



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 02:20 PM UTC

PDB ID : 7JMJ / pdb_00007jnj
EMDB ID : EMD-22396
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots
- Frame 37 - State 5 (S5)
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

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:

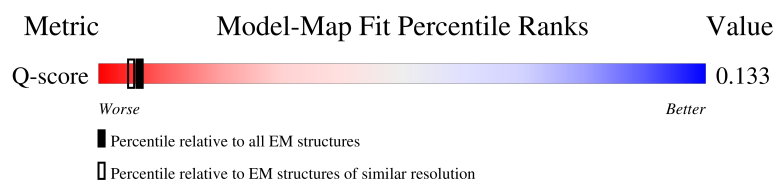
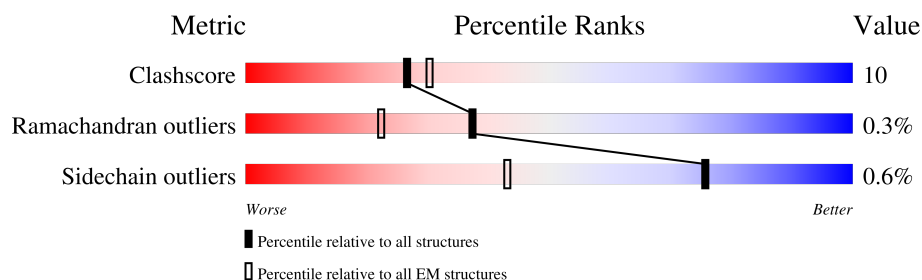
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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

Mol	Chain	Length	Quality of chain
1	A	107	36% 69% 30% .
1	F	107	52% 73% 26% .
1	H	107	52% 71% 28% .
1	J	107	52% 72% 26% .

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Mol	Chain	Length	Quality of chain
2	B	4687	39% 69% 19% 11%
2	E	4687	44% 70% 19% 11%
2	G	4687	49% 69% 19% 11%
2	I	4687	48% 70% 19% 11%

2 Entry composition [i](#)

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 (CCD ID: 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 (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest")

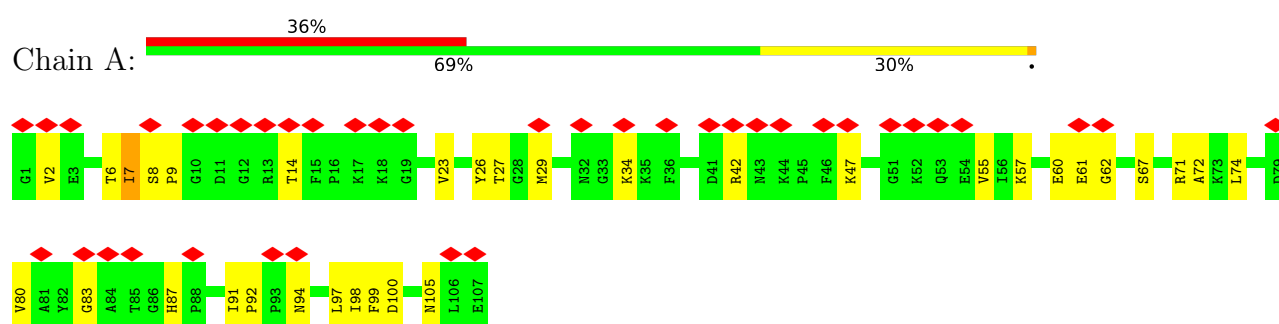
by depositor).

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

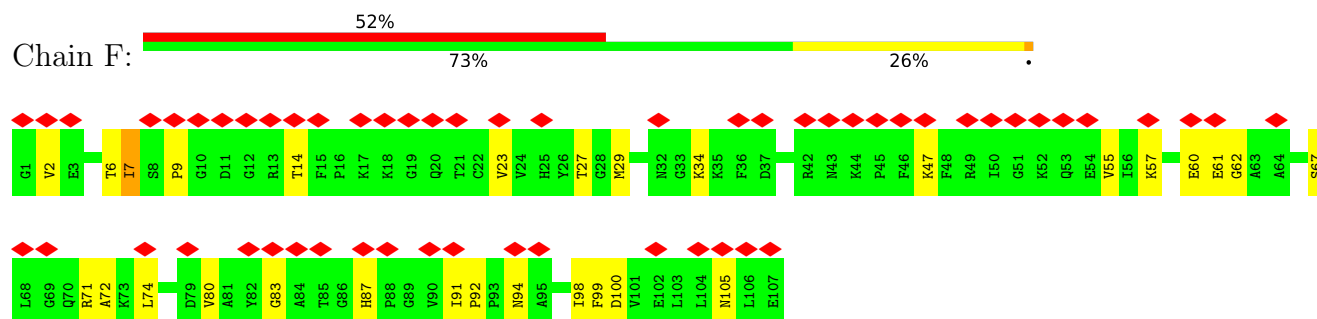
3 Residue-property plots [i](#)

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.

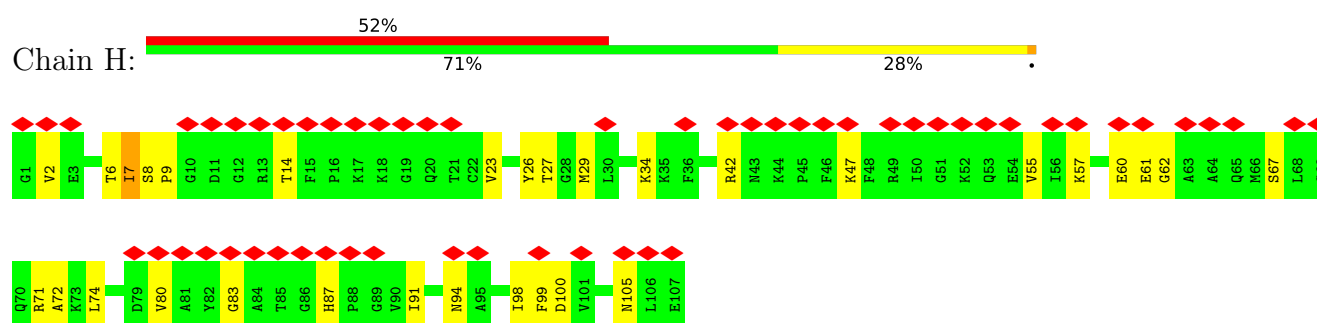
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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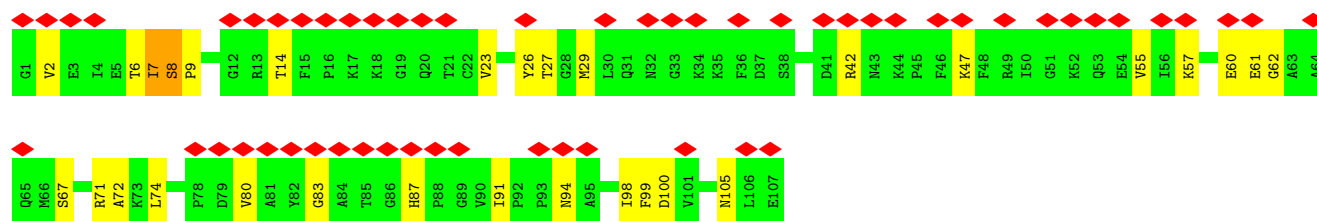


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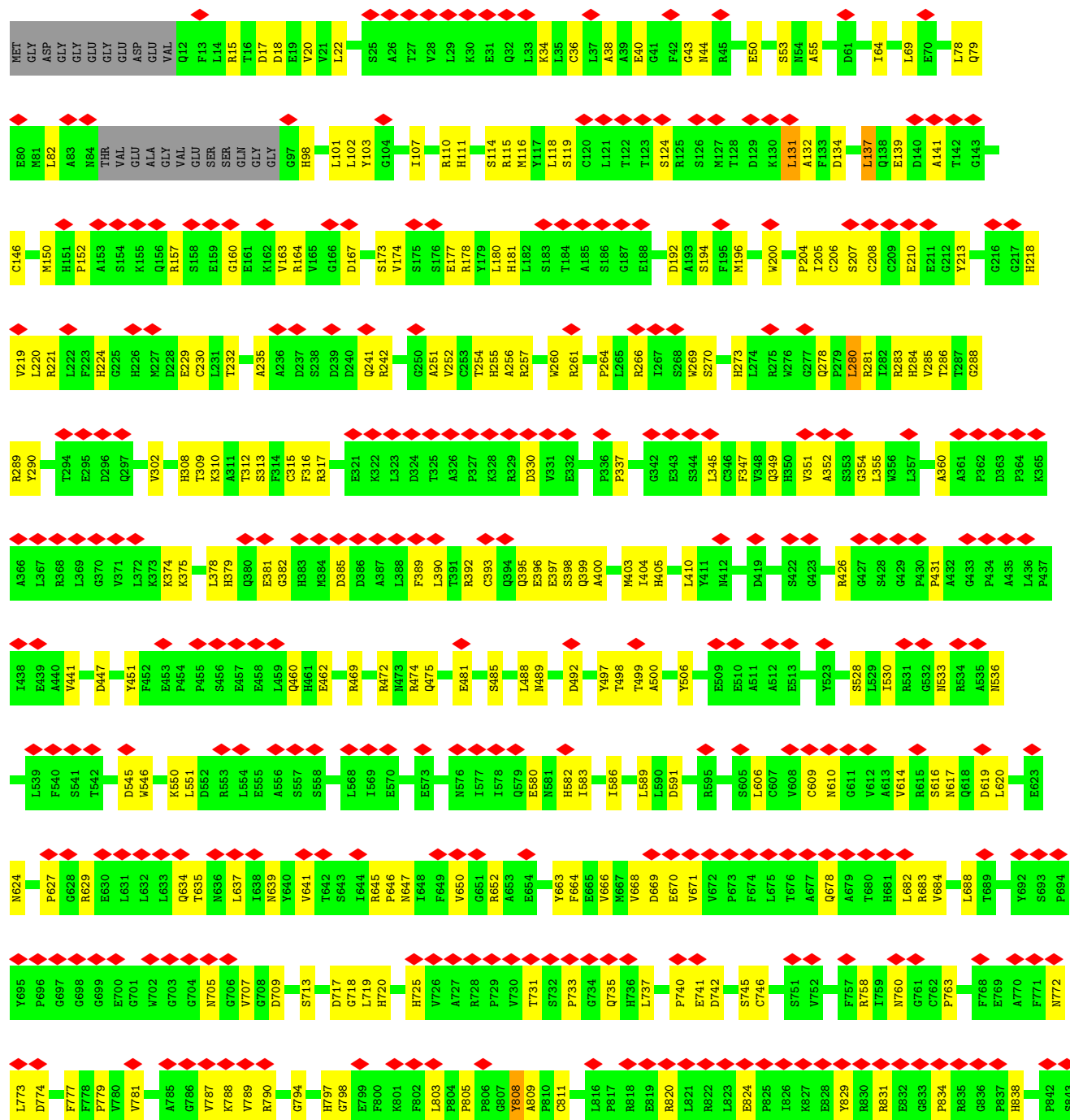
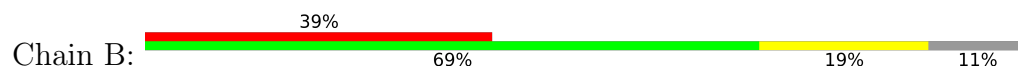


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

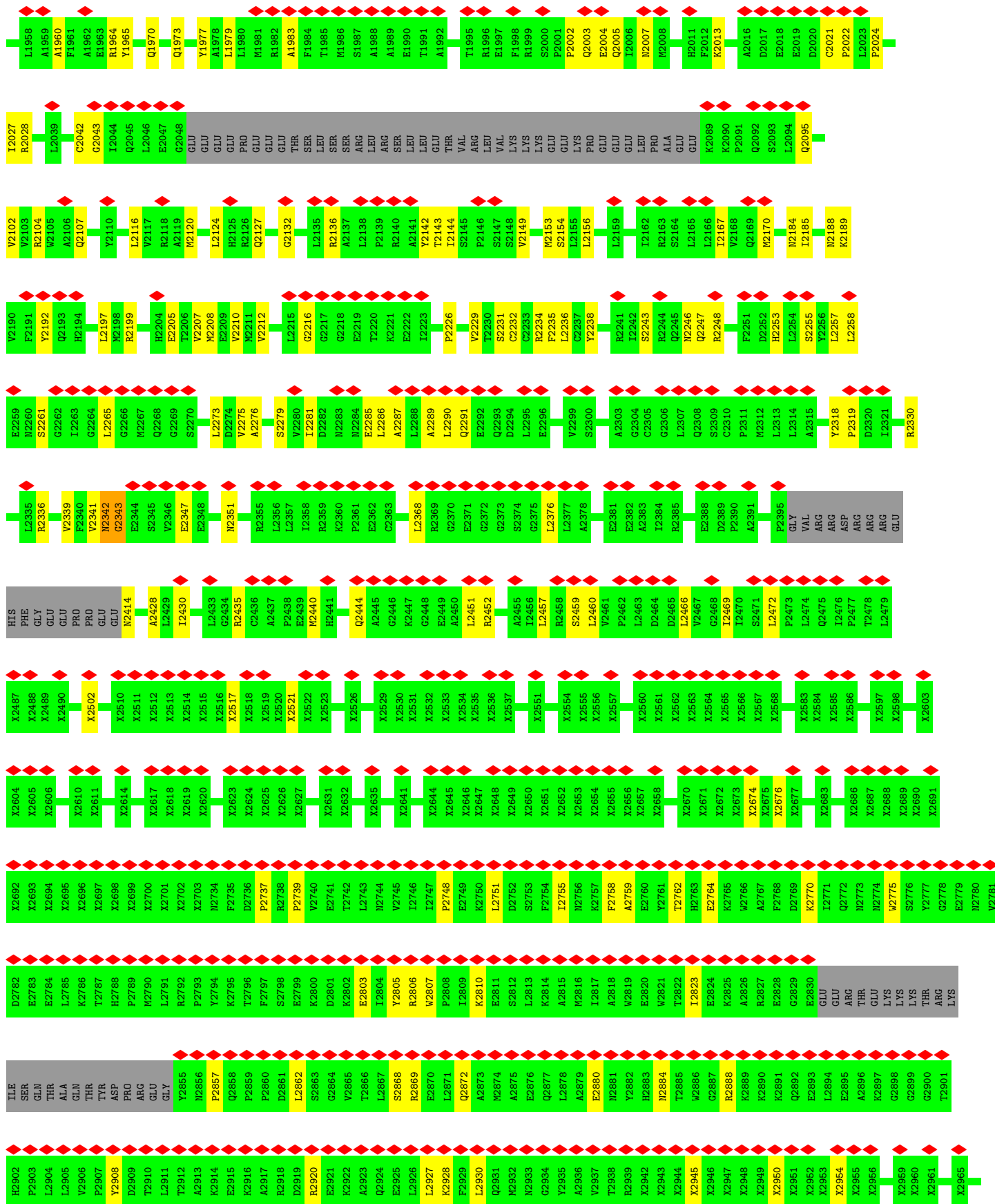


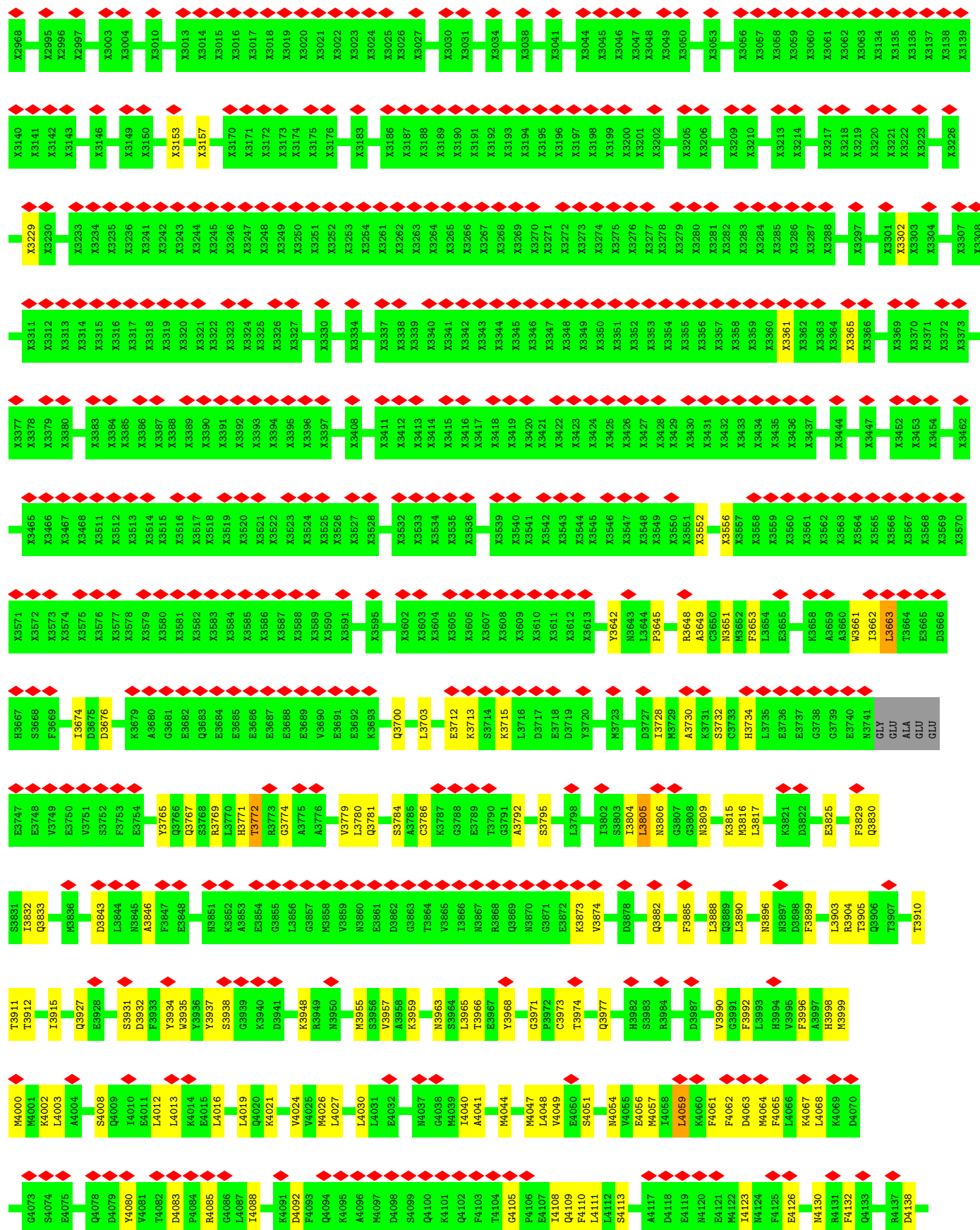


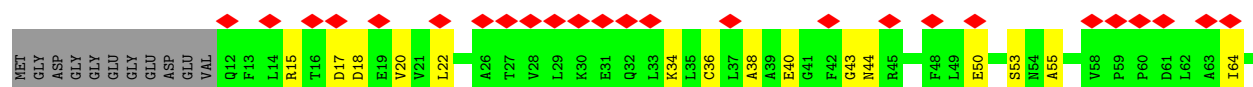
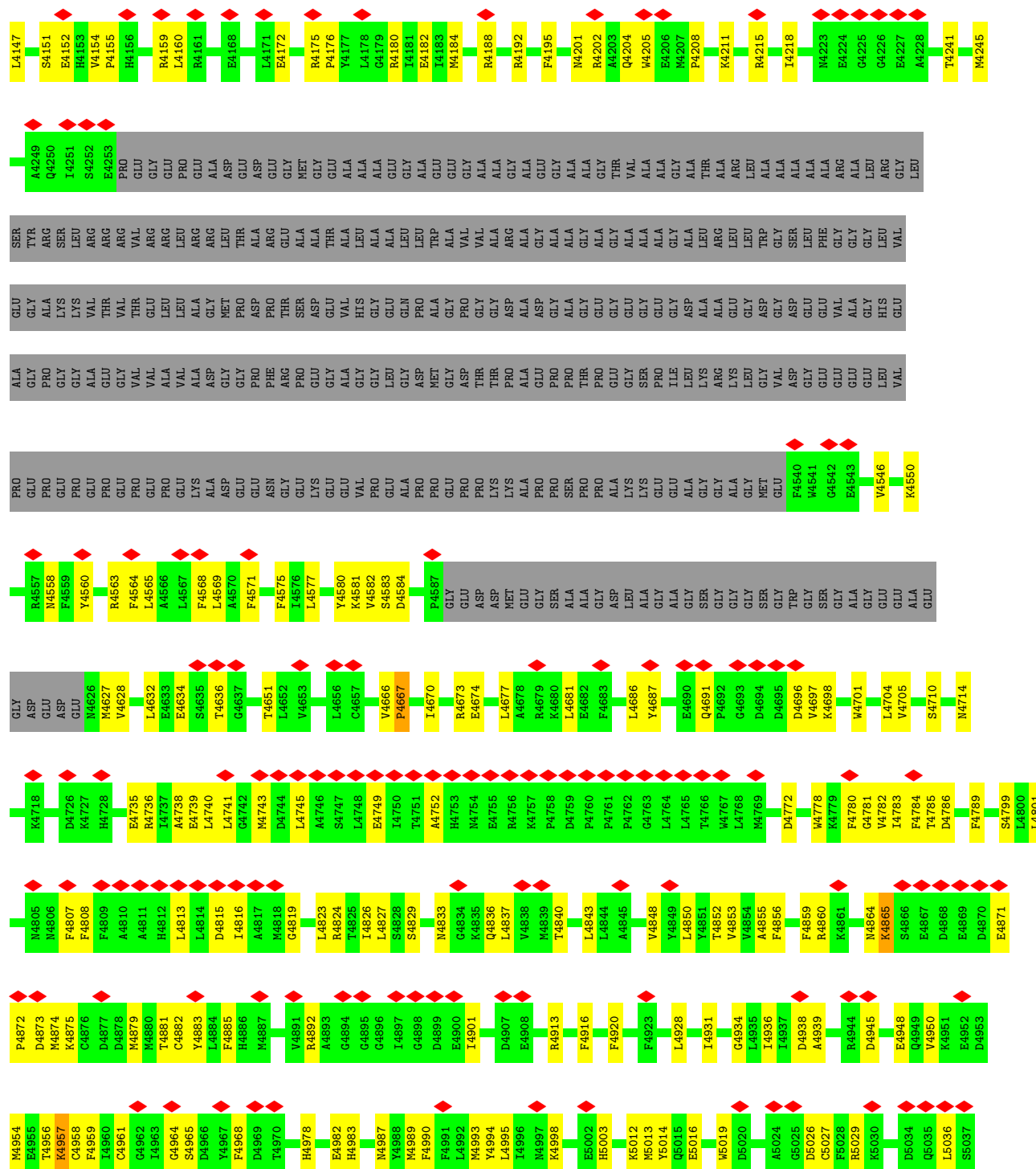
• Molecule 2: ryanodine receptor type 1



GLU	R844	R916	A980	E1054	A1117	L1202	T1263	X1514	S1606	R1671	R1743	E1817
GLU	C945	E917	Q981	PRO	D1118	N1203	V1264	X1515	R1607	L1676	F1748	D1821
GLU	L846	R918	T982	PRO	E1119	L1204	D1265	X1516	M1608	G1677	P1749	G1822
ASP	S947	R919	T983	ASP	L1120	G1205	P1268	X1519	P1609	G1678	P1750	G1823
GLU	H848	N920	R987	GLN	A1121	Q1206	C1269	X1520	N1610	N1679	G1751	G1824
GLU	T849	Y920	R988	GLU	V1122	D1207	R1270	X1521	H1611	N1680	G1752	H1825
GLU	D850	Q923	A989	PRO	V1123	V1208	L1271	X1522	F1612	F1681	R1753	H1826
LYS	F851	S925	G992	GLN	F1124	S1209	L1272	X1523	L1614	A1682	G1754	L1827
GLU	V852	M924	G992	VAL	G1140	S1210	A1273	X1524	V1615	H1683	G1755	D1828
ASP	P853	S926	G992	ASN	F1139	S1211	X1279	X1525	GLU	D1690	M1756	P1829
GLU	D857	T928	A1002	GLN	G1141	L1212	X1280	X1526	THR	G1693	A1757	V1830
GLU	THR	L929	Q1003	ARG	Q1144	R1213	X1281	X1527	ARG	L1694	L1762	G1832
GLU	VAL	L930	G1004	TRP	S1145	F1214	X1282	X1528	ALA	L1695	G1763	G1832
LYS	I861	K930	W1005	D1070	D1146	A1215	X1283	X1529	GLY	H1696	P1764	E1835
GLU	V862	L932	Y1007	R1071	D1147	L1216	X1289	X1530	E1622	A1697	G1765	F1836
GLU	L863	L933	S1008	Y1073	V1148	C1217	X1290	X1531	R1623	L1698	V1766	Q1837
GLU	P864	L935	A1009	I1074	V1149	G1218	X1291	X1532	G1625	L1699	G1767	F1838
GLU	P865	L936	VAL	I1075	M1152	L1219	X1292	X1533	W1626	E1699	L1768	V1839
GLU	H866	C937	GLN	F1076	I1153	Q1220	X1293	X1534	A1627	A1701	L1771	P1840
GLU	L867	C937	ILE	A1077	I1161	E1221	X1294	X1543	V1628	H1702	R1772	V1841
GLU	E868	H938	ALA	E1078	F1162	G1222	X1430	X1544	Q1629	L1703	P1773	L1842
GLU	R869	V939	ARG	K1079	T1163	F1223	X1440	X1545	C1630	P1704	P1774	K1843
GLU	I870	G940	ASN	Y1081	L1164	F1226	X1441	X1546	Q1631	L1707	H1775	L1844
GLU	N877	M941	PRO	Y1082	M1165	A1227	X1442	X1547	D1632	R1708	H1776	L1848
GLU	I878	A942	R1020	V1083	V1168	L1228	X1443	X1548	P1633	A1709	G1777	V1850
GLU	H879	D943	Y1024	Q1084	L1169	N1229	X1444	X1549	L1634	G1710	F1778	M1851
GLU	E880	E944	R1025	S1085	M1170	Q1230	X1445	X1550	L1635	Y1711	S1778	G1852
GLU	L881	K945	D1028	W1088	D1172	R1233	X1446	X1551	M1636	Y1712	P1779	I1853
GLU	L884	A946	E1029	Y1089	S1173	P1233	X1449	X1552	M1637	D1713	G1781	F1854
GLU	T885	E947	A1030	E1091	G1174	V1234	X1450	X1553	E1644	S1717	C1782	G1855
GLU	R886	N949	T1031	F1092	S1175	T1235	X1451	X1554	R1646	I1718	V1783	D1858
GLU	I887	L950	K1032	E1093	E1176	F1238	X1452	X1577	M1648	H1719	A1784	V1859
GLU	E888	K951	D1033	E1094	R1180	S1239	X1453	A1578	D1649	L1720	G1785	L1862
GLU	Q889	K952	S1034	A1094	E1181	X1240	X1454	M1579	L1650	E1721	L1786	M1865
GLU	G890	T953	N1035	V1095	I1182	S1241	X1455	F1580	L1651	S1722	P1787	I1866
GLU	W891	K954	R1036	T1096	E1183	P1243	X1469	L1581	R1647	R1725	A1788	M1866
GLU	T892	L955	D1037	L1097	I1184	Q1244	X1470	S1582	M1648	R1726	ALA	I1866
GLU	Y893	P956	S1038	R1101	G1185	F1245	X1471	E1583	D1649	R1727	GLY	M1866
GLU	G894	K957	L1039	V1102	D1186	E1246	X1471	L1584	L1652	S1728	VAL	F1871
GLU	P895	T958	L1039	G1103	G1187	P1247	X1489	N1585	L1653	S1729	ALA	T1872
GLU	V896	Y959	Q1041	W1104	F1188	P1247	X1499	N1586	R1656	M1730	E1793	E1874
GLU	R897	M960	A1042	L1105	L1189	V1248	X1500	P1587	L1657	L1731	P1795	GLU
GLU	D898	M961	V1043	P1106	L1189	P1249	X1504	Q1590	L1657	S1732	A1796	GLU
GLU	D899	N961	R1044	P1107	P1190	P1250	X1505	C1591	D1658	E1733	R1797	GLU
GLU	S962	N963	T1045	E1108	V1191	E1251	X1506	R1594	L1659	Y1734	L1798	GLU
GLU	N900	G964	L1046	L1109	C1192	H1252	X1507	L1595	Q1660	I1735	S1799	GLU
GLU	K901	A968	L1047	R1110	S1193	P1253	X1508	L1599	R1661	W1736	I1802	GLU
GLU	R902	D971	G1048	P1111	P1196	P1254	X1509	R1599	L1662	P1737	P1803	GLU
GLU	L903	L972	Y1049	D1112	Q1198	H1255	X1510	L1595	S1663	L1738	L1804	GLU
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GLU	S912	R976	I1053	G1116		D1261		S1604	R1668		R1808	GLU
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GLU	P914	T978										
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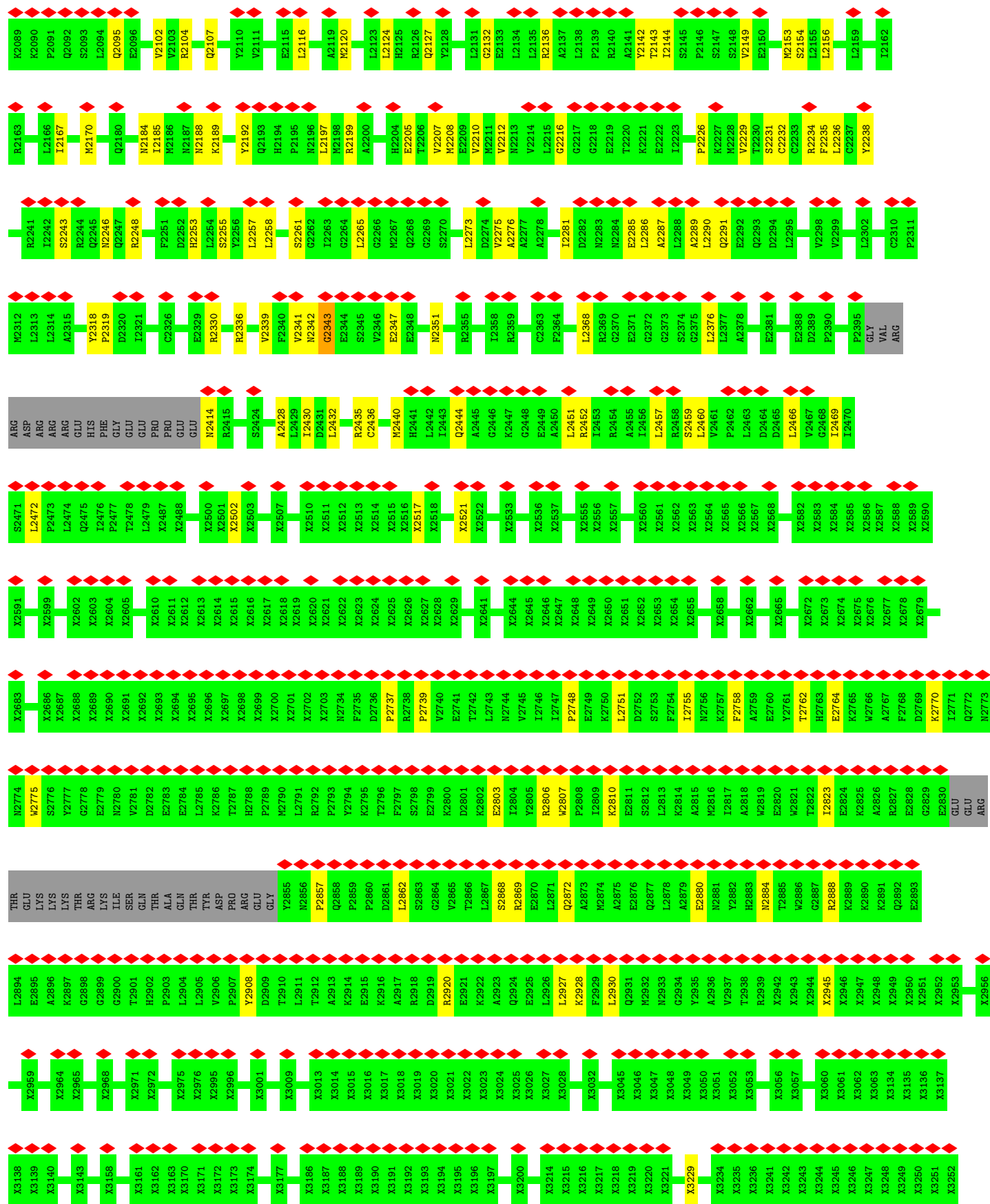




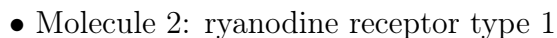




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E2018	L1931	F1871	P1903	T1739	M1608	X1530	X1443	K1240	F1179	T1097	R1036
E2019	P1932	T1872	L1804	P1740	P1609	X1531	X1444	S1241	R1180	R1101	D1037
D2020	V1935	E1873	E1905	R1743	M1610	X1532	X1445	L1242	E1181	G1103	S1038
C2021	K1936	E1874	A1906	A1744	F1611	X1533	X1446	Q1244	I1182	W1104	L1039
P2022	L1937	G1877	L1807	T1745	H1612	X1534	X1447	Q1244	E1183	A1105	C1040
L2023	C1940	R1878	R1908	L1746	L1613	X1535	X1448	F1245	I1184	R1106	Q1041
P2024	F1946	R1879	D1809	L1747	Q1614	X1536	X1449	E1246	I1185	P1107	A1042
E2025	E1960	L1812	L1812	F1748	V1615	X1537	X1450	P1247	D1186	E1108	V1043
E2026	L1951	R1813	R1813	P1749	THR	X1538	X1451	V1248	G1187	L1109	R1044
L2027	H1952	G1816	G1816	ARG	ARG	X1539	X1452	P1249	F1188	R1110	T1045
B2028	H1953	E1817	E1817	ARG	ALA	X1540	X1453	P1250	L1189	P1111	L1046
C2042	R1954	R1820	R1820	ALA	GLY	X1541	X1454	E1251	P1190	D1112	L1047
G2043	V1955	D1821	D1821	GLY	GLY	X1542	X1455	H1252	V1191	V1113	G1048
T2044	A1960	G1822	G1822	K1753	E1622	X1543	X1456	P1253	C1192	E1114	G1049
Q2045	R1964	G1823	G1823	G1755	R1623	X1544	X1457	H1254	S1193	L1115	Y1051
E2047	Y1965	Q1824	Q1824	N1756	L1624	X1545	X1458	E1255	P1196	G1116	N1052
G2048	Q1970	Q1825	Q1825	A1757	G1625	X1546	X1459	E1256	G1197	A1117	I1053
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GLU	GLU	A1825	A1825	GLU	A1627	X1548	X1471	A1258	P1199	D1118	PRO
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GLU	GLU	G1831	G1831	G1766	P1633	X1562	X1493	W1264	L1204	GLN	GLN
GLU	GLU	F1835	F1835	T1768	L1634	X1563	X1497	D1265	GLU	F1139	VAL
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GLU	GLU	V1838	V1838	GLU	M1637	P1574	X1500	L1270	W1143	W1143	SER
GLU	GLU	P1840	P1840	GLU	A1638	L1575	X1501	R1271	X1210	Q1144	ARG
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GLU	GLU	K1843	K1843	GLU	P1642	A1578	X1504	H1274	F1213	D1147	R1071
GLU	GLU	L1844	L1844	GLU	E1643	M1579	X1505	X1278	F1214	V1148	V1072
GLU	GLU	V1845	V1845	GLU	E1644	F1580	X1506	X1279	A1215	V1149	R1073
GLU	GLU	L1848	L1848	GLU	M1645	L1581	X1507	X1280	I1216	M1152	F1074
GLU	GLU	L1849	L1849	GLU	R1646	L1582	X1508	X1281	G1217	I1153	F1075
GLU	GLU	V1850	V1850	GLU	C1647	E1583	X1509	X1282	G1218	I1161	E1078
GLU	GLU	M1851	M1851	GLU	D1649	R1584	X1510	X1283	L1219	F1162	K1079
GLU	GLU	G1852	G1852	GLU	E1721	K1585	X1511	X1286	L1219	T1163	S1080
GLU	GLU	F1854	F1854	GLU	L1651	M1586	X1512	X1289	Q1220	L1164	S1081
GLU	GLU	G1855	G1855	GLU	E1652	P1587	X1513	X1290	E1221	N1165	T1082
GLU	GLU	D1856	D1856	GLU	L1653	Q1590	X1514	X1291	G1222	G1166	V1083
GLU	GLU	E1857	E1857	GLU	E1655	C1591	X1515	X1292	E1223	E1167	Q1084
GLU	GLU	L1858	L1858	GLU	R1657	R1594	X1516	X1293	F1225	V1168	Q1085
GLU	GLU	V1859	V1859	GLU	D1658	L1595	X1517	X1294	F1226	L1169	G1086
GLU	GLU	K1860	K1860	GLU	Q1660	E1596	X1518	X1295	I1228	M1170	R1087
GLU	GLU	Q1861	Q1861	GLU	H1663	Y1734	X1519	X1296	L1229	S1171	V1089
GLU	GLU	M1865	M1865	GLU	S1664	I1735	X1520	X1297	M1229	F1090	F1091
GLU	GLU	I1866	I1866	GLU	T1665	Q1597	X1521	X1300	M1230	D1172	F1092
GLU	GLU	E1867	E1867	GLU	H1666	L1600	X1522	X1301	Q1231	S1173	E1093
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GLU	GLU	P1800	P1800	GLU	L1667	S1606	X1525	X1304	V1234	E1176	
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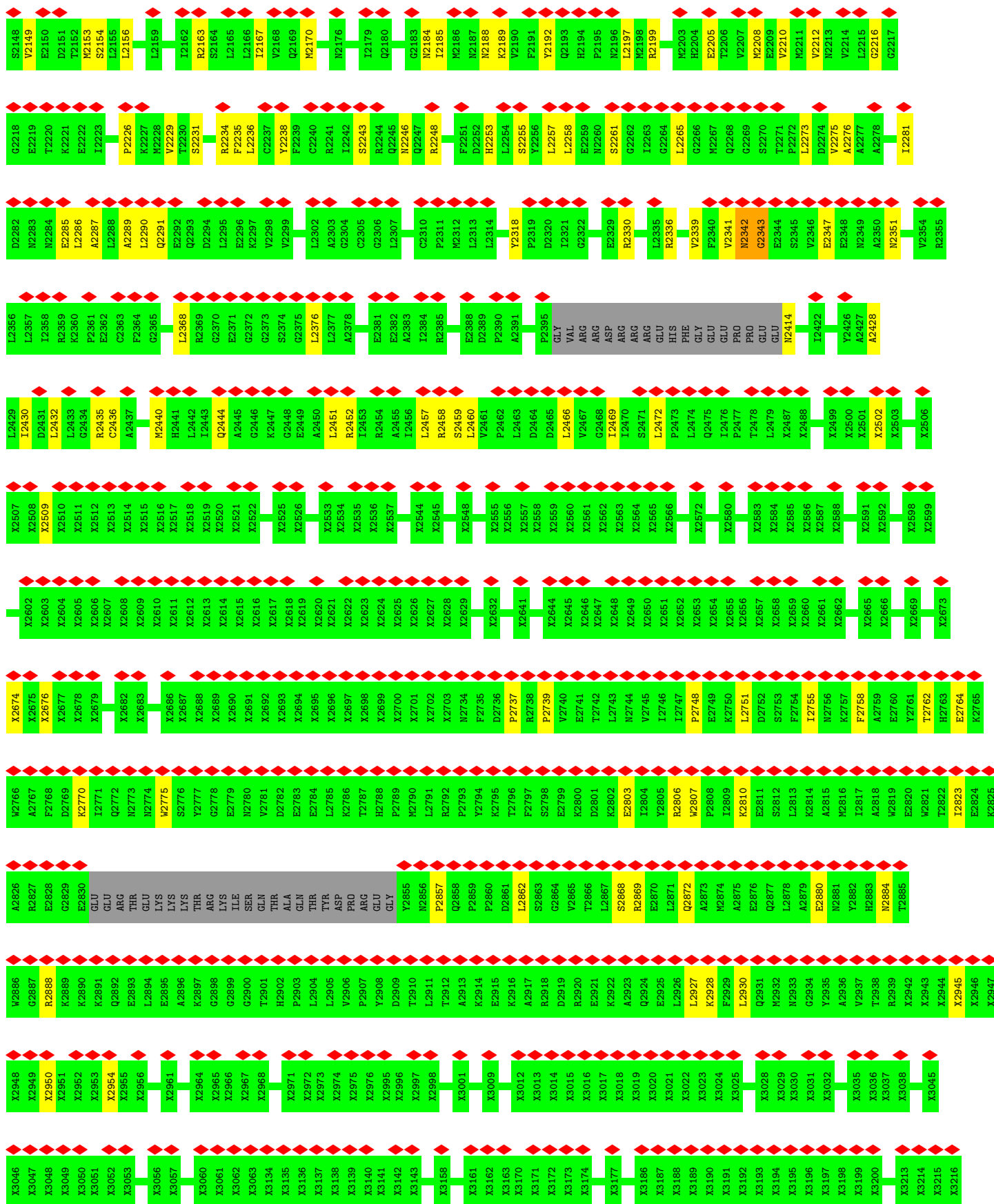


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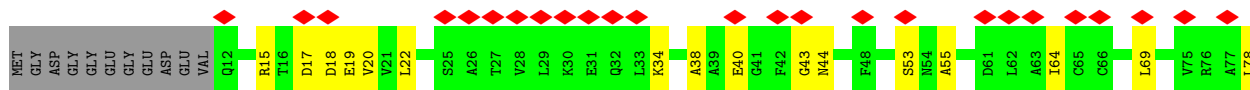


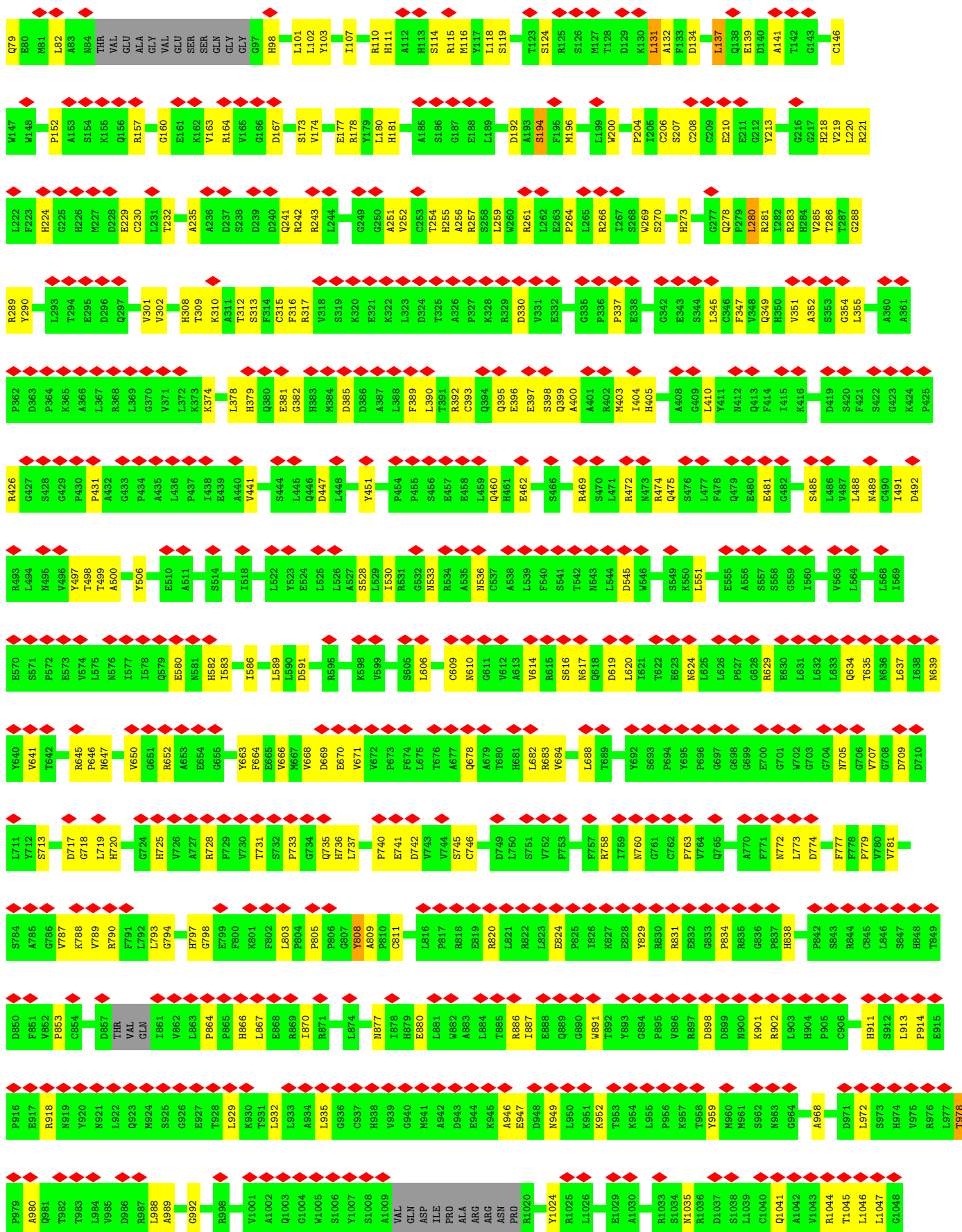
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	L4014	T4082	E3943	L3728	L3663	X3564	X3425	X3356	X3287
	K4014	D4083	V3944	N3729	T3664	X3565	X3426	X3357	X3288
	E4015	P4084	E3944	A3730	E3665	X3566	X3427	X3358	X3289
	L4016	R4085	E3945	R3731	D3666	X3567	X3428	X3359	X3290
				S3732	H3667	X3568	X3429	X3360	X3291
				C3733	F3668	X3569	X3430	X3361	X3292
				T3797	E3670	X3570	X3431	X3362	X3293
				L3735		X3571	X3432	X3363	X3294
						X3572	X3433	X3364	X3295
						X3573	X3434	X3365	X3296
						X3574	X3435	X3366	X3297







X2975	X2976	X2985	X2986	X2997	X2998	X3001	X3002	X3003	X3004	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3031	X3032	X3035	X3038	X3041	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3134	X3135									
P2903	L2904	L2905	V2906	L2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	A2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	R2932	N2933	Q2934	V2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2961	X2964	X2965	X2968				
SFR	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	N2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	A2876	Q2877	L2878	A2879	E2880	N2881	H2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	A2895	A2896	K2897	G2898	G2899	T2900	T2901	H2902
E2783	E2784	L2785	K2786	L2787	H2788	P2789	M2790	L2791	R2792	P2793	V2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	P2807	R2808	L2809	K2810	E2811	D2812	L2813	R2814	K2815	A2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	E2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE
X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	N2735	D2736	P2737	R2738	V2739	E2740	T2742	L2743	N2744	V2745	L2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	
X2613	X2614	X2615	X2616	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2629	X2632	X2641	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2656	X2657	X2658	X2659	X2662	X2666	X2669	X2673	X2674	X2675	X2676	X2677	X2678	X2683	X2686	X2687	X2688	X2689	X2690	X2691	X2692										
X2521	X2522	X2523	E2524	X2525	X2526	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2544	X2545	X2548	X2551	X2552	X2553	X2554	X2555	X2556	X2557	X2558	X2559	X2560	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2583	X2584	X2585	X2586	X2594	X2598	X2603	X2604	X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612								
G2446	K2447	G2448	E2449	L2450	L2451	R2452	L2453	R2454	A2455	L2456	L2457	R2458	S2459	L2460	V2461	P2462	L2463	D2464	D2465	L2466	V2467	G2468	L2469	L2470	S2471	L2472	P2473	Q2475	T2476	P2477	T2478	L2479	X2487	X2488	X2489	X2490	X2499	X2500	X2501	X2502	X2503	X2506	X2507	X2508	X2509	X2510	X2511	X2512	X2513	X2514	X2515	X2516	X2517	X2518	X2519	X2520			
G2373	S2374	G2375	L2376	L2377	A2378	E2381	E2382	A2383	I2384	R2385	E2388	D2389	P2390	A2391	R2392	P2395	VAL	ARG	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	N2414	M2423	A2427	A2428	L2429	L2430	L2433	G2434	R2435	G2436	A2437	P2438	E2439	M2440	H2441	L2442	L2443	Q2444	A2445									
V2298	V2299	S2300	Y2301	L2302	A2303	G2304	C2305	G2306	L2307	M2312	L2313	L2314	A2315	Y2318	P2319	D2320	L2321	G2322	R2330	L2331	L2332	L2335	R2336	V2339	F2340	N2341	N2342	G2343	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	V2354	R2355	L2356	L2357	L2358	R2359	K2360	P2361	E2362	C2363	F2364	L2368	R2369	G2370	E2371	G2372							
L2236	G2237	Y2238	F2239	C2240	R2241	L2242	S2243	R2244	Q2245	N2246	Q2247	R2248	F2251	D2252	H2253	L2254	S2255	Y2256	L2257	L2258	E2259	N2260	S2261	Q2262	L2263	Q2264	L2265	Q2266	M2267	Q2268	G2269	S2270	T2271	P2272	L2273	D2274	V2275	A2276	S2279	V2280	L2281	D2282	N2283	L2284	E2285	L2286	A2287	L2288	A2289	L2290	Y2291	E2292	Q2293	D2294	L2295	E2296	K2297		
R2104	W2105	A2106	Q2107	V2110	Q2111	Q2112	S2113	P2114	E2115	L2116	V2117	R2118	A2119	M2120	F2121	S2122	L2123	L2124	H2125	R2126	Q2127	V2128	D2129	G2130	L2131	G2132	L2135	R2136	A2137	L2138	E2209	V2210	M2211	V2212	N2213	V2214	L2215	G2216	G2217	G2218	E2219	T2220	K2221	E2222	I2223	R2224	F2225	P2226	K2227	M2228	V2229	Y2230	S2231	C2232	C2233	R2234	F2235		

D4083	K3136	X3462	X3572	L3674	G3738	S3803	K3948	L4013	D4083
P4084	X3137	X3463	X3573	D3675	G3739	I3804	K3949	K4014	P4084
R4085	X3138	X3464	X3574	D3676	E3740	L3805	N3950	E4015	R4085
I4088	X3139	X3465	X3575	A3680	I3741	N3806	N3951	L4016	I4088
K4091	X3140	X3466	X3576	G3681	GLU	G3807	F3952	L4017	K4091
D4092	X3141	X3467	X3577	E3682	ALA	G3808	K3953	D4018	D4092
F4093	X3142	X3468	X3578	Q3683	GLU	N3809	A3954	L4019	F4093
Q4094	X3143	X3469	X3579	E3684	GLU	K3815	N3955	Q4020	Q4094
K4095	X3146	X3470	X3580	E3685	GLU	M3816	S3956	K4021	K4095
A4096	X3146	X3471	X3581	E3686	GLU	L3817	F3957	V4024	A4096
M4097	X3162	X3472	X3582	E3687	E3747	L3820	A3958	L4027	M4097
D4098	X3163	X3473	X3583	E3688	E3748	K3821	K3959	L4028	D4098
S4099	X3170	X3474	X3584	E3689	V3749	L3822	F3962	S4029	S4099
Q4100	X3171	X3475	X3585	V3690	E3750	K3824	N3963	L4030	Q4100
K4101	X3172	X3476	X3586	E3691	E3751	E3825	S3964	M4037	K4101
F4103	X3173	X3477	X3587	E3692	F3753	F3829	L3965	I4040	F4103
T4104	X3174	X3478	X3588	E3693	E3754	Q3830	E3967	A4041	T4104
G4105	X3183	X3479	X3589	K3694	E3755	S3831	T3968	R4042	G4105
E4106	X3184	X3480	X3590	P3695	K3756	Q3833	T3969	Q4043	E4106
A4107	X3186	X3481	X3591	L3696	E3759	M3836	I3969	M4044	A4107
I4108	X3187	X3482	X3602	H3699	K3760	Q3837	Q3970	V4045	I4108
Q4109	X3188	X3483	X3603	Q3700	L3763	T3838	G3971	D4046	Q4109
F4110	X3189	X3484	X3604	L3701	L3764	G3839	N3972	M4047	F4110
L4111	X3189	X3485	X3605	V3702	V3765	C3839	C3973	V4048	L4111
S4112	X3190	X3486	X3606	L3703	Q3766	L3842	Q3974	L4049	S4112
A4117	X3191	X3487	X3607	H3704	Q3767	D3843	Q3977	V4050	A4117
D4118	X3192	X3488	X3608	F3705	S3768	L3844	Q3978	E4051	D4118
E4119	X3193	X3489	X3609	S3706	R3769	N3845	A3981	S4051	E4119
M4120	X3194	X3490	X3610	S3707	L3770	N3846	H3982	R4052	M4120
E4121	X3195	X3491	X3611	T3708	H3771	Q3847	S3983	M4053	E4121
N4122	X3196	X3492	X3612	A3709	T3772	F3848	R3984	V4054	N4122
I4123	X3197	X3493	X3613	L3710	R3774	E3849	D3987	M4055	I4123
F4125	X3198	X3494	X3614	E3711	A3775	R3850	V3990	L4056	F4125
E4126	X3199	X3495	X3615	K3713	A3776	Q3851	G3991	O4057	E4126
M4130	X3201	X3496	X3616	S3714	V3779	K3852	L4059	A4058	M4130
F4131	X3202	X3497	X3617	K3715	L3780	L3853	G3992	F4060	F4131
F4132	X3205	X3498	X3618	L3716	Q3781	E3854	F3993	F4061	F4132
Q4133	X3206	X3499	X3619	D3717	M3782	G3855	H3994	D4062	Q4133
A4136	X3209	X3500	X3620	E3718	I3783	G3856	F3995	D4063	A4136
R4137	X3210	X3501	X3621	S3719	S3784	L3857	A3997	M4064	R4137
D4138	X3214	X3502	X3622	K3651	C3786	G3858	H3998	F4065	D4138
G4140	X3217	X3503	X3623	M3652	K3787	M3859	M4000	L4066	G4140
A4144	X3218	X3504	X3624	A3724	G3788	V3859	M4001	K4067	A4144
L4147	X3219	X3505	X3625	S3725	E3789	N3860	K4002	L4068	L4147
S4151	X3220	X3506	X3626	A3726	E3790	E3861	A4004	D4069	S4151
F4152	X3222	X3507	X3627	L3727	T3791	D3862	Q4005	D4070	F4152
V4154	X3223	X3508	X3628	I3728	G3791	G3863	Q4008	G4073	V4154
	X3226	X3509	X3629	M3729	M3793	T3864	I4009	S4074	
	X3229	X3510	X3630	K3731	V3794	V3865	Q4009	E4075	
	X3230	X3511	X3631	S3732	S3795	N3867	I4010	A4076	
				E3733	L3798	R3868	E4011		
				L3735	K3799	Q3869	L4012		
				E3736	I3802	G3871			
				E3737		E3872			



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	0.466	Depositor
Minimum map value	-0.266	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	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	0.27	0/834	0.64	3/1123 (0.3%)
1	F	0.27	0/834	0.64	2/1123 (0.2%)
1	H	0.27	0/834	0.63	3/1123 (0.3%)
1	J	0.27	0/834	0.64	3/1123 (0.3%)
2	B	0.36	0/25428	0.67	1/34534 (0.0%)
2	E	0.36	0/25428	0.67	1/34534 (0.0%)
2	G	0.36	0/25428	0.67	1/34534 (0.0%)
2	I	0.36	0/25428	0.67	1/34534 (0.0%)
All	All	0.36	0/105048	0.67	15/142628 (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	19
2	E	0	19
2	G	0	19
2	I	0	20
All	All	0	77

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4872	PRO	N-CA-C	-6.67	104.64	113.65
2	B	4872	PRO	N-CA-C	-6.62	104.72	113.65
2	G	4872	PRO	N-CA-C	-6.46	104.55	113.53
2	I	4872	PRO	N-CA-C	-6.39	104.65	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	7	ILE	CA-C-N	5.92	128.40	120.58
1	F	7	ILE	C-N-CA	5.92	128.40	120.58
1	A	8	SER	N-CA-C	5.36	120.21	113.25
1	J	8	SER	N-CA-C	5.32	120.16	113.25
1	H	8	SER	N-CA-C	5.26	120.09	113.25
1	H	7	ILE	CA-C-N	5.10	128.51	120.97
1	H	7	ILE	C-N-CA	5.10	128.51	120.97
1	J	7	ILE	CA-C-N	5.08	128.49	120.97
1	J	7	ILE	C-N-CA	5.08	128.49	120.97
1	A	7	ILE	CA-C-N	5.02	128.40	120.97
1	A	7	ILE	C-N-CA	5.02	128.40	120.97

There are no chirality outliers.

All (77) 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	2291	GLN	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3786	CYS	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4696	ASP	Peptide
2	B	4807	PHE	Peptide
2	B	4865	LYS	Peptide
2	B	4873	ASP	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	2291	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	E	2342	ASN	Peptide
2	E	2343	GLY	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	4865	LYS	Peptide
2	E	4873	ASP	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	2291	GLN	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
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	4865	LYS	Peptide
2	G	4873	ASP	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	2291	GLN	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide

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Mol	Chain	Res	Type	Group
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	4865	LYS	Peptide
2	I	4873	ASP	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	21	0
1	F	818	0	824	19	0
1	H	818	0	824	19	0
1	J	818	0	824	20	0
2	B	29369	0	24716	551	0
2	E	29369	0	24712	538	0
2	G	29369	0	24713	551	0
2	I	29369	0	24713	546	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	2235	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 10.

All (2235) 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:4860:ARG:HD2	2:I:4582:VAL:HG11	1.65	0.79
2:B:853:PRO:HB3	2:B:1024:TYR:H	1.51	0.76
2:B:379:HIS:HD2	2:B:382:GLY:H	1.35	0.75
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.51	0.75
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.51	0.75
2:G:379:HIS:HD2	2:G:382:GLY:H	1.35	0.75
2:G:853:PRO:HB3	2:G:1024:TYR:H	1.51	0.74
2:I:379:HIS:HD2	2:I:382:GLY:H	1.35	0.74
2:E:379:HIS:HD2	2:E:382:GLY:H	1.35	0.72
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.23	0.72
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.23	0.72
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.23	0.72
2:I:111:HIS:HD2	2:I:114:SER:H	1.36	0.71
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.23	0.71
2:B:111:HIS:HD2	2:B:114:SER:H	1.36	0.70
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.73	0.70
2:E:111:HIS:HD2	2:E:114:SER:H	1.36	0.70
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.74	0.69
2:G:111:HIS:HD2	2:G:114:SER:H	1.36	0.69
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.74	0.69
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.74	0.69
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.74	0.69
2:E:221:ARG:NH2	2:E:255:HIS:O	2.27	0.68
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.76	0.68
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.76	0.68
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.60	0.67
2:I:221:ARG:NH2	2:I:255:HIS:O	2.27	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.76	0.67
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.60	0.67
2:G:221:ARG:NH2	2:G:255:HIS:O	2.27	0.67
2:B:221:ARG:NH2	2:B:255:HIS:O	2.27	0.67
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.60	0.67
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.76	0.67
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.76	0.67
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.76	0.67
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.76	0.66
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.76	0.66
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.77	0.66
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.60	0.66
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.76	0.66
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.78	0.66
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.76	0.66
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.61	0.66
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.29	0.66
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.77	0.66
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.76	0.66
2:E:829:TYR:HB3	2:E:1073:ARG:HH11	1.61	0.66
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.77	0.66
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.78	0.65
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.76	0.65
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.78	0.65
2:E:4176:PRO:O	2:E:4202:ARG:NH2	2.30	0.65
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.78	0.65
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.78	0.65
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.29	0.65
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.77	0.65
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.78	0.65
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.77	0.65
2:E:3767:GLN:HB3	2:E:3772:THR:HG22	1.78	0.65
2:G:3767:GLN:HB3	2:G:3772:THR:HG22	1.77	0.65
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.77	0.65
2:G:4176:PRO:O	2:G:4202:ARG:NH2	2.30	0.65
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.79	0.65
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.79	0.65
2:B:829:TYR:HB3	2:B:1073:ARG:HH11	1.61	0.65
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.29	0.65
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.78	0.65
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.78	0.65
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.29	0.65
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.77	0.65
2:B:4176:PRO:O	2:B:4202:ARG:NH2	2.30	0.65
2:G:829:TYR:HB3	2:G:1073:ARG:HH11	1.61	0.65
2:I:4176:PRO:O	2:I:4202:ARG:NH2	2.30	0.64
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.79	0.64
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.77	0.64
2:I:829:TYR:HB3	2:I:1073:ARG:HH11	1.61	0.64
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.61	0.64
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.78	0.64
2:B:3767:GLN:HB3	2:B:3772:THR:HG22	1.78	0.64
2:E:1232:ARG:HH21	2:E:1701:ALA:HB1	1.63	0.64
2:G:606:LEU:O	2:G:617:ASN:ND2	2.31	0.64
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.80	0.64
2:B:606:LEU:O	2:B:617:ASN:ND2	2.31	0.64
2:B:1830:VAL:HB	2:B:1837:GLN:HA	1.80	0.64
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.61	0.64
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.80	0.64
2:B:1232:ARG:HH21	2:B:1701:ALA:HB1	1.63	0.64
2:I:132:ALA:HA	2:I:194:SER:HB2	1.79	0.64
2:I:3767:GLN:HB3	2:I:3772:THR:HG22	1.78	0.64
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.31	0.64
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.80	0.64
2:E:1830:VAL:HB	2:E:1837:GLN:HA	1.80	0.64
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.79	0.63
2:E:132:ALA:HA	2:E:194:SER:HB2	1.78	0.63
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.80	0.63
2:E:606:LEU:O	2:E:617:ASN:ND2	2.31	0.63
2:B:132:ALA:HA	2:B:194:SER:HB2	1.79	0.63
2:G:1232:ARG:HH21	2:G:1701:ALA:HB1	1.63	0.63
2:I:17:ASP:HB2	2:I:98:HIS:HE1	1.64	0.63
2:I:606:LEU:O	2:I:617:ASN:ND2	2.31	0.63
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.80	0.63
2:G:132:ALA:HA	2:G:194:SER:HB2	1.79	0.63
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.80	0.63
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.31	0.63
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.32	0.63
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.80	0.63
2:E:4741:LEU:HB2	2:E:4743:MET:HE2	1.81	0.63
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.80	0.63
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.81	0.63
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.81	0.63
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.80	0.63
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.32	0.63
2:G:4704:LEU:HD22	2:G:4778:TRP:HB2	1.81	0.63
2:I:1830:VAL:HB	2:I:1837:GLN:HA	1.80	0.63
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.81	0.63
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.81	0.63
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.80	0.63
2:I:1232:ARG:HH21	2:I:1701:ALA:HB1	1.63	0.63
2:B:4741:LEU:HB2	2:B:4743:MET:HE2	1.81	0.62
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.80	0.62
2:E:4704:LEU:HD22	2:E:4778:TRP:HB2	1.81	0.62
2:B:4824:ARG:HG3	2:B:4827:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.81	0.62
2:I:4824:ARG:HG3	2:I:4827:LEU:HD23	1.81	0.62
1:A:6:THR:HA	1:A:72:ALA:HA	1.81	0.62
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.81	0.62
2:E:18:ASP:HB2	2:E:69:LEU:HD12	1.82	0.62
2:G:17:ASP:HB2	2:G:98:HIS:HE1	1.64	0.62
2:B:17:ASP:HB2	2:B:98:HIS:HE1	1.64	0.62
2:G:18:ASP:HB2	2:G:69:LEU:HD12	1.82	0.62
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.82	0.62
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.64	0.62
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.31	0.62
2:E:4581:LYS:HB2	2:E:4632:LEU:HB2	1.81	0.62
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.32	0.62
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.82	0.62
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.64	0.62
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.81	0.62
2:E:1973:GLN:O	2:E:1977:TYR:N	2.33	0.62
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.80	0.62
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.98	0.62
2:B:4581:LYS:HB2	2:B:4632:LEU:HB2	1.81	0.62
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.73	0.62
2:G:1830:VAL:HB	2:G:1837:GLN:HA	1.80	0.62
2:G:1973:GLN:O	2:G:1977:TYR:N	2.33	0.62
2:I:261:ARG:HB3	2:I:283:ARG:HB3	1.82	0.62
2:I:4741:LEU:HB2	2:I:4743:MET:HE2	1.81	0.62
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.32	0.62
2:E:17:ASP:HB2	2:E:98:HIS:HE1	1.64	0.62
2:G:4741:LEU:HB2	2:G:4743:MET:HE2	1.81	0.62
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.73	0.62
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.80	0.62
2:E:4824:ARG:HG3	2:E:4827:LEU:HD23	1.81	0.61
1:F:6:THR:HA	1:F:72:ALA:HA	1.81	0.61
2:G:728:ARG:NH2	2:G:1527:UNK:O	2.33	0.61
2:B:4704:LEU:HD22	2:B:4778:TRP:HB2	1.81	0.61
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.73	0.61
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.64	0.61
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.81	0.61
2:G:4581:LYS:HB2	2:G:4632:LEU:HB2	1.81	0.61
2:I:4704:LEU:HD22	2:I:4778:TRP:HB2	1.81	0.61
2:B:261:ARG:HB3	2:B:283:ARG:HB3	1.82	0.61
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:639:ASN:H	2:G:678:GLN:HE22	1.49	0.61
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.82	0.61
2:G:4824:ARG:HG3	2:G:4827:LEU:HD23	1.81	0.61
2:I:18:ASP:HB2	2:I:69:LEU:HD12	1.82	0.61
2:B:639:ASN:H	2:B:678:GLN:HE22	1.48	0.61
2:E:1271:ARG:HA	2:E:1471:UNK:HA	1.83	0.61
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.33	0.61
2:B:1271:ARG:HA	2:B:1471:UNK:HA	1.81	0.61
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.64	0.61
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.82	0.61
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.81	0.61
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.73	0.61
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.81	0.61
2:E:639:ASN:H	2:E:678:GLN:HE22	1.48	0.61
2:E:4184:MET:HE2	2:E:4188:ARG:HA	1.82	0.61
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.34	0.61
2:I:4855:ALA:HA	2:I:4859:PHE:HB2	1.83	0.61
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.82	0.61
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.98	0.61
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.80	0.61
2:I:1973:GLN:O	2:I:1977:TYR:N	2.33	0.61
1:J:6:THR:HA	1:J:72:ALA:HA	1.81	0.61
2:B:18:ASP:HB2	2:B:69:LEU:HD12	1.82	0.61
2:B:1973:GLN:O	2:B:1977:TYR:N	2.33	0.61
2:E:34:LYS:H	2:E:53:SER:HG	1.49	0.61
2:G:4184:MET:HE2	2:G:4188:ARG:HA	1.82	0.61
2:I:4581:LYS:HB2	2:I:4632:LEU:HB2	1.81	0.61
2:E:609:CYS:SG	2:E:610:ASN:N	2.74	0.61
1:H:6:THR:HA	1:H:72:ALA:HA	1.81	0.61
2:G:261:ARG:HB3	2:G:283:ARG:HB3	1.82	0.61
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.34	0.61
2:G:4855:ALA:HA	2:G:4859:PHE:HB2	1.83	0.61
2:I:609:CYS:SG	2:I:610:ASN:N	2.74	0.61
2:I:1211:LEU:HD11	2:I:1225:PRO:HB3	1.83	0.61
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.83	0.60
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.74	0.60
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.83	0.60
2:B:609:CYS:SG	2:B:610:ASN:N	2.74	0.60
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.83	0.60
2:B:4184:MET:HE2	2:B:4188:ARG:HA	1.82	0.60
2:G:1211:LEU:HD11	2:G:1225:PRO:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.83	0.60
2:E:4855:ALA:HA	2:E:4859:PHE:HB2	1.83	0.60
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.98	0.60
2:I:1777:PHE:HA	2:I:1799:SER:HB2	1.84	0.60
2:E:261:ARG:HB3	2:E:283:ARG:HB3	1.82	0.60
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.35	0.60
2:E:1211:LEU:HD11	2:E:1225:PRO:HB3	1.83	0.60
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.34	0.60
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.83	0.60
2:B:4855:ALA:HA	2:B:4859:PHE:HB2	1.83	0.60
2:E:1721:GLU:O	2:E:1725:ARG:NH2	2.35	0.60
2:I:639:ASN:H	2:I:678:GLN:HE22	1.49	0.60
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.34	0.60
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.98	0.60
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.83	0.60
2:B:1721:GLU:O	2:B:1725:ARG:NH2	2.35	0.60
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.34	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.60
2:G:1777:PHE:HA	2:G:1799:SER:HB2	1.84	0.60
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.82	0.60
2:G:3732:SER:O	2:G:3769:ARG:NH2	2.35	0.60
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.74	0.60
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.34	0.60
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.35	0.59
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.34	0.59
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.84	0.59
2:I:4184:MET:HE2	2:I:4188:ARG:HA	1.82	0.59
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.83	0.59
2:B:1218:GLY:HA2	2:B:1223:PHE:HB2	1.84	0.59
2:B:3732:SER:O	2:B:3769:ARG:NH2	2.35	0.59
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.68	0.59
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.35	0.59
2:E:1218:GLY:HA2	2:E:1223:PHE:HB2	1.84	0.59
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.35	0.59
2:G:1101:ARG:HE	2:G:1115:LEU:HB3	1.67	0.59
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.84	0.59
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.84	0.59
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.84	0.59
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.84	0.59
2:I:1721:GLU:O	2:I:1725:ARG:NH2	2.35	0.59
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1211:LEU:HD11	2:B:1225:PRO:HB3	1.83	0.59
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.67	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.83	0.59
2:B:1721:GLU:HG2	2:B:1725:ARG:HH12	1.67	0.59
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.84	0.59
2:I:3732:SER:O	2:I:3769:ARG:NH2	2.35	0.59
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.85	0.59
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.84	0.59
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.84	0.59
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.85	0.59
2:E:1101:ARG:HE	2:E:1115:LEU:HB3	1.67	0.59
2:E:1721:GLU:HG2	2:E:1725:ARG:HH12	1.67	0.59
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.84	0.59
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.84	0.59
2:B:232:THR:HB	2:B:252:VAL:HG11	1.85	0.59
2:E:4056:GLU:HA	2:E:4059:LEU:HB2	1.85	0.59
2:G:1721:GLU:O	2:G:1725:ARG:NH2	2.35	0.59
2:E:315:CYS:SG	2:E:316:PHE:N	2.76	0.59
2:E:1091:GLU:HB3	2:E:1203:ASN:HB3	1.85	0.59
2:E:3990:VAL:HG13	2:E:4051:SER:HB2	1.84	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.74	0.59
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.84	0.59
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.84	0.59
2:E:3732:SER:O	2:E:3769:ARG:NH2	2.35	0.59
2:G:3990:VAL:HG13	2:G:4051:SER:HB2	1.84	0.59
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.67	0.59
2:I:34:LYS:H	2:I:53:SER:HG	1.49	0.59
2:I:3990:VAL:HG13	2:I:4051:SER:HB2	1.84	0.59
2:B:1777:PHE:HA	2:B:1799:SER:HB2	1.84	0.58
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.58
2:I:1865:MET:N	2:I:1865:MET:SD	2.76	0.58
2:I:4083:ASP:HA	2:I:4085:ARG:HH11	1.68	0.58
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.68	0.58
2:B:34:LYS:H	2:B:53:SER:HG	1.49	0.58
2:B:157:ARG:NH2	2:B:167:ASP:OD1	2.36	0.58
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.68	0.58
2:E:1777:PHE:HA	2:E:1799:SER:HB2	1.84	0.58
2:E:2440:MET:O	2:E:2444:GLN:N	2.36	0.58
2:G:315:CYS:SG	2:G:316:PHE:N	2.76	0.58
2:G:1091:GLU:HB3	2:G:1203:ASN:HB3	1.85	0.58
2:G:1218:GLY:HA2	2:G:1223:PHE:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1721:GLU:HG2	2:G:1725:ARG:HH12	1.67	0.58
2:G:4083:ASP:HA	2:G:4085:ARG:HH11	1.68	0.58
2:I:736:HIS:HB3	1:J:8:SER:H	1.68	0.58
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.58
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.84	0.58
2:I:157:ARG:NH2	2:I:167:ASP:OD1	2.36	0.58
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.34	0.58
2:B:3843:ASP:H	2:B:3874:VAL:HG13	1.69	0.58
2:B:4843:LEU:HD12	2:E:4823:LEU:HD21	1.85	0.58
2:G:157:ARG:NH2	2:G:167:ASP:OD1	2.36	0.58
2:G:731:THR:OG1	2:G:1519:UNK:O	2.20	0.58
1:H:27:THR:HB	1:H:100:ASP:HB3	1.86	0.58
2:I:1101:ARG:HE	2:I:1115:LEU:HB3	1.67	0.58
2:I:1218:GLY:HA2	2:I:1223:PHE:HB2	1.84	0.58
2:E:2281:ILE:HG23	2:E:2341:VAL:HG11	1.86	0.58
2:E:4105:GLY:HA2	2:E:4108:ILE:HD12	1.86	0.58
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.74	0.58
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.68	0.58
2:I:315:CYS:SG	2:I:316:PHE:N	2.76	0.58
2:I:2281:ILE:HG23	2:I:2341:VAL:HG11	1.86	0.58
2:I:3843:ASP:H	2:I:3874:VAL:HG13	1.69	0.58
2:B:1091:GLU:HB3	2:B:1203:ASN:HB3	1.85	0.58
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.84	0.58
2:B:1865:MET:N	2:B:1865:MET:SD	2.77	0.58
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.84	0.58
2:G:2281:ILE:HG23	2:G:2341:VAL:HG11	1.86	0.58
2:I:1271:ARG:HA	2:I:1471:UNK:HA	1.85	0.58
2:I:1721:GLU:HG2	2:I:1725:ARG:HH12	1.67	0.58
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.84	0.58
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.84	0.58
2:G:4056:GLU:HA	2:G:4059:LEU:HB2	1.84	0.58
2:I:2440:MET:O	2:I:2444:GLN:N	2.36	0.58
1:J:27:THR:HB	1:J:100:ASP:HB3	1.86	0.58
2:B:315:CYS:SG	2:B:316:PHE:N	2.76	0.58
2:B:3990:VAL:HG13	2:B:4051:SER:HB2	1.85	0.58
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.85	0.58
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.34	0.58
2:G:4105:GLY:HA2	2:G:4108:ILE:HD12	1.86	0.58
2:I:645:ARG:N	2:I:824:GLU:O	2.37	0.58
1:A:27:THR:HB	1:A:100:ASP:HB3	1.86	0.58
2:B:4105:GLY:HA2	2:B:4108:ILE:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.84	0.58
2:E:157:ARG:NH2	2:E:167:ASP:OD1	2.36	0.58
2:E:232:THR:HB	2:E:252:VAL:HG11	1.85	0.58
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.85	0.58
2:G:1865:MET:N	2:G:1865:MET:SD	2.76	0.58
2:G:3843:ASP:H	2:G:3874:VAL:HG13	1.69	0.58
2:G:4918:ILE:HD13	2:I:4892:ARG:HD3	1.85	0.58
2:I:232:THR:HB	2:I:252:VAL:HG11	1.85	0.58
2:B:4056:GLU:HA	2:B:4059:LEU:HB2	1.85	0.57
2:E:3843:ASP:H	2:E:3874:VAL:HG13	1.69	0.57
1:F:27:THR:HB	1:F:100:ASP:HB3	1.86	0.57
2:G:1727:ARG:HH12	2:G:1772:ARG:HB3	1.69	0.57
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.57
2:I:4056:GLU:HA	2:I:4059:LEU:HB2	1.85	0.57
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.86	0.57
2:B:1101:ARG:HE	2:B:1115:LEU:HB3	1.67	0.57
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.85	0.57
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.86	0.57
2:E:1865:MET:N	2:E:1865:MET:SD	2.76	0.57
2:I:1091:GLU:HB3	2:I:1203:ASN:HB3	1.85	0.57
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.68	0.57
2:G:650:VAL:HB	2:G:777:PHE:HB2	1.87	0.57
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.37	0.57
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.86	0.57
2:B:2281:ILE:HG23	2:B:2341:VAL:HG11	1.86	0.57
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.87	0.57
2:I:1727:ARG:HH12	2:I:1772:ARG:HB3	1.70	0.57
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.68	0.57
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.37	0.57
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.38	0.57
2:G:232:THR:HB	2:G:252:VAL:HG11	1.85	0.57
2:I:650:VAL:HB	2:I:777:PHE:HB2	1.87	0.57
2:E:4151:SER:HA	2:E:4160:LEU:HD21	1.86	0.57
2:E:4899:ASP:OD1	2:G:4892:ARG:NH2	2.32	0.57
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.70	0.57
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.37	0.57
2:I:4105:GLY:HA2	2:I:4108:ILE:HD12	1.86	0.57
2:B:4083:ASP:HA	2:B:4085:ARG:HH11	1.68	0.57
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.57
2:I:488:LEU:O	2:I:492:ASP:N	2.37	0.57
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:VAL:HB	2:B:777:PHE:HB2	1.87	0.57
2:B:1727:ARG:HH12	2:B:1772:ARG:HB3	1.70	0.57
2:E:650:VAL:HB	2:E:777:PHE:HB2	1.87	0.57
2:E:4012:LEU:O	2:E:4016:LEU:N	2.38	0.57
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.74	0.57
2:E:4083:ASP:HA	2:E:4085:ARG:HH11	1.68	0.57
2:G:4151:SER:HA	2:G:4160:LEU:HD21	1.86	0.57
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.70	0.57
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.86	0.56
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.56
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.38	0.56
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.88	0.56
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.56
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.37	0.56
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.88	0.56
2:G:488:LEU:O	2:G:492:ASP:N	2.37	0.56
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.87	0.56
1:A:34:LYS:NZ	2:B:635:THR:O	2.37	0.56
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.68	0.56
2:B:396:GLU:O	2:B:400:ALA:N	2.36	0.56
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.56
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.70	0.56
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.88	0.56
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.38	0.56
2:E:4054:ASN:ND2	2:E:4057:MET:SD	2.79	0.56
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.38	0.56
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.88	0.56
2:B:1636:MET:HE2	2:B:1638:ALA:HB2	1.88	0.56
2:B:4054:ASN:ND2	2:B:4057:MET:SD	2.79	0.56
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.39	0.56
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.88	0.56
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.38	0.56
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.86	0.56
2:E:1727:ARG:HH12	2:E:1772:ARG:HB3	1.70	0.56
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.88	0.56
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.39	0.56
1:A:62:GLY:HA3	1:A:74:LEU:HD21	1.87	0.56
1:H:62:GLY:HA3	1:H:74:LEU:HD21	1.87	0.56
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.38	0.56
2:B:451:TYR:O	2:B:474:ARG:NH1	2.39	0.56
2:E:645:ARG:N	2:E:824:GLU:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.70	0.56
2:G:451:TYR:O	2:G:474:ARG:NH1	2.39	0.56
2:I:4054:ASN:ND2	2:I:4057:MET:SD	2.79	0.56
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.39	0.56
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.87	0.56
2:E:635:THR:O	1:F:34:LYS:NZ	2.36	0.56
2:B:3992:PHE:O	2:B:3996:PHE:N	2.36	0.56
2:B:4151:SER:HA	2:B:4160:LEU:HD21	1.86	0.56
1:F:62:GLY:HA3	1:F:74:LEU:HD21	1.87	0.56
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.86	0.56
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.38	0.56
1:J:62:GLY:HA3	1:J:74:LEU:HD21	1.87	0.56
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.38	0.55
2:E:451:TYR:O	2:E:474:ARG:NH1	2.39	0.55
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.39	0.55
2:G:4054:ASN:ND2	2:G:4057:MET:SD	2.79	0.55
2:I:1713:ASP:O	2:I:1717:SER:N	2.39	0.55
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.89	0.55
2:G:4012:LEU:O	2:G:4016:LEU:N	2.38	0.55
2:I:736:HIS:HB2	1:J:7:ILE:HG23	1.87	0.55
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.88	0.55
2:B:647:ASN:ND2	2:B:820:ARG:O	2.39	0.55
2:E:488:LEU:O	2:E:492:ASP:N	2.37	0.55
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.55
2:E:728:ARG:NH2	2:E:1527:UNK:O	2.39	0.55
2:G:1636:MET:HE2	2:G:1638:ALA:HB2	1.88	0.55
2:I:4151:SER:HA	2:I:4160:LEU:HD21	1.86	0.55
2:E:1667:LEU:O	2:E:1671:ARG:NH1	2.40	0.55
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.87	0.55
2:E:4958:CYS:SG	2:E:4959:PHE:N	2.79	0.55
2:I:1636:MET:HE2	2:I:1638:ALA:HB2	1.88	0.55
2:E:396:GLU:O	2:E:400:ALA:N	2.36	0.55
2:E:1231:GLN:NE2	2:E:1821:ASP:O	2.40	0.55
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.89	0.55
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.55
2:B:4012:LEU:O	2:B:4016:LEU:N	2.38	0.55
2:G:2013:LYS:HA	2:G:2028:ARG:HB2	1.89	0.55
2:E:1241:SER:HA	2:E:1603:VAL:HA	1.88	0.55
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.55
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.87	0.55
2:B:2440:MET:O	2:B:2444:GLN:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1231:GLN:NE2	2:G:1821:ASP:O	2.40	0.55
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.89	0.55
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.37	0.55
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.88	0.55
2:E:4152:GLU:OE1	2:E:4192:ARG:NH1	2.40	0.55
2:E:4215:ARG:HA	2:E:4218:ILE:HD12	1.89	0.55
2:G:4958:CYS:SG	2:G:4959:PHE:N	2.80	0.55
2:I:451:TYR:O	2:I:474:ARG:NH1	2.39	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.55
2:B:1241:SER:HA	2:B:1603:VAL:HA	1.88	0.55
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.37	0.55
2:B:4958:CYS:SG	2:B:4959:PHE:N	2.79	0.55
2:E:4218:ILE:HG23	2:E:4954:MET:HE3	1.89	0.55
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.89	0.55
2:G:1667:LEU:O	2:G:1671:ARG:NH1	2.40	0.55
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.89	0.55
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.40	0.55
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.88	0.55
2:I:4012:LEU:O	2:I:4016:LEU:N	2.38	0.55
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.87	0.55
2:B:1667:LEU:O	2:B:1671:ARG:NH1	2.40	0.54
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.89	0.54
2:E:731:THR:OG1	2:E:1519:UNK:O	2.25	0.54
2:E:3992:PHE:O	2:E:3996:PHE:N	2.36	0.54
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.40	0.54
2:G:2185:ILE:HA	2:G:2188:ASN:HD21	1.72	0.54
2:G:2440:MET:O	2:G:2444:GLN:N	2.36	0.54
2:G:4201:ASN:O	2:G:4205:TRP:N	2.39	0.54
2:I:4958:CYS:SG	2:I:4959:PHE:N	2.79	0.54
2:B:1231:GLN:NE2	2:B:1821:ASP:O	2.40	0.54
2:B:2013:LYS:HA	2:B:2028:ARG:HB2	1.89	0.54
2:E:1636:MET:HE2	2:E:1638:ALA:HB2	1.88	0.54
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.89	0.54
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.40	0.54
2:G:34:LYS:H	2:G:53:SER:HG	1.53	0.54
2:G:1241:SER:HA	2:G:1603:VAL:HA	1.88	0.54
2:I:1241:SER:HA	2:I:1603:VAL:HA	1.88	0.54
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.89	0.54
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.40	0.54
2:E:627:PRO:HB2	1:F:92:PRO:HD3	1.89	0.54
2:G:1258:ALA:HB3	2:G:1271:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1258:ALA:HB3	2:I:1271:ARG:HB3	1.90	0.54
2:I:1667:LEU:O	2:I:1671:ARG:NH1	2.40	0.54
2:I:2013:LYS:HA	2:I:2028:ARG:HB2	1.89	0.54
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.40	0.54
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.40	0.54
2:I:2185:ILE:HA	2:I:2188:ASN:HD21	1.73	0.54
2:I:4961:CYS:SG	2:I:4978:HIS:NE2	2.80	0.54
2:B:1713:ASP:O	2:B:1717:SER:N	2.39	0.54
2:B:4215:ARG:HA	2:B:4218:ILE:HD12	1.89	0.54
2:E:647:ASN:ND2	2:E:820:ARG:O	2.39	0.54
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	1.89	0.54
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.90	0.54
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.89	0.54
2:I:1231:GLN:NE2	2:I:1821:ASP:O	2.40	0.54
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.89	0.54
2:B:4201:ASN:O	2:B:4205:TRP:N	2.39	0.54
2:E:1854:PHE:HD1	2:E:1858:ASP:HB3	1.73	0.54
2:E:2185:ILE:HA	2:E:2188:ASN:HD21	1.72	0.54
1:F:87:HIS:N	1:F:91:ILE:O	2.41	0.54
1:H:87:HIS:N	1:H:91:ILE:O	2.41	0.54
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.54
1:J:87:HIS:N	1:J:91:ILE:O	2.41	0.54
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.90	0.54
2:E:4546:VAL:O	2:E:4550:LYS:N	2.38	0.54
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	1.88	0.54
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.40	0.54
2:B:4152:GLU:OE1	2:B:4192:ARG:NH1	2.40	0.54
2:G:4961:CYS:SG	2:G:4978:HIS:NE2	2.80	0.54
2:B:1258:ALA:HB3	2:B:1271:ARG:HB3	1.90	0.54
2:B:4558:ASN:OD1	2:B:4558:ASN:N	2.39	0.54
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.90	0.54
2:E:3806:ASN:HA	2:E:3890:LEU:HD13	1.90	0.54
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.90	0.54
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.89	0.54
2:G:4215:ARG:HA	2:G:4218:ILE:HD12	1.89	0.54
2:I:396:GLU:O	2:I:400:ALA:N	2.36	0.54
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.90	0.53
2:B:4961:CYS:SG	2:B:4978:HIS:NE2	2.80	0.53
2:E:206:CYS:SG	2:E:207:SER:N	2.82	0.53
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.91	0.53
2:I:4152:GLU:OE1	2:I:4192:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.73	0.53
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.42	0.53
2:B:4218:ILE:HG23	2:B:4954:MET:HE3	1.89	0.53
2:B:4546:VAL:O	2:B:4550:LYS:N	2.38	0.53
2:E:682:LEU:HD13	2:E:787:VAL:HG11	1.91	0.53
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.90	0.53
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.41	0.53
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.90	0.53
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	1.90	0.53
2:I:3806:ASN:HA	2:I:3890:LEU:HD13	1.90	0.53
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.41	0.53
1:A:87:HIS:N	1:A:91:ILE:O	2.41	0.53
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.90	0.53
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	1.90	0.53
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.89	0.53
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.89	0.53
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.42	0.53
2:G:1854:PHE:HD1	2:G:1858:ASP:HB3	1.73	0.53
2:G:3932:ASP:HA	2:G:3935:TRP:HD1	1.73	0.53
2:G:3992:PHE:O	2:G:3996:PHE:N	2.36	0.53
2:G:4218:ILE:HG23	2:G:4954:MET:HE3	1.89	0.53
2:B:206:CYS:SG	2:B:207:SER:N	2.82	0.53
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.34	0.53
2:G:206:CYS:SG	2:G:207:SER:N	2.82	0.53
2:G:637:LEU:HG	2:G:1693:GLN:HB3	1.91	0.53
2:G:1713:ASP:O	2:G:1717:SER:N	2.39	0.53
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.73	0.53
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.90	0.53
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.90	0.53
2:I:4218:ILE:HG23	2:I:4954:MET:HE3	1.89	0.53
2:B:3806:ASN:HA	2:B:3890:LEU:HD13	1.90	0.53
2:E:1258:ALA:HB3	2:E:1271:ARG:HB3	1.90	0.53
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.90	0.53
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.90	0.53
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.42	0.53
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.41	0.53
2:I:4215:ARG:HA	2:I:4218:ILE:HD12	1.89	0.53
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	1.88	0.53
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.73	0.53
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.89	0.53
2:G:682:LEU:HD13	2:G:787:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2132:GLY:O	2:B:2136:ARG:N	2.42	0.53
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.90	0.53
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.90	0.53
2:I:1854:PHE:HD1	2:I:1858:ASP:HB3	1.73	0.53
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.90	0.53
2:E:2368:LEU:HD13	2:E:2376:LEU:HB2	1.91	0.53
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.42	0.53
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.73	0.53
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.74	0.53
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.90	0.53
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.42	0.53
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.42	0.53
2:B:1854:PHE:HD1	2:B:1858:ASP:HB3	1.73	0.53
2:E:278:GLN:N	2:E:315:CYS:SG	2.82	0.53
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	1.90	0.53
2:E:1773:PRO:HB3	2:E:2153:MET:HE1	1.91	0.53
2:E:2013:LYS:HA	2:E:2028:ARG:HB2	1.89	0.53
2:E:3552:UNK:O	2:E:3556:UNK:N	2.42	0.53
2:I:637:LEU:HG	2:I:1693:GLN:HB3	1.91	0.53
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.74	0.53
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.91	0.53
2:B:1659:LEU:O	2:B:1663:HIS:N	2.40	0.53
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.90	0.53
2:E:4560:TYR:O	2:E:4564:PHE:N	2.40	0.53
2:G:124:SER:HA	2:G:132:ALA:HB3	1.91	0.53
2:G:3904:ARG:NH2	2:G:3973:CYS:SG	2.82	0.53
2:G:4152:GLU:OE1	2:G:4192:ARG:NH1	2.40	0.53
2:I:124:SER:HA	2:I:132:ALA:HB3	1.91	0.53
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	1.89	0.53
2:B:682:LEU:HD13	2:B:787:VAL:HG11	1.90	0.52
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.74	0.52
2:E:637:LEU:HG	2:E:1693:GLN:HB3	1.91	0.52
2:E:1713:ASP:O	2:E:1717:SER:N	2.39	0.52
2:E:4201:ASN:O	2:E:4205:TRP:N	2.39	0.52
2:I:278:GLN:N	2:I:315:CYS:SG	2.82	0.52
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.91	0.52
2:B:2185:ILE:HA	2:B:2188:ASN:HD21	1.72	0.52
2:B:3552:UNK:O	2:B:3556:UNK:N	2.42	0.52
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.41	0.52
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.42	0.52
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4956:THR:O	2:E:4965:SER:N	2.42	0.52
2:G:645:ARG:N	2:G:824:GLU:O	2.37	0.52
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.92	0.52
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.42	0.52
2:G:3882:GLN:HB2	2:G:3957:VAL:HG22	1.91	0.52
2:G:4780:PHE:O	2:G:4784:PHE:N	2.40	0.52
2:I:2132:GLY:O	2:I:2136:ARG:N	2.42	0.52
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.42	0.52
2:B:4780:PHE:O	2:B:4784:PHE:N	2.40	0.52
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.91	0.52
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.90	0.52
2:E:3932:ASP:HA	2:E:3935:TRP:HD1	1.73	0.52
2:G:396:GLU:O	2:G:400:ALA:N	2.36	0.52
2:G:1046:LEU:HB3	2:G:1051:TYR:HB2	1.92	0.52
2:G:2257:LEU:O	2:G:2261:SER:N	2.43	0.52
2:G:3552:UNK:O	2:G:3556:UNK:N	2.43	0.52
2:G:4040:ILE:O	2:G:4044:MET:N	2.43	0.52
2:G:4998:LYS:HB3	2:G:5003:HIS:HE1	1.74	0.52
2:I:206:CYS:SG	2:I:207:SER:N	2.82	0.52
2:I:1694:LEU:O	2:I:1712:TYR:OH	2.21	0.52
2:I:1773:PRO:HB3	2:I:2153:MET:HE1	1.91	0.52
2:I:3904:ARG:NH2	2:I:3973:CYS:SG	2.82	0.52
2:B:488:LEU:O	2:B:492:ASP:N	2.36	0.52
2:B:1071:ARG:HD3	2:B:1241:SER:HB3	1.92	0.52
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.42	0.52
2:B:2336:ARG:HD3	2:B:2435:ARG:HD2	1.92	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.42	0.52
2:E:4745:LEU:O	2:E:4749:GLU:N	2.41	0.52
2:E:4913:ARG:HA	2:E:4916:PHE:HB3	1.92	0.52
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.21	0.52
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.91	0.52
2:G:2132:GLY:O	2:G:2136:ARG:N	2.42	0.52
2:I:242:ARG:O	2:I:289:ARG:NH1	2.43	0.52
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.91	0.52
2:B:124:SER:HA	2:B:132:ALA:HB3	1.91	0.52
2:B:4913:ARG:HA	2:B:4916:PHE:HB3	1.91	0.52
2:E:1046:LEU:HB3	2:E:1051:TYR:HB2	1.92	0.52
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.92	0.52
2:G:647:ASN:ND2	2:G:820:ARG:O	2.39	0.52
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.42	0.52
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1046:LEU:HB3	2:I:1051:TYR:HB2	1.92	0.52
2:B:645:ARG:N	2:B:824:GLU:O	2.37	0.52
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.43	0.52
2:B:1046:LEU:HB3	2:B:1051:TYR:HB2	1.92	0.52
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.91	0.52
2:B:3932:ASP:HA	2:B:3935:TRP:HD1	1.73	0.52
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.91	0.52
2:B:4956:THR:O	2:B:4965:SER:N	2.42	0.52
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.74	0.52
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.91	0.52
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.91	0.52
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	1.92	0.52
2:I:2336:ARG:HD3	2:I:2435:ARG:HD2	1.92	0.52
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.43	0.52
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.92	0.52
2:E:2336:ARG:HD3	2:E:2435:ARG:HD2	1.92	0.52
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	1.90	0.52
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.37	0.52
2:I:4201:ASN:O	2:I:4205:TRP:N	2.39	0.52
2:I:4998:LYS:HB3	2:I:5003:HIS:HE1	1.74	0.52
2:B:637:LEU:HG	2:B:1693:GLN:HB3	1.91	0.52
2:B:2368:LEU:HD13	2:B:2376:LEU:HB2	1.91	0.52
2:B:4998:LYS:HB3	2:B:5003:HIS:HE1	1.74	0.52
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	1.92	0.52
2:E:3882:GLN:HB2	2:E:3957:VAL:HG22	1.91	0.52
2:G:139:GLU:O	2:G:141:ALA:N	2.43	0.52
2:G:1773:PRO:HB3	2:G:2153:MET:HE1	1.91	0.52
2:G:3806:ASN:HA	2:G:3890:LEU:HD13	1.90	0.52
2:I:682:LEU:HD13	2:I:787:VAL:HG11	1.91	0.52
2:I:731:THR:OG1	2:I:1519:UNK:O	2.27	0.52
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.92	0.52
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.91	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.24	0.52
2:B:1773:PRO:HB3	2:B:2153:MET:HE1	1.91	0.52
2:B:3882:GLN:HB2	2:B:3957:VAL:HG22	1.91	0.52
2:G:22:LEU:HD22	2:G:200:TRP:HB3	1.92	0.52
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	1.92	0.52
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.91	0.52
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.40	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.52
2:I:3932:ASP:HA	2:I:3935:TRP:HD1	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:LEU:HD22	2:B:200:TRP:HB3	1.92	0.52
2:E:124:SER:HA	2:E:132:ALA:HB3	1.91	0.52
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.43	0.52
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.42	0.52
2:G:43:GLY:N	2:G:447:ASP:OD2	2.43	0.52
2:G:278:GLN:N	2:G:315:CYS:SG	2.82	0.52
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.43	0.52
2:G:1271:ARG:HA	2:G:1471:UNK:HA	1.92	0.52
2:I:880:GLU:OE1	2:I:968:ALA:N	2.43	0.52
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	1.92	0.52
2:B:709:ASP:O	2:B:725:HIS:ND1	2.43	0.51
2:B:880:GLU:OE1	2:B:968:ALA:N	2.43	0.51
2:E:22:LEU:HD22	2:E:200:TRP:HB3	1.92	0.51
2:E:3904:ARG:NH2	2:E:3973:CYS:SG	2.82	0.51
1:F:7:ILE:HG22	1:F:9:PRO:HD2	1.92	0.51
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.51
2:I:709:ASP:O	2:I:725:HIS:ND1	2.43	0.51
2:I:1659:LEU:O	2:I:1663:HIS:N	2.40	0.51
2:I:3552:UNK:O	2:I:3556:UNK:N	2.43	0.51
2:I:4109:GLN:O	2:I:4113:SER:N	2.42	0.51
2:I:4956:THR:O	2:I:4965:SER:N	2.42	0.51
2:E:139:GLU:O	2:E:141:ALA:N	2.43	0.51
2:E:242:ARG:O	2:E:289:ARG:NH1	2.43	0.51
2:E:709:ASP:O	2:E:725:HIS:ND1	2.43	0.51
2:E:1071:ARG:HD3	2:E:1241:SER:HB3	1.92	0.51
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.92	0.51
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.91	0.51
2:E:4998:LYS:HB3	2:E:5003:HIS:HE1	1.74	0.51
2:G:2336:ARG:HD3	2:G:2435:ARG:HD2	1.92	0.51
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.92	0.51
2:I:2257:LEU:O	2:I:2261:SER:N	2.43	0.51
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	1.92	0.51
2:B:139:GLU:O	2:B:141:ALA:N	2.43	0.51
2:B:4697:VAL:O	2:B:4701:TRP:N	2.42	0.51
2:E:742:ASP:OD1	2:E:760:ASN:ND2	2.44	0.51
2:G:111:HIS:CD2	2:G:114:SER:H	2.24	0.51
2:G:2368:LEU:HD13	2:G:2376:LEU:HB2	1.91	0.51
2:I:139:GLU:O	2:I:141:ALA:N	2.43	0.51
2:I:2368:LEU:HD13	2:I:2376:LEU:HB2	1.91	0.51
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.51
2:I:4780:PHE:O	2:I:4784:PHE:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HG22	1:A:9:PRO:HD2	1.92	0.51
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.91	0.51
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.74	0.51
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.51
2:B:3904:ARG:NH2	2:B:3973:CYS:SG	2.82	0.51
2:B:4044:MET:HA	2:B:4047:MET:HG2	1.92	0.51
2:G:242:ARG:O	2:G:289:ARG:NH1	2.43	0.51
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.91	0.51
2:B:278:GLN:N	2:B:315:CYS:SG	2.82	0.51
2:B:742:ASP:OD1	2:B:760:ASN:ND2	2.44	0.51
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.92	0.51
2:E:1778:SER:N	2:E:1799:SER:O	2.44	0.51
2:E:4040:ILE:O	2:E:4044:MET:N	2.43	0.51
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.37	0.51
2:G:4204:GLN:NE2	2:G:4245:MET:SD	2.84	0.51
2:B:242:ARG:O	2:B:289:ARG:NH1	2.43	0.51
2:E:880:GLU:OE1	2:E:968:ALA:N	2.42	0.51
2:E:2257:LEU:O	2:E:2261:SER:N	2.43	0.51
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.51
2:E:4697:VAL:O	2:E:4701:TRP:N	2.42	0.51
2:G:709:ASP:O	2:G:725:HIS:ND1	2.43	0.51
2:G:1071:ARG:HD3	2:G:1241:SER:HB3	1.92	0.51
1:H:7:ILE:HG22	1:H:9:PRO:HD2	1.92	0.51
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.92	0.51
2:B:4560:TYR:O	2:B:4564:PHE:N	2.40	0.51
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.76	0.51
2:E:2235:PHE:HA	2:E:2238:TYR:HD2	1.75	0.51
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.76	0.51
2:G:4913:ARG:HA	2:G:4916:PHE:HB3	1.92	0.51
2:I:647:ASN:ND2	2:I:820:ARG:O	2.39	0.51
2:I:742:ASP:OD1	2:I:760:ASN:ND2	2.44	0.51
2:I:3882:GLN:HB2	2:I:3957:VAL:HG22	1.91	0.51
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.76	0.51
2:B:2257:LEU:O	2:B:2261:SER:N	2.43	0.51
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.93	0.51
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	1.92	0.51
2:E:4041:ALA:HA	2:E:4044:MET:HB2	1.93	0.51
2:G:1778:SER:N	2:G:1799:SER:O	2.44	0.51
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	1.92	0.51
2:E:173:SER:HB3	2:E:178:ARG:H	1.76	0.51
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4044:MET:HA	2:E:4047:MET:HG2	1.92	0.51
2:G:252:VAL:HA	2:G:255:HIS:HB2	1.93	0.51
2:I:22:LEU:HD22	2:I:200:TRP:HB3	1.92	0.51
2:I:173:SER:HB3	2:I:178:ARG:H	1.76	0.51
2:I:1071:ARG:HD3	2:I:1241:SER:HB3	1.92	0.51
1:J:7:ILE:HG22	1:J:9:PRO:HD2	1.92	0.51
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.91	0.51
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.51
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	1.92	0.51
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.76	0.51
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.93	0.51
2:G:4044:MET:HA	2:G:4047:MET:HG2	1.92	0.51
2:I:4204:GLN:NE2	2:I:4245:MET:SD	2.83	0.51
2:I:4546:VAL:O	2:I:4550:LYS:N	2.38	0.51
2:B:4204:GLN:NE2	2:B:4245:MET:SD	2.84	0.50
2:E:252:VAL:HA	2:E:255:HIS:HB2	1.93	0.50
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	1.93	0.50
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.91	0.50
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.93	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.50
2:I:111:HIS:CD2	2:I:114:SER:H	2.24	0.50
2:G:118:LEU:HD12	2:G:137:LEU:HB3	1.94	0.50
2:G:742:ASP:OD1	2:G:760:ASN:ND2	2.44	0.50
2:G:932:LEU:HD23	2:G:935:LEU:HD12	1.94	0.50
2:G:4041:ALA:HA	2:G:4044:MET:HB2	1.93	0.50
2:G:4064:MET:HA	2:G:4067:LYS:HG2	1.93	0.50
2:I:43:GLY:N	2:I:447:ASP:OD2	2.43	0.50
2:I:4913:ARG:HA	2:I:4916:PHE:HB3	1.92	0.50
2:B:173:SER:HB3	2:B:178:ARG:H	1.76	0.50
2:B:252:VAL:HA	2:B:255:HIS:HB2	1.93	0.50
2:B:1778:SER:N	2:B:1799:SER:O	2.44	0.50
2:B:4041:ALA:HA	2:B:4044:MET:HB2	1.93	0.50
2:E:932:LEU:HD23	2:E:935:LEU:HD12	1.94	0.50
2:G:914:PRO:O	2:G:918:ARG:N	2.45	0.50
2:G:4546:VAL:O	2:G:4550:LYS:N	2.38	0.50
2:I:4040:ILE:O	2:I:4044:MET:N	2.43	0.50
2:E:988:LEU:O	2:E:992:GLY:N	2.44	0.50
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.93	0.50
2:E:4782:VAL:O	2:E:4785:THR:OG1	2.29	0.50
2:E:4934:GLY:HA3	2:G:4937:ILE:HD12	1.94	0.50
2:G:78:LEU:O	2:G:82:LEU:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1203:ASN:ND2	2:G:1210:SER:O	2.45	0.50
2:B:118:LEU:HD12	2:B:137:LEU:HB3	1.94	0.50
2:B:2235:PHE:HA	2:B:2238:TYR:HD2	1.75	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.76	0.50
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.93	0.50
2:G:395:GLN:HG3	2:G:397:GLU:H	1.76	0.50
2:G:635:THR:O	1:H:34:LYS:NZ	2.44	0.50
2:G:2235:PHE:HA	2:G:2238:TYR:HD2	1.76	0.50
2:G:4560:TYR:O	2:G:4564:PHE:N	2.40	0.50
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	1.93	0.50
2:I:932:LEU:HD23	2:I:935:LEU:HD12	1.94	0.50
2:I:1778:SER:N	2:I:1799:SER:O	2.44	0.50
2:I:1817:GLU:O	2:I:1821:ASP:N	2.42	0.50
2:I:2205:GLU:HG2	2:I:2253:HIS:HE1	1.77	0.50
2:I:2235:PHE:HA	2:I:2238:TYR:HD2	1.75	0.50
2:I:4044:MET:HA	2:I:4047:MET:HG2	1.92	0.50
2:B:43:GLY:N	2:B:447:ASP:OD2	2.43	0.50
2:B:131:LEU:HB3	2:E:2459:SER:HB2	1.93	0.50
2:B:4745:LEU:O	2:B:4749:GLU:N	2.41	0.50
2:E:43:GLY:N	2:E:447:ASP:OD2	2.43	0.50
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.92	0.50
2:I:118:LEU:HD12	2:I:137:LEU:HB3	1.94	0.50
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.92	0.50
2:E:317:ARG:N	2:E:347:PHE:O	2.45	0.50
2:E:4064:MET:HA	2:E:4067:LYS:HG2	1.93	0.50
2:G:880:GLU:OE1	2:G:968:ALA:N	2.42	0.50
2:G:1647:CYS:SG	2:G:1648:MET:N	2.85	0.50
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.43	0.50
2:I:4041:ALA:HA	2:I:4044:MET:HB2	1.93	0.50
2:I:4558:ASN:OD1	2:I:4558:ASN:N	2.39	0.50
2:I:4990:PHE:O	2:I:4994:TYR:N	2.43	0.50
2:B:4565:LEU:O	2:B:4569:LEU:N	2.37	0.50
2:E:78:LEU:O	2:E:82:LEU:N	2.43	0.50
2:E:1970:GLN:HB2	2:E:3642:TYR:HA	1.94	0.50
2:G:173:SER:HB3	2:G:178:ARG:H	1.76	0.50
2:B:731:THR:OG1	2:B:1519:UNK:O	2.30	0.50
2:B:1647:CYS:SG	2:B:1648:MET:N	2.85	0.50
2:E:1659:LEU:O	2:E:1663:HIS:N	2.40	0.50
2:E:2132:GLY:O	2:E:2136:ARG:N	2.42	0.50
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.94	0.50
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2205:GLU:HG2	2:G:2253:HIS:HE1	1.77	0.50
2:G:4956:THR:O	2:G:4965:SER:N	2.42	0.50
2:I:252:VAL:HA	2:I:255:HIS:HB2	1.93	0.50
2:I:1647:CYS:SG	2:I:1648:MET:N	2.85	0.50
2:I:3992:PHE:O	2:I:3996:PHE:N	2.36	0.50
2:B:932:LEU:HD23	2:B:935:LEU:HD12	1.94	0.49
2:B:1203:ASN:ND2	2:B:1210:SER:O	2.45	0.49
2:B:2205:GLU:HG2	2:B:2253:HIS:HE1	1.77	0.49
2:E:330:ASP:OD1	2:E:330:ASP:N	2.45	0.49
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	1.94	0.49
2:E:3974:THR:HA	2:E:3977:GLN:HB2	1.94	0.49
2:G:229:GLU:OE2	2:G:374:LYS:NZ	2.41	0.49
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.93	0.49
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.94	0.49
2:E:2205:GLU:HG2	2:E:2253:HIS:HE1	1.77	0.49
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.48	0.49
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.94	0.49
2:B:1294:UNK:HA	2:B:1455:UNK:HA	1.95	0.49
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.94	0.49
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.94	0.49
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.45	0.49
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.93	0.49
2:I:4745:LEU:O	2:I:4749:GLU:N	2.41	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.77	0.49
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.94	0.49
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.45	0.49
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.46	0.49
2:B:4040:ILE:O	2:B:4044:MET:N	2.43	0.49
2:B:4823:LEU:HD21	2:I:4843:LEU:HD12	1.94	0.49
2:E:5014:TYR:HD1	2:E:5019:TRP:HH2	1.60	0.49
2:G:1659:LEU:O	2:G:1663:HIS:N	2.40	0.49
2:G:1817:GLU:O	2:G:1821:ASP:N	2.42	0.49
2:G:3974:THR:HA	2:G:3977:GLN:HB2	1.94	0.49
2:I:988:LEU:O	2:I:992:GLY:N	2.44	0.49
2:B:317:ARG:N	2:B:347:PHE:O	2.45	0.49
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.47	0.49
2:B:4815:ASP:O	2:B:4819:GLY:N	2.44	0.49
2:E:1203:ASN:ND2	2:E:1210:SER:O	2.45	0.49
2:E:1647:CYS:SG	2:E:1648:MET:N	2.85	0.49
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.45	0.49
2:G:4945:ASP:HA	2:G:4948:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:78:LEU:O	2:I:82:LEU:N	2.43	0.49
2:I:914:PRO:O	2:I:918:ARG:N	2.45	0.49
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.78	0.49
2:I:4934:GLY:O	2:I:4938:ASP:N	2.41	0.49
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.93	0.49
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.78	0.49
2:B:4782:VAL:O	2:B:4785:THR:OG1	2.29	0.49
2:B:5014:TYR:HD1	2:B:5019:TRP:HH2	1.60	0.49
2:E:475:GLN:NE2	2:E:528:SER:O	2.46	0.49
2:E:914:PRO:O	2:E:918:ARG:N	2.45	0.49
2:E:4710:SER:OG	2:E:4772:ASP:OD2	2.29	0.49
2:G:911:HIS:O	2:G:918:ARG:NH2	2.44	0.49
2:G:1970:GLN:HB2	2:G:3642:TYR:HA	1.94	0.49
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.95	0.49
2:I:728:ARG:NH2	2:I:1527:UNK:O	2.46	0.49
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.46	0.49
2:I:4064:MET:HA	2:I:4067:LYS:HG2	1.93	0.49
2:B:988:LEU:O	2:B:992:GLY:N	2.44	0.49
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.94	0.49
2:E:177:GLU:HG3	2:G:2452:ARG:HH12	1.78	0.49
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.78	0.49
2:G:475:GLN:NE2	2:G:528:SER:O	2.46	0.49
2:G:1693:GLN:HA	2:G:1696:HIS:HB3	1.95	0.49
2:I:1203:ASN:ND2	2:I:1210:SER:O	2.45	0.49
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	1.93	0.49
2:E:118:LEU:HD12	2:E:137:LEU:HB3	1.94	0.49
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.94	0.49
2:E:1693:GLN:HA	2:E:1696:HIS:HB3	1.94	0.49
2:E:4990:PHE:O	2:E:4994:TYR:N	2.43	0.49
2:G:988:LEU:O	2:G:992:GLY:N	2.44	0.49
2:G:2265:LEU:HB3	2:G:2330:ARG:HG2	1.95	0.49
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.28	0.49
2:I:4065:PHE:CE2	2:I:4132:PHE:HB3	2.48	0.49
2:B:261:ARG:HD3	2:B:283:ARG:HD3	1.95	0.49
2:B:1817:GLU:O	2:B:1821:ASP:N	2.42	0.49
2:E:111:HIS:CD2	2:E:114:SER:H	2.24	0.49
2:E:3905:THR:HA	2:E:3912:THR:HG23	1.95	0.49
2:E:4945:ASP:HA	2:E:4948:GLU:HG2	1.95	0.49
2:G:317:ARG:N	2:G:347:PHE:O	2.45	0.49
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.95	0.49
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.46	0.49
2:G:3905:THR:HA	2:G:3912:THR:HG23	1.95	0.49
2:I:395:GLN:HG3	2:I:397:GLU:H	1.76	0.49
2:B:911:HIS:O	2:B:918:ARG:NH2	2.44	0.49
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.95	0.49
2:B:1970:GLN:HB2	2:B:3642:TYR:HA	1.94	0.49
2:B:4109:GLN:O	2:B:4113:SER:N	2.42	0.49
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	1.93	0.49
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.45	0.49
2:E:2265:LEU:HB3	2:E:2330:ARG:HG2	1.95	0.49
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.95	0.49
2:G:4782:VAL:O	2:G:4785:THR:OG1	2.29	0.49
2:I:475:GLN:NE2	2:I:528:SER:O	2.46	0.49
2:B:4064:MET:HA	2:B:4067:LYS:HG2	1.93	0.48
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.95	0.48
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.94	0.48
2:G:1965:TYR:OH	2:G:2027:ILE:O	2.24	0.48
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.95	0.48
2:I:4916:PHE:O	2:I:4920:PHE:N	2.46	0.48
2:B:475:GLN:NE2	2:B:528:SER:O	2.46	0.48
2:B:2265:LEU:HB3	2:B:2330:ARG:HG2	1.95	0.48
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.47	0.48
2:E:4895:GLY:O	2:G:4892:ARG:NH2	2.38	0.48
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.49	0.48
2:I:2265:LEU:HB3	2:I:2330:ARG:HG2	1.95	0.48
2:I:4571:PHE:O	2:I:4575:PHE:N	2.46	0.48
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.78	0.48
2:I:4697:VAL:O	2:I:4701:TRP:N	2.42	0.48
2:I:4945:ASP:HA	2:I:4948:GLU:HG2	1.95	0.48
2:B:914:PRO:O	2:B:918:ARG:N	2.45	0.48
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.95	0.48
2:I:3905:THR:HA	2:I:3912:THR:HG23	1.95	0.48
2:I:4735:GLU:O	2:I:4739:GLU:N	2.47	0.48
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.78	0.48
2:B:4945:ASP:HA	2:B:4948:GLU:HG2	1.95	0.48
2:E:652:ARG:HB3	2:E:773:LEU:HD13	1.96	0.48
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.46	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.95	0.48
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.48	0.48
2:G:4670:ILE:O	2:G:4674:GLU:N	2.38	0.48
2:G:4735:GLU:O	2:G:4739:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.94	0.48
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.96	0.48
2:E:229:GLU:OE2	2:E:374:LYS:NZ	2.41	0.48
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.79	0.48
2:E:2347:GLU:O	2:E:2351:ASN:N	2.36	0.48
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.94	0.48
2:G:4065:PHE:CE2	2:G:4132:PHE:HB3	2.48	0.48
2:G:5014:TYR:HD1	2:G:5019:TRP:HH2	1.60	0.48
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.47	0.48
2:I:1196:PRO:O	2:I:1198:GLN:NE2	2.44	0.48
2:I:2170:MET:HE1	2:I:2210:VAL:HG23	1.96	0.48
2:I:3974:THR:HA	2:I:3977:GLN:HB2	1.94	0.48
2:I:4560:TYR:O	2:I:4564:PHE:N	2.40	0.48
2:I:5014:TYR:HD1	2:I:5019:TRP:HH2	1.60	0.48
2:B:652:ARG:HB3	2:B:773:LEU:HD13	1.96	0.48
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.79	0.48
2:B:2170:MET:HE1	2:B:2210:VAL:HG23	1.96	0.48
2:E:4204:GLN:NE2	2:E:4245:MET:SD	2.84	0.48
2:E:4670:ILE:O	2:E:4674:GLU:N	2.37	0.48
2:G:4916:PHE:O	2:G:4920:PHE:N	2.46	0.48
2:I:261:ARG:HD3	2:I:283:ARG:HD3	1.95	0.48
2:I:1970:GLN:HB2	2:I:3642:TYR:HA	1.94	0.48
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.49	0.48
2:B:3974:THR:HA	2:B:3977:GLN:HB2	1.94	0.48
2:B:4990:PHE:O	2:B:4994:TYR:N	2.44	0.48
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.49	0.48
2:E:4735:GLU:O	2:E:4739:GLU:N	2.47	0.48
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.48
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.79	0.48
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.96	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.95	0.48
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.48
2:E:261:ARG:HD3	2:E:283:ARG:HD3	1.95	0.48
2:E:4065:PHE:CE2	2:E:4132:PHE:HB3	2.48	0.48
2:E:4780:PHE:O	2:E:4784:PHE:N	2.40	0.48
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.43	0.48
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.34	0.48
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.79	0.48
2:G:4697:VAL:O	2:G:4701:TRP:N	2.42	0.48
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.79	0.48
2:I:4822:THR:O	2:I:4825:THR:OG1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.49	0.48
2:B:4065:PHE:CE2	2:B:4132:PHE:HB3	2.48	0.48
2:B:4916:PHE:O	2:B:4920:PHE:N	2.46	0.48
2:E:1663:HIS:O	2:E:1667:LEU:N	2.45	0.48
2:E:4916:PHE:O	2:E:4920:PHE:N	2.46	0.48
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	1.96	0.48
2:G:385:ASP:OD1	2:G:385:ASP:N	2.47	0.48
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.96	0.48
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.49	0.48
2:I:317:ARG:N	2:I:347:PHE:O	2.45	0.48
2:B:1693:GLN:HA	2:B:1696:HIS:HB3	1.94	0.48
2:B:3905:THR:HA	2:B:3912:THR:HG23	1.95	0.48
2:B:4088:ILE:HG23	2:B:4123:ILE:HB	1.95	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.48
2:I:652:ARG:HB3	2:I:773:LEU:HD13	1.96	0.48
2:B:264:PRO:HA	2:B:280:LEU:HA	1.96	0.47
2:B:1931:LEU:HD22	2:B:1935:VAL:HG11	1.96	0.47
2:B:1950:GLU:OE2	2:B:1954:ARG:NH2	2.43	0.47
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.96	0.47
2:B:4833:ASN:ND2	2:B:4939:ALA:HB2	2.29	0.47
2:B:4848:VAL:HG23	2:B:4883:TYR:HE1	1.79	0.47
2:E:1965:TYR:OH	2:E:2027:ILE:O	2.24	0.47
2:G:426:ARG:HG2	2:G:431:PRO:HA	1.96	0.47
2:G:2212:VAL:O	2:G:2216:GLY:N	2.46	0.47
2:G:4558:ASN:OD1	2:G:4558:ASN:N	2.39	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.46	0.47
2:G:4815:ASP:O	2:G:4819:GLY:N	2.44	0.47
2:I:1668:ARG:HA	2:I:1671:ARG:HH11	1.79	0.47
2:I:1693:GLN:HA	2:I:1696:HIS:HB3	1.94	0.47
2:I:1931:LEU:HD22	2:I:1935:VAL:HG11	1.96	0.47
2:I:1952:GLN:HA	2:I:1955:VAL:HG12	1.96	0.47
2:I:2457:LEU:HD23	2:I:2460:LEU:HD12	1.96	0.47
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.96	0.47
2:I:4110:PHE:HA	2:I:4113:SER:HB3	1.96	0.47
2:I:4782:VAL:O	2:I:4785:THR:OG1	2.29	0.47
2:E:2286:LEU:HA	2:E:2289:ALA:HB3	1.97	0.47
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.96	0.47
2:E:5012:LYS:O	2:E:5016:GLU:N	2.43	0.47
2:G:261:ARG:HD3	2:G:283:ARG:HD3	1.95	0.47
2:G:2286:LEU:HA	2:G:2289:ALA:HB3	1.97	0.47
2:G:3771:HIS:O	2:G:3774:GLY:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.46	0.47
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.78	0.47
2:G:3840:SER:OG	2:G:3875:MET:O	2.29	0.47
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.96	0.47
2:G:4110:PHE:HA	2:G:4113:SER:HB3	1.96	0.47
2:I:15:ARG:HD3	2:I:98:HIS:HB3	1.95	0.47
2:I:385:ASP:N	2:I:385:ASP:OD1	2.47	0.47
2:B:111:HIS:N	2:B:116:MET:O	2.37	0.47
2:B:460:GLN:HG2	2:B:462:GLU:H	1.80	0.47
2:B:1044:ARG:HA	2:B:1047:LEU:HD12	1.97	0.47
2:B:2286:LEU:HA	2:B:2289:ALA:HB3	1.97	0.47
2:B:4580:TYR:HB2	2:I:4879:MET:HB2	1.95	0.47
2:B:4813:LEU:HA	2:B:4816:ILE:HG12	1.96	0.47
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.49	0.47
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.49	0.47
2:E:1668:ARG:HA	2:E:1671:ARG:HH11	1.79	0.47
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.47
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.78	0.47
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.49	0.47
2:G:1668:ARG:HA	2:G:1671:ARG:HH11	1.79	0.47
2:G:2170:MET:HE1	2:G:2210:VAL:HG23	1.96	0.47
2:G:4833:ASN:ND2	2:G:4939:ALA:HB2	2.29	0.47
2:G:4848:VAL:HG23	2:G:4883:TYR:HE1	1.79	0.47
2:I:264:PRO:HA	2:I:280:LEU:HA	1.96	0.47
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.49	0.47
2:B:1952:GLN:HA	2:B:1955:VAL:HG12	1.96	0.47
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.96	0.47
2:E:4957:LYS:HE3	2:E:4957:LYS:HB3	1.73	0.47
2:G:4172:GLU:OE1	2:G:4175:ARG:NH1	2.47	0.47
2:I:379:HIS:CD2	2:I:382:GLY:H	2.25	0.47
2:I:4833:ASN:ND2	2:I:4939:ALA:HB2	2.29	0.47
2:B:15:ARG:HD3	2:B:98:HIS:HB3	1.95	0.47
2:B:18:ASP:H	2:B:69:LEU:HB2	1.80	0.47
2:B:870:ILE:HD11	2:B:1049:TYR:CG	2.49	0.47
2:B:2457:LEU:HD23	2:B:2460:LEU:HD12	1.96	0.47
2:E:15:ARG:HD3	2:E:98:HIS:HB3	1.95	0.47
2:E:1240:LYS:O	2:E:1604:SER:N	2.46	0.47
2:E:1931:LEU:HD22	2:E:1935:VAL:HG11	1.97	0.47
2:E:4833:ASN:ND2	2:E:4939:ALA:HB2	2.29	0.47
2:G:15:ARG:HD3	2:G:98:HIS:HB3	1.95	0.47
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1044:ARG:HA	2:G:1047:LEU:HD12	1.97	0.47
2:G:4705:VAL:HB	2:G:4778:TRP:CG	2.49	0.47
2:I:18:ASP:H	2:I:69:LEU:HB2	1.80	0.47
2:I:207:SER:OG	2:I:208:CYS:N	2.48	0.47
2:B:1229:ASN:O	2:B:1827:ARG:N	2.40	0.47
2:B:2869:ARG:HH12	2:B:2945:UNK:C	2.27	0.47
2:B:4705:VAL:HB	2:B:4778:TRP:CG	2.49	0.47
2:B:4928:LEU:HA	2:B:4931:ILE:HD12	1.96	0.47
2:E:18:ASP:H	2:E:69:LEU:HB2	1.80	0.47
2:G:1931:LEU:HD22	2:G:1935:VAL:HG11	1.96	0.47
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.38	0.47
2:G:2457:LEU:HD23	2:G:2460:LEU:HD12	1.96	0.47
2:G:4088:ILE:HG23	2:G:4123:ILE:HB	1.95	0.47
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.47
2:I:4705:VAL:HB	2:I:4778:TRP:CG	2.49	0.47
2:B:164:ARG:N	2:B:167:ASP:OD2	2.47	0.47
2:B:213:TYR:CG	2:B:337:PRO:HB2	2.50	0.47
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.30	0.47
2:B:1245:PHE:HE1	2:B:1600:LEU:HD23	1.80	0.47
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.21	0.47
2:B:4061:PHE:C	2:B:4063:ASP:H	2.22	0.47
2:B:4735:GLU:O	2:B:4739:GLU:N	2.47	0.47
2:E:38:ALA:HB1	2:E:64:ILE:HG13	1.96	0.47
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.47	0.47
2:E:1044:ARG:HA	2:E:1047:LEU:HD12	1.97	0.47
2:E:2170:MET:HE1	2:E:2210:VAL:HG23	1.96	0.47
2:E:4241:THR:HG22	2:E:4245:MET:HE2	1.97	0.47
2:E:4837:LEU:HD21	2:E:4936:ILE:HD11	1.96	0.47
2:E:4848:VAL:HG23	2:E:4883:TYR:HE1	1.79	0.47
2:G:111:HIS:N	2:G:116:MET:O	2.37	0.47
2:G:251:ALA:O	2:G:254:THR:OG1	2.30	0.47
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.30	0.47
2:G:652:ARG:HB3	2:G:773:LEU:HD13	1.96	0.47
2:G:1516:UNK:N	2:G:1529:UNK:O	2.48	0.47
2:G:4875:LYS:HB3	2:G:4882:CYS:HA	1.97	0.47
2:I:426:ARG:HG2	2:I:431:PRO:HA	1.97	0.47
2:I:1229:ASN:O	2:I:1827:ARG:N	2.40	0.47
2:I:1245:PHE:HE1	2:I:1600:LEU:HD23	1.80	0.47
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.48	0.47
2:I:2286:LEU:HA	2:I:2289:ALA:HB3	1.97	0.47
2:I:4061:PHE:C	2:I:4063:ASP:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.47	0.47
2:B:1663:HIS:O	2:B:1667:LEU:N	2.46	0.47
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.38	0.47
2:B:4241:THR:HG22	2:B:4245:MET:HE2	1.97	0.47
2:B:4670:ILE:O	2:B:4674:GLU:N	2.37	0.47
2:E:4813:LEU:HA	2:E:4816:ILE:HG12	1.96	0.47
2:G:38:ALA:HB1	2:G:64:ILE:HG13	1.96	0.47
2:G:1196:PRO:O	2:G:1198:GLN:NE2	2.44	0.47
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.48	0.47
2:G:4241:THR:HG22	2:G:4245:MET:HE2	1.97	0.47
2:I:580:GLU:OE2	2:I:624:ASN:ND2	2.47	0.47
2:I:1649:ASP:OD1	2:I:1650:ILE:N	2.48	0.47
2:I:4024:VAL:HG23	2:I:4027:LEU:HD12	1.97	0.47
2:I:4088:ILE:HG23	2:I:4123:ILE:HB	1.95	0.47
2:B:426:ARG:HG2	2:B:431:PRO:HA	1.97	0.47
2:B:580:GLU:OE2	2:B:624:ASN:ND2	2.48	0.47
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.46	0.47
2:E:213:TYR:CG	2:E:337:PRO:HB2	2.50	0.47
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.96	0.47
2:E:4875:LYS:HB3	2:E:4882:CYS:HA	1.97	0.47
2:G:533:ASN:HB3	2:G:536:ASN:HB2	1.97	0.47
2:G:1577:ALA:HB1	2:G:1584:ARG:HA	1.97	0.47
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.46	0.47
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.48	0.47
2:B:3805:LEU:H	2:B:3805:LEU:HG	1.51	0.47
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.44	0.47
2:E:243:ARG:NH1	2:E:301:VAL:O	2.39	0.47
2:E:426:ARG:HG2	2:E:431:PRO:HA	1.97	0.47
2:E:639:ASN:HD22	2:E:1635:THR:HA	1.80	0.47
2:E:2869:ARG:HH12	2:E:2945:UNK:C	2.28	0.47
2:G:330:ASP:N	2:G:330:ASP:OD1	2.44	0.47
2:G:4735:GLU:HA	2:G:4738:ALA:HB3	1.97	0.47
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	1.96	0.47
2:I:213:TYR:CG	2:I:337:PRO:HB2	2.50	0.47
2:I:639:ASN:HD22	2:I:1635:THR:HA	1.80	0.47
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.97	0.47
2:I:4670:ILE:O	2:I:4674:GLU:N	2.37	0.47
2:I:4735:GLU:HA	2:I:4738:ALA:HB3	1.97	0.47
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.97	0.46
2:B:4110:PHE:HA	2:B:4113:SER:HB3	1.96	0.46
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1952:GLN:HA	2:E:1955:VAL:HG12	1.96	0.46
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.47	0.46
2:G:18:ASP:H	2:G:69:LEU:HB2	1.80	0.46
2:G:639:ASN:HD22	2:G:1635:THR:HA	1.80	0.46
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.49	0.46
2:G:4813:LEU:HA	2:G:4816:ILE:HG12	1.96	0.46
2:I:55:ALA:O	2:I:281:ARG:NH1	2.48	0.46
2:I:460:GLN:HG2	2:I:462:GLU:H	1.80	0.46
2:I:629:ARG:HB3	2:I:634:GLN:NE2	2.30	0.46
2:I:1294:UNK:HA	2:I:1455:UNK:HA	1.97	0.46
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.98	0.46
2:I:4241:THR:HG22	2:I:4245:MET:HE2	1.97	0.46
2:I:4848:VAL:HG23	2:I:4883:TYR:HE1	1.79	0.46
2:B:69:LEU:HD22	2:B:107:ILE:HD11	1.98	0.46
2:B:1196:PRO:O	2:B:1198:GLN:NE2	2.44	0.46
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.97	0.46
2:B:2459:SER:HB2	2:I:131:LEU:HB3	1.96	0.46
2:E:264:PRO:HA	2:E:280:LEU:HA	1.96	0.46
2:E:1649:ASP:OD1	2:E:1650:ILE:N	2.48	0.46
2:E:2212:VAL:O	2:E:2216:GLY:N	2.46	0.46
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.98	0.46
2:E:4088:ILE:HG23	2:E:4123:ILE:HB	1.96	0.46
2:E:4110:PHE:HA	2:E:4113:SER:HB3	1.96	0.46
2:E:4735:GLU:HA	2:E:4738:ALA:HB3	1.97	0.46
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.97	0.46
2:G:946:ALA:HA	2:G:949:ASN:HB2	1.98	0.46
2:G:2336:ARG:NH2	2:G:2428:ALA:O	2.49	0.46
2:G:4565:LEU:O	2:G:4569:LEU:N	2.37	0.46
2:I:1044:ARG:HA	2:I:1047:LEU:HD12	1.97	0.46
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.97	0.46
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.98	0.46
2:B:1704:PRO:HG2	2:B:1707:LEU:HB2	1.98	0.46
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.97	0.46
2:B:2950:UNK:O	2:B:2954:UNK:N	2.49	0.46
2:B:4710:SER:OG	2:B:4772:ASP:OD2	2.29	0.46
2:B:4934:GLY:O	2:B:4938:ASP:N	2.41	0.46
2:E:207:SER:OG	2:E:208:CYS:N	2.48	0.46
2:E:460:GLN:HG2	2:E:462:GLU:H	1.80	0.46
2:E:684:VAL:HA	2:E:781:VAL:HA	1.98	0.46
2:E:2457:LEU:HD23	2:E:2460:LEU:HD12	1.96	0.46
2:E:4705:VAL:HB	2:E:4778:TRP:CG	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:69:LEU:HD22	2:G:107:ILE:HD11	1.98	0.46
2:G:213:TYR:CG	2:G:337:PRO:HB2	2.50	0.46
2:G:866:HIS:O	2:G:1051:TYR:OH	2.32	0.46
2:G:1773:PRO:HD3	2:G:2156:LEU:HD21	1.97	0.46
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.97	0.46
2:I:911:HIS:O	2:I:918:ARG:NH2	2.44	0.46
2:B:639:ASN:HD22	2:B:1635:THR:HA	1.80	0.46
2:B:1841:VAL:HA	2:B:1844:LEU:HB3	1.98	0.46
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.98	0.46
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.49	0.46
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	1.97	0.46
2:E:1577:ALA:HB1	2:E:1584:ARG:HA	1.98	0.46
2:G:1676:LEU:HD22	2:G:2167:ILE:HG13	1.98	0.46
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.98	0.46
2:G:3649:ALA:O	2:G:3653:PHE:N	2.45	0.46
1:H:14:THR:N	1:H:67:SER:OG	2.49	0.46
1:H:29:MET:HB3	1:H:98:ILE:HB	1.98	0.46
2:I:1841:VAL:HA	2:I:1844:LEU:HB3	1.98	0.46
2:B:385:ASP:OD1	2:B:385:ASP:N	2.47	0.46
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.97	0.46
2:B:4040:ILE:HG22	2:B:4044:MET:HE3	1.98	0.46
2:B:4875:LYS:HA	2:B:4881:THR:HG22	1.98	0.46
2:E:1676:LEU:HD22	2:E:2167:ILE:HG13	1.98	0.46
2:E:1950:GLU:OE2	2:E:1954:ARG:NH2	2.43	0.46
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.38	0.46
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.96	0.46
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.49	0.46
1:F:14:THR:N	1:F:67:SER:OG	2.49	0.46
2:G:164:ARG:N	2:G:167:ASP:OD2	2.47	0.46
2:G:684:VAL:HA	2:G:781:VAL:HA	1.98	0.46
2:G:1286:UNK:HA	2:G:1461:UNK:HA	1.97	0.46
2:G:4040:ILE:HG22	2:G:4044:MET:HE3	1.98	0.46
2:I:69:LEU:HD22	2:I:107:ILE:HD11	1.98	0.46
2:I:1704:PRO:HG2	2:I:1707:LEU:HB2	1.98	0.46
2:I:4928:LEU:HA	2:I:4931:ILE:HD12	1.96	0.46
2:B:1240:LYS:O	2:B:1604:SER:N	2.46	0.46
2:B:1676:LEU:HD22	2:B:2167:ILE:HG13	1.98	0.46
2:E:164:ARG:N	2:E:167:ASP:OD2	2.47	0.46
2:E:583:ILE:HA	2:E:586:ILE:HD12	1.98	0.46
2:E:614:VAL:HG22	2:E:616:SER:H	1.81	0.46
2:E:1245:PHE:HE1	2:E:1600:LEU:HD23	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:264:PRO:HA	2:G:280:LEU:HA	1.96	0.46
2:G:273:HIS:CE1	2:G:337:PRO:HB3	2.51	0.46
2:G:1649:ASP:OD1	2:G:1650:ILE:N	2.48	0.46
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.97	0.46
2:G:1952:GLN:HA	2:G:1955:VAL:HG12	1.96	0.46
1:J:14:THR:N	1:J:67:SER:OG	2.49	0.46
2:B:78:LEU:O	2:B:82:LEU:N	2.43	0.46
2:B:330:ASP:OD1	2:B:330:ASP:N	2.44	0.46
2:B:614:VAL:HG22	2:B:616:SER:H	1.81	0.46
2:B:684:VAL:HA	2:B:781:VAL:HA	1.98	0.46
2:B:946:ALA:HA	2:B:949:ASN:HB2	1.98	0.46
2:B:1649:ASP:OD1	2:B:1650:ILE:N	2.48	0.46
2:B:1668:ARG:HA	2:B:1671:ARG:HH11	1.79	0.46
2:B:3771:HIS:O	2:B:3774:GLY:N	2.45	0.46
2:B:4195:PHE:HZ	2:B:4987:ASN:HB3	1.81	0.46
2:E:69:LEU:HD22	2:E:107:ILE:HD11	1.98	0.46
2:E:580:GLU:OE2	2:E:624:ASN:ND2	2.47	0.46
2:E:1773:PRO:HD3	2:E:2156:LEU:HD21	1.97	0.46
2:G:670:GLU:H	2:G:740:PRO:HB3	1.81	0.46
2:G:1663:HIS:O	2:G:1667:LEU:N	2.45	0.46
2:G:4195:PHE:HZ	2:G:4987:ASN:HB3	1.81	0.46
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.97	0.46
2:I:946:ALA:HA	2:I:949:ASN:HB2	1.98	0.46
2:I:1773:PRO:HD3	2:I:2156:LEU:HD21	1.97	0.46
2:I:2336:ARG:NH2	2:I:2428:ALA:O	2.49	0.46
2:I:4813:LEU:HA	2:I:4816:ILE:HG12	1.96	0.46
1:A:23:VAL:HB	1:A:105:ASN:HA	1.98	0.46
2:B:38:ALA:HB1	2:B:64:ILE:HG13	1.96	0.46
2:B:2347:GLU:O	2:B:2351:ASN:N	2.36	0.46
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.81	0.46
2:E:670:GLU:H	2:E:740:PRO:HB3	1.81	0.46
2:E:1516:UNK:N	2:E:1529:UNK:O	2.49	0.46
2:E:1817:GLU:O	2:E:1821:ASP:N	2.42	0.46
2:E:3927:GLN:O	2:E:3931:SER:N	2.44	0.46
1:F:23:VAL:HB	1:F:105:ASN:HA	1.98	0.46
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.47	0.46
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.97	0.46
2:G:1841:VAL:HA	2:G:1844:LEU:HB3	1.98	0.46
2:G:2149:VAL:O	2:G:2153:MET:N	2.46	0.46
2:G:4745:LEU:O	2:G:4749:GLU:N	2.41	0.46
2:I:614:VAL:HG22	2:I:616:SER:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG23	1:A:60:GLU:HB2	1.98	0.46
2:B:583:ILE:HA	2:B:586:ILE:HD12	1.98	0.46
2:B:1577:ALA:HB1	2:B:1584:ARG:HA	1.97	0.46
2:E:79:GLN:HA	2:E:82:LEU:HB2	1.98	0.46
2:E:4109:GLN:O	2:E:4113:SER:N	2.42	0.46
2:E:4172:GLU:OE1	2:E:4175:ARG:NH1	2.47	0.46
2:E:4571:PHE:O	2:E:4575:PHE:N	2.46	0.46
2:E:4875:LYS:HA	2:E:4881:THR:HG22	1.97	0.46
1:F:29:MET:HB3	1:F:98:ILE:HB	1.98	0.46
2:G:40:GLU:H	2:G:44:ASN:HD22	1.64	0.46
2:G:207:SER:OG	2:G:208:CYS:N	2.48	0.46
2:G:1245:PHE:HE1	2:G:1600:LEU:HD23	1.80	0.46
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.81	0.46
2:I:533:ASN:HB3	2:I:536:ASN:HB2	1.97	0.46
2:I:3963:ASN:O	2:I:3966:THR:OG1	2.30	0.46
2:I:4021:LYS:HA	2:I:4024:VAL:HG12	1.98	0.46
2:B:379:HIS:CD2	2:B:382:GLY:H	2.25	0.46
2:B:533:ASN:HB3	2:B:536:ASN:HB2	1.97	0.46
2:B:3663:LEU:H	2:B:3663:LEU:HG	1.39	0.46
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.97	0.46
2:B:4024:VAL:HG23	2:B:4027:LEU:HD12	1.97	0.46
2:E:273:HIS:CE1	2:E:337:PRO:HB3	2.51	0.46
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.98	0.46
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.48	0.46
2:E:3903:LEU:HG	2:E:3915:ILE:HD12	1.98	0.46
2:E:4195:PHE:HZ	2:E:4987:ASN:HB3	1.81	0.46
2:G:4109:GLN:O	2:G:4113:SER:N	2.42	0.46
2:I:4815:ASP:O	2:I:4819:GLY:N	2.44	0.46
2:I:4875:LYS:HB3	2:I:4882:CYS:HA	1.97	0.46
2:B:273:HIS:CE1	2:B:337:PRO:HB3	2.51	0.45
2:B:670:GLU:H	2:B:740:PRO:HB3	1.81	0.45
2:B:797:HIS:HB3	2:B:1625:GLY:H	1.81	0.45
2:B:1227:ALA:HB1	2:B:1230:MET:HG3	1.98	0.45
2:B:2243:SER:HB3	2:B:2246:ASN:H	1.81	0.45
2:B:4875:LYS:HB3	2:B:4882:CYS:HA	1.97	0.45
2:E:809:ALA:O	2:E:811:CYS:N	2.48	0.45
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.97	0.45
2:E:1841:VAL:HA	2:E:1844:LEU:HB3	1.98	0.45
2:E:4040:ILE:HG22	2:E:4044:MET:HE3	1.98	0.45
2:E:4565:LEU:O	2:E:4569:LEU:N	2.37	0.45
2:E:4934:GLY:O	2:E:4938:ASP:N	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:VAL:HG23	1:F:60:GLU:HB2	1.98	0.45
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.81	0.45
2:G:460:GLN:HG2	2:G:462:GLU:H	1.80	0.45
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.97	0.45
2:G:1704:PRO:HG2	2:G:1707:LEU:HB2	1.98	0.45
2:G:2347:GLU:O	2:G:2351:ASN:N	2.36	0.45
2:G:4024:VAL:HG23	2:G:4027:LEU:HD12	1.97	0.45
2:I:2243:SER:HB3	2:I:2246:ASN:H	1.81	0.45
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.45	0.45
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.97	0.45
2:I:4837:LEU:HD21	2:I:4936:ILE:HD11	1.98	0.45
2:I:5012:LYS:O	2:I:5016:GLU:N	2.43	0.45
1:J:7:ILE:N	1:J:71:ARG:O	2.46	0.45
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.98	0.45
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.99	0.45
2:E:55:ALA:O	2:E:281:ARG:NH1	2.48	0.45
2:E:251:ALA:O	2:E:254:THR:OG1	2.30	0.45
2:E:913:LEU:HD13	2:E:918:ARG:HA	1.99	0.45
2:E:1704:PRO:HG2	2:E:1707:LEU:HB2	1.98	0.45
1:F:83:GLY:O	1:F:94:ASN:N	2.50	0.45
2:G:809:ALA:O	2:G:811:CYS:N	2.48	0.45
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.98	0.45
2:G:2248:ARG:NH2	2:G:2285:GLU:OE1	2.49	0.45
2:G:3903:LEU:HG	2:G:3915:ILE:HD12	1.98	0.45
2:I:38:ALA:HB1	2:I:64:ILE:HG13	1.96	0.45
2:I:273:HIS:CE1	2:I:337:PRO:HB3	2.51	0.45
2:I:670:GLU:H	2:I:740:PRO:HB3	1.81	0.45
2:I:1577:ALA:HB1	2:I:1584:ARG:HA	1.98	0.45
2:I:2154:SER:O	2:I:2184:ASN:ND2	2.49	0.45
2:I:2212:VAL:O	2:I:2216:GLY:N	2.46	0.45
1:A:29:MET:HB3	1:A:98:ILE:HB	1.98	0.45
2:B:1965:TYR:OH	2:B:2027:ILE:O	2.24	0.45
2:B:2154:SER:O	2:B:2184:ASN:ND2	2.49	0.45
2:B:4021:LYS:HA	2:B:4024:VAL:HG12	1.98	0.45
2:B:4865:LYS:HG2	2:B:4874:MET:HA	1.98	0.45
2:E:40:GLU:H	2:E:44:ASN:HD22	1.65	0.45
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.97	0.45
2:G:583:ILE:HA	2:G:586:ILE:HD12	1.98	0.45
2:G:2243:SER:HB3	2:G:2246:ASN:H	1.81	0.45
2:G:4021:LYS:HA	2:G:4024:VAL:HG12	1.98	0.45
2:I:684:VAL:HA	2:I:781:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.98	0.45
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.49	0.45
2:I:4040:ILE:HG22	2:I:4044:MET:HE3	1.98	0.45
2:I:4865:LYS:HG2	2:I:4874:MET:HA	1.98	0.45
2:I:4875:LYS:HA	2:I:4881:THR:HG22	1.97	0.45
2:I:4957:LYS:HE3	2:I:4957:LYS:HB3	1.73	0.45
2:B:79:GLN:HA	2:B:82:LEU:HB2	1.98	0.45
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.98	0.45
2:E:4024:VAL:HG23	2:E:4027:LEU:HD12	1.97	0.45
2:G:286:THR:HA	2:G:405:HIS:HB2	1.99	0.45
2:G:379:HIS:CD2	2:G:382:GLY:H	2.25	0.45
2:G:614:VAL:HG22	2:G:616:SER:H	1.81	0.45
2:I:913:LEU:HD13	2:I:918:ARG:HA	1.98	0.45
2:I:1227:ALA:HB1	2:I:1230:MET:HG3	1.98	0.45
2:I:1676:LEU:HD22	2:I:2167:ILE:HG13	1.98	0.45
2:I:2950:UNK:O	2:I:2954:UNK:N	2.50	0.45
1:J:23:VAL:HB	1:J:105:ASN:HA	1.98	0.45
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.81	0.45
2:B:207:SER:OG	2:B:208:CYS:N	2.48	0.45
2:B:1773:PRO:HD3	2:B:2156:LEU:HD21	1.97	0.45
2:B:2149:VAL:O	2:B:2153:MET:N	2.46	0.45
2:B:3903:LEU:HG	2:B:3915:ILE:HD12	1.98	0.45
2:E:2154:SER:O	2:E:2184:ASN:ND2	2.49	0.45
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.99	0.45
2:G:3927:GLN:O	2:G:3931:SER:N	2.44	0.45
2:I:40:GLU:H	2:I:44:ASN:HD22	1.64	0.45
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.99	0.45
2:I:4710:SER:OG	2:I:4772:ASP:OD2	2.29	0.45
2:I:4736:ARG:O	2:I:4740:LEU:N	2.50	0.45
1:J:55:VAL:HG23	1:J:60:GLU:HB2	1.98	0.45
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.98	0.45
2:B:266:ARG:NH2	2:B:269:TRP:O	2.50	0.45
2:B:4182:GLU:HA	2:B:4192:ARG:HA	1.99	0.45
2:E:241:GLN:O	2:E:289:ARG:NH1	2.44	0.45
2:E:668:VAL:HG22	2:E:789:VAL:HG23	1.99	0.45
2:E:790:ARG:HG2	2:E:1627:ALA:HA	1.98	0.45
2:E:1227:ALA:HB1	2:E:1230:MET:HG3	1.98	0.45
2:E:2248:ARG:NH2	2:E:2285:GLU:OE1	2.49	0.45
2:E:2336:ARG:NH2	2:E:2428:ALA:O	2.48	0.45
2:E:3885:PHE:HA	2:E:3888:LEU:HD12	1.99	0.45
2:G:3885:PHE:HA	2:G:3888:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:668:VAL:O	2:I:741:GLU:N	2.49	0.45
2:I:3998:HIS:CE1	2:I:4054:ASN:HD21	2.35	0.45
2:I:4182:GLU:HA	2:I:4192:ARG:HA	1.99	0.45
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.99	0.45
2:B:251:ALA:O	2:B:254:THR:OG1	2.30	0.45
2:B:668:VAL:O	2:B:741:GLU:N	2.49	0.45
2:B:733:PRO:HD2	2:B:763:PRO:HD2	1.99	0.45
2:B:4837:LEU:HD21	2:B:4936:ILE:HD11	1.98	0.45
2:E:134:ASP:HA	2:E:192:ASP:HA	1.98	0.45
2:E:286:THR:HA	2:E:405:HIS:HB2	1.99	0.45
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.82	0.45
2:G:1105:ALA:O	2:G:1189:LEU:N	2.50	0.45
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.48	0.45
2:G:4710:SER:OG	2:G:4772:ASP:OD2	2.29	0.45
2:G:4875:LYS:HA	2:G:4881:THR:HG22	1.97	0.45
2:G:4934:GLY:O	2:G:4938:ASP:N	2.41	0.45
2:G:4990:PHE:O	2:G:4994:TYR:N	2.43	0.45
1:H:83:GLY:O	1:H:94:ASN:N	2.50	0.45
2:I:266:ARG:NH2	2:I:269:TRP:O	2.50	0.45
2:I:583:ILE:HA	2:I:586:ILE:HD12	1.98	0.45
2:I:1950:GLU:OE2	2:I:1954:ARG:NH2	2.43	0.45
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.99	0.45
1:A:14:THR:N	1:A:67:SER:OG	2.49	0.45
2:B:1516:UNK:N	2:B:1529:UNK:O	2.49	0.45
2:B:1740:PRO:HA	2:B:1743:ARG:HB3	1.99	0.45
2:E:911:HIS:O	2:E:918:ARG:NH2	2.44	0.45
2:E:1694:LEU:O	2:E:1712:TYR:OH	2.21	0.45
2:E:4815:ASP:O	2:E:4819:GLY:N	2.44	0.45
2:G:79:GLN:HA	2:G:82:LEU:HB2	1.98	0.45
2:G:3934:TYR:O	2:G:3938:SER:N	2.50	0.45
2:G:3998:HIS:CE1	2:G:4054:ASN:HD21	2.35	0.45
1:H:55:VAL:HG23	1:H:60:GLU:HB2	1.98	0.45
2:I:79:GLN:HA	2:I:82:LEU:HB2	1.98	0.45
2:I:134:ASP:HA	2:I:192:ASP:HA	1.98	0.45
2:I:797:HIS:HB3	2:I:1625:GLY:H	1.81	0.45
2:I:1268:PRO:HB2	2:I:1591:CYS:HB2	1.99	0.45
2:I:4195:PHE:HZ	2:I:4987:ASN:HB3	1.81	0.45
1:A:83:GLY:O	1:A:94:ASN:N	2.50	0.45
2:B:40:GLU:H	2:B:44:ASN:HD22	1.65	0.45
2:B:1105:ALA:O	2:B:1189:LEU:N	2.50	0.45
2:B:1268:PRO:HB2	2:B:1591:CYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1679:ASN:O	2:B:1683:HIS:ND1	2.36	0.45
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.48	0.45
2:B:3885:PHE:HA	2:B:3888:LEU:HD12	1.99	0.45
2:B:4571:PHE:O	2:B:4575:PHE:N	2.46	0.45
2:E:266:ARG:NH2	2:E:269:TRP:O	2.50	0.45
2:E:385:ASP:OD1	2:E:385:ASP:N	2.47	0.45
2:E:533:ASN:HB3	2:E:536:ASN:HB2	1.97	0.45
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.99	0.45
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.99	0.45
2:G:5012:LYS:O	2:G:5016:GLU:N	2.43	0.45
2:I:218:HIS:HB3	2:I:392:ARG:HD3	1.99	0.45
2:I:3846:ALA:HB1	2:I:3873:LYS:HG2	1.99	0.45
2:I:3927:GLN:O	2:I:3931:SER:N	2.44	0.45
2:B:134:ASP:HA	2:B:192:ASP:HA	1.98	0.45
2:B:668:VAL:HG22	2:B:789:VAL:HG23	1.99	0.45
2:B:2336:ARG:NH2	2:B:2428:ALA:O	2.48	0.45
2:B:3934:TYR:O	2:B:3938:SER:N	2.50	0.45
2:E:666:VAL:HG21	2:E:684:VAL:HG21	1.99	0.45
2:E:797:HIS:HB3	2:E:1625:GLY:H	1.81	0.45
2:E:946:ALA:HA	2:E:949:ASN:HB2	1.98	0.45
2:E:2243:SER:HB3	2:E:2246:ASN:H	1.81	0.45
2:E:3676:ASP:OD1	2:E:3676:ASP:N	2.49	0.45
2:E:4865:LYS:HG2	2:E:4874:MET:HA	1.98	0.45
2:G:40:GLU:H	2:G:44:ASN:ND2	2.15	0.45
2:G:134:ASP:HA	2:G:192:ASP:HA	1.98	0.45
2:G:266:ARG:NH2	2:G:269:TRP:O	2.50	0.45
2:G:668:VAL:HG22	2:G:789:VAL:HG23	1.99	0.45
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.50	0.45
2:G:913:LEU:HD13	2:G:918:ARG:HA	1.99	0.45
2:G:2869:ARG:HH12	2:G:2945:UNK:C	2.29	0.45
2:G:2950:UNK:O	2:G:2954:UNK:N	2.50	0.45
2:I:111:HIS:N	2:I:116:MET:O	2.37	0.45
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.99	0.45
2:I:1240:LYS:O	2:I:1604:SER:N	2.46	0.45
2:I:2248:ARG:NH2	2:I:2285:GLU:OE1	2.49	0.45
2:I:3903:LEU:HG	2:I:3915:ILE:HD12	1.98	0.45
1:J:29:MET:HB3	1:J:98:ILE:HB	1.98	0.45
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.99	0.44
2:B:530:ILE:HA	2:B:536:ASN:HB3	1.99	0.44
2:B:666:VAL:HG21	2:B:684:VAL:HG21	1.99	0.44
2:B:1737:PRO:HG2	2:B:1739:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2248:ARG:NH2	2:B:2285:GLU:OE1	2.49	0.44
2:B:2880:GLU:O	2:B:2884:ASN:N	2.47	0.44
2:B:4853:VAL:HA	2:B:4856:PHE:HB3	1.99	0.44
2:E:1684:ALA:HA	2:E:1782:PHE:HZ	1.82	0.44
2:E:3771:HIS:O	2:E:3774:GLY:N	2.45	0.44
2:E:3934:TYR:O	2:E:3938:SER:N	2.50	0.44
2:G:790:ARG:HG2	2:G:1627:ALA:HA	1.98	0.44
2:G:1774:PRO:HG2	2:G:1776:HIS:CE1	2.52	0.44
2:G:3846:ALA:HB1	2:G:3873:LYS:HG2	1.99	0.44
2:I:40:GLU:H	2:I:44:ASN:ND2	2.15	0.44
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.98	0.44
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.86	0.44
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.82	0.44
2:I:1774:PRO:HG2	2:I:1776:HIS:CE1	2.52	0.44
2:B:790:ARG:HG2	2:B:1627:ALA:HA	1.98	0.44
2:B:2212:VAL:O	2:B:2216:GLY:N	2.46	0.44
2:B:3713:LYS:HG2	2:B:3715:LYS:H	1.82	0.44
2:E:218:HIS:HB3	2:E:392:ARG:HD3	1.99	0.44
2:E:1105:ALA:O	2:E:1189:LEU:N	2.50	0.44
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.44
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.98	0.44
2:G:3963:ASN:O	2:G:3966:THR:OG1	2.30	0.44
2:I:2869:ARG:HH12	2:I:2945:UNK:C	2.30	0.44
2:I:3885:PHE:HA	2:I:3888:LEU:HD12	1.99	0.44
1:J:83:GLY:O	1:J:94:ASN:N	2.50	0.44
2:B:286:THR:HA	2:B:405:HIS:HB2	1.99	0.44
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.82	0.44
2:B:1774:PRO:HG2	2:B:1776:HIS:CE1	2.52	0.44
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.98	0.44
2:B:4172:GLU:OE1	2:B:4175:ARG:NH1	2.47	0.44
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.98	0.44
2:E:1740:PRO:HA	2:E:1743:ARG:HB3	1.99	0.44
2:E:4021:LYS:HA	2:E:4024:VAL:HG12	1.98	0.44
2:G:243:ARG:NH1	2:G:301:VAL:O	2.39	0.44
2:G:797:HIS:HB3	2:G:1625:GLY:H	1.81	0.44
2:G:1227:ALA:HB1	2:G:1230:MET:HG3	1.98	0.44
2:G:2154:SER:O	2:G:2184:ASN:ND2	2.49	0.44
2:G:4182:GLU:HA	2:G:4192:ARG:HA	1.99	0.44
2:I:229:GLU:OE2	2:I:374:LYS:NZ	2.41	0.44
2:I:243:ARG:NH1	2:I:301:VAL:O	2.39	0.44
2:I:485:SER:O	2:I:489:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1269:CYS:HA	2:I:1473:UNK:HA	1.99	0.44
2:I:4826:ILE:O	2:I:4829:SER:OG	2.33	0.44
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.98	0.44
2:B:1091:GLU:O	2:B:1203:ASN:N	2.40	0.44
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.46	0.44
2:E:4000:MET:HE2	2:E:4061:PHE:CD2	2.53	0.44
2:E:4182:GLU:HA	2:E:4192:ARG:HA	1.99	0.44
2:G:55:ALA:O	2:G:281:ARG:NH1	2.48	0.44
2:G:1268:PRO:HB2	2:G:1591:CYS:HB2	1.99	0.44
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	2.00	0.44
1:H:23:VAL:HB	1:H:105:ASN:HA	1.98	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.47	0.44
2:I:790:ARG:HG2	2:I:1627:ALA:HA	1.98	0.44
2:I:2142:TYR:CG	2:I:2197:LEU:HD13	2.53	0.44
2:I:3934:TYR:O	2:I:3938:SER:N	2.50	0.44
2:I:4565:LEU:O	2:I:4569:LEU:N	2.37	0.44
2:B:913:LEU:HD13	2:B:918:ARG:HA	1.98	0.44
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	2.00	0.44
2:B:4201:ASN:ND2	2:B:4993:MET:SD	2.91	0.44
2:E:1032:LYS:O	2:E:1036:ARG:N	2.45	0.44
2:E:1737:PRO:HG2	2:E:1739:THR:HG23	1.99	0.44
2:E:2142:TYR:CG	2:E:2197:LEU:HD13	2.53	0.44
2:E:4068:LEU:HD23	2:E:4132:PHE:HE2	1.82	0.44
2:G:666:VAL:HG21	2:G:684:VAL:HG21	1.99	0.44
2:G:1497:UNK:HA	2:G:1535:UNK:HA	1.99	0.44
2:G:4201:ASN:ND2	2:G:4993:MET:SD	2.91	0.44
2:G:4853:VAL:HA	2:G:4856:PHE:HB3	1.99	0.44
2:I:668:VAL:HG22	2:I:789:VAL:HG23	1.99	0.44
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.50	0.44
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.99	0.44
2:I:2770:LYS:O	2:I:2775:TRP:N	2.42	0.44
2:I:4968:PHE:HE1	2:I:5029:ARG:HD3	1.82	0.44
2:B:40:GLU:H	2:B:44:ASN:ND2	2.15	0.44
2:E:1268:PRO:HB2	2:E:1591:CYS:HB2	1.99	0.44
2:E:3846:ALA:HB1	2:E:3873:LYS:HG2	2.00	0.44
2:G:668:VAL:O	2:G:741:GLU:N	2.49	0.44
2:G:2142:TYR:CG	2:G:2197:LEU:HD13	2.53	0.44
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.49	0.44
2:G:4068:LEU:HD23	2:G:4132:PHE:HE2	1.82	0.44
2:G:4837:LEU:HD21	2:G:4936:ILE:HD11	1.98	0.44
2:G:4957:LYS:HB3	2:G:4964:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:286:THR:HA	2:I:405:HIS:HB2	1.99	0.44
2:I:392:ARG:HH12	2:I:398:SER:HB2	1.83	0.44
2:I:2908:TYR:OH	2:I:2920:ARG:NE	2.45	0.44
2:I:4201:ASN:ND2	2:I:4993:MET:SD	2.91	0.44
2:I:4989:MET:HB3	2:I:4989:MET:HE2	1.81	0.44
2:B:55:ALA:O	2:B:281:ARG:NH1	2.48	0.44
2:B:102:LEU:HB3	2:B:160:GLY:HA2	1.99	0.44
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.51	0.44
2:E:733:PRO:HD2	2:E:763:PRO:HD2	1.99	0.44
2:E:1196:PRO:O	2:E:1198:GLN:NE2	2.44	0.44
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.99	0.44
2:E:2444:GLN:HA	2:E:2451:LEU:HD21	2.00	0.44
2:E:4824:ARG:O	2:E:4828:SER:N	2.47	0.44
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.98	0.44
2:G:218:HIS:HB3	2:G:392:ARG:HD3	1.99	0.44
2:G:831:ARG:HD3	2:G:1199:VAL:HG12	1.99	0.44
2:G:4000:MET:HE2	2:G:4061:PHE:CD2	2.53	0.44
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.48	0.44
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	2.00	0.44
2:B:218:HIS:HB3	2:B:392:ARG:HD3	1.99	0.44
2:B:392:ARG:HH12	2:B:398:SER:HB2	1.83	0.44
2:B:3846:ALA:HB1	2:B:3873:LYS:HG2	1.99	0.44
2:B:4147:LEU:O	2:B:4151:SER:OG	2.30	0.44
2:B:5012:LYS:O	2:B:5016:GLU:N	2.43	0.44
2:E:379:HIS:CD2	2:E:382:GLY:H	2.25	0.44
2:E:392:ARG:HH12	2:E:398:SER:HB2	1.83	0.44
2:E:2149:VAL:O	2:E:2153:MET:N	2.46	0.44
2:E:2255:SER:HA	2:E:2258:LEU:HB3	2.00	0.44
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	1.99	0.44
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.00	0.44
2:G:379:HIS:CD2	2:G:381:GLU:H	2.36	0.44
2:G:580:GLU:OE2	2:G:624:ASN:ND2	2.47	0.44
2:G:1092:PHE:O	2:G:1149:VAL:N	2.49	0.44
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.82	0.44
2:G:1229:ASN:O	2:G:1827:ARG:N	2.40	0.44
2:G:1240:LYS:O	2:G:1604:SER:N	2.46	0.44
2:G:1269:CYS:HA	2:G:1473:UNK:HA	1.99	0.44
2:G:4822:THR:O	2:G:4825:THR:OG1	2.28	0.44
2:G:4865:LYS:HG2	2:G:4874:MET:HA	1.98	0.44
2:I:102:LEU:HB3	2:I:160:GLY:HA2	2.00	0.44
2:I:545:ASP:HA	2:I:582:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:733:PRO:HD2	2:I:763:PRO:HD2	1.99	0.44
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.99	0.44
2:B:2116:LEU:O	2:B:2120:MET:N	2.48	0.44
2:B:3998:HIS:CE1	2:B:4054:ASN:HD21	2.35	0.44
2:E:668:VAL:O	2:E:741:GLU:N	2.49	0.44
2:E:1229:ASN:O	2:E:1827:ARG:N	2.40	0.44
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	2.00	0.44
2:E:4968:PHE:HE1	2:E:5029:ARG:HD3	1.82	0.44
2:G:485:SER:O	2:G:489:ASN:N	2.50	0.44
2:G:530:ILE:HA	2:G:536:ASN:HB3	1.99	0.44
2:G:4061:PHE:C	2:G:4063:ASP:H	2.25	0.44
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.98	0.44
2:I:530:ILE:HA	2:I:536:ASN:HB3	1.98	0.44
2:I:1232:ARG:HD3	2:I:1702:HIS:HB3	2.00	0.44
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	2.00	0.44
2:I:3713:LYS:HG2	2:I:3715:LYS:H	1.82	0.44
2:I:4172:GLU:OE1	2:I:4175:ARG:NH1	2.47	0.44
2:I:4957:LYS:HB3	2:I:4964:GLY:HA2	2.00	0.44
2:B:410:LEU:HD21	2:B:441:VAL:HA	2.00	0.43
2:B:838:HIS:CE1	2:B:1201:HIS:HD2	2.36	0.43
2:B:2142:TYR:CG	2:B:2197:LEU:HD13	2.53	0.43
2:B:4885:PHE:HE2	2:B:4901:ILE:HD11	1.83	0.43
2:B:4968:PHE:HE1	2:B:5029:ARG:HD3	1.82	0.43
2:E:545:ASP:HA	2:E:582:HIS:CE1	2.53	0.43
2:E:4885:PHE:HE2	2:E:4901:ILE:HD11	1.83	0.43
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.53	0.43
2:G:2255:SER:HA	2:G:2258:LEU:HB3	2.00	0.43
2:G:4568:PHE:HA	2:G:4571:PHE:HD2	1.83	0.43
2:I:867:LEU:HD22	2:I:929:LEU:HD22	2.00	0.43
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.01	0.43
2:I:3771:HIS:O	2:I:3774:GLY:N	2.45	0.43
1:A:97:LEU:HD13	1:A:97:LEU:HA	1.88	0.43
2:B:831:ARG:HD3	2:B:1199:VAL:HG12	1.99	0.43
2:B:1232:ARG:HD3	2:B:1702:HIS:HB3	2.00	0.43
2:B:2444:GLN:HA	2:B:2451:LEU:HD21	2.00	0.43
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.43
2:B:3825:GLU:OE1	2:B:3825:GLU:N	2.52	0.43
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.00	0.43
2:E:40:GLU:H	2:E:44:ASN:ND2	2.16	0.43
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.99	0.43
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	2.00	0.43
2:E:3649:ALA:O	2:E:3653:PHE:N	2.45	0.43
2:E:3953:LYS:O	2:E:3956:SER:OG	2.29	0.43
2:G:392:ARG:HH12	2:G:398:SER:HB2	1.83	0.43
2:G:545:ASP:HA	2:G:582:HIS:CE1	2.53	0.43
2:G:838:HIS:CE1	2:G:1201:HIS:HD2	2.37	0.43
2:G:1684:ALA:HA	2:G:1782:PHE:HZ	1.82	0.43
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.99	0.43
2:G:1737:PRO:HG2	2:G:1739:THR:HG23	1.99	0.43
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	2.00	0.43
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.35	0.43
2:I:330:ASP:N	2:I:330:ASP:OD1	2.45	0.43
2:I:666:VAL:HG21	2:I:684:VAL:HG21	1.99	0.43
2:I:1105:ALA:O	2:I:1189:LEU:N	2.50	0.43
2:I:3676:ASP:N	2:I:3676:ASP:OD1	2.49	0.43
2:B:229:GLU:OE2	2:B:374:LYS:NZ	2.41	0.43
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.99	0.43
2:E:831:ARG:HD3	2:E:1199:VAL:HG12	1.99	0.43
2:E:838:HIS:CE1	2:E:1201:HIS:HD2	2.37	0.43
2:E:3825:GLU:OE1	2:E:3825:GLU:N	2.51	0.43
2:E:3998:HIS:CE1	2:E:4054:ASN:HD21	2.35	0.43
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.00	0.43
2:G:3713:LYS:HG2	2:G:3715:LYS:H	1.82	0.43
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.54	0.43
2:I:1116:GLY:HA3	2:I:1123:VAL:HG12	2.00	0.43
2:I:1679:ASN:O	2:I:1683:HIS:ND1	2.36	0.43
2:I:2444:GLN:HA	2:I:2451:LEU:HD21	2.00	0.43
2:B:794:GLY:H	2:B:798:GLY:HA3	1.84	0.43
2:B:867:LEU:HD22	2:B:929:LEU:HD22	2.00	0.43
2:B:1116:GLY:HA3	2:B:1123:VAL:HG12	2.00	0.43
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.00	0.43
2:B:4000:MET:HE2	2:B:4061:PHE:CD2	2.53	0.43
2:B:4736:ARG:O	2:B:4740:LEU:N	2.50	0.43
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.54	0.43
2:E:4061:PHE:C	2:E:4063:ASP:H	2.26	0.43
2:E:4201:ASN:ND2	2:E:4993:MET:SD	2.91	0.43
2:E:4957:LYS:HB3	2:E:4964:GLY:HA2	2.00	0.43
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.99	0.43
2:G:1116:GLY:HA3	2:G:1123:VAL:HG12	2.00	0.43
2:G:1740:PRO:HA	2:G:1743:ARG:HB3	1.99	0.43
2:G:3361:UNK:O	2:G:3365:UNK:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:ILE:N	1:H:71:ARG:O	2.46	0.43
2:I:1965:TYR:OH	2:I:2027:ILE:O	2.24	0.43
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.38	0.43
2:I:2880:GLU:O	2:I:2884:ASN:N	2.47	0.43
2:I:4853:VAL:HA	2:I:4856:PHE:HB3	1.99	0.43
2:B:545:ASP:HA	2:B:582:HIS:CE1	2.53	0.43
2:B:809:ALA:O	2:B:811:CYS:N	2.48	0.43
2:B:4957:LYS:HB3	2:B:4964:GLY:HA2	2.00	0.43
2:E:76:ARG:HB3	2:G:3935:TRP:HB3	2.01	0.43
2:E:410:LEU:HD21	2:E:441:VAL:HA	2.00	0.43
2:E:4000:MET:HE2	2:E:4061:PHE:HD2	1.84	0.43
2:E:4853:VAL:HA	2:E:4856:PHE:HB3	1.99	0.43
2:G:220:LEU:HD11	2:G:390:LEU:HD22	2.00	0.43
2:G:4968:PHE:HE1	2:G:5029:ARG:HD3	1.82	0.43
2:I:809:ALA:O	2:I:811:CYS:N	2.48	0.43
2:I:3229:UNK:HA	2:I:3302:UNK:HA	2.01	0.43
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.49	0.43
2:B:3927:GLN:O	2:B:3931:SER:N	2.44	0.43
2:B:4068:LEU:HD23	2:B:4132:PHE:HE2	1.82	0.43
2:B:4780:PHE:HA	2:B:4783:ILE:HD12	2.00	0.43
2:E:102:LEU:HB3	2:E:160:GLY:HA2	1.99	0.43
2:E:530:ILE:HA	2:E:536:ASN:HB3	1.98	0.43
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.51	0.43
2:E:1774:PRO:HG2	2:E:1776:HIS:CE1	2.52	0.43
2:E:2908:TYR:OH	2:E:2920:ARG:NE	2.45	0.43
2:E:3361:UNK:O	2:E:3365:UNK:N	2.52	0.43
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	2.00	0.43
2:G:102:LEU:HB3	2:G:160:GLY:HA2	1.99	0.43
2:G:345:LEU:HD23	2:G:389:PHE:HB3	2.00	0.43
2:G:867:LEU:HD22	2:G:929:LEU:HD22	2.00	0.43
2:G:978:THR:HB	2:G:980:ALA:H	1.84	0.43
2:G:3934:TYR:HB2	2:G:3999:MET:HE3	2.01	0.43
2:G:4000:MET:HE2	2:G:4061:PHE:HD2	1.84	0.43
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	1.99	0.43
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.00	0.43
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	1.99	0.43
2:I:4780:PHE:HA	2:I:4783:ILE:HD12	2.00	0.43
1:A:87:HIS:HB3	1:A:91:ILE:H	1.84	0.43
2:B:1684:ALA:HA	2:B:1782:PHE:HZ	1.82	0.43
2:B:4108:ILE:HA	2:B:4111:LEU:HD12	2.01	0.43
2:B:4568:PHE:HA	2:B:4571:PHE:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4801:LEU:HB3	2:B:4808:PHE:CG	2.54	0.43
2:B:4850:LEU:HD22	2:E:4814:LEU:HD21	2.01	0.43
2:B:4957:LYS:HB3	2:B:4957:LYS:HE3	1.73	0.43
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.99	0.43
2:G:733:PRO:HD2	2:G:763:PRO:HD2	1.99	0.43
2:G:794:GLY:H	2:G:798:GLY:HA3	1.84	0.43
2:G:2144:ILE:H	2:G:2144:ILE:HG13	1.74	0.43
2:I:831:ARG:HD3	2:I:1199:VAL:HG12	1.99	0.43
2:I:1658:ASP:N	2:I:1658:ASP:OD1	2.52	0.43
2:I:2758:PHE:O	2:I:2762:THR:N	2.46	0.43
2:I:4686:LEU:O	2:I:4691:GLN:N	2.52	0.43
2:B:313:SER:HB3	2:B:352:ALA:H	1.84	0.43
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	2.00	0.43
2:E:485:SER:O	2:E:489:ASN:N	2.50	0.43
2:E:1094:ALA:HA	2:E:1200:GLY:HA2	2.01	0.43
2:E:4108:ILE:HA	2:E:4111:LEU:HD12	2.01	0.43
2:G:1094:ALA:HA	2:G:1200:GLY:HA2	2.01	0.43
2:G:3825:GLU:OE1	2:G:3825:GLU:N	2.51	0.43
2:I:313:SER:HB3	2:I:352:ALA:H	1.84	0.43
2:I:410:LEU:HD21	2:I:441:VAL:HA	2.00	0.43
2:I:1684:ALA:HA	2:I:1782:PHE:HZ	1.82	0.43
2:B:379:HIS:CD2	2:B:381:GLU:H	2.36	0.43
2:E:379:HIS:CD2	2:E:381:GLU:H	2.36	0.43
2:E:4995:LEU:HA	2:E:4995:LEU:HD22	1.82	0.43
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.01	0.43
2:G:4928:LEU:HD13	2:G:4931:ILE:HD12	2.01	0.43
2:I:758:ARG:NH2	2:I:803:LEU:O	2.52	0.43
2:I:838:HIS:CE1	2:I:1201:HIS:HD2	2.36	0.43
2:I:1740:PRO:HA	2:I:1743:ARG:HB3	1.99	0.43
2:I:2255:SER:HA	2:I:2258:LEU:HB3	2.00	0.43
2:I:3700:GLN:HA	2:I:3703:LEU:HD12	2.01	0.43
2:I:4000:MET:HE2	2:I:4061:PHE:CD2	2.53	0.43
2:B:241:GLN:O	2:B:289:ARG:NH1	2.44	0.43
2:B:1658:ASP:OD1	2:B:1658:ASP:N	2.52	0.43
2:E:758:ARG:NH2	2:E:803:LEU:O	2.52	0.43
2:E:1116:GLY:HA3	2:E:1123:VAL:HG12	2.00	0.43
2:E:1679:ASN:O	2:E:1683:HIS:ND1	2.36	0.43
2:E:3713:LYS:HG2	2:E:3715:LYS:H	1.82	0.43
2:E:3934:TYR:HB2	2:E:3999:MET:HE3	2.01	0.43
2:E:4780:PHE:HA	2:E:4783:ILE:HD12	2.00	0.43
2:G:4824:ARG:O	2:G:4828:SER:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5026:ASP:OD1	2:G:5027:CYS:N	2.52	0.43
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.01	0.43
2:I:379:HIS:CD2	2:I:381:GLU:H	2.36	0.43
2:I:794:GLY:H	2:I:798:GLY:HA3	1.84	0.43
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.00	0.43
2:I:4801:LEU:HB3	2:I:4808:PHE:CG	2.54	0.43
2:B:290:TYR:O	2:B:302:VAL:N	2.52	0.42
2:B:758:ARG:NH2	2:B:803:LEU:O	2.52	0.42
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	1.99	0.42
2:E:345:LEU:HD23	2:E:389:PHE:HB3	2.00	0.42
2:G:410:LEU:HD21	2:G:441:VAL:HA	2.00	0.42
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.37	0.42
2:I:2149:VAL:O	2:I:2153:MET:N	2.46	0.42
1:J:57:LYS:HB2	1:J:80:VAL:HB	2.01	0.42
1:A:57:LYS:HB2	1:A:80:VAL:HB	2.01	0.42
2:B:2255:SER:HA	2:B:2258:LEU:HB3	2.00	0.42
2:B:3700:GLN:HA	2:B:3703:LEU:HD12	2.01	0.42
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.01	0.42
2:B:4836:GLN:O	2:B:4840:THR:OG1	2.28	0.42
2:B:5026:ASP:OD1	2:B:5027:CYS:N	2.52	0.42
2:E:313:SER:HB3	2:E:352:ALA:H	1.84	0.42
2:E:349:GLN:HE21	2:E:354:GLY:HA2	1.85	0.42
2:E:463:GLU:O	2:E:466:SER:OG	2.34	0.42
2:E:978:THR:HB	2:E:980:ALA:H	1.84	0.42
2:E:1232:ARG:HD3	2:E:1702:HIS:HB3	2.00	0.42
2:E:4801:LEU:HB3	2:E:4808:PHE:CG	2.54	0.42
2:G:313:SER:HB3	2:G:351:VAL:HB	2.01	0.42
2:G:334:MET:HE3	2:G:334:MET:HB3	1.89	0.42
2:G:3229:UNK:HA	2:G:3302:UNK:HA	2.00	0.42
2:G:4885:PHE:HE2	2:G:4901:ILE:HD11	1.83	0.42
2:I:251:ALA:O	2:I:254:THR:OG1	2.30	0.42
2:I:1516:UNK:N	2:I:1529:UNK:O	2.52	0.42
2:I:3825:GLU:OE1	2:I:3825:GLU:N	2.51	0.42
2:I:4568:PHE:HA	2:I:4571:PHE:HD2	1.84	0.42
2:B:2517:UNK:O	2:B:2521:UNK:N	2.52	0.42
2:B:3361:UNK:O	2:B:3365:UNK:N	2.52	0.42
2:B:4000:MET:HE2	2:B:4061:PHE:HD2	1.83	0.42
2:E:220:LEU:HD11	2:E:390:LEU:HD22	2.00	0.42
2:E:290:TYR:O	2:E:302:VAL:N	2.52	0.42
2:E:867:LEU:HD22	2:E:929:LEU:HD22	2.00	0.42
1:F:87:HIS:HB3	1:F:91:ILE:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:758:ARG:NH2	2:G:803:LEU:O	2.52	0.42
2:G:2444:GLN:HA	2:G:2451:LEU:HD21	2.00	0.42
2:G:4667:PRO:O	2:G:4714:ASN:ND2	2.52	0.42
2:I:220:LEU:HD11	2:I:390:LEU:HD22	2.00	0.42
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.38	0.42
2:I:4885:PHE:HE2	2:I:4901:ILE:HD11	1.83	0.42
2:B:891:TRP:HA	2:B:902:ARG:HB3	2.01	0.42
2:B:947:GLU:HG3	2:B:1049:TYR:HD1	1.85	0.42
2:B:1866:ILE:HG13	2:B:1926:LEU:HB3	2.02	0.42
2:E:299:LEU:HD12	2:E:299:LEU:HA	1.87	0.42
2:E:355:LEU:HB3	2:E:378:LEU:HB3	2.01	0.42
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.37	0.42
2:G:4780:PHE:HA	2:G:4783:ILE:HD12	2.00	0.42
2:I:1737:PRO:HG2	2:I:1739:THR:HG23	1.99	0.42
2:I:1866:ILE:HG13	2:I:1926:LEU:HB3	2.02	0.42
2:I:5026:ASP:OD1	2:I:5027:CYS:N	2.52	0.42
2:B:1497:UNK:HA	2:B:1535:UNK:HA	2.02	0.42
2:B:4989:MET:HE2	2:B:4989:MET:HB3	1.81	0.42
2:E:111:HIS:N	2:E:116:MET:O	2.37	0.42
2:E:498:THR:OG1	2:E:499:THR:N	2.53	0.42
2:E:1092:PHE:O	2:E:1149:VAL:N	2.49	0.42
2:E:1658:ASP:OD1	2:E:1658:ASP:N	2.52	0.42
2:E:1979:LEU:HA	2:E:1983:ALA:HB3	2.02	0.42
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	2.01	0.42
2:E:4822:THR:O	2:E:4825:THR:OG1	2.28	0.42
2:G:891:TRP:HA	2:G:902:ARG:HB3	2.01	0.42
2:G:3674:ILE:HG13	2:G:3732:SER:HB3	2.01	0.42
2:G:4686:LEU:O	2:G:4691:GLN:N	2.52	0.42
2:G:4843:LEU:HD12	2:I:4823:LEU:HD21	2.02	0.42
2:I:17:ASP:HB2	2:I:98:HIS:CE1	2.50	0.42
2:I:4068:LEU:HD23	2:I:4132:PHE:HE2	1.82	0.42
2:B:349:GLN:HE21	2:B:354:GLY:HA2	1.85	0.42
2:B:546:TRP:O	2:B:550:LYS:NZ	2.35	0.42
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.38	0.42
2:E:281:ARG:HA	2:E:312:THR:HG21	2.02	0.42
2:E:1207:ASP:HB3	2:E:1210:SER:HB3	2.02	0.42
2:G:1207:ASP:HB3	2:G:1210:SER:HB3	2.02	0.42
2:G:5013:MET:HA	2:G:5016:GLU:HB3	2.01	0.42
2:I:264:PRO:HG2	2:I:270:SER:HB2	2.02	0.42
2:I:498:THR:OG1	2:I:499:THR:N	2.53	0.42
2:I:4864:ASN:H	2:I:4874:MET:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	2.02	0.42
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.45	0.42
2:B:3649:ALA:O	2:B:3653:PHE:N	2.45	0.42
2:B:4026:MET:O	2:B:4030:LEU:N	2.52	0.42
2:B:4048:LEU:HD23	2:B:4048:LEU:HA	1.87	0.42
2:B:4701:TRP:CZ2	2:B:4781:GLY:HA3	2.55	0.42
2:E:794:GLY:H	2:E:798:GLY:HA3	1.84	0.42
2:E:1866:ILE:HG13	2:E:1926:LEU:HB3	2.01	0.42
2:E:3229:UNK:HA	2:E:3302:UNK:HA	2.01	0.42
2:G:290:TYR:O	2:G:302:VAL:N	2.52	0.42
2:G:349:GLN:HE21	2:G:354:GLY:HA2	1.84	0.42
2:G:2021:CYS:HA	2:G:2022:PRO:HD3	1.91	0.42
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.02	0.42
2:G:3700:GLN:HA	2:G:3703:LEU:HD12	2.01	0.42
2:G:4048:LEU:HD23	2:G:4048:LEU:HA	1.87	0.42
2:G:4864:ASN:H	2:G:4874:MET:HG2	1.85	0.42
2:I:866:HIS:O	2:I:1051:TYR:OH	2.32	0.42
2:I:947:GLU:HG3	2:I:1049:TYR:HD1	1.85	0.42
2:I:1207:ASP:HB3	2:I:1210:SER:HB3	2.02	0.42
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.02	0.42
2:I:5013:MET:HA	2:I:5016:GLU:HB3	2.01	0.42
2:B:345:LEU:HD23	2:B:389:PHE:HB3	2.00	0.42
2:B:498:THR:OG1	2:B:499:THR:N	2.53	0.42
2:B:4864:ASN:H	2:B:4874:MET:HG2	1.84	0.42
2:B:5013:MET:HA	2:B:5016:GLU:HB3	2.01	0.42
2:E:2517:UNK:O	2:E:2521:UNK:N	2.53	0.42
2:E:4568:PHE:HA	2:E:4571:PHE:HD2	1.84	0.42
2:G:180:LEU:HD22	2:G:200:TRP:NE1	2.35	0.42
2:G:313:SER:HB3	2:G:352:ALA:H	1.84	0.42
2:G:4801:LEU:HB3	2:G:4808:PHE:CG	2.54	0.42
2:I:891:TRP:HA	2:I:902:ARG:HB3	2.01	0.42
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	2.02	0.42
2:I:3934:TYR:HB2	2:I:3999:MET:HE3	2.01	0.42
2:I:3953:LYS:O	2:I:3956:SER:OG	2.29	0.42
2:I:4928:LEU:HD13	2:I:4931:ILE:HD12	2.01	0.42
2:B:264:PRO:HG2	2:B:270:SER:HB2	2.02	0.42
2:B:355:LEU:HB3	2:B:378:LEU:HB3	2.01	0.42
2:B:3934:TYR:HB2	2:B:3999:MET:HE3	2.01	0.42
2:E:947:GLU:HG3	2:E:1049:TYR:HD1	1.85	0.42
2:E:3927:GLN:NE2	2:E:3988:ALA:O	2.49	0.42
2:E:4174:PHE:HD1	2:E:4174:PHE:HA	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5013:MET:HA	2:E:5016:GLU:HB3	2.01	0.42
2:E:5026:ASP:OD1	2:E:5027:CYS:N	2.52	0.42
2:G:947:GLU:HG3	2:G:1049:TYR:HD1	1.85	0.42
2:I:180:LEU:HD22	2:I:200:TRP:NE1	2.35	0.42
2:I:313:SER:HB3	2:I:351:VAL:HB	2.01	0.42
2:I:1663:HIS:O	2:I:1667:LEU:N	2.46	0.42
2:I:1703:LEU:HD21	2:I:1830:VAL:HG13	2.02	0.42
2:I:1979:LEU:HA	2:I:1983:ALA:HB3	2.02	0.42
2:I:2116:LEU:O	2:I:2120:MET:N	2.48	0.42
2:I:3674:ILE:HG13	2:I:3732:SER:HB3	2.01	0.42
2:I:4639:MET:HE2	2:I:4639:MET:HB3	1.90	0.42
2:I:4667:PRO:O	2:I:4714:ASN:ND2	2.52	0.42
2:B:220:LEU:HD11	2:B:390:LEU:HD22	2.00	0.42
2:B:4686:LEU:O	2:B:4691:GLN:N	2.52	0.42
2:G:635:THR:HB	2:G:1639:LEU:HD23	2.02	0.42
2:G:1232:ARG:HD3	2:G:1702:HIS:HB3	2.00	0.42
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.00	0.42
2:G:4026:MET:O	2:G:4030:LEU:N	2.52	0.42
2:G:4736:ARG:O	2:G:4740:LEU:N	2.50	0.42
2:I:290:TYR:O	2:I:302:VAL:N	2.52	0.42
2:I:349:GLN:HE21	2:I:354:GLY:HA2	1.85	0.42
1:J:87:HIS:HB3	1:J:91:ILE:H	1.84	0.42
2:B:36:CYS:O	2:B:50:GLU:N	2.53	0.41
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.02	0.41
2:B:3229:UNK:HA	2:B:3302:UNK:HA	2.01	0.41
2:E:101:LEU:HB2	2:E:163:VAL:HB	2.02	0.41
2:E:3674:ILE:HG13	2:E:3732:SER:HB3	2.01	0.41
2:G:119:SER:HA	2:G:146:CYS:HA	2.03	0.41
2:I:241:GLN:O	2:I:289:ARG:NH1	2.44	0.41
2:I:1094:ALA:HA	2:I:1200:GLY:HA2	2.01	0.41
2:I:2347:GLU:O	2:I:2351:ASN:N	2.36	0.41
2:I:4000:MET:HE2	2:I:4061:PHE:HD2	1.83	0.41
2:I:4701:TRP:CZ2	2:I:4781:GLY:HA3	2.55	0.41
2:I:4852:THR:HG21	2:I:4883:TYR:HB2	2.01	0.41
2:B:1094:ALA:HA	2:B:1200:GLY:HA2	2.01	0.41
2:B:4928:LEU:HD13	2:B:4931:ILE:HD12	2.01	0.41
2:E:635:THR:HB	2:E:1639:LEU:HD23	2.02	0.41
2:E:891:TRP:HA	2:E:902:ARG:HB3	2.01	0.41
2:E:2116:LEU:O	2:E:2120:MET:N	2.48	0.41
2:E:4736:ARG:O	2:E:4740:LEU:N	2.50	0.41
2:E:4928:LEU:HD13	2:E:4931:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1657:LEU:HD13	2:G:1657:LEU:HA	1.91	0.41
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	2.02	0.41
2:I:3361:UNK:O	2:I:3365:UNK:N	2.52	0.41
2:B:288:GLY:HA3	2:B:405:HIS:CE1	2.54	0.41
2:B:360:ALA:N	2:B:375:LYS:O	2.53	0.41
2:B:1207:ASP:HB3	2:B:1210:SER:HB3	2.02	0.41
2:B:1703:LEU:HD21	2:B:1830:VAL:HG13	2.01	0.41
2:B:2318:TYR:HA	2:B:2319:PRO:HD3	1.88	0.41
2:B:3792:ALA:HA	2:B:3795:SER:HB3	2.02	0.41
2:E:131:LEU:HB3	2:G:2459:SER:HB2	2.03	0.41
2:E:313:SER:HB3	2:E:351:VAL:HB	2.01	0.41
2:E:1090:PHE:CD2	2:E:1202:LEU:HD11	2.56	0.41
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	2.02	0.41
2:G:1088:TRP:HB2	2:G:1153:ILE:HG22	2.02	0.41
2:G:1866:ILE:HG13	2:G:1926:LEU:HB3	2.01	0.41
2:G:2116:LEU:O	2:G:2120:MET:N	2.48	0.41
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	2.02	0.41
2:G:4108:ILE:HA	2:G:4111:LEU:HD12	2.01	0.41
2:I:101:LEU:HB2	2:I:163:VAL:HB	2.02	0.41
2:I:4108:ILE:HA	2:I:4111:LEU:HD12	2.01	0.41
2:B:180:LEU:HD22	2:B:200:TRP:NE1	2.35	0.41
2:B:635:THR:HB	2:B:1639:LEU:HD23	2.02	0.41
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.03	0.41
2:B:978:THR:HB	2:B:980:ALA:H	1.84	0.41
2:B:983:THR:O	2:B:987:ARG:N	2.52	0.41
2:B:1090:PHE:CD2	2:B:1202:LEU:HD11	2.56	0.41
2:B:1092:PHE:O	2:B:1149:VAL:N	2.49	0.41
2:B:3674:ILE:HG13	2:B:3732:SER:HB3	2.02	0.41
2:B:4583:SER:O	2:B:4628:VAL:N	2.44	0.41
2:B:4826:ILE:O	2:B:4829:SER:OG	2.33	0.41
2:E:36:CYS:O	2:E:50:GLU:N	2.53	0.41
2:E:180:LEU:HD22	2:E:200:TRP:NE1	2.35	0.41
2:E:4852:THR:HG21	2:E:4883:TYR:HB2	2.02	0.41
2:G:281:ARG:HA	2:G:312:THR:HG21	2.02	0.41
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.02	0.41
2:G:2458:ARG:NH2	2:G:2509:UNK:O	2.42	0.41
2:I:635:THR:HA	2:I:1639:LEU:HA	2.03	0.41
2:I:978:THR:HB	2:I:980:ALA:H	1.84	0.41
2:I:1041:GLN:O	2:I:1045:THR:OG1	2.29	0.41
2:I:4824:ARG:O	2:I:4828:SER:N	2.47	0.41
2:B:2770:LYS:O	2:B:2775:TRP:N	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4852:THR:HG21	2:B:4883:TYR:HB2	2.01	0.41
2:B:4879:MET:HB2	2:E:4580:TYR:HB2	2.02	0.41
2:E:264:PRO:HG2	2:E:270:SER:HB2	2.02	0.41
2:E:4686:LEU:O	2:E:4691:GLN:N	2.52	0.41
2:E:4864:ASN:H	2:E:4874:MET:HG2	1.84	0.41
2:G:224:HIS:H	2:G:230:CYS:HA	1.86	0.41
2:G:1679:ASN:O	2:G:1683:HIS:ND1	2.36	0.41
2:G:1950:GLU:OE2	2:G:1954:ARG:NH2	2.43	0.41
2:G:2880:GLU:O	2:G:2884:ASN:N	2.47	0.41
2:G:3953:LYS:O	2:G:3956:SER:OG	2.29	0.41
2:G:4701:TRP:CZ2	2:G:4781:GLY:HA3	2.55	0.41
2:G:4826:ILE:O	2:G:4829:SER:OG	2.33	0.41
2:I:345:LEU:HD23	2:I:389:PHE:HB3	2.00	0.41
2:I:1095:VAL:HA	2:I:1146:GLY:H	1.85	0.41
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	2.01	0.41
2:B:485:SER:O	2:B:489:ASN:N	2.50	0.41
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	2.03	0.41
2:E:22:LEU:HD23	2:E:22:LEU:HA	1.92	0.41
2:E:805:PRO:HB2	2:E:808:TYR:CE2	2.56	0.41
2:E:3792:ALA:HA	2:E:3795:SER:HB3	2.02	0.41
2:E:3915:ILE:H	2:E:3915:ILE:HG13	1.56	0.41
2:G:1948:ASP:O	2:G:1952:GLN:N	2.44	0.41
2:G:3998:HIS:CD2	2:G:4057:MET:HE1	2.56	0.41
2:G:4852:THR:HG21	2:G:4883:TYR:HB2	2.02	0.41
1:H:87:HIS:HB3	1:H:91:ILE:H	1.84	0.41
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.85	0.41
2:I:4174:PHE:HD1	2:I:4174:PHE:HA	1.71	0.41
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.28	0.41
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.35	0.41
1:A:7:ILE:HB	1:A:71:ARG:HB3	2.03	0.41
2:B:224:HIS:H	2:B:230:CYS:HA	1.86	0.41
2:B:313:SER:HB3	2:B:351:VAL:HB	2.01	0.41
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.41
2:B:3730:ALA:O	2:B:3734:HIS:N	2.41	0.41
2:B:3963:ASN:O	2:B:3966:THR:OG1	2.30	0.41
2:B:4667:PRO:O	2:B:4714:ASN:ND2	2.52	0.41
2:B:4824:ARG:HA	2:B:4827:LEU:HB3	2.03	0.41
2:E:119:SER:HA	2:E:146:CYS:HA	2.03	0.41
2:E:308:HIS:CE1	2:E:310:LYS:HD2	2.56	0.41
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.02	0.41
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3700:GLN:HA	2:E:3703:LEU:HD12	2.01	0.41
2:E:3765:TYR:CD2	2:E:3769:ARG:HD3	2.56	0.41
2:G:173:SER:OG	2:G:174:VAL:N	2.54	0.41
2:G:360:ALA:N	2:G:375:LYS:O	2.53	0.41
2:G:1032:LYS:O	2:G:1036:ARG:N	2.45	0.41
2:G:2674:UNK:O	2:G:2676:UNK:N	2.54	0.41
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.86	0.41
2:G:4563:ARG:HH12	2:G:4815:ASP:CG	2.29	0.41
2:I:355:LEU:HB3	2:I:378:LEU:HB3	2.01	0.41
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.03	0.41
2:I:2517:UNK:O	2:I:2521:UNK:N	2.54	0.41
2:I:4563:ARG:HH12	2:I:4815:ASP:CG	2.29	0.41
2:I:4824:ARG:HA	2:I:4827:LEU:HB3	2.03	0.41
2:B:281:ARG:HA	2:B:312:THR:HG21	2.01	0.41
2:B:308:HIS:CE1	2:B:310:LYS:HD2	2.56	0.41
2:B:2021:CYS:HA	2:B:2022:PRO:HD3	1.91	0.41
2:B:2908:TYR:OH	2:B:2920:ARG:NE	2.45	0.41
2:E:181:HIS:CD2	2:E:196:MET:HB2	2.56	0.41
2:E:793:LEU:HD12	2:E:797:HIS:HB2	2.02	0.41
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.03	0.41
2:E:1088:TRP:HB2	2:E:1153:ILE:HG22	2.02	0.41
2:E:3963:ASN:O	2:E:3966:THR:OG1	2.30	0.41
2:E:4563:ARG:HH12	2:E:4815:ASP:CG	2.29	0.41
2:E:4701:TRP:CZ2	2:E:4781:GLY:HA3	2.55	0.41
2:G:1979:LEU:HA	2:G:1983:ALA:HB3	2.02	0.41
2:G:4705:VAL:HB	2:G:4778:TRP:CD1	2.56	0.41
2:I:119:SER:HA	2:I:146:CYS:HA	2.03	0.41
2:I:635:THR:HB	2:I:1639:LEU:HD23	2.02	0.41
2:I:1657:LEU:HD13	2:I:1657:LEU:HA	1.90	0.41
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.54	0.41
2:B:181:HIS:CD2	2:B:196:MET:HB2	2.56	0.41
2:B:205:ILE:HD12	2:B:205:ILE:HA	1.94	0.41
2:B:635:THR:HA	2:B:1639:LEU:HA	2.03	0.41
2:B:805:PRO:HB2	2:B:808:TYR:CE2	2.56	0.41
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.54	0.41
2:B:1979:LEU:HA	2:B:1983:ALA:HB3	2.01	0.41
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	2.02	0.41
2:B:2265:LEU:HD21	2:B:2273:LEU:HD13	2.02	0.41
2:B:3965:LEU:HA	2:B:3968:TYR:CD2	2.56	0.41
2:B:4705:VAL:HB	2:B:4778:TRP:CD1	2.56	0.41
2:E:1095:VAL:HA	2:E:1146:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1703:LEU:HD21	2:E:1830:VAL:HG13	2.02	0.41
2:E:2880:GLU:O	2:E:2884:ASN:N	2.47	0.41
2:E:3646:THR:O	2:E:3650:CYS:N	2.49	0.41
2:E:4701:TRP:HE1	2:E:4782:VAL:HG23	1.86	0.41
2:E:4705:VAL:HB	2:E:4778:TRP:CD1	2.56	0.41
1:F:7:ILE:HB	1:F:71:ARG:HB3	2.03	0.41
2:G:36:CYS:O	2:G:50:GLU:N	2.53	0.41
2:G:259:LEU:HD23	2:G:259:LEU:HA	1.83	0.41
2:G:355:LEU:HB3	2:G:378:LEU:HB3	2.01	0.41
2:G:488:LEU:HA	2:G:491:ILE:HB	2.03	0.41
2:G:805:PRO:HB2	2:G:808:TYR:CE2	2.56	0.41
2:G:1090:PHE:CD2	2:G:1202:LEU:HD11	2.56	0.41
2:G:1658:ASP:OD1	2:G:1658:ASP:N	2.52	0.41
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	2.03	0.41
2:G:3805:LEU:H	2:G:3805:LEU:HG	1.51	0.41
2:G:4702:ASP:HA	2:G:4778:TRP:HE1	1.86	0.41
1:H:7:ILE:HB	1:H:71:ARG:HB3	2.03	0.41
2:I:181:HIS:CD2	2:I:196:MET:HB2	2.56	0.41
2:I:663:TYR:HB2	2:I:808:TYR:HB3	2.03	0.41
2:I:2247:GLN:O	2:I:2279:SER:OG	2.39	0.41
2:I:2674:UNK:O	2:I:2676:UNK:N	2.54	0.41
2:I:3965:LEU:HA	2:I:3968:TYR:CD2	2.56	0.41
2:I:3998:HIS:CD2	2:I:4057:MET:HE1	2.56	0.41
2:I:4705:VAL:HB	2:I:4778:TRP:CD1	2.56	0.41
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.35	0.41
2:B:119:SER:HA	2:B:146:CYS:HA	2.02	0.41
2:B:870:ILE:HA	2:B:870:ILE:HD12	1.86	0.41
2:B:1088:TRP:HB2	2:B:1153:ILE:HG22	2.02	0.41
2:E:710:ASP:OD1	2:E:710:ASP:N	2.52	0.41
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	2.03	0.41
2:E:2021:CYS:HA	2:E:2022:PRO:HD3	1.91	0.41
2:E:2265:LEU:HD21	2:E:2273:LEU:HD13	2.02	0.41
2:E:3645:PRO:HB2	2:E:3648:ARG:HB3	2.03	0.41
1:F:7:ILE:N	1:F:71:ARG:O	2.46	0.41
2:G:793:LEU:HD12	2:G:797:HIS:HB2	2.02	0.41
2:G:1729:SER:O	2:G:2163:ARG:NH1	2.54	0.41
2:G:3765:TYR:CD2	2:G:3769:ARG:HD3	2.56	0.41
2:G:3965:LEU:HA	2:G:3968:TYR:CD2	2.56	0.41
2:G:4824:ARG:HA	2:G:4827:LEU:HB3	2.03	0.41
2:I:173:SER:OG	2:I:174:VAL:N	2.54	0.41
2:I:224:HIS:H	2:I:230:CYS:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:788:LYS:HG2	2:I:1630:CYS:N	2.33	0.41
2:I:2207:VAL:HG13	2:I:2232:CYS:HB2	2.03	0.41
2:I:2759:ALA:HB1	2:I:2805:TYR:HB3	2.03	0.41
2:I:3805:LEU:H	2:I:3805:LEU:HG	1.51	0.41
2:I:4701:TRP:HE1	2:I:4782:VAL:HG23	1.86	0.41
1:A:7:ILE:N	1:A:71:ARG:O	2.46	0.40
2:B:150:MET:HE2	2:B:150:MET:HB3	1.98	0.40
2:B:4563:ARG:HH12	2:B:4815:ASP:CG	2.29	0.40
2:B:4701:TRP:HE1	2:B:4782:VAL:HG23	1.86	0.40
2:E:836:GLY:HA3	2:E:1201:HIS:ND1	2.36	0.40
2:E:1936:LYS:O	2:E:1940:CYS:N	2.50	0.40
2:E:4824:ARG:HA	2:E:4827:LEU:HB3	2.03	0.40
2:G:101:LEU:HB2	2:G:163:VAL:HB	2.03	0.40
2:G:635:THR:HA	2:G:1639:LEU:HA	2.03	0.40
2:G:1095:VAL:HA	2:G:1146:GLY:H	1.85	0.40
2:G:1096:THR:OG1	2:G:1199:VAL:O	2.39	0.40
2:G:2770:LYS:O	2:G:2775:TRP:N	2.42	0.40
2:G:4701:TRP:HE1	2:G:4782:VAL:HG23	1.86	0.40
2:I:103:TYR:HB3	2:I:152:PRO:HD3	2.04	0.40
2:I:793:LEU:HD12	2:I:797:HIS:HB2	2.03	0.40
2:I:1948:ASP:O	2:I:1952:GLN:N	2.44	0.40
2:B:103:TYR:HB3	2:B:152:PRO:HD3	2.04	0.40
2:B:173:SER:OG	2:B:174:VAL:N	2.54	0.40
2:B:663:TYR:HB2	2:B:808:TYR:HB3	2.03	0.40
2:B:2207:VAL:HG13	2:B:2232:CYS:HB2	2.03	0.40
2:B:3153:UNK:O	2:B:3157:UNK:N	2.54	0.40
2:B:3765:TYR:CD2	2:B:3769:ARG:HD3	2.56	0.40
2:B:4677:LEU:HD13	2:B:4677:LEU:HA	1.94	0.40
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.54	0.40
2:E:2207:VAL:HG13	2:E:2232:CYS:HB2	2.03	0.40
2:E:4182:GLU:HB3	2:E:4192:ARG:HG3	2.04	0.40
2:E:4859:PHE:HZ	2:E:4912:TYR:HB2	1.86	0.40
2:G:264:PRO:HG2	2:G:270:SER:HB2	2.02	0.40
2:G:864:PRO:HA	2:G:865:PRO:HD3	1.97	0.40
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.02	0.40
2:G:4570:ALA:O	2:G:4574:ASN:ND2	2.55	0.40
2:I:1088:TRP:HB2	2:I:1153:ILE:HG22	2.02	0.40
2:I:2265:LEU:HD21	2:I:2273:LEU:HD13	2.02	0.40
2:I:3663:LEU:H	2:I:3663:LEU:HG	1.40	0.40
2:I:3765:TYR:CD2	2:I:3769:ARG:HD3	2.56	0.40
1:J:7:ILE:HB	1:J:71:ARG:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ASP:HB2	2:B:98:HIS:CE1	2.50	0.40
2:B:101:LEU:HB2	2:B:163:VAL:HB	2.02	0.40
2:B:1256:GLU:HG2	2:B:1273:ALA:HB3	2.03	0.40
2:B:4580:TYR:H	2:I:4879:MET:HB3	1.86	0.40
2:B:4651:THR:HA	2:B:4799:SER:HB3	2.04	0.40
2:E:3998:HIS:CD2	2:E:4057:MET:HE1	2.56	0.40
2:E:4667:PRO:O	2:E:4714:ASN:ND2	2.52	0.40
2:G:17:ASP:HB2	2:G:98:HIS:CE1	2.50	0.40
2:G:836:GLY:HA3	2:G:1201:HIS:ND1	2.36	0.40
2:G:983:THR:O	2:G:987:ARG:N	2.52	0.40
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.54	0.40
2:G:1936:LYS:O	2:G:1940:CYS:N	2.50	0.40
2:G:4174:PHE:HD1	2:G:4174:PHE:HA	1.71	0.40
2:G:4207:MET:HA	2:G:4208:PRO:HD3	1.96	0.40
2:I:308:HIS:CE1	2:I:310:LYS:HD2	2.56	0.40
2:I:488:LEU:HA	2:I:491:ILE:HB	2.03	0.40
2:I:805:PRO:HB2	2:I:808:TYR:CE2	2.56	0.40
2:I:1497:UNK:HA	2:I:1535:UNK:HA	2.02	0.40
2:I:4091:LYS:HA	2:I:4091:LYS:HD3	1.85	0.40
2:I:4147:LEU:O	2:I:4151:SER:OG	2.30	0.40
2:I:4924:VAL:O	2:I:4928:LEU:N	2.37	0.40
2:B:260:TRP:CE2	2:B:284:HIS:HD2	2.40	0.40
2:B:3645:PRO:HB2	2:B:3648:ARG:HB3	2.03	0.40
2:E:173:SER:OG	2:E:174:VAL:N	2.54	0.40
2:E:663:TYR:HB2	2:E:808:TYR:HB3	2.03	0.40
2:E:4570:ALA:O	2:E:4574:ASN:ND2	2.55	0.40
2:G:181:HIS:CD2	2:G:196:MET:HB2	2.56	0.40
2:G:308:HIS:CE1	2:G:310:LYS:HD2	2.56	0.40
2:G:663:TYR:HB2	2:G:808:TYR:HB3	2.03	0.40
2:G:1703:LEU:HD21	2:G:1830:VAL:HG13	2.01	0.40
2:G:3661:TRP:HB3	2:G:3662:ILE:H	1.77	0.40
2:G:4795:TYR:CZ	2:G:4812:HIS:HD2	2.40	0.40
2:G:4961:CYS:HB2	2:G:4963:ILE:HD12	2.04	0.40
2:B:975:VAL:O	2:B:1044:ARG:NH2	2.52	0.40
2:B:1032:LYS:O	2:B:1036:ARG:N	2.45	0.40
2:B:2247:GLN:O	2:B:2279:SER:OG	2.39	0.40
2:B:2759:ALA:HB1	2:B:2805:TYR:HB3	2.04	0.40
2:B:3661:TRP:HB3	2:B:3662:ILE:H	1.77	0.40
2:B:3998:HIS:CD2	2:B:4057:MET:HE1	2.56	0.40
2:B:4080:TYR:CD1	2:B:4092:ASP:HB2	2.57	0.40
2:E:224:HIS:H	2:E:230:CYS:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:488:LEU:HA	2:E:491:ILE:HB	2.03	0.40
2:E:1497:UNK:HA	2:E:1535:UNK:HA	2.03	0.40
2:E:2318:TYR:HA	2:E:2319:PRO:HD3	1.88	0.40
2:E:2432:LEU:O	2:E:2436:CYS:N	2.55	0.40
2:E:3965:LEU:HA	2:E:3968:TYR:CD2	2.56	0.40
2:E:4651:THR:HA	2:E:4799:SER:HB3	2.04	0.40
2:G:463:GLU:O	2:G:466:SER:OG	2.34	0.40
2:G:1034:SER:O	2:G:1038:SER:N	2.54	0.40
2:G:2265:LEU:HD21	2:G:2273:LEU:HD13	2.02	0.40
2:G:2432:LEU:O	2:G:2436:CYS:N	2.55	0.40
2:G:4064:MET:HA	2:G:4067:LYS:HE3	2.04	0.40
2:I:19:GLU:HB2	2:I:206:CYS:HB3	2.04	0.40
2:I:131:LEU:H	2:I:131:LEU:HG	1.58	0.40
2:I:259:LEU:HD23	2:I:259:LEU:HA	1.83	0.40
2:I:281:ARG:HA	2:I:312:THR:HG21	2.02	0.40
2:I:1090:PHE:CD2	2:I:1202:LEU:HD11	2.56	0.40
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.03	0.40
2:I:3694:LYS:HA	2:I:3695:PRO:HD3	1.98	0.40
2:I:4080:TYR:CD1	2:I:4092:ASP:HB2	2.57	0.40
2:I:4680:LYS:HB3	2:I:4686:LEU:HD22	2.03	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	3235/4687 (69%)	2859 (88%)	367 (11%)	9 (0%)	36	71
2	E	3235/4687 (69%)	2860 (88%)	367 (11%)	8 (0%)	43	77
2	G	3235/4687 (69%)	2859 (88%)	367 (11%)	9 (0%)	36	71
2	I	3235/4687 (69%)	2860 (88%)	366 (11%)	9 (0%)	36	71
All	All	13360/19176 (70%)	11818 (88%)	1507 (11%)	35 (0%)	37	71

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3772	THR
2	B	4667	PRO
2	E	3772	THR
2	E	4667	PRO
2	G	3772	THR
2	G	4667	PRO
2	I	3772	THR
2	I	4667	PRO
2	B	1708	ARG
2	B	1829	PRO
2	B	1932	PRO
2	B	4062	PHE
2	E	1708	ARG
2	E	1829	PRO
2	E	1932	PRO
2	G	1708	ARG
2	G	1829	PRO
2	G	1932	PRO
2	I	1708	ARG
2	I	1829	PRO
2	I	1932	PRO
2	I	4062	PHE
2	B	1840	PRO
2	E	1840	PRO
2	G	553	ARG
2	G	1840	PRO
2	I	1840	PRO
2	B	834	PRO
2	G	834	PRO
2	I	834	PRO
2	B	2343	GLY
2	E	834	PRO

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Mol	Chain	Res	Type
2	E	2343	GLY
2	G	2343	GLY
2	I	2343	GLY

5.3.2 Protein sidechains [i](#)

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%)	2477 (99%)	16 (1%)	78	80
2	E	2493/3209 (78%)	2477 (99%)	16 (1%)	78	80
2	G	2493/3209 (78%)	2477 (99%)	16 (1%)	78	80
2	I	2493/3209 (78%)	2477 (99%)	16 (1%)	78	80
All	All	10324/13188 (78%)	10260 (99%)	64 (1%)	76	80

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	280	LEU
2	B	688	LEU
2	B	978	THR
2	B	2144	ILE
2	B	2339	VAL
2	B	3663	LEU
2	B	3805	LEU
2	B	3896	ASN
2	B	4059	LEU
2	B	4154	VAL
2	B	4180	ARG

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Mol	Chain	Res	Type
2	B	4871	GLU
2	B	4950	VAL
2	B	4957	LYS
2	B	4995	LEU
2	E	131	LEU
2	E	280	LEU
2	E	688	LEU
2	E	978	THR
2	E	2144	ILE
2	E	2339	VAL
2	E	3663	LEU
2	E	3805	LEU
2	E	3896	ASN
2	E	4059	LEU
2	E	4154	VAL
2	E	4180	ARG
2	E	4871	GLU
2	E	4950	VAL
2	E	4957	LYS
2	E	4995	LEU
2	G	131	LEU
2	G	280	LEU
2	G	688	LEU
2	G	978	THR
2	G	2144	ILE
2	G	2339	VAL
2	G	3663	LEU
2	G	3805	LEU
2	G	3896	ASN
2	G	4059	LEU
2	G	4154	VAL
2	G	4180	ARG
2	G	4871	GLU
2	G	4950	VAL
2	G	4957	LYS
2	G	4995	LEU
2	I	131	LEU
2	I	280	LEU
2	I	688	LEU
2	I	978	THR
2	I	2144	ILE
2	I	2339	VAL

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Mol	Chain	Res	Type
2	I	3663	LEU
2	I	3805	LEU
2	I	3896	ASN
2	I	4059	LEU
2	I	4154	VAL
2	I	4180	ARG
2	I	4871	GLU
2	I	4950	VAL
2	I	4957	LYS
2	I	4995	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (240) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	44	ASN
2	B	111	HIS
2	B	113	HIS
2	B	138	GLN
2	B	151	HIS
2	B	201	ASN
2	B	255	HIS
2	B	273	HIS
2	B	308	HIS
2	B	379	HIS
2	B	395	GLN
2	B	405	HIS
2	B	413	GLN
2	B	495	ASN
2	B	639	ASN
2	B	678	GLN
2	B	765	GLN
2	B	797	HIS
2	B	838	HIS
2	B	877	ASN
2	B	1035	ASN
2	B	1158	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1696	HIS
2	B	1719	HIS
2	B	1775	HIS

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Mol	Chain	Res	Type
2	B	1776	HIS
2	B	1837	GLN
2	B	1861	GLN
2	B	1941	ASN
2	B	1949	GLN
2	B	2005	GLN
2	B	2011	HIS
2	B	2188	ASN
2	B	2291	GLN
2	B	2858	GLN
2	B	3767	GLN
2	B	3771	HIS
2	B	3814	GLN
2	B	3882	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3960	GLN
2	B	3963	ASN
2	B	3978	GLN
2	B	3982	HIS
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4201	ASN
2	B	4209	GLN
2	B	4246	GLN
2	B	4553	ASN
2	B	4691	GLN
2	B	4728	HIS
2	B	4833	ASN
2	B	4886	HIS
2	B	4984	ASN
2	B	4987	ASN
2	E	44	ASN
2	E	111	HIS
2	E	113	HIS
2	E	138	GLN
2	E	151	HIS
2	E	201	ASN
2	E	255	HIS
2	E	273	HIS

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Mol	Chain	Res	Type
2	E	379	HIS
2	E	395	GLN
2	E	405	HIS
2	E	413	GLN
2	E	495	ASN
2	E	639	ASN
2	E	678	GLN
2	E	765	GLN
2	E	797	HIS
2	E	838	HIS
2	E	877	ASN
2	E	1035	ASN
2	E	1158	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1691	GLN
2	E	1696	HIS
2	E	1719	HIS
2	E	1775	HIS
2	E	1776	HIS
2	E	1837	GLN
2	E	1861	GLN
2	E	1941	ASN
2	E	1949	GLN
2	E	2005	GLN
2	E	2011	HIS
2	E	2188	ASN
2	E	2291	GLN
2	E	2858	GLN
2	E	3766	GLN
2	E	3767	GLN
2	E	3771	HIS
2	E	3814	GLN
2	E	3882	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3960	GLN
2	E	3963	ASN
2	E	3978	GLN
2	E	3982	HIS
2	E	4034	ASN
2	E	4054	ASN

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Mol	Chain	Res	Type
2	E	4120	ASN
2	E	4130	ASN
2	E	4201	ASN
2	E	4209	GLN
2	E	4246	GLN
2	E	4553	ASN
2	E	4728	HIS
2	E	4806	ASN
2	E	4886	HIS
2	E	4984	ASN
2	E	4987	ASN
2	E	5031	GLN
2	G	44	ASN
2	G	111	HIS
2	G	113	HIS
2	G	138	GLN
2	G	151	HIS
2	G	201	ASN
2	G	255	HIS
2	G	273	HIS
2	G	308	HIS
2	G	379	HIS
2	G	395	GLN
2	G	405	HIS
2	G	413	GLN
2	G	495	ASN
2	G	639	ASN
2	G	765	GLN
2	G	797	HIS
2	G	838	HIS
2	G	877	ASN
2	G	1035	ASN
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN
2	G	1696	HIS
2	G	1719	HIS
2	G	1775	HIS
2	G	1837	GLN
2	G	1861	GLN
2	G	1941	ASN
2	G	1949	GLN

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Mol	Chain	Res	Type
2	G	2005	GLN
2	G	2011	HIS
2	G	2188	ASN
2	G	2858	GLN
2	G	3766	GLN
2	G	3767	GLN
2	G	3771	HIS
2	G	3814	GLN
2	G	3882	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	3978	GLN
2	G	3982	HIS
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4209	GLN
2	G	4246	GLN
2	G	4553	ASN
2	G	4691	GLN
2	G	4728	HIS
2	G	4886	HIS
2	G	4984	ASN
2	G	4987	ASN
2	G	5031	GLN
2	I	44	ASN
2	I	111	HIS
2	I	113	HIS
2	I	138	GLN
2	I	151	HIS
2	I	201	ASN
2	I	255	HIS
2	I	273	HIS
2	I	308	HIS
2	I	379	HIS
2	I	395	GLN
2	I	405	HIS
2	I	413	GLN
2	I	495	ASN

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Mol	Chain	Res	Type
2	I	639	ASN
2	I	678	GLN
2	I	797	HIS
2	I	838	HIS
2	I	877	ASN
2	I	1035	ASN
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1696	HIS
2	I	1719	HIS
2	I	1775	HIS
2	I	1776	HIS
2	I	1837	GLN
2	I	1861	GLN
2	I	1941	ASN
2	I	1949	GLN
2	I	2005	GLN
2	I	2188	ASN
2	I	2291	GLN
2	I	2858	GLN
2	I	3767	GLN
2	I	3771	HIS
2	I	3814	GLN
2	I	3882	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3960	GLN
2	I	3963	ASN
2	I	3978	GLN
2	I	3982	HIS
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4130	ASN
2	I	4201	ASN
2	I	4209	GLN
2	I	4246	GLN
2	I	4553	ASN
2	I	4691	GLN
2	I	4728	HIS
2	I	4886	HIS

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Mol	Chain	Res	Type
2	I	4984	ASN
2	I	4987	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 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	G	12

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	3613:UNK	C	3639:THR	N	44.11
1	I	3613:UNK	C	3639:THR	N	44.00
1	B	3613:UNK	C	3639:THR	N	43.94
1	E	3613:UNK	C	3639:THR	N	43.92
1	B	3163:UNK	C	3170:UNK	N	16.36
1	E	3163:UNK	C	3170:UNK	N	16.33
1	G	3163:UNK	C	3170:UNK	N	16.33
1	I	3163:UNK	C	3170:UNK	N	16.30
1	G	3468:UNK	C	3511:UNK	N	14.94
1	I	3468:UNK	C	3511:UNK	N	14.93
1	E	3468:UNK	C	3511:UNK	N	14.92
1	B	3468:UNK	C	3511:UNK	N	14.86
1	I	2703:UNK	C	2734:ASN	N	14.67
1	I	3063:UNK	C	3134:UNK	N	14.51
1	G	3063:UNK	C	3134:UNK	N	14.49
1	G	2703:UNK	C	2734:ASN	N	14.48
1	E	2703:UNK	C	2734:ASN	N	14.47
1	E	3063:UNK	C	3134:UNK	N	14.47
1	B	3063:UNK	C	3134:UNK	N	14.44
1	B	2703:UNK	C	2734:ASN	N	14.42
1	G	3236:UNK	C	3241:UNK	N	13.22
1	I	3236:UNK	C	3241:UNK	N	13.18
1	B	3236:UNK	C	3241:UNK	N	13.14
1	E	3236:UNK	C	3241:UNK	N	13.10
1	I	1564:UNK	C	1573:MET	N	12.99
1	B	1564:UNK	C	1573:MET	N	12.92
1	E	1564:UNK	C	1573:MET	N	12.81
1	G	1564:UNK	C	1573:MET	N	12.78
1	B	2976:UNK	C	2995:UNK	N	12.16
1	E	2976:UNK	C	2995:UNK	N	12.16
1	G	2976:UNK	C	2995:UNK	N	12.08
1	I	2976:UNK	C	2995:UNK	N	12.05
1	B	3254:UNK	C	3261:UNK	N	8.60
1	I	3254:UNK	C	3261:UNK	N	8.60
1	E	3254:UNK	C	3261:UNK	N	8.59
1	G	3254:UNK	C	3261:UNK	N	8.59

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	1297:UNK	C	1430:UNK	N	5.77
1	B	1297:UNK	C	1430:UNK	N	5.73
1	G	1297:UNK	C	1430:UNK	N	5.66
1	I	1297:UNK	C	1430:UNK	N	5.38
1	B	2479:LEU	C	2487:UNK	N	3.76
1	G	2939:ARG	C	2942:UNK	N	3.69
1	G	2479:LEU	C	2487:UNK	N	3.65
1	I	2479:LEU	C	2487:UNK	N	3.63
1	E	2479:LEU	C	2487:UNK	N	3.60
1	I	2939:ARG	C	2942:UNK	N	3.46
1	E	2939:ARG	C	2942:UNK	N	3.43
1	B	2939:ARG	C	2942:UNK	N	3.42

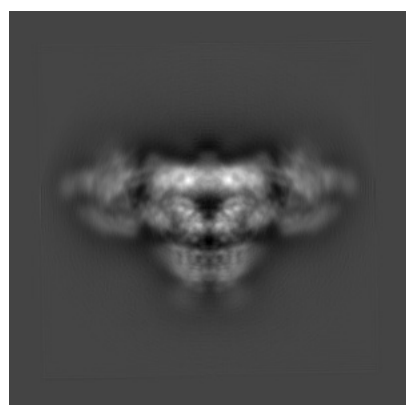
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22396. These allow visual inspection of the internal detail of the map and identification of artifacts.

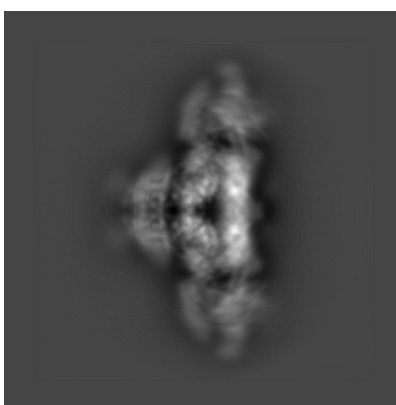
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

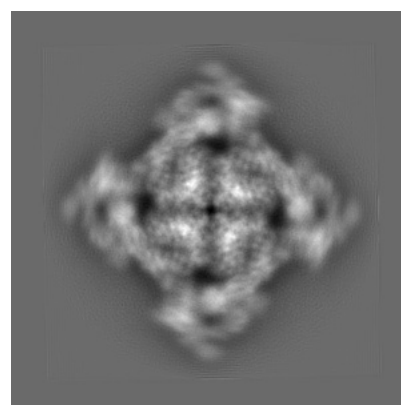
6.1.1 Primary map



X



Y

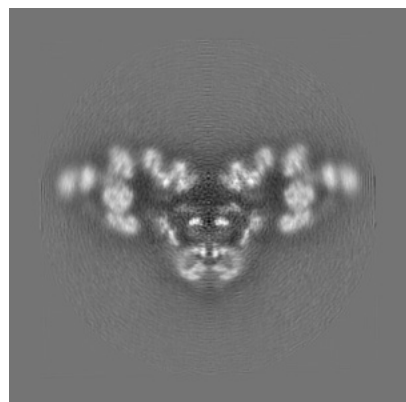


Z

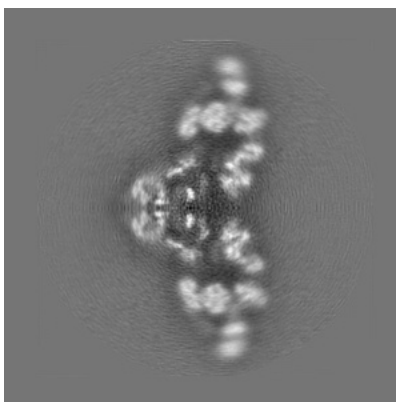
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

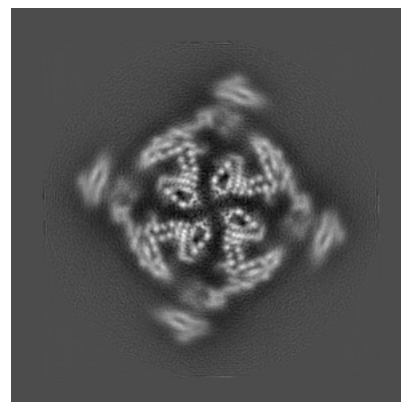
6.2.1 Primary map



X Index: 200



Y Index: 200

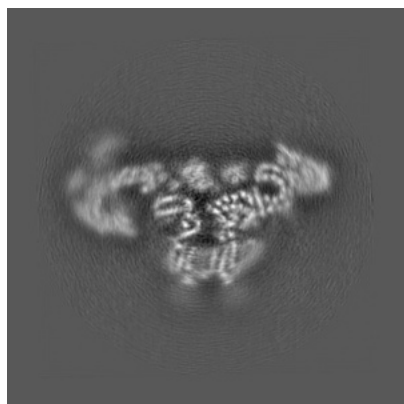


Z Index: 200

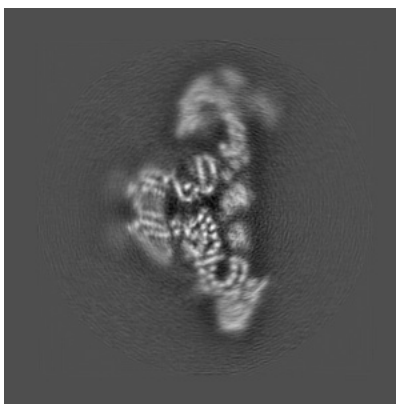
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

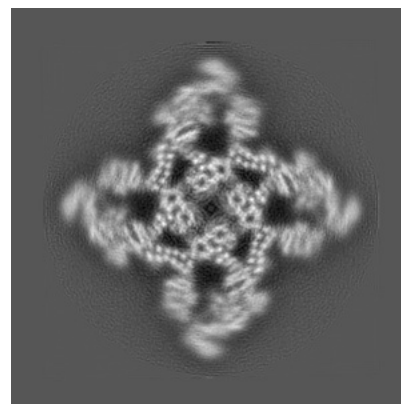
6.3.1 Primary map



X Index: 177



Y Index: 177

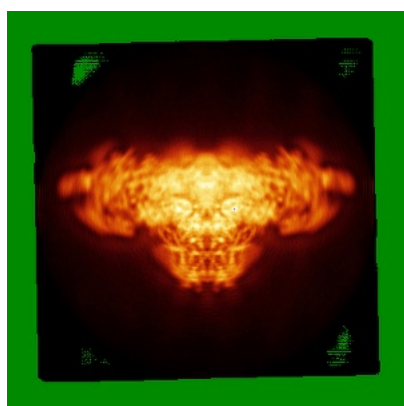


Z Index: 227

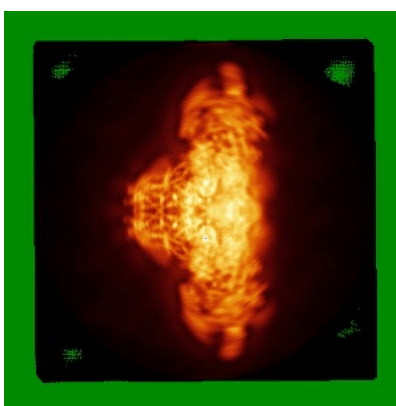
The images above show the largest variance slices of the map in three orthogonal directions.

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

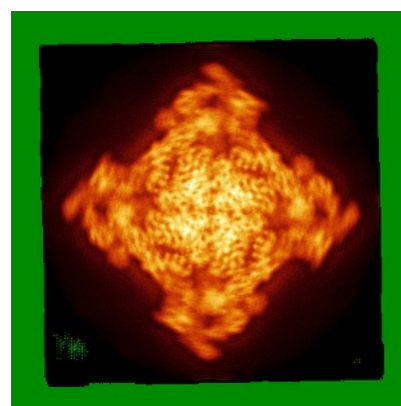
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

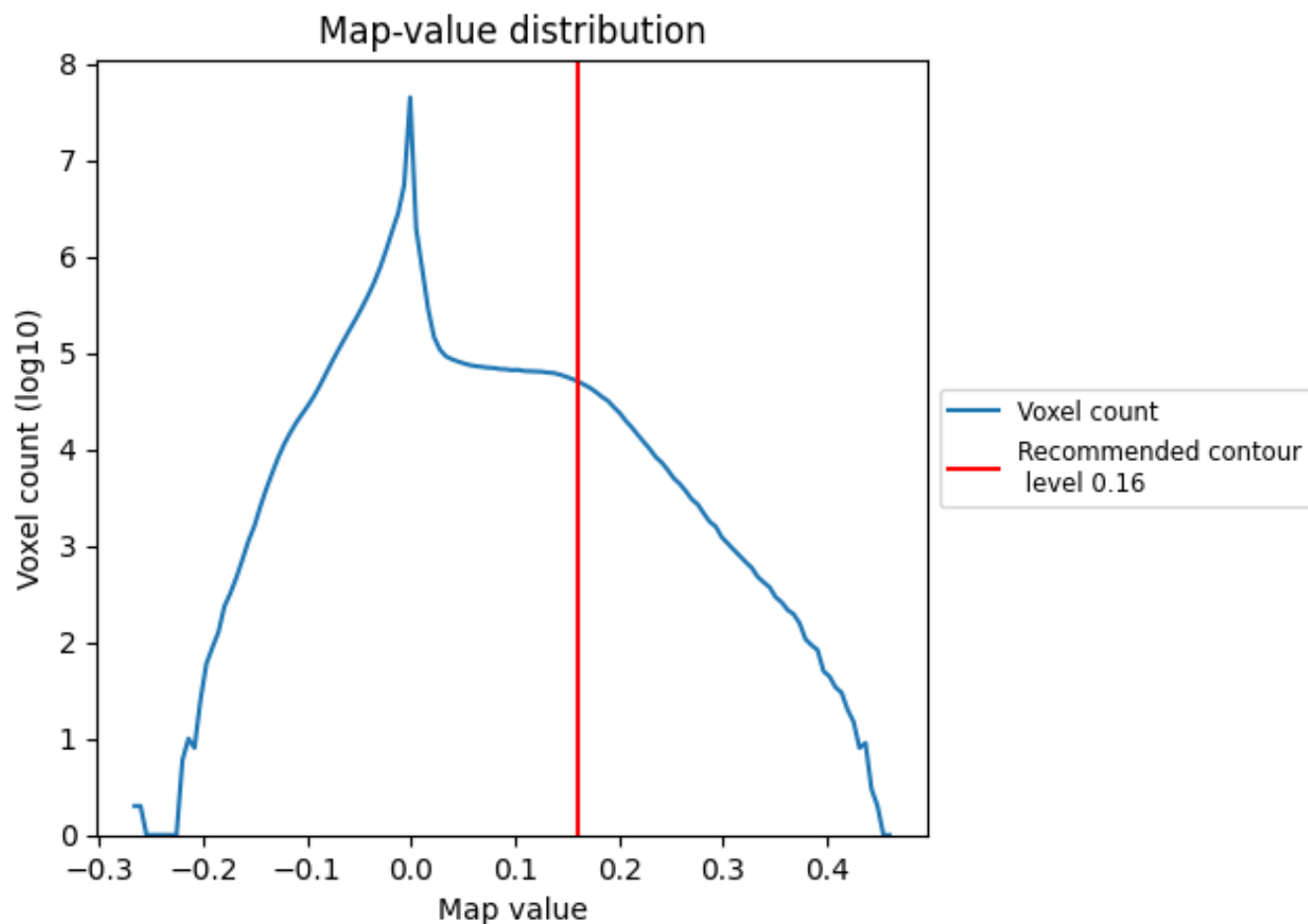
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

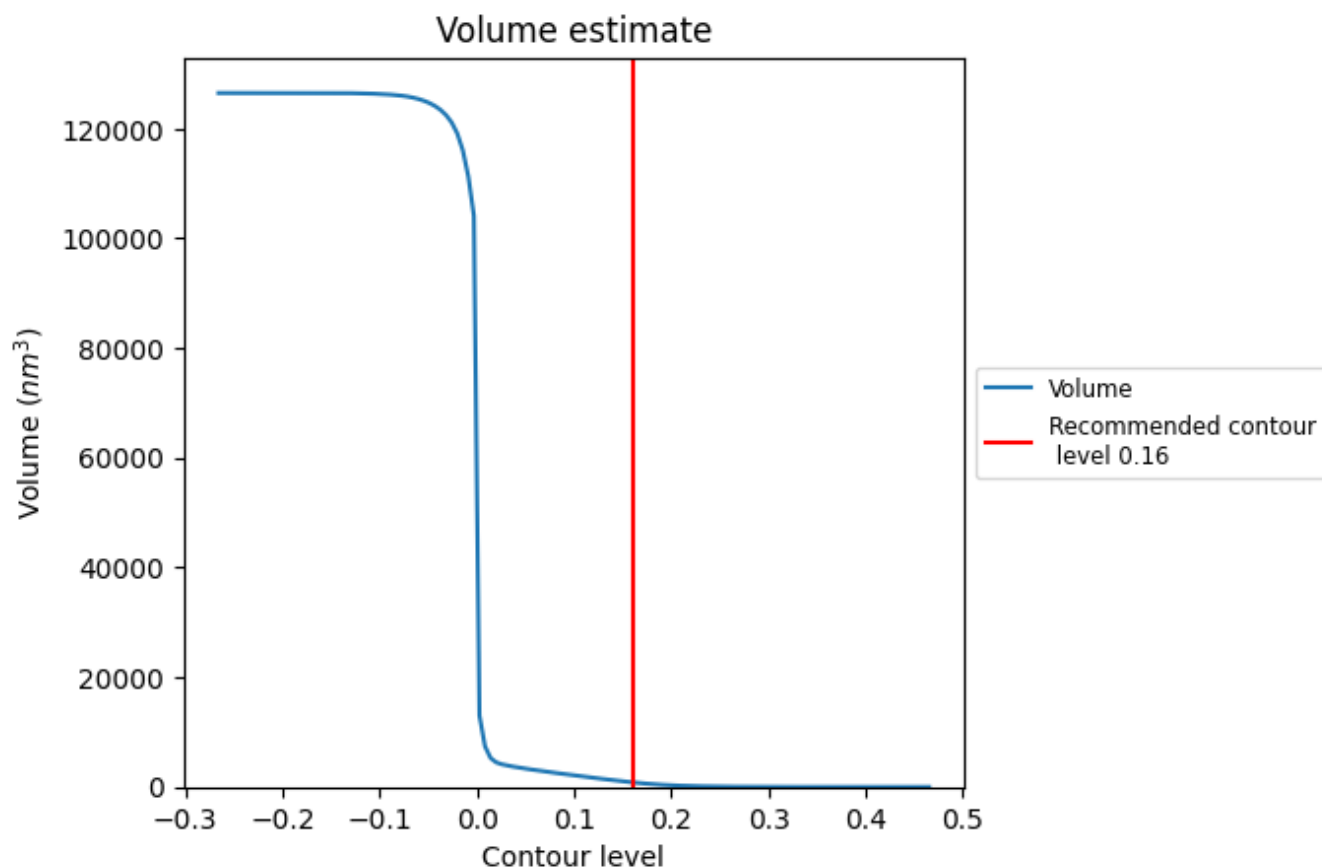
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

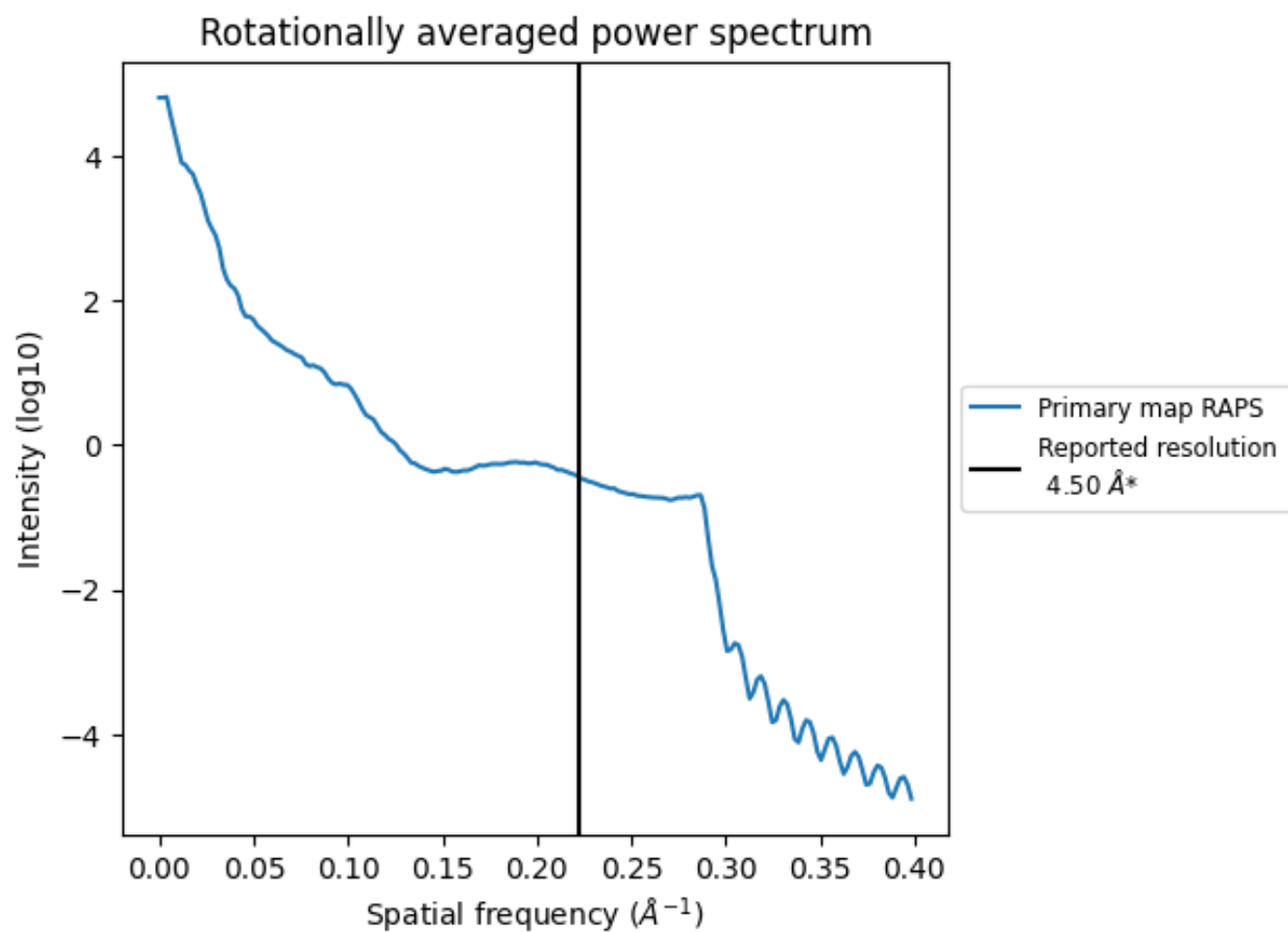
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 846 nm^3 ; this corresponds to an approximate mass of 764 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⁻¹

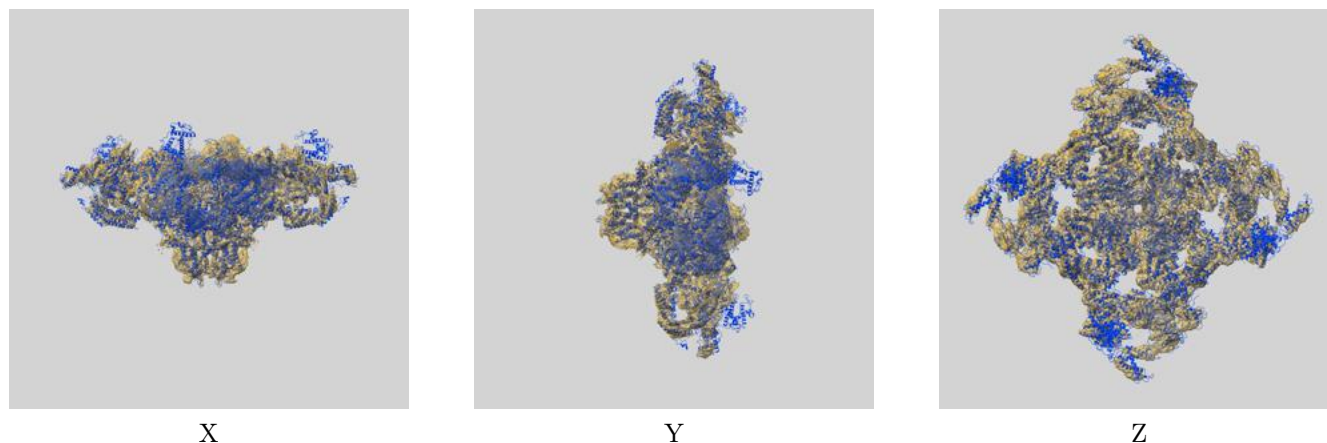
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

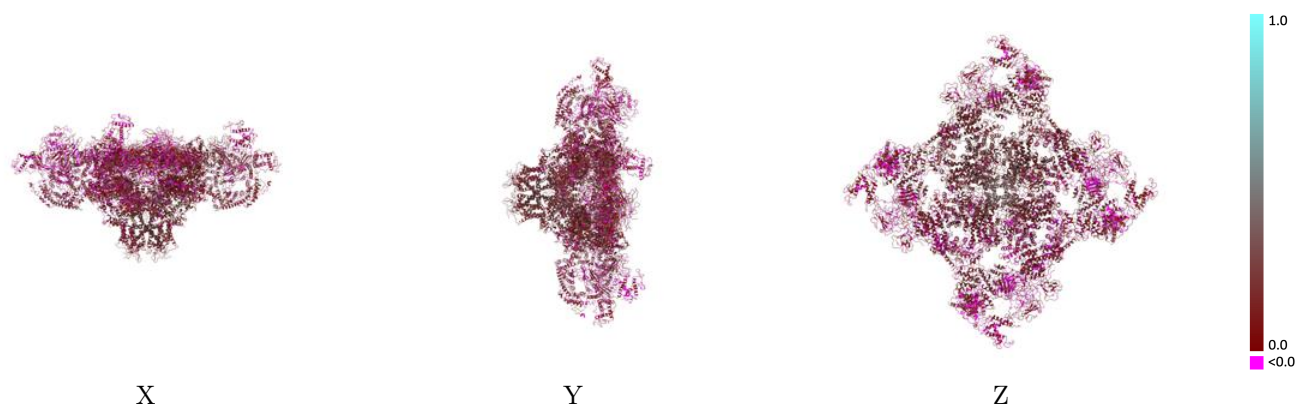
This section contains information regarding the fit between EMDB map EMD-22396 and PDB model 7JMJ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



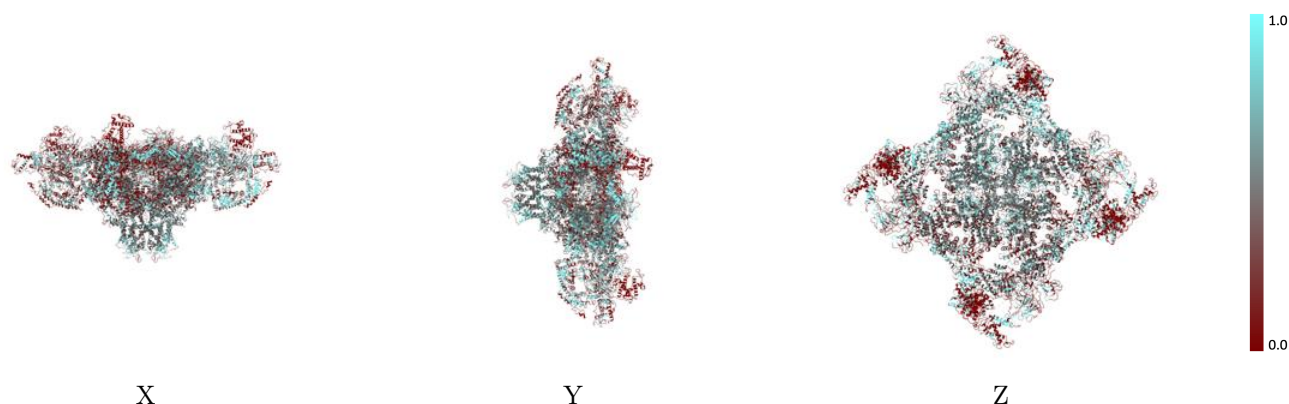
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



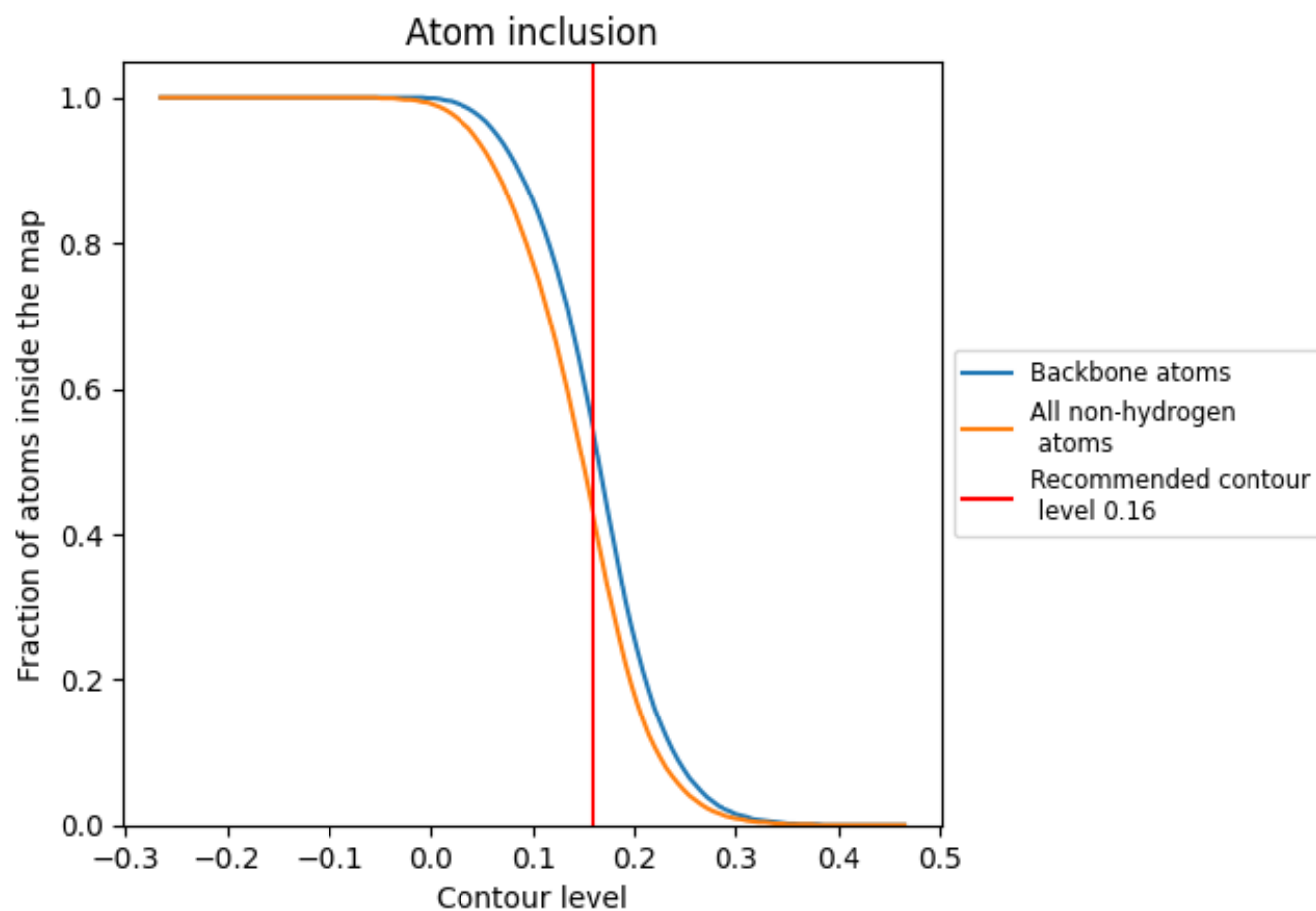
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 54% of all backbone atoms, 42% 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	0.4250	0.1330
A	0.4530	0.1410
B	0.4630	0.1670
E	0.4320	0.1360
F	0.4260	0.1110
G	0.3980	0.1060
H	0.3920	0.1210
I	0.4060	0.1230
J	0.4020	0.1150

1.0

0.0

<0.0