



Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 04:14 AM EDT

PDB ID : 5TAN
EMDB ID : EMD-8380
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.30 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

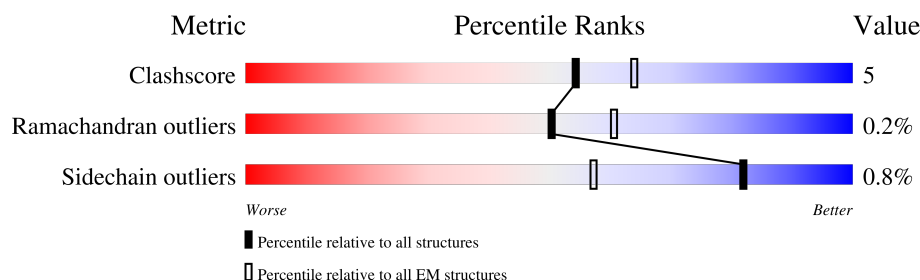
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>58%</div> <div>81%19%.</div> </div>
1	F	108	<div> <div>59%</div> <div>81%19%.</div> </div>
1	H	108	<div> <div>60%</div> <div>81%19%.</div> </div>
1	J	108	<div> <div>58%</div> <div>81%19%.</div> </div>
2	B	4416	<div> <div>46%</div> <div>84%11%5%</div> </div>
2	E	4416	<div> <div>46%</div> <div>83%11%5%</div> </div>
2	G	4416	<div> <div>46%</div> <div>83%11%5%</div> </div>
2	I	4416	<div> <div>46%</div> <div>84%11%5%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 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.

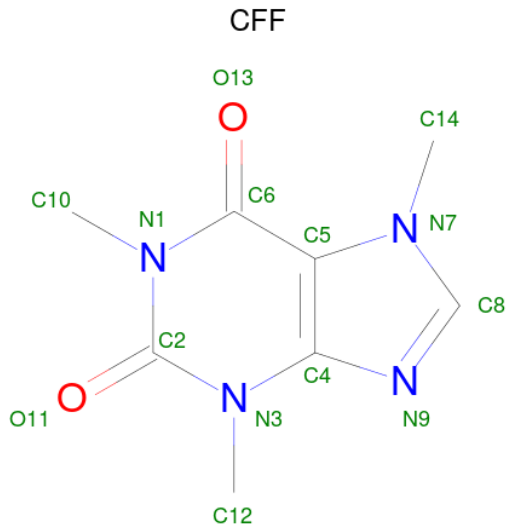
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

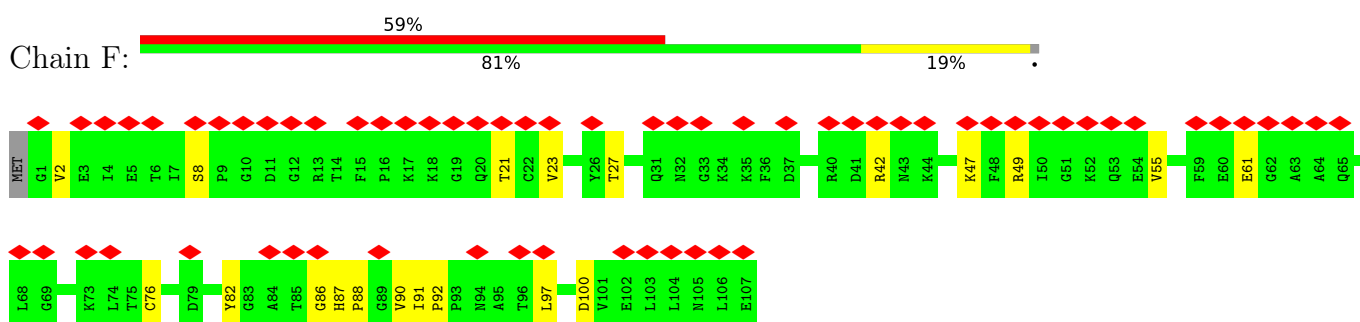
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

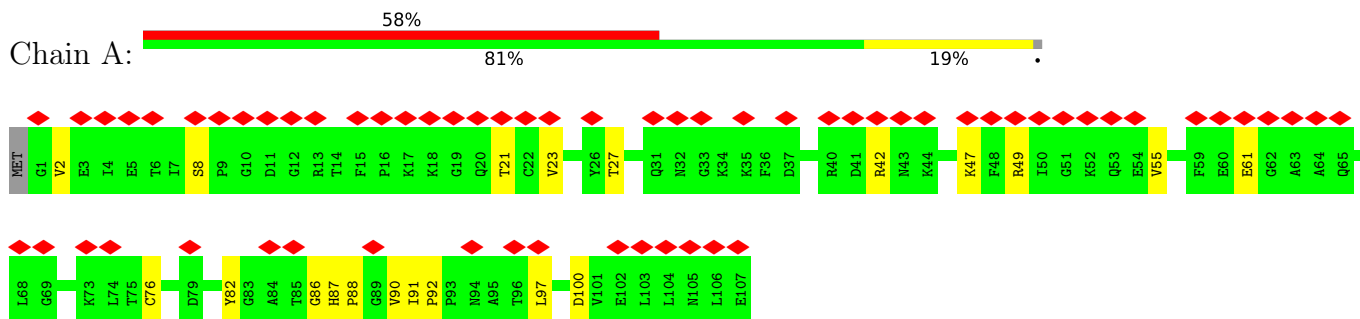
3 Residue-property plots [i](#)

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.

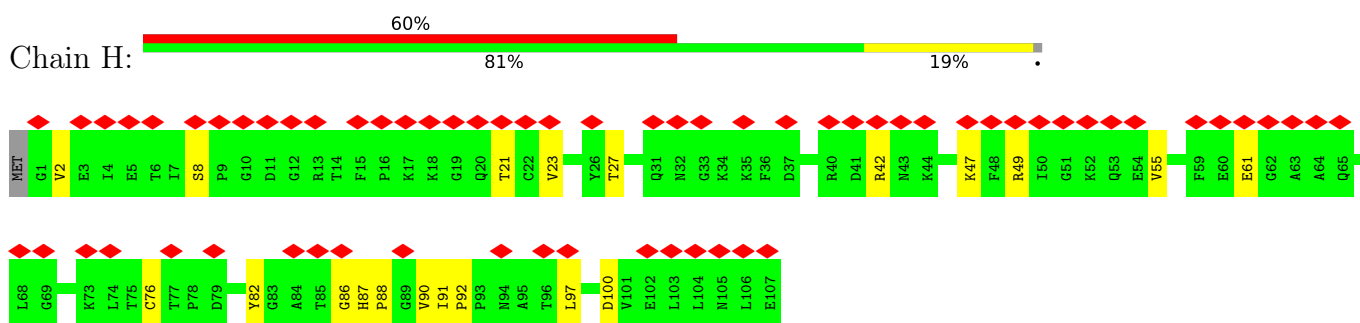
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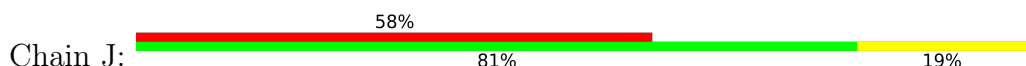
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

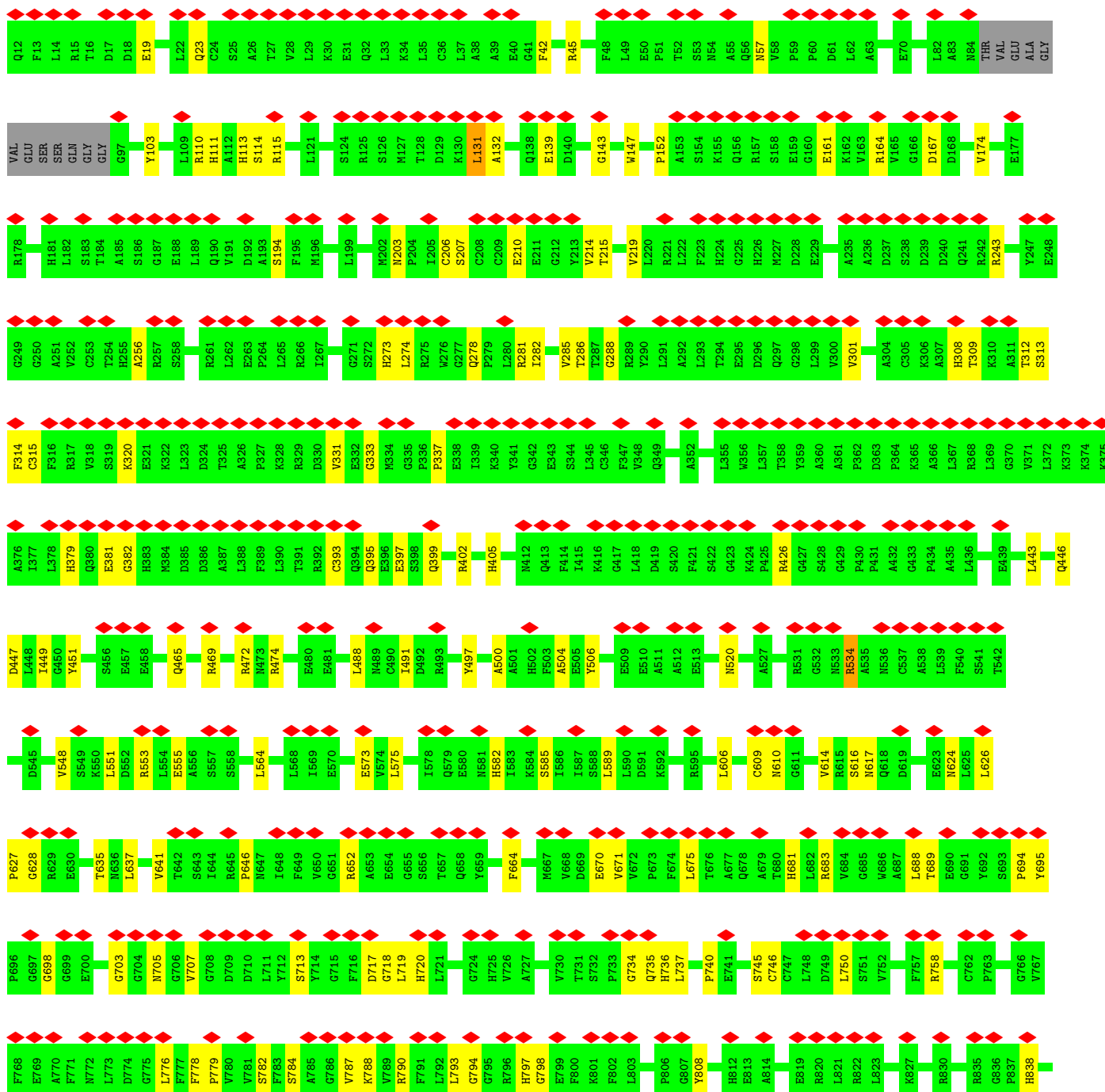


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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

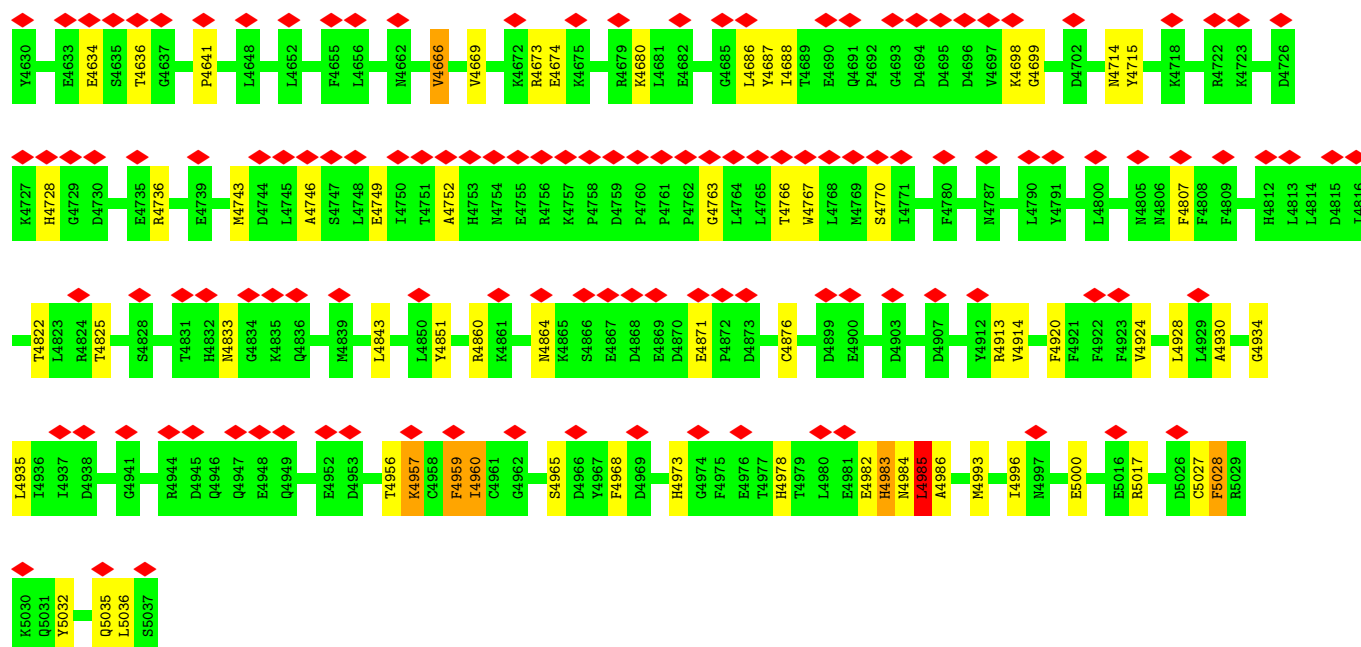




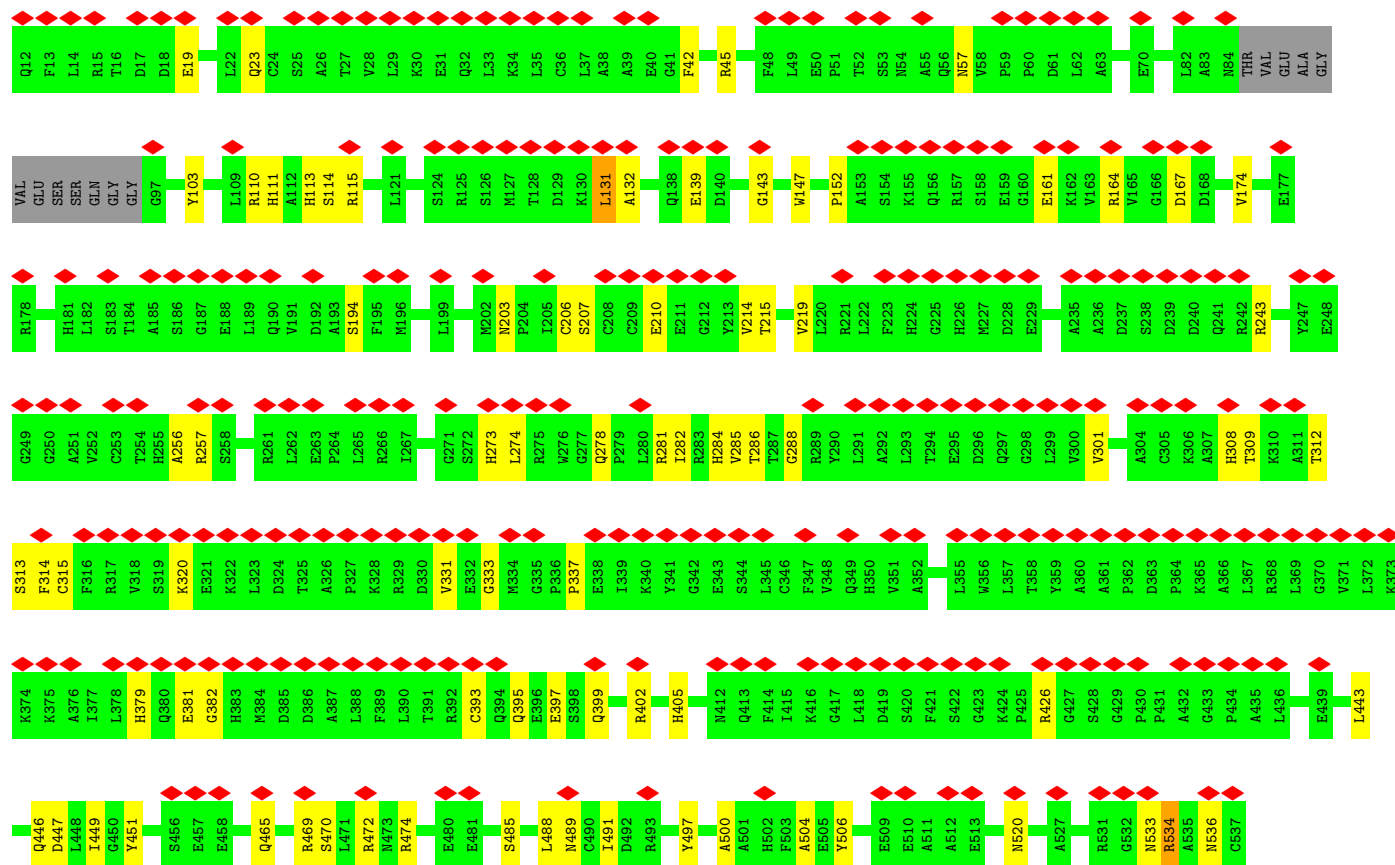
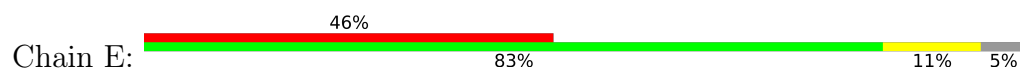
F1961	G1961	K901	M961	S1034	E1099	A1178	R1271	X1537	E1644	S1732	I1802	GLU	F1961
A1962	P842	R902	S962	N1035	M1100	F1179	L1272	X1543	E1644	E1733	E1805	GLU	A1962
E1963	S843	L903	N963	N1036	R1101	R1180	A1273	X1544	N1645	Y1734	A1806	GLU	E1963
R1964	R844	H904	G964	D1037	V1102	E1181	H1274	X1545	E1655	I1735	R1808	GLU	R1964
Y1965	C845	P905	K966	S1038	W1104	T1184	R1275	X1546	R1656	P1740	R1808	GLU	Y1965
K1968	L846	L906	K966	L1039	A1105	G1186	X1276	X1547	L1657	E1741	R1813	ASP	K1968
L1969	S847	L907	P967	C1040	P1107	D1186	X1277	X1548	L1658	T1742	M1814	GLU	L1969
Q1970	H848	V908	A968	Q1041	G1187	F1187	X1278	X1549	D1658	R1743	L1815	GLU	Q1970
A1971	T849	N909	P969	A1042	E1108	F1188	X1279	X1549	H1663	A1744	G1816	LYS	A1971
N1972	D850	F910	L970	V1043	L1109	L1189	X1280	X1550	S1664	I1745	E1817	GLU	N1972
Q1973	F851	H911	D971	R1044	P1111	V1199	X1281	M1573	H1665	F1748	Q1973	ASP	Q1973
R1974	S852	S912	L972	T1045	D1112	G1200	X1282	P1574	T1666	P1749	R1974	ASP	R1974
S1975	P853	L913	S973	L1046	L1115	H1201	X1283	L1575	R1668	P1750	D1821	GLU	S1975
R1976	C854	P914	H974	L1047	L1115	G1202	X1284	S1576	L1669	G1751	L1822	GLU	R1976
Y1977	P855	E915	V975	G1048	D1118	N1203	X1291	M1579	Y1670	R1752	Q1824	GLU	Y1977
A1978	V856	P916	R976	Y1049	E1119	L1204	X1430	F1580	L1671	K1753	H1825	LYS	A1978
L1979	D857	E917	L977	G1050	L1120	G1206	X1441	E1583	L1676	G1754	A1826	GLU	L1979
L1980	THR	R918	T978	Y1051	V1123	D1207	X1442	F1589	N1679	H1755	R1827	ASP	L1980
M1981	GLN	N919	P979	N1052	F1124	Q1210	X1447	Q1590	R1680	H1756	D1828	ALA	M1981
R1982	I861	Y920	A980	I1053	R1126	L1211	X1466	P1589	L1685	A1757	G1831	LYS	R1982
A1983	V862	N921	Q981	E1054	G1129	R1212	X1466	Q1590	L1685	R1758	Q1837	GLU	A1983
F1984	L863	Q923	T982	PRO	Q1130	F1213	X1467	P1593	H1688	H1759	F1838	GLU	F1984
T1985	P864	M924	T983	ASP	R1131	F1214	X1467	R1594	V1689	H1760	V1839	GLU	T1985
T1986	P865	S925	V985	GLU	L1134	F1215	X1468	L1595	D1690	G1761	P1840	ALA	T1986
S1987	H866	R926	D986	PRO	L1135	I1216	X1475	L1600	Q1691	P1763	V1845	GLU	S1987
A1988	L867	E927	R987	GLN	S1136	C1217	X1476	L1600	L1694	G1764	L1848	GLY	A1988
A1989	R868	R927	R988	VAL	G1136	G1218	X1477	W1605	L1695	V1765	L1848	GLU	A1989
E1990	R869	T928	L988	GLU	S1136	L1219	X1478	S1606	H1696	G1766	L1848	LYS	E1990
T1991	I870	L929	A989	ASN	F1139	Q1220	X1480	R1607	A1697	T1768	I1853	ASP	T1991
A1992	R871	K930	A997	GLN	R1141	E1221	X1481	H1611	A1701	L1771	D1856	GLU	A1992
R1993	K873	T931	R998	GLN	S1145	F1223	X1486	Q1614	H1702	A1772	V1859	GLU	R1993
R1994	L874	L932	D999	TRP	G1140	F1222	X1486	V1615	H1702	P1773	K1860	LYS	R1994
T1995	A875	L933	Q1003	D1070	R1071	E1223	X1504	GLU	R1708	H1775	Q1862	GLU	T1995
R1996	E876	L935	A1009	R1072	V1073	Q1231	X1505	THR	A1709	G1776	Q1864	GLU	R1996
E1997	I877	G936	VAL	R1076	R1073	R1232	X1505	ARG	G1710	P1777	M1865	GLU	E1997
F1998	H879	C937	GLN	A1077	E1078	E1251	X1516	ALA	Y1711	F1782	V1870	GLU	F1998
R1999	E880	H938	ILE	A1077	E1078	H1254	X1517	E1622	D1713	V1783	F1871	GLU	R1999
S2000	L881	V939	PRO	A1077	E1078	Y1255	X1518	R1623	H1718	A1784	T1872	GLU	S2000
P2001	W882	G940	ALA	Y1081	L1155	E1256	X1519	E1627	H1719	A1785	L1873	GLU	P2001
Q2003	A883	M941	ARG	Y1081	L1156	E1256	X1520	V1628	L1720	L1786	E1874	GLU	Q2003
E2004	L884	A942	ASN	S1080	E1157	E1256	X1521	Q1629	E1721	P1787	GLU	E2004	
Q2006	T885	D943	PRO	S1085	M1158	R1259	X1522	C1630	R1725	A1788	GLU	Q2006	
N2007	R886	E944	R1020	G1086	I1161	M1260	X1523	Q1631	S1726	ALA	GLU	N2007	
W2008	I887	K945	L1021	F1087	F1162	M1260	X1524	D1632	R1727	GLY	GLU	W2008	
L2009	E888	A946	V1022	Y1088	T1163	D1261	X1525	P1633	H1728	VAL	GLU	L2009	
L2010	Q889	E947	R1025	L1026	D1172	G1262	X1526	L1634	S1729	ALA	GLU	L2010	
H2011	G890	D948	L1026	L1027	G1173	T1263	X1527	L1634	Y1731	E1793	GLU	H2011	
F2012	W891	N949	L1027	D1028	S1174	V1264	X1528	M1637	L1731	A1794	GLU	F2012	
K2013	T892	K951	K952	A1029	S1175	D1266	X1529	L1639		P1795	GLU	K2013	
D2014	Y893	K952	K953	A1030	E1176	T1266	X1530			A1796	GLU	D2014	
E2015	G894	T953	K954	T1031	F1177	C1269	X1531			R1797	GLU	E2015	
A2016	P895	L955	L956	K1032		L1270				L1798	GLU	A2016	
D2017	R897	T958	P956	K1033								GLU	D2017
E2018	D898	K957	T958										E2018
A2019	D899	Y959	M960										A2019
D2020	N900												D2020
C2021													C2021

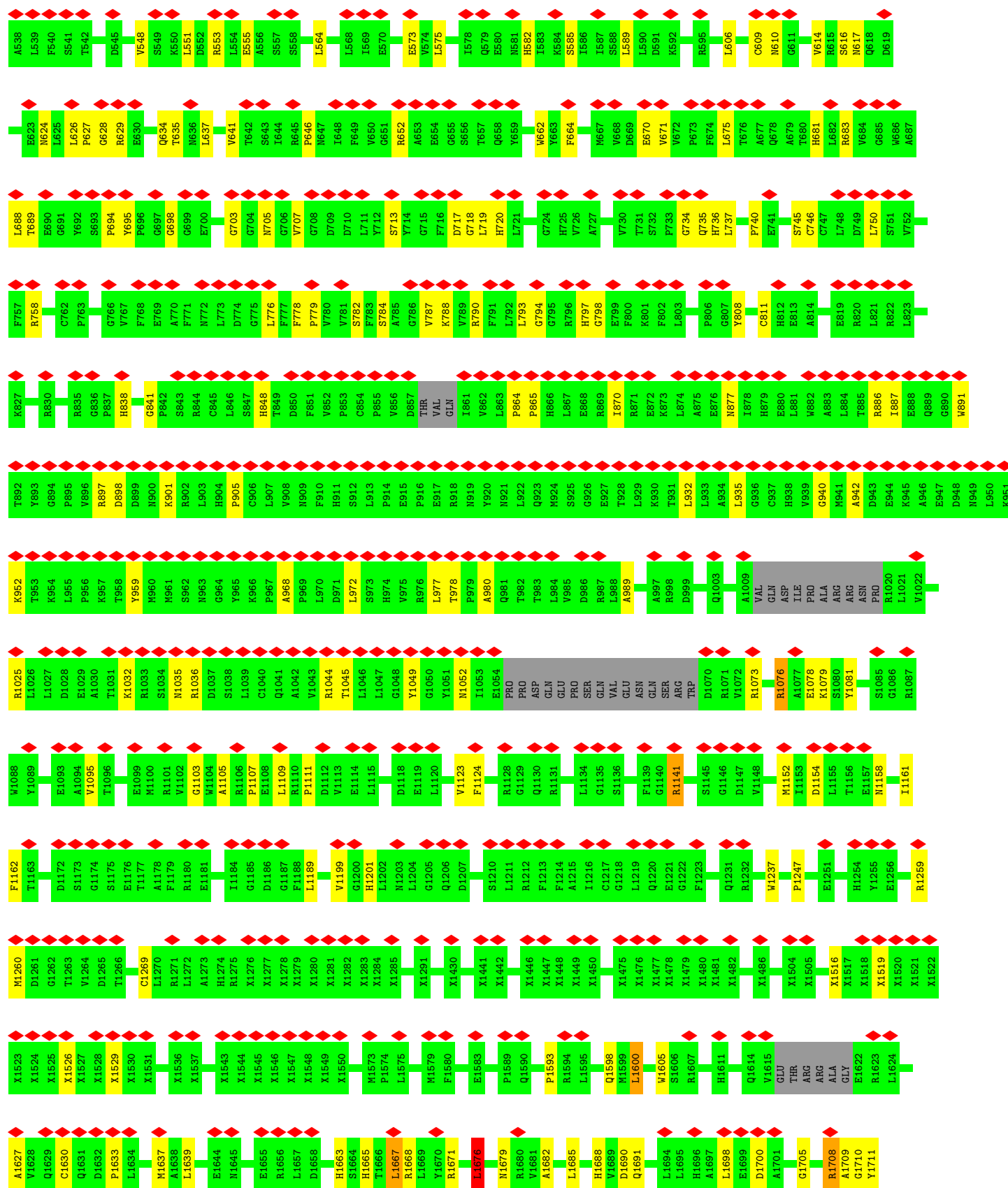






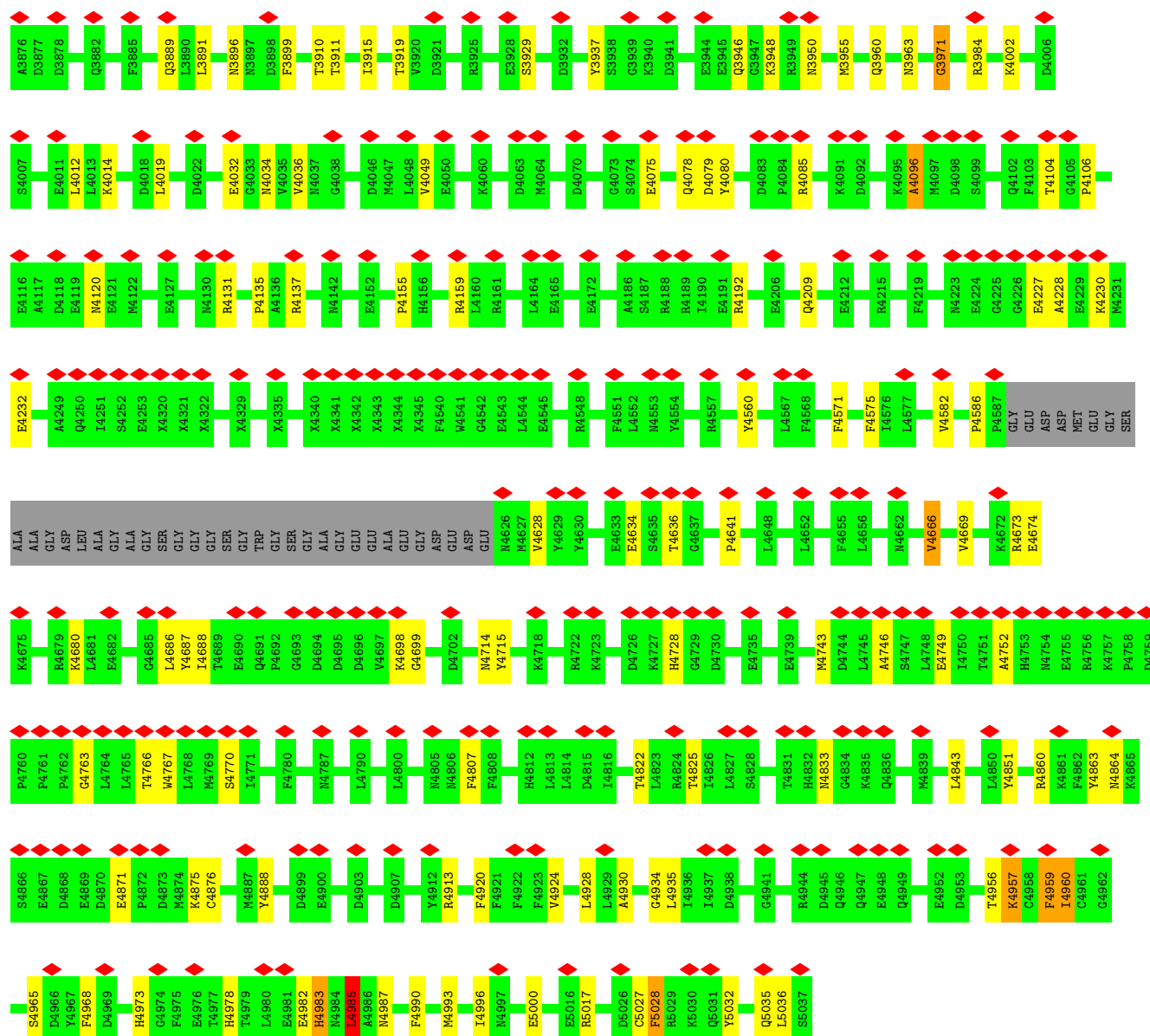
• Molecule 2: Ryanodine receptor 1



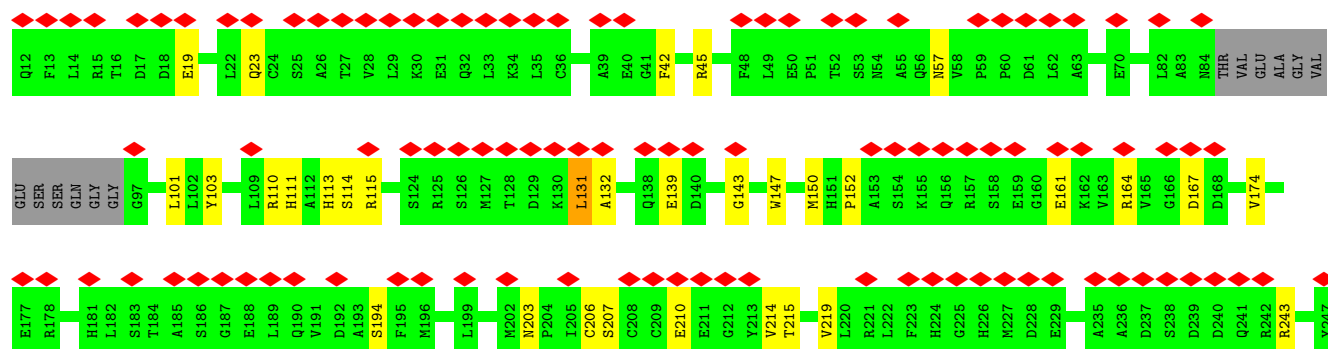
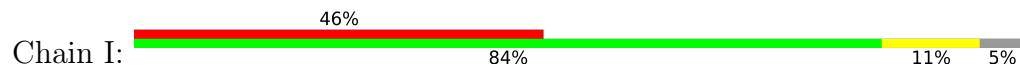




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X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593			
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X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3323	X3324	X3325	X3326	X3327	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344			
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X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3142	X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3151	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3182	X3183	X3186	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3201	X3204	X3205						
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ASP	PRU	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	Q2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909



• Molecule 2: Ryanodine receptor 1






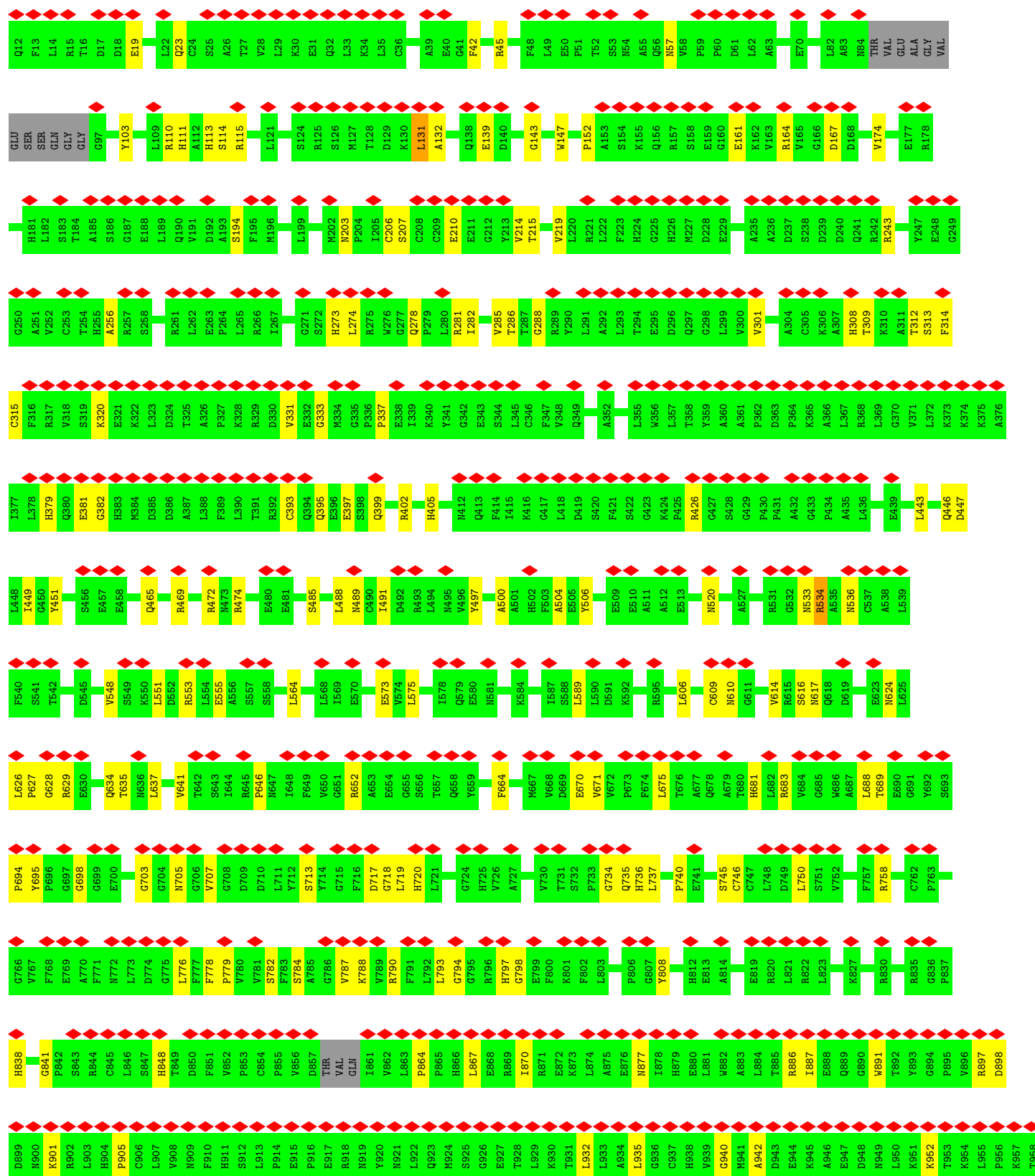
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					L4544	E4152	E4032	F3885	K3787	E3691	X3607
					E4545	E4152	E4032	F3885	K3787	E3691	X3608
					R4546	E4152	E4032	F3885	K3787	E3691	X3609
						E4172	E4032	F3885	K3787	E3691	X3610
							E4032	F3885	K3787	E3691	X3611
							E4032	F3885	K3787	E3691	X3612
							E4032	F3885	K3787	E3691	X3613
							E4032	F3885	K3787	E3691	X3614
							E4032	F3885	K3787	E3691	X3615
							E4032	F3885	K3787	E3691	X3616
							E4032	F3885	K3787	E3691	X3617
							E4032	F3885	K3787	E3691	X3618
							E4032	F3885	K3787	E3691	X3619
							E4032	F3885	K3787	E3691	X3620
							E4032	F3885	K3787	E3691	X3621
							E4032	F3885	K3787	E3691	X3622
							E4032	F3885	K3787	E3691	X3623
							E4032	F3885	K3787	E3691	X3624
							E4032	F3885	K3787	E3691	X3625
							E4032	F3885	K3787	E3691	X3626
							E4032	F3885	K3787	E3691	X3627
							E4032	F3885	K3787	E3691	X3628
							E4032	F3885	K3787	E3691	X3629
							E4032	F3885	K3787	E3691	X3630
							E4032	F3885	K3787	E3691	X3631
							E4032	F3885	K3787	E3691	X3632
							E4032	F3885	K3787	E3691	X3633
							E4032	F3885	K3787	E3691	X3634
							E4032	F3885	K3787	E3691	X3635
							E4032	F3885	K3787	E3691	X3636
							E4032	F3885	K3787	E3691	X3637
							E4032	F3885	K3787	E3691	X3638
							E4032	F3885	K3787	E3691	X3639
							E4032	F3885	K3787	E3691	X3640
							E4032	F3885	K3787	E3691	X3641
							E4032	F3885	K3787	E3691	X3642
							E4032	F3885	K3787	E3691	X3643
							E4032	F3885	K3787	E3691	X3644
							E4032	F3885	K3787	E3691	X3645
							E4032	F3885	K3787	E3691	X3646
							E4032	F3885	K3787	E3691	X3647
							E4032	F3885	K3787	E3691	X3648

● Molecule 2: Ryanodine receptor 1

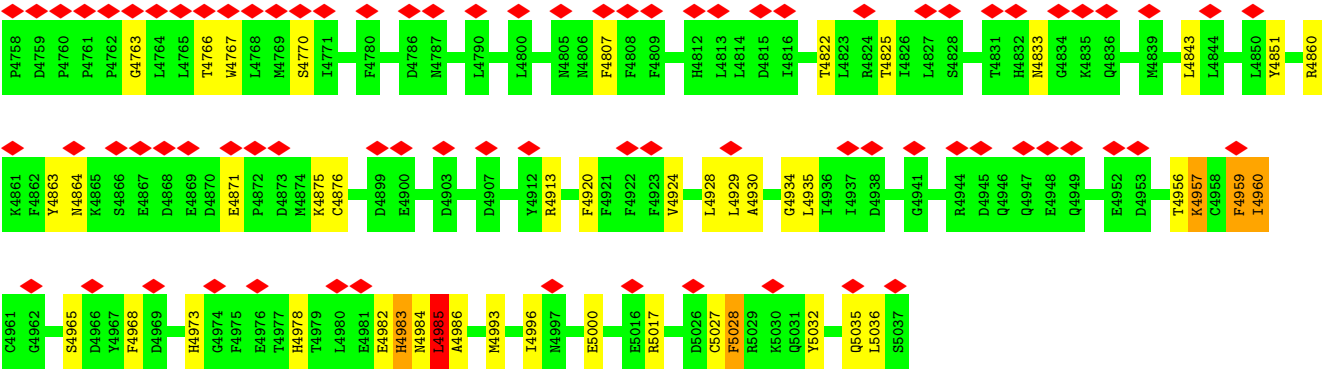
Chain G: 





X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3237	X3238	X3239	X3240	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3255	X3256	X3257	X3258	X3259	X3260	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277																																																																																												
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X3134	X3135	X3136	X3137	X3138	X3143										X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3151	X3152	X3153	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3182										X3183	X3184	X3185	X3186	X3190										X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200										X3201	X3204										X3205	X3206	X3207																																																														
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L2273	D2274	V2275	A2276	A2277	E2285										L2288	A2289	L2290	Q2291	E2292	V2214	D2293	D2294	L2295	E2296	K2297	V2298	V2299	S2300	Y2301	L2302	A2303	G2304	L2307										Q2308	S2309	C2310	M2312	L2313	L2314	A2315	K2316	G2317	Y2318	P2319	D2320	I2321	C2326										G2327	R2330										ARG	L2332	S2333	F2334	L2335	R2336	F2337	F2340										V2341	N2342	G2343	E2344	S2345																																																															
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SER	ALA	ALA	GLY	ASP	LEU	ALA	GLY	ALA	GLY	SER	GLY	GLY	GLY	GLY	TRP	SER	GLY	ALA	GLY	GLY	GLU	GLU	M4626	M4627	V4628	Y4629	Y4630	E4633	E4634	S4635	T4636	Q4637	P4641	L4648	L4652	F4655	L4656	G4660	V4666	V4669	K4672	R4673	GLY	GLY	ASP	ASP	GLY	GLY								
E4227	A4228	E4229	K4230	M4231	E4232	A4249	Q4250	I4251	S4252	E4253	A4320	X4321	X4322	X4329	X4340	X4341	X4342	X4343	X4344	X4345	F4540	W4541	G4542	E4543	L4544	E4545	R4548	F4551	L4552	S4187	R4188	R4189	I4190	E4191	R4192	E4196	E4206	Q4209	E4212	R4215	F4219	M4223	E4224	G4225	G4226											
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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	0.070	Depositor
Minimum map value	-0.034	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: ATP, ZN, CA, CFF

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	0.32	0/834	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.31	0/25428	0.55	8/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	32/142628 (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
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	76

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.10	133.92	115.30
2	B	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	E	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	G	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	I	4985	LEU	CA-CB-CG	6.89	131.16	115.30
2	B	1600	LEU	CA-CB-CG	6.89	131.15	115.30
2	G	1600	LEU	CA-CB-CG	6.88	131.14	115.30
2	E	1600	LEU	CA-CB-CG	6.88	131.12	115.30
2	G	4985	LEU	CA-CB-CG	6.88	131.12	115.30
2	B	4985	LEU	CA-CB-CG	6.88	131.11	115.30
2	I	1600	LEU	CA-CB-CG	6.87	131.11	115.30
2	E	4985	LEU	CA-CB-CG	6.86	131.08	115.30
2	B	1676	LEU	CA-CB-CG	6.77	130.87	115.30
2	I	1676	LEU	CA-CB-CG	6.77	130.87	115.30
2	E	1676	LEU	CA-CB-CG	6.76	130.85	115.30
2	G	1676	LEU	CA-CB-CG	6.76	130.85	115.30
2	G	977	LEU	CA-CB-CG	6.08	129.29	115.30
2	E	977	LEU	CA-CB-CG	6.07	129.27	115.30
2	B	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	I	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	E	2290	LEU	CA-CB-CG	5.73	128.48	115.30
2	G	2290	LEU	CA-CB-CG	5.72	128.47	115.30
2	B	2290	LEU	CA-CB-CG	5.72	128.46	115.30
2	I	2290	LEU	CA-CB-CG	5.71	128.44	115.30
2	I	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	B	688	LEU	CA-CB-CG	5.40	127.71	115.30
2	E	688	LEU	CA-CB-CG	5.39	127.69	115.30
2	G	688	LEU	CA-CB-CG	5.38	127.68	115.30
2	B	1667	LEU	CA-CB-CG	5.20	127.25	115.30
2	E	1667	LEU	CA-CB-CG	5.20	127.26	115.30
2	G	1667	LEU	CA-CB-CG	5.20	127.25	115.30
2	I	1667	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide

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Mol	Chain	Res	Type	Group
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	4096	ALA	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	624	ASN	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	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
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4096	ALA	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	624	ASN	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	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

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Mol	Chain	Res	Type	Group
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4096	ALA	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	624	ASN	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	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	4096	ALA	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	624	ASN	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	12	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	12	0
2	B	29499	0	24753	296	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	29499	0	24753	305	0
2	G	29499	0	24753	299	0
2	I	29499	0	24753	295	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102396	1213	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 (1213) 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:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.32	1.18
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.32	1.17
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.32	1.17
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.32	1.16
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.64	1.16
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	1.64	1.15
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	1.64	1.14
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	1.64	1.14
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.67	1.12
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.67	1.11
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.67	1.10
2:G:5028:PHE:HE1	2:G:5032:TYR:CD2	1.67	1.09
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.54	0.94
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	1.81	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	1.81	0.92
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.54	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	1.81	0.92
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.54	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.54	0.91
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.05	0.90
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.05	0.90
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.05	0.90
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.05	0.90
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	1.81	0.89
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.16	0.81
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.16	0.81
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.16	0.80
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.16	0.80
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	1.96	0.78
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	1.96	0.78
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	1.96	0.78
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	1.96	0.78
2:E:4192:ARG:HH11	2:E:5028:PHE:HD2	1.36	0.74
2:B:4192:ARG:HH11	2:B:5028:PHE:HD2	1.36	0.73
2:G:4192:ARG:HH11	2:G:5028:PHE:HD2	1.36	0.73
2:I:4192:ARG:HH11	2:I:5028:PHE:HD2	1.36	0.72
2:B:111:HIS:HD2	2:B:114:SER:H	1.41	0.69
2:G:111:HIS:HD2	2:G:114:SER:H	1.41	0.68
2:E:111:HIS:HD2	2:E:114:SER:H	1.41	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.68
2:E:4957:LYS:NZ	2:E:4957:LYS:HB2	2.08	0.68
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.58	0.68
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.58	0.68
2:G:4957:LYS:HB2	2:G:4957:LYS:NZ	2.08	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.68
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.58	0.68
2:I:111:HIS:HD2	2:I:114:SER:H	1.41	0.68
2:B:4957:LYS:HB2	2:B:4957:LYS:NZ	2.08	0.67
2:E:5028:PHE:HE1	2:E:5032:TYR:HE2	1.39	0.67
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.58	0.67
2:I:4957:LYS:HB2	2:I:4957:LYS:NZ	2.08	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.66
2:E:4230:LYS:HG2	2:E:4959:PHE:HE1	1.60	0.66
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.78	0.66
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.78	0.65
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.15	0.65
2:B:4230:LYS:HG2	2:B:4959:PHE:HE1	1.60	0.65
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.78	0.65
2:I:4230:LYS:HG2	2:I:4959:PHE:HE1	1.60	0.65
2:G:4230:LYS:HD2	2:G:4959:PHE:HD1	1.62	0.65
2:E:161:GLU:HA	2:G:3984:ARG:HH22	1.62	0.64
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.15	0.64
2:I:4230:LYS:CD	2:I:4959:PHE:CE1	2.81	0.64
2:G:4230:LYS:HG2	2:G:4959:PHE:HE1	1.61	0.64
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.31	0.64
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.80	0.64
2:B:3984:ARG:HH22	2:I:161:GLU:HA	1.63	0.64
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.31	0.64
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.78	0.63
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.80	0.63
2:B:4230:LYS:CD	2:B:4959:PHE:CE1	2.81	0.63
2:I:4230:LYS:HD2	2:I:4959:PHE:HD1	1.62	0.63
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.15	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.63
2:E:4230:LYS:CD	2:E:4959:PHE:CE1	2.81	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.63
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.80	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.63
2:G:4230:LYS:CD	2:G:4959:PHE:CE1	2.81	0.63
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.15	0.62
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.32	0.62
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.32	0.62
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.33	0.62
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.31	0.62
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.31	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.32	0.62
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.32	0.62
2:B:331:VAL:HG12	2:B:333:GLY:H	1.65	0.62
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.81	0.62
2:B:4228:ALA:HB2	2:E:4973:HIS:HE1	1.64	0.62
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.81	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.61
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.81	0.61
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.65	0.61
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.81	0.61
2:E:331:VAL:HG12	2:E:333:GLY:H	1.65	0.61
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.33	0.61
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.81	0.61
2:I:331:VAL:HG12	2:I:333:GLY:H	1.65	0.61
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.33	0.61
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.80	0.61
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.83	0.61
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.61
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.33	0.61
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.61
2:E:4230:LYS:CG	2:E:4959:PHE:CE1	2.82	0.61
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.83	0.61
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.61
2:B:5028:PHE:HE1	2:B:5032:TYR:HE2	1.39	0.61
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.61
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.83	0.61
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.81	0.61
2:G:5028:PHE:HE1	2:G:5032:TYR:HE2	1.39	0.61
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.34	0.61
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.33	0.61
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.83	0.60
2:G:4230:LYS:CG	2:G:4959:PHE:CE1	2.83	0.60
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.34	0.60
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.33	0.60
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.84	0.60
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.60
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.66	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.65	0.60
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.81	0.60
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.66	0.60
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.84	0.60
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.90	0.60
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.84	0.60
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.84	0.60
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.84	0.60
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.84	0.60
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.84	0.60
2:I:5028:PHE:HE1	2:I:5032:TYR:HE2	1.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.84	0.60
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.84	0.60
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.60
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.66	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.84	0.59
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.84	0.59
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.84	0.59
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.36	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.59
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.84	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.59
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.90	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.85	0.59
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.90	0.59
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.84	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.66	0.59
2:B:4230:LYS:HD2	2:B:4959:PHE:HD1	1.62	0.59
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.84	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.66	0.59
2:B:4973:HIS:HE1	2:I:4228:ALA:HB2	1.67	0.59
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.85	0.59
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.58
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.37	0.58
2:E:4228:ALA:HB2	2:G:4973:HIS:HE1	1.68	0.58
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.37	0.58
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.85	0.58
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.35	0.58
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.90	0.58
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.84	0.58
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.36	0.58
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.37	0.58
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.37	0.58
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.86	0.58
2:B:4230:LYS:CG	2:B:4959:PHE:CE1	2.83	0.58
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.85	0.58
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.58
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.37	0.58
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.86	0.58
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.85	0.58
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.36	0.58
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.85	0.58
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.58
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.36	0.58
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.77	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.57
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.37	0.57
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.87	0.57
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.86	0.57
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.86	0.57
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.77	0.57
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.86	0.57
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.87	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.57
2:I:4973:HIS:HE1	2:G:4228:ALA:HB2	1.68	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.68	0.57
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.86	0.57
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.73	0.57
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.87	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.70	0.57
2:I:4230:LYS:CG	2:I:4959:PHE:CE1	2.82	0.57
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.77	0.57
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.73	0.57
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.70	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.56
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.87	0.56
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.87	0.56
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.87	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.70	0.56
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.87	0.56
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.87	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.68	0.56
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.87	0.56
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.87	0.56
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.39	0.56
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.87	0.56
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.87	0.56
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.86	0.56
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.70	0.56
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.39	0.56
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.73	0.56
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.39	0.56
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.36	0.56
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.87	0.56
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.56
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.39	0.56
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.87	0.55
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.89	0.55
2:B:3770:LEU:HD21	2:B:3775:ALA:HB3	1.88	0.55
2:E:4230:LYS:HD2	2:E:4959:PHE:HD1	1.62	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.87	0.55
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.89	0.55
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.70	0.55
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.88	0.55
2:G:626:LEU:HG	2:G:628:GLY:H	1.71	0.55
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.87	0.55
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.86	0.55
2:I:626:LEU:HG	2:I:628:GLY:H	1.72	0.55
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.40	0.55
2:B:626:LEU:HG	2:B:628:GLY:H	1.71	0.55
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.40	0.55
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.87	0.55
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.38	0.55
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.87	0.55
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.88	0.55
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.36	0.55
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.89	0.55
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.40	0.55
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.89	0.55
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.88	0.55
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.40	0.55
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.89	0.55
2:E:626:LEU:HG	2:E:628:GLY:H	1.72	0.55
2:I:3770:LEU:HD21	2:I:3775:ALA:HB3	1.88	0.54
2:G:3770:LEU:HD21	2:G:3775:ALA:HB3	1.88	0.54
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.88	0.54
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.41	0.54
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.90	0.54
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.81	0.54
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.90	0.54
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.40	0.54
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.72	0.54
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.73	0.54
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.40	0.54
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.23	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.41	0.54
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.90	0.54
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.40	0.54
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.73	0.54
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.38	0.54
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.88	0.54
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.72	0.54
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.73	0.54
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.54
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.90	0.54
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.41	0.54
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.89	0.54
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.81	0.54
2:B:309:THR:O	2:B:313:SER:OG	2.26	0.54
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.54
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.90	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:B:4230:LYS:CD	2:B:4959:PHE:HE1	2.20	0.54
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.41	0.54
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.73	0.54
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.41	0.54
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.23	0.54
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.73	0.54
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.41	0.54
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.90	0.54
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.41	0.54
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.54
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.90	0.54
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.89	0.53
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.73	0.53
2:E:309:THR:O	2:E:313:SER:OG	2.26	0.53
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.81	0.53
2:E:3770:LEU:HD21	2:E:3775:ALA:HB3	1.88	0.53
2:E:5028:PHE:CD1	2:E:5032:TYR:CD2	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:309:THR:O	2:G:313:SER:OG	2.26	0.53
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.90	0.53
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.42	0.53
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.91	0.53
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.41	0.53
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.90	0.53
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.53
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.41	0.53
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.90	0.53
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.90	0.53
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.90	0.53
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.91	0.53
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.90	0.53
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.73	0.53
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.41	0.53
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.40	0.53
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.73	0.53
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.91	0.53
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.22	0.53
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.91	0.53
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.91	0.53
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.91	0.53
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.38	0.53
2:G:2347:GLU:O	2:G:2351:ASN:N	2.36	0.53
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.91	0.53
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.91	0.53
2:E:4230:LYS:CD	2:E:4959:PHE:HE1	2.20	0.53
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.90	0.53
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.91	0.53
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.91	0.53
2:G:978:THR:HB	2:G:980:ALA:H	1.74	0.53
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.91	0.52
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.52
2:E:978:THR:HB	2:E:980:ALA:H	1.74	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.52
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.91	0.52
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.91	0.52
2:B:4960:ILE:N	2:B:4960:ILE:HD13	2.23	0.52
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.90	0.52
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.36	0.52
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.52
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.40	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.52
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.43	0.52
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.52
2:B:5028:PHE:CD1	2:B:5032:TYR:CD2	2.96	0.52
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.38	0.52
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.92	0.52
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.92	0.52
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.92	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.52
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.91	0.52
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.91	0.52
2:I:309:THR:O	2:I:313:SER:OG	2.26	0.52
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.91	0.52
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.92	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.52
2:B:3760:LYS:NZ	2:B:5000:GLU:OE1	2.41	0.52
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.43	0.52
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.91	0.52
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.43	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.91	0.52
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.43	0.52
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.91	0.52
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.91	0.52
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.90	0.52
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.43	0.52
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.91	0.52
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.40	0.52
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.43	0.52
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.40	0.52
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.92	0.52
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.36	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.91	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.52
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.40	0.52
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.92	0.52
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.91	0.51
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.91	0.51
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:132:ALA:HA	2:I:194:SER:HB2	1.91	0.51
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.93	0.51
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.51
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.92	0.51
2:E:3891:LEU:HB3	2:E:3899:PHE:HE2	1.76	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.91	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.92	0.51
2:G:3891:LEU:HB3	2:G:3899:PHE:HE2	1.76	0.51
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.91	0.51
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.92	0.51
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.91	0.51
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.44	0.51
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.91	0.51
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.92	0.51
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.92	0.51
2:G:5028:PHE:CD1	2:G:5032:TYR:CD2	2.95	0.51
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.93	0.51
2:B:978:THR:HB	2:B:980:ALA:H	1.74	0.51
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.91	0.51
2:G:132:ALA:HA	2:G:194:SER:HB2	1.91	0.51
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.51
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.93	0.51
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.93	0.51
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.36	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.91	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.91	0.51
2:B:132:ALA:HA	2:B:194:SER:HB2	1.91	0.51
2:E:132:ALA:HA	2:E:194:SER:HB2	1.91	0.51
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.76	0.51
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.84	0.51
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.44	0.51
2:I:3891:LEU:HB3	2:I:3899:PHE:HE2	1.76	0.51
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.92	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.51
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.76	0.51
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.43	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.51
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.44	0.51
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.92	0.51
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.44	0.51
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.51
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.77	0.51
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.43	0.51
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.77	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.44	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.50
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.46	0.50
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.93	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.44	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.50
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.76	0.50
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.92	0.50
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.92	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.50
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.77	0.50
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.92	0.50
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.77	0.50
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.93	0.50
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.92	0.50
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.84	0.50
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.44	0.50
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.44	0.50
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.46	0.50
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.94	0.50
2:I:395:GLN:HG3	2:I:397:GLU:H	1.76	0.50
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.77	0.50
2:B:3891:LEU:HB3	2:B:3899:PHE:HE2	1.76	0.50
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.77	0.50
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.93	0.50
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.92	0.50
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.84	0.50
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.94	0.50
2:I:4956:THR:O	2:I:4965:SER:N	2.42	0.50
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.94	0.50
2:I:5028:PHE:CD1	2:I:5032:TYR:CD2	2.96	0.50
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.77	0.50
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.50
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.77	0.50
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.44	0.50
2:I:1516:UNK:N	2:I:1529:UNK:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.94	0.50
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.40	0.50
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.45	0.49
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.77	0.49
2:G:395:GLN:HG3	2:G:397:GLU:H	1.76	0.49
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.76	0.49
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.94	0.49
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.93	0.49
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.46	0.49
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.95	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.36	0.49
2:E:3760:LYS:NZ	2:E:5000:GLU:OE1	2.41	0.49
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.93	0.49
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.95	0.49
1:A:21:THR:HA	1:A:49:ARG:HA	1.95	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.94	0.49
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.94	0.49
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.93	0.49
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.84	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.45	0.49
2:B:320:LYS:NZ	2:B:381:GLU:O	2.42	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.76	0.49
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.94	0.49
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.94	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.49
2:E:548:VAL:HG12	2:E:564:LEU:HD22	1.95	0.49
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	1.95	0.49
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.94	0.49
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.49
1:F:21:THR:HA	1:F:49:ARG:HA	1.95	0.49
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.95	0.49
1:J:21:THR:HA	1:J:49:ARG:HA	1.95	0.49
2:B:794:GLY:H	2:B:798:GLY:HA3	1.78	0.49
2:G:548:VAL:HG12	2:G:564:LEU:HD22	1.95	0.49
2:G:794:GLY:H	2:G:798:GLY:HA3	1.78	0.49
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.46	0.49
2:E:794:GLY:H	2:E:798:GLY:HA3	1.78	0.49
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.95	0.49
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.78	0.49
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.77	0.49
2:I:794:GLY:H	2:I:798:GLY:HA3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.94	0.49
2:I:3760:LYS:NZ	2:I:5000:GLU:OE1	2.41	0.49
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.78	0.49
2:B:548:VAL:HG12	2:B:564:LEU:HD22	1.95	0.49
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	1.95	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.95	0.49
2:I:548:VAL:HG12	2:I:564:LEU:HD22	1.95	0.49
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.95	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.36	0.49
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.77	0.49
1:H:21:THR:HA	1:H:49:ARG:HA	1.95	0.48
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.95	0.48
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.78	0.48
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.78	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.95	0.48
2:G:4956:THR:O	2:G:4965:SER:N	2.42	0.48
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.94	0.48
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.95	0.48
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.95	0.48
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.95	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.77	0.48
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.43	0.48
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	1.96	0.48
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.95	0.48
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.39	0.48
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.46	0.48
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.95	0.48
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.95	0.48
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.95	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.48
2:I:776:LEU:HG	2:I:848:HIS:HA	1.95	0.48
2:G:776:LEU:HG	2:G:848:HIS:HA	1.95	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.45	0.48
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.96	0.48
2:E:4957:LYS:NZ	2:E:4957:LYS:CB	2.77	0.48
2:G:164:ARG:N	2:G:167:ASP:OD2	2.46	0.48
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.95	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.45	0.48
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.48
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.95	0.48
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.46	0.48
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.95	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.48
2:E:164:ARG:N	2:E:167:ASP:OD2	2.46	0.48
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.79	0.48
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.95	0.48
2:I:2758:PHE:O	2:I:2762:THR:N	2.46	0.48
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.46	0.48
2:B:776:LEU:HG	2:B:848:HIS:HA	1.95	0.48
2:E:776:LEU:HG	2:E:848:HIS:HA	1.95	0.48
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.95	0.48
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.96	0.48
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	1.96	0.48
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.48
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.32	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.48
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.95	0.48
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.79	0.48
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.31	0.48
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.79	0.48
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.47	0.48
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.48
2:I:4571:PHE:O	2:I:4575:PHE:N	2.47	0.48
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.47	0.48
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.96	0.47
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	1.96	0.47
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.96	0.47
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.95	0.47
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.32	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.47	0.47
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.96	0.47
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.96	0.47
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.95	0.47
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.95	0.47
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.47
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	1.95	0.47
2:I:4957:LYS:HB2	2:I:4957:LYS:HZ1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.95	0.47
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.32	0.47
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.80	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.47
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.47	0.47
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.31	0.47
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.79	0.47
2:I:4230:LYS:CD	2:I:4959:PHE:HE1	2.20	0.47
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	1.95	0.47
1:F:27:THR:HB	1:F:100:ASP:HB3	1.97	0.47
1:A:27:THR:HB	1:A:100:ASP:HB3	1.97	0.47
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.96	0.47
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.96	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.95	0.47
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.47
2:G:4230:LYS:CD	2:G:4959:PHE:HE1	2.20	0.47
2:G:4957:LYS:NZ	2:G:4957:LYS:CB	2.77	0.47
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.95	0.47
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.32	0.47
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.95	0.47
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.39	0.47
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.79	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.95	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.96	0.47
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.39	0.47
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.96	0.47
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.95	0.47
2:I:164:ARG:N	2:I:167:ASP:OD2	2.46	0.47
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.47
2:B:164:ARG:N	2:B:167:ASP:OD2	2.46	0.47
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.95	0.47
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.47	0.47
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.95	0.47
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.80	0.47
2:G:320:LYS:NZ	2:G:381:GLU:O	2.42	0.47
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.47
2:G:3760:LYS:NZ	2:G:5000:GLU:OE1	2.41	0.47
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.95	0.47
2:E:243:ARG:NH1	2:E:301:VAL:O	2.43	0.47
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.48	0.47
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.80	0.47
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.97	0.47
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.48	0.47
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.48	0.47
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.47
2:I:215:THR:HG22	2:I:273:HIS:HA	1.97	0.47
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.47	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.80	0.47
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.47	0.47
2:B:3915:ILE:O	2:B:3919:THR:N	2.47	0.47
2:I:320:LYS:NZ	2:I:381:GLU:O	2.42	0.47
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.95	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.96	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.47
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.95	0.46
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.38	0.46
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.98	0.46
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.97	0.46
2:G:379:HIS:CD2	2:G:381:GLU:H	2.33	0.46
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.48	0.46
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.98	0.46
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.97	0.46
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.31	0.46
2:I:4822:THR:O	2:I:4825:THR:OG1	2.29	0.46
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.43	0.46
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.48	0.46
2:B:215:THR:HG22	2:B:273:HIS:HA	1.97	0.46
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.97	0.46
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	1.96	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.48	0.46
2:I:379:HIS:CD2	2:I:381:GLU:H	2.33	0.46
2:I:485:SER:O	2:I:489:ASN:N	2.38	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.47	0.46
2:I:4957:LYS:NZ	2:I:4957:LYS:CB	2.77	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.80	0.46
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.98	0.46
2:E:215:THR:HG22	2:E:273:HIS:HA	1.97	0.46
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.98	0.46
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.48	0.46
2:E:4930:ALA:O	2:E:4934:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.46
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.96	0.46
1:J:27:THR:HB	1:J:100:ASP:HB3	1.97	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.46
2:G:215:THR:HG22	2:G:273:HIS:HA	1.97	0.46
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.98	0.46
1:H:27:THR:HB	1:H:100:ASP:HB3	1.97	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.43	0.46
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.97	0.46
2:E:1991:THR:O	2:E:1995:THR:OG1	2.34	0.46
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.98	0.46
2:G:940:GLY:O	2:G:1052:ASN:N	2.49	0.46
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.98	0.46
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.97	0.46
2:G:4930:ALA:O	2:G:4934:GLY:N	2.49	0.46
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.97	0.46
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.98	0.46
2:B:4957:LYS:NZ	2:B:4957:LYS:CB	2.77	0.46
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.96	0.46
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.98	0.46
2:I:4930:ALA:O	2:I:4934:GLY:N	2.49	0.46
1:H:87:HIS:H	1:H:91:ILE:HB	1.81	0.46
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.98	0.46
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.98	0.46
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.98	0.46
2:G:1991:THR:O	2:G:1995:THR:OG1	2.34	0.46
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.98	0.46
2:G:3915:ILE:O	2:G:3919:THR:N	2.47	0.46
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.98	0.46
1:F:87:HIS:H	1:F:91:ILE:HB	1.81	0.46
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.97	0.46
1:J:87:HIS:H	1:J:91:ILE:HB	1.81	0.46
2:B:793:LEU:HB2	2:B:797:HIS:H	1.81	0.46
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.98	0.46
2:B:4822:THR:O	2:B:4825:THR:OG1	2.29	0.46
2:B:4930:ALA:O	2:B:4934:GLY:N	2.49	0.46
2:I:940:GLY:O	2:I:1052:ASN:N	2.49	0.46
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.98	0.46
2:G:243:ARG:NH1	2:G:301:VAL:O	2.43	0.46
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.98	0.46
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.97	0.46
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.45
2:E:451:TYR:O	2:E:474:ARG:NH1	2.47	0.45
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.98	0.45
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.97	0.45
2:I:243:ARG:NH1	2:I:301:VAL:O	2.43	0.45
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.98	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.45
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.48	0.45
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.98	0.45
2:B:1936:LYS:O	2:B:1940:CYS:N	2.46	0.45
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.43	0.45
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.98	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.99	0.45
2:G:451:TYR:O	2:G:474:ARG:NH1	2.47	0.45
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.45
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.45
2:E:2347:GLU:O	2:E:2351:ASN:N	2.36	0.45
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.45
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.32	0.45
2:E:4822:THR:O	2:E:4825:THR:OG1	2.29	0.45
2:I:451:TYR:O	2:I:474:ARG:NH1	2.47	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.64	0.45
2:G:793:LEU:HB2	2:G:797:HIS:H	1.81	0.45
1:A:87:HIS:H	1:A:91:ILE:HB	1.81	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.33	0.45
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.98	0.45
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.98	0.45
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.98	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.98	0.45
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.97	0.45
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.98	0.45
2:G:4978:HIS:CD2	2:G:4982:GLU:HB2	2.52	0.45
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.80	0.45
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.45
2:I:793:LEU:HB2	2:I:797:HIS:H	1.81	0.45
2:G:206:CYS:SG	2:G:207:SER:N	2.89	0.45
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.31	0.45
2:E:3948:LYS:HG2	2:E:4012:LEU:HD22	1.99	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.97	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.99	0.45
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.98	0.45
2:B:940:GLY:O	2:B:1052:ASN:N	2.49	0.45
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.45
2:B:3829:PHE:HD1	2:B:3915:ILE:HD11	1.82	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.33	0.45
2:E:793:LEU:HB2	2:E:797:HIS:H	1.81	0.45
2:I:4978:HIS:CD2	2:I:4982:GLU:HB2	2.52	0.45
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.98	0.45
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.32	0.45
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.98	0.45
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.50	0.45
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.64	0.45
2:B:4851:TYR:HD2	2:B:4920:PHE:HD1	1.65	0.45
2:I:1991:THR:O	2:I:1995:THR:OG1	2.34	0.45
2:I:3829:PHE:HD1	2:I:3915:ILE:HD11	1.82	0.45
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.45
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.99	0.45
2:B:1991:THR:O	2:B:1995:THR:OG1	2.34	0.45
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.82	0.45
2:B:3948:LYS:HG2	2:B:4012:LEU:HD22	1.99	0.45
2:E:206:CYS:SG	2:E:207:SER:N	2.89	0.45
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.64	0.45
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.98	0.45
2:G:3948:LYS:HG2	2:G:4012:LEU:HD22	1.99	0.45
2:B:451:TYR:O	2:B:474:ARG:NH1	2.47	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.45
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.98	0.45
2:G:485:SER:O	2:G:489:ASN:N	2.38	0.45
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.45
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.98	0.44
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.98	0.44
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.50	0.44
2:E:1105:ALA:N	2:E:1189:LEU:O	2.51	0.44
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.82	0.44
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.44
2:E:3829:PHE:HD1	2:E:3915:ILE:HD11	1.82	0.44
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.98	0.44
2:I:4851:TYR:HD2	2:I:4920:PHE:HD1	1.65	0.44
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.82	0.44
2:B:379:HIS:NE2	2:B:381:GLU:OE1	2.50	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.38	0.44
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.82	0.44
2:E:940:GLY:O	2:E:1052:ASN:N	2.49	0.44
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.82	0.44
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.00	0.44
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.47	0.44
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.32	0.44
2:E:257:ARG:O	2:E:284:HIS:NE2	2.48	0.44
2:E:4571:PHE:O	2:E:4575:PHE:N	2.47	0.44
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.82	0.44
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.39	0.44
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.64	0.44
2:B:1105:ALA:N	2:B:1189:LEU:O	2.51	0.44
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.00	0.44
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.00	0.44
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.99	0.44
2:B:4978:HIS:CD2	2:B:4982:GLU:HB2	2.52	0.44
2:E:5028:PHE:CG	2:E:5028:PHE:O	2.70	0.44
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.83	0.44
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.98	0.44
2:B:206:CYS:SG	2:B:207:SER:N	2.89	0.44
2:B:1663:HIS:O	2:B:1667:LEU:N	2.51	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.44
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.44
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.99	0.44
2:I:3948:LYS:HG2	2:I:4012:LEU:HD22	1.99	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.99	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.44
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.98	0.44
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.50	0.44
2:E:379:HIS:NE2	2:E:381:GLU:OE1	2.50	0.44
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.00	0.44
2:I:379:HIS:NE2	2:I:381:GLU:OE1	2.50	0.44
2:G:379:HIS:NE2	2:G:381:GLU:OE1	2.50	0.44
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.99	0.44
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.00	0.44
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.53	0.44
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	2.00	0.44
2:E:4851:TYR:HD2	2:E:4920:PHE:HD1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.00	0.44
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.98	0.44
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.83	0.44
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.00	0.44
2:G:1105:ALA:N	2:G:1189:LEU:O	2.51	0.44
2:B:282:ILE:HD12	2:B:314:PHE:HD2	1.83	0.44
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	2.00	0.44
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.00	0.44
2:B:4571:PHE:O	2:B:4575:PHE:N	2.47	0.44
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	2.00	0.44
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.53	0.44
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.00	0.44
2:G:4851:TYR:HD2	2:G:4920:PHE:HD1	1.65	0.44
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.00	0.43
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.99	0.43
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.83	0.43
2:E:4978:HIS:CD2	2:E:4982:GLU:HB2	2.52	0.43
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.83	0.43
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.43
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.83	0.43
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	2.00	0.43
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.00	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.83	0.43
2:G:4822:THR:O	2:G:4825:THR:OG1	2.29	0.43
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.90	0.43
1:A:82:TYR:O	1:A:86:GLY:N	2.51	0.43
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.82	0.43
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.42	0.43
2:B:4956:THR:O	2:B:4965:SER:N	2.42	0.43
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.51	0.43
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.00	0.43
2:I:606:LEU:O	2:I:617:ASN:ND2	2.51	0.43
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.00	0.43
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	2.00	0.43
2:G:606:LEU:O	2:G:617:ASN:ND2	2.51	0.43
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.00	0.43
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	2.00	0.43
2:B:606:LEU:O	2:B:617:ASN:ND2	2.51	0.43
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.43
2:B:4996:ILE:HG12	4:B:5102:CFF:H123	2.00	0.43
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.00	0.43
2:G:282:ILE:HD12	2:G:314:PHE:HD2	1.83	0.43
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	2.00	0.43
2:G:3829:PHE:HD1	2:G:3915:ILE:HD11	1.82	0.43
2:G:5028:PHE:CG	2:G:5028:PHE:O	2.70	0.43
1:F:82:TYR:O	1:F:86:GLY:N	2.51	0.43
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.83	0.43
2:E:282:ILE:HD12	2:E:314:PHE:HD2	1.83	0.43
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.00	0.43
2:I:446:GLN:HA	2:I:449:ILE:HD12	2.01	0.43
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.00	0.43
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.00	0.43
2:G:1663:HIS:O	2:G:1667:LEU:N	2.51	0.43
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.99	0.43
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.99	0.43
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.49	0.43
2:E:606:LEU:O	2:E:617:ASN:ND2	2.51	0.43
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.00	0.43
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.82	0.43
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.53	0.43
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.99	0.43
2:G:1154:ASP:O	2:G:1158:ASN:N	2.52	0.43
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.52	0.43
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.99	0.43
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	2.00	0.43
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.82	0.43
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.83	0.43
2:I:534:ARG:NH2	2:I:573:GLU:OE2	2.52	0.43
2:I:1154:ASP:O	2:I:1158:ASN:N	2.52	0.43
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.52	0.43
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	2.00	0.43
2:G:446:GLN:HA	2:G:449:ILE:HD12	2.01	0.43
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.82	0.43
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.83	0.43
2:E:485:SER:O	2:E:489:ASN:N	2.38	0.43
2:G:1936:LYS:O	2:G:1940:CYS:N	2.46	0.43
2:E:278:GLN:N	2:E:315:CYS:SG	2.92	0.43
2:E:446:GLN:HA	2:E:449:ILE:HD12	2.01	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.82	0.43
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	2.00	0.43
2:I:101:LEU:HB3	2:I:150:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.01	0.43
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.43
2:E:689:THR:H	2:E:778:PHE:HE2	1.67	0.43
2:E:1032:LYS:O	2:E:1036:ARG:N	2.47	0.43
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.01	0.43
2:E:4957:LYS:HB2	2:E:4957:LYS:HZ1	1.83	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:3915:ILE:O	2:I:3919:THR:N	2.47	0.43
2:B:446:GLN:HA	2:B:449:ILE:HD12	2.01	0.43
2:B:1973:GLN:O	2:B:1977:TYR:N	2.44	0.43
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.00	0.43
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	2.01	0.43
2:E:4996:ILE:HG12	4:E:5102:CFF:H123	2.00	0.43
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.54	0.42
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.49	0.42
2:E:1936:LYS:O	2:E:1940:CYS:N	2.46	0.42
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.53	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.42
2:I:689:THR:H	2:I:778:PHE:HE2	1.66	0.42
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.84	0.42
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.83	0.42
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.54	0.42
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.53	0.42
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	2.01	0.42
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.00	0.42
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.84	0.42
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.54	0.42
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.83	0.42
2:I:1973:GLN:O	2:I:1977:TYR:N	2.44	0.42
2:G:534:ARG:NH2	2:G:573:GLU:OE2	2.52	0.42
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.42
1:J:82:TYR:O	1:J:86:GLY:N	2.51	0.42
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.83	0.42
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.52	0.42
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	2.01	0.42
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.85	0.42
2:I:1105:ALA:N	2:I:1189:LEU:O	2.51	0.42
2:I:2138:LEU:HD11	2:I:3654:LEU:HD11	2.01	0.42
2:I:4996:ILE:HG12	4:I:5102:CFF:H123	2.00	0.42
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	2.01	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.90	0.42
2:B:113:HIS:O	2:B:399:GLN:NE2	2.53	0.42
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	2.02	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	2.01	0.42
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.52	0.42
2:E:2138:LEU:HD11	2:E:3654:LEU:HD11	2.01	0.42
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.84	0.42
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	2.00	0.42
2:G:4996:ILE:HG12	4:G:5102:CFF:H123	2.00	0.42
1:H:82:TYR:O	1:H:86:GLY:N	2.51	0.42
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.01	0.42
2:E:113:HIS:O	2:E:399:GLN:NE2	2.53	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.02	0.42
2:I:1663:HIS:O	2:I:1667:LEU:N	2.51	0.42
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.01	0.42
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	2.02	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.84	0.42
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.01	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:B:4984:ASN:C	2:B:4986:ALA:H	2.23	0.42
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.02	0.42
2:E:1154:ASP:O	2:E:1158:ASN:N	2.52	0.42
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.85	0.42
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.77	0.42
2:I:1936:LYS:O	2:I:1940:CYS:N	2.46	0.42
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	2.01	0.42
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.53	0.42
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.02	0.42
2:B:1154:ASP:O	2:B:1158:ASN:N	2.52	0.42
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.42
2:B:4736:ARG:NH1	2:E:4079:ASP:OD1	2.53	0.42
2:E:670:GLU:HG3	2:E:787:VAL:HG13	2.01	0.42
2:E:1124:PHE:HB2	2:E:1162:PHE:CE2	2.55	0.42
2:I:282:ILE:HD12	2:I:314:PHE:HD2	1.83	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.02	0.42
2:B:2138:LEU:HD11	2:B:3654:LEU:HD11	2.01	0.42
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3677:LEU:O	2:B:3698:LEU:N	2.52	0.42
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.53	0.42
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	2.02	0.42
2:I:1124:PHE:HB2	2:I:1162:PHE:CE2	2.55	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.01	0.42
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	2.02	0.42
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.32	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.42
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.53	0.42
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.02	0.42
2:B:689:THR:H	2:B:778:PHE:HE2	1.67	0.42
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.53	0.42
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.84	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.02	0.42
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.83	0.42
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.50	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	2.02	0.42
2:G:278:GLN:N	2:G:315:CYS:SG	2.92	0.42
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.77	0.42
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	2.02	0.42
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.84	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.90	0.42
2:B:551:LEU:HD21	2:B:589:LEU:HB2	2.02	0.42
2:B:1124:PHE:HB2	2:B:1162:PHE:CE2	2.55	0.42
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.85	0.42
2:I:1032:LYS:O	2:I:1036:ARG:N	2.47	0.42
2:G:614:VAL:HA	2:G:2169:GLN:HB3	2.02	0.42
2:G:1124:PHE:HB2	2:G:1162:PHE:CE2	2.55	0.42
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	2.01	0.42
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.50	0.42
2:B:670:GLU:HG3	2:B:787:VAL:HG13	2.01	0.41
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	2.02	0.41
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	2.02	0.41
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.02	0.41
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	2.01	0.41
2:E:3915:ILE:O	2:E:3919:THR:N	2.47	0.41
2:E:4228:ALA:O	2:E:4232:GLU:N	2.52	0.41
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.85	0.41
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.53	0.41
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.85	0.41
2:B:278:GLN:N	2:B:315:CYS:SG	2.92	0.41
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.84	0.41
2:E:614:VAL:HA	2:E:2169:GLN:HB3	2.02	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.01	0.41
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.01	0.41
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.84	0.41
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	2.02	0.41
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.01	0.41
2:G:2138:LEU:HD11	2:G:3654:LEU:HD11	2.01	0.41
2:G:4080:TYR:CZ	2:G:4096:ALA:HB3	2.55	0.41
2:B:614:VAL:HA	2:B:2169:GLN:HB3	2.02	0.41
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.01	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.85	0.41
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.01	0.41
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.01	0.41
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.53	0.41
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.01	0.41
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.01	0.41
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	2.01	0.41
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.41
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.92	0.41
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.38	0.41
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.85	0.41
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.86	0.41
2:G:113:HIS:O	2:G:399:GLN:NE2	2.53	0.41
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.56	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.86	0.41
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.77	0.41
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.86	0.41
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.53	0.41
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.50	0.41
2:E:4586:PRO:HA	2:E:4628:VAL:HG11	2.02	0.41
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.86	0.41
2:I:614:VAL:HA	2:I:2169:GLN:HB3	2.02	0.41
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.54	0.41
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	2.01	0.41
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.84	0.41
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.02	0.41
2:G:689:THR:H	2:G:778:PHE:HE2	1.66	0.41
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	2.02	0.41
2:G:4984:ASN:C	2:G:4986:ALA:H	2.23	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.41
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.52	0.41
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.53	0.41
2:I:4863:TYR:HD2	2:I:4875:LYS:HB2	1.86	0.41
2:I:4984:ASN:C	2:I:4986:ALA:H	2.23	0.41
2:I:5027:CYS:SG	2:I:5027:CYS:O	2.79	0.41
2:G:1032:LYS:O	2:G:1036:ARG:N	2.47	0.41
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.90	0.41
2:B:1032:LYS:O	2:B:1036:ARG:N	2.47	0.41
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.03	0.41
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.56	0.41
2:E:320:LYS:NZ	2:E:381:GLU:O	2.42	0.41
2:E:734:GLY:O	2:E:736:HIS:ND1	2.52	0.41
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	2.02	0.41
2:I:113:HIS:O	2:I:399:GLN:NE2	2.53	0.41
2:I:670:GLU:HG3	2:I:787:VAL:HG13	2.02	0.41
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.01	0.41
2:I:4014:LYS:HE2	2:I:4135:PRO:HG3	2.03	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.95	0.41
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.41
2:G:5027:CYS:SG	2:G:5027:CYS:O	2.79	0.41
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.53	0.41
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	2.02	0.41
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.53	0.41
2:E:698:GLY:HA2	2:E:703:GLY:HA2	2.03	0.41
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.03	0.41
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	2.02	0.41
2:E:4014:LYS:HE2	2:E:4135:PRO:HG3	2.03	0.41
2:E:4080:TYR:CZ	2:E:4096:ALA:HB3	2.55	0.41
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	2.02	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.02	0.41
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.03	0.41
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.01	0.41
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.86	0.41
2:B:4914:VAL:HG23	2:E:4888:TYR:CD1	2.56	0.41
2:E:1663:HIS:O	2:E:1667:LEU:N	2.51	0.41
2:E:3706:SER:OG	2:E:3781:GLN:NE2	2.54	0.41
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.02	0.41
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.49	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.85	0.41
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	2.02	0.41
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.01	0.41
2:G:4863:TYR:HD2	2:G:4875:LYS:HB2	1.86	0.41
2:B:698:GLY:HA2	2:B:703:GLY:HA2	2.03	0.41
2:B:4014:LYS:HE2	2:B:4135:PRO:HG3	2.03	0.41
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.86	0.41
2:E:534:ARG:NH2	2:E:573:GLU:OE2	2.52	0.41
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.85	0.41
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	2.02	0.41
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.84	0.41
2:I:257:ARG:O	2:I:284:HIS:NE2	2.48	0.41
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.03	0.41
2:I:4586:PRO:HA	2:I:4628:VAL:HG11	2.02	0.41
2:G:670:GLU:HG3	2:G:787:VAL:HG13	2.02	0.41
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.85	0.41
2:G:4586:PRO:HA	2:G:4628:VAL:HG11	2.02	0.41
2:B:288:GLY:HA3	2:B:405:HIS:CE1	2.56	0.41
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	2.02	0.41
2:E:470:SER:O	2:E:474:ARG:NE	2.50	0.41
2:E:4956:THR:O	2:E:4965:SER:N	2.42	0.41
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.56	0.41
2:I:4080:TYR:CZ	2:I:4096:ALA:HB3	2.55	0.41
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.86	0.41
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.56	0.41
2:G:551:LEU:HD21	2:G:589:LEU:HB2	2.02	0.41
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.03	0.41
2:B:4957:LYS:HB2	2:B:4957:LYS:HZ1	1.82	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.56	0.40
2:E:551:LEU:HD21	2:E:589:LEU:HB2	2.02	0.40
2:E:582:HIS:O	2:E:585:SER:OG	2.30	0.40
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.56	0.40
2:I:551:LEU:HD21	2:I:589:LEU:HB2	2.02	0.40
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.56	0.40
2:G:1973:GLN:O	2:G:1977:TYR:N	2.44	0.40
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	2.02	0.40
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	2.02	0.40
2:G:4929:LEU:HD13	2:G:4929:LEU:HA	1.92	0.40
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.40
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:582:HIS:O	2:B:585:SER:OG	2.30	0.40
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.87	0.40
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.02	0.40
2:B:3706:SER:OG	2:B:3781:GLN:NE2	2.54	0.40
2:B:4080:TYR:CZ	2:B:4096:ALA:HB3	2.55	0.40
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.87	0.40
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.87	0.40
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.84	0.40
2:B:734:GLY:O	2:B:736:HIS:ND1	2.52	0.40
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.02	0.40
2:B:3847:PHE:HE1	2:B:3950:ASN:HD22	1.70	0.40
2:B:5027:CYS:SG	2:B:5027:CYS:O	2.79	0.40
2:B:5028:PHE:CD1	2:B:5028:PHE:O	2.75	0.40
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.86	0.40
2:E:662:TRP:HZ3	2:E:811:CYS:HA	1.87	0.40
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.03	0.40
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.03	0.40
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.04	0.40
2:E:4987:ASN:HA	2:E:4990:PHE:HD2	1.87	0.40
2:E:5028:PHE:CD1	2:E:5028:PHE:O	2.75	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.87	0.40
2:G:864:PRO:HD2	2:G:867:LEU:HD12	2.03	0.40
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.55	0.40
2:B:870:ILE:HD12	2:B:870:ILE:HA	1.92	0.40
2:B:4586:PRO:HA	2:B:4628:VAL:HG11	2.02	0.40
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.04	0.40
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	2.02	0.40
2:E:1705:GLY:HA2	2:E:1709:ALA:HB3	2.04	0.40
2:E:3677:LEU:O	2:E:3698:LEU:N	2.52	0.40
2:E:5027:CYS:O	2:E:5027:CYS:SG	2.79	0.40
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.86	0.40
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.01	0.40
2:I:2029:GLN:O	2:I:2033:ASP:N	2.48	0.40
2:I:2298:VAL:HA	2:I:2301:TYR:HB2	2.03	0.40
2:I:3805:LEU:H	2:I:3805:LEU:HG	1.77	0.40
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.49	0.40
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.04	0.40
2:G:4014:LYS:HE2	2:G:4135:PRO:HG3	2.03	0.40
2:B:534:ARG:NH2	2:B:573:GLU:OE2	2.52	0.40
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.55	0.40
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4863:TYR:HD2	2:E:4875:LYS:HB2	1.86	0.40
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.40
2:I:278:GLN:N	2:I:315:CYS:SG	2.92	0.40
2:I:698:GLY:HA2	2:I:703:GLY:HA2	2.03	0.40
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.86	0.40
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.04	0.40
2:G:698:GLY:HA2	2:G:703:GLY:HA2	2.03	0.40
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.56	0.40
2:G:2298:VAL:HA	2:G:2301:TYR:HB2	2.03	0.40
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	47	81
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	47	81
2	G	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	47	81
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	47	81
All	All	13360/18096 (74%)	11941 (89%)	1395 (10%)	24 (0%)	50	81

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	B	4641	PRO
2	B	4985	LEU
2	E	1932	PRO
2	E	4641	PRO
2	E	4985	LEU
2	I	1932	PRO
2	I	4641	PRO
2	I	4985	LEU
2	G	1932	PRO
2	G	4641	PRO
2	G	4985	LEU
2	B	1840	PRO
2	E	1840	PRO
2	I	1840	PRO
2	G	1840	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%)	2473 (99%)	20 (1%)	81	89
2	E	2493/3022 (82%)	2473 (99%)	20 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	2493/3022 (82%)	2473 (99%)	20 (1%)	81	89
2	I	2493/3022 (82%)	2473 (99%)	20 (1%)	81	89
All	All	10324/12444 (83%)	10244 (99%)	80 (1%)	82	89

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4137	ARG
2	B	4913	ARG
2	B	4957	LYS
2	B	4959	PHE
2	B	4960	ILE
2	B	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG

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Mol	Chain	Res	Type
2	E	4137	ARG
2	E	4913	ARG
2	E	4957	LYS
2	E	4959	PHE
2	E	4960	ILE
2	E	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4137	ARG
2	I	4913	ARG
2	I	4957	LYS
2	I	4959	PHE
2	I	4960	ILE
2	I	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4137	ARG
2	G	4913	ARG

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Mol	Chain	Res	Type
2	G	4957	LYS
2	G	4959	PHE
2	G	4960	ILE
2	G	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	25	HIS
1	F	87	HIS
1	A	25	HIS
1	A	87	HIS
1	H	25	HIS
1	H	87	HIS
1	J	25	HIS
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	405	HIS
2	B	413	GLN
2	B	520	ASN
2	B	797	HIS
2	B	838	HIS
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2007	ASN
2	B	2127	GLN
2	B	2291	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN

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Mol	Chain	Res	Type
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4209	GLN
2	B	4806	ASN
2	B	4933	GLN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	405	HIS
2	E	413	GLN
2	E	520	ASN
2	E	797	HIS
2	E	838	HIS
2	E	1598	GLN
2	E	1679	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	2127	GLN
2	E	2291	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	3976	ASN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4201	ASN

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Mol	Chain	Res	Type
2	E	4209	GLN
2	E	4806	ASN
2	E	4933	GLN
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	405	HIS
2	I	413	GLN
2	I	520	ASN
2	I	797	HIS
2	I	838	HIS
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2127	GLN
2	I	2291	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4201	ASN
2	I	4209	GLN
2	I	4806	ASN
2	I	4933	GLN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS

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Mol	Chain	Res	Type
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	405	HIS
2	G	413	GLN
2	G	520	ASN
2	G	797	HIS
2	G	838	HIS
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2127	GLN
2	G	2291	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	3976	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4142	ASN
2	G	4201	ASN
2	G	4209	GLN
2	G	4806	ASN
2	G	4933	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ATP	E	5101	-	26,33,33	0.85	1 (3%)	31,52,52	1.55	6 (19%)
3	ATP	B	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.55	6 (19%)
3	ATP	G	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.56	6 (19%)
4	CFF	B	5102	-	8,15,15	2.49	3 (37%)	8,23,23	1.24	1 (12%)
4	CFF	G	5102	-	8,15,15	2.49	3 (37%)	8,23,23	1.24	1 (12%)
3	ATP	I	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.55	6 (19%)
4	CFF	E	5102	-	8,15,15	2.50	3 (37%)	8,23,23	1.23	1 (12%)
4	CFF	I	5102	-	8,15,15	2.48	3 (37%)	8,23,23	1.23	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	E	5101	-	-	4/18/38/38	0/3/3/3
3	ATP	B	5101	-	-	4/18/38/38	0/3/3/3
3	ATP	G	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	I	5102	-	-	-	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C5-C4	-4.67	1.33	1.39
4	B	5102	CFF	C5-C4	-4.60	1.33	1.39
4	I	5102	CFF	C5-C4	-4.60	1.33	1.39
4	G	5102	CFF	C5-C4	-4.60	1.33	1.39
4	E	5102	CFF	C6-N1	-3.99	1.32	1.38
4	B	5102	CFF	C6-N1	-3.98	1.32	1.38
4	G	5102	CFF	C6-N1	-3.95	1.32	1.38
4	I	5102	CFF	C6-N1	-3.92	1.32	1.38
4	E	5102	CFF	O13-C6	-2.32	1.18	1.24
4	B	5102	CFF	O13-C6	-2.32	1.18	1.24
4	I	5102	CFF	O13-C6	-2.32	1.18	1.24
4	G	5102	CFF	O13-C6	-2.32	1.18	1.24
3	E	5101	ATP	C5-C4	2.17	1.46	1.40
3	B	5101	ATP	C5-C4	2.15	1.46	1.40
3	G	5101	ATP	C5-C4	2.15	1.46	1.40
3	I	5101	ATP	C5-C4	2.14	1.46	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	PB-O3B-PG	-3.60	120.46	132.83
3	E	5101	ATP	PB-O3B-PG	-3.60	120.47	132.83
3	G	5101	ATP	PB-O3B-PG	-3.60	120.48	132.83
3	B	5101	ATP	PB-O3B-PG	-3.60	120.48	132.83
3	G	5101	ATP	N3-C2-N1	-3.48	123.24	128.68
3	B	5101	ATP	N3-C2-N1	-3.47	123.26	128.68
3	I	5101	ATP	N3-C2-N1	-3.47	123.26	128.68
3	E	5101	ATP	N3-C2-N1	-3.47	123.26	128.68
3	B	5101	ATP	PA-O3A-PB	-3.18	121.91	132.83
3	G	5101	ATP	PA-O3A-PB	-3.18	121.91	132.83
3	I	5101	ATP	PA-O3A-PB	-3.18	121.92	132.83
3	E	5101	ATP	PA-O3A-PB	-3.18	121.93	132.83
4	E	5102	CFF	C14-N7-C8	-2.82	111.86	125.43
4	B	5102	CFF	C14-N7-C8	-2.82	111.88	125.43
4	I	5102	CFF	C14-N7-C8	-2.81	111.91	125.43
4	G	5102	CFF	C14-N7-C8	-2.81	111.91	125.43
3	G	5101	ATP	C3'-C2'-C1'	2.57	104.84	100.98
3	E	5101	ATP	C3'-C2'-C1'	2.55	104.81	100.98
3	B	5101	ATP	C3'-C2'-C1'	2.54	104.80	100.98
3	I	5101	ATP	C3'-C2'-C1'	2.51	104.76	100.98
3	B	5101	ATP	C4-C5-N7	-2.09	107.22	109.40
3	E	5101	ATP	C4-C5-N7	-2.07	107.24	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	C4-C5-N7	-2.07	107.24	109.40
3	G	5101	ATP	C4-C5-N7	-2.07	107.25	109.40
3	G	5101	ATP	C2-N1-C6	2.05	122.26	118.75
3	E	5101	ATP	C2-N1-C6	2.04	122.24	118.75
3	B	5101	ATP	C2-N1-C6	2.03	122.23	118.75
3	I	5101	ATP	C2-N1-C6	2.03	122.23	118.75

There are no chirality outliers.

All (16) torsion outliers are listed below:

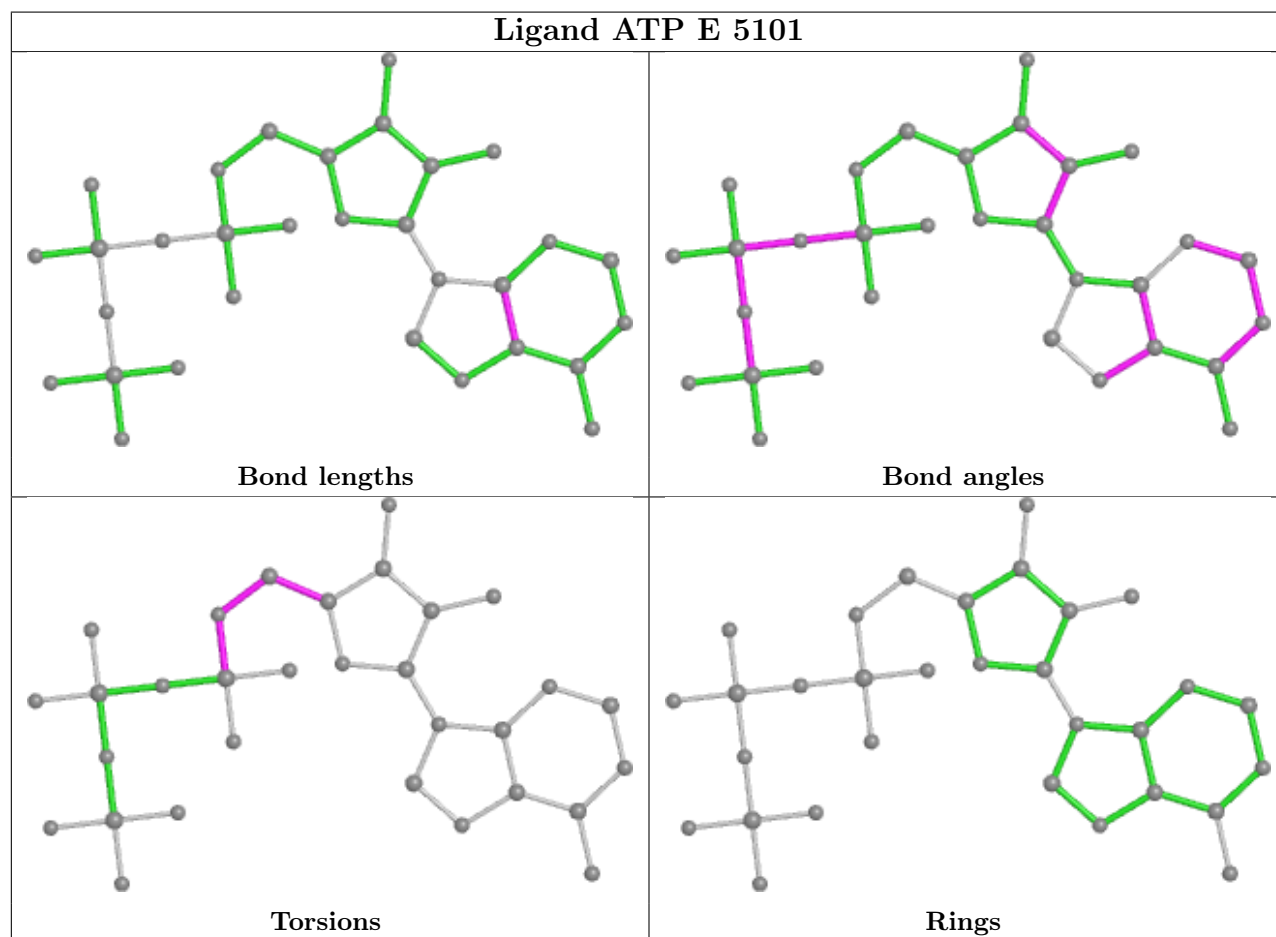
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	C4'-C5'-O5'-PA
3	E	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA
3	G	5101	ATP	C4'-C5'-O5'-PA
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'

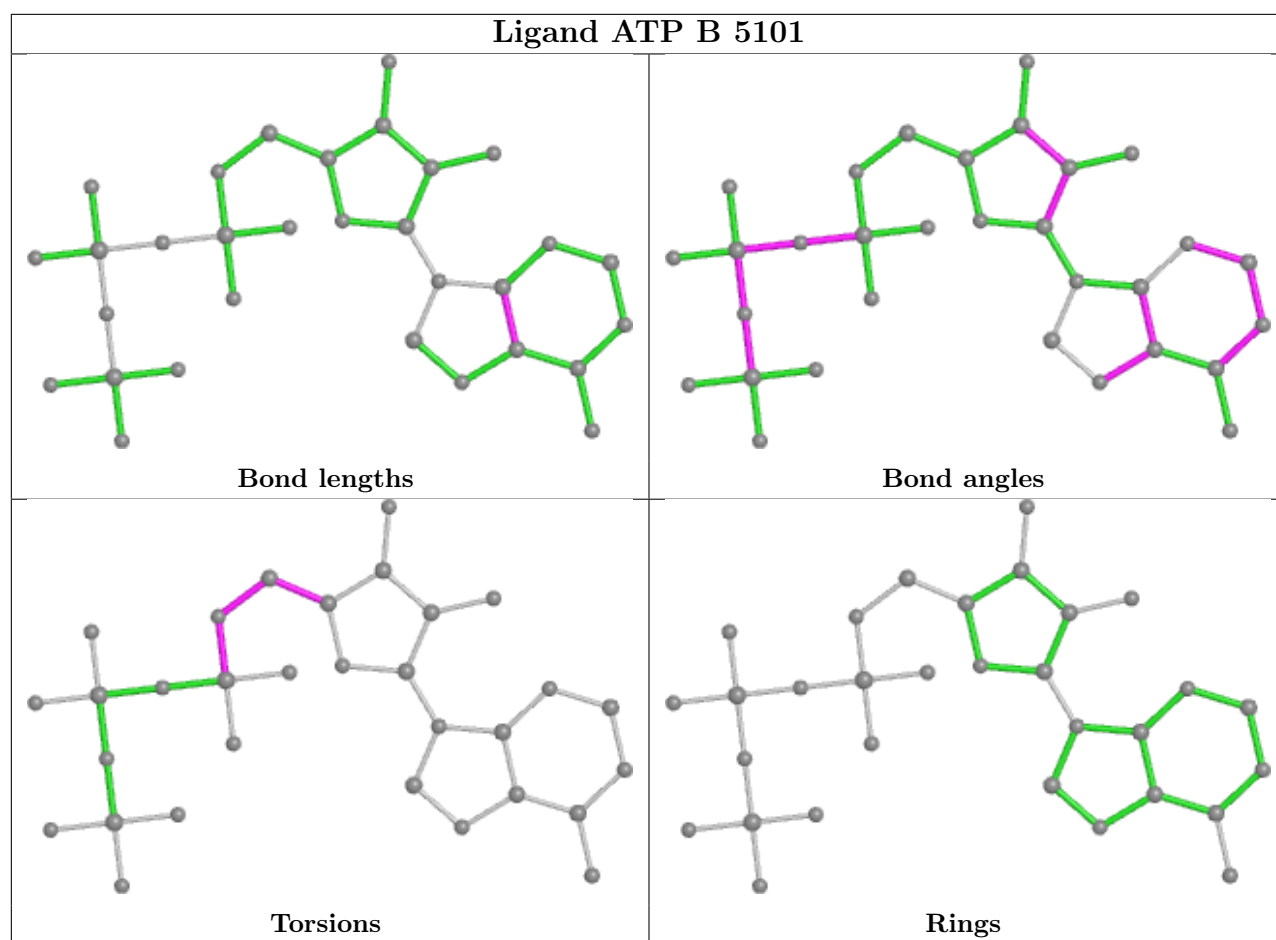
There are no ring outliers.

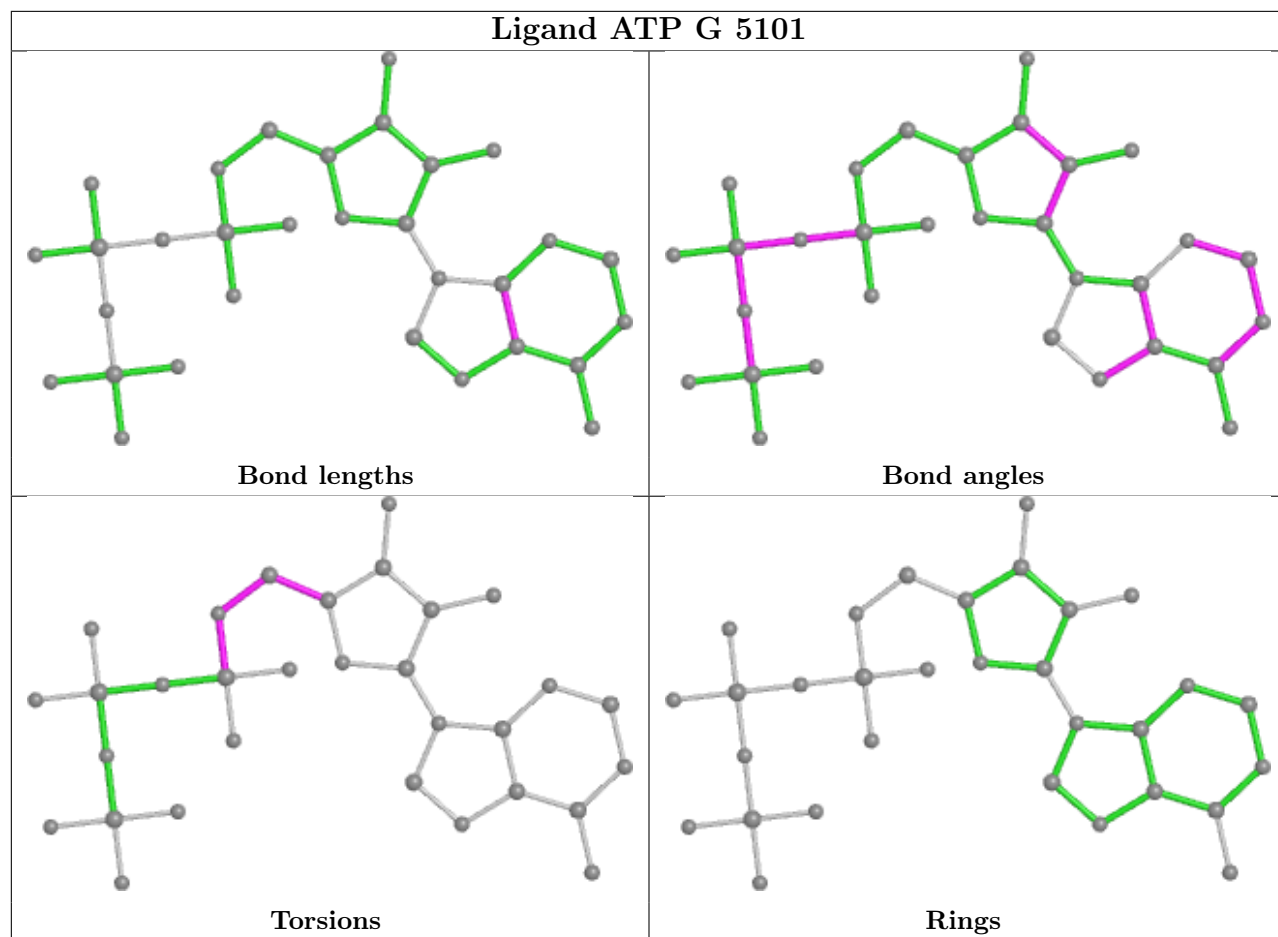
8 monomers are involved in 8 short contacts:

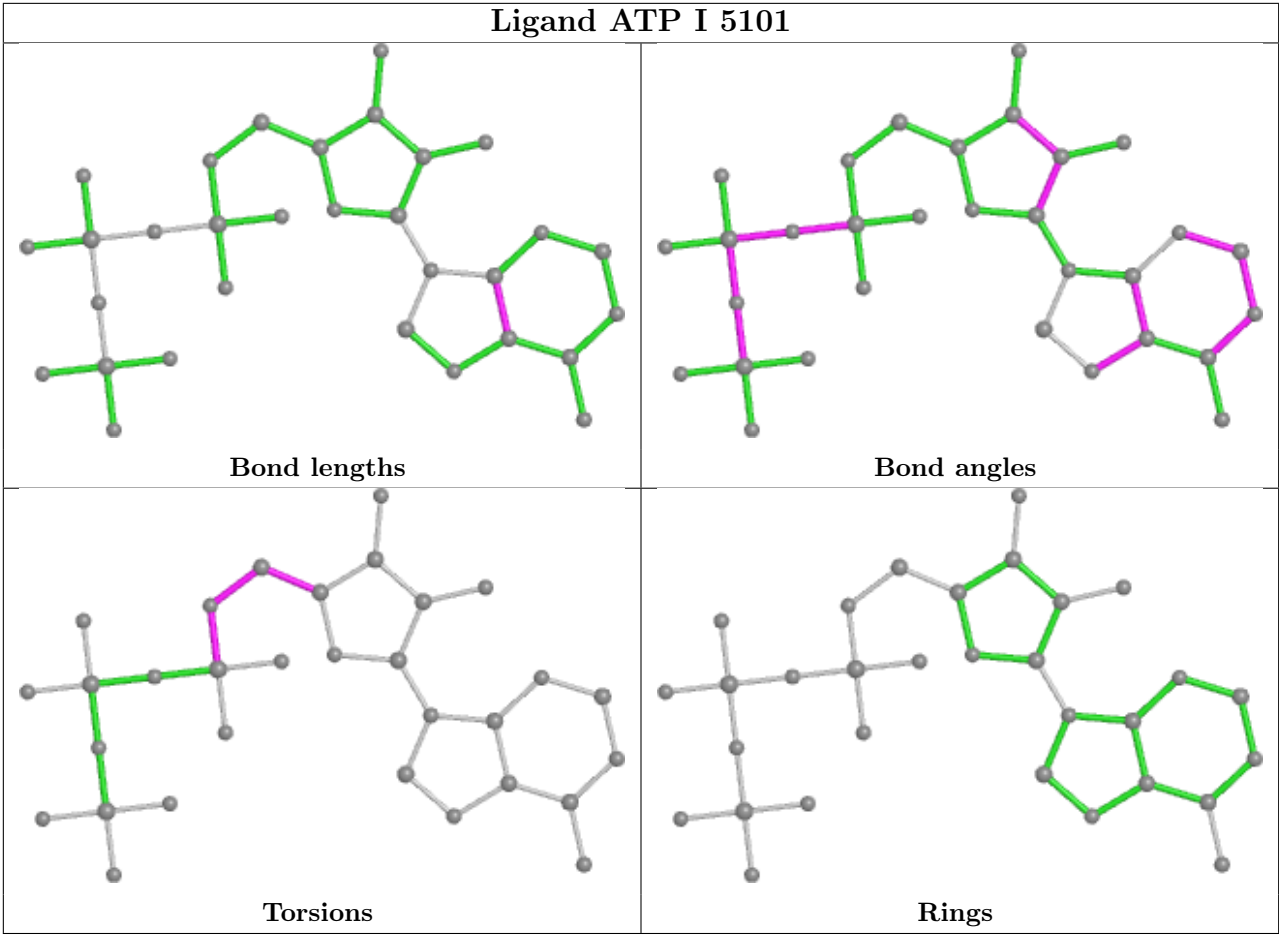
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	1	0
3	B	5101	ATP	1	0
3	G	5101	ATP	1	0
4	B	5102	CFF	1	0
4	G	5102	CFF	1	0
3	I	5101	ATP	1	0
4	E	5102	CFF	1	0
4	I	5102	CFF	1	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	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	72.44
1	E	4345:UNK	C	4540:PHE	N	72.44

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.44
1	G	4345:UNK	C	4540:PHE	N	72.44
1	B	3613:UNK	C	3639:THR	N	42.93
1	E	3613:UNK	C	3639:THR	N	42.93
1	I	3613:UNK	C	3639:THR	N	42.93
1	G	3613:UNK	C	3639:THR	N	42.93
1	B	4253:GLU	C	4320:UNK	N	27.35
1	E	4253:GLU	C	4320:UNK	N	27.35
1	I	4253:GLU	C	4320:UNK	N	27.35
1	G	4253:GLU	C	4320:UNK	N	27.35
1	B	3163:UNK	C	3170:UNK	N	16.17
1	E	3163:UNK	C	3170:UNK	N	16.17
1	I	3163:UNK	C	3170:UNK	N	16.17
1	G	3163:UNK	C	3170:UNK	N	16.17
1	B	3063:UNK	C	3134:UNK	N	14.81
1	E	3063:UNK	C	3134:UNK	N	14.81
1	I	3063:UNK	C	3134:UNK	N	14.81
1	G	3063:UNK	C	3134:UNK	N	14.81
1	B	2703:UNK	C	2734:ASN	N	14.74
1	E	2703:UNK	C	2734:ASN	N	14.74
1	I	2703:UNK	C	2734:ASN	N	14.74
1	G	2703:UNK	C	2734:ASN	N	14.74
1	B	3468:UNK	C	3511:UNK	N	14.16
1	E	3468:UNK	C	3511:UNK	N	14.16
1	I	3468:UNK	C	3511:UNK	N	14.16
1	G	3468:UNK	C	3511:UNK	N	14.16
1	B	3236:UNK	C	3241:UNK	N	13.24
1	E	3236:UNK	C	3241:UNK	N	13.24
1	I	3236:UNK	C	3241:UNK	N	13.24
1	G	3236:UNK	C	3241:UNK	N	13.24
1	B	2976:UNK	C	2995:UNK	N	12.70
1	E	2976:UNK	C	2995:UNK	N	12.70
1	I	2976:UNK	C	2995:UNK	N	12.70
1	G	2976:UNK	C	2995:UNK	N	12.70
1	B	1564:UNK	C	1573:MET	N	12.34
1	E	1564:UNK	C	1573:MET	N	12.34
1	I	1564:UNK	C	1573:MET	N	12.34
1	G	1564:UNK	C	1573:MET	N	12.34
1	B	3254:UNK	C	3261:UNK	N	8.53
1	E	3254:UNK	C	3261:UNK	N	8.53
1	I	3254:UNK	C	3261:UNK	N	8.53
1	G	3254:UNK	C	3261:UNK	N	8.53

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	6.12
1	E	1297:UNK	C	1430:UNK	N	6.12
1	I	1297:UNK	C	1430:UNK	N	6.12
1	G	1297:UNK	C	1430:UNK	N	6.12
1	B	2479:LEU	C	2487:UNK	N	3.24
1	E	2479:LEU	C	2487:UNK	N	3.24
1	I	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24
1	B	2939:ARG	C	2942:UNK	N	3.23
1	E	2939:ARG	C	2942:UNK	N	3.23
1	G	2939:ARG	C	2942:UNK	N	3.23
1	I	2939:ARG	C	2942:UNK	N	3.22

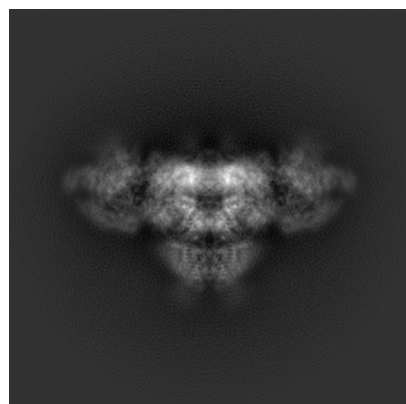
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8380. These allow visual inspection of the internal detail of the map and identification of artifacts.

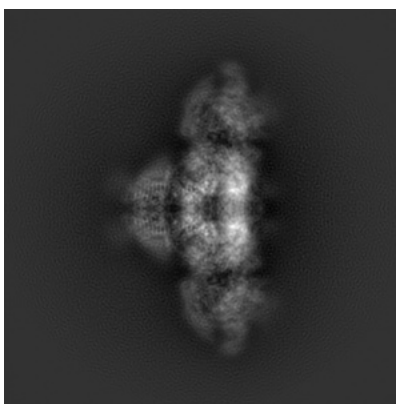
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

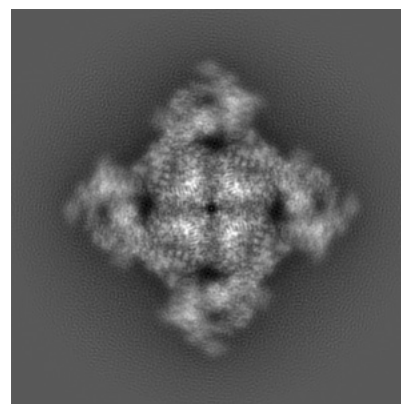
6.1.1 Primary map



X

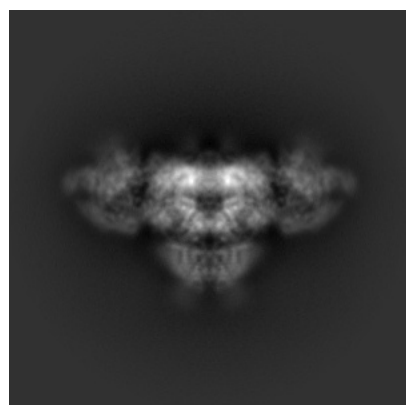


Y

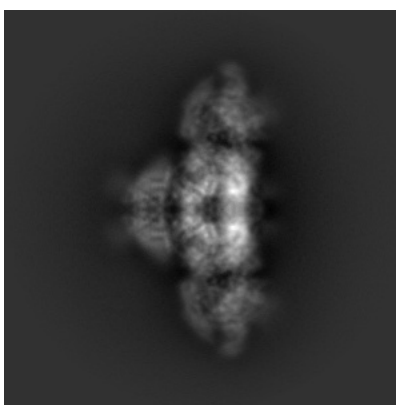


Z

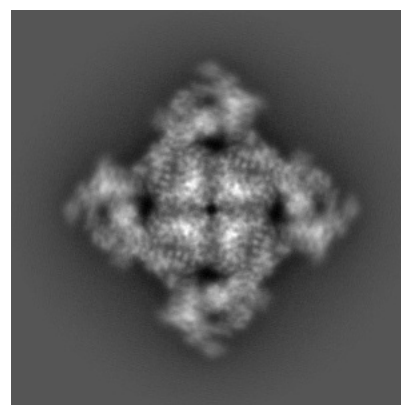
6.1.2 Raw map



X



Y

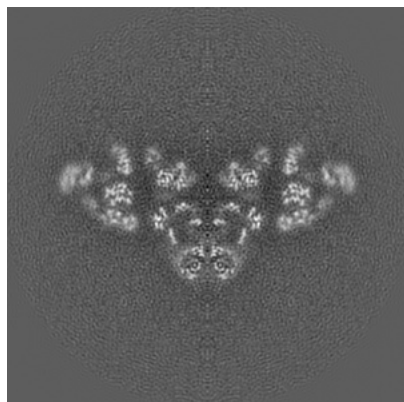


Z

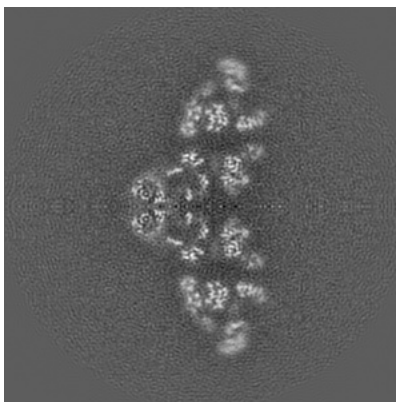
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

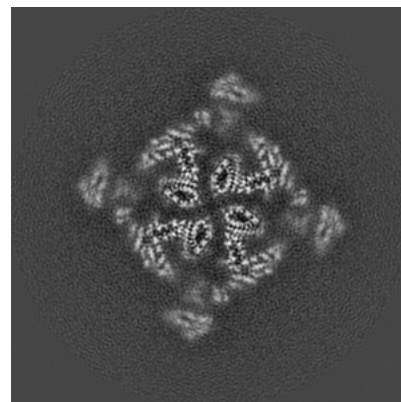
6.2.1 Primary map



X Index: 200

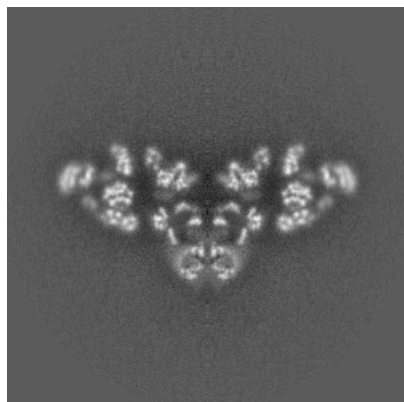


Y Index: 200

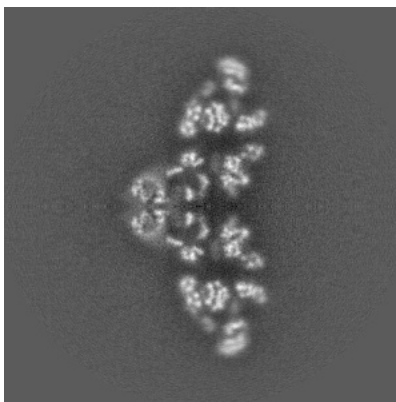


Z Index: 200

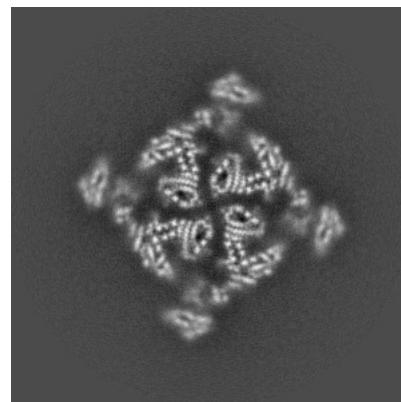
6.2.2 Raw map



X Index: 200



Y Index: 200

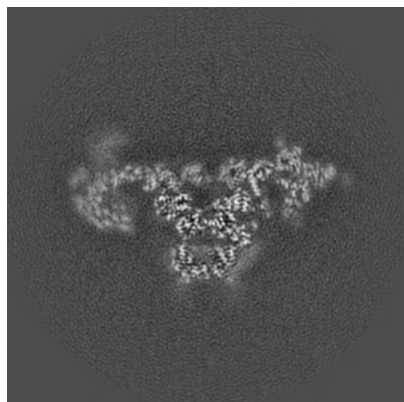


Z Index: 200

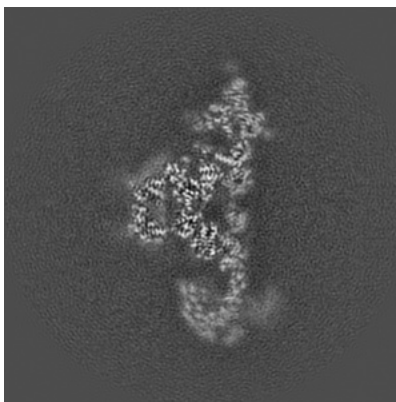
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

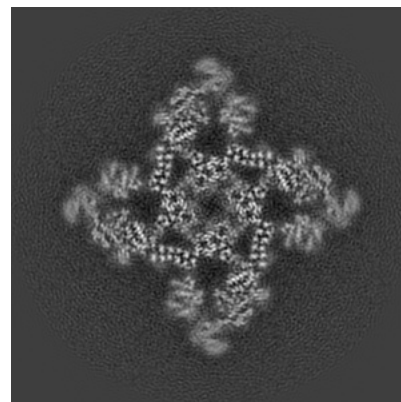
6.3.1 Primary map



X Index: 183

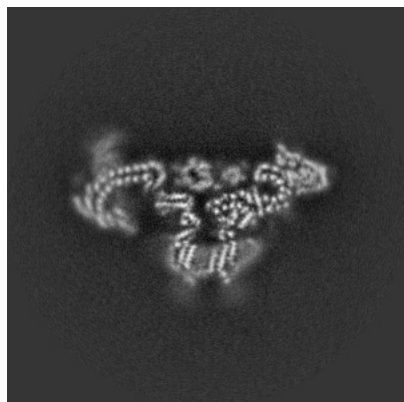


Y Index: 217

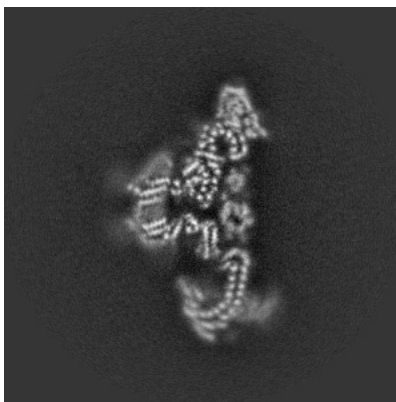


Z Index: 226

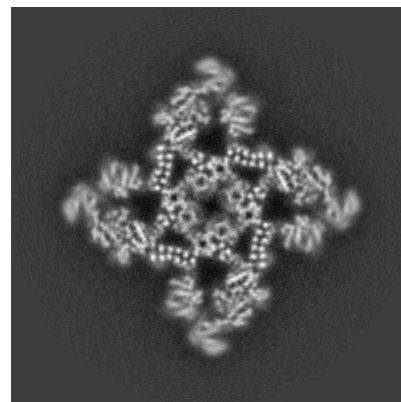
6.3.2 Raw map



X Index: 176



Y Index: 224

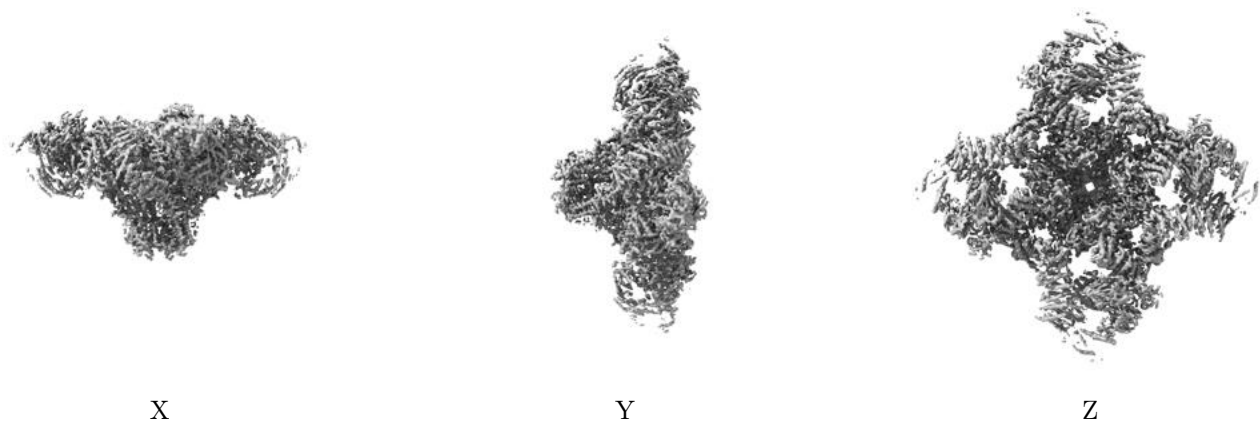


Z Index: 226

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



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.

6.4.2 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.

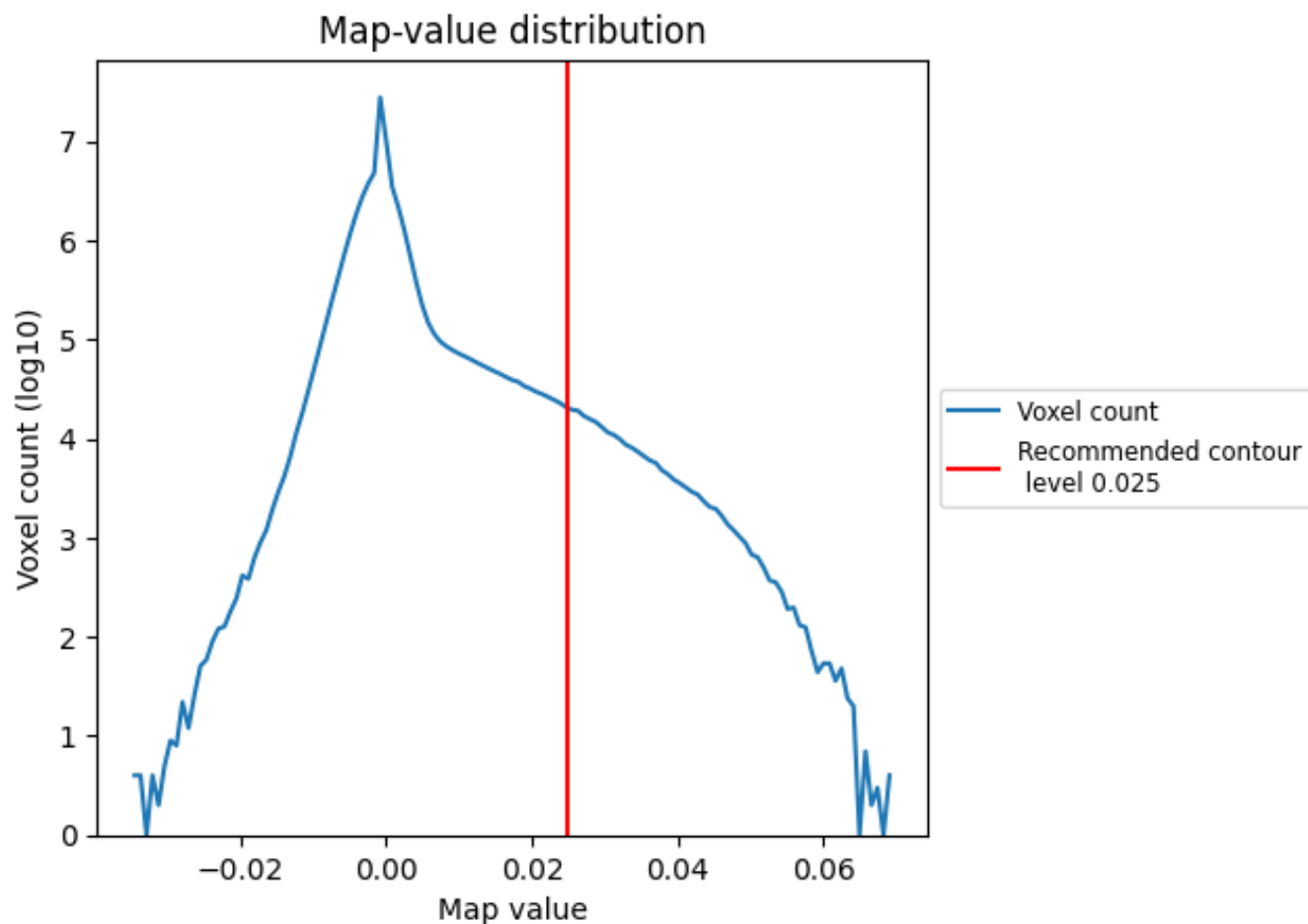
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

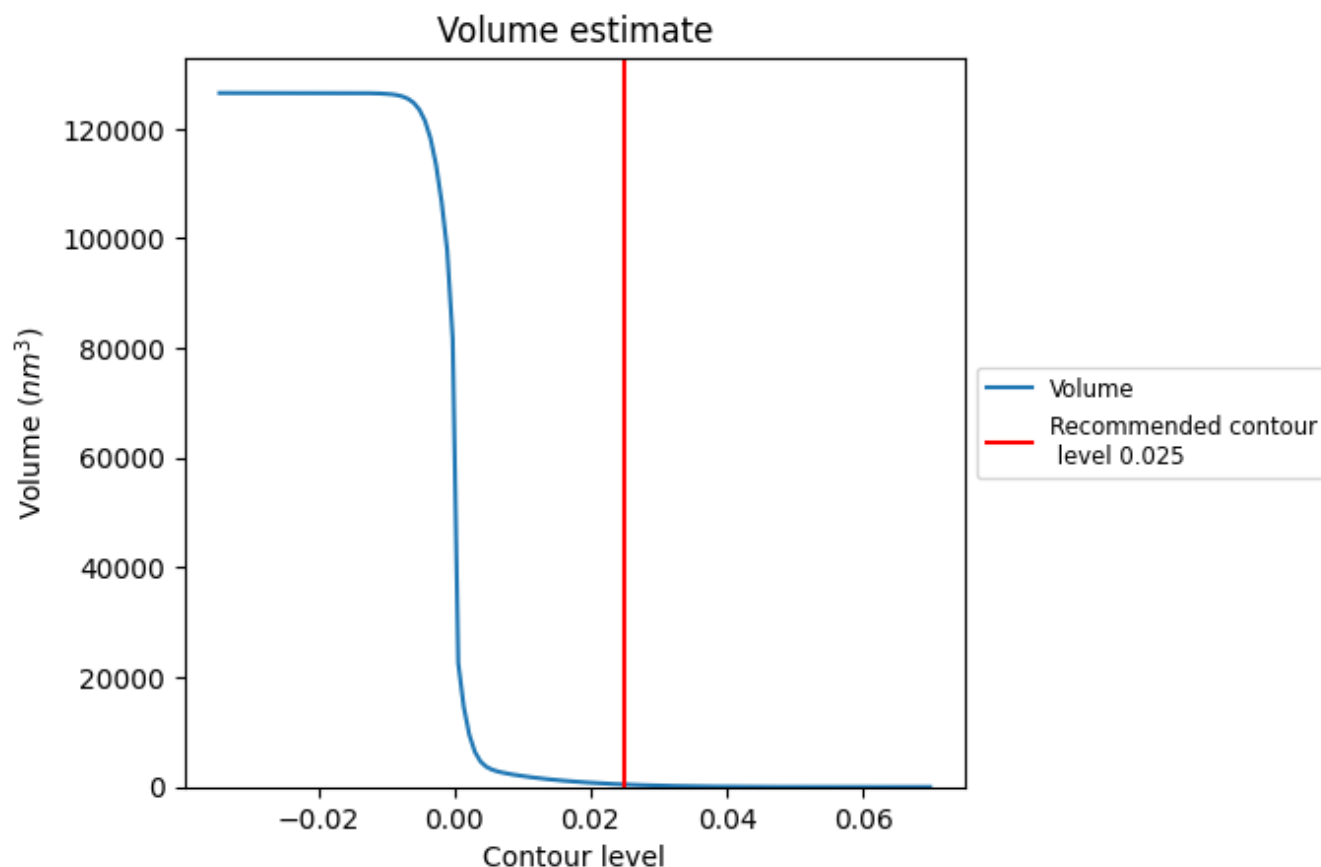
This section contains the results of statistical analysis of the map.

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.

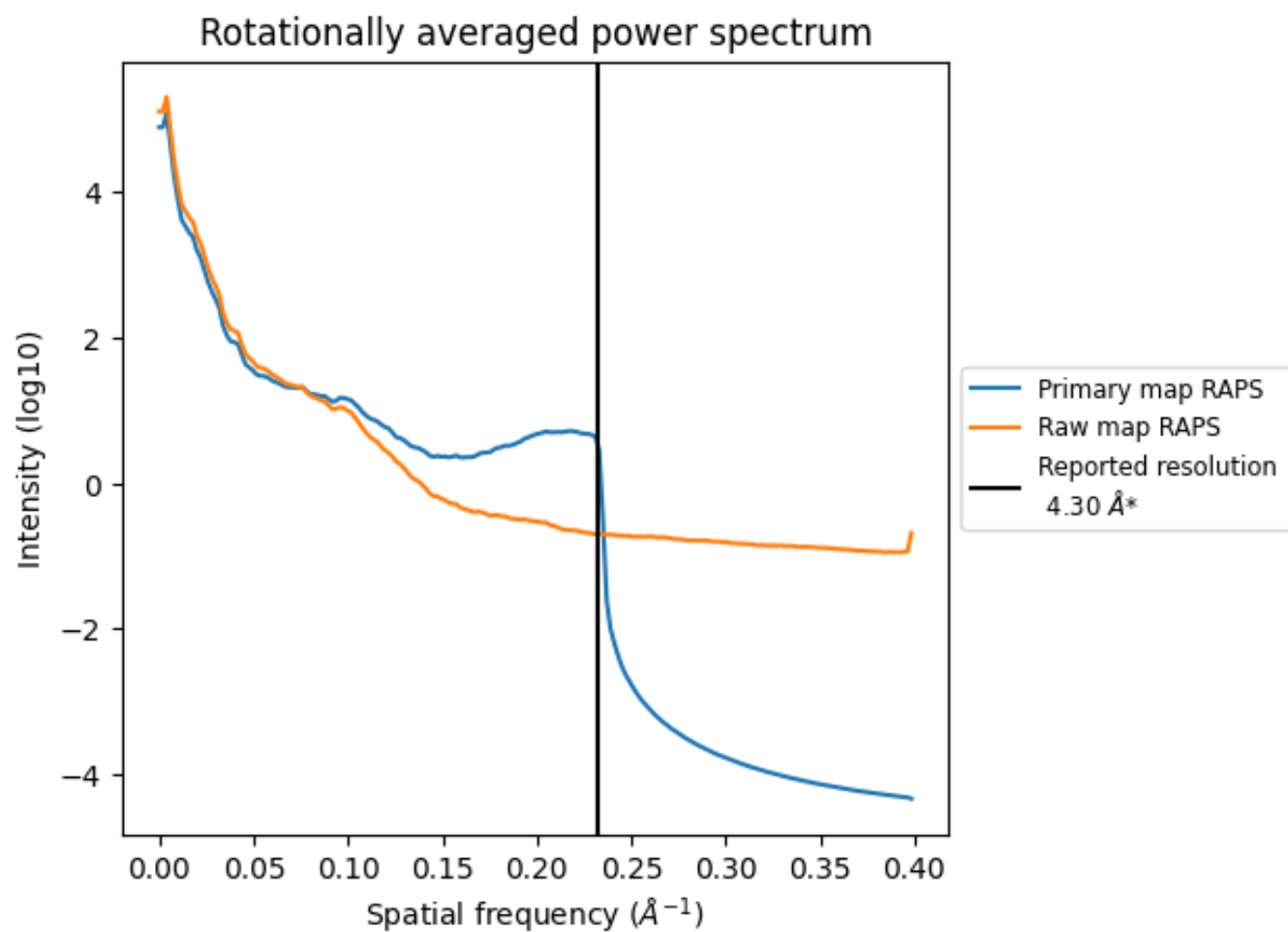
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 452 nm³; this corresponds to an approximate mass of 408 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 ⓘ

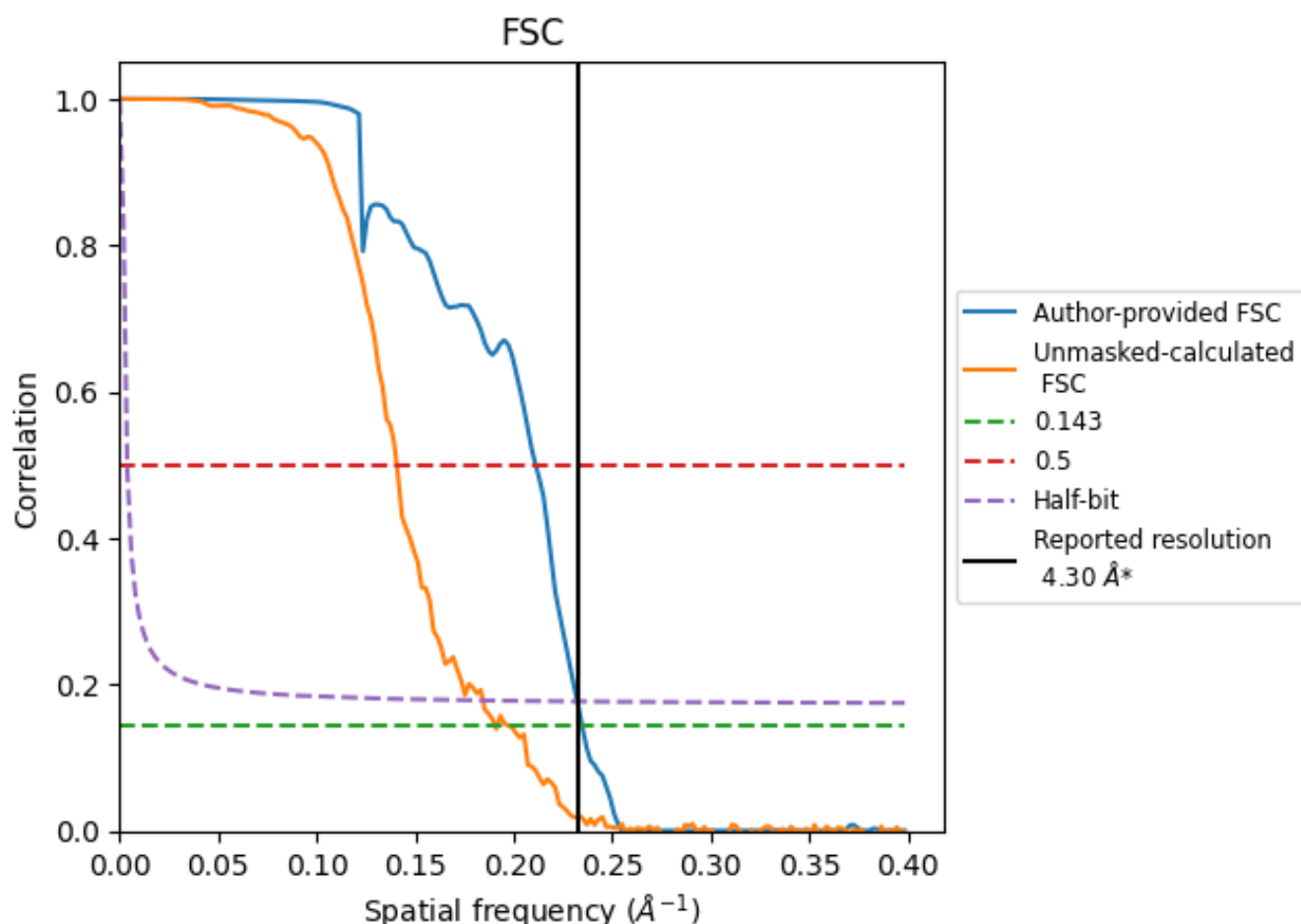


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 \AA^{-1}

8.2 Resolution estimates [i](#)

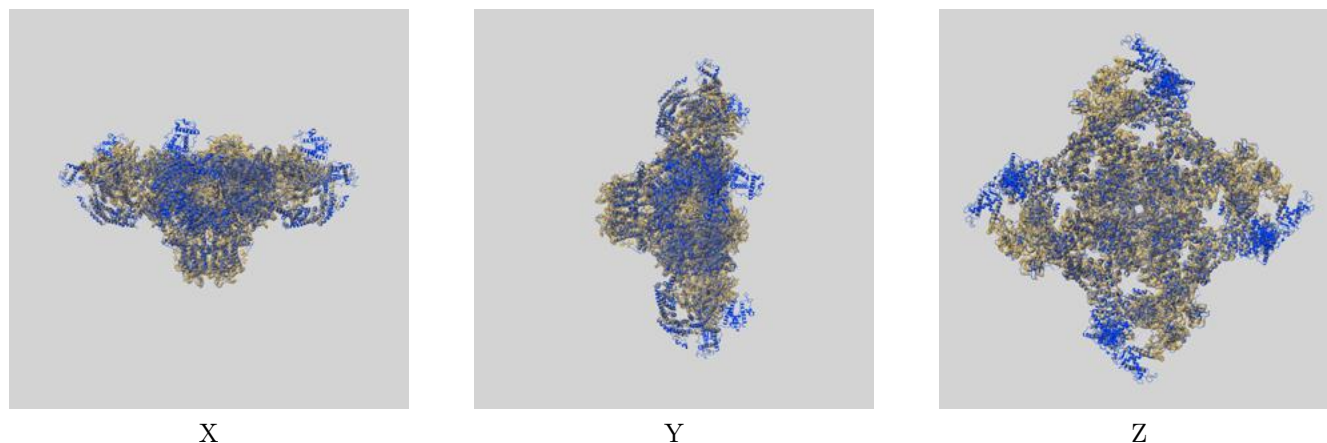
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.26	4.74	4.31
Unmasked-calculated*	5.24	7.11	5.43

*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 5.24 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

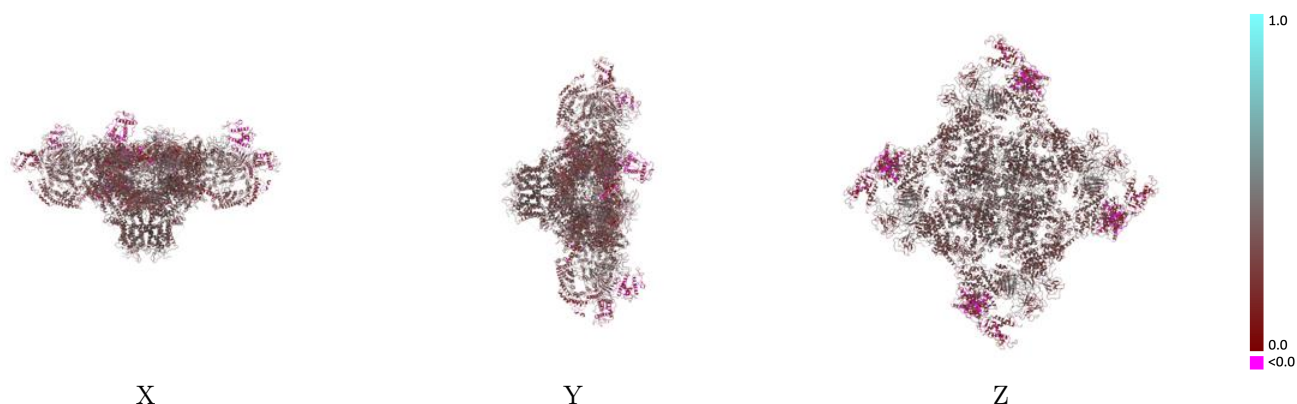
This section contains information regarding the fit between EMDB map EMD-8380 and PDB model 5TAN. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



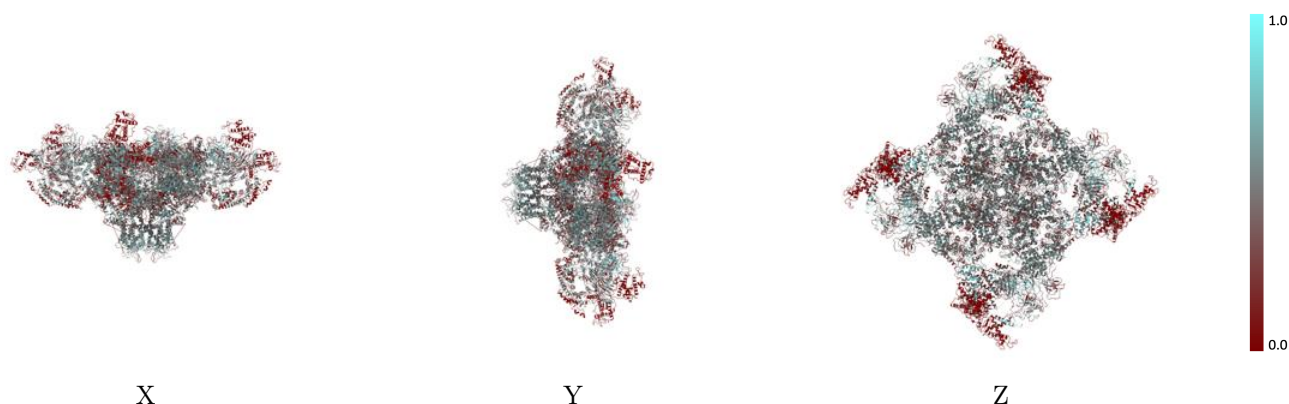
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



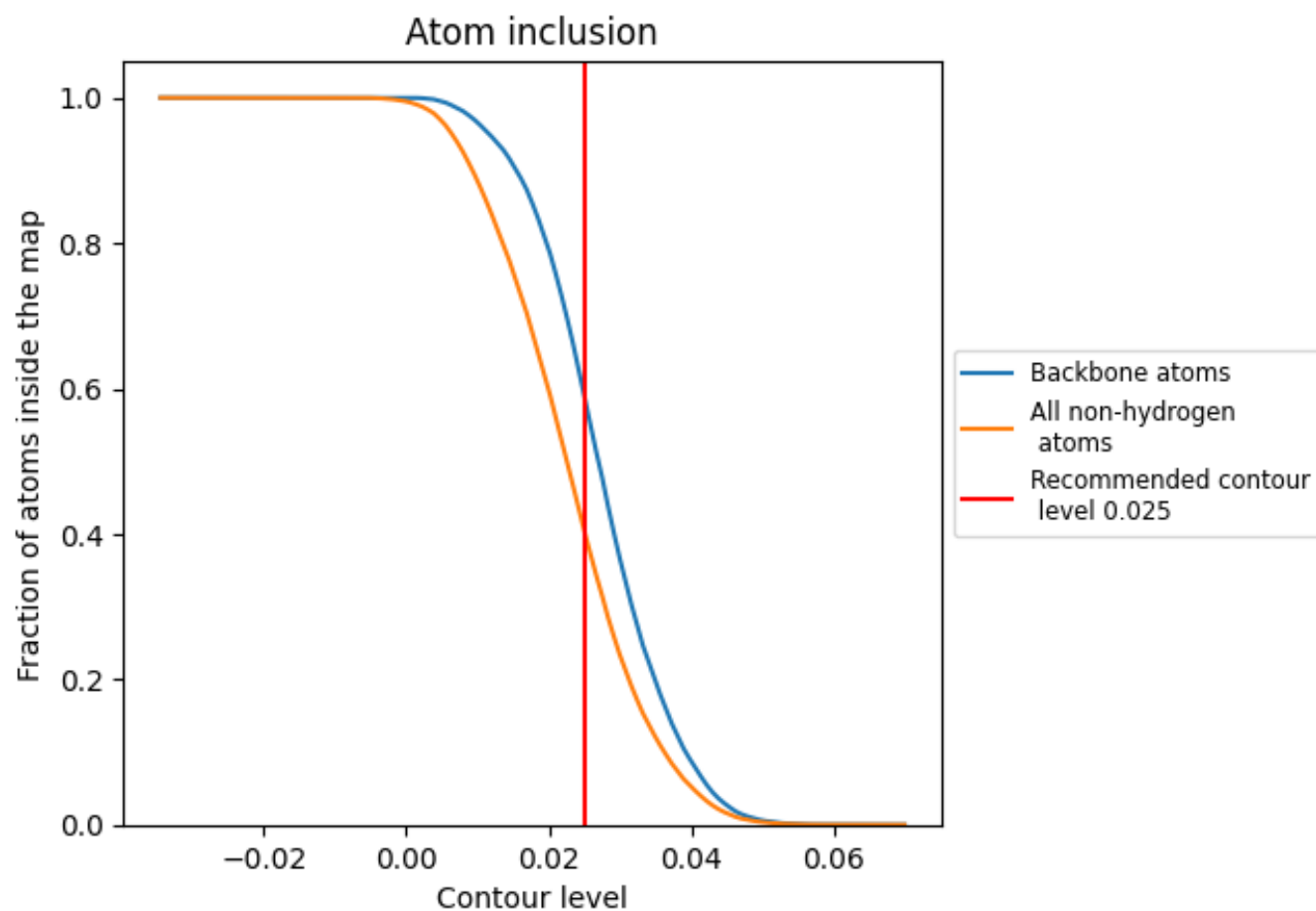
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 40% 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	<div></div> 0.4022	<div></div> 0.3150
A	<div></div> 0.3499	<div></div> 0.3180
B	<div></div> 0.4043	<div></div> 0.3140
E	<div></div> 0.4032	<div></div> 0.3140
F	<div></div> 0.3449	<div></div> 0.3230
G	<div></div> 0.4031	<div></div> 0.3140
H	<div></div> 0.3474	<div></div> 0.3230
I	<div></div> 0.4041	<div></div> 0.3140
J	<div></div> 0.3499	<div></div> 0.3190

1.0

0.0

<0.0