



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 02:39 PM UTC

PDB ID : 5TB1 / pdb_00005tb1
EMDB ID : EMD-8392
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

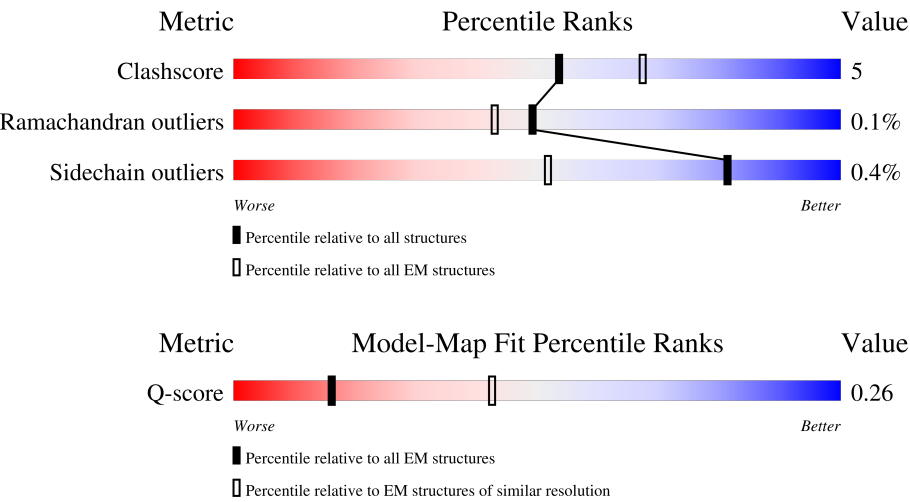
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	2407 (4.10 - 5.10)

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	108	82% 73%26%
1	F	108	83% 70%29%
1	H	108	81% 73%26%
1	J	108	82% 74%25%

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Mol	Chain	Length	Quality of chain
2	B	4416	70% 83% 11% 5%
2	E	4416	71% 83% 12% 5%
2	G	4416	70% 83% 11% 5%
2	I	4416	70% 83% 11% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 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	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

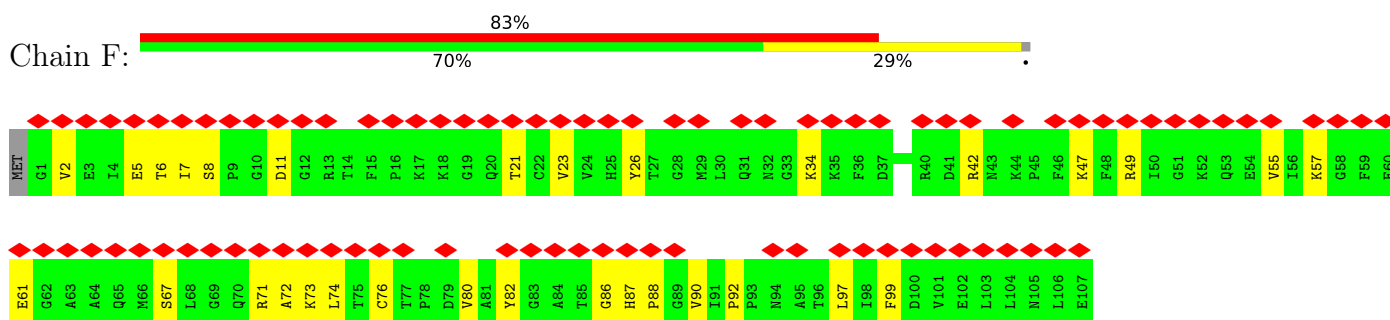
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

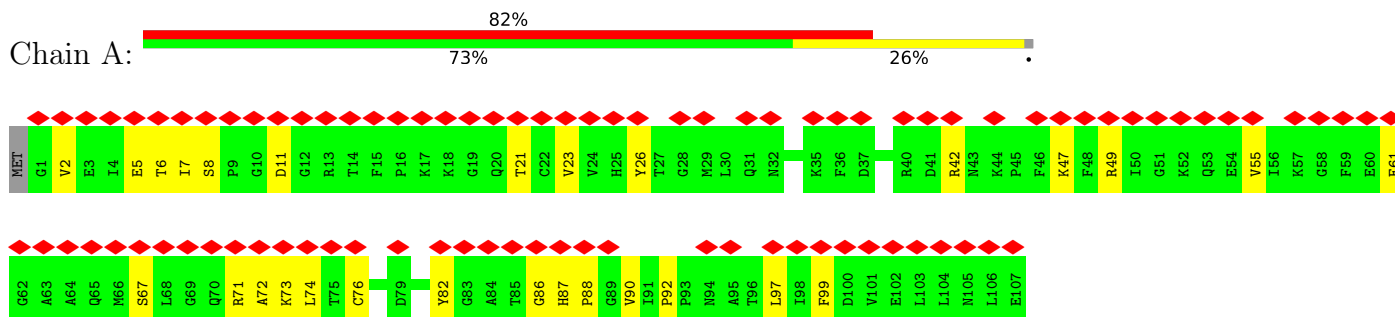
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

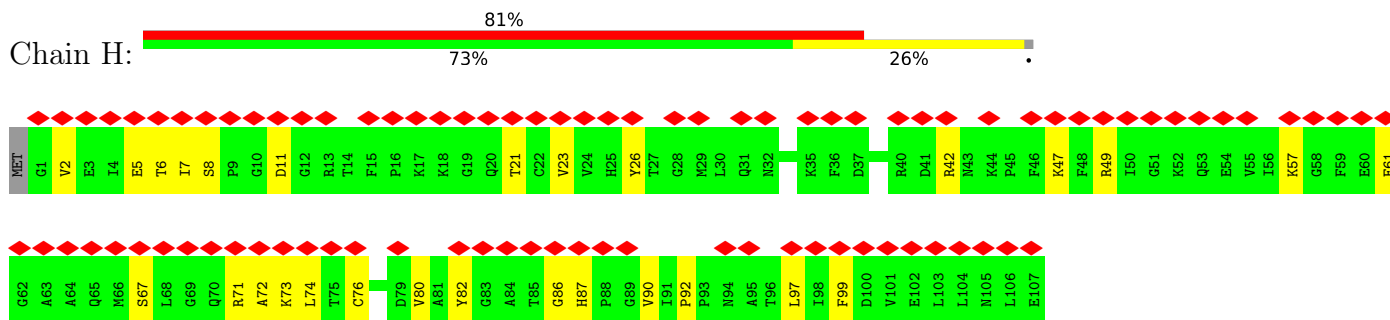
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



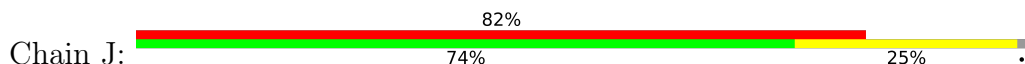
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

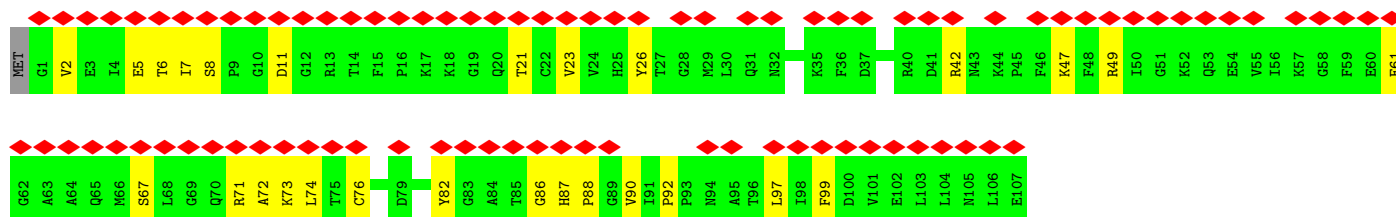


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

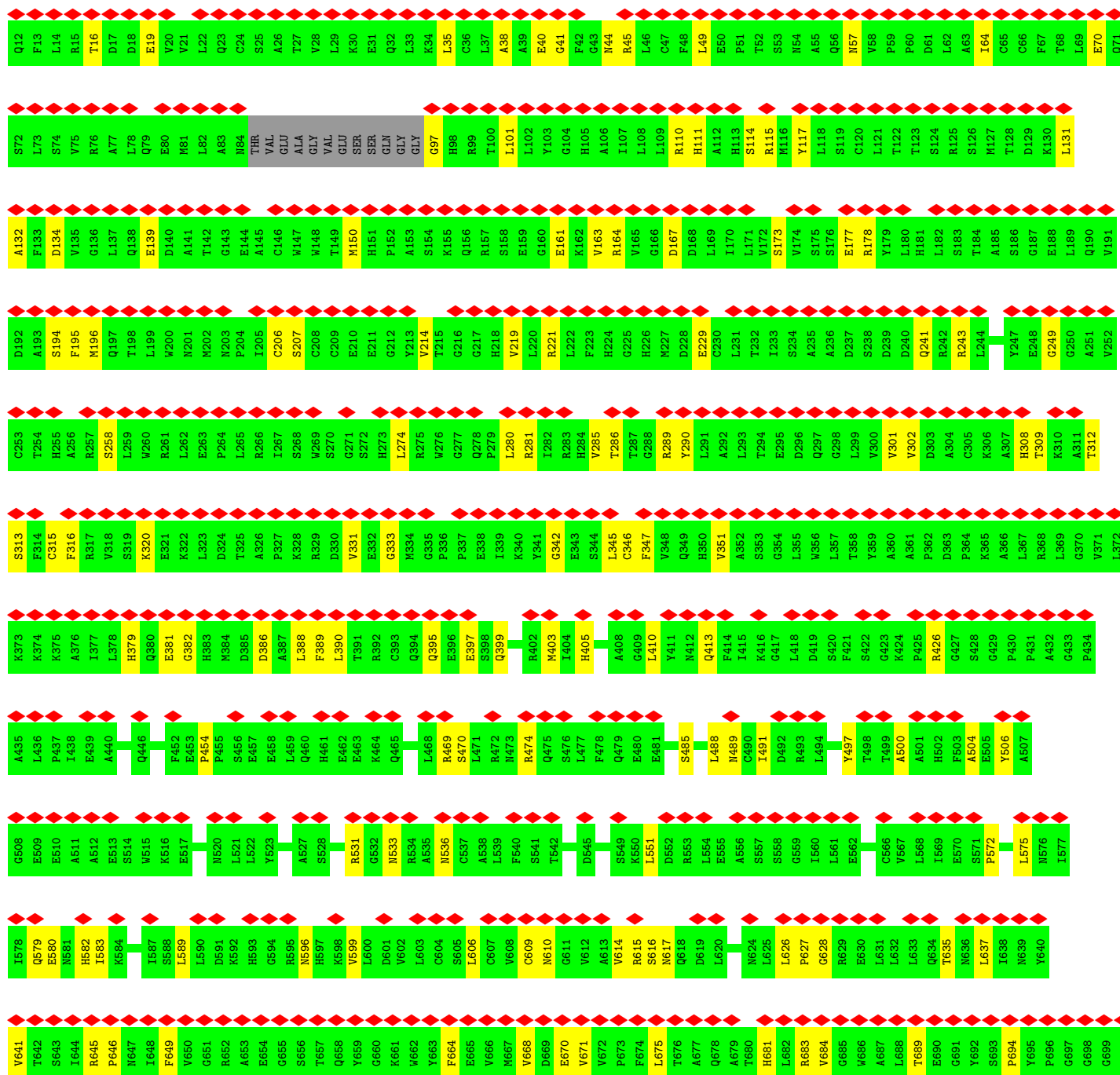
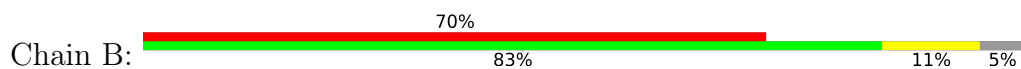


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 2: Ryanodine receptor 1

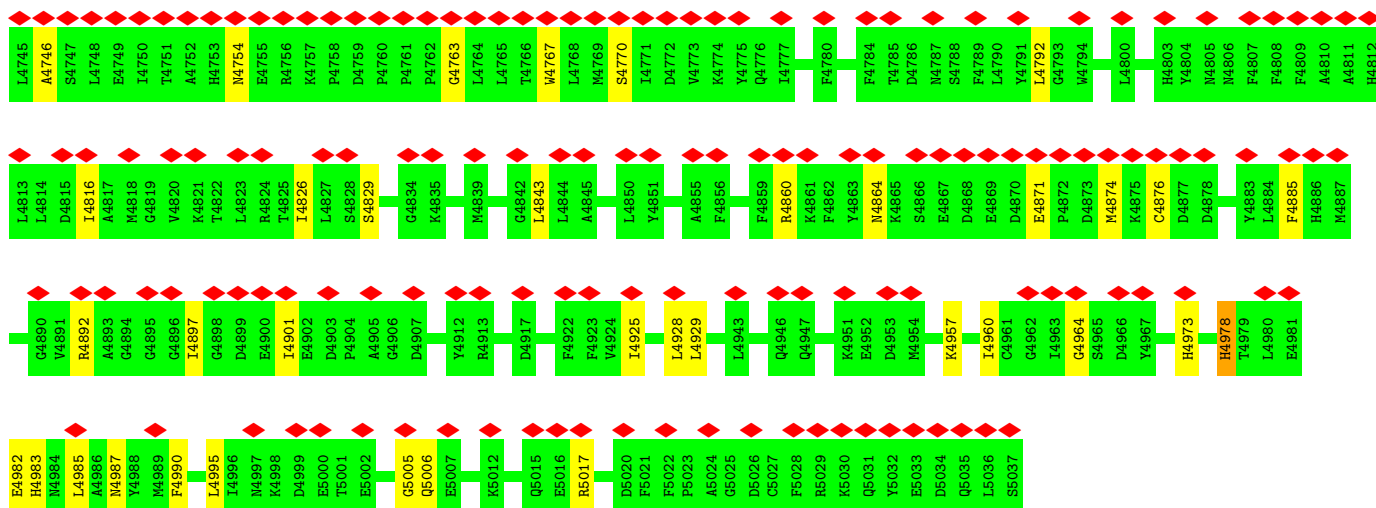


G701	G702	G703	G704	N705	G706	G707	G708	G709	D710	L711	L712	S713	Y714	G715	F716	D717	G718	L719	H720	L721	F722	T723	A724	H725	V726	A727	R728	P729	V730	S732	P733	G734	Q735	H736	L737	L738	A739	P740	E741	D742	P743	V744	S745	G746	C747	L748	D749	L750	S751	V752	P753	S754	I755	S756	F757	R758	L759	N760			
G761	C762	P763			G766	V767	F768	E769	A770	F771	N772	L773	D774	G775	L776	F777	F778	P779	V780	Y781	S782	F783	S784	A785	G786	H787	K788	V789	R790	F791	L792	L793	G794	G795	R796	H797	G798	E799	F800	K801	F802	L803	P804	P805	P806	G807	Y808	A809			H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822
L823	E824	P825	I826	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	V840	G841	P842	S843	R844	C845	L846	S847	H848	T849	D850	F851	V852	P853	C854	P855	V856	THR	VAL	GLN	I861	V862	L863	P864	P865	H866	L867	E868	R869	L870	R871	E872	K873	L874	A875	E876	N877	L878	H879	E880	L881	W882			
A883	L884	T885	R886	I887	E888	Q889	G890	W891	T892	Y893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	R904	C905	C906	L907	V908	N909	F910	F911	V912	P913	L914	P915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	M941	A942		
D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M960	M961	S962	N963	C964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	Y975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	E990	N991			A997	R998	D999	R1000	V1001	A1002	Q1003	G1004	W1005	S1006	
Y1007	S1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	M1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	M1052	I1053	E1054	PRO	ASP	GLN	PRO	ASP	GLU	GLN	VAL	GLU	ASN	GLN				
SER	ARG	TRP	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	Y1081	Q1084	S1085	G1086	R1087	W1088	Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	W1104	A1105	P1107	E1108	R1109	P1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	V1123	F1124	N1125	G1126	H1127					
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X1448	X1449	X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1461	X1462	X1463	X1464	X1468	X1471	X1472	X1473	X1474	X1475	X1476	X1477	X1478	X1479	X1480	X1481	X1482	X1483	X1484	X1485	X1486	X1487	X1488	X1489	X1492	X1493	X1494	X1495	X1496	X1497	X1502	X1503	X1504	X1505	X1506	X1507	X1508	X1509	X1510	X1511	X1512	X1513	X1514						
X1515	X1516	X1519	X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1535	X1536	X1537	X1538	X1539	X1540	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1558	M1573	P1574	S1575	A1577	A1578	M1579	F1580	E1583	R1584	K1585	M1586	P1587	A1588	P1589						
Q1590	C1591	P1592	L1595	E1596	V1597	Q1598	M1599	L1600	V1603	S1604	W1605	P1606	R1607	M1608	F1612	L1613	Q1614	V1615	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	Q1629	C1630	Q1631	D1632	P1633	L1634	M1635	M1636	M1637	A1638	L1639	H1640	E1643	E1644	N1645	R1646	C1647	M1648	D1649	I1650	L1653	S1654	E1655							

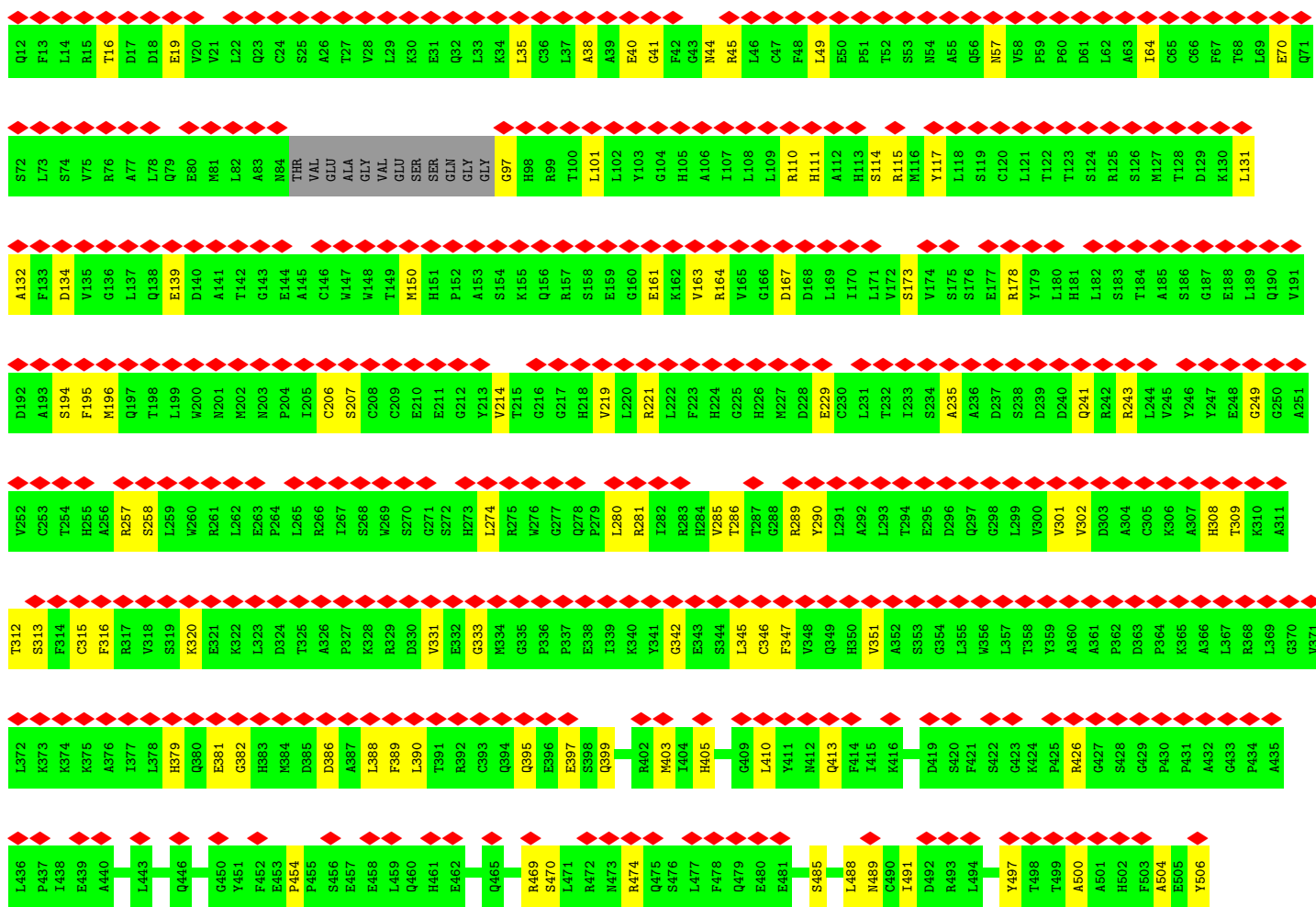
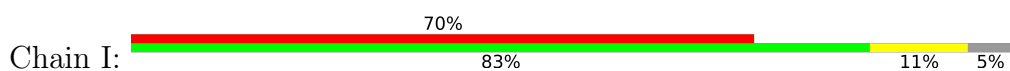
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	E2296			F2226	F2226	S2147	P2001	L1937	E1874	ALA	M1732	L1668
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	L2302			M2228	M2228	E2150	Q2003	Q1939		ALA	M1734	L1670
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	S2309			L2156	L2156	L2156	F2012	Y1945		ALA	T1742	N1679
	C2310			L2156	L2156	L2156	F2013	F1946		ALA	R1743	R1680
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	P2320			L2156	L2156	L2156	P2022	A1963		ALA	G1755	D1690
	G2321			L2156	L2156	L2156	P2024	R1964		ALA	G1756	Q1691
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	P2324			L2156	L2156	L2156	T2027	D1967		ALA	L1694	L1694
	P2325			L2156	L2156	L2156	R2028	K1968		ALA	R1758	L1695
	C2326			L2156	L2156	L2156	Q2029	L1969		ALA	R1759	H1696
	G2327			L2156	L2156	L2156	D2033	Q1970		ALA	H1760	A1697
	E2328			L2156	L2156	L2156	F2034	A1971		ALA	L1762	L1698
	E2329			L2156	L2156	L2156	H2035	Q1973		ALA	G1764	E1699
	E2330			L2156	L2156	L2156	Q2036	L1974		ALA	V1765	D1700
	L2332			L2156	L2156	L2156	A2040	S1975		ALA	G1766	A1701
	D2333			L2156	L2156	L2156	C2042	S1976		ALA	P1767	H1702
	F2334			L2156	L2156	L2156	Q2043	Y1977		ALA	T1768	L1703
	F2337			L2156	L2156	L2156	G2043	A1978		ALA	T1769	G1705
	A2338			L2156	L2156	L2156	L2044	L1979		ALA	L1770	P1706
	V2339			L2156	L2156	L2156	Q2045	L1980		ALA	L1771	L1707
	F2340			L2156	L2156	L2156	L2046	M1981		ALA	R1772	R1708
	N2341			L2156	L2156	L2156	E2047	M1982		ALA	H1775	G1710
	Q2342			L2156	L2156	L2156	G2048	A1983		ALA	H1776	Y1711
	G2343			L2156	L2156	L2156	GLU	A1984		ALA	F1777	Y1712
	E2344			L2156	L2156	L2156	GLU	T1985		ALA	P1780	D1713
	S2345			L2156	L2156	L2156	GLU	M1986		ALA	C1781	H1718
	S2346			L2156	L2156	L2156	PRO	S1987		ALA	F1782	H1719
	E2347			L2156	L2156	L2156	GLU	A1988		ALA	V1783	L1720
	E2348			L2156	L2156	L2156	GLU	A1989		ALA		

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• Molecule 2: Ryanodine receptor 1

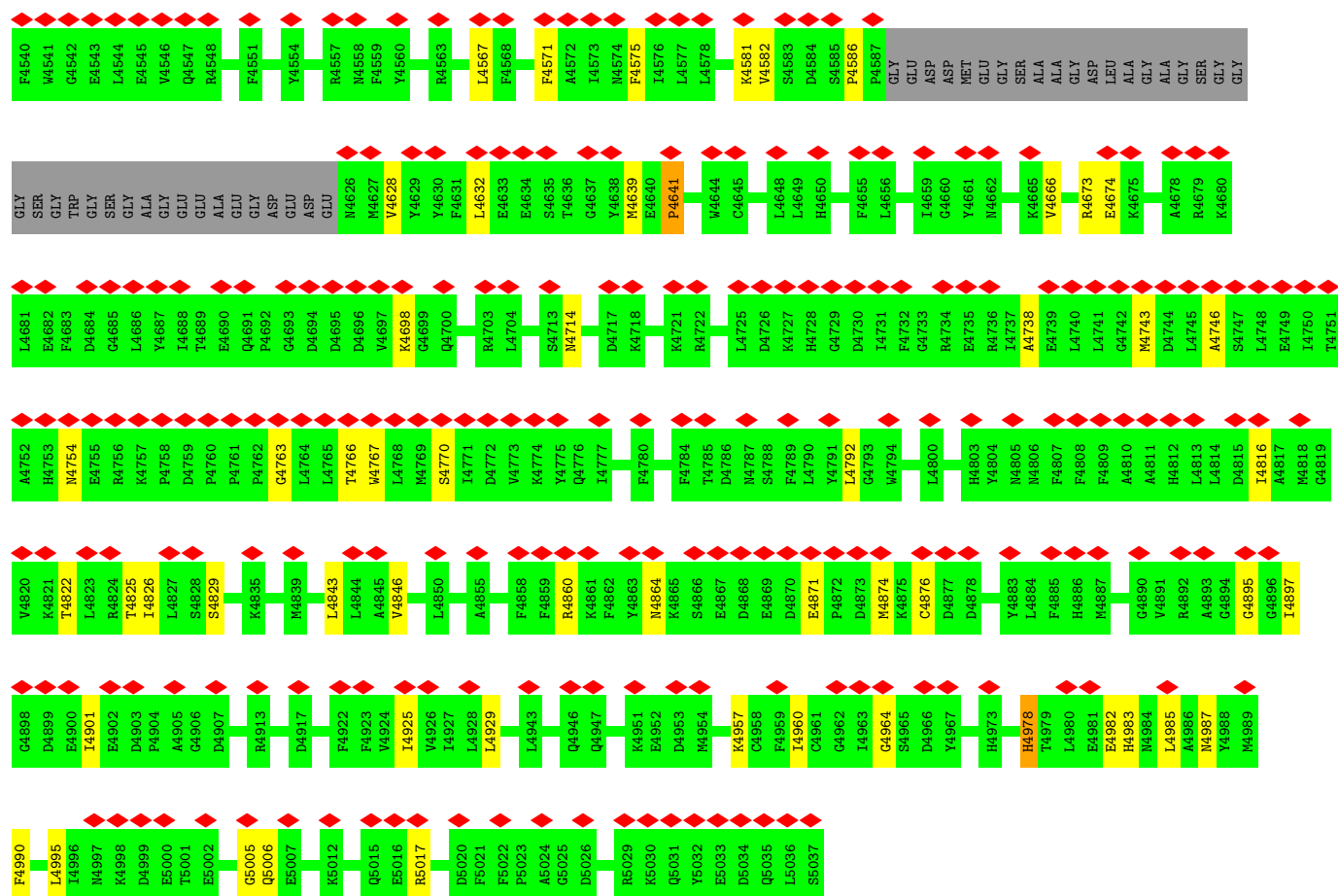


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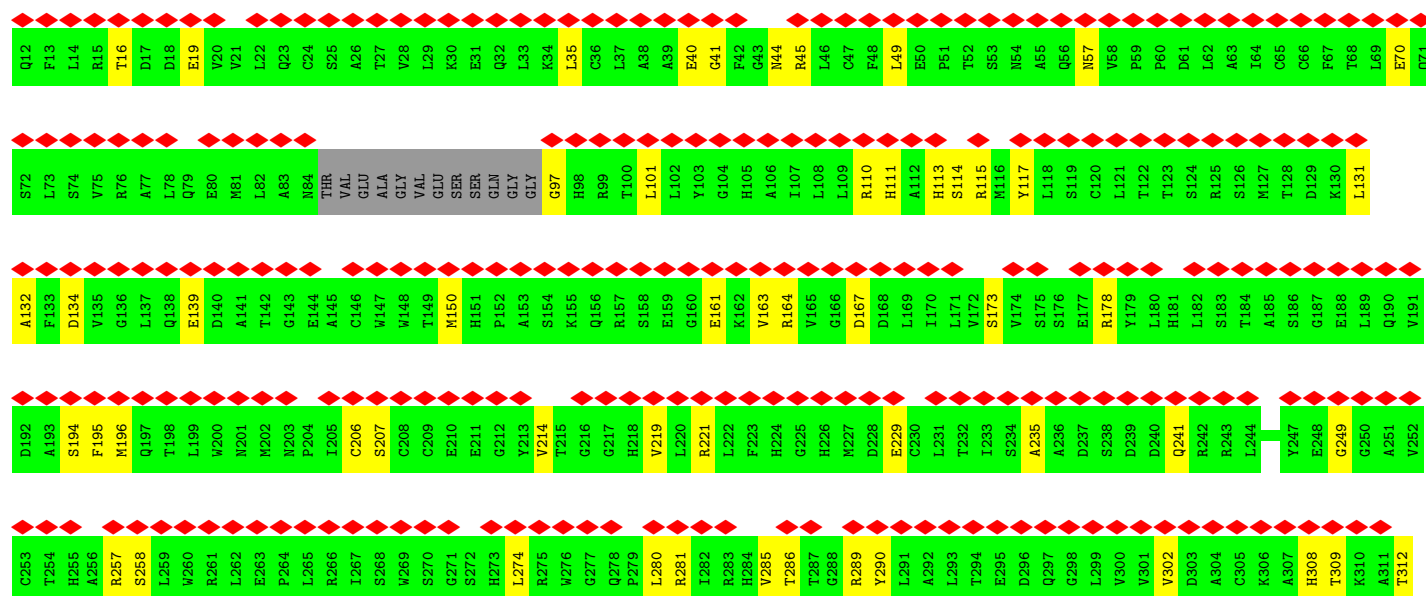
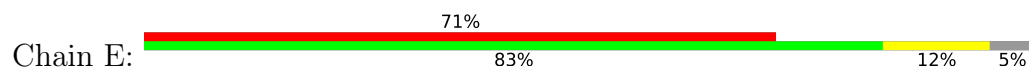
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F2340	X1504	G1705	G1768	L1849	LVS	T1987	L2046	N2208	A2279	F2340
V2341	X1505	L1706	T1769	G1852	ASP	S1987	E2047	E2209	G2280	V2341
G2342	X1506	L1707	L1770	I1853	E1923	M1988	G2048	V2210	N2283	G2342
C2343	X1507	Q1708	Q1771	F1854	E1924	F1989	G2049	Q2127	N2284	C2343
E2344	X1508	A1709	R1771	G1855	E1925	T1991	L2046	Y2128	E2285	E2344
S2345	X1509	Y1711	R1772	G1856	E1926	A1992	E2047	G2129	L2286	S2345
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D2347	X1511	D1713	F1776	D1858	GLU	R1994	G2049	L2131	A2287	D2347
E2348	X1512	I1653	I1718	V1859	GLU	T1995	G2049	R2136	L2288	E2348
N2349	X1513	S1654	H1719	K1860	GLU	A1996	G2049	GLU	G2216	N2349
L2350	X1514	E1655	H1720	Q1861	GLU	R1997	G2049	GLU	G2217	L2350
K2351	X1515	E1656	L1720	L1862	ASP	R1998	G2049	GLU	G2218	K2351
R2355	X1516	R1657	E1721	L1863	E1926	T1999	G2049	GLU	E2219	R2355
L2356	X1517	D1658	F1722	K1864	L1926	R1996	G2049	GLU	E2220	L2356
L2357	X1518	P1587	A1723			R1997	G2049	GLU		L2357
C1591	X1519	Q1589	A1784			F1998	G2049	GLU		C1591

X3231	X3171	X3035	X2957	X2895	GLU	W2775	X2685	X2625	X2563	X2493	G2419	R2369
X3232	X3172	X3036	X2958	A2895	LVS	S2776	X2686	X2626	X2564	X2494	I2422	R2360
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X3234	X3174	X3038	X2960	G2898	THR	G2778	X2688	X2628	X2566	X2497	S2424	C2363
X3235	X3175	X3039	X2961	G2899	ARG	E2779	X2689	X2629	X2567	X2498	F2425	F2364
X3236	X3176	X3040	X2962	G2900	LVS	X2780	X2690	X2630	X2568	X2499	Y2426	Q2365
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X3244	X3180	X3044	X2966	L2904	ALA	E2784	X2694	X2634	X2572		L2429	R2368
X3245	X3181	X3045	X2967	L2905	GLN	X2785	X2695	X2635	X2573		I2430	L2369
X3246	X3182	X3046	X2968	V2906	THR	L2786	X2696	X2636	X2574	X2506	D2431	G2370
X3247	X3183	X3047	X2969	V2907	TTR	X2787	X2697	X2637	X2575	X2511	L2432	E2371
X3248	X3184	X3048	X2970	P2907	ASP	X2788	X2698	X2638	X2576	X2512	L2433	G2372
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X3250	X3186	X3050	X2972	D2909	GLU	X2789	X2700	X2640	X2580	X2514	R2435	S2374
X3251	X3187	X3051	X2973	T2910	GLY	M2790	X2701	X2641	X2581	X2515	C2436	G2375
X3252	X3188	X3052	X2974	L2911		L2791	X2702	X2642	X2582	X2516	A2437	L2376
X3253	X3189	X3053	X2975	T2912		R2792	X2703	X2643	X2583	X2517	P2438	L2377
X3254	X3190	X3054	X2976	G2913		X2793	X2704	X2644	X2584	X2518	H2441	A2378
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X3263	X3194	X3058	X2980	D2861		F2797	R2737	X2648	X2588	X2522	K2448	E2382
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X3270	X3201	X3134	X3004	S2868		I2804	L2744	X2655	X2595	X2529	R2454	D2389
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X3277	X3208	X3141	X3011	L2930		E2811	L2751	X2662	X2602	X2536	L2463	GLY
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X3279	X3210	X3143	X3013	M2932		L2813	G2753	X2664	X2604	X2538	D2465	ARG
X3280	X3211	X3144	X3014	G2933		K2814	F2754	X2665	X2605	X2539	L2466	ARG
X3281	X3212	X3145	X3015	Q2934		A2815	L2755	X2666	X2606	X2540	G2467	ASP
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X3284	X3215	X3148	X3018	V2937		I2818	F2758	X2669	X2609	X2543	I2470	GLU
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X3290	X3221	X3154	X3024	X2945		I2824	H2764	X2675	X2615		I2476	PRO
X3291	X3222	X3155	X3025	X2946		E2825	K2765	X2676	X2616	X2555	P2477	GLU
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X3297	X3228	X3161	X3031	X2952		GLU	I2771	E2831	X2622	X2561		
X3298	X3229	X3162	X3032	X2953		GLU	Q2772	X2882	X2623	X2562		
X3299	X3230	X3163	X3033	X2954		ARG	N2773	X2883	X2624			
X3300		X3170	X3034	X2955		THR	M2774	X2884	X2625			

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• Molecule 2: Ryanodine receptor 1

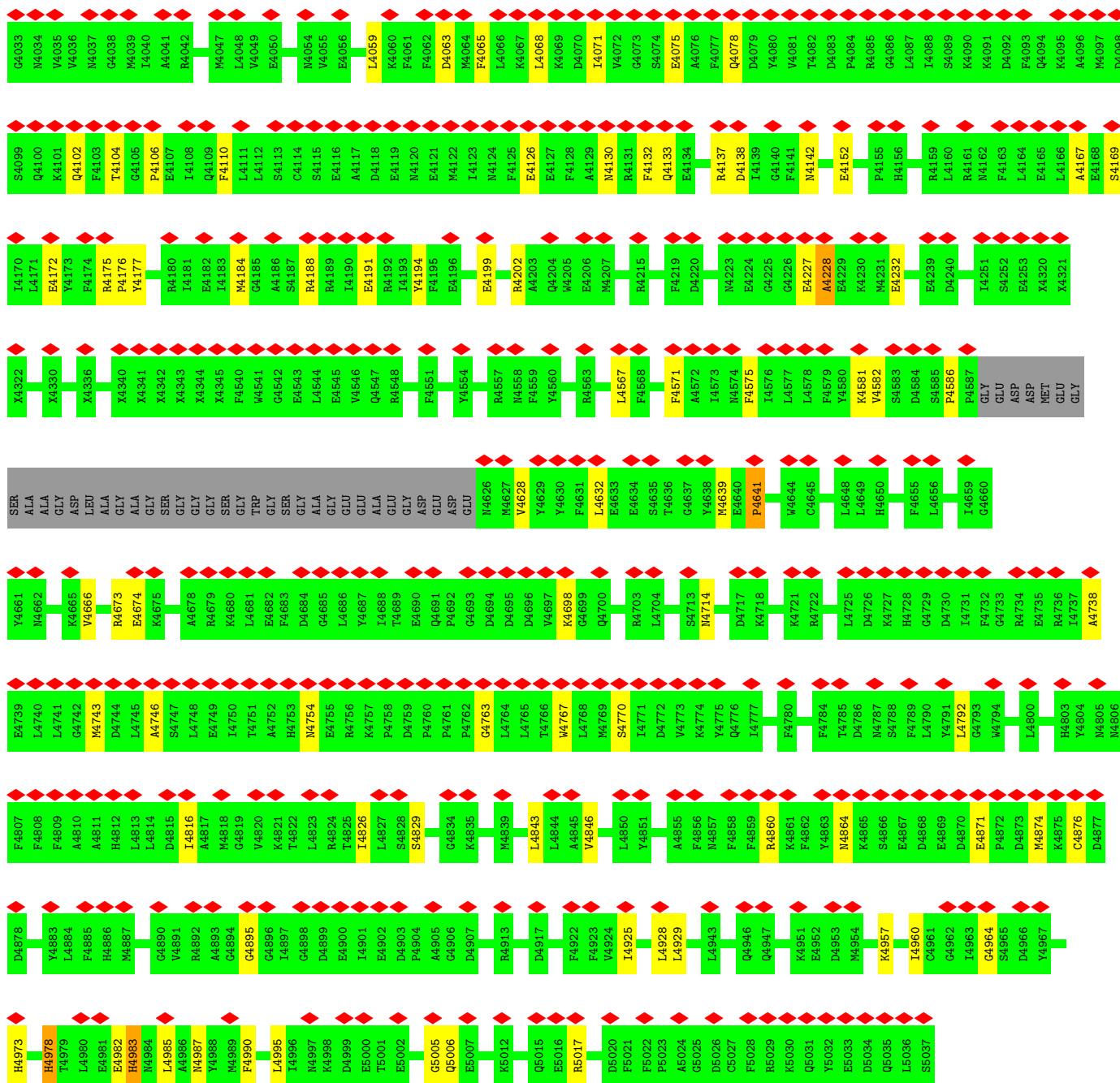


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SER	R1071	Y1007	D943	A883	L823	G761	G701	V641	Q579	E509	L436	K374	F314
ARG	V1072	S1008	E944	L884	E824	C762	W702	T642	E580	E510	P437	K375	C315
TRP	V1073	A1009	K945	T885	P825	P763	G703	S643	N581	A511	I438	A376	F316
		VAL	A946	R886	I826	G766	G704	T644	H582	A512	E439	I377	R317
		GLN	E947	T887	K827	V767	N705	P646	K584	S514	A440	L378	V318
		ASP	D948	E888	E828	F768	G706	R645	S585	S515	Q446	H379	S319
		ILE	N949	Q889	Y829	E769	V707	G647	T586	W515		Q380	K320
		PRO	R830	Q890	R830	F769	G708	T648	I587	K316		E321	K321
		ALA	L950	G890	R831	A770	G709	F649	S588	W517		G382	K322
		ARG	K951	W891	F771	F771	D710	P650	L589	E517		H383	L323
		ASN	K952	T892	E832	F771	D711	G651	L590	N520		M384	D324
		PRO	T953	W893	G833	L773	L711	R652	D591	L521		D385	T325
			K954	G894	P834	L773	Y712	R652	K592	L522		D386	A326
			L955	P895	R835	D774	S713	A653	H593	Y523		A387	P327
			P956	W896	G836	G775	Y714	E654	G594	A527		L388	K328
			K957	R897	P837	L776	G715	G655	R595	S528		F389	R329
			Y958	D898	H838	F777	F716	S656	N596			L390	D330
			Y959	D899	L839	F778	D717	T657	H597			L391	V331
			M960	W900	V840	P779	G718	Q658	K598	R531		R392	E332
			M961	K901	G841	W780	L719	V659	V599	N533		C393	G333
			S962	R902	P842	V781	H720	G660	L600	N533		Q394	M334
			N963	L903	S843	S782	L721	G661	D601	R534		Q395	G335
			G964	R904	R844	F783	W722	W662	V602	A535		E396	P336
			Y965	P905	C845	W784	W723	W663	L603	N536		E397	E338
			K1031	C906	L846	A785	G724	Y664	C604	C537		S470	I339
			K1032	C906	S847	G786	H725	P664	S605	L471		R402	K340
			R1033	L907	H848	W787	V726	E665	L606	R472		M403	Y341
			S1034	V908	T849	K788	A727	V666	C607	R474		I404	G342
			N1035	W909	D849	V789	R728	W667	V608	Q475		H405	E343
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			D1037	R910	F851	R790	P729	D669	N610	S477		G409	C346
			S1038	S912	W852	L792	W730	E670	G611	T542		L410	F347
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			E915	P916	P855	G794	P733	W672	A613	S549		Q413	Q349
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			Q981	N921	W862	K801	P740	A679	L620	A556		S420	L357
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			T983	Q923	P864	L803	D742	H681	L625	T498		S422	Y359
			L984	N924	P865	P804	W743	L682	L626	T499		G423	A360
			V985	S925	H866	P805	V744	R683	P627	A500		K424	A361
			D986	G926	L867	P806	V744	V684	G628	A501		R426	P362
			R987	E927	E868	G807	S745	G685	R629	H502		G427	D363
			L988	T928	R869	Y808	G746	W686	E630	F503		S428	K365
			A989	L929	I870	A809	C747	A687	L631	P572		G429	A366
			E990	K930	R871	H812	L748	L688	L632	Y506		P430	L367
			N991	T931	E872	E813	D749	L688	L633	A507		A432	R368
			A997	L932	K873	A814	S751	T689	L633	H502		G433	L369
			R998	L933	L874	W815	V752	E690	Q634	F503		P434	G370
			D999	A934	A875	L816	P753	G691	Q634	A504			V371
			F1124	L935	E876	P817	S754	W692	N636	Y506			L372
			N1125	G936	R877	E818	S756	S693	L638	A507			
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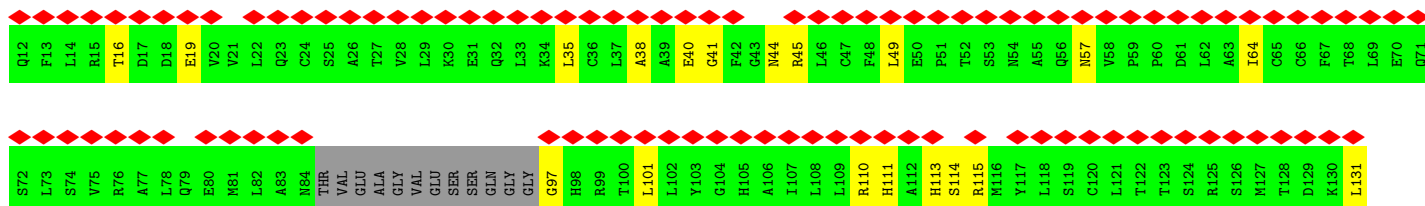
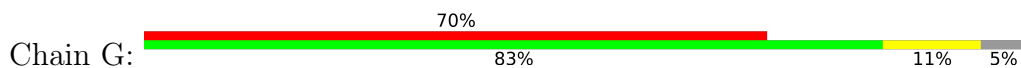
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THR	G1925	A1785	Q1861	A1785	S1722	D1658	L1595	X1521	X1453	M1260	L1194	H133
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N3809	A3810	K3815	F3816	L3817	N3741	GLU	GLU	GLU	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	F3758	E3759	K3760	Q3761	R3762	L3763	L3764	E3691	Q3766	Q3767	S3768	R3769	L3770	F3778	V3779	E3712	K3713	S3714	K3715	L3716	D3717	E3718	R3719	Y3720	L3721	Y3722	K3723	A3724	A3725	K3731	H3734	L3735	E3736						
D3883	L3884	F3885	R3886	F3887	L3888	Q3889	E3893	N3897	D3898	F3899	Y3902	L3903	R3904	L3905	Q3906	T3907	G3908	N3909	T3910	T3911	T3912	I3913	Y3922	L3923	L3924	R3925	E3928	S3929	L3930	S3931	D3932	F3933	V3934	Y3935	Y3936	Y3937	S3938	G3939	K3940	D3941	V3942	I3943	E3944	E3945	Q3946	G3947	K3948	R3949	N3950	A3954	M3955	E4032							
K3959	Q3960	F3961	N3963	E3967	Q3970	G3971	F3972	C3973	N3976	Q3977	A3981	H3982	S3983	R3984	L3985	W3986	F3992	L3993	H3994	V3995	F3996	A3997	H3998	K3999	M4000	M4001	K4002	L4003	A4004	Q4005	D4006	D4007	S4007	A4008	Q4009	L4010	E4011	L4012	L4013	L4014	E4015	L4016	L4017	D4018	L4019	Q4020	K4021	D4022	L4027	L4030	L4031	E4032							



• Molecule 2: Ryanodine receptor 1



K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M960	M961	S962	N963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	A988	A989	N991	A997	R998	D999	R1000	V1001	A1002	Q1003	G1004	V1005	S1006	Y1007	S1008		
P825	T826	R827	P828	Y829	R830	R831	K952	E832	G833	P834	R835	G836	P837	H838	L839	V840	G841	P842	S843	R844	C845	L846	S847	H848	T849	D850	P851	W852	P853	C854	P855	W856	D857	THR	VAL	R861	W862	L863	P864	P865	R866	L867	E868	R869	R870	R871	E872	R873	L874	A875	E876	M877	L878	E880	L881	W882	A883	L884	
F763	G766	F767	F768	E769	A770	F771	F772	L773	D774	G775	L776	F777	F778	F779	W780	Y781	S782	F783	S784	A785	G786	W787	K788	W789	R790	F791	L792	L793	G794	G795	R796	H797	G798	E799	F800	R801	F802	L803	P804	P805	P806	G807	Y808	A809	H812	E813	A814	W815	L816	P817	R818	E819	R820	L821	R822	L823	E824		
G703	G704	N705	G706	V707	G708	D709	D710	L711	V712	S713	V714	G715	F716	D717	G718	L719	H720	L721	W722	G723	G724	H725	V726	A727	R728	P729	W730	T731	S732	P733	G734	Q735	H736	L737	L738	A739	P740	E741	D742	V743	P744	S745	C746	C747	L748	D749	L750	S751	V752	F753	S754	T755	W756	F757	R758	L759	N760	G761	G762
S643	T644	R645	P646	R647	T648	F649	V650	G651	R652	A653	G654	G655	S656	T657	Q658	Y659	G660	R661	W662	T663	F664	E665	V666	R667	W668	D669	E670	V671	V672	P673	F674	L675	T676	A677	G678	A679	T680	H681	L682	R683	V684	G685	W686	A687	L688	T689	E690	G691	S692	P693	P694	V695	P696	W697	E698	G699	E700	G701	W702
Q579	E580	N581	H582	I583	K584	L587	S588	L589	H593	G594	R595	N596	H597	K598	V599	L600	D601	V602	L603	C604	S605	L606	C607	V608	C609	N610	G611	V612	A613	V614	R615	S616	N617	Q618	D619	L620	M624	L625	L626	P627	G628	R629	E630	L631	L632	L633	Q634	T635	N636	L637	L638	V639	Y640	V641	T642				
E510	A511	A512	E513	S514	M515	K516	E517	N520	L521	L522	Y523	A527	S528	R531	G532	N533	R534	A535	N536	C537	A538	L539	F540	S541	T542	D545	S549	K550	L551	D552	R553	L554	A555	S557	S558	D559	G559	T560	L561	E562	C566	V567	L568	L569	E570	S571	P572	E573	V574	L575	N576	L577	I578						
K373	K374	K375	A376	I377	L378	H379	Q380	E381	G382	H383	M384	D385	D386	A387	L388	F389	L390	T391	R392	C393	Q394	Q395	E396	E397	S398	Q399	R402	M403	I404	H405	A408	G409	L410	Y411	N412	Q413	F414	I415	K416	G417	L418	D419	S420	F421	S422	G423	R426	G427	S428	G429	P430	P431	A432	G433	P434	A435			
C253	T254	H255	A256	R257	S258	L259	W260	R261	L262	E263	P264	L265	R266	I267	S268	W269	T270	G271	S272	H273	L274	R275	W276	G277	Q278	P279	L280	R281	I282	R283	H284	V285	T286	T287	G288	R289	Y290	L291	A292	L293	T294	E295	D296	Q297	G298	L299	V300	V301	V302	D303	A304	C305	K306	A307	H308	T309	K310	A311	T312
S313	F314	C315	F316	R317	V318	S319	K320	E321	K322	L323	D324	T325	A326	P327	K328	R329	D330	V331	E332	G333	M334	G335	P336	P337	E338	I339	K340	Y341	G342	E343	H344	L345	C346	F347	V348	Q349	H350	V351	A352	S353	G354	L355	W356	L357	T358	V359	A360	A361	P362	D363	P364	K365	A366	L367	R368	L369	G370	V371	L372
D192	A193	S194	F195	M196	Q197	T198	L199	W200	K201	M202	N203	P204	E205	C206	S207	C208	W209	T210	E211	G212	Y213	T214	G216	G217	H218	V219	L220	R221	L222	F223	H224	G225	H226	M227	D228	E229	C230	L231	L232	T232	T233	S234	A235	A236	S238	D239	D240	Q241	R242	K243	L244	Y247	E248	C249	G250	A251	V252		



LYS	E1997	E2222	E2361	E2422	X2497	X2568	X2691	V2781	L2855
ILE	F1998	I2223	E2362	M2423	X2498	X2569	X2692	D2782	N2856
SER	R1999	R2224	C2363	S2424	X2499	X2570	X2693	E2783	P2857
GLN	S2000	F2225	F2364	F2425	X2500	X2571	X2694	E2784	Q2858
ALA	P2001	P2226	C2365	Y2426	X2501	X2572	X2695	L2785	Q2859
GLN	P2002	K2227	P2366	A2427	X2502	X2573	X2696	K2786	P2859
THR	Q2003	K2228	A2367	A2428	X2506	X2574	X2697	T2787	Y2855
ASP	E2004	V2229	L2368	A2429	X2507	X2575	X2698	H2788	Y2856
ARG	Q2005	E2230	R2369	I2430	X2508	X2576	X2699	P2789	Y2857
LEU	Q2006	F2231	G2370	G2434	X2509	X2577	X2700	M2790	Y2858
LEU	Q2007	R2232	E2371	R2435	X2510	X2578	X2701	L2791	Y2859
LYS	L2010	M2153	G2372	P2436	X2511	X2579	X2702	R2792	Y2860
LYS	L2011	L2155	G2373	H2441	X2512	X2580	X2703	Q2793	Y2861
GLU	H2011	L2156	S2374	L2442	X2513	X2581	X2704	T2794	Y2862
LYS	F2012	Q2161	S2375	H2443	X2514	X2582	X2705	N2794	Y2863
LYS	K2013	R2162	G2376	G2446	X2515	X2583	X2706	F2735	Y2864
GLU	K2014	R2163	L2376	K2447	X2516	X2584	X2707	D2736	Y2865
GLU	D2014	L2166	L2377	K2448	X2517	X2585	X2708	Y2737	Y2866
LEU	E2015	L2167	A2378	E2449	X2518	X2586	X2709	R2738	Y2867
LEU	A2016	Q2169	I2379	E2450	X2519	X2587	X2710	V2739	Y2868
ALA	D2017	M2170	I2380	A2451	X2520	X2588	X2711	E2740	Y2869
GLU	E2018	Q2171	E2381	R2452	X2521	X2589	X2712	T2741	Y2870
LEU	E2019	P2172	E2382	L2453	X2522	X2590	X2713	L2742	Y2871
LEU	D2020	Q2173	L2383	L2454	X2523	X2591	X2714	L2743	Y2872
LEU	C2021	Q2174	R2384	R2455	X2524	X2592	X2715	N2744	Y2873
LEU	P2022	I2179	R2385	A2456	X2525	X2593	X2716	V2745	Y2874
LEU	L2023	L2257	E2386	L2457	X2526	X2594	X2717	L2746	Y2875
LEU	P2024	E2258	I2257	L2458	X2527	X2595	X2718	L2747	Y2876
LEU	E2025	E2096	M2260	R2459	X2528	X2596	X2719	E2748	Y2877
LEU	D2026	E2104	S2261	R2460	X2529	X2597	X2720	K2749	Y2878
LEU	I2027	R2105	G2262	L2461	X2530	X2598	X2721	E2750	Y2879
LEU	R2028	A2106	I2263	L2462	X2531	X2599	X2722	L2751	Y2880
LEU	Q2029	Q2107	G2264	L2463	X2532	X2600	X2723	D2752	Y2881
LEU	F2034	Y2110	G2265	L2464	X2533	X2601	X2724	S2753	Y2882
LEU	H2035	Q2193	G2266	L2465	X2534	X2602	X2725	L2754	Y2883
LEU	H2036	Q2194	G2267	L2466	X2535	X2603	X2726	F2755	Y2884
LEU	A2040	N2196	G2268	L2467	X2536	X2604	X2727	L2756	Y2885
LEU	H2041	E2115	P2272	G2468	X2537	X2605	X2728	N2757	Y2886
LEU	C2042	R2199	L2273	I2469	X2538	X2606	X2729	K2758	Y2887
LEU	G2043	A2200	D2274	I2470	X2539	X2607	X2730	A2759	Y2888
LEU	I2044	H2204	V2275	S2471	X2540	X2608	X2731	E2760	Y2889
LEU	Q2045	F2121	A2277	L2472	X2541	X2609	X2732	X2761	Y2890
LEU	L2046	M2208	A2278	P2473	X2542	X2610	X2733	T2762	Y2891
LEU	E2047	E2209	G2283	L2474	X2543	X2611	X2734	H2763	Y2892
LEU	Q2048	V2210	N2284	Q2475	X2544	X2612	X2735	X2764	Y2893
LEU	GLU	V2211	E2285	Q2476	X2545	X2613	X2736	X2765	Y2894
LEU	GLU	N2212	E2286	Q2477	X2546	X2614	X2737	X2766	Y2895
LEU	PRO	N2213	L2287	P2478	X2547	X2615	X2738	X2767	Y2896
LEU	GLU	V2214	A2287	T2479	X2548	X2616	X2739	X2768	Y2897
LEU	GLU	L2215	L2288	L2480	X2549	X2617	X2740	F2769	Y2898
LEU	GLU	G2216	A2289	X2488	X2550	X2618	X2741	X2770	Y2899
LEU	GLU	G2217	L2290	X2489	X2551	X2619	X2742	K2771	Y2900
LEU	THR	Q2218	Q2291	V2416	X2552	X2620	X2743	L2772	
LEU	SER	E2219	E2292	H2417	X2553	X2621	X2744	Q2773	
LEU	SER	T2220	Q2293	L2418	X2554	X2622	X2745	N2774	
LEU	ARG	K2221	D2294	G2419	X2555	X2623	X2746	W2775	
LEU			L2295	X2496	X2556	X2624	X2747	S2776	
LEU					X2557	X2625	X2748	Y2777	
LEU					X2558	X2626	X2749	G2778	
LEU					X2559	X2627	X2750	E2779	
LEU					X2560	X2628	X2751		
LEU					X2561	X2629	X2752		
LEU					X2562	X2630	X2753		
LEU					X2563	X2631	X2754		
LEU					X2564	X2632	X2755		
LEU					X2565	X2633	X2756		
LEU					X2566	X2634	X2757		
LEU					X2567	X2635	X2758		
LEU					X2568	X2636	X2759		
LEU					X2569	X2637	X2760		
LEU					X2570	X2638	X2761		
LEU					X2571	X2639	X2762		
LEU					X2572	X2640	X2763		
LEU					X2573	X2641	X2764		
LEU					X2574	X2642	X2765		
LEU					X2575	X2643	X2766		
LEU					X2576	X2644	X2767		
LEU					X2577	X2645	X2768		
LEU					X2578	X2646	X2769		
LEU					X2579	X2647	X2770		
LEU					X2580	X2648	X2771		
LEU					X2581	X2649	X2772		
LEU					X2582	X2650	X2773		
LEU					X2583	X2651	X2774		
LEU					X2584	X2652	X2775		
LEU					X2585	X2653	X2776		
LEU					X2586	X2654	X2777		
LEU					X2587	X2655	X2778		
LEU					X2588	X2656	X2779		
LEU					X2589	X2657	X2780		
LEU					X2590	X2658	X2781		
LEU					X2591	X2659	X2782		
LEU					X2592	X2660	X2783		
LEU					X2593	X2661	X2784		
LEU					X2594	X2662	X2785		
LEU					X2595	X2663	X2786		
LEU					X2596	X2664	X2787		
LEU					X2597	X2665	X2788		
LEU					X2598	X2666	X2789		
LEU					X2599	X2667	X2790		
LEU					X2600	X2668	X2791		
LEU					X2601	X2669	X2792		
LEU					X2602	X2670	X2793		
LEU					X2603	X2671	X2794		
LEU					X2604	X2672	X2795		
LEU					X2605	X2673	X2796		
LEU					X2606	X2674	X2797		
LEU					X2607	X2675	X2798		
LEU					X2608	X2676	X2799		
LEU					X2609	X2677	X2800		
LEU					X2610	X2678	X2801		
LEU					X2611	X2679	X2802		
LEU					X2612	X2680	X2803		
LEU					X2613	X2681	X2804		
LEU					X2614	X2682	X2805		
LEU					X2615	X2683	X2806		
LEU					X2616	X2684	X2807		
LEU					X2617	X2685	X2808		
LEU					X2618	X2686	X2809		
LEU					X2619	X2687	X2810		
LEU					X2620	X2688	X2811		
LEU					X2621	X2689	X2812		
LEU					X2622	X2690	X2813		
LEU					X2623	X2691	X2814		
LEU					X2624	X2692	X2815		
LEU					X2625	X2693	X2816		
LEU					X2626	X2694	X2817		
LEU					X2627	X2695	X2818		
LEU					X2628	X2696	X2819		
LEU					X2629	X2697	X2820		
LEU					X2630	X2698	X2821		
LEU					X2631	X2699	X2822		
LEU					X2632	X2700	X2823		
LEU					X2633	X2701	X2824		
LEU					X2634	X2702	X2825		
LEU					X2635	X2703	X2826		
LEU					X2636	X2704	X2827		
LEU					X2637	X2705	X2828		
LEU					X2638	X2706	X2829		
LEU					X2639	X2707	X2830		
LEU					X2640	X2708	X2831		
LEU					X2641	X2709	X2832		
LEU					X2642	X2710	X2833		
LEU					X2643	X2711	X2834		
LEU					X2644	X2712	X2835		
LEU					X2645	X2713	X2836		
LEU					X2646	X2714	X2837		
LEU					X2647	X2715	X2838		
LEU					X2648	X2716	X2839		
LEU					X2649	X2717	X2840		
LEU					X2650	X2718	X2841		
LEU					X2651	X2719	X2842		
LEU					X2652	X2720	X2843		
LEU					X2653	X2721	X2844		
LEU					X2654	X2722	X2845		
LEU					X2655	X2723	X2846		
LEU					X2656	X2724	X2847		
LEU					X2657	X2725	X2848		
LEU					X2658	X2726	X2849		
LEU					X2659	X2727	X2850		
LEU					X2660	X2728	X2851		
LEU					X2661	X2729	X2852		
LEU					X2662	X2730	X2853		
LEU					X2663	X2731	X2854		
LEU					X2664	X2732	X2855		
LEU					X2665	X2733	X2856		
LEU					X2666	X2734	X2857		
LEU					X2667	X2735	X2858		
LEU					X2668	X2736	X2859		
LEU					X2669	X2737			





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	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	0.058	Depositor
Minimum map value	-0.029	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	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

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	0.20	0/834	0.51	1/1123 (0.1%)
1	F	0.20	0/834	0.51	1/1123 (0.1%)
1	H	0.20	0/834	0.51	1/1123 (0.1%)
1	J	0.20	0/834	0.51	1/1123 (0.1%)
2	B	0.21	0/25428	0.52	3/34534 (0.0%)
2	E	0.21	0/25428	0.52	3/34534 (0.0%)
2	G	0.21	0/25428	0.52	3/34534 (0.0%)
2	I	0.21	0/25428	0.52	3/34534 (0.0%)
All	All	0.21	0/105048	0.52	16/142628 (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	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	64

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	8	SER	N-CA-C	5.50	120.40	113.25
1	A	8	SER	N-CA-C	5.45	120.33	113.25
1	J	8	SER	N-CA-C	5.44	120.33	113.25
1	F	8	SER	N-CA-C	5.44	120.32	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1829	PRO	N-CA-C	5.31	119.56	111.11
2	B	1829	PRO	N-CA-C	5.29	119.52	111.11
2	G	1829	PRO	N-CA-C	5.29	119.52	111.11
2	I	1829	PRO	N-CA-C	5.27	119.49	111.11
2	I	4639	MET	CA-C-N	5.05	134.12	121.80
2	I	4639	MET	C-N-CA	5.05	134.12	121.80
2	B	4639	MET	CA-C-N	5.03	134.07	121.80
2	B	4639	MET	C-N-CA	5.03	134.07	121.80
2	G	4639	MET	CA-C-N	5.02	134.04	121.80
2	G	4639	MET	C-N-CA	5.02	134.04	121.80
2	E	4639	MET	CA-C-N	5.01	134.02	121.80
2	E	4639	MET	C-N-CA	5.01	134.02	121.80

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4228	ALA	Peptide
2	B	4641	PRO	Peptide
2	B	4666	VAL	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide

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Mol	Chain	Res	Type	Group
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4228	ALA	Peptide
2	E	4641	PRO	Peptide
2	E	4666	VAL	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4228	ALA	Peptide
2	G	4641	PRO	Peptide
2	G	4666	VAL	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4228	ALA	Peptide
2	I	4641	PRO	Peptide
2	I	4666	VAL	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	16	0
1	F	818	0	824	19	0
1	H	818	0	824	16	0
1	J	818	0	824	15	0
2	B	29499	0	24746	281	0
2	E	29499	0	24746	286	0
2	G	29499	0	24746	275	0
2	I	29499	0	24746	273	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
All	All	121272	0	102280	1154	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 5.

All (1154) 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:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.68
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.67
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.67
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.66
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.61	0.65
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.61	0.65
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.61	0.65
2:I:3773:ARG:HG3	2:I:3815:LYS:HZ3	1.62	0.64
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.61	0.64
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.79	0.64
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.61	0.64
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.79	0.64
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.81	0.63
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.81	0.63
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.79	0.62
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.79	0.62
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.81	0.62
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.62
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.82	0.61
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.61
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.82	0.61
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.32	0.61
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.32	0.61
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.33	0.61
2:E:331:VAL:HG12	2:E:333:GLY:H	1.65	0.61
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.82	0.61
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.32	0.61
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.82	0.61
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.83	0.61
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.83	0.61
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.82	0.61
2:G:3755:GLU:O	2:G:3762:ARG:NH2	2.34	0.61
2:I:3755:GLU:O	2:I:3762:ARG:NH2	2.34	0.61
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.83	0.61
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.83	0.60
2:B:3755:GLU:O	2:B:3762:ARG:NH2	2.34	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.65	0.60
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.83	0.60
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.82	0.60
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.83	0.60
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.82	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.83	0.60
2:E:3755:GLU:O	2:E:3762:ARG:NH2	2.34	0.60
2:E:4184:MET:HE2	2:E:4188:ARG:HA	1.83	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.65	0.60
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.82	0.60
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.35	0.60
2:I:683:ARG:NH1	2:I:707:VAL:O	2.34	0.60
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.35	0.60
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.60
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.35	0.60
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.83	0.59
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.84	0.59
2:I:331:VAL:HG12	2:I:333:GLY:H	1.66	0.59
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.59
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.83	0.59
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.83	0.59
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.83	0.59
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.82	0.59
2:G:4184:MET:HE2	2:G:4188:ARG:HA	1.83	0.59
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.85	0.59
2:E:683:ARG:NH1	2:E:707:VAL:O	2.34	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.59
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.85	0.58
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.85	0.58
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.58
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.35	0.58
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.84	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.58
2:I:4184:MET:HE2	2:I:4188:ARG:HA	1.83	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.58
2:B:4184:MET:HE2	2:B:4188:ARG:HA	1.83	0.58
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.58
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.85	0.58
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.58
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.86	0.58
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.58
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.37	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.57
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.57
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.37	0.57
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.38	0.57
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.85	0.57
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.87	0.57
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.37	0.57
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.37	0.57
2:I:4172:GLU:HA	2:I:4175:ARG:HE	1.69	0.57
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.87	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.57
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.87	0.57
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.86	0.57
2:E:132:ALA:HA	2:E:194:SER:HB2	1.87	0.57
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.37	0.57
2:G:614:VAL:HG22	2:G:616:SER:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:614:VAL:HG22	2:B:616:SER:H	1.69	0.56
2:I:614:VAL:HG22	2:I:616:SER:H	1.69	0.56
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.86	0.56
2:G:4172:GLU:HA	2:G:4175:ARG:HE	1.69	0.56
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.87	0.56
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.86	0.56
2:E:4172:GLU:HA	2:E:4175:ARG:HE	1.69	0.56
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.87	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.56
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.86	0.56
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.88	0.56
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.88	0.56
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.87	0.56
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.86	0.56
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.39	0.56
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.39	0.56
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.39	0.56
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.86	0.56
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.39	0.56
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.87	0.56
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.87	0.56
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.86	0.56
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.39	0.56
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.39	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.87	0.56
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.88	0.56
1:A:5:GLU:HB2	1:A:73:LYS:HB3	1.88	0.56
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.87	0.56
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.87	0.56
2:I:132:ALA:HA	2:I:194:SER:HB2	1.87	0.56
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.88	0.56
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.87	0.56
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.88	0.56
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.88	0.56
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.88	0.56
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.88	0.56
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.87	0.56
2:G:1271:ARG:HA	2:G:1471:UNK:HA	1.88	0.56
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.88	0.56
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.88	0.55
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.88	0.55
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.87	0.55
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.89	0.55
2:I:1271:ARG:HA	2:I:1471:UNK:HA	1.88	0.55
2:E:1271:ARG:HA	2:E:1471:UNK:HA	1.88	0.55
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.39	0.55
2:G:2347:GLU:O	2:G:2351:ASN:N	2.39	0.55
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.89	0.55
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.89	0.55
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.39	0.55
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.40	0.55
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.39	0.55
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.87	0.55
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.88	0.55
2:B:683:ARG:NH1	2:B:707:VAL:O	2.34	0.55
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.89	0.55
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.89	0.55
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.39	0.55
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.55
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.72	0.55
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.55
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.89	0.55
1:F:5:GLU:HB2	1:F:73:LYS:HB3	1.88	0.55
2:E:614:VAL:HG22	2:E:616:SER:H	1.69	0.55
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.40	0.55
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.39	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.89	0.55
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.39	0.55
2:B:4172:GLU:HA	2:B:4175:ARG:HE	1.69	0.55
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.88	0.55
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.40	0.55
2:I:241:GLN:O	2:I:289:ARG:NH1	2.37	0.55
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.38	0.55
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.89	0.55
2:B:1271:ARG:HA	2:B:1471:UNK:HA	1.88	0.55
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.72	0.55
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.40	0.55
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.40	0.55
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.88	0.55
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.89	0.55
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.72	0.55
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.88	0.54
2:I:164:ARG:N	2:I:167:ASP:OD2	2.41	0.54
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.89	0.54
2:G:683:ARG:NH1	2:G:707:VAL:O	2.33	0.54
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.72	0.54
1:H:5:GLU:HB2	1:H:73:LYS:HB3	1.88	0.54
1:J:5:GLU:HB2	1:J:73:LYS:HB3	1.88	0.54
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.54
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.89	0.54
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.40	0.54
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.89	0.54
2:E:4763:GLY:H	2:E:4767:TRP:HE1	1.56	0.54
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.41	0.54
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.88	0.54
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.90	0.54
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.41	0.54
2:B:4763:GLY:H	2:B:4767:TRP:HE1	1.56	0.54
2:E:609:CYS:SG	2:E:610:ASN:N	2.80	0.54
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.89	0.54
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.89	0.54
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.72	0.54
2:G:4763:GLY:H	2:G:4767:TRP:HE1	1.56	0.54
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.90	0.54
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.40	0.54
2:G:164:ARG:N	2:G:167:ASP:OD2	2.41	0.54
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.88	0.54
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.90	0.54
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.54
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.90	0.54
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.90	0.53
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.90	0.53
2:G:241:GLN:O	2:G:289:ARG:NH1	2.37	0.53
2:G:609:CYS:SG	2:G:610:ASN:N	2.80	0.53
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.73	0.53
2:B:609:CYS:SG	2:B:610:ASN:N	2.80	0.53
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.91	0.53
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.41	0.53
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.74	0.53
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2347:GLU:O	2:I:2351:ASN:N	2.39	0.53
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.73	0.53
2:I:609:CYS:SG	2:I:610:ASN:N	2.80	0.53
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.74	0.53
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.73	0.53
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.90	0.53
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.73	0.53
2:I:4763:GLY:H	2:I:4767:TRP:HE1	1.56	0.53
2:E:164:ARG:N	2:E:167:ASP:OD2	2.41	0.53
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.74	0.53
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.90	0.53
2:E:978:THR:HB	2:E:980:ALA:H	1.74	0.53
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.82	0.53
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.53
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.41	0.53
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.82	0.53
2:E:2347:GLU:O	2:E:2351:ASN:N	2.39	0.53
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.73	0.53
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.91	0.53
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.53
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.42	0.53
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.91	0.53
2:B:978:THR:HB	2:B:980:ALA:H	1.74	0.53
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.82	0.53
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.74	0.53
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.91	0.53
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.41	0.53
2:B:164:ARG:N	2:B:167:ASP:OD2	2.41	0.52
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.40	0.52
2:G:290:TYR:O	2:G:302:VAL:N	2.43	0.52
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.90	0.52
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.74	0.52
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.74	0.52
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.74	0.52
2:G:645:ARG:N	2:G:824:GLU:O	2.40	0.52
2:B:2347:GLU:O	2:B:2351:ASN:N	2.39	0.52
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.91	0.52
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.75	0.52
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.73	0.52
2:G:978:THR:HB	2:G:980:ALA:H	1.74	0.52
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.42	0.52
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.52
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.92	0.52
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.92	0.52
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.92	0.52
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.42	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.92	0.52
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.92	0.52
2:E:290:TYR:O	2:E:302:VAL:N	2.42	0.52
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.92	0.52
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.75	0.52
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.41	0.52
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.43	0.52
2:I:290:TYR:O	2:I:302:VAL:N	2.42	0.52
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.74	0.52
2:E:1660:GLN:HG3	2:E:1707:LEU:HD13	1.92	0.52
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.82	0.52
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.43	0.52
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.91	0.52
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.43	0.52
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.43	0.52
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.92	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.74	0.52
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.42	0.52
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.91	0.52
2:B:1660:GLN:HG3	2:B:1707:LEU:HD13	1.92	0.52
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.74	0.52
2:G:101:LEU:HB3	2:G:150:MET:HE1	1.92	0.52
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.74	0.52
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.91	0.51
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.92	0.51
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.91	0.51
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.44	0.51
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.93	0.51
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.92	0.51
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.93	0.51
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.43	0.51
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.43	0.51
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.91	0.51
2:B:290:TYR:O	2:B:302:VAL:N	2.43	0.51
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3984:ARG:HH22	2:I:161:GLU:HG2	1.74	0.51
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.43	0.51
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.43	0.51
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.93	0.51
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.92	0.51
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.75	0.51
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.25	0.51
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.43	0.51
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.92	0.51
2:I:645:ARG:N	2:I:824:GLU:O	2.40	0.51
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.93	0.51
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.93	0.51
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.75	0.51
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.92	0.51
2:B:241:GLN:O	2:B:289:ARG:NH1	2.37	0.51
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.39	0.51
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.44	0.51
2:I:315:CYS:SG	2:I:316:PHE:N	2.84	0.51
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.92	0.51
2:G:1636:MET:HE2	2:G:1638:ALA:HB2	1.93	0.51
2:G:1660:GLN:HG3	2:G:1707:LEU:HD13	1.92	0.51
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.91	0.51
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.93	0.51
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.41	0.51
2:I:2452:ARG:HH12	2:G:177:GLU:HG3	1.76	0.51
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.93	0.51
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.51
2:B:1636:MET:HE2	2:B:1638:ALA:HB2	1.93	0.51
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.43	0.51
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.93	0.51
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.75	0.51
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.92	0.51
2:E:101:LEU:HB3	2:E:150:MET:HE1	1.92	0.51
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.44	0.51
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.75	0.51
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.93	0.51
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.43	0.51
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	1.93	0.51
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.92	0.50
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.43	0.50
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.92	0.50
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.93	0.50
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.93	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.45	0.50
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.75	0.50
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.92	0.50
2:G:470:SER:O	2:G:474:ARG:NE	2.40	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.45	0.50
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.42	0.50
2:I:1636:MET:HE2	2:I:1638:ALA:HB2	1.93	0.50
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.92	0.50
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.94	0.50
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.93	0.50
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.75	0.50
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.92	0.50
2:B:315:CYS:SG	2:B:316:PHE:N	2.84	0.50
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.92	0.50
2:E:315:CYS:SG	2:E:316:PHE:N	2.84	0.50
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.93	0.50
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.93	0.50
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.92	0.50
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.91	0.50
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.92	0.50
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.94	0.50
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.93	0.50
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.94	0.50
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.92	0.50
2:E:1636:MET:HE2	2:E:1638:ALA:HB2	1.93	0.50
2:E:4065:PHE:HB3	2:E:4132:PHE:CE2	2.47	0.50
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.45	0.50
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	1.93	0.50
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.94	0.50
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.94	0.50
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.45	0.50
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.93	0.50
2:G:315:CYS:SG	2:G:316:PHE:N	2.84	0.50
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.93	0.50
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.92	0.50
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.44	0.50
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.94	0.50
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.50
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.44	0.50
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.93	0.50
2:G:4065:PHE:HB3	2:G:4132:PHE:CE2	2.47	0.50
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.45	0.50
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.94	0.50
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.93	0.50
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.93	0.50
2:B:4065:PHE:HB3	2:B:4132:PHE:CE2	2.47	0.50
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.92	0.50
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.94	0.50
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	1.93	0.50
2:I:1660:GLN:HG3	2:I:1707:LEU:HD13	1.92	0.50
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	1.94	0.50
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.94	0.50
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.93	0.50
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.93	0.50
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.44	0.50
2:B:470:SER:O	2:B:474:ARG:NE	2.40	0.49
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	1.94	0.49
2:I:3762:ARG:H	2:I:4754:ASN:HA	1.77	0.49
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.77	0.49
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.45	0.49
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	1.93	0.49
2:E:173:SER:HB3	2:E:178:ARG:H	1.77	0.49
2:E:241:GLN:O	2:E:289:ARG:NH1	2.37	0.49
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.43	0.49
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.93	0.49
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.45	0.49
2:B:3762:ARG:H	2:B:4754:ASN:HA	1.77	0.49
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.77	0.49
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.46	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.92	0.49
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.46	0.49
1:A:82:TYR:O	1:A:86:GLY:N	2.43	0.49
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.93	0.49
2:B:1171:SER:HG	2:B:1175:SER:H	1.61	0.49
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.44	0.49
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.49
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.92	0.49
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	1.94	0.49
2:B:309:THR:O	2:B:313:SER:OG	2.31	0.49
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.94	0.49
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.46	0.49
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.94	0.49
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.94	0.49
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.94	0.49
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.44	0.49
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	1.94	0.49
2:G:309:THR:O	2:G:313:SER:OG	2.31	0.49
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.94	0.49
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.94	0.49
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.78	0.49
2:B:286:THR:HA	2:B:405:HIS:HB2	1.95	0.49
2:I:286:THR:HA	2:I:405:HIS:HB2	1.95	0.49
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.78	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.95	0.49
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.94	0.49
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.44	0.49
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.46	0.49
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.93	0.49
2:B:645:ARG:N	2:B:824:GLU:O	2.40	0.49
2:B:999:ASP:O	2:B:1004:GLY:N	2.46	0.49
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.78	0.49
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.94	0.49
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.94	0.49
2:E:999:ASP:O	2:E:1004:GLY:N	2.46	0.49
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.45	0.49
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.45	0.49
2:I:309:THR:O	2:I:313:SER:OG	2.31	0.49
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.78	0.49
2:E:1694:LEU:O	2:E:1712:TYR:OH	2.25	0.49
2:E:3762:ARG:H	2:E:4754:ASN:HA	1.77	0.49
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.93	0.49
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.78	0.49
1:F:11:ASP:OD1	1:F:67:SER:OG	2.30	0.49
1:H:6:THR:HA	1:H:72:ALA:HA	1.94	0.49
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.45	0.49
2:B:173:SER:HB3	2:B:178:ARG:H	1.77	0.49
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.95	0.49
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:134:ASP:OD1	2:I:134:ASP:N	2.46	0.49
2:I:999:ASP:O	2:I:1004:GLY:N	2.46	0.49
2:E:286:THR:HA	2:E:405:HIS:HB2	1.95	0.49
2:E:309:THR:O	2:E:313:SER:OG	2.31	0.49
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.46	0.49
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.78	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.93	0.49
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.93	0.49
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.94	0.49
2:G:286:THR:HA	2:G:405:HIS:HB2	1.95	0.49
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.30	0.49
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.46	0.49
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.94	0.49
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.94	0.49
2:I:16:THR:OG1	2:I:97:GLY:O	2.31	0.49
2:I:173:SER:HB3	2:I:178:ARG:H	1.77	0.49
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	1.95	0.49
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.46	0.49
2:I:4065:PHE:HB3	2:I:4132:PHE:CE2	2.47	0.49
2:G:999:ASP:O	2:G:1004:GLY:N	2.46	0.49
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.77	0.49
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.44	0.49
1:A:6:THR:HA	1:A:72:ALA:HA	1.94	0.48
1:H:11:ASP:OD1	1:H:67:SER:OG	2.30	0.48
2:I:4138:ASP:O	2:I:4142:ASN:ND2	2.46	0.48
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.78	0.48
2:E:606:LEU:O	2:E:617:ASN:ND2	2.46	0.48
2:E:3767:GLN:NE2	2:E:3803:SER:O	2.46	0.48
1:F:6:THR:HA	1:F:72:ALA:HA	1.94	0.48
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.42	0.48
2:B:4826:ILE:O	2:B:4829:SER:OG	2.29	0.48
2:I:3767:GLN:NE2	2:I:3803:SER:O	2.46	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.46	0.48
2:E:4987:ASN:HA	2:E:4990:PHE:HD2	1.78	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.48
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.96	0.48
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.79	0.48
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.47	0.48
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.96	0.48
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.47	0.48
2:I:4987:ASN:HA	2:I:4990:PHE:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.85	0.48
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.46	0.48
2:G:4138:ASP:O	2:G:4142:ASN:ND2	2.47	0.48
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	1.95	0.48
2:B:4071:ILE:HD11	2:B:4102:GLN:HE21	1.79	0.48
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.94	0.48
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.95	0.48
2:G:1270:LEU:O	2:G:1472:UNK:N	2.47	0.48
2:G:3762:ARG:H	2:G:4754:ASN:HA	1.77	0.48
2:I:1270:LEU:O	2:I:1472:UNK:N	2.47	0.48
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.46	0.48
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.39	0.48
2:E:1270:LEU:O	2:E:1472:UNK:N	2.47	0.48
2:E:4138:ASP:O	2:E:4142:ASN:ND2	2.47	0.48
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	1.95	0.48
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.96	0.48
2:I:606:LEU:O	2:I:617:ASN:ND2	2.46	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.48
2:E:150:MET:HE3	2:E:163:VAL:HG21	1.96	0.48
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.47	0.48
2:E:4071:ILE:HD11	2:E:4102:GLN:HE21	1.79	0.48
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.48
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.78	0.48
2:B:606:LEU:O	2:B:617:ASN:ND2	2.46	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.48
2:B:1991:THR:O	2:B:1995:THR:OG1	2.32	0.48
2:I:150:MET:HE3	2:I:163:VAL:HG21	1.96	0.48
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.96	0.48
2:I:1991:THR:O	2:I:1995:THR:OG1	2.32	0.48
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	1.95	0.48
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.39	0.48
2:G:606:LEU:O	2:G:617:ASN:ND2	2.46	0.48
1:J:6:THR:HA	1:J:72:ALA:HA	1.94	0.48
2:B:280:LEU:HD21	2:B:316:PHE:HE2	1.78	0.48
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.43	0.48
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.96	0.48
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.30	0.48
2:G:16:THR:OG1	2:G:97:GLY:O	2.31	0.48
2:G:4987:ASN:HA	2:G:4990:PHE:HD2	1.78	0.48
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.96	0.48
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.96	0.48
2:G:4071:ILE:HD11	2:G:4102:GLN:HE21	1.79	0.48
1:F:82:TYR:O	1:F:86:GLY:N	2.43	0.48
2:B:150:MET:HE3	2:B:163:VAL:HG21	1.96	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.48
2:B:1270:LEU:O	2:B:1472:UNK:N	2.47	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.46	0.48
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.96	0.48
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.96	0.48
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.96	0.48
2:G:134:ASP:OD1	2:G:134:ASP:N	2.46	0.48
1:J:11:ASP:OD1	1:J:67:SER:OG	2.30	0.47
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.96	0.47
2:I:280:LEU:HD21	2:I:316:PHE:HE2	1.78	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.47
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.96	0.47
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.77	0.47
2:G:173:SER:HB3	2:G:178:ARG:H	1.77	0.47
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.96	0.47
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.96	0.47
1:J:82:TYR:O	1:J:86:GLY:N	2.43	0.47
2:B:134:ASP:OD1	2:B:134:ASP:N	2.46	0.47
2:B:3767:GLN:NE2	2:B:3803:SER:O	2.46	0.47
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.96	0.47
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	1.96	0.47
2:I:4071:ILE:HD11	2:I:4102:GLN:HE21	1.79	0.47
2:G:1171:SER:HG	2:G:1175:SER:H	1.59	0.47
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.96	0.47
2:G:1991:THR:O	2:G:1995:THR:OG1	2.32	0.47
2:G:4826:ILE:O	2:G:4829:SER:OG	2.29	0.47
2:B:16:THR:OG1	2:B:97:GLY:O	2.31	0.47
2:B:4138:ASP:O	2:B:4142:ASN:ND2	2.46	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.33	0.47
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.97	0.47
2:B:4987:ASN:HA	2:B:4990:PHE:HD2	1.78	0.47
2:I:485:SER:O	2:I:489:ASN:N	2.43	0.47
2:I:579:GLN:H	2:I:582:HIS:HD2	1.63	0.47
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	1.97	0.47
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.47	0.47
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.47
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.47
2:I:1457:UNK:N	2:I:1497:UNK:O	2.47	0.47
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.96	0.47
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.96	0.47
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.47
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.95	0.47
2:G:1457:UNK:N	2:G:1497:UNK:O	2.47	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.48	0.47
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	1.96	0.47
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.88	0.47
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.48	0.47
2:E:280:LEU:HD21	2:E:316:PHE:HE2	1.78	0.47
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.42	0.47
2:G:150:MET:HE3	2:G:163:VAL:HG21	1.96	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.43	0.47
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.88	0.47
2:I:4571:PHE:O	2:I:4575:PHE:N	2.48	0.47
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.96	0.47
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.80	0.47
2:G:3767:GLN:NE2	2:G:3803:SER:O	2.46	0.47
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.80	0.47
2:B:1457:UNK:N	2:B:1497:UNK:O	2.47	0.47
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.96	0.47
2:I:4228:ALA:O	2:I:4232:GLU:N	2.48	0.47
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.97	0.47
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.80	0.47
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.97	0.47
2:E:4571:PHE:O	2:E:4575:PHE:N	2.48	0.47
2:G:280:LEU:HD21	2:G:316:PHE:HE2	1.78	0.47
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.80	0.47
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	1.97	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.96	0.47
2:B:342:GLY:N	2:B:390:LEU:O	2.48	0.47
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.47
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.96	0.47
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.96	0.47
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.30	0.47
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.79	0.47
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.96	0.47
2:B:4892:ARG:NH2	2:I:4895:GLY:O	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.80	0.47
2:E:16:THR:OG1	2:E:97:GLY:O	2.31	0.47
2:E:670:GLU:HG3	2:E:787:VAL:HG13	1.97	0.47
2:G:579:GLN:H	2:G:582:HIS:HD2	1.63	0.47
1:A:11:ASP:OD1	1:A:67:SER:OG	2.30	0.47
2:B:579:GLN:H	2:B:582:HIS:HD2	1.63	0.47
2:B:670:GLU:HG3	2:B:787:VAL:HG13	1.97	0.47
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.96	0.47
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.96	0.47
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.80	0.46
2:G:342:GLY:N	2:G:390:LEU:O	2.48	0.46
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.97	0.46
2:G:4228:ALA:O	2:G:4232:GLU:N	2.48	0.46
2:E:134:ASP:N	2:E:134:ASP:OD1	2.46	0.46
2:E:161:GLU:HG2	2:G:3984:ARG:HH22	1.80	0.46
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.88	0.46
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.97	0.46
2:B:2208:MET:SD	2:B:2253:HIS:ND1	2.85	0.46
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.88	0.46
2:E:1457:UNK:N	2:E:1497:UNK:O	2.47	0.46
2:E:2208:MET:SD	2:E:2253:HIS:ND1	2.85	0.46
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.96	0.46
2:B:4191:GLU:OE1	2:B:5006:GLN:NE2	2.48	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.48	0.46
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.98	0.46
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.80	0.46
2:E:579:GLN:H	2:E:582:HIS:HD2	1.63	0.46
2:E:4191:GLU:OE1	2:E:5006:GLN:NE2	2.48	0.46
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.97	0.46
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.80	0.46
2:B:221:ARG:NE	2:B:258:SER:OG	2.43	0.46
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.46	0.46
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.96	0.46
2:I:3771:HIS:O	2:I:3774:GLY:N	2.45	0.46
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.98	0.46
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.48	0.46
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.97	0.46
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.98	0.46
2:B:4228:ALA:O	2:B:4232:GLU:N	2.48	0.46
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.98	0.46
2:E:4227:GLU:OE2	2:G:4973:HIS:ND1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.97	0.46
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.80	0.46
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.85	0.46
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.81	0.46
2:B:2810:LYS:O	2:B:2814:LYS:N	2.45	0.46
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.97	0.46
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.33	0.46
2:E:342:GLY:N	2:E:390:LEU:O	2.48	0.46
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.98	0.46
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.81	0.46
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.80	0.46
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.96	0.46
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.98	0.46
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.80	0.46
2:E:221:ARG:NE	2:E:258:SER:OG	2.44	0.46
2:E:3759:GLU:OE1	2:E:3762:ARG:NH2	2.43	0.46
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.98	0.46
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.46
2:G:689:THR:H	2:G:778:PHE:HE2	1.64	0.46
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.97	0.46
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.81	0.46
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.48	0.46
2:G:4191:GLU:OE1	2:G:5006:GLN:NE2	2.48	0.46
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.98	0.46
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.80	0.46
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.97	0.46
2:I:4191:GLU:OE1	2:I:5006:GLN:NE2	2.48	0.46
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.46	0.46
2:G:3759:GLU:OE1	2:G:3762:ARG:NH2	2.43	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.82	0.45
2:B:4005:GLN:HE21	2:B:4110:PHE:HE1	1.64	0.45
2:I:346:CYS:N	2:I:388:LEU:O	2.49	0.45
2:I:681:HIS:HE2	2:I:683:ARG:NE	2.14	0.45
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.98	0.45
2:E:485:SER:O	2:E:489:ASN:N	2.43	0.45
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.98	0.45
2:G:395:GLN:HG3	2:G:397:GLU:H	1.81	0.45
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.49	0.45
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.46	0.45
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.99	0.45
2:I:2208:MET:SD	2:I:2253:HIS:ND1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.98	0.45
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.98	0.45
2:E:395:GLN:HG3	2:E:397:GLU:H	1.81	0.45
2:E:681:HIS:HE2	2:E:683:ARG:NE	2.14	0.45
2:E:4005:GLN:HE21	2:E:4110:PHE:HE1	1.64	0.45
2:G:346:CYS:N	2:G:388:LEU:O	2.49	0.45
2:G:4005:GLN:HE21	2:G:4110:PHE:HE1	1.64	0.45
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.98	0.45
2:I:670:GLU:HG3	2:I:787:VAL:HG13	1.97	0.45
2:I:689:THR:H	2:I:778:PHE:HE2	1.64	0.45
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.30	0.45
2:I:4826:ILE:O	2:I:4829:SER:OG	2.29	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.45
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.80	0.45
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.52	0.45
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.81	0.45
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	1.99	0.45
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.45
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.81	0.45
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.99	0.45
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.98	0.45
1:H:82:TYR:O	1:H:86:GLY:N	2.43	0.45
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.99	0.45
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.49	0.45
2:I:320:LYS:NZ	2:I:381:GLU:O	2.36	0.45
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	1.99	0.45
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.98	0.45
2:E:689:THR:H	2:E:778:PHE:HE2	1.64	0.45
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.33	0.45
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.98	0.45
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.30	0.45
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.99	0.45
2:B:346:CYS:N	2:B:388:LEU:O	2.49	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.97	0.45
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.98	0.45
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.49	0.45
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.98	0.45
2:G:670:GLU:HG3	2:G:787:VAL:HG13	1.97	0.45
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.99	0.45
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.48	0.45
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.98	0.45
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.98	0.45
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.97	0.45
2:E:346:CYS:N	2:E:388:LEU:O	2.49	0.45
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.97	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.99	0.45
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.98	0.45
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.98	0.45
2:I:342:GLY:N	2:I:390:LEU:O	2.48	0.45
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.98	0.45
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.98	0.45
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	1.99	0.45
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.82	0.45
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.81	0.45
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.52	0.45
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.85	0.45
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.99	0.45
2:E:2908:TYR:OH	2:E:2920:ARG:NE	2.48	0.45
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.98	0.45
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.99	0.45
2:B:41:GLY:O	2:B:45:ARG:NH1	2.50	0.45
2:B:4047:MET:HE3	2:B:4047:MET:HB2	1.89	0.45
2:B:395:GLN:HG3	2:B:397:GLU:H	1.81	0.45
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.97	0.45
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	1.99	0.45
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.99	0.45
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.81	0.45
2:E:2810:LYS:O	2:E:2814:LYS:N	2.45	0.45
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.99	0.45
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.98	0.45
2:G:41:GLY:O	2:G:45:ARG:NH1	2.50	0.45
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.52	0.45
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.99	0.45
2:G:3771:HIS:O	2:G:3774:GLY:N	2.45	0.45
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.81	0.44
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.52	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.50	0.44
2:I:395:GLN:HG3	2:I:397:GLU:H	1.81	0.44
2:E:4228:ALA:O	2:E:4232:GLU:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.81	0.44
2:G:3759:GLU:HG3	2:G:3763:LEU:HD22	1.99	0.44
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.98	0.44
2:B:689:THR:H	2:B:778:PHE:HE2	1.64	0.44
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.83	0.44
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.99	0.44
2:E:645:ARG:N	2:E:824:GLU:O	2.40	0.44
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.82	0.44
2:B:243:ARG:NH1	2:B:301:VAL:O	2.44	0.44
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.85	0.44
2:B:2381:GLU:HA	2:B:2384:ILE:HD12	2.00	0.44
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.99	0.44
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.53	0.44
2:E:3766:GLN:HG3	2:E:3769:ARG:HH12	1.83	0.44
2:I:793:LEU:HD22	2:I:821:LEU:HD13	2.00	0.44
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.53	0.44
2:I:4005:GLN:HE21	2:I:4110:PHE:HE1	1.64	0.44
2:E:41:GLY:O	2:E:45:ARG:NH1	2.50	0.44
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.98	0.44
2:G:3766:GLN:HG3	2:G:3769:ARG:HH12	1.83	0.44
2:I:3759:GLU:HG3	2:I:3763:LEU:HD22	1.99	0.44
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.49	0.44
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.98	0.44
2:G:2810:LYS:O	2:G:2814:LYS:N	2.45	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.50	0.44
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.98	0.44
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.30	0.44
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.44
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.82	0.44
2:B:793:LEU:HD22	2:B:821:LEU:HD13	2.00	0.44
2:B:3552:UNK:O	2:B:3556:UNK:N	2.51	0.44
2:B:3766:GLN:HG3	2:B:3769:ARG:HH12	1.83	0.44
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.99	0.44
2:E:4895:GLY:O	2:G:4892:ARG:NH2	2.43	0.44
2:G:111:HIS:CD2	2:G:114:SER:H	2.36	0.44
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.44
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.82	0.44
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.00	0.44
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.99	0.44
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	1.99	0.44
2:I:2950:UNK:O	2:I:2954:UNK:N	2.51	0.44
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.83	0.44
2:E:793:LEU:HD12	2:E:797:HIS:HB2	2.00	0.44
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.99	0.44
2:B:668:VAL:O	2:B:741:GLU:N	2.49	0.44
2:B:2950:UNK:O	2:B:2954:UNK:N	2.51	0.44
2:E:2381:GLU:HA	2:E:2384:ILE:HD12	2.00	0.44
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.83	0.44
2:G:2381:GLU:HA	2:G:2384:ILE:HD12	2.00	0.44
2:G:2950:UNK:O	2:G:2954:UNK:N	2.51	0.44
2:B:111:HIS:CD2	2:B:114:SER:H	2.36	0.43
2:B:793:LEU:HD12	2:B:797:HIS:HB2	2.00	0.43
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.53	0.43
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.43
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.99	0.43
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.00	0.43
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.83	0.43
2:I:111:HIS:CD2	2:I:114:SER:H	2.36	0.43
2:E:626:LEU:HG	2:E:628:GLY:H	1.83	0.43
2:E:1936:LYS:O	2:E:1940:CYS:N	2.47	0.43
2:E:2758:PHE:O	2:E:2762:THR:N	2.52	0.43
2:B:626:LEU:HG	2:B:628:GLY:H	1.83	0.43
2:E:2950:UNK:O	2:E:2954:UNK:N	2.51	0.43
2:G:793:LEU:HD12	2:G:797:HIS:HB2	2.00	0.43
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.84	0.43
2:I:1105:ALA:N	2:I:1189:LEU:O	2.51	0.43
2:I:3766:GLN:HG3	2:I:3769:ARG:HH12	1.83	0.43
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.46	0.43
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.43
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.43
2:G:4065:PHE:HD1	2:G:4068:LEU:HD22	1.83	0.43
1:A:55:VAL:HA	2:B:1784:ALA:HA	2.00	0.43
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.54	0.43
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.00	0.43
2:B:2758:PHE:O	2:B:2762:THR:N	2.52	0.43
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.00	0.43
2:I:2467:VAL:HA	2:I:2470:ILE:HD12	2.01	0.43
2:I:4065:PHE:HD1	2:I:4068:LEU:HD22	1.83	0.43
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.53	0.43
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.99	0.43
1:A:21:THR:HA	1:A:49:ARG:HA	2.01	0.43
2:I:313:SER:HB3	2:I:351:VAL:HB	2.01	0.43
2:I:4864:ASN:HA	2:I:4874:MET:HG2	2.01	0.43
2:E:111:HIS:CD2	2:E:114:SER:H	2.36	0.43
2:E:668:VAL:O	2:E:741:GLU:N	2.49	0.43
2:E:1105:ALA:N	2:E:1189:LEU:O	2.51	0.43
2:G:793:LEU:HD22	2:G:821:LEU:HD13	2.00	0.43
2:G:2467:VAL:HA	2:G:2470:ILE:HD12	2.01	0.43
2:B:4586:PRO:HA	2:B:4628:VAL:HG11	2.01	0.43
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	2.01	0.43
2:I:2381:GLU:HA	2:I:2384:ILE:HD12	2.00	0.43
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.54	0.43
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.84	0.43
2:E:4864:ASN:HA	2:E:4874:MET:HG2	2.01	0.43
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.54	0.43
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	2.01	0.43
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.83	0.43
2:G:4586:PRO:HA	2:G:4628:VAL:HG11	2.01	0.43
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.01	0.43
2:I:41:GLY:O	2:I:45:ARG:NH1	2.50	0.43
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.54	0.43
2:I:793:LEU:HD12	2:I:797:HIS:HB2	2.00	0.43
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.01	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.84	0.43
2:I:4586:PRO:HA	2:I:4628:VAL:HG11	2.01	0.43
2:E:3759:GLU:HG3	2:E:3763:LEU:HD22	1.99	0.43
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.33	0.43
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.84	0.43
2:B:2257:LEU:O	2:B:2261:SER:N	2.52	0.43
2:B:3771:HIS:O	2:B:3774:GLY:N	2.45	0.43
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.84	0.43
2:B:4864:ASN:HA	2:B:4874:MET:HG2	2.01	0.43
2:B:4973:HIS:ND1	2:I:4227:GLU:OE2	2.51	0.43
2:E:793:LEU:HD22	2:E:821:LEU:HD13	2.00	0.43
1:F:21:THR:HA	1:F:49:ARG:HA	2.01	0.43
1:J:7:ILE:HB	1:J:71:ARG:HB3	2.01	0.43
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.01	0.43
2:B:3759:GLU:HG3	2:B:3763:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4065:PHE:HD1	2:B:4068:LEU:HD22	1.83	0.43
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.83	0.43
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.00	0.43
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.84	0.43
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.84	0.43
2:G:2257:LEU:O	2:G:2261:SER:N	2.52	0.43
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.01	0.42
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.01	0.42
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.00	0.42
2:E:313:SER:HB3	2:E:351:VAL:HB	2.01	0.42
2:E:615:ARG:NH2	2:E:1677:GLY:O	2.52	0.42
2:E:4586:PRO:HA	2:E:4628:VAL:HG11	2.01	0.42
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	2.01	0.42
2:G:3361:UNK:O	2:G:3365:UNK:N	2.52	0.42
1:A:7:ILE:HB	1:A:71:ARG:HB3	2.01	0.42
1:J:21:THR:HA	1:J:49:ARG:HA	2.01	0.42
2:B:1105:ALA:N	2:B:1189:LEU:O	2.51	0.42
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.84	0.42
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.84	0.42
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	2.02	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.01	0.42
2:E:2257:LEU:O	2:E:2261:SER:N	2.52	0.42
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.83	0.42
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.84	0.42
2:I:626:LEU:HG	2:I:628:GLY:H	1.83	0.42
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	2.02	0.42
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.01	0.42
2:G:313:SER:HB3	2:G:351:VAL:HB	2.01	0.42
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.00	0.42
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.01	0.42
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.01	0.42
2:G:4047:MET:HE3	2:G:4047:MET:HB2	1.89	0.42
2:G:4864:ASN:HA	2:G:4874:MET:HG2	2.01	0.42
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.01	0.42
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	2.01	0.42
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.01	0.42
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.84	0.42
2:I:4822:THR:O	2:I:4825:THR:OG1	2.34	0.42
2:E:582:HIS:O	2:E:585:SER:OG	2.32	0.42
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.01	0.42
2:E:2467:VAL:HA	2:E:2470:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4065:PHE:HD1	2:E:4068:LEU:HD22	1.83	0.42
2:G:626:LEU:HG	2:G:628:GLY:H	1.83	0.42
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.01	0.42
2:I:221:ARG:NE	2:I:258:SER:OG	2.43	0.42
2:I:2257:LEU:O	2:I:2261:SER:N	2.52	0.42
2:I:2447:LYS:HG3	2:I:2450:ALA:H	1.84	0.42
2:I:3759:GLU:OE1	2:I:3762:ARG:NH2	2.43	0.42
2:G:2447:LYS:HG3	2:G:2450:ALA:H	1.84	0.42
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.00	0.42
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.84	0.42
2:B:1770:SER:OG	2:B:1772:ARG:NE	2.53	0.42
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	2.02	0.42
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	2.02	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.00	0.42
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.02	0.42
2:I:3361:UNK:O	2:I:3365:UNK:N	2.52	0.42
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.42
2:E:2208:MET:HE2	2:E:2208:MET:HB3	1.97	0.42
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	2.02	0.42
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	2.02	0.42
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.84	0.42
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.30	0.42
2:G:668:VAL:O	2:G:741:GLU:N	2.49	0.42
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.84	0.42
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	2.02	0.42
2:B:1171:SER:OG	2:B:1175:SER:N	2.45	0.42
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	2.02	0.42
2:E:788:LYS:HG2	2:E:1629:GLN:HA	2.01	0.42
2:G:221:ARG:NE	2:G:258:SER:OG	2.43	0.42
2:G:2908:TYR:OH	2:G:2920:ARG:NE	2.48	0.42
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	2.02	0.42
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	2.02	0.42
2:B:2447:LYS:HG3	2:B:2450:ALA:H	1.84	0.42
2:B:3361:UNK:O	2:B:3365:UNK:N	2.52	0.42
2:E:2447:LYS:HG3	2:E:2450:ALA:H	1.84	0.42
2:E:3361:UNK:O	2:E:3365:UNK:N	2.52	0.42
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.02	0.42
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.50	0.42
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	2.02	0.42
2:B:313:SER:HB3	2:B:351:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	2.02	0.42
2:I:1770:SER:OG	2:I:1772:ARG:NE	2.53	0.42
2:I:4177:TYR:CE1	2:I:4199:GLU:HB3	2.55	0.42
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.02	0.42
1:H:21:THR:HA	1:H:49:ARG:HA	2.01	0.42
2:I:788:LYS:HG2	2:I:1629:GLN:HA	2.02	0.42
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.85	0.42
2:E:1663:HIS:O	2:E:1667:LEU:N	2.52	0.42
2:E:3771:HIS:O	2:E:3774:GLY:N	2.45	0.42
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.85	0.42
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.52	0.42
2:G:788:LYS:HG2	2:G:1629:GLN:HA	2.01	0.42
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.84	0.42
1:F:71:ARG:HH22	2:E:679:ALA:HB2	1.85	0.41
1:H:7:ILE:HB	1:H:71:ARG:HB3	2.01	0.41
2:I:195:PHE:HB3	2:I:196:MET:HG2	2.02	0.41
2:I:776:LEU:HG	2:I:848:HIS:HA	2.02	0.41
2:I:2758:PHE:O	2:I:2762:THR:N	2.52	0.41
2:I:4027:LEU:HA	2:I:4030:LEU:HD12	2.02	0.41
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.02	0.41
2:G:1105:ALA:N	2:G:1189:LEU:O	2.51	0.41
1:F:55:VAL:HA	2:E:1784:ALA:HA	2.02	0.41
2:B:3759:GLU:OE1	2:B:3762:ARG:NH2	2.43	0.41
2:I:615:ARG:NH2	2:I:1677:GLY:O	2.52	0.41
2:I:684:VAL:HA	2:I:781:VAL:HA	2.02	0.41
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	2.03	0.41
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.01	0.41
2:G:776:LEU:HG	2:G:848:HIS:HA	2.02	0.41
2:G:1770:SER:OG	2:G:1772:ARG:NE	2.53	0.41
2:B:161:GLU:HG2	2:E:3984:ARG:HH22	1.85	0.41
2:B:2908:TYR:OH	2:B:2920:ARG:NE	2.48	0.41
2:B:4177:TYR:CE1	2:B:4199:GLU:HB3	2.55	0.41
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	2.01	0.41
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.02	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.85	0.41
2:I:914:PRO:O	2:I:918:ARG:N	2.49	0.41
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	2.02	0.41
2:E:914:PRO:O	2:E:918:ARG:N	2.49	0.41
2:E:1770:SER:OG	2:E:1772:ARG:NE	2.53	0.41
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	2.03	0.41
2:G:4547:GLN:O	2:G:4551:PHE:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.93	0.41
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.01	0.41
2:B:788:LYS:HG2	2:B:1629:GLN:HA	2.01	0.41
2:B:1936:LYS:O	2:B:1940:CYS:N	2.47	0.41
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.85	0.41
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	2.02	0.41
2:E:195:PHE:HB3	2:E:196:MET:HG2	2.02	0.41
2:E:4826:ILE:O	2:E:4829:SER:OG	2.29	0.41
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	2.03	0.41
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	2.02	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.01	0.41
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	2.02	0.41
2:G:2208:MET:SD	2:G:2253:HIS:ND1	2.85	0.41
2:G:4177:TYR:CE1	2:G:4199:GLU:HB3	2.55	0.41
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	2.03	0.41
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.93	0.41
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.01	0.41
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.02	0.41
2:B:4897:ILE:HG12	2:B:4901:ILE:HD13	2.02	0.41
2:E:745:SER:N	2:E:758:ARG:O	2.43	0.41
2:E:2034:PHE:O	2:E:2038:LEU:N	2.54	0.41
2:E:4027:LEU:HA	2:E:4030:LEU:HD12	2.02	0.41
2:G:2758:PHE:O	2:G:2762:THR:N	2.52	0.41
2:B:2208:MET:HE2	2:B:2208:MET:HB3	1.97	0.41
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.02	0.41
2:E:1973:GLN:O	2:E:1977:TYR:N	2.54	0.41
2:E:2742:THR:OG1	2:E:2811:GLU:OE1	2.36	0.41
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.01	0.41
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	2.03	0.41
2:I:347:PHE:HE1	2:I:386:ASP:HB2	1.86	0.41
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.01	0.41
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	2.02	0.41
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.02	0.41
2:E:2810:LYS:HE2	2:E:2814:LYS:HE3	2.03	0.41
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.41
1:F:7:ILE:HB	1:F:71:ARG:HB3	2.01	0.41
1:H:71:ARG:HH22	2:G:679:ALA:HB2	1.86	0.41
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.78	0.41
2:B:2874:MET:O	2:B:2878:LEU:N	2.44	0.41
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.02	0.41
2:I:2908:TYR:OH	2:I:2920:ARG:NE	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4897:ILE:HG12	2:I:4901:ILE:HD13	2.02	0.41
2:E:70:GLU:HG3	2:E:117:TYR:HE1	1.86	0.41
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.94	0.41
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	2.02	0.41
2:E:4133:GLN:HE22	2:E:4137:ARG:HG3	1.86	0.41
2:E:4177:TYR:CE1	2:E:4199:GLU:HB3	2.55	0.41
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.02	0.41
2:G:1973:GLN:O	2:G:1977:TYR:N	2.54	0.41
2:G:4027:LEU:HA	2:G:4030:LEU:HD12	2.02	0.41
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	2.02	0.41
2:G:4897:ILE:HG12	2:G:4901:ILE:HD13	2.02	0.41
2:B:195:PHE:HB3	2:B:196:MET:HG2	2.02	0.41
2:B:4133:GLN:HE22	2:B:4137:ARG:HG3	1.86	0.41
2:I:70:GLU:HG3	2:I:117:TYR:HE1	1.86	0.41
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.02	0.41
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.42	0.41
2:I:4133:GLN:HE22	2:I:4137:ARG:HG3	1.86	0.41
2:B:70:GLU:HG3	2:B:117:TYR:HE1	1.86	0.40
2:B:206:CYS:SG	2:B:207:SER:N	2.94	0.40
2:B:615:ARG:NH2	2:B:1677:GLY:O	2.52	0.40
2:B:1639:LEU:N	2:B:1648:MET:O	2.54	0.40
2:B:4227:GLU:OE2	2:E:4973:HIS:ND1	2.55	0.40
2:I:206:CYS:SG	2:I:207:SER:N	2.94	0.40
2:I:4843:LEU:HA	2:I:4846:VAL:HG12	2.03	0.40
2:E:206:CYS:SG	2:E:207:SER:N	2.94	0.40
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	2.04	0.40
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.02	0.40
2:G:4053:SER:HA	2:G:4056:GLU:HB2	2.03	0.40
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.04	0.40
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	2.04	0.40
2:E:776:LEU:HG	2:E:848:HIS:HA	2.02	0.40
2:G:684:VAL:HA	2:G:781:VAL:HA	2.03	0.40
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.40
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.93	0.40
2:B:38:ALA:HB1	2:B:64:ILE:HG13	2.04	0.40
2:B:347:PHE:HE1	2:B:386:ASP:HB2	1.86	0.40
2:B:583:ILE:H	2:B:583:ILE:HG13	1.69	0.40
2:B:870:ILE:HD11	2:B:1049:TYR:CG	2.57	0.40
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	2.03	0.40
2:I:1739:THR:H	2:I:1742:THR:HB	1.87	0.40
2:I:2034:PHE:O	2:I:2038:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.57	0.40
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.57	0.40
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.50	0.40
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.39	0.40
2:E:4843:LEU:HA	2:E:4846:VAL:HG12	2.03	0.40
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.57	0.40
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.04	0.40
2:B:684:VAL:HA	2:B:781:VAL:HA	2.03	0.40
2:B:776:LEU:HG	2:B:848:HIS:HA	2.02	0.40
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.39	0.40
2:B:4547:GLN:O	2:B:4551:PHE:N	2.49	0.40
2:I:243:ARG:NH1	2:I:301:VAL:O	2.44	0.40
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	2.03	0.40
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.02	0.40
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	2.04	0.40
2:E:347:PHE:HE1	2:E:386:ASP:HB2	1.86	0.40
2:E:684:VAL:HA	2:E:781:VAL:HA	2.03	0.40
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	2.03	0.40
2:E:4982:GLU:HB3	2:E:4983:HIS:H	1.77	0.40
2:G:38:ALA:HB1	2:G:64:ILE:HG13	2.04	0.40
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.36	0.40
2:B:320:LYS:NZ	2:B:381:GLU:O	2.36	0.40
2:B:485:SER:O	2:B:489:ASN:N	2.43	0.40
2:B:4885:PHE:HE2	2:B:4901:ILE:HD11	1.87	0.40
2:I:38:ALA:HB1	2:I:64:ILE:HG13	2.04	0.40
2:I:1171:SER:OG	2:I:1175:SER:N	2.45	0.40
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.39	0.40
2:I:1973:GLN:O	2:I:1977:TYR:N	2.54	0.40
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.53	0.40
2:G:320:LYS:NZ	2:G:381:GLU:O	2.36	0.40
2:G:1189:LEU:HD12	2:G:1190:PRO:HD2	2.04	0.40
2:G:3722:TYR:CZ	2:G:3782:MET:HE3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	F	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	H	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	J	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
2	B	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	48	83
2	E	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	48	83
2	G	3235/4416 (73%)	2887 (89%)	344 (11%)	4 (0%)	48	83
2	I	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	48	83
All	All	13360/18096 (74%)	11919 (89%)	1425 (11%)	16 (0%)	49	83

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	I	1932	PRO
2	E	1932	PRO
2	G	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	I	1840	PRO
2	I	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	G	1840	PRO
2	G	4641	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2483 (100%)	10 (0%)	84	82
2	E	2493/3022 (82%)	2482 (100%)	11 (0%)	84	82
2	G	2493/3022 (82%)	2482 (100%)	11 (0%)	84	82
2	I	2493/3022 (82%)	2482 (100%)	11 (0%)	84	82
All	All	10324/12444 (83%)	10281 (100%)	43 (0%)	81	82

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	1600	LEU
2	B	1676	LEU
2	B	2010	LEU
2	B	3663	LEU
2	B	3805	LEU
2	B	4792	LEU
2	B	4978	HIS
2	B	4983	HIS
2	B	4995	LEU
2	I	131	LEU
2	I	719	LEU
2	I	1600	LEU
2	I	1676	LEU
2	I	2010	LEU
2	I	3663	LEU
2	I	3805	LEU
2	I	4792	LEU
2	I	4978	HIS
2	I	4983	HIS
2	I	4995	LEU
2	E	131	LEU
2	E	719	LEU
2	E	1600	LEU

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Mol	Chain	Res	Type
2	E	1676	LEU
2	E	2010	LEU
2	E	3663	LEU
2	E	3805	LEU
2	E	4792	LEU
2	E	4978	HIS
2	E	4983	HIS
2	E	4995	LEU
2	G	131	LEU
2	G	719	LEU
2	G	1600	LEU
2	G	1676	LEU
2	G	2010	LEU
2	G	3663	LEU
2	G	3805	LEU
2	G	4792	LEU
2	G	4978	HIS
2	G	4983	HIS
2	G	4995	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (220) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	32	ASN
1	F	87	HIS
1	A	32	ASN
1	A	87	HIS
1	H	32	ASN
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	113	HIS
2	B	151	HIS
2	B	201	ASN
2	B	273	HIS
2	B	379	HIS
2	B	399	GLN
2	B	412	ASN
2	B	413	GLN
2	B	461	HIS
2	B	479	GLN
2	B	582	HIS

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Mol	Chain	Res	Type
2	B	593	HIS
2	B	797	HIS
2	B	838	HIS
2	B	866	HIS
2	B	949	ASN
2	B	1220	GLN
2	B	1598	GLN
2	B	1678	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	1949	GLN
2	B	1953	HIS
2	B	1972	ASN
2	B	1973	GLN
2	B	2127	GLN
2	B	2260	ASN
2	B	2773	ASN
2	B	3700	GLN
2	B	3767	GLN
2	B	3781	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3963	ASN
2	B	3976	ASN
2	B	3994	HIS
2	B	4005	GLN
2	B	4034	ASN
2	B	4054	ASN
2	B	4102	GLN
2	B	4109	GLN
2	B	4130	ASN
2	B	4133	GLN
2	B	4142	ASN
2	B	4700	GLN

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Mol	Chain	Res	Type
2	B	4776	GLN
2	B	4947	GLN
2	I	57	ASN
2	I	113	HIS
2	I	151	HIS
2	I	201	ASN
2	I	273	HIS
2	I	379	HIS
2	I	412	ASN
2	I	413	GLN
2	I	461	HIS
2	I	479	GLN
2	I	593	HIS
2	I	797	HIS
2	I	866	HIS
2	I	949	ASN
2	I	1220	GLN
2	I	1598	GLN
2	I	1678	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1949	GLN
2	I	1953	HIS
2	I	1973	GLN
2	I	2127	GLN
2	I	2260	ASN
2	I	3700	GLN
2	I	3767	GLN
2	I	3781	GLN
2	I	3809	ASN
2	I	3814	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3963	ASN

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Mol	Chain	Res	Type
2	I	3976	ASN
2	I	3994	HIS
2	I	4005	GLN
2	I	4034	ASN
2	I	4037	ASN
2	I	4054	ASN
2	I	4102	GLN
2	I	4130	ASN
2	I	4133	GLN
2	I	4142	ASN
2	I	4691	GLN
2	I	4776	GLN
2	I	4947	GLN
2	E	57	ASN
2	E	113	HIS
2	E	151	HIS
2	E	201	ASN
2	E	273	HIS
2	E	379	HIS
2	E	412	ASN
2	E	413	GLN
2	E	461	HIS
2	E	479	GLN
2	E	582	HIS
2	E	593	HIS
2	E	797	HIS
2	E	838	HIS
2	E	866	HIS
2	E	949	ASN
2	E	1220	GLN
2	E	1598	GLN
2	E	1678	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	1949	GLN
2	E	1953	HIS
2	E	1972	ASN
2	E	2260	ASN

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Mol	Chain	Res	Type
2	E	2881	ASN
2	E	3700	GLN
2	E	3767	GLN
2	E	3781	GLN
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3963	ASN
2	E	3976	ASN
2	E	3994	HIS
2	E	4005	GLN
2	E	4034	ASN
2	E	4037	ASN
2	E	4054	ASN
2	E	4102	GLN
2	E	4109	GLN
2	E	4130	ASN
2	E	4133	GLN
2	E	4142	ASN
2	E	4947	GLN
2	G	57	ASN
2	G	113	HIS
2	G	151	HIS
2	G	201	ASN
2	G	273	HIS
2	G	379	HIS
2	G	412	ASN
2	G	413	GLN
2	G	461	HIS
2	G	582	HIS
2	G	593	HIS
2	G	797	HIS
2	G	866	HIS
2	G	949	ASN
2	G	1220	GLN
2	G	1598	GLN
2	G	1678	ASN
2	G	1688	HIS
2	G	1691	GLN

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Mol	Chain	Res	Type
2	G	1693	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	1949	GLN
2	G	1953	HIS
2	G	1972	ASN
2	G	1973	GLN
2	G	2260	ASN
2	G	2773	ASN
2	G	2856	ASN
2	G	2881	ASN
2	G	3700	GLN
2	G	3767	GLN
2	G	3781	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	3976	ASN
2	G	4005	GLN
2	G	4034	ASN
2	G	4037	ASN
2	G	4054	ASN
2	G	4102	GLN
2	G	4109	GLN
2	G	4130	ASN
2	G	4133	GLN
2	G	4142	ASN
2	G	4947	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	I	14
2	E	14
2	G	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.36
1	I	4345:UNK	C	4540:PHE	N	73.36
1	E	4345:UNK	C	4540:PHE	N	73.36
1	G	4345:UNK	C	4540:PHE	N	73.36
1	B	3613:UNK	C	3639:THR	N	46.46
1	I	3613:UNK	C	3639:THR	N	46.46
1	E	3613:UNK	C	3639:THR	N	46.46
1	G	3613:UNK	C	3639:THR	N	46.46
1	B	4253:GLU	C	4320:UNK	N	27.46

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4253:GLU	C	4320:UNK	N	27.46
1	E	4253:GLU	C	4320:UNK	N	27.46
1	G	4253:GLU	C	4320:UNK	N	27.46
1	B	3163:UNK	C	3170:UNK	N	15.87
1	I	3163:UNK	C	3170:UNK	N	15.87
1	E	3163:UNK	C	3170:UNK	N	15.87
1	G	3163:UNK	C	3170:UNK	N	15.87
1	B	3063:UNK	C	3134:UNK	N	14.92
1	I	3063:UNK	C	3134:UNK	N	14.92
1	E	3063:UNK	C	3134:UNK	N	14.92
1	G	3063:UNK	C	3134:UNK	N	14.92
1	B	3468:UNK	C	3511:UNK	N	14.79
1	I	3468:UNK	C	3511:UNK	N	14.79
1	E	3468:UNK	C	3511:UNK	N	14.79
1	G	3468:UNK	C	3511:UNK	N	14.79
1	B	2703:UNK	C	2734:ASN	N	13.42
1	I	2703:UNK	C	2734:ASN	N	13.42
1	E	2703:UNK	C	2734:ASN	N	13.42
1	G	2703:UNK	C	2734:ASN	N	13.42
1	B	3236:UNK	C	3241:UNK	N	13.13
1	I	3236:UNK	C	3241:UNK	N	13.13
1	E	3236:UNK	C	3241:UNK	N	13.13
1	G	3236:UNK	C	3241:UNK	N	13.13
1	B	1564:UNK	C	1573:MET	N	12.39
1	I	1564:UNK	C	1573:MET	N	12.39
1	E	1564:UNK	C	1573:MET	N	12.39
1	G	1564:UNK	C	1573:MET	N	12.39
1	B	2976:UNK	C	2995:UNK	N	12.28
1	I	2976:UNK	C	2995:UNK	N	12.28
1	E	2976:UNK	C	2995:UNK	N	12.28
1	G	2976:UNK	C	2995:UNK	N	12.28
1	B	3254:UNK	C	3261:UNK	N	8.43
1	I	3254:UNK	C	3261:UNK	N	8.43
1	E	3254:UNK	C	3261:UNK	N	8.43
1	G	3254:UNK	C	3261:UNK	N	8.43
1	B	1297:UNK	C	1430:UNK	N	6.02
1	I	1297:UNK	C	1430:UNK	N	6.02
1	E	1297:UNK	C	1430:UNK	N	6.02
1	G	1297:UNK	C	1430:UNK	N	6.02
1	B	2939:ARG	C	2942:UNK	N	3.58
1	I	2939:ARG	C	2942:UNK	N	3.58
1	E	2939:ARG	C	2942:UNK	N	3.58

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2939:ARG	C	2942:UNK	N	3.58
1	B	2479:LEU	C	2487:UNK	N	3.25
1	I	2479:LEU	C	2487:UNK	N	3.25
1	E	2479:LEU	C	2487:UNK	N	3.25
1	G	2479:LEU	C	2487:UNK	N	3.25

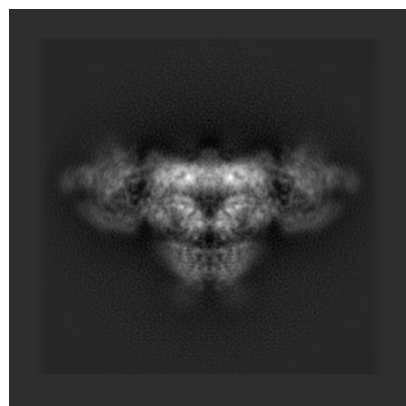
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8392. These allow visual inspection of the internal detail of the map and identification of artifacts.

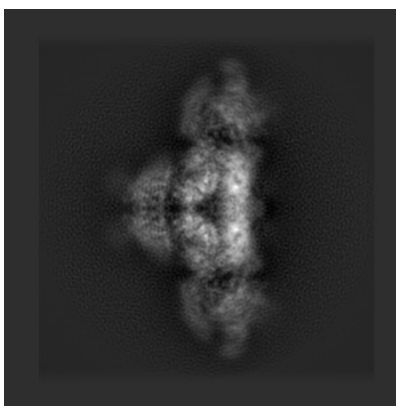
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

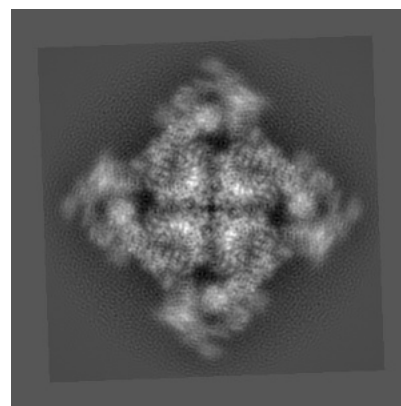
6.1.1 Primary map



X

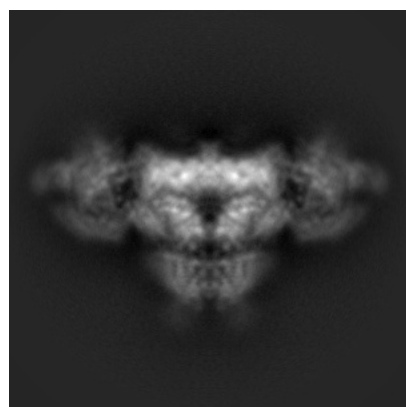


Y

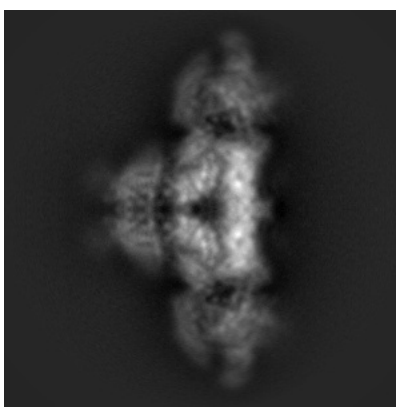


Z

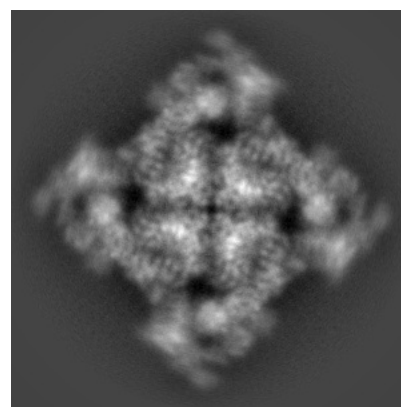
6.1.2 Raw map



X



Y

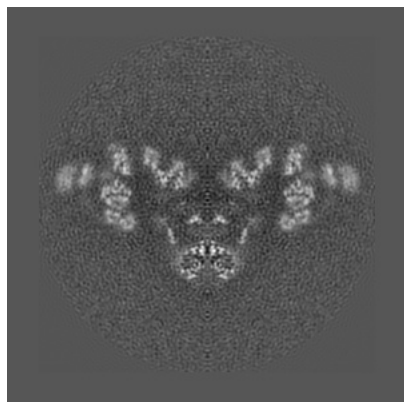


Z

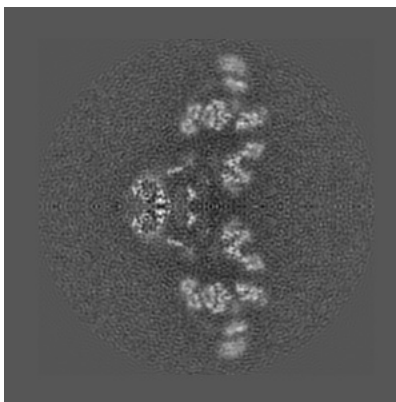
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

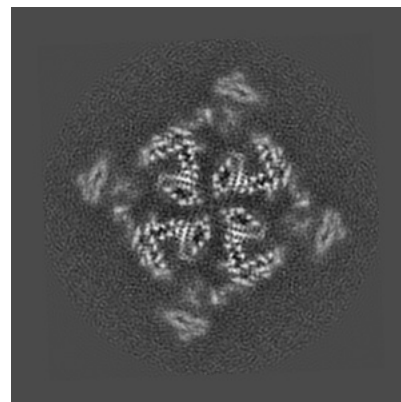
6.2.1 Primary map



X Index: 200

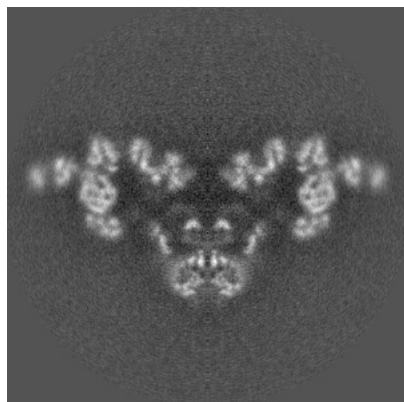


Y Index: 200

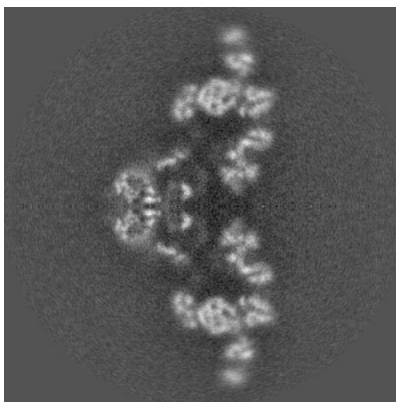


Z Index: 200

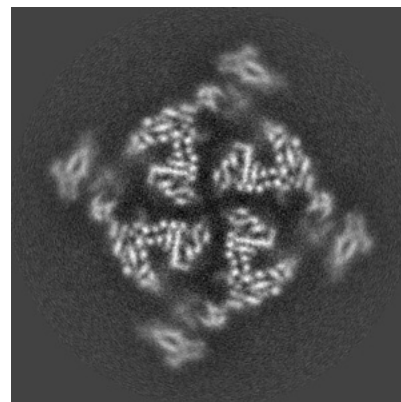
6.2.2 Raw map



X Index: 168



Y Index: 168

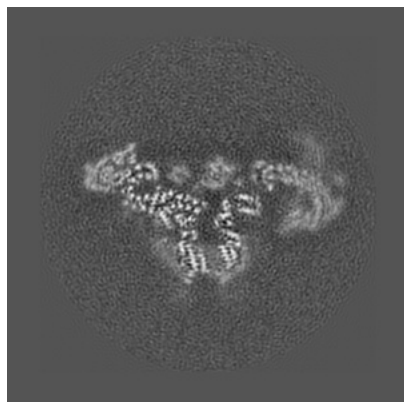


Z Index: 168

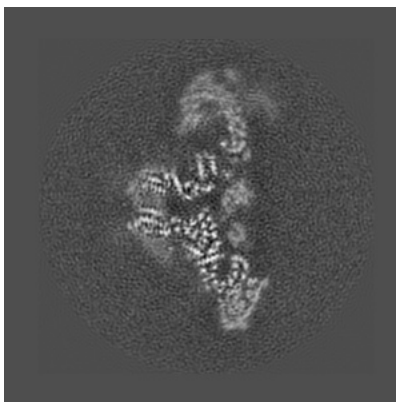
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

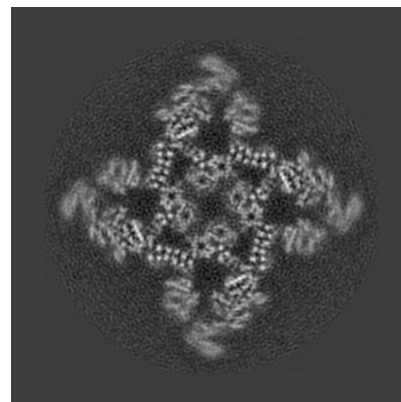
6.3.1 Primary map



X Index: 224

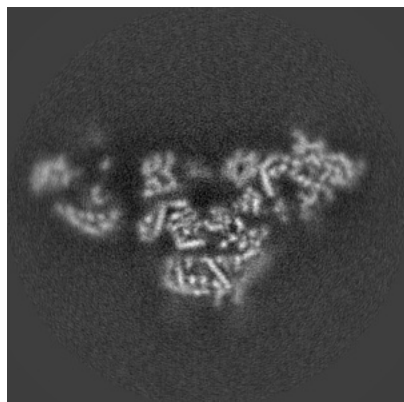


Y Index: 177

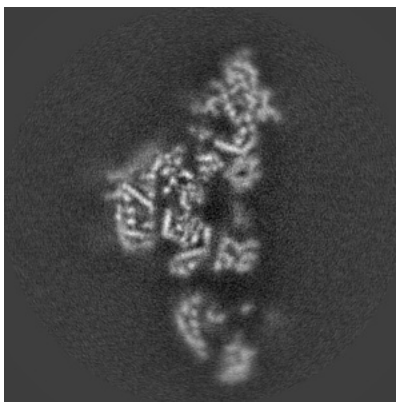


Z Index: 227

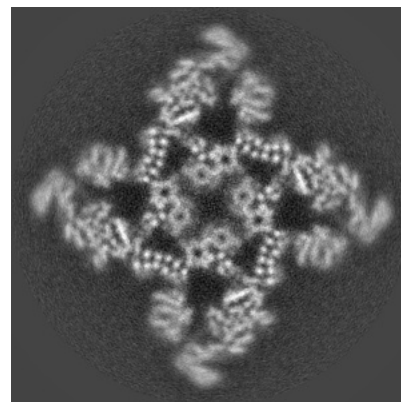
6.3.2 Raw map



X Index: 154



Y Index: 182

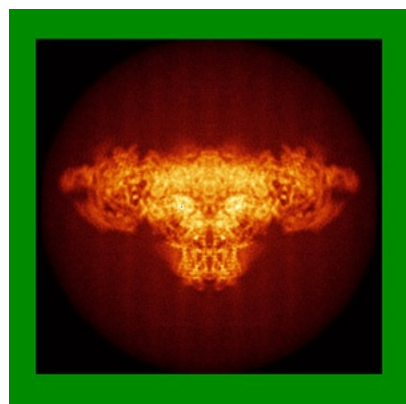


Z Index: 192

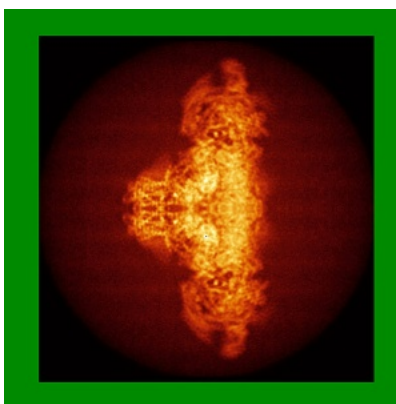
The images above show the largest variance slices of the map in three orthogonal directions.

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

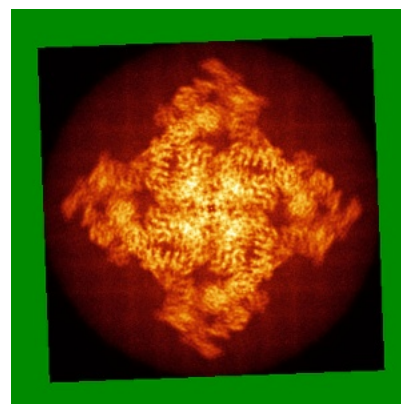
6.4.1 Primary map



X

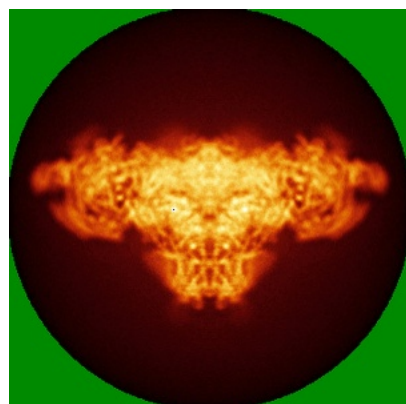


Y

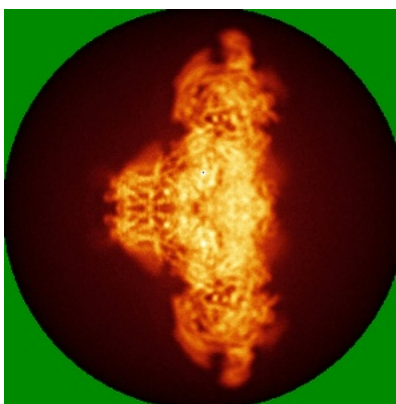


Z

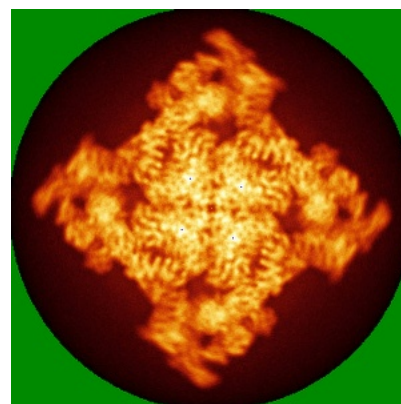
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

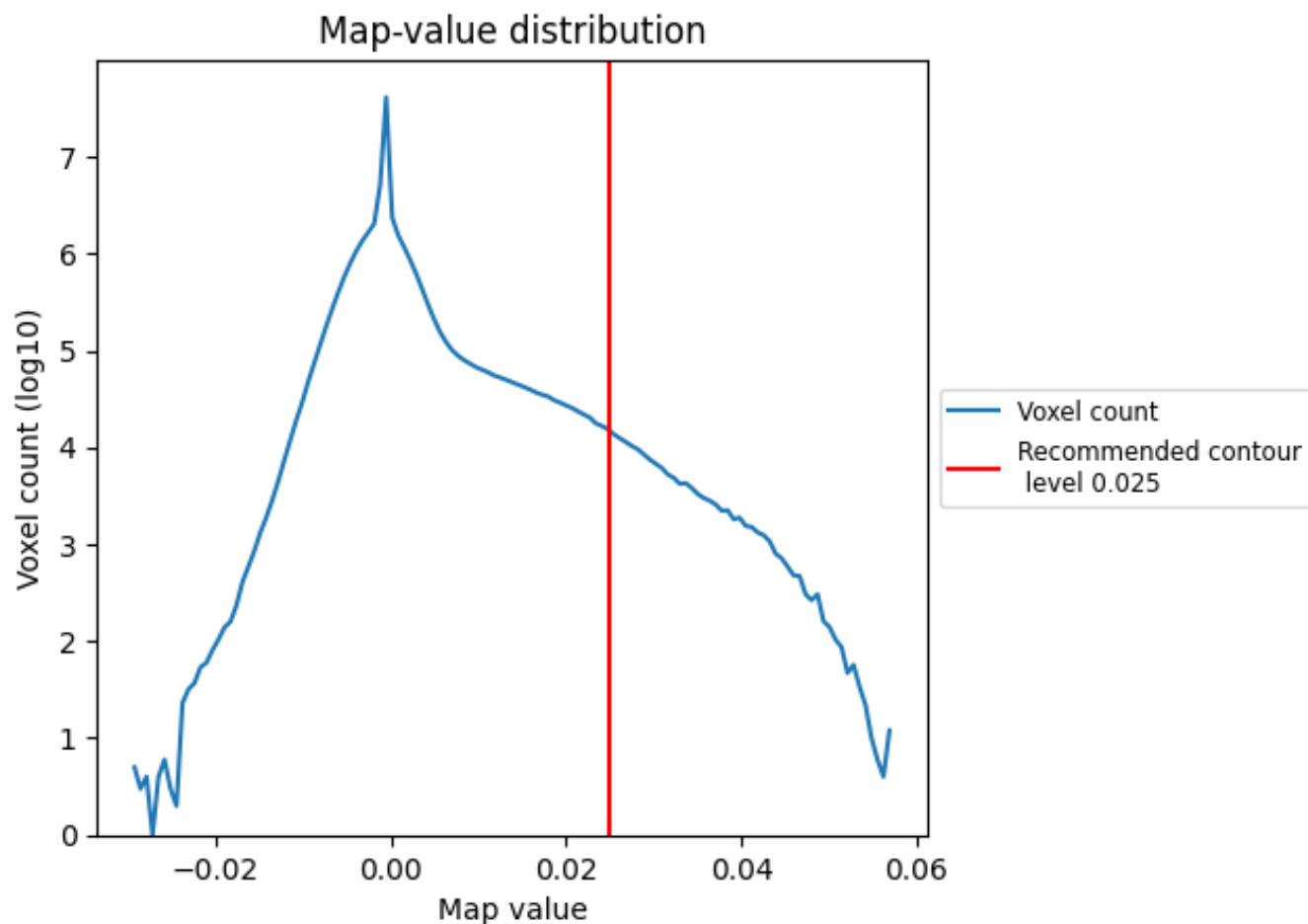
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

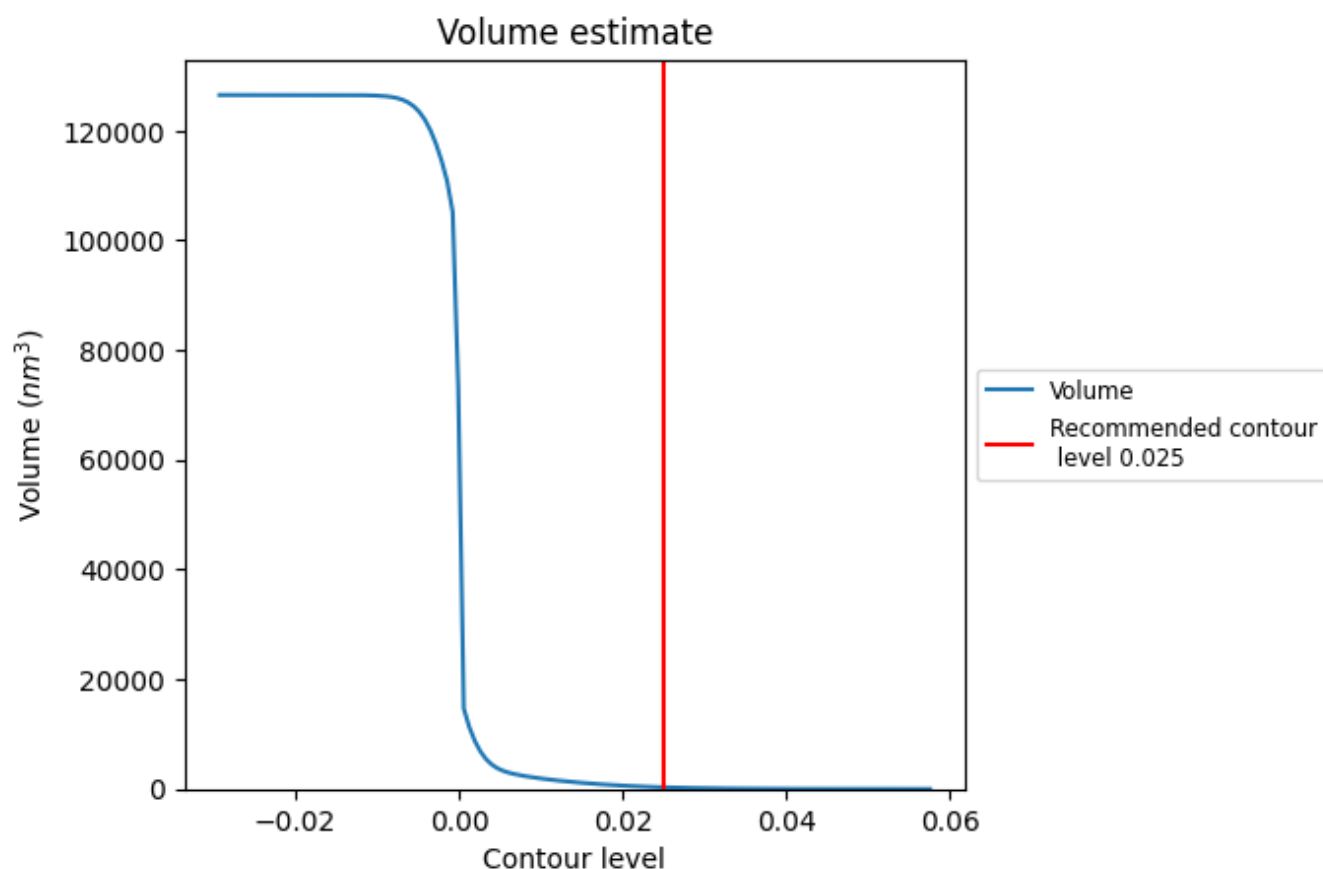
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

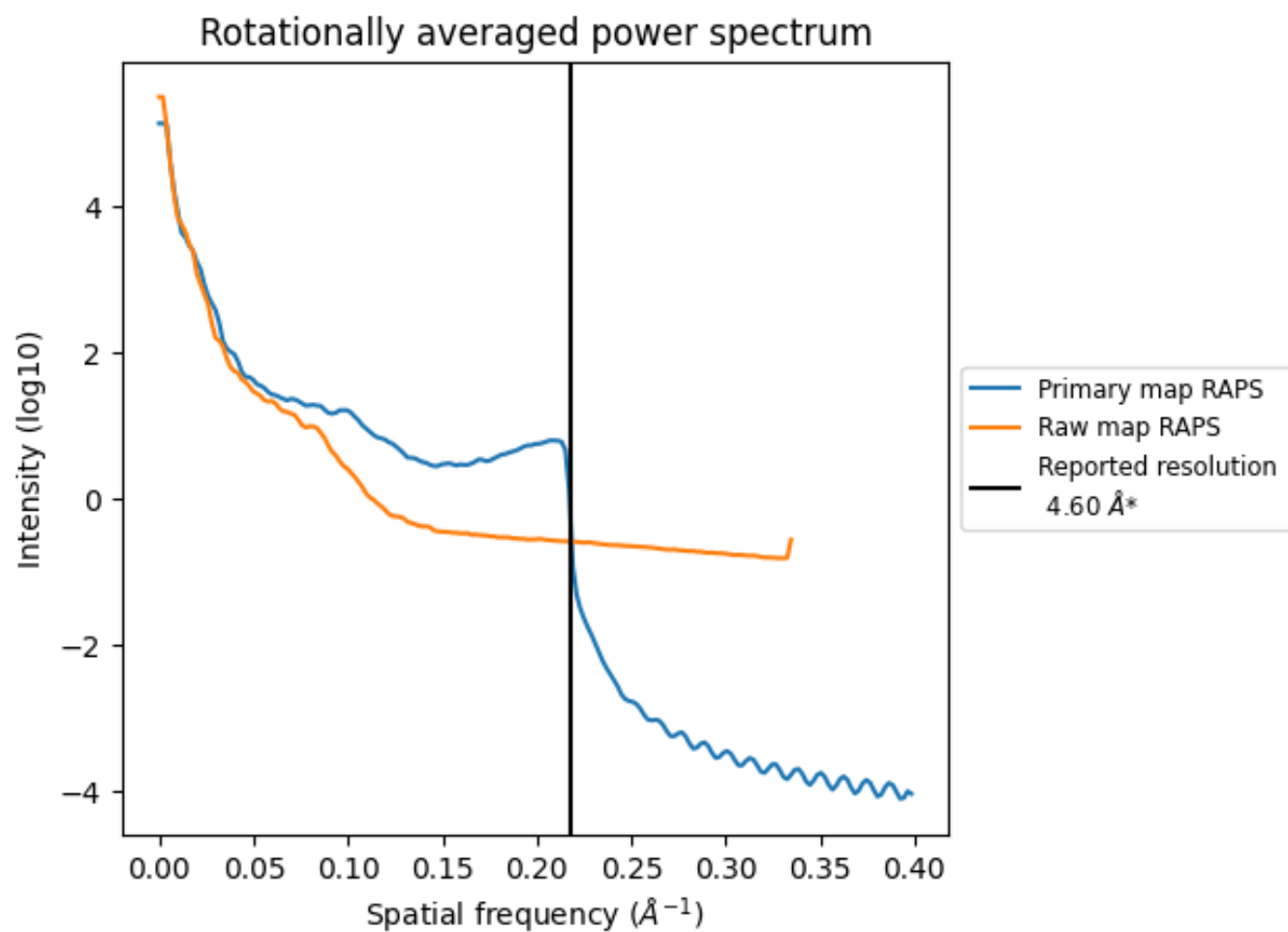
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 298 nm^3 ; this corresponds to an approximate mass of 269 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 ⓘ

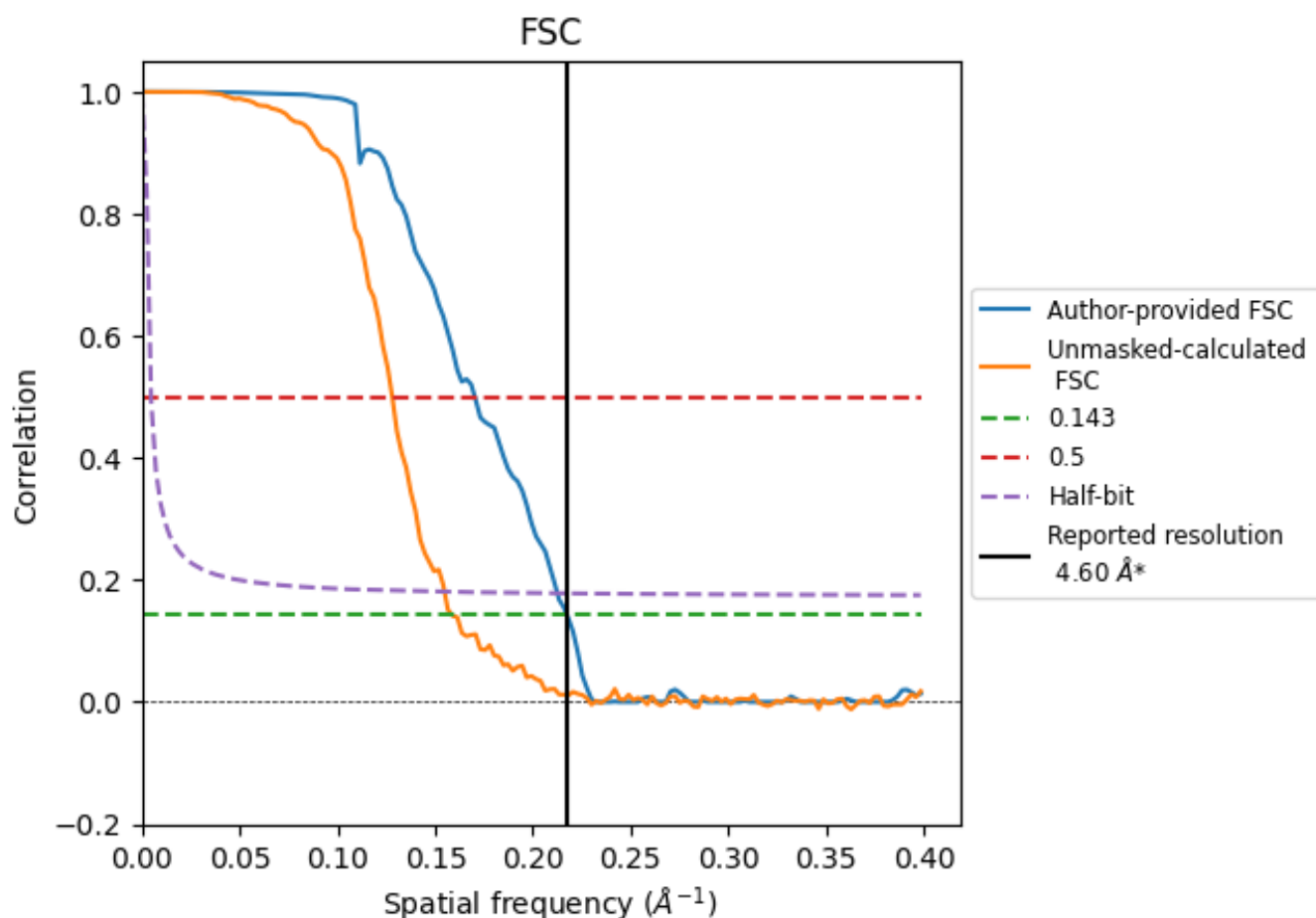


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

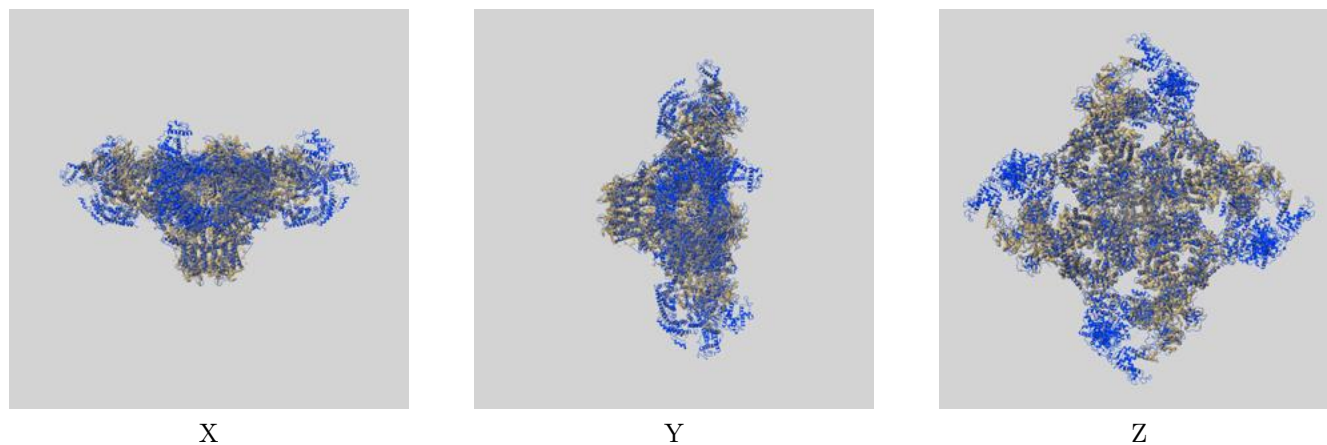
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.60	5.87	4.71
Unmasked-calculated*	6.31	7.81	6.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.31 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

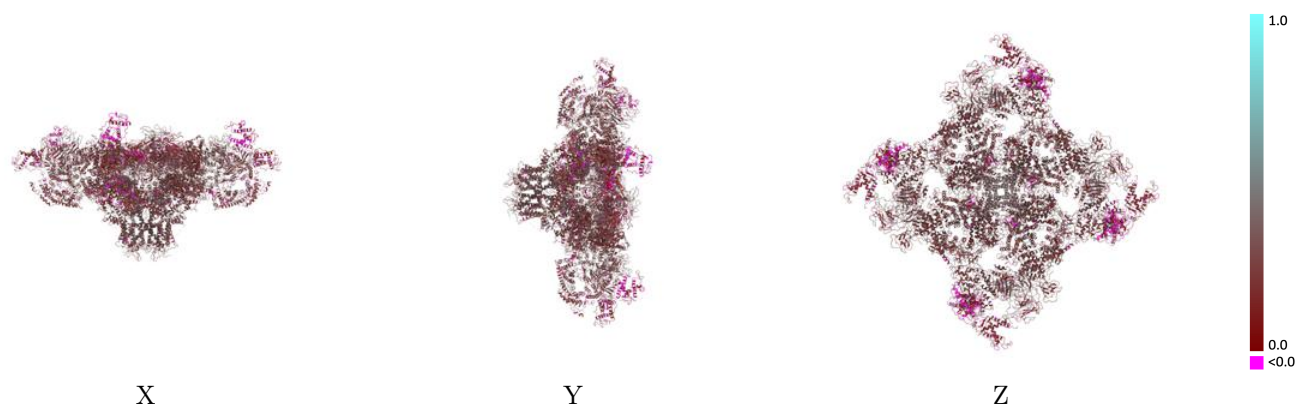
This section contains information regarding the fit between EMDB map EMD-8392 and PDB model 5TB1. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



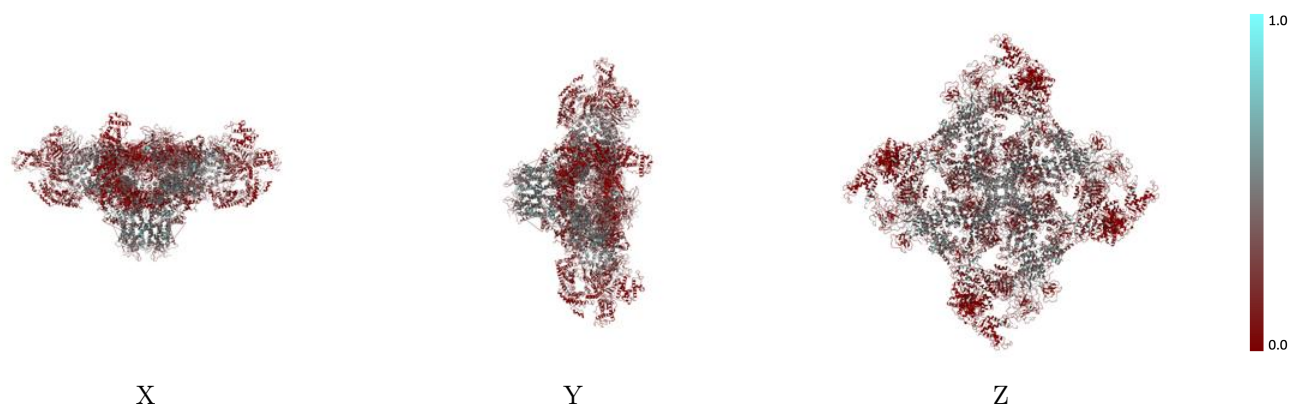
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



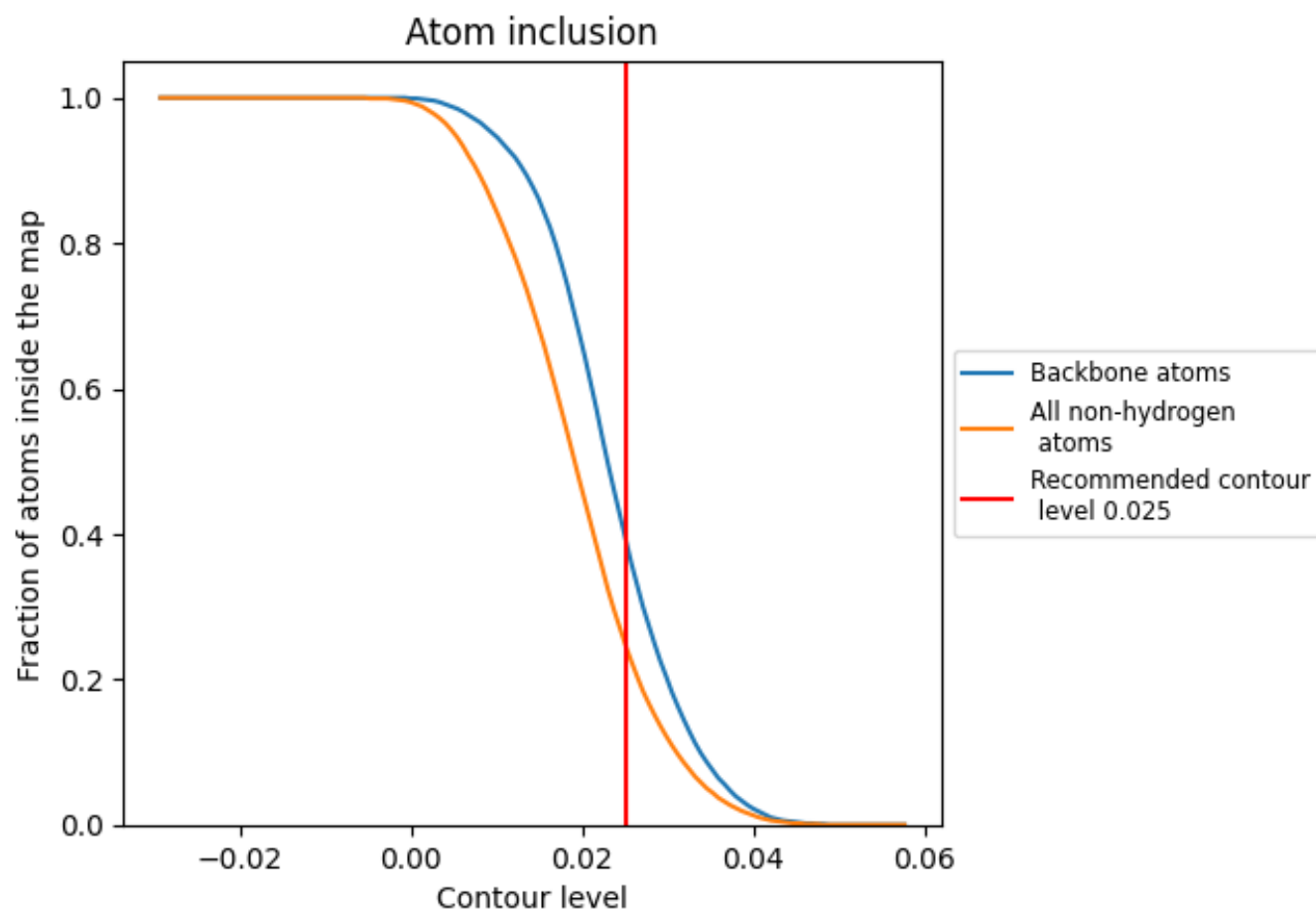
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 25% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2490	0.2600
A	0.1890	0.2650
B	0.2510	0.2600
E	0.2510	0.2600
F	0.1840	0.2700
G	0.2510	0.2600
H	0.1890	0.2670
I	0.2510	0.2590
J	0.1890	0.2640

