:N	1:A:91:ILE:O	2.44	0.51
2:B:317:ARG:HB2	2:B:347:PHE:HB2	1.92	0.51
2:B:1727:ARG:HH12	2:B:1772:ARG:HB3	1.76	0.51
2:E:2190:VAL:HA	2:E:2193:GLN:HB2	1.93	0.51
2:E:4780:PHE:O	2:E:4784:PHE:N	2.42	0.51
2:E:4998:LYS:HB3	2:E:5003:HIS:HE1	1.76	0.51
2:I:792:LEU:HD22	2:I:799:GLU:H	1.76	0.51
2:I:2368:LEU:HD13	2:I:2376:LEU:HB2	1.91	0.51
1:J:57:LYS:HB2	1:J:80:VAL:HB	1.92	0.51
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.51
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.93	0.51
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.42	0.51
2:E:3552:UNK:O	2:E:3556:UNK:N	2.43	0.51
2:G:728:ARG:NH2	2:G:1527:UNK:O	2.44	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.28	0.51
2:B:792:LEU:HD22	2:B:799:GLU:H	1.76	0.51
2:B:2758:PHE:O	2:B:2762:THR:N	2.43	0.51
2:E:43:GLY:N	2:E:447:ASP:OD2	2.44	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:111:HIS:N	2:E:116:MET:O	2.36	0.51
2:E:792:LEU:HD22	2:E:799:GLU:H	1.76	0.51
2:E:4899:ASP:OD1	2:G:4892:ARG:NH2	2.37	0.51
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.93	0.51
2:G:3552:UNK:O	2:G:3556:UNK:N	2.44	0.51
2:G:4918:ILE:HD13	2:I:4892:ARG:HD3	1.92	0.51
2:I:3756:LYS:O	2:I:3760:LYS:NZ	2.37	0.51
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.92	0.51
2:B:2265:LEU:HB3	2:B:2330:ARG:HG2	1.92	0.51
2:B:3552:UNK:O	2:B:3556:UNK:N	2.44	0.51
2:B:4934:GLY:HA3	2:E:4937:ILE:HD12	1.92	0.51
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.51
2:G:639:ASN:H	2:G:678:GLN:HE22	1.59	0.51
2:G:1727:ARG:HH12	2:G:1772:ARG:HB3	1.76	0.51
2:G:2235:PHE:HA	2:G:2238:TYR:HD2	1.76	0.51
2:G:4859:PHE:CA	2:G:4862:PHE:CD2	2.75	0.51
2:I:2235:PHE:HA	2:I:2238:TYR:HD2	1.76	0.51
2:I:2265:LEU:HB3	2:I:2330:ARG:HG2	1.92	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.93	0.51
1:J:29:MET:HB3	1:J:98:ILE:HB	1.93	0.51
2:B:4855:ALA:HA	2:B:4859:PHE:HB2	1.92	0.51
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.92	0.51
2:E:880:GLU:OE1	2:E:968:ALA:N	2.43	0.51
2:E:1713:ASP:O	2:E:1717:SER:N	2.41	0.51
2:E:2248:ARG:NH2	2:E:2285:GLU:OE1	2.44	0.51
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	1.93	0.51
2:G:1778:SER:N	2:G:1799:SER:O	2.44	0.51
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.42	0.51
2:B:709:ASP:O	2:B:725:HIS:ND1	2.44	0.51
2:B:1071:ARG:HD3	2:B:1241:SER:HB3	1.93	0.51
2:B:2248:ARG:NH2	2:B:2285:GLU:OE1	2.44	0.51
2:B:3904:ARG:NH2	2:B:3973:CYS:SG	2.84	0.51
2:E:317:ARG:HB2	2:E:347:PHE:HB2	1.92	0.51
2:E:2013:LYS:HA	2:E:2028:ARG:HB2	1.93	0.51
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.93	0.51
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.93	0.51
2:E:4745:LEU:O	2:E:4749:GLU:N	2.43	0.51
2:I:43:GLY:N	2:I:447:ASP:OD2	2.43	0.51
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.93	0.51
2:I:731:THR:OG1	2:I:1519:UNK:O	2.29	0.51
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2190:VAL:HA	2:I:2193:GLN:HB2	1.93	0.51
2:I:4570:ALA:O	2:I:4574:ASN:ND2	2.44	0.51
2:B:639:ASN:H	2:B:678:GLN:HE22	1.59	0.50
2:B:1684:ALA:HA	2:B:1782:PHE:HZ	1.75	0.50
2:E:639:ASN:H	2:E:678:GLN:HE22	1.59	0.50
2:I:2248:ARG:NH2	2:I:2285:GLU:OE1	2.44	0.50
2:I:4998:LYS:HB3	2:I:5003:HIS:HE1	1.76	0.50
2:B:134:ASP:HA	2:B:192:ASP:HA	1.94	0.50
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.94	0.50
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.94	0.50
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.94	0.50
2:E:4570:ALA:O	2:E:4574:ASN:ND2	2.44	0.50
1:F:25:HIS:HB3	1:F:40:ARG:HD3	1.92	0.50
2:G:1071:ARG:HD3	2:G:1241:SER:HB3	1.92	0.50
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	1.93	0.50
2:I:396:GLU:O	2:I:400:ALA:N	2.40	0.50
2:I:1659:LEU:O	2:I:1663:HIS:N	2.41	0.50
2:B:932:LEU:HD23	2:B:935:LEU:HD12	1.94	0.50
2:B:4998:LYS:HB3	2:B:5003:HIS:HE1	1.76	0.50
2:E:54:ASN:O	2:E:58:VAL:N	2.43	0.50
2:E:1241:SER:HA	2:E:1603:VAL:HA	1.92	0.50
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.45	0.50
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.92	0.50
2:G:709:ASP:O	2:G:725:HIS:ND1	2.44	0.50
2:I:395:GLN:HG3	2:I:397:GLU:H	1.74	0.50
2:I:932:LEU:HD23	2:I:935:LEU:HD12	1.94	0.50
2:B:2235:PHE:HA	2:B:2238:TYR:HD2	1.76	0.50
2:B:4570:ALA:O	2:B:4574:ASN:ND2	2.44	0.50
2:E:69:LEU:HD22	2:E:107:ILE:HD11	1.93	0.50
2:E:134:ASP:HA	2:E:192:ASP:HA	1.94	0.50
2:E:232:THR:HB	2:E:252:VAL:HG11	1.93	0.50
2:E:1727:ARG:HH12	2:E:1772:ARG:HB3	1.76	0.50
2:E:2235:PHE:HA	2:E:2238:TYR:HD2	1.76	0.50
2:G:2248:ARG:NH2	2:G:2285:GLU:OE1	2.44	0.50
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.93	0.50
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.44	0.50
2:I:4109:GLN:O	2:I:4113:SER:N	2.43	0.50
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	1.93	0.50
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.93	0.50
2:E:1684:ALA:HA	2:E:1782:PHE:HZ	1.76	0.50
2:E:1778:SER:N	2:E:1799:SER:O	2.44	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2457:LEU:HD23	2:E:2460:LEU:HD12	1.92	0.50
2:G:880:GLU:OE1	2:G:968:ALA:N	2.43	0.50
2:G:2190:VAL:HA	2:G:2193:GLN:HB2	1.93	0.50
2:G:4855:ALA:HA	2:G:4859:PHE:HB2	1.92	0.50
1:H:29:MET:HB3	1:H:98:ILE:HB	1.93	0.50
2:I:2013:LYS:HA	2:I:2028:ARG:HB2	1.93	0.50
2:B:1241:SER:HA	2:B:1603:VAL:HA	1.92	0.50
2:B:3765:TYR:O	2:B:3769:ARG:N	2.36	0.50
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.94	0.50
2:G:932:LEU:HD23	2:G:935:LEU:HD12	1.94	0.50
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.93	0.50
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.94	0.50
2:G:2257:LEU:O	2:G:2261:SER:N	2.45	0.50
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	1.94	0.50
2:G:3904:ARG:NH2	2:G:3973:CYS:SG	2.84	0.50
2:I:2758:PHE:O	2:I:2762:THR:N	2.43	0.50
2:B:1721:GLU:O	2:B:1725:ARG:NH2	2.45	0.50
2:B:1778:SER:N	2:B:1799:SER:O	2.44	0.50
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.93	0.50
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.77	0.50
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.93	0.50
2:E:1071:ARG:HD3	2:E:1241:SER:HB3	1.92	0.50
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	1.94	0.50
2:G:69:LEU:HD22	2:G:107:ILE:HD11	1.93	0.50
2:G:1721:GLU:O	2:G:1725:ARG:NH2	2.45	0.50
2:G:2013:LYS:HA	2:G:2028:ARG:HB2	1.93	0.50
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.94	0.50
2:G:4998:LYS:HB3	2:G:5003:HIS:HE1	1.76	0.50
2:I:639:ASN:H	2:I:678:GLN:HE22	1.59	0.50
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.94	0.50
2:I:3552:UNK:O	2:I:3556:UNK:N	2.44	0.50
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.77	0.50
2:B:488:LEU:O	2:B:492:ASP:N	2.39	0.50
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.93	0.50
2:B:2013:LYS:HA	2:B:2028:ARG:HB2	1.93	0.50
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	1.93	0.50
2:E:932:LEU:HD23	2:E:935:LEU:HD12	1.94	0.50
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.94	0.50
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.94	0.50
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.77	0.50
1:H:25:HIS:HB3	1:H:40:ARG:HD3	1.92	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:134:ASP:HA	2:I:192:ASP:HA	1.94	0.50
2:I:709:ASP:O	2:I:725:HIS:ND1	2.44	0.50
2:I:1721:GLU:O	2:I:1725:ARG:NH2	2.45	0.50
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.93	0.50
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.45	0.50
2:E:124:SER:HA	2:E:132:ALA:HB3	1.93	0.50
2:E:1721:GLU:O	2:E:1725:ARG:NH2	2.45	0.50
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.77	0.50
2:G:670:GLU:H	2:G:740:PRO:HB3	1.77	0.50
2:G:1241:SER:HA	2:G:1603:VAL:HA	1.92	0.50
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.33	0.50
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.45	0.50
2:I:379:HIS:CD2	2:I:382:GLY:H	2.27	0.50
2:I:1778:SER:N	2:I:1799:SER:O	2.44	0.50
2:B:4571:PHE:O	2:B:4575:PHE:N	2.43	0.49
2:E:684:VAL:HG23	2:E:781:VAL:HB	1.94	0.49
2:E:709:ASP:O	2:E:725:HIS:ND1	2.44	0.49
2:E:3904:ARG:NH2	2:E:3973:CYS:SG	2.84	0.49
2:E:4571:PHE:O	2:E:4575:PHE:N	2.43	0.49
2:G:134:ASP:HA	2:G:192:ASP:HA	1.94	0.49
2:G:3761:GLN:HB3	2:G:4754:ASN:HA	1.93	0.49
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.44	0.49
2:G:4560:TYR:O	2:G:4564:PHE:N	2.45	0.49
2:G:5012:LYS:O	2:G:5016:GLU:N	2.44	0.49
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.94	0.49
2:I:2257:LEU:O	2:I:2261:SER:N	2.45	0.49
2:I:4924:VAL:O	2:I:4928:LEU:N	2.35	0.49
1:J:87:HIS:N	1:J:91:ILE:O	2.44	0.49
2:B:2132:GLY:O	2:B:2136:ARG:N	2.46	0.49
2:B:3756:LYS:O	2:B:3760:LYS:NZ	2.37	0.49
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.94	0.49
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.94	0.49
2:G:546:TRP:O	2:G:550:LYS:NZ	2.31	0.49
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.92	0.49
2:I:1241:SER:HA	2:I:1603:VAL:HA	1.92	0.49
2:I:3904:ARG:NH2	2:I:3973:CYS:SG	2.84	0.49
1:A:25:HIS:HB3	1:A:40:ARG:HD3	1.92	0.49
2:B:124:SER:HA	2:B:132:ALA:HB3	1.94	0.49
2:B:670:GLU:H	2:B:740:PRO:HB3	1.77	0.49
2:E:670:GLU:H	2:E:740:PRO:HB3	1.77	0.49
2:E:2257:LEU:O	2:E:2261:SER:N	2.45	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2758:PHE:O	2:E:2762:THR:N	2.44	0.49
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.93	0.49
2:E:4875:LYS:HB3	2:E:4882:CYS:HA	1.95	0.49
2:G:124:SER:HA	2:G:132:ALA:HB3	1.94	0.49
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.78	0.49
2:G:4875:LYS:HB3	2:G:4882:CYS:HA	1.95	0.49
2:I:670:GLU:H	2:I:740:PRO:HB3	1.77	0.49
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	1.94	0.49
2:B:684:VAL:HG23	2:B:781:VAL:HB	1.94	0.49
2:B:2190:VAL:HA	2:B:2193:GLN:HB2	1.93	0.49
2:B:3761:GLN:HB3	2:B:4754:ASN:HA	1.93	0.49
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.93	0.49
2:E:4040:ILE:O	2:E:4044:MET:N	2.41	0.49
2:E:4546:VAL:O	2:E:4550:LYS:N	2.42	0.49
2:G:232:THR:HB	2:G:252:VAL:HG11	1.93	0.49
2:G:4570:ALA:O	2:G:4574:ASN:ND2	2.44	0.49
2:I:124:SER:HA	2:I:132:ALA:HB3	1.94	0.49
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.94	0.49
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.94	0.49
2:B:5012:LYS:O	2:B:5016:GLU:N	2.44	0.49
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.94	0.49
2:G:2132:GLY:O	2:G:2136:ARG:N	2.46	0.49
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.93	0.49
2:I:164:ARG:N	2:I:167:ASP:OD2	2.46	0.49
2:I:1071:ARG:HD3	2:I:1241:SER:HB3	1.93	0.49
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.94	0.49
2:I:2132:GLY:O	2:I:2136:ARG:N	2.46	0.49
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.45	0.49
2:I:5012:LYS:O	2:I:5016:GLU:N	2.44	0.49
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.44	0.49
2:B:4863:TYR:HB2	2:B:4874:MET:HE2	1.95	0.49
1:F:29:MET:HB3	1:F:98:ILE:HB	1.93	0.49
2:G:43:GLY:N	2:G:447:ASP:OD2	2.43	0.49
2:I:252:VAL:HA	2:I:255:HIS:HB2	1.94	0.49
2:I:988:LEU:O	2:I:992:GLY:N	2.44	0.49
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.94	0.49
2:I:4875:LYS:HB3	2:I:4882:CYS:HA	1.95	0.49
2:B:988:LEU:O	2:B:992:GLY:N	2.45	0.49
2:E:3761:GLN:HB3	2:E:4754:ASN:HA	1.93	0.49
2:E:3765:TYR:O	2:E:3769:ARG:N	2.36	0.49
2:G:78:LEU:O	2:G:82:LEU:N	2.44	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.94	0.49
2:I:1841:VAL:HA	2:I:1844:LEU:HB3	1.95	0.49
2:I:3761:GLN:HB3	2:I:4754:ASN:HA	1.93	0.49
2:B:1841:VAL:HA	2:B:1844:LEU:HB3	1.95	0.49
2:B:3840:SER:OG	2:B:3875:MET:O	2.25	0.49
2:E:495:ASN:HD21	2:E:550:LYS:HD2	1.77	0.49
2:E:1841:VAL:HA	2:E:1844:LEU:HB3	1.95	0.49
2:I:69:LEU:HD22	2:I:107:ILE:HD11	1.93	0.49
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.94	0.49
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.94	0.49
2:I:3905:THR:HA	2:I:3912:THR:HG23	1.95	0.49
2:I:4241:THR:HB	2:I:4989:MET:HE1	1.93	0.49
2:I:4560:TYR:O	2:I:4564:PHE:N	2.45	0.49
2:B:396:GLU:O	2:B:400:ALA:N	2.40	0.49
2:B:867:LEU:HD22	2:B:929:LEU:HD22	1.95	0.49
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	1.94	0.49
2:B:4875:LYS:HB3	2:B:4882:CYS:HA	1.95	0.49
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.78	0.49
2:E:1229:ASN:O	2:E:1827:ARG:N	2.42	0.49
2:E:1737:PRO:HG2	2:E:1739:THR:HG23	1.95	0.49
2:E:3756:LYS:O	2:E:3760:LYS:NZ	2.37	0.49
2:G:1841:VAL:HA	2:G:1844:LEU:HB3	1.95	0.49
2:I:2336:ARG:NH2	2:I:2428:ALA:O	2.46	0.49
2:B:379:HIS:CD2	2:B:382:GLY:H	2.27	0.49
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.38	0.49
2:B:2257:LEU:O	2:B:2261:SER:N	2.45	0.49
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.94	0.49
1:H:7:ILE:HG22	1:H:9:PRO:HD2	1.94	0.49
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.78	0.49
2:I:1663:HIS:O	2:I:1667:LEU:N	2.46	0.49
2:I:3840:SER:OG	2:I:3875:MET:O	2.25	0.49
2:B:232:THR:HB	2:B:252:VAL:HG11	1.93	0.48
2:B:252:VAL:HA	2:B:255:HIS:HB2	1.95	0.48
2:B:797:HIS:HB3	2:B:1625:GLY:H	1.78	0.48
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.94	0.48
2:G:54:ASN:O	2:G:58:VAL:N	2.43	0.48
2:G:867:LEU:HD22	2:G:929:LEU:HD22	1.95	0.48
2:G:988:LEU:O	2:G:992:GLY:N	2.45	0.48
2:I:867:LEU:HD22	2:I:929:LEU:HD22	1.95	0.48
2:I:1952:GLN:HA	2:I:1955:VAL:HG12	1.95	0.48
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2868:SER:O	2:I:2872:GLN:N	2.46	0.48
1:A:7:ILE:HG22	1:A:9:PRO:HD2	1.94	0.48
2:B:164:ARG:N	2:B:167:ASP:OD2	2.46	0.48
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.29	0.48
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.78	0.48
2:E:2868:SER:O	2:E:2872:GLN:N	2.46	0.48
2:G:1229:ASN:O	2:G:1827:ARG:N	2.42	0.48
2:G:4863:TYR:HB2	2:G:4874:MET:HE2	1.94	0.48
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.45	0.48
1:A:29:MET:HB3	1:A:98:ILE:HB	1.93	0.48
2:B:54:ASN:O	2:B:58:VAL:N	2.43	0.48
2:B:69:LEU:HD22	2:B:107:ILE:HD11	1.93	0.48
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.94	0.48
2:B:1952:GLN:HA	2:B:1955:VAL:HG12	1.95	0.48
2:E:1659:LEU:O	2:E:1663:HIS:N	2.40	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.46	0.48
2:I:266:ARG:NH2	2:I:269:TRP:O	2.46	0.48
2:I:1294:UNK:HA	2:I:1455:UNK:HA	1.96	0.48
2:E:913:LEU:HD13	2:E:918:ARG:HA	1.96	0.48
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.44	0.48
1:F:7:ILE:HG22	1:F:9:PRO:HD2	1.94	0.48
2:G:266:ARG:NH2	2:G:269:TRP:O	2.46	0.48
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.28	0.48
2:I:485:SER:O	2:I:489:ASN:N	2.46	0.48
2:I:495:ASN:HD21	2:I:550:LYS:HD2	1.77	0.48
2:I:4863:TYR:HB2	2:I:4874:MET:HE2	1.95	0.48
2:B:1227:ALA:HB1	2:B:1230:MET:HG3	1.95	0.48
2:E:988:LEU:O	2:E:992:GLY:N	2.45	0.48
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.45	0.48
2:E:4705:VAL:HB	2:E:4778:TRP:CG	2.48	0.48
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.48	0.48
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.95	0.48
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	1.95	0.48
2:I:913:LEU:HD13	2:I:918:ARG:HA	1.96	0.48
2:I:4705:VAL:HB	2:I:4778:TRP:CG	2.49	0.48
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.95	0.48
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.45	0.48
2:B:2868:SER:O	2:B:2872:GLN:N	2.46	0.48
2:E:266:ARG:NH2	2:E:269:TRP:O	2.47	0.48
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.29	0.48
2:E:867:LEU:HD22	2:E:929:LEU:HD22	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3993:LEU:HA	2:E:3996:PHE:HB2	1.96	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.48
2:I:232:THR:HB	2:I:252:VAL:HG11	1.93	0.48
2:I:1668:ARG:HA	2:I:1671:ARG:HH11	1.79	0.48
2:I:3992:PHE:O	2:I:3996:PHE:N	2.38	0.48
2:I:4745:LEU:O	2:I:4749:GLU:N	2.43	0.48
2:B:266:ARG:NH2	2:B:269:TRP:O	2.46	0.48
2:B:4705:VAL:HB	2:B:4778:TRP:CG	2.49	0.48
2:E:164:ARG:N	2:E:167:ASP:OD2	2.46	0.48
2:E:1668:ARG:HA	2:E:1671:ARG:HH11	1.79	0.48
2:G:164:ARG:N	2:G:167:ASP:OD2	2.46	0.48
2:G:252:VAL:HA	2:G:255:HIS:HB2	1.95	0.48
2:G:396:GLU:O	2:G:400:ALA:N	2.41	0.48
2:G:495:ASN:HD21	2:G:550:LYS:HD2	1.77	0.48
2:G:684:VAL:HG23	2:G:781:VAL:HB	1.94	0.48
2:G:1203:ASN:ND2	2:G:1210:SER:O	2.47	0.48
2:G:1952:GLN:HA	2:G:1955:VAL:HG12	1.95	0.48
2:G:4705:VAL:HB	2:G:4778:TRP:CG	2.48	0.48
2:I:668:VAL:HG22	2:I:789:VAL:HG23	1.96	0.48
2:I:1227:ALA:HB1	2:I:1230:MET:HG3	1.95	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
1:J:7:ILE:HG22	1:J:9:PRO:HD2	1.94	0.48
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.46	0.48
2:B:4745:LEU:O	2:B:4749:GLU:N	2.43	0.48
2:E:220:LEU:HD11	2:E:390:LEU:HD22	1.95	0.48
2:E:2336:ARG:NH2	2:E:2428:ALA:O	2.46	0.48
2:G:220:LEU:HD11	2:G:390:LEU:HD22	1.95	0.48
2:G:485:SER:O	2:G:489:ASN:N	2.46	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.48
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.79	0.48
2:B:495:ASN:HD21	2:B:550:LYS:HD2	1.77	0.48
2:B:1203:ASN:ND2	2:B:1210:SER:O	2.47	0.48
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.96	0.48
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.48
2:E:914:PRO:O	2:E:918:ARG:N	2.46	0.48
2:E:1854:PHE:HD1	2:E:1858:ASP:HB3	1.79	0.48
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	1.95	0.48
2:G:637:LEU:HG	2:G:1693:GLN:HB3	1.96	0.48
2:G:797:HIS:HB3	2:G:1625:GLY:H	1.78	0.48
2:G:1659:LEU:O	2:G:1663:HIS:N	2.41	0.48
2:G:1976:ARG:NH1	2:G:1997:GLU:OE2	2.35	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:78:LEU:O	2:I:82:LEU:N	2.44	0.48
2:I:684:VAL:HG23	2:I:781:VAL:HB	1.94	0.48
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.96	0.48
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.96	0.48
2:B:1668:ARG:HA	2:B:1671:ARG:HH11	1.79	0.48
2:E:252:VAL:HA	2:E:255:HIS:HB2	1.95	0.48
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.96	0.48
2:E:1952:GLN:HA	2:E:1955:VAL:HG12	1.95	0.48
2:E:3905:THR:HA	2:E:3912:THR:HG23	1.95	0.48
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.49	0.48
2:G:379:HIS:CD2	2:G:382:GLY:H	2.27	0.48
2:G:1668:ARG:HA	2:G:1671:ARG:HH11	1.79	0.48
2:I:54:ASN:O	2:I:58:VAL:N	2.43	0.48
2:I:637:LEU:HG	2:I:1693:GLN:HB3	1.96	0.48
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.49	0.48
2:I:797:HIS:HB3	2:I:1625:GLY:H	1.78	0.48
2:I:4942:GLU:O	2:I:4946:GLN:N	2.43	0.48
2:B:2336:ARG:NH2	2:B:2428:ALA:O	2.46	0.47
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.79	0.47
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.96	0.47
2:E:546:TRP:O	2:E:550:LYS:NZ	2.31	0.47
2:E:637:LEU:HG	2:E:1693:GLN:HB3	1.96	0.47
2:E:668:VAL:HG22	2:E:789:VAL:HG23	1.96	0.47
2:E:1203:ASN:ND2	2:E:1210:SER:O	2.47	0.47
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	1.95	0.47
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.96	0.47
2:I:1203:ASN:ND2	2:I:1210:SER:O	2.47	0.47
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	1.95	0.47
2:I:4928:LEU:HA	2:I:4931:ILE:HD12	1.96	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:4560:TYR:O	2:B:4564:PHE:N	2.45	0.47
2:G:1227:ALA:HB1	2:G:1230:MET:HG3	1.95	0.47
2:G:3905:THR:HA	2:G:3912:THR:HG23	1.95	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.43	0.47
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.96	0.47
2:I:1737:PRO:HG2	2:I:1739:THR:HG23	1.95	0.47
2:B:913:LEU:HD13	2:B:918:ARG:HA	1.95	0.47
2:B:1229:ASN:O	2:B:1827:ARG:N	2.42	0.47
2:B:1737:PRO:HG2	2:B:1739:THR:HG23	1.95	0.47
2:E:809:ALA:O	2:E:811:CYS:N	2.47	0.47
2:E:1227:ALA:HB1	2:E:1230:MET:HG3	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:139:GLU:O	2:G:141:ALA:N	2.47	0.47
2:G:4780:PHE:O	2:G:4784:PHE:N	2.42	0.47
2:I:629:ARG:HB3	2:I:634:GLN:NE2	2.29	0.47
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.97	0.47
2:B:288:GLY:HA3	2:B:405:HIS:CE1	2.49	0.47
2:B:668:VAL:HG22	2:B:789:VAL:HG23	1.96	0.47
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.96	0.47
2:B:1817:GLU:O	2:B:1821:ASP:N	2.45	0.47
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.97	0.47
2:E:1663:HIS:O	2:E:1667:LEU:N	2.46	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.48	0.47
2:E:4056:GLU:HA	2:E:4059:LEU:HB2	1.97	0.47
2:G:173:SER:OG	2:G:174:VAL:N	2.48	0.47
2:G:410:LEU:HD21	2:G:441:VAL:HA	1.96	0.47
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.96	0.47
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.50	0.47
2:G:913:LEU:HD13	2:G:918:ARG:HA	1.96	0.47
2:G:1044:ARG:HA	2:G:1047:LEU:HD12	1.97	0.47
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.96	0.47
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	1.95	0.47
2:I:652:ARG:HB3	2:I:773:LEU:HD13	1.97	0.47
2:B:173:SER:OG	2:B:174:VAL:N	2.47	0.47
2:B:4928:LEU:HA	2:B:4931:ILE:HD12	1.96	0.47
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.49	0.47
2:E:797:HIS:HB3	2:E:1625:GLY:H	1.78	0.47
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.47
2:E:3927:GLN:O	2:E:3931:SER:N	2.43	0.47
2:G:1737:PRO:HG2	2:G:1739:THR:HG23	1.95	0.47
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.45	0.47
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.48	0.47
2:I:4896:GLY:HA2	2:I:4921:PHE:HB2	1.97	0.47
2:B:220:LEU:HD11	2:B:390:LEU:HD22	1.95	0.47
2:B:637:LEU:HG	2:B:1693:GLN:HB3	1.96	0.47
2:B:2154:SER:O	2:B:2184:ASN:ND2	2.47	0.47
2:B:3674:ILE:HG13	2:B:3732:SER:HB3	1.96	0.47
2:B:3993:LEU:HA	2:B:3996:PHE:HB2	1.96	0.47
2:B:4546:VAL:O	2:B:4550:LYS:N	2.42	0.47
2:E:4059:LEU:O	2:E:4063:ASP:N	2.47	0.47
2:E:4858:PHE:O	2:E:4862:PHE:HE2	1.98	0.47
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.95	0.47
2:G:4172:GLU:HA	2:G:4175:ARG:HE	1.79	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.47
2:I:1044:ARG:HA	2:I:1047:LEU:HD12	1.97	0.47
2:B:118:LEU:HD12	2:B:137:LEU:HB3	1.97	0.47
2:B:410:LEU:HD21	2:B:441:VAL:HA	1.96	0.47
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.47
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.49	0.47
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.97	0.47
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.95	0.47
2:B:4021:LYS:HA	2:B:4024:VAL:HG12	1.97	0.47
2:B:4109:GLN:O	2:B:4113:SER:N	2.43	0.47
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	1.96	0.47
2:B:4710:SER:OG	2:B:4772:ASP:OD2	2.28	0.47
2:B:4896:GLY:HA2	2:B:4921:PHE:HB2	1.97	0.47
2:E:652:ARG:HB3	2:E:773:LEU:HD13	1.97	0.47
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.49	0.47
2:E:1046:LEU:HB3	2:E:1051:TYR:HB2	1.97	0.47
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.48	0.47
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.95	0.47
2:E:2132:GLY:O	2:E:2136:ARG:N	2.45	0.47
2:E:2154:SER:O	2:E:2184:ASN:ND2	2.47	0.47
2:E:4021:LYS:HA	2:E:4024:VAL:HG12	1.97	0.47
2:G:118:LEU:HD12	2:G:137:LEU:HB3	1.97	0.47
2:G:652:ARG:HB3	2:G:773:LEU:HD13	1.97	0.47
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.96	0.47
2:G:1516:UNK:N	2:G:1529:UNK:O	2.47	0.47
2:G:4056:GLU:HA	2:G:4059:LEU:HB2	1.97	0.47
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.46	0.47
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	1.96	0.47
2:I:220:LEU:HD11	2:I:390:LEU:HD22	1.95	0.47
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.95	0.47
2:I:4172:GLU:HA	2:I:4175:ARG:HE	1.79	0.47
2:B:139:GLU:O	2:B:141:ALA:N	2.47	0.47
2:B:914:PRO:O	2:B:918:ARG:N	2.46	0.47
2:B:3905:THR:HA	2:B:3912:THR:HG23	1.95	0.47
2:E:139:GLU:O	2:E:141:ALA:N	2.47	0.47
2:E:485:SER:O	2:E:489:ASN:N	2.46	0.47
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.97	0.47
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	1.96	0.47
2:G:668:VAL:HG22	2:G:789:VAL:HG23	1.96	0.47
2:G:809:ALA:O	2:G:811:CYS:N	2.47	0.47
2:G:1046:LEU:HB3	2:G:1051:TYR:HB2	1.97	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1854:PHE:HD1	2:G:1858:ASP:HB3	1.79	0.47
2:G:4201:ASN:ND2	2:G:4993:MET:SD	2.88	0.47
2:I:118:LEU:HD12	2:I:137:LEU:HB3	1.97	0.47
2:I:218:HIS:HB3	2:I:392:ARG:HD3	1.97	0.47
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.97	0.47
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.97	0.47
2:B:475:GLN:NE2	2:B:528:SER:O	2.48	0.47
2:B:1046:LEU:HB3	2:B:1051:TYR:HB2	1.97	0.47
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.97	0.47
2:B:1854:PHE:HD1	2:B:1858:ASP:HB3	1.79	0.47
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.97	0.47
2:E:4083:ASP:HA	2:E:4085:ARG:HH11	1.80	0.47
2:E:4201:ASN:ND2	2:E:4993:MET:SD	2.88	0.47
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.97	0.47
2:E:4863:TYR:HB2	2:E:4874:MET:HE2	1.95	0.47
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.96	0.47
2:I:546:TRP:O	2:I:550:LYS:NZ	2.31	0.47
2:I:3765:TYR:O	2:I:3769:ARG:N	2.36	0.47
1:A:23:VAL:HB	1:A:105:ASN:HA	1.97	0.47
2:B:176:SER:HB2	2:B:178:ARG:HD3	1.97	0.47
2:B:652:ARG:HB3	2:B:773:LEU:HD13	1.97	0.47
2:B:1044:ARG:HA	2:B:1047:LEU:HD12	1.97	0.47
2:E:173:SER:OG	2:E:174:VAL:N	2.48	0.47
2:E:410:LEU:HD21	2:E:441:VAL:HA	1.96	0.47
2:E:702:TRP:O	2:E:705:ASN:ND2	2.46	0.47
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.46	0.47
2:G:176:SER:HB2	2:G:178:ARG:HD3	1.97	0.47
2:G:241:GLN:O	2:G:289:ARG:NH1	2.42	0.47
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.47
2:G:2154:SER:O	2:G:2184:ASN:ND2	2.47	0.47
2:G:4896:GLY:HA2	2:G:4921:PHE:HB2	1.97	0.47
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.80	0.47
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.46	0.47
2:B:460:GLN:HG2	2:B:462:GLU:H	1.80	0.46
2:E:379:HIS:CD2	2:E:382:GLY:H	2.27	0.46
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.96	0.46
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.97	0.46
1:F:23:VAL:HB	1:F:105:ASN:HA	1.97	0.46
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.80	0.46
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.48	0.46
2:G:3674:ILE:HG13	2:G:3732:SER:HB3	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3927:GLN:O	2:G:3931:SER:N	2.43	0.46
2:G:4083:ASP:HA	2:G:4085:ARG:HH11	1.80	0.46
2:G:4858:PHE:O	2:G:4862:PHE:HE2	1.98	0.46
2:I:139:GLU:O	2:I:141:ALA:N	2.48	0.46
2:I:173:SER:OG	2:I:174:VAL:N	2.47	0.46
2:I:410:LEU:HD21	2:I:441:VAL:HA	1.96	0.46
2:I:1046:LEU:HB3	2:I:1051:TYR:HB2	1.97	0.46
2:I:1149:VAL:HG22	2:I:1164:LEU:HD13	1.97	0.46
2:I:1976:ARG:NH1	2:I:1997:GLU:OE2	2.35	0.46
2:I:3993:LEU:HA	2:I:3996:PHE:HB2	1.96	0.46
2:B:34:LYS:N	2:B:53:SER:OG	2.43	0.46
2:B:1149:VAL:HG22	2:B:1164:LEU:HD13	1.97	0.46
2:B:2880:GLU:O	2:B:2884:ASN:N	2.45	0.46
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	1.95	0.46
2:B:4083:ASP:HA	2:B:4085:ARG:HH11	1.80	0.46
2:E:118:LEU:HD12	2:E:137:LEU:HB3	1.97	0.46
2:E:218:HIS:HB3	2:E:392:ARG:HD3	1.97	0.46
2:E:1098:GLY:HA2	2:E:1127:HIS:CD2	2.51	0.46
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	1.96	0.46
2:G:111:HIS:N	2:G:116:MET:O	2.36	0.46
2:G:385:ASP:OD1	2:G:385:ASP:N	2.48	0.46
2:G:1098:GLY:HA2	2:G:1127:HIS:CD2	2.51	0.46
2:G:4563:ARG:NH1	2:G:4815:ASP:OD2	2.36	0.46
2:I:460:GLN:HG2	2:I:462:GLU:H	1.80	0.46
2:B:4172:GLU:HA	2:B:4175:ARG:HE	1.79	0.46
2:E:396:GLU:O	2:E:400:ALA:N	2.40	0.46
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.96	0.46
2:E:3674:ILE:HG13	2:E:3732:SER:HB3	1.97	0.46
2:E:4172:GLU:HA	2:E:4175:ARG:HE	1.80	0.46
2:G:2336:ARG:NH2	2:G:2428:ALA:O	2.46	0.46
2:I:475:GLN:NE2	2:I:528:SER:O	2.48	0.46
2:I:3674:ILE:HG13	2:I:3732:SER:HB3	1.97	0.46
2:I:4056:GLU:HA	2:I:4059:LEU:HB2	1.97	0.46
2:E:176:SER:HB2	2:E:178:ARG:HD3	1.97	0.46
2:E:2212:VAL:O	2:E:2216:GLY:N	2.46	0.46
2:E:4896:GLY:HA2	2:E:4921:PHE:HB2	1.97	0.46
2:G:426:ARG:HG2	2:G:431:PRO:HA	1.98	0.46
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.97	0.46
2:G:2758:PHE:O	2:G:2762:THR:N	2.44	0.46
2:I:1854:PHE:HD1	2:I:1858:ASP:HB3	1.79	0.46
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:ARG:HG2	2:B:431:PRO:HA	1.98	0.46
2:B:702:TRP:O	2:B:705:ASN:ND2	2.46	0.46
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.48	0.46
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.98	0.46
2:B:4824:ARG:O	2:B:4828:SER:N	2.38	0.46
2:G:742:ASP:OD1	2:G:760:ASN:ND2	2.49	0.46
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.97	0.46
2:G:4021:LYS:HA	2:G:4024:VAL:HG12	1.97	0.46
2:I:176:SER:HB2	2:I:178:ARG:HD3	1.97	0.46
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.49	0.46
2:I:4546:VAL:O	2:I:4550:LYS:N	2.42	0.46
2:B:485:SER:O	2:B:489:ASN:N	2.46	0.46
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.46
2:B:1663:HIS:O	2:B:1667:LEU:N	2.46	0.46
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.97	0.46
2:G:264:PRO:HA	2:G:280:LEU:HA	1.97	0.46
2:G:355:LEU:HB3	2:G:378:LEU:HB3	1.97	0.46
2:G:1149:VAL:HG22	2:G:1164:LEU:HD13	1.97	0.46
2:G:3993:LEU:HA	2:G:3996:PHE:HB2	1.96	0.46
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.98	0.46
2:I:2154:SER:O	2:I:2184:ASN:ND2	2.47	0.46
2:I:4021:LYS:HA	2:I:4024:VAL:HG12	1.97	0.46
2:I:4853:VAL:HA	2:I:4856:PHE:HB3	1.98	0.46
2:B:583:ILE:HA	2:B:586:ILE:HD12	1.98	0.46
2:E:426:ARG:HG2	2:E:431:PRO:HA	1.98	0.46
2:E:475:GLN:NE2	2:E:528:SER:O	2.48	0.46
2:E:1149:VAL:HG22	2:E:1164:LEU:HD13	1.97	0.46
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.98	0.46
2:G:218:HIS:HB3	2:G:392:ARG:HD3	1.97	0.46
1:H:14:THR:N	1:H:67:SER:OG	2.49	0.46
2:I:34:LYS:N	2:I:53:SER:OG	2.43	0.46
2:I:385:ASP:N	2:I:385:ASP:OD1	2.48	0.46
2:I:426:ARG:HG2	2:I:431:PRO:HA	1.98	0.46
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.38	0.46
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.98	0.46
2:E:1044:ARG:HA	2:E:1047:LEU:HD12	1.97	0.46
2:E:2158:CYS:HB2	2:E:2184:ASN:HD22	1.81	0.46
2:E:4105:GLY:HA2	2:E:4108:ILE:HD12	1.98	0.46
2:G:1647:CYS:SG	2:G:1648:MET:N	2.89	0.46
2:G:4934:GLY:HA3	2:I:4937:ILE:HD12	1.97	0.46
2:I:1098:GLY:HA2	2:I:1127:HIS:CD2	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4083:ASP:HA	2:I:4085:ARG:HH11	1.80	0.46
2:B:218:HIS:HB3	2:B:392:ARG:HD3	1.97	0.46
2:B:650:VAL:HB	2:B:777:PHE:HB2	1.98	0.46
2:B:2158:CYS:HB2	2:B:2184:ASN:HD22	1.81	0.46
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.49	0.46
2:E:583:ILE:HA	2:E:586:ILE:HD12	1.98	0.46
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.98	0.46
2:G:34:LYS:N	2:G:53:SER:OG	2.43	0.46
2:I:742:ASP:OD1	2:I:760:ASN:ND2	2.49	0.46
2:I:1661:ARG:O	2:I:1664:SER:OG	2.32	0.46
2:I:1817:GLU:O	2:I:1821:ASP:N	2.45	0.46
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.98	0.46
2:I:4201:ASN:ND2	2:I:4993:MET:SD	2.88	0.46
2:B:278:GLN:N	2:B:315:CYS:SG	2.89	0.46
2:B:4056:GLU:HA	2:B:4059:LEU:HB2	1.97	0.46
2:B:4201:ASN:ND2	2:B:4993:MET:SD	2.88	0.46
2:B:4942:GLU:O	2:B:4946:GLN:N	2.43	0.46
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	1.98	0.46
2:G:475:GLN:NE2	2:G:528:SER:O	2.48	0.46
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.81	0.46
2:G:4059:LEU:O	2:G:4063:ASP:N	2.49	0.46
2:I:264:PRO:HA	2:I:280:LEU:HA	1.97	0.46
2:I:355:LEU:HB3	2:I:378:LEU:HB3	1.97	0.46
2:I:1647:CYS:SG	2:I:1648:MET:N	2.89	0.46
2:I:2243:SER:HB3	2:I:2246:ASN:H	1.81	0.46
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	1.98	0.46
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.97	0.46
2:B:666:VAL:HG21	2:B:684:VAL:HG21	1.98	0.45
2:B:1647:CYS:SG	2:B:1648:MET:N	2.89	0.45
2:B:3805:LEU:H	2:B:3805:LEU:HG	1.61	0.45
2:E:1965:TYR:HE1	2:E:2027:ILE:HB	1.82	0.45
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.81	0.45
2:E:4813:LEU:HA	2:E:4816:ILE:HG12	1.99	0.45
1:F:14:THR:N	1:F:67:SER:OG	2.49	0.45
2:G:583:ILE:HA	2:G:586:ILE:HD12	1.98	0.45
2:G:650:VAL:HB	2:G:777:PHE:HB2	1.98	0.45
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.24	0.45
2:G:4853:VAL:HA	2:G:4856:PHE:HB3	1.98	0.45
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.81	0.45
2:I:668:VAL:O	2:I:741:GLU:N	2.49	0.45
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.81	0.45
2:B:742:ASP:OD1	2:B:760:ASN:ND2	2.49	0.45
2:B:2869:ARG:HH12	2:B:2945:UNK:C	2.29	0.45
2:B:4895:GLY:O	2:E:4892:ARG:NH2	2.48	0.45
2:E:355:LEU:HB3	2:E:378:LEU:HB3	1.97	0.45
2:E:5012:LYS:O	2:E:5016:GLU:N	2.44	0.45
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.81	0.45
2:G:2243:SER:HB3	2:G:2246:ASN:H	1.81	0.45
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	1.98	0.45
2:G:4105:GLY:HA2	2:G:4108:ILE:HD12	1.98	0.45
2:G:4109:GLN:O	2:G:4113:SER:N	2.43	0.45
2:I:3927:GLN:O	2:I:3931:SER:N	2.43	0.45
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.51	0.45
1:J:14:THR:N	1:J:67:SER:OG	2.49	0.45
2:B:264:PRO:HA	2:B:280:LEU:HA	1.97	0.45
2:B:668:VAL:O	2:B:741:GLU:N	2.49	0.45
2:B:2243:SER:HB3	2:B:2246:ASN:H	1.81	0.45
2:B:4041:ALA:HA	2:B:4044:MET:HB2	1.99	0.45
2:B:4813:LEU:HA	2:B:4816:ILE:HG12	1.98	0.45
2:E:264:PRO:HA	2:E:280:LEU:HA	1.97	0.45
2:E:460:GLN:HG2	2:E:462:GLU:H	1.80	0.45
2:E:742:ASP:OD1	2:E:760:ASN:ND2	2.49	0.45
2:E:1516:UNK:N	2:E:1529:UNK:O	2.50	0.45
2:G:702:TRP:O	2:G:705:ASN:ND2	2.46	0.45
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.38	0.45
2:G:4041:ALA:HA	2:G:4044:MET:HB2	1.99	0.45
2:G:4546:VAL:O	2:G:4550:LYS:N	2.42	0.45
2:I:278:GLN:N	2:I:315:CYS:SG	2.89	0.45
2:I:583:ILE:HA	2:I:586:ILE:HD12	1.98	0.45
2:I:2869:ARG:HH12	2:I:2945:UNK:C	2.29	0.45
2:I:3676:ASP:N	2:I:3676:ASP:OD1	2.49	0.45
2:I:4813:LEU:HA	2:I:4816:ILE:HG12	1.98	0.45
2:B:983:THR:O	2:B:987:ARG:N	2.48	0.45
2:B:1098:GLY:HA2	2:B:1127:HIS:CD2	2.51	0.45
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	1.98	0.45
2:B:4780:PHE:HA	2:B:4783:ILE:HD12	1.99	0.45
2:E:983:THR:O	2:E:987:ARG:N	2.48	0.45
2:E:4041:ALA:HA	2:E:4044:MET:HB2	1.99	0.45
2:E:4780:PHE:HA	2:E:4783:ILE:HD12	1.99	0.45
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.52	0.45
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4780:PHE:HA	2:G:4783:ILE:HD12	1.99	0.45
1:H:23:VAL:HB	1:H:105:ASN:HA	1.97	0.45
2:I:838:HIS:CE1	2:I:1201:HIS:HD2	2.35	0.45
2:I:2212:VAL:O	2:I:2216:GLY:N	2.46	0.45
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.98	0.45
2:I:2880:GLU:O	2:I:2884:ASN:N	2.45	0.45
2:I:4044:MET:HA	2:I:4047:MET:HG2	1.98	0.45
2:B:838:HIS:CE1	2:B:1201:HIS:HD2	2.35	0.45
2:B:1245:PHE:HE1	2:B:1600:LEU:HD23	1.82	0.45
2:B:2908:TYR:OH	2:B:2920:ARG:NE	2.44	0.45
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.82	0.45
2:B:4105:GLY:HA2	2:B:4108:ILE:HD12	1.98	0.45
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.81	0.45
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.38	0.45
2:E:2869:ARG:HH12	2:E:2945:UNK:C	2.29	0.45
2:G:278:GLN:N	2:G:315:CYS:SG	2.89	0.45
2:G:1663:HIS:O	2:G:1667:LEU:N	2.46	0.45
2:G:1817:GLU:O	2:G:1821:ASP:N	2.45	0.45
2:G:2158:CYS:HB2	2:G:2184:ASN:HD22	1.81	0.45
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.49	0.45
1:J:23:VAL:HB	1:J:105:ASN:HA	1.97	0.45
1:A:14:THR:N	1:A:67:SER:OG	2.49	0.45
2:B:78:LEU:O	2:B:82:LEU:N	2.44	0.45
2:B:684:VAL:HA	2:B:781:VAL:HA	1.99	0.45
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.81	0.45
2:B:4044:MET:HA	2:B:4047:MET:HG2	1.98	0.45
2:E:838:HIS:CE1	2:E:1201:HIS:HD2	2.35	0.45
2:E:1647:CYS:SG	2:E:1648:MET:N	2.89	0.45
2:E:1694:LEU:O	2:E:1712:TYR:OH	2.24	0.45
2:G:684:VAL:HA	2:G:781:VAL:HA	1.99	0.45
2:G:4044:MET:HA	2:G:4047:MET:HG2	1.98	0.45
2:I:1245:PHE:HE1	2:I:1600:LEU:HD23	1.82	0.45
2:I:4780:PHE:HA	2:I:4783:ILE:HD12	1.99	0.45
2:B:1092:PHE:N	2:B:1149:VAL:O	2.37	0.45
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.82	0.45
2:E:278:GLN:N	2:E:315:CYS:SG	2.89	0.45
2:E:666:VAL:HG21	2:E:684:VAL:HG21	1.98	0.45
2:E:4853:VAL:HA	2:E:4856:PHE:HB3	1.98	0.45
2:G:3649:ALA:O	2:G:3653:PHE:N	2.47	0.45
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.82	0.45
2:G:4031:LEU:HB3	2:G:4034:ASN:HB2	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2158:CYS:HB2	2:I:2184:ASN:HD22	1.81	0.45
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	1.98	0.45
2:B:809:ALA:O	2:B:811:CYS:N	2.47	0.45
2:B:1679:ASN:O	2:B:1683:HIS:ND1	2.36	0.45
2:B:3927:GLN:O	2:B:3931:SER:N	2.43	0.45
2:B:4031:LEU:HB3	2:B:4034:ASN:HB2	1.99	0.45
2:E:684:VAL:HA	2:E:781:VAL:HA	1.99	0.45
2:E:840:VAL:HB	2:E:1199:VAL:HG12	1.99	0.45
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.98	0.45
2:E:2950:UNK:O	2:E:2954:UNK:N	2.50	0.45
2:G:666:VAL:HG21	2:G:684:VAL:HG21	1.98	0.45
2:G:840:VAL:HB	2:G:1199:VAL:HG12	1.99	0.45
2:G:4942:GLU:O	2:G:4946:GLN:N	2.43	0.45
2:I:4105:GLY:HA2	2:I:4108:ILE:HD12	1.98	0.45
2:B:349:GLN:HA	2:B:356:TRP:HA	1.99	0.45
2:B:355:LEU:HB3	2:B:378:LEU:HB3	1.97	0.45
2:B:870:ILE:HD11	2:B:1049:TYR:CG	2.52	0.45
2:B:4853:VAL:HA	2:B:4856:PHE:HB3	1.98	0.45
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.51	0.45
2:E:1817:GLU:O	2:E:1821:ASP:N	2.45	0.45
2:E:4031:LEU:HB3	2:E:4034:ASN:HB2	1.99	0.45
2:E:4169:SER:HA	2:E:4172:GLU:HB3	1.99	0.45
2:G:4813:LEU:HA	2:G:4816:ILE:HG12	1.99	0.45
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.51	0.45
2:I:666:VAL:HG21	2:I:684:VAL:HG21	1.98	0.45
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.82	0.45
2:I:3963:ASN:O	2:I:3966:THR:OG1	2.28	0.45
2:I:4735:GLU:HA	2:I:4738:ALA:HB3	1.99	0.45
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.99	0.45
2:B:2950:UNK:O	2:B:2954:UNK:N	2.50	0.45
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.81	0.45
2:G:349:GLN:HA	2:G:356:TRP:HA	1.99	0.45
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.99	0.45
2:G:2950:UNK:O	2:G:2954:UNK:N	2.50	0.45
2:G:4735:GLU:HA	2:G:4738:ALA:HB3	1.99	0.45
2:G:4859:PHE:C	2:G:4862:PHE:HD2	2.20	0.45
2:I:4031:LEU:HB3	2:I:4034:ASN:HB2	1.99	0.45
2:I:4968:PHE:HE1	2:I:5029:ARG:HD3	1.82	0.45
2:B:317:ARG:N	2:B:347:PHE:O	2.50	0.44
2:B:385:ASP:OD1	2:B:385:ASP:N	2.48	0.44
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.98	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1679:ASN:O	2:E:1683:HIS:ND1	2.36	0.44
2:E:2116:LEU:O	2:E:2120:MET:N	2.46	0.44
2:E:4109:GLN:O	2:E:4113:SER:N	2.43	0.44
2:E:4735:GLU:HA	2:E:4738:ALA:HB3	1.99	0.44
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.51	0.44
2:E:4968:PHE:HE1	2:E:5029:ARG:HD3	1.82	0.44
2:G:1965:TYR:HE1	2:G:2027:ILE:HB	1.82	0.44
2:G:3963:ASN:O	2:G:3966:THR:OG1	2.29	0.44
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.52	0.44
2:E:317:ARG:N	2:E:347:PHE:O	2.50	0.44
2:E:650:VAL:HB	2:E:777:PHE:HB2	1.98	0.44
2:E:1245:PHE:HE1	2:E:1600:LEU:HD23	1.82	0.44
2:E:2243:SER:HB3	2:E:2246:ASN:H	1.81	0.44
2:E:2908:TYR:OH	2:E:2920:ARG:NE	2.44	0.44
2:E:3974:THR:HA	2:E:3977:GLN:HB2	1.99	0.44
2:G:281:ARG:HA	2:G:312:THR:HG21	2.00	0.44
2:G:460:GLN:HG2	2:G:462:GLU:H	1.80	0.44
2:G:983:THR:O	2:G:987:ARG:N	2.48	0.44
2:G:1245:PHE:HE1	2:G:1600:LEU:HD23	1.82	0.44
2:G:1497:UNK:HA	2:G:1535:UNK:HA	1.99	0.44
2:G:2116:LEU:O	2:G:2120:MET:N	2.46	0.44
2:G:4169:SER:HA	2:G:4172:GLU:HB3	1.99	0.44
2:G:4558:ASN:HB2	2:G:4561:THR:HB	2.00	0.44
2:I:392:ARG:HH12	2:I:398:SER:HB2	1.83	0.44
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.99	0.44
2:I:2950:UNK:O	2:I:2954:UNK:N	2.50	0.44
2:B:264:PRO:HG2	2:B:270:SER:HB2	2.00	0.44
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	1.99	0.44
2:E:349:GLN:HA	2:E:356:TRP:HA	1.99	0.44
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.52	0.44
2:E:4560:TYR:O	2:E:4564:PHE:N	2.45	0.44
2:G:317:ARG:N	2:G:347:PHE:O	2.50	0.44
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.99	0.44
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.81	0.44
2:I:349:GLN:HA	2:I:356:TRP:HA	1.99	0.44
2:I:4041:ALA:HA	2:I:4044:MET:HB2	1.99	0.44
2:B:1965:TYR:HE1	2:B:2027:ILE:HB	1.82	0.44
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.83	0.44
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	2.00	0.44
2:E:1965:TYR:OH	2:E:2027:ILE:O	2.26	0.44
2:G:392:ARG:HH12	2:G:398:SER:HB2	1.83	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4568:PHE:HA	2:G:4571:PHE:HD2	1.83	0.44
2:G:4968:PHE:HE1	2:G:5029:ARG:HD3	1.83	0.44
2:I:684:VAL:HA	2:I:781:VAL:HA	1.99	0.44
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.99	0.44
2:I:4568:PHE:HA	2:I:4571:PHE:HD2	1.82	0.44
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.81	0.44
2:B:392:ARG:HH12	2:B:398:SER:HB2	1.83	0.44
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.50	0.44
2:B:1931:LEU:HD22	2:B:1935:VAL:HG11	2.00	0.44
2:B:2212:VAL:O	2:B:2216:GLY:N	2.46	0.44
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.50	0.44
2:E:3361:UNK:O	2:E:3365:UNK:N	2.51	0.44
2:E:4139:ILE:HA	2:E:4142:ASN:HD22	1.82	0.44
2:G:360:ALA:N	2:G:375:LYS:O	2.50	0.44
2:I:650:VAL:HB	2:I:777:PHE:HB2	1.98	0.44
2:I:1931:LEU:HD22	2:I:1935:VAL:HG11	2.00	0.44
2:I:4558:ASN:HB2	2:I:4561:THR:HB	2.00	0.44
2:B:4139:ILE:HA	2:B:4142:ASN:HD22	1.82	0.44
2:B:4990:PHE:O	2:B:4994:TYR:N	2.48	0.44
2:E:16:THR:OG1	2:E:97:GLY:O	2.35	0.44
2:E:392:ARG:HH12	2:E:398:SER:HB2	1.83	0.44
2:E:1976:ARG:NH1	2:E:1997:GLU:OE2	2.35	0.44
2:E:2142:TYR:CG	2:E:2197:LEU:HD13	2.53	0.44
2:G:978:THR:HB	2:G:980:ALA:H	1.83	0.44
2:G:3974:THR:HA	2:G:3977:GLN:HB2	1.99	0.44
2:I:264:PRO:HG2	2:I:270:SER:HB2	2.00	0.44
2:I:283:ARG:HH21	2:I:402:ARG:HH12	1.65	0.44
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.35	0.44
2:B:4059:LEU:O	2:B:4063:ASP:N	2.50	0.44
2:E:876:GLU:O	2:E:880:GLU:N	2.48	0.44
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.82	0.44
2:G:668:VAL:O	2:G:741:GLU:N	2.49	0.44
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.83	0.44
2:G:4745:LEU:O	2:G:4749:GLU:N	2.43	0.44
2:I:840:VAL:HB	2:I:1199:VAL:HG12	1.99	0.44
2:I:1965:TYR:HE1	2:I:2027:ILE:HB	1.82	0.44
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.99	0.44
2:B:1497:UNK:HA	2:B:1535:UNK:HA	2.00	0.44
2:B:3361:UNK:O	2:B:3365:UNK:N	2.50	0.44
2:E:38:ALA:HB1	2:E:64:ILE:HG13	1.99	0.44
2:E:668:VAL:O	2:E:741:GLU:N	2.49	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4044:MET:HA	2:E:4047:MET:HG2	1.98	0.44
2:G:533:ASN:HB3	2:G:536:ASN:HB2	2.00	0.44
2:G:838:HIS:CE1	2:G:1201:HIS:HD2	2.35	0.44
2:G:3361:UNK:O	2:G:3365:UNK:N	2.51	0.44
2:I:983:THR:O	2:I:987:ARG:N	2.48	0.44
2:I:1232:ARG:HD3	2:I:1702:HIS:HB3	2.00	0.44
2:B:283:ARG:HH21	2:B:402:ARG:HH12	1.65	0.44
2:B:840:VAL:HB	2:B:1199:VAL:HG12	1.99	0.44
2:B:1661:ARG:O	2:B:1664:SER:OG	2.32	0.44
2:B:3713:LYS:HG2	2:B:3715:LYS:H	1.83	0.44
2:B:4169:SER:HA	2:B:4172:GLU:HB3	1.99	0.44
2:B:4968:PHE:HE1	2:B:5029:ARG:HD3	1.83	0.44
2:E:385:ASP:OD1	2:E:385:ASP:N	2.48	0.44
2:E:1676:LEU:HD22	2:E:2167:ILE:HG13	2.00	0.44
2:E:1779:PRO:HG2	1:F:44:LYS:HE3	2.00	0.44
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.98	0.44
2:I:281:ARG:HA	2:I:312:THR:HG21	2.00	0.44
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.51	0.44
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.00	0.44
2:I:1676:LEU:HD22	2:I:2167:ILE:HG13	2.00	0.44
2:I:2142:TYR:CG	2:I:2197:LEU:HD13	2.53	0.44
2:B:635:THR:HB	2:B:1639:LEU:HD23	2.00	0.43
2:B:2142:TYR:CG	2:B:2197:LEU:HD13	2.53	0.43
2:E:177:GLU:HG3	2:G:2452:ARG:HH12	1.83	0.43
2:E:1577:ALA:HB1	2:E:1584:ARG:HA	2.00	0.43
2:E:4215:ARG:HA	2:E:4218:ILE:HD12	2.00	0.43
2:E:4942:GLU:O	2:E:4946:GLN:N	2.43	0.43
2:G:1232:ARG:HD3	2:G:1702:HIS:HB3	1.99	0.43
2:G:1286:UNK:HA	2:G:1461:UNK:HA	1.99	0.43
2:I:702:TRP:O	2:I:705:ASN:ND2	2.46	0.43
2:I:4139:ILE:HA	2:I:4142:ASN:HD22	1.82	0.43
2:B:213:TYR:CG	2:B:337:PRO:HB2	2.53	0.43
2:B:1294:UNK:HA	2:B:1455:UNK:HA	1.98	0.43
2:E:4568:PHE:HA	2:E:4571:PHE:HD2	1.83	0.43
2:G:113:HIS:CE1	2:G:399:GLN:HA	2.53	0.43
2:G:1577:ALA:HB1	2:G:1584:ARG:HA	2.01	0.43
2:I:655:GLY:HA2	2:I:1002:ALA:HB2	2.01	0.43
2:I:4989:MET:HE2	2:I:4989:MET:HB3	1.91	0.43
2:B:1738:LEU:H	2:B:2146:PRO:HD3	1.83	0.43
2:B:4918:ILE:HD13	2:E:4892:ARG:HD3	2.01	0.43
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:38:ALA:HB1	2:G:64:ILE:HG13	1.99	0.43
2:G:530:ILE:HA	2:G:536:ASN:HB3	2.00	0.43
2:G:914:PRO:O	2:G:918:ARG:N	2.46	0.43
2:G:3731:LYS:O	2:G:3735:LEU:N	2.50	0.43
2:I:113:HIS:CE1	2:I:399:GLN:HA	2.53	0.43
2:I:261:ARG:N	2:I:283:ARG:O	2.44	0.43
2:I:360:ALA:N	2:I:375:LYS:O	2.50	0.43
2:I:4059:LEU:O	2:I:4063:ASP:N	2.51	0.43
1:J:2:VAL:HG21	1:J:61:GLU:HB2	2.00	0.43
2:B:655:GLY:HA2	2:B:1002:ALA:HB2	2.01	0.43
2:B:831:ARG:HH21	2:B:840:VAL:HG11	1.84	0.43
2:B:3953:LYS:O	2:B:3956:SER:OG	2.29	0.43
2:B:4558:ASN:HB2	2:B:4561:THR:HB	1.99	0.43
2:B:4568:PHE:HA	2:B:4571:PHE:HD2	1.83	0.43
2:E:113:HIS:CE1	2:E:399:GLN:HA	2.53	0.43
2:E:3731:LYS:O	2:E:3735:LEU:N	2.50	0.43
2:E:4651:THR:HA	2:E:4799:SER:HB3	2.00	0.43
2:G:215:THR:HG22	2:G:273:HIS:HA	2.00	0.43
2:G:2142:TYR:CG	2:G:2197:LEU:HD13	2.53	0.43
2:G:4139:ILE:HA	2:G:4142:ASN:HD22	1.82	0.43
2:I:213:TYR:CG	2:I:337:PRO:HB2	2.53	0.43
2:I:658:GLN:O	2:I:662:TRP:NE1	2.51	0.43
2:I:1738:LEU:H	2:I:2146:PRO:HD3	1.83	0.43
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.00	0.43
2:B:733:PRO:HD2	2:B:763:PRO:HD2	2.00	0.43
2:B:1516:UNK:N	2:B:1529:UNK:O	2.51	0.43
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	2.01	0.43
2:E:281:ARG:HA	2:E:312:THR:HG21	2.00	0.43
2:E:978:THR:HB	2:E:980:ALA:H	1.83	0.43
2:E:1232:ARG:HD3	2:E:1702:HIS:HB3	1.99	0.43
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.83	0.43
2:G:264:PRO:HG2	2:G:270:SER:HB2	1.99	0.43
2:G:1738:LEU:H	2:G:2146:PRO:HD3	1.83	0.43
2:G:2869:ARG:HH12	2:G:2945:UNK:C	2.32	0.43
2:G:2880:GLU:O	2:G:2884:ASN:N	2.45	0.43
2:I:215:THR:HG22	2:I:273:HIS:HA	2.01	0.43
2:I:317:ARG:N	2:I:347:PHE:O	2.50	0.43
2:B:1232:ARG:HD3	2:B:1702:HIS:HB3	1.99	0.43
2:B:1577:ALA:HB1	2:B:1584:ARG:HA	2.01	0.43
2:B:4215:ARG:HA	2:B:4218:ILE:HD12	2.00	0.43
2:E:264:PRO:HG2	2:E:270:SER:HB2	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:635:THR:O	1:F:34:LYS:NZ	2.49	0.43
2:E:2286:LEU:HA	2:E:2289:ALA:HB3	2.01	0.43
2:E:4918:ILE:HD11	2:G:4888:TYR:HA	2.01	0.43
2:G:379:HIS:CD2	2:G:381:GLU:H	2.37	0.43
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.00	0.43
2:G:2155:LEU:HD23	2:G:2185:ILE:HG22	2.01	0.43
2:G:2286:LEU:HA	2:G:2289:ALA:HB3	2.01	0.43
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	2.01	0.43
2:I:545:ASP:HA	2:I:582:HIS:CE1	2.54	0.43
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.01	0.43
2:I:3713:LYS:HG2	2:I:3715:LYS:H	1.83	0.43
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.83	0.43
2:I:4169:SER:HA	2:I:4172:GLU:HB3	1.99	0.43
1:J:7:ILE:N	1:J:71:ARG:O	2.47	0.43
2:B:342:GLY:HA2	2:B:389:PHE:HD2	1.83	0.43
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.51	0.43
2:B:614:VAL:HG22	2:B:616:SER:H	1.84	0.43
2:B:1229:ASN:HB3	2:B:1826:ALA:HA	2.01	0.43
2:E:215:THR:HG22	2:E:273:HIS:HA	2.01	0.43
2:E:360:ALA:N	2:E:375:LYS:O	2.50	0.43
2:E:2155:LEU:HD23	2:E:2185:ILE:HG22	2.01	0.43
2:E:3676:ASP:OD1	2:E:3676:ASP:N	2.49	0.43
2:G:213:TYR:CG	2:G:337:PRO:HB2	2.53	0.43
2:G:313:SER:HB3	2:G:352:ALA:H	1.84	0.43
2:G:2185:ILE:HA	2:G:2188:ASN:HD21	1.84	0.43
2:G:3953:LYS:O	2:G:3956:SER:OG	2.29	0.43
2:G:4791:TYR:HD2	2:G:4792:LEU:HD22	1.84	0.43
2:G:4895:GLY:O	2:I:4892:ARG:NH2	2.50	0.43
2:I:38:ALA:HB1	2:I:64:ILE:HG13	1.99	0.43
2:I:831:ARG:HH21	2:I:840:VAL:HG11	1.84	0.43
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	2.01	0.43
2:B:2286:LEU:HA	2:B:2289:ALA:HB3	2.01	0.43
2:E:283:ARG:HH21	2:E:402:ARG:HH12	1.66	0.43
2:E:655:GLY:HA2	2:E:1002:ALA:HB2	2.01	0.43
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.50	0.43
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.00	0.43
2:G:5026:ASP:OD1	2:G:5027:CYS:N	2.52	0.43
2:I:530:ILE:HA	2:I:536:ASN:HB3	2.00	0.43
2:I:809:ALA:O	2:I:811:CYS:N	2.47	0.43
2:I:1229:ASN:HB3	2:I:1826:ALA:HA	2.01	0.43
2:I:1649:ASP:OD1	2:I:1650:ILE:N	2.52	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3974:THR:HA	2:I:3977:GLN:HB2	1.99	0.43
2:B:38:ALA:HB1	2:B:64:ILE:HG13	1.99	0.43
2:B:313:SER:HB3	2:B:352:ALA:H	1.84	0.43
2:B:530:ILE:HA	2:B:536:ASN:HB3	2.00	0.43
2:B:5026:ASP:OD1	2:B:5027:CYS:N	2.52	0.43
2:E:213:TYR:CG	2:E:337:PRO:HB2	2.53	0.43
2:E:313:SER:HB3	2:E:352:ALA:H	1.84	0.43
2:E:342:GLY:HA2	2:E:389:PHE:HD2	1.83	0.43
2:E:703:GLY:H	2:E:1647:CYS:HB3	1.84	0.43
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	2.01	0.43
2:E:4558:ASN:HB2	2:E:4561:THR:HB	2.00	0.43
2:G:342:GLY:HA2	2:G:389:PHE:HD2	1.83	0.43
2:G:635:THR:HB	2:G:1639:LEU:HD23	2.00	0.43
2:G:831:ARG:HH21	2:G:840:VAL:HG11	1.84	0.43
2:G:3713:LYS:HG2	2:G:3715:LYS:H	1.83	0.43
1:H:16:PRO:HD2	1:H:64:ALA:HA	2.01	0.43
2:I:1152:MET:HB2	2:I:1161:ILE:HB	2.01	0.43
2:I:1229:ASN:O	2:I:1827:ARG:N	2.42	0.43
2:I:1577:ALA:HB1	2:I:1584:ARG:HA	2.01	0.43
2:I:2286:LEU:HA	2:I:2289:ALA:HB3	2.01	0.43
1:J:16:PRO:HD2	1:J:64:ALA:HA	2.00	0.43
2:B:113:HIS:CE1	2:B:399:GLN:HA	2.53	0.43
2:B:281:ARG:HA	2:B:312:THR:HG21	2.00	0.43
2:B:978:THR:HB	2:B:980:ALA:H	1.83	0.43
2:B:2185:ILE:HA	2:B:2188:ASN:HD21	1.84	0.43
2:B:3974:THR:HA	2:B:3977:GLN:HB2	1.99	0.43
2:E:530:ILE:HA	2:E:536:ASN:HB3	1.99	0.43
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.99	0.43
2:E:635:THR:HB	2:E:1639:LEU:HD23	2.01	0.43
2:E:1738:LEU:H	2:E:2146:PRO:HD3	1.83	0.43
2:E:1931:LEU:HD22	2:E:1935:VAL:HG11	2.00	0.43
2:E:2880:GLU:O	2:E:2884:ASN:N	2.45	0.43
2:E:3805:LEU:H	2:E:3805:LEU:HG	1.61	0.43
2:E:4990:PHE:O	2:E:4994:TYR:N	2.48	0.43
2:E:4995:LEU:HA	2:E:4995:LEU:HD22	1.81	0.43
2:G:1676:LEU:HD22	2:G:2167:ILE:HG13	2.00	0.43
2:G:2006:ILE:O	2:G:2010:LEU:N	2.45	0.43
2:G:4651:THR:HA	2:G:4799:SER:HB3	2.00	0.43
2:G:4670:ILE:O	2:G:4674:GLU:N	2.44	0.43
1:H:2:VAL:HG21	1:H:61:GLU:HB2	2.00	0.43
2:I:313:SER:HB3	2:I:352:ALA:H	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1516:UNK:N	2:I:1529:UNK:O	2.52	0.43
2:I:3731:LYS:O	2:I:3735:LEU:N	2.50	0.43
2:I:3825:GLU:OE1	2:I:3825:GLU:N	2.52	0.43
2:I:4990:PHE:O	2:I:4994:TYR:N	2.48	0.43
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.39	0.43
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.01	0.42
2:E:545:ASP:HA	2:E:582:HIS:CE1	2.54	0.42
2:E:614:VAL:HG22	2:E:616:SER:H	1.84	0.42
2:E:831:ARG:HH21	2:E:840:VAL:HG11	1.84	0.42
2:E:1649:ASP:OD1	2:E:1650:ILE:N	2.52	0.42
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.01	0.42
2:E:3649:ALA:O	2:E:3653:PHE:N	2.48	0.42
1:F:83:GLY:O	1:F:94:ASN:N	2.52	0.42
2:G:283:ARG:HH21	2:G:402:ARG:HH12	1.65	0.42
2:G:545:ASP:HA	2:G:582:HIS:CE1	2.54	0.42
2:G:4215:ARG:HA	2:G:4218:ILE:HD12	2.00	0.42
2:I:342:GLY:HA2	2:I:389:PHE:HD2	1.83	0.42
2:I:703:GLY:H	2:I:1647:CYS:HB3	1.84	0.42
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.01	0.42
2:E:345:LEU:HD23	2:E:389:PHE:HB3	2.01	0.42
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.51	0.42
2:G:655:GLY:HA2	2:G:1002:ALA:HB2	2.01	0.42
2:G:733:PRO:HD2	2:G:763:PRO:HD2	2.00	0.42
2:I:379:HIS:CD2	2:I:381:GLU:H	2.37	0.42
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.01	0.42
2:I:947:GLU:HG3	2:I:1049:TYR:HD1	1.84	0.42
2:I:3361:UNK:O	2:I:3365:UNK:N	2.52	0.42
2:I:5026:ASP:OD1	2:I:5027:CYS:N	2.52	0.42
2:B:215:THR:HG22	2:B:273:HIS:HA	2.01	0.42
2:B:545:ASP:HA	2:B:582:HIS:CE1	2.54	0.42
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.00	0.42
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.01	0.42
2:G:1931:LEU:HD22	2:G:1935:VAL:HG11	1.99	0.42
2:G:3880:PHE:O	2:G:3884:LEU:N	2.52	0.42
2:I:614:VAL:HG22	2:I:616:SER:H	1.84	0.42
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.50	0.42
2:I:2185:ILE:HA	2:I:2188:ASN:HD21	1.84	0.42
2:I:3229:UNK:HA	2:I:3302:UNK:HA	2.02	0.42
2:B:260:TRP:CE2	2:B:284:HIS:HD2	2.38	0.42
2:B:533:ASN:HB3	2:B:536:ASN:HB2	2.00	0.42
2:B:703:GLY:H	2:B:1647:CYS:HB3	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:947:GLU:HG3	2:B:1049:TYR:HD1	1.85	0.42
2:B:1152:MET:HB2	2:B:1161:ILE:HB	2.01	0.42
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.83	0.42
2:B:3825:GLU:OE1	2:B:3825:GLU:N	2.52	0.42
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.01	0.42
2:E:733:PRO:HD2	2:E:763:PRO:HD2	2.00	0.42
2:E:3880:PHE:O	2:E:3884:LEU:N	2.52	0.42
2:E:4670:ILE:O	2:E:4674:GLU:N	2.44	0.42
2:E:4791:TYR:HD2	2:E:4792:LEU:HD22	1.84	0.42
2:G:703:GLY:H	2:G:1647:CYS:HB3	1.84	0.42
2:G:1649:ASP:OD1	2:G:1650:ILE:N	2.52	0.42
2:G:2212:VAL:O	2:G:2216:GLY:N	2.46	0.42
2:I:16:THR:OG1	2:I:97:GLY:O	2.35	0.42
2:I:533:ASN:HB3	2:I:536:ASN:HB2	2.00	0.42
2:I:733:PRO:HD2	2:I:763:PRO:HD2	2.00	0.42
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.87	0.42
2:I:4651:THR:HA	2:I:4799:SER:HB3	2.00	0.42
2:I:4791:TYR:HD2	2:I:4792:LEU:HD22	1.84	0.42
1:A:2:VAL:HG21	1:A:61:GLU:HB2	2.00	0.42
2:B:1649:ASP:OD1	2:B:1650:ILE:N	2.52	0.42
2:B:2144:ILE:H	2:B:2144:ILE:HG13	1.72	0.42
2:B:2155:LEU:HD23	2:B:2185:ILE:HG22	2.01	0.42
2:B:3880:PHE:O	2:B:3884:LEU:N	2.52	0.42
2:E:119:SER:HA	2:E:146:CYS:HA	2.01	0.42
2:E:379:HIS:CD2	2:E:381:GLU:H	2.37	0.42
2:E:3825:GLU:OE1	2:E:3825:GLU:N	2.52	0.42
1:F:2:VAL:HG21	1:F:61:GLU:HB2	2.00	0.42
1:F:55:VAL:HG23	1:F:60:GLU:HB2	2.02	0.42
2:G:614:VAL:HG22	2:G:616:SER:H	1.84	0.42
2:G:1771:LEU:HD11	2:G:2149:VAL:HB	2.01	0.42
2:I:260:TRP:CE2	2:I:284:HIS:HD2	2.38	0.42
2:I:873:LYS:HB3	2:I:1049:TYR:CZ	2.55	0.42
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.02	0.42
2:I:2155:LEU:HD23	2:I:2185:ILE:HG22	2.01	0.42
1:A:16:PRO:HD2	1:A:64:ALA:HA	2.00	0.42
2:B:1676:LEU:HD22	2:B:2167:ILE:HG13	2.00	0.42
2:B:4651:THR:HA	2:B:4799:SER:HB3	2.00	0.42
2:E:273:HIS:CE1	2:E:337:PRO:HB3	2.55	0.42
1:F:16:PRO:HD2	1:F:64:ALA:HA	2.00	0.42
2:G:3663:LEU:H	2:G:3663:LEU:HG	1.64	0.42
2:I:345:LEU:HD23	2:I:389:PHE:HB3	2.01	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1771:LEU:HD11	2:I:2149:VAL:HB	2.01	0.42
2:I:4960:ILE:HD12	2:I:4983:HIS:HB3	2.02	0.42
2:B:119:SER:HA	2:B:146:CYS:HA	2.01	0.42
2:B:345:LEU:HD23	2:B:389:PHE:HB3	2.01	0.42
2:B:3770:LEU:HD22	2:B:3804:ILE:HD11	2.01	0.42
2:B:4960:ILE:HD12	2:B:4983:HIS:HB3	2.02	0.42
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.02	0.42
2:E:1229:ASN:HB3	2:E:1826:ALA:HA	2.01	0.42
2:E:2185:ILE:HA	2:E:2188:ASN:HD21	1.84	0.42
2:E:3713:LYS:HG2	2:E:3715:LYS:H	1.83	0.42
2:G:345:LEU:HD23	2:G:389:PHE:HB3	2.01	0.42
2:G:1152:MET:HB2	2:G:1161:ILE:HB	2.01	0.42
1:H:7:ILE:N	1:H:71:ARG:O	2.47	0.42
1:H:83:GLY:O	1:H:94:ASN:N	2.52	0.42
2:I:4215:ARG:HA	2:I:4218:ILE:HD12	2.00	0.42
1:A:55:VAL:HG23	1:A:60:GLU:HB2	2.02	0.42
2:B:273:HIS:CE1	2:B:337:PRO:HB3	2.55	0.42
2:B:2318:TYR:HA	2:B:2319:PRO:HD3	1.87	0.42
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	2.02	0.42
2:E:260:TRP:CE2	2:E:284:HIS:HD2	2.38	0.42
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	2.02	0.42
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.02	0.42
2:G:1229:ASN:HB3	2:G:1826:ALA:HA	2.01	0.42
2:G:3770:LEU:HD22	2:G:3804:ILE:HD11	2.01	0.42
2:G:3825:GLU:OE1	2:G:3825:GLU:N	2.52	0.42
2:G:4692:PRO:HG2	2:G:4703:ARG:HH21	1.84	0.42
2:G:4852:THR:HG21	2:G:4883:TYR:HB2	2.02	0.42
2:I:102:LEU:HB3	2:I:160:GLY:HA2	2.02	0.42
2:I:241:GLN:O	2:I:289:ARG:NH1	2.42	0.42
2:B:379:HIS:CD2	2:B:381:GLU:H	2.37	0.42
2:B:1771:LEU:HD11	2:B:2149:VAL:HB	2.02	0.42
2:B:1976:ARG:NH1	2:B:1997:GLU:OE2	2.35	0.42
2:B:3963:ASN:O	2:B:3966:THR:OG1	2.29	0.42
2:E:533:ASN:HB3	2:E:536:ASN:HB2	2.00	0.42
2:E:1152:MET:HB2	2:E:1161:ILE:HB	2.01	0.42
2:E:1936:LYS:O	2:E:1940:CYS:N	2.48	0.42
2:E:4736:ARG:O	2:E:4740:LEU:N	2.53	0.42
2:E:4960:ILE:HD12	2:E:4983:HIS:HB3	2.02	0.42
2:E:5026:ASP:OD1	2:E:5027:CYS:N	2.52	0.42
2:G:349:GLN:HE21	2:G:354:GLY:HA2	1.85	0.42
2:G:873:LYS:HB3	2:G:1049:TYR:CZ	2.55	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1936:LYS:O	2:G:1940:CYS:N	2.48	0.42
2:G:4736:ARG:O	2:G:4740:LEU:N	2.53	0.42
2:B:3716:LEU:HD22	2:B:3785:ALA:HB1	2.02	0.42
2:B:3927:GLN:NE2	2:B:3988:ALA:O	2.46	0.42
2:B:4791:TYR:HD2	2:B:4792:LEU:HD22	1.84	0.42
2:E:488:LEU:HA	2:E:491:ILE:HB	2.02	0.42
2:E:947:GLU:HG3	2:E:1049:TYR:HD1	1.84	0.42
2:G:35:LEU:HD13	2:G:49:LEU:HD13	2.02	0.42
2:G:131:LEU:HD22	2:G:178:ARG:NH1	2.35	0.42
2:G:4859:PHE:HA	2:G:4862:PHE:CE2	2.47	0.42
2:G:4956:THR:O	2:G:4965:SER:N	2.52	0.42
2:I:273:HIS:CE1	2:I:337:PRO:HB3	2.55	0.42
2:I:349:GLN:HE21	2:I:354:GLY:HA2	1.84	0.42
1:A:83:GLY:O	1:A:94:ASN:N	2.52	0.41
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.02	0.41
2:B:102:LEU:HB3	2:B:160:GLY:HA2	2.02	0.41
2:B:110:ARG:NH2	2:B:115:ARG:HB3	2.35	0.41
2:B:873:LYS:HB3	2:B:1049:TYR:CZ	2.55	0.41
2:B:946:ALA:HA	2:B:949:ASN:HB2	2.02	0.41
2:B:1256:GLU:HG2	2:B:1273:ALA:HB3	2.02	0.41
2:B:3766:GLN:O	2:B:3770:LEU:N	2.50	0.41
2:B:3773:ARG:HG2	2:B:3815:LYS:HD3	2.03	0.41
2:B:4167:ALA:HA	2:B:4170:ILE:HD12	2.02	0.41
2:E:261:ARG:N	2:E:283:ARG:O	2.44	0.41
2:E:658:GLN:O	2:E:662:TRP:NE1	2.51	0.41
2:E:3716:LEU:HD22	2:E:3785:ALA:HB1	2.02	0.41
2:E:3770:LEU:HD22	2:E:3804:ILE:HD11	2.01	0.41
2:E:4167:ALA:HA	2:E:4170:ILE:HD12	2.02	0.41
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.02	0.41
2:G:260:TRP:CE2	2:G:284:HIS:HD2	2.38	0.41
2:G:273:HIS:CE1	2:G:337:PRO:HB3	2.55	0.41
2:G:488:LEU:HA	2:G:491:ILE:HB	2.02	0.41
2:G:947:GLU:HG3	2:G:1049:TYR:HD1	1.84	0.41
2:G:1661:ARG:O	2:G:1664:SER:OG	2.32	0.41
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	2.02	0.41
2:G:4960:ILE:HD12	2:G:4983:HIS:HB3	2.02	0.41
2:I:110:ARG:NH2	2:I:115:ARG:HB3	2.35	0.41
2:I:978:THR:HB	2:I:980:ALA:H	1.83	0.41
2:I:3880:PHE:O	2:I:3884:LEU:N	2.52	0.41
1:J:83:GLY:O	1:J:94:ASN:N	2.52	0.41
1:A:34:LYS:NZ	2:B:634:GLN:HB3	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:LEU:HD12	2:B:299:LEU:HA	1.89	0.41
2:B:1268:PRO:HB2	2:B:1591:CYS:HB2	2.03	0.41
2:E:639:ASN:HD22	2:E:1635:THR:HA	1.85	0.41
2:E:873:LYS:HB3	2:E:1049:TYR:CZ	2.55	0.41
2:E:1771:LEU:HD11	2:E:2149:VAL:HB	2.02	0.41
2:E:3901:ASN:OD1	2:E:3904:ARG:NH1	2.49	0.41
2:I:488:LEU:HA	2:I:491:ILE:HB	2.02	0.41
2:I:639:ASN:HD22	2:I:1635:THR:HA	1.85	0.41
2:I:1679:ASN:O	2:I:1683:HIS:ND1	2.36	0.41
2:I:3770:LEU:HD22	2:I:3804:ILE:HD11	2.01	0.41
2:I:4692:PRO:HG2	2:I:4703:ARG:HH21	1.84	0.41
2:I:4852:THR:HG21	2:I:4883:TYR:HB2	2.02	0.41
2:B:1041:GLN:O	2:B:1045:THR:OG1	2.30	0.41
2:E:131:LEU:HB3	2:G:2459:SER:HB2	2.01	0.41
2:E:3963:ASN:O	2:E:3966:THR:OG1	2.29	0.41
2:G:639:ASN:HD22	2:G:1635:THR:HA	1.85	0.41
2:G:658:GLN:O	2:G:662:TRP:NE1	2.51	0.41
2:G:3646:THR:O	2:G:3650:CYS:N	2.51	0.41
2:G:3716:LEU:HD22	2:G:3785:ALA:HB1	2.02	0.41
2:G:3756:LYS:O	2:G:3760:LYS:NZ	2.37	0.41
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.02	0.41
2:I:635:THR:HB	2:I:1639:LEU:HD23	2.00	0.41
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.02	0.41
2:I:1268:PRO:HB2	2:I:1591:CYS:HB2	2.03	0.41
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	2.02	0.41
2:I:3964:SER:HG	2:I:3968:TYR:HH	1.67	0.41
1:J:55:VAL:HG23	1:J:60:GLU:HB2	2.02	0.41
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.39	0.41
2:B:728:ARG:NH2	2:B:1527:UNK:O	2.53	0.41
2:B:3915:ILE:H	2:B:3915:ILE:HG13	1.63	0.41
2:B:4692:PRO:HG2	2:B:4703:ARG:HH21	1.84	0.41
2:B:4736:ARG:O	2:B:4740:LEU:N	2.53	0.41
2:B:4801:LEU:HB3	2:B:4808:PHE:CG	2.56	0.41
2:E:78:LEU:O	2:E:82:LEU:N	2.44	0.41
2:E:241:GLN:O	2:E:289:ARG:NH1	2.42	0.41
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.02	0.41
2:G:2265:LEU:HD21	2:G:2273:LEU:HD13	2.02	0.41
2:G:3927:GLN:NE2	2:G:3988:ALA:O	2.46	0.41
2:I:1256:GLU:HG2	2:I:1273:ALA:HB3	2.02	0.41
2:B:131:LEU:HD22	2:B:178:ARG:NH1	2.35	0.41
2:B:639:ASN:HD22	2:B:1635:THR:HA	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.02	0.41
2:B:4195:PHE:HZ	2:B:4987:ASN:HB3	1.86	0.41
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.02	0.41
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.02	0.41
2:E:3645:PRO:O	2:E:3649:ALA:N	2.53	0.41
2:E:4692:PRO:HG2	2:E:4703:ARG:HH21	1.84	0.41
2:E:4801:LEU:HB3	2:E:4808:PHE:CG	2.56	0.41
2:G:119:SER:HA	2:G:146:CYS:HA	2.01	0.41
2:G:3229:UNK:HA	2:G:3302:UNK:HA	2.02	0.41
1:H:55:VAL:HG23	1:H:60:GLU:HB2	2.02	0.41
2:I:914:PRO:O	2:I:918:ARG:N	2.46	0.41
2:I:3773:ARG:HG2	2:I:3815:LYS:HD3	2.02	0.41
2:B:349:GLN:HE21	2:B:354:GLY:HA2	1.85	0.41
2:B:4707:ASN:OD1	2:B:4742:GLY:N	2.49	0.41
2:B:4822:THR:O	2:B:4825:THR:OG1	2.30	0.41
2:B:4957:LYS:HE3	2:B:4957:LYS:HB3	1.83	0.41
2:E:131:LEU:HD22	2:E:178:ARG:NH1	2.35	0.41
2:E:1497:UNK:HA	2:E:1535:UNK:HA	2.02	0.41
2:G:110:ARG:NH2	2:G:115:ARG:HB3	2.35	0.41
2:G:1256:GLU:HG2	2:G:1273:ALA:HB3	2.02	0.41
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	2.02	0.41
2:G:2908:TYR:OH	2:G:2920:ARG:NE	2.44	0.41
2:I:876:GLU:O	2:I:880:GLU:N	2.48	0.41
2:B:1088:TRP:HB2	2:B:1153:ILE:HG22	2.03	0.41
2:B:3649:ALA:O	2:B:3653:PHE:N	2.48	0.41
2:E:110:ARG:NH2	2:E:115:ARG:HB3	2.35	0.41
2:E:1116:GLY:HA3	2:E:1123:VAL:HG12	2.02	0.41
2:E:1270:LEU:HD11	2:E:1595:LEU:HB3	2.03	0.41
2:G:16:THR:OG1	2:G:97:GLY:O	2.35	0.41
2:G:946:ALA:HA	2:G:949:ASN:HB2	2.02	0.41
2:G:4990:PHE:O	2:G:4994:TYR:N	2.48	0.41
2:B:805:PRO:HA	2:B:806:PRO:HD3	1.95	0.41
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	2.03	0.41
2:E:34:LYS:N	2:E:53:SER:OG	2.43	0.41
2:E:308:HIS:CE1	2:E:310:LYS:HB2	2.56	0.41
2:E:349:GLN:HE21	2:E:354:GLY:HA2	1.85	0.41
2:E:2144:ILE:H	2:E:2144:ILE:HG13	1.72	0.41
2:E:3773:ARG:HG2	2:E:3815:LYS:HD3	2.03	0.41
2:E:4195:PHE:HZ	2:E:4987:ASN:HB3	1.86	0.41
2:E:4847:VAL:HG11	2:E:4924:VAL:HG11	2.03	0.41
2:G:102:LEU:HB3	2:G:160:GLY:HA2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:805:PRO:HA	2:G:806:PRO:HD3	1.94	0.41
2:G:1088:TRP:HB2	2:G:1153:ILE:HG22	2.03	0.41
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	2.03	0.41
2:G:3921:ASP:HA	2:G:3924:LEU:HB3	2.03	0.41
2:G:4847:VAL:HG11	2:G:4924:VAL:HG11	2.03	0.41
2:I:119:SER:HA	2:I:146:CYS:HA	2.01	0.41
2:I:3915:ILE:H	2:I:3915:ILE:HG13	1.63	0.41
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	2.03	0.41
2:B:17:ASP:HB2	2:B:98:HIS:CE1	2.55	0.41
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.02	0.41
2:B:1116:GLY:HA3	2:B:1123:VAL:HG12	2.02	0.41
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.39	0.41
2:B:2265:LEU:HD21	2:B:2273:LEU:HD13	2.02	0.41
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.54	0.41
2:B:3153:UNK:O	2:B:3157:UNK:N	2.54	0.41
2:B:3921:ASP:HA	2:B:3924:LEU:HB3	2.03	0.41
2:B:4852:THR:HG21	2:B:4883:TYR:HB2	2.02	0.41
2:E:259:LEU:HA	2:E:259:LEU:HD23	1.87	0.41
2:E:913:LEU:O	2:E:918:ARG:NH2	2.54	0.41
2:E:1088:TRP:HB2	2:E:1153:ILE:HG22	2.03	0.41
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	2.03	0.41
2:E:3229:UNK:HA	2:E:3302:UNK:HA	2.02	0.41
2:E:3663:LEU:H	2:E:3663:LEU:HG	1.64	0.41
2:E:4958:CYS:SG	2:E:4959:PHE:N	2.94	0.41
2:G:259:LEU:HD23	2:G:259:LEU:HA	1.87	0.41
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.02	0.41
2:G:1116:GLY:HA3	2:G:1123:VAL:HG12	2.02	0.41
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.02	0.41
2:G:3773:ARG:HG2	2:G:3815:LYS:HD3	2.03	0.41
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	2.03	0.41
2:G:4957:LYS:HE3	2:G:4957:LYS:HB3	1.83	0.41
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.54	0.41
2:I:728:ARG:NH2	2:I:1527:UNK:O	2.54	0.41
2:I:946:ALA:HA	2:I:949:ASN:HB2	2.02	0.41
2:I:1088:TRP:HB2	2:I:1153:ILE:HG22	2.03	0.41
2:I:1116:GLY:HA3	2:I:1123:VAL:HG12	2.02	0.41
2:I:1497:UNK:HA	2:I:1535:UNK:HA	2.02	0.41
2:I:2116:LEU:O	2:I:2120:MET:N	2.46	0.41
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.39	0.41
2:I:2265:LEU:HD21	2:I:2273:LEU:HD13	2.02	0.41
2:I:2384:ILE:O	2:I:2388:GLU:N	2.54	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3663:LEU:H	2:I:3663:LEU:HG	1.64	0.41
2:I:3716:LEU:HD22	2:I:3785:ALA:HB1	2.02	0.41
2:I:4167:ALA:HA	2:I:4170:ILE:HD12	2.02	0.41
2:I:4195:PHE:HZ	2:I:4987:ASN:HB3	1.86	0.41
2:I:4707:ASN:OD1	2:I:4742:GLY:N	2.49	0.41
2:I:4736:ARG:O	2:I:4740:LEU:N	2.53	0.41
2:I:4847:VAL:HG11	2:I:4924:VAL:HG11	2.03	0.41
2:I:4957:LYS:HB3	2:I:4957:LYS:HE3	1.83	0.41
2:I:5013:MET:HA	2:I:5016:GLU:HB3	2.03	0.41
2:B:308:HIS:CE1	2:B:310:LYS:HB2	2.56	0.41
2:B:1092:PHE:HE2	2:B:1094:ALA:HB2	1.85	0.41
2:B:1936:LYS:O	2:B:1940:CYS:N	2.48	0.41
2:B:2116:LEU:O	2:B:2120:MET:N	2.46	0.41
2:B:2517:UNK:O	2:B:2521:UNK:N	2.54	0.41
2:B:4191:GLU:OE1	2:B:5006:GLN:NE2	2.54	0.41
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.03	0.41
2:B:4958:CYS:SG	2:B:4959:PHE:N	2.94	0.41
2:B:5013:MET:HA	2:B:5016:GLU:HB3	2.03	0.41
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.02	0.41
2:E:1256:GLU:HG2	2:E:1273:ALA:HB3	2.02	0.41
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	2.03	0.41
2:E:4191:GLU:OE1	2:E:5006:GLN:NE2	2.54	0.41
1:F:7:ILE:N	1:F:71:ARG:O	2.47	0.41
2:G:1270:LEU:HD11	2:G:1595:LEU:HB3	2.03	0.41
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.54	0.41
2:G:4191:GLU:OE1	2:G:5006:GLN:NE2	2.54	0.41
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.41
2:I:131:LEU:HD22	2:I:178:ARG:NH1	2.35	0.41
2:I:308:HIS:CE1	2:I:310:LYS:HB2	2.56	0.41
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	2.03	0.41
2:I:3362:UNK:O	2:I:3366:UNK:N	2.54	0.41
2:I:4191:GLU:OE1	2:I:5006:GLN:NE2	2.54	0.41
2:I:4204:GLN:NE2	2:I:4245:MET:SD	2.94	0.41
2:I:4569:LEU:HD11	2:I:4646:LEU:HD22	2.03	0.41
2:I:4801:LEU:HB3	2:I:4808:PHE:CG	2.56	0.41
2:B:488:LEU:HA	2:B:491:ILE:HB	2.02	0.40
2:B:4091:LYS:HD3	2:B:4091:LYS:HA	1.90	0.40
2:B:4581:LYS:HD2	2:B:4632:LEU:HD13	2.04	0.40
2:E:17:ASP:HB2	2:E:98:HIS:CE1	2.55	0.40
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.54	0.40
2:E:3645:PRO:HB2	2:E:3648:ARG:HB3	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.56	0.40
2:E:3921:ASP:HA	2:E:3924:LEU:HB3	2.03	0.40
2:E:3953:LYS:O	2:E:3956:SER:OG	2.29	0.40
2:E:4138:ASP:O	2:E:4142:ASN:ND2	2.54	0.40
2:E:4852:THR:HG21	2:E:4883:TYR:HB2	2.02	0.40
2:G:414:PHE:HE1	2:G:436:LEU:HB3	1.86	0.40
2:G:4569:LEU:HD11	2:G:4646:LEU:HD22	2.03	0.40
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.02	0.40
2:I:4930:ALA:HA	2:I:4933:GLN:HB3	2.03	0.40
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.40
2:B:2006:ILE:O	2:B:2010:LEU:N	2.45	0.40
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.54	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.40
2:B:3645:PRO:HB2	2:B:3648:ARG:HB3	2.03	0.40
2:E:320:LYS:HG2	2:E:356:TRP:CD1	2.57	0.40
2:E:627:PRO:HB2	1:F:92:PRO:HD3	2.04	0.40
2:E:836:GLY:HA3	2:E:1201:HIS:ND1	2.37	0.40
2:E:1693:GLN:HA	2:E:1696:HIS:HB3	2.04	0.40
2:E:2255:SER:HA	2:E:2258:LEU:HB3	2.04	0.40
2:E:4837:LEU:HD11	2:E:4936:ILE:HD11	2.03	0.40
2:G:1092:PHE:HE2	2:G:1094:ALA:HB2	1.85	0.40
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.39	0.40
2:G:3771:HIS:O	2:G:3774:GLY:N	2.52	0.40
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.02	0.40
2:I:2810:LYS:O	2:I:2814:LYS:N	2.52	0.40
2:B:414:PHE:HE1	2:B:436:LEU:HB3	1.86	0.40
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.54	0.40
2:B:688:LEU:HB3	2:B:777:PHE:CE1	2.57	0.40
2:B:1270:LEU:HD11	2:B:1595:LEU:HB3	2.03	0.40
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	2.03	0.40
2:B:4847:VAL:HG11	2:B:4924:VAL:HG11	2.03	0.40
2:B:4875:LYS:HA	2:B:4881:THR:HG22	2.03	0.40
2:E:946:ALA:HA	2:E:949:ASN:HB2	2.02	0.40
2:E:1092:PHE:HE2	2:E:1094:ALA:HB2	1.85	0.40
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.39	0.40
2:E:2318:TYR:HA	2:E:2319:PRO:HD3	1.88	0.40
2:E:3921:ASP:O	2:E:3925:ARG:N	2.51	0.40
2:E:4114:CYS:HB3	2:E:4131:ARG:HH22	1.86	0.40
2:G:149:THR:N	2:G:172:VAL:O	2.55	0.40
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.54	0.40
2:G:913:LEU:O	2:G:918:ARG:NH2	2.54	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2023:LEU:O	2:G:2025:GLU:N	2.54	0.40
2:G:2384:ILE:O	2:G:2388:GLU:N	2.54	0.40
2:G:2674:UNK:O	2:G:2676:UNK:N	2.55	0.40
2:G:4138:ASP:O	2:G:4142:ASN:ND2	2.55	0.40
2:G:4801:LEU:HB3	2:G:4808:PHE:CG	2.56	0.40
2:G:5013:MET:HA	2:G:5016:GLU:HB3	2.03	0.40
2:I:414:PHE:HE1	2:I:436:LEU:HB3	1.86	0.40
2:I:716:PHE:HE2	2:I:759:ILE:HD11	1.86	0.40
2:I:1092:PHE:HE2	2:I:1094:ALA:HB2	1.85	0.40
2:I:1270:LEU:HD11	2:I:1595:LEU:HB3	2.03	0.40
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	2.04	0.40
2:I:3766:GLN:O	2:I:3770:LEU:N	2.50	0.40
2:I:3832:ILE:O	2:I:3836:MET:N	2.45	0.40
2:I:3921:ASP:HA	2:I:3924:LEU:HB3	2.03	0.40
2:B:221:ARG:NH2	2:B:255:HIS:O	2.55	0.40
2:B:360:ALA:N	2:B:375:LYS:O	2.50	0.40
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.02	0.40
2:B:4850:LEU:HD22	2:E:4814:LEU:HD21	2.03	0.40
2:E:102:LEU:HB3	2:E:160:GLY:HA2	2.02	0.40
2:E:688:LEU:HB3	2:E:777:PHE:CE1	2.57	0.40
2:E:776:LEU:HG	2:E:848:HIS:HA	2.04	0.40
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.54	0.40
2:E:3363:UNK:O	2:E:3367:UNK:N	2.55	0.40
2:E:3915:ILE:H	2:E:3915:ILE:HG13	1.63	0.40
2:E:4956:THR:O	2:E:4965:SER:N	2.52	0.40
2:G:308:HIS:CE1	2:G:310:LYS:HB2	2.56	0.40
2:G:716:PHE:HE2	2:G:759:ILE:HD11	1.86	0.40
2:G:836:GLY:HA3	2:G:1201:HIS:ND1	2.37	0.40
2:G:1268:PRO:HB2	2:G:1591:CYS:HB2	2.03	0.40
2:G:1294:UNK:HA	2:G:1455:UNK:HA	2.03	0.40
2:G:4195:PHE:HZ	2:G:4987:ASN:HB3	1.86	0.40
2:G:4204:GLN:NE2	2:G:4245:MET:SD	2.94	0.40
2:I:913:LEU:O	2:I:918:ARG:NH2	2.54	0.40
2:I:2674:UNK:O	2:I:2676:UNK:N	2.55	0.40
2:I:4138:ASP:O	2:I:4142:ASN:ND2	2.55	0.40
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.02	0.40
2:B:716:PHE:HE2	2:B:759:ILE:HD11	1.86	0.40
2:E:1268:PRO:HB2	2:E:1591:CYS:HB2	2.03	0.40
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	2.03	0.40
2:E:2265:LEU:HD21	2:E:2273:LEU:HD13	2.02	0.40
2:G:151:HIS:HB2	2:G:170:ILE:HB	2.04	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:663:TYR:HB2	2:G:808:TYR:HB3	2.04	0.40
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.54	0.40
2:G:2255:SER:HA	2:G:2258:LEU:HB3	2.04	0.40
2:G:4167:ALA:HA	2:G:4170:ILE:HD12	2.02	0.40
2:I:4236:SER:O	2:I:4240:ASP:N	2.45	0.40
2:I:4978:HIS:O	2:I:4983:HIS:N	2.47	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	F	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	H	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	J	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4687 (69%)	2848 (88%)	382 (12%)	5 (0%)	47	81
2	E	3235/4687 (69%)	2849 (88%)	381 (12%)	5 (0%)	47	81
2	G	3235/4687 (69%)	2848 (88%)	382 (12%)	5 (0%)	47	81
2	I	3235/4687 (69%)	2850 (88%)	380 (12%)	5 (0%)	47	81
All	All	13360/19176 (70%)	11775 (88%)	1565 (12%)	20 (0%)	54	85

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	I	1708	ARG

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1932	PRO
2	E	1932	PRO
2	G	1932	PRO
2	I	1932	PRO
2	B	4667	PRO
2	E	4667	PRO
2	G	4667	PRO
2	I	4667	PRO
2	B	1840	PRO
2	E	1840	PRO
2	G	1840	PRO
2	I	1840	PRO
2	B	4641	PRO
2	E	4641	PRO
2	G	4641	PRO
2	I	4641	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	88/88 (100%)	88 (100%)	0	100	100
1	F	88/88 (100%)	88 (100%)	0	100	100
1	H	88/88 (100%)	88 (100%)	0	100	100
1	J	88/88 (100%)	88 (100%)	0	100	100
2	B	2493/3209 (78%)	2473 (99%)	20 (1%)	81	89
2	E	2493/3209 (78%)	2473 (99%)	20 (1%)	81	89
2	G	2493/3209 (78%)	2472 (99%)	21 (1%)	81	89
2	I	2493/3209 (78%)	2473 (99%)	20 (1%)	81	89
All	All	10324/13188 (78%)	10243 (99%)	81 (1%)	82	89

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	534	ARG
2	B	553	ARG
2	B	688	LEU
2	B	1076	ARG
2	B	1141	ARG
2	B	1964	ARG
2	B	3663	LEU
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4137	ARG
2	B	4798	MET
2	B	4871	GLU
2	B	4913	ARG
2	B	4957	LYS
2	B	4984	ASN
2	B	4995	LEU
2	E	534	ARG
2	E	553	ARG
2	E	688	LEU
2	E	1076	ARG
2	E	1141	ARG
2	E	1964	ARG
2	E	3663	LEU
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4137	ARG
2	E	4798	MET
2	E	4871	GLU
2	E	4913	ARG
2	E	4957	LYS
2	E	4984	ASN
2	E	4995	LEU
2	G	534	ARG
2	G	553	ARG
2	G	688	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1964	ARG
2	G	3663	LEU
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4137	ARG
2	G	4798	MET
2	G	4871	GLU
2	G	4913	ARG
2	G	4957	LYS
2	G	4984	ASN
2	G	4995	LEU
2	I	534	ARG
2	I	553	ARG
2	I	688	LEU
2	I	1076	ARG
2	I	1141	ARG
2	I	1964	ARG
2	I	3663	LEU
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4137	ARG
2	I	4798	MET
2	I	4871	GLU
2	I	4913	ARG
2	I	4957	LYS
2	I	4984	ASN
2	I	4995	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (164) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
2	B	57	ASN
2	B	111	HIS
2	B	151	HIS
2	B	218	HIS
2	B	224	HIS
2	B	273	HIS
2	B	308	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	405	HIS
2	B	479	GLN
2	B	495	ASN
2	B	838	HIS
2	B	1035	ASN
2	B	1158	ASN
2	B	1231	GLN
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1941	ASN
2	B	1973	GLN
2	B	2005	GLN
2	B	2127	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3963	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4142	ASN
2	B	4728	HIS
2	B	4886	HIS
2	B	4984	ASN
2	B	4987	ASN
2	B	5003	HIS
2	E	57	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	111	HIS
2	E	151	HIS
2	E	218	HIS
2	E	224	HIS
2	E	273	HIS
2	E	308	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	405	HIS
2	E	479	GLN
2	E	495	ASN
2	E	838	HIS
2	E	1035	ASN
2	E	1158	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1941	ASN
2	E	1973	GLN
2	E	2005	GLN
2	E	2127	GLN
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3963	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4142	ASN
2	E	4728	HIS
2	E	4886	HIS
2	E	4984	ASN
2	E	4987	ASN
2	E	5003	HIS
1	F	25	HIS
2	G	57	ASN
2	G	111	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	113	HIS
2	G	218	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	405	HIS
2	G	479	GLN
2	G	495	ASN
2	G	838	HIS
2	G	1035	ASN
2	G	1158	ASN
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1941	ASN
2	G	1973	GLN
2	G	2005	GLN
2	G	2127	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4142	ASN
2	G	4728	HIS
2	G	4886	HIS
2	G	4984	ASN
2	G	4987	ASN
2	G	5003	HIS
1	H	25	HIS
2	I	57	ASN
2	I	111	HIS
2	I	151	HIS
2	I	218	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	I	224	HIS
2	I	273	HIS
2	I	308	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	405	HIS
2	I	479	GLN
2	I	495	ASN
2	I	838	HIS
2	I	1035	ASN
2	I	1158	ASN
2	I	1231	GLN
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1941	ASN
2	I	1973	GLN
2	I	2005	GLN
2	I	2127	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3963	ASN
2	I	4120	ASN
2	I	4130	ASN
2	I	4142	ASN
2	I	4728	HIS
2	I	4886	HIS
2	I	4984	ASN
2	I	4987	ASN
2	I	5003	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	12
2	I	12
2	E	12
2	G	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	44.41
1	I	3613:UNK	C	3639:THR	N	44.36
1	E	3613:UNK	C	3639:THR	N	44.35
1	G	3613:UNK	C	3639:THR	N	44.35

*Continued on next page...*



*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3163:UNK	C	3170:UNK	N	16.42
1	E	3163:UNK	C	3170:UNK	N	16.36
1	G	3163:UNK	C	3170:UNK	N	16.35
1	I	3163:UNK	C	3170:UNK	N	16.29
1	G	3468:UNK	C	3511:UNK	N	14.86
1	E	3468:UNK	C	3511:UNK	N	14.84
1	I	3468:UNK	C	3511:UNK	N	14.84
1	B	3468:UNK	C	3511:UNK	N	14.79
1	I	3063:UNK	C	3134:UNK	N	14.53
1	G	3063:UNK	C	3134:UNK	N	14.50
1	G	2703:UNK	C	2734:ASN	N	14.49
1	E	3063:UNK	C	3134:UNK	N	14.48
1	I	2703:UNK	C	2734:ASN	N	14.48
1	B	3063:UNK	C	3134:UNK	N	14.46
1	B	2703:UNK	C	2734:ASN	N	14.44
1	E	2703:UNK	C	2734:ASN	N	14.34
1	B	3236:UNK	C	3241:UNK	N	13.22
1	G	3236:UNK	C	3241:UNK	N	13.20
1	E	3236:UNK	C	3241:UNK	N	13.17
1	I	3236:UNK	C	3241:UNK	N	13.16
1	I	1564:UNK	C	1573:MET	N	12.84
1	B	1564:UNK	C	1573:MET	N	12.82
1	E	1564:UNK	C	1573:MET	N	12.72
1	G	1564:UNK	C	1573:MET	N	12.61
1	B	2976:UNK	C	2995:UNK	N	12.18
1	E	2976:UNK	C	2995:UNK	N	12.15
1	I	2976:UNK	C	2995:UNK	N	12.07
1	G	2976:UNK	C	2995:UNK	N	12.06
1	G	3254:UNK	C	3261:UNK	N	8.57
1	I	3254:UNK	C	3261:UNK	N	8.57
1	B	3254:UNK	C	3261:UNK	N	8.56
1	E	3254:UNK	C	3261:UNK	N	8.53
1	E	1297:UNK	C	1430:UNK	N	5.79
1	I	1297:UNK	C	1430:UNK	N	5.74
1	G	1297:UNK	C	1430:UNK	N	5.65
1	B	1297:UNK	C	1430:UNK	N	5.48
1	B	2479:LEU	C	2487:UNK	N	3.92
1	E	2479:LEU	C	2487:UNK	N	3.92
1	I	2479:LEU	C	2487:UNK	N	3.89
1	G	2479:LEU	C	2487:UNK	N	3.81
1	G	2939:ARG	C	2942:UNK	N	3.63
1	I	2939:ARG	C	2942:UNK	N	3.56

*Continued on next page...*

*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2939:ARG	C	2942:UNK	N	3.53
1	E	2939:ARG	C	2942:UNK	N	3.53

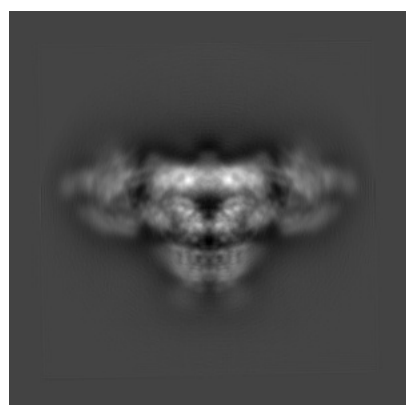
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22394. These allow visual inspection of the internal detail of the map and identification of artifacts.

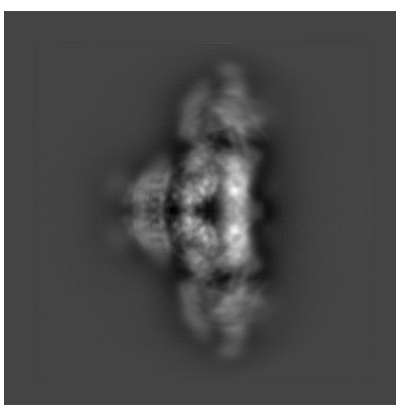
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

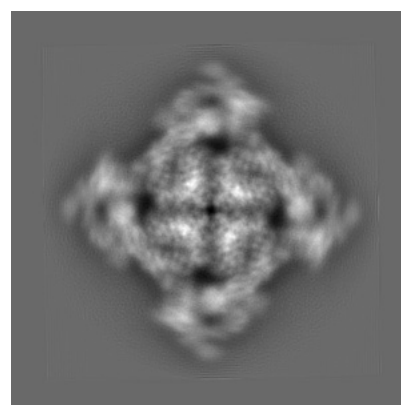
#### 6.1.1 Primary map



X



Y

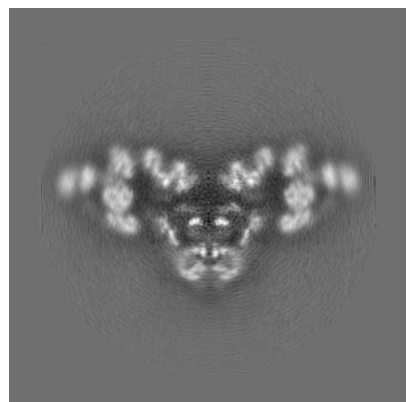


Z

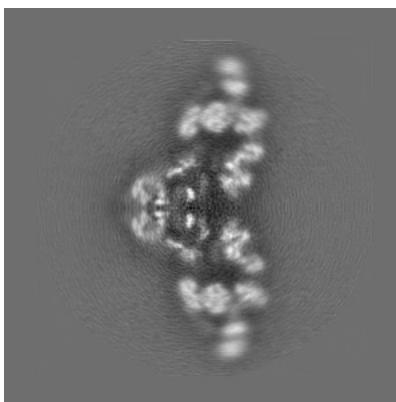
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

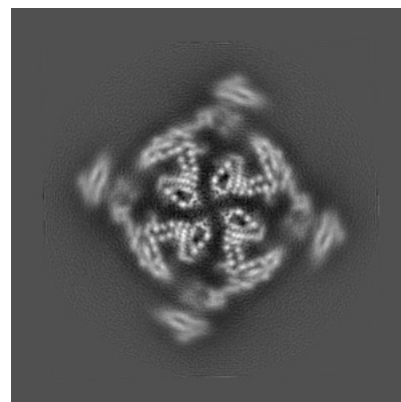
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

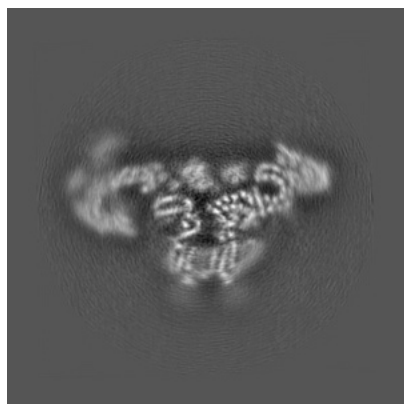


Z Index: 200

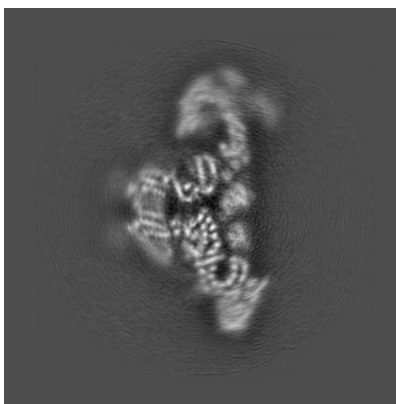
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

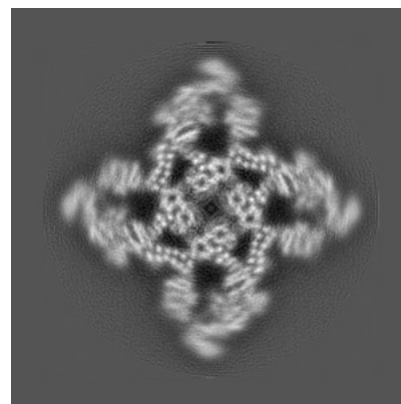
### 6.3.1 Primary map



X Index: 177



Y Index: 177



Z Index: 227

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

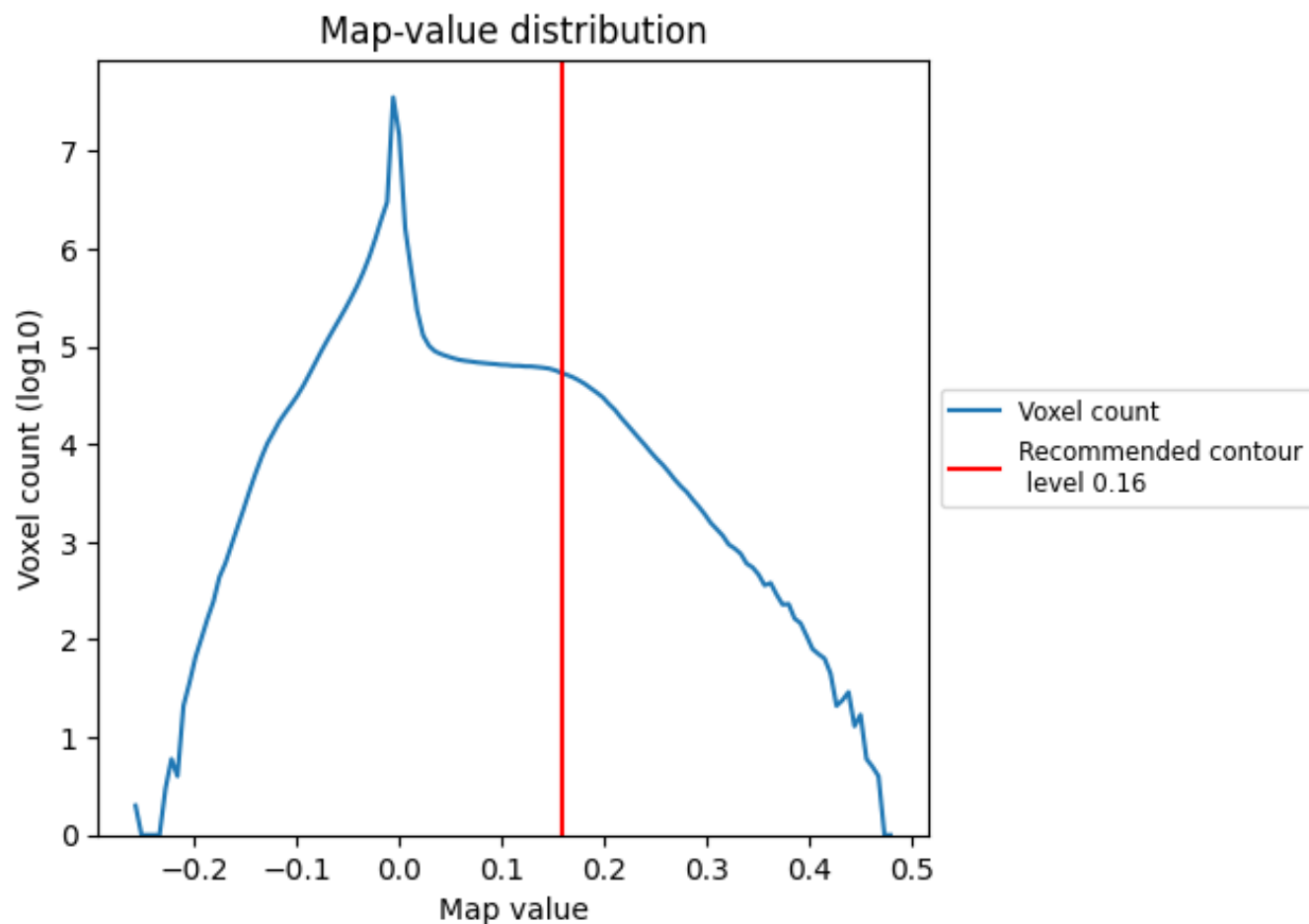
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

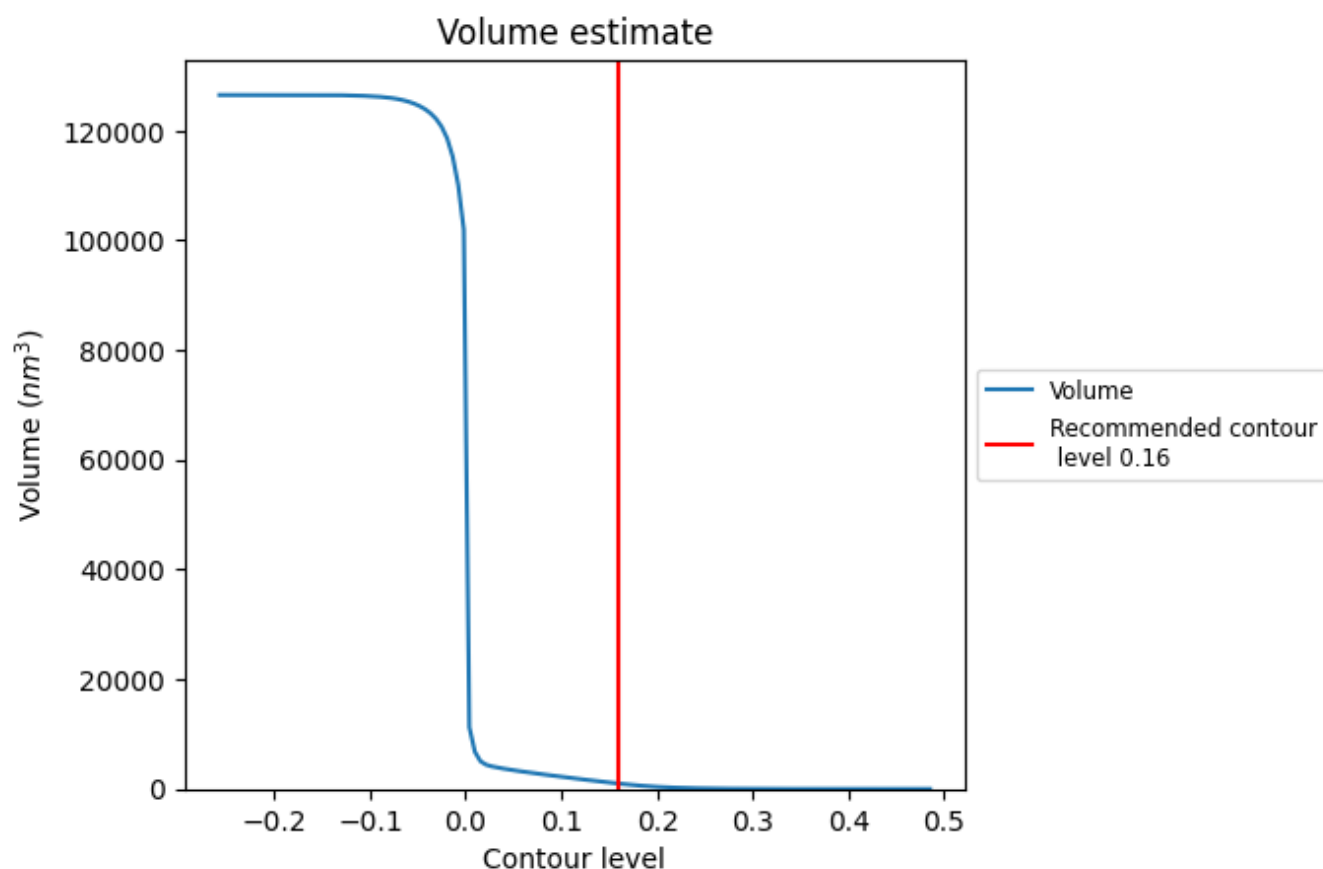
This section contains the results of statistical analysis of the map.

### 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.

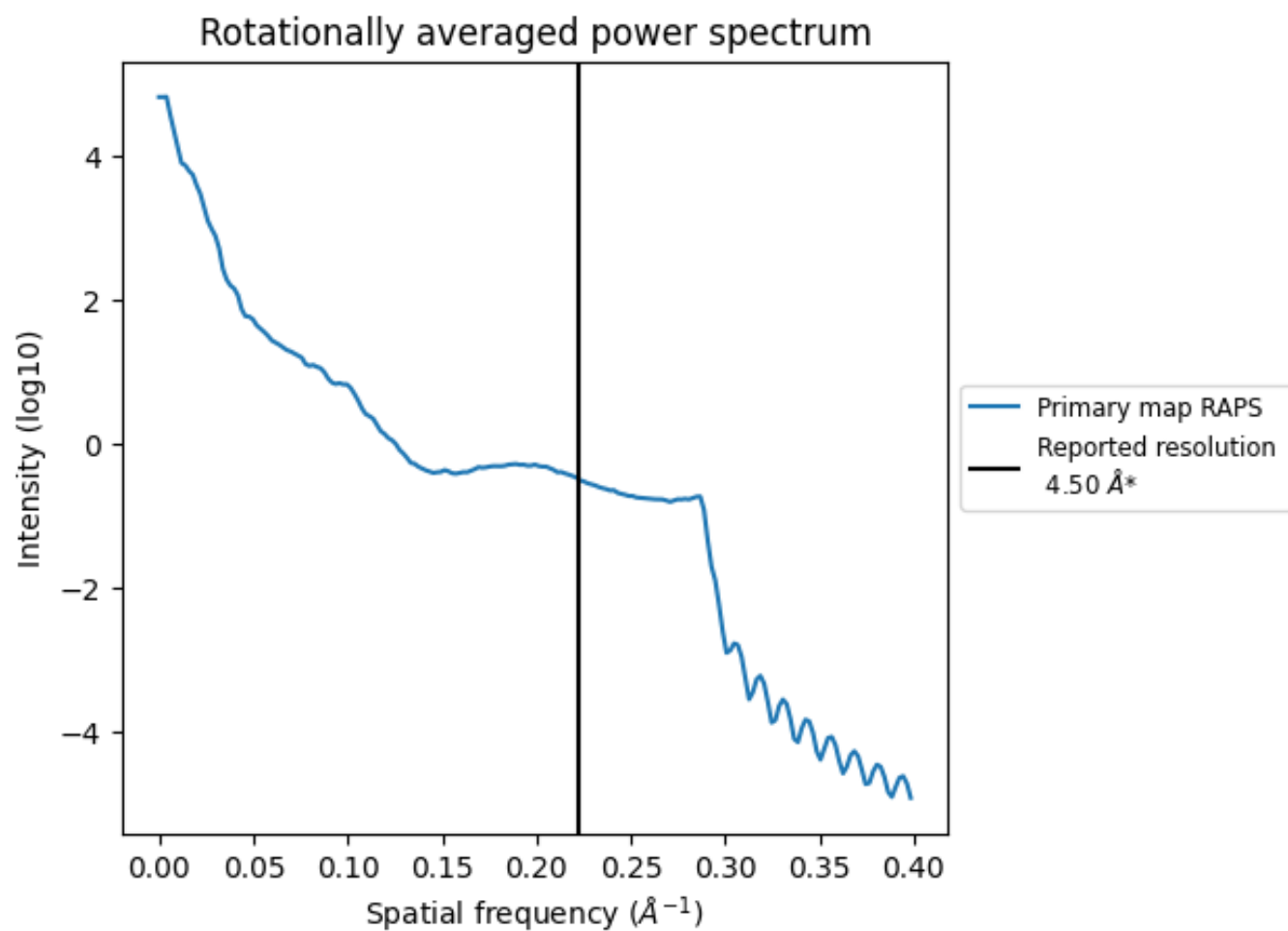
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 979 nm<sup>3</sup>; this corresponds to an approximate mass of 884 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 0.222 Å<sup>-1</sup>



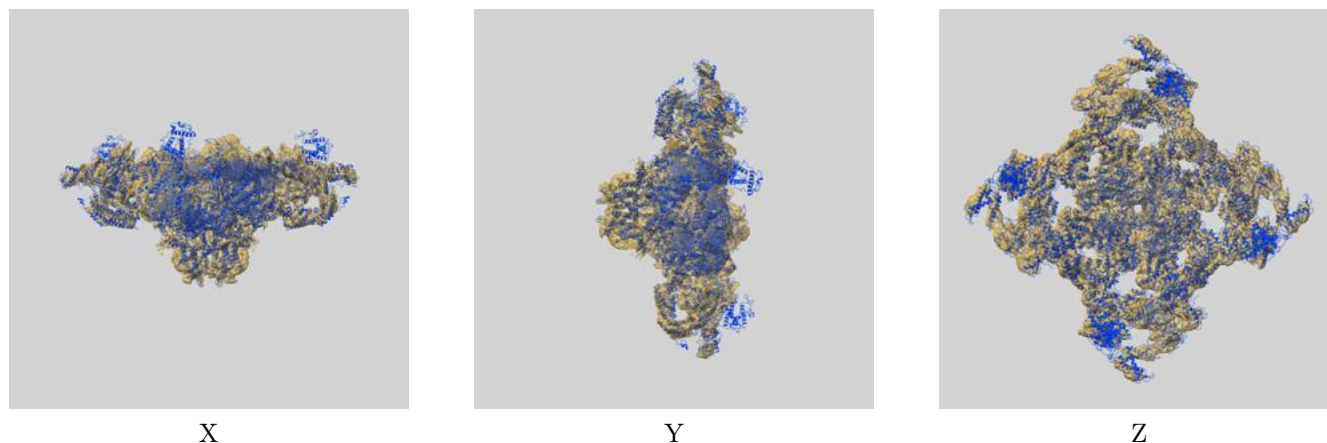
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

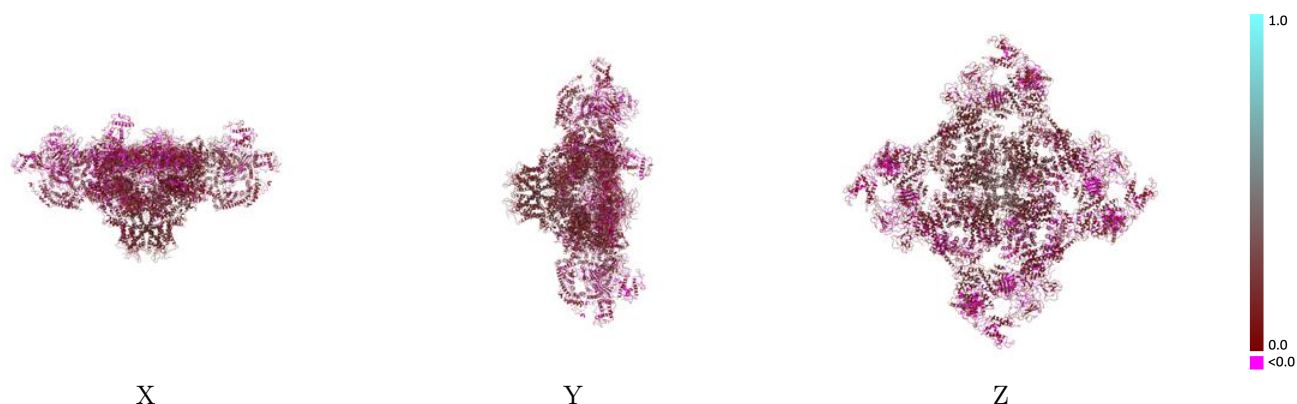
This section contains information regarding the fit between EMDB map EMD-22394 and PDB model 7JMH. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlay [i](#)



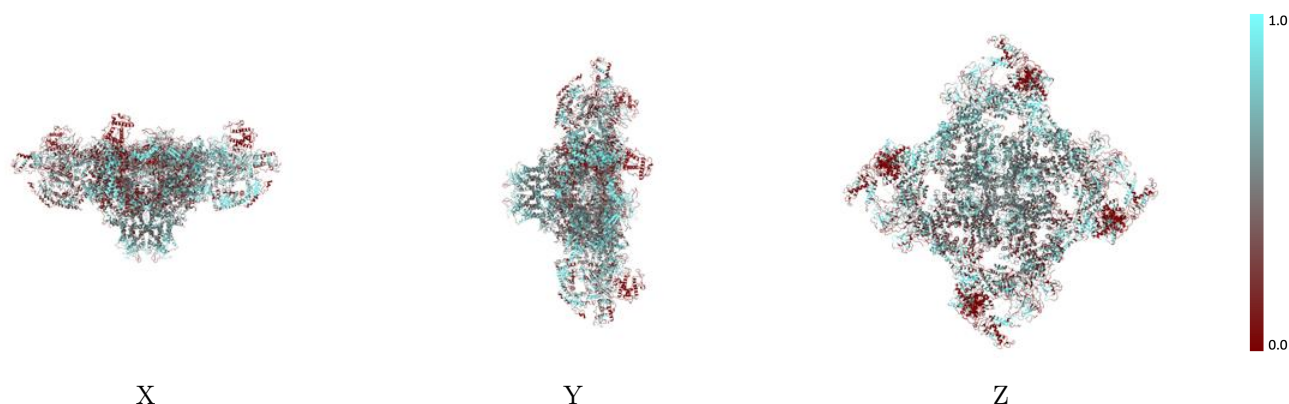
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



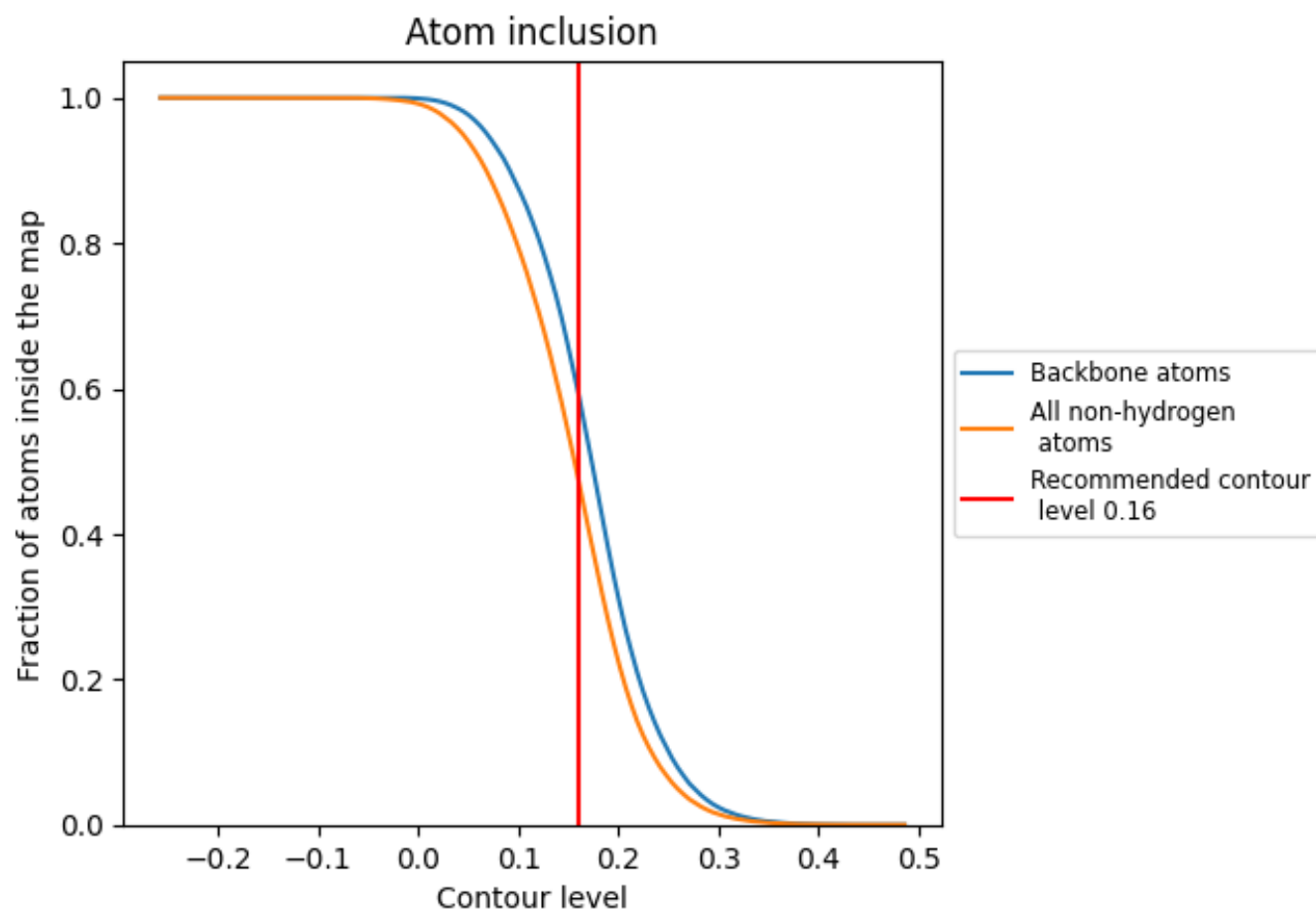
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 47% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.4748	<div><div></div></div> 0.1320
A	<div><div></div></div> 0.5620	<div><div></div></div> 0.1390
B	<div><div></div></div> 0.5148	<div><div></div></div> 0.1680
E	<div><div></div></div> 0.4812	<div><div></div></div> 0.1330
F	<div><div></div></div> 0.4888	<div><div></div></div> 0.1070
G	<div><div></div></div> 0.4453	<div><div></div></div> 0.1070
H	<div><div></div></div> 0.4529	<div><div></div></div> 0.1190
I	<div><div></div></div> 0.4560	<div><div></div></div> 0.1230
J	<div><div></div></div> 0.4690	<div><div></div></div> 0.1180

1.0

0.0

<0.0