



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:30 PM UTC

PDB ID : 5TA3 / pdb_00005ta3
EMDB ID : EMD-8377
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

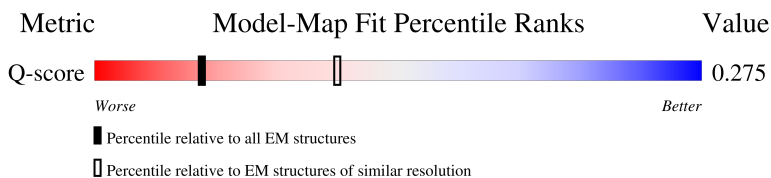
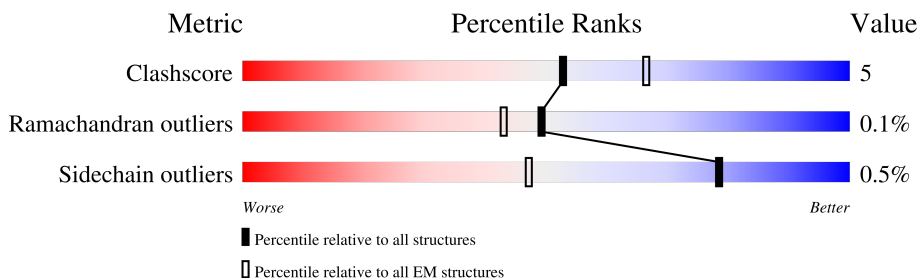
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	69% 76% 23% .
1	F	108	69% 72% 27% .
1	H	108	69% 73% 26% .
1	J	108	69% 71% 28% .

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Mol	Chain	Length	Quality of chain
2	B	4416	64% 83% 11% 5%
2	E	4416	63% 83% 12% 5%
2	G	4416	63% 83% 11% 5%
2	I	4416	63% 83% 12% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	B	5102	-	X	-	-
4	CFF	E	5102	-	X	-	-
4	CFF	G	5102	-	X	-	-
4	CFF	I	5102	-	X	-	-

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.

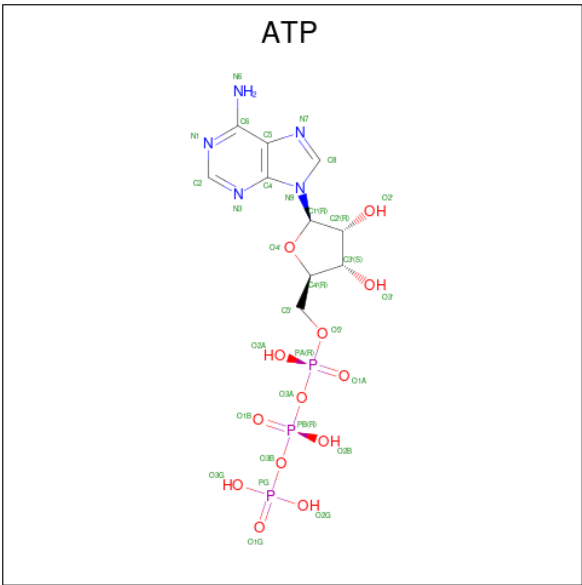
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

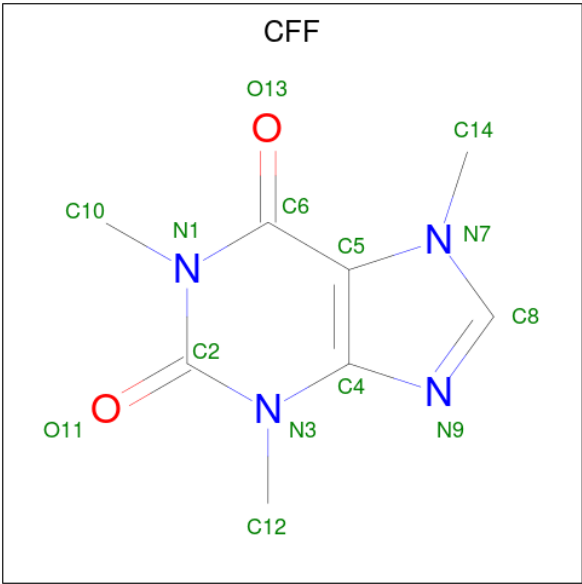
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

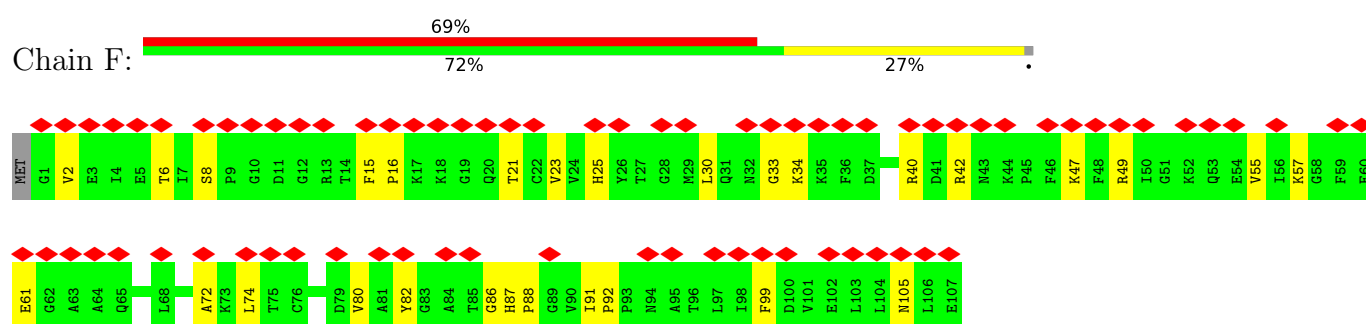
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

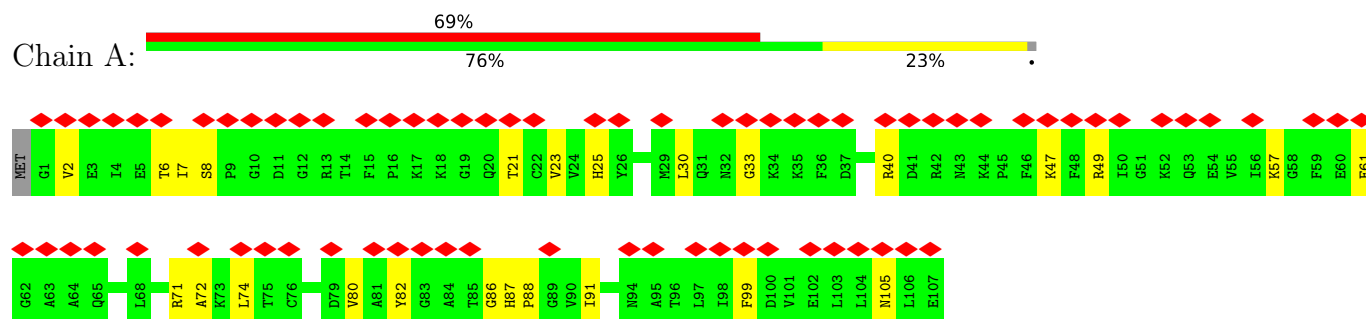
3 Residue-property plots [i](#)

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.

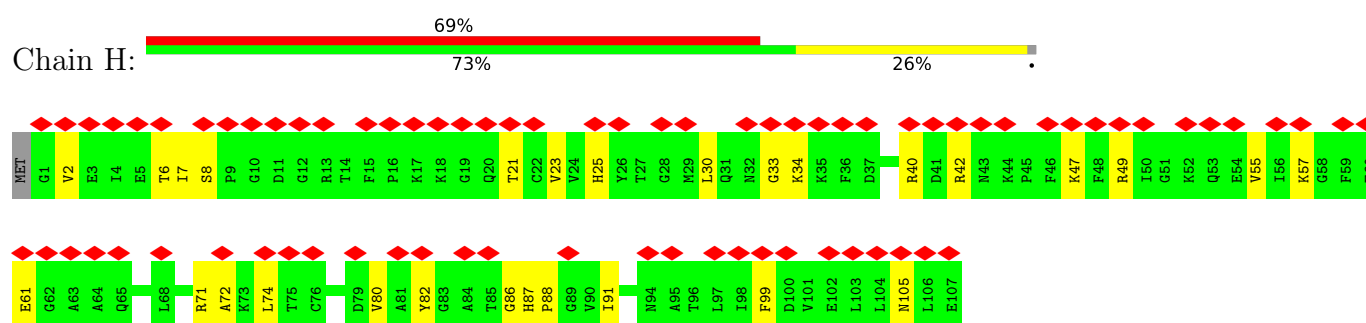
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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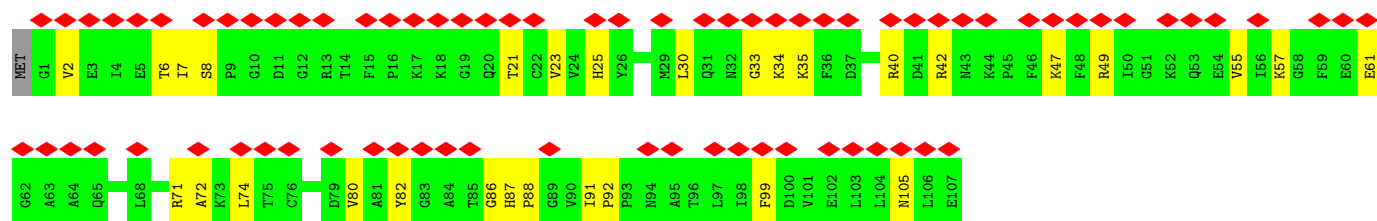


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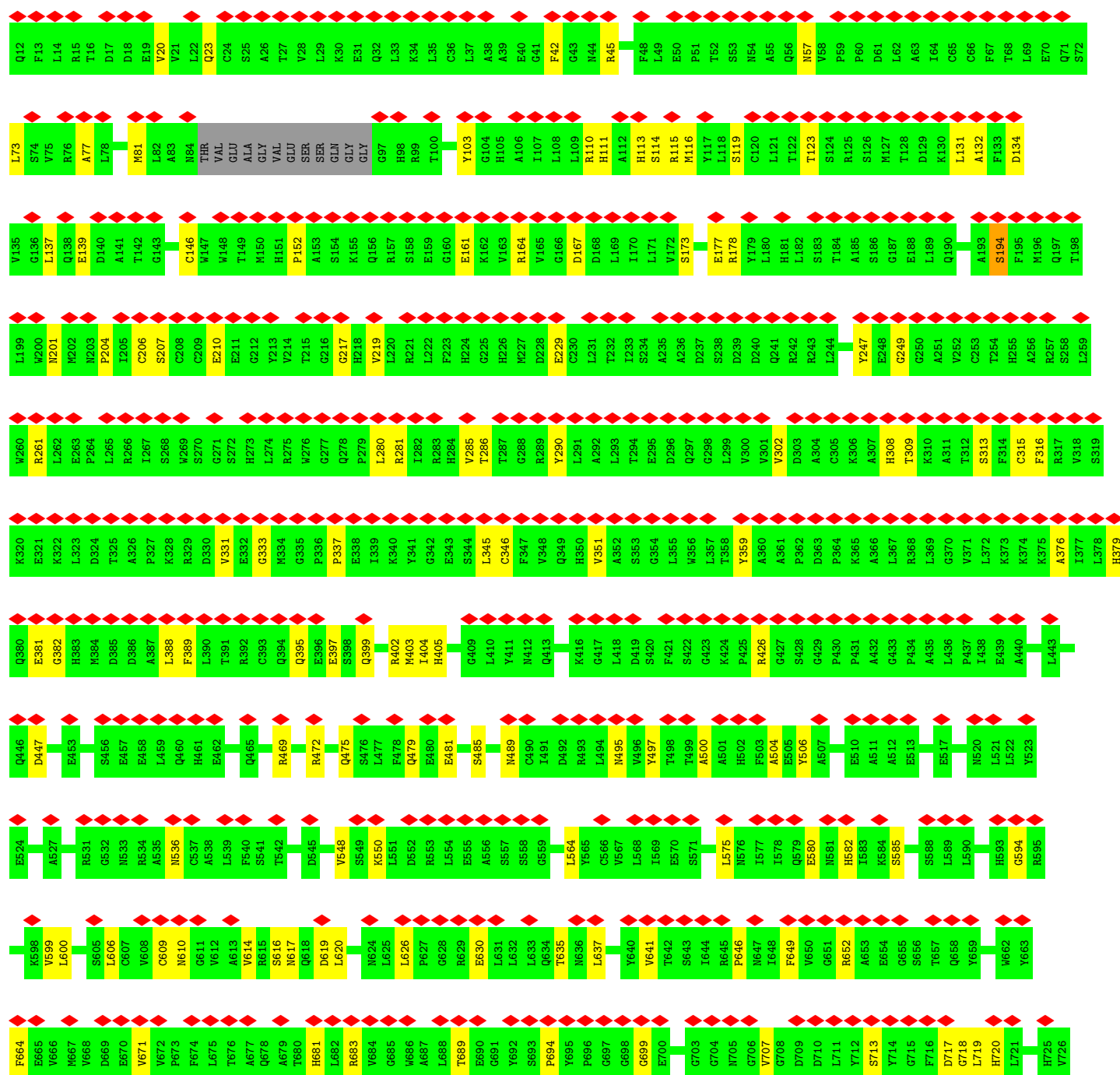
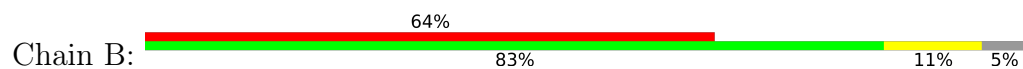


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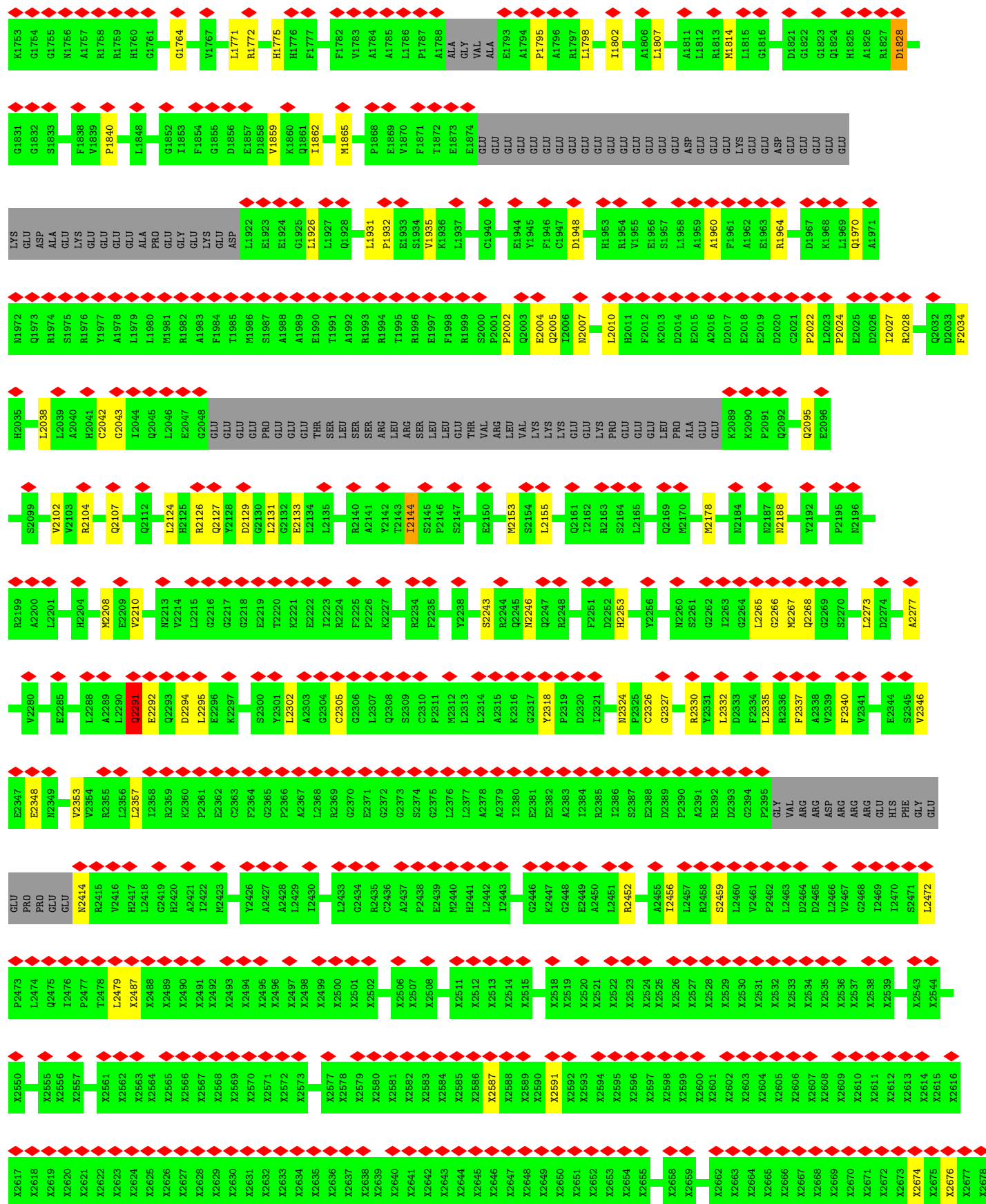




• Molecule 2: Ryanodine receptor 1

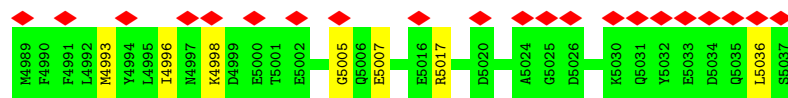


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M1608	F1612	L1613	Q1614	V1615	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	Q1629	C1630	Q1631	D1632	P1633	L1634	T1635	M1636	M1637	A1638	L1639	E1643	E1644	N1645	R1646	C1647	M1648	D1649	L1650	L1651	L1653	S1654	E1655	R1656	L1657	Q1660	R1661	H1665	T1666	L1667	R1671	A1672	V1673	C1674	A1675								
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I1228	N1229	M1230	Q1231	R1232	T1235	T1236	K1240	S1241	L1242	P1243	Q1244	F1245	E1251	H1254	E1256	V1257	A1258	R1259	M1260	D1261	T1262	T1263	V1264	D1265	T1266	P1267	P1268	C1269	L1270	R1271	L1272	L1273	H1274	R1275	X1276	X1277	X1278	X1279	X1280	X1281	X1282	X1283	X1284	X1285	X1286	X1287	X1297	X1430	X1434	X1435	X1436	X1437							
T1163	L1164	M1165	G1166	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	I1182	E1183	I1184	G1185	D1186	G1187	F1188	V1191	C1192	S1193	L1194	G1195	Q1198	V1199	G1200	H1201	L1202	L1203	L1204	G1205	Q1206	D1207	V1208	S1209	S1210	L1211	R1212	F1213	F1214	A1215	I1216	C1217	G1218	L1219	Q1220	E1221	G1222	F1223	A1227				
G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	Y1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	V1123	F1124	M1125	G1126	H1127	R1128	G1129	Q1130	R1131	W1132	H1133	L1134	G1135	S1136	E1137	P1138	F1139	G1140	R1141	P1142	W1143	S1145	G1146	D1147	V1148	V1149	G1150	C1151	M1152	I1153	L1155	T1156	E1157	M1158	T1159	I1160	I1161	F1162		
Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	SER	ARG	TRP	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Q1084	S1085	G1086	R1087	W1088	Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	V1102				
H974	V975	R976	L977	T978	P979	Q981	T982	T983	L984	V985	D986	R987	L988	A989	E990	R991	G992	A997	R998	D999	R1000	V1001	A1002	Q1003	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040				
C954	P955	V956	D957	THR	VAL	GLN	I961	V962	L963	P964	P965	H966	L967	R968	R969	I970	R971	E972	K973	L974	A975	E976	N977	I978	H979	E980	L981	W982	A983	L984	T985	R986	I987	E988	Q989	G990	W991	T992	Y993	G994	P995	V996	R997	D998	D999	N990	K991	R992	L993	H994	C995	L996	S997	H998	T999	D999	P999	L999	
P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	N941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M960	N961	S962	N963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973
A727	R728	P729	V730	T731	S732	P733	Q734	Q735	H736	L737	L738	A739	P740	E741	L803	D742	S745	C746	C747	L748	D749	L750	V751	V752	P753	S754	F757	R758	I759	N760	G761	C762	P763	V764	Q765	G766	V767	F768	E769	A770	F771	N772	L773	D774	G775	L776	F777	F778	P779	V780	V781	S782	F783	S784	A785	G786	V787	K788	
V789	R790	F791	L792	G793	G795	R796	H797	G798	E799	F800	K801	F802	P804	P805	P806	G807	Y808	H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	E824	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	S843	R844	C845	L846	S847	H848	T849	D850	P851	V852	P853					

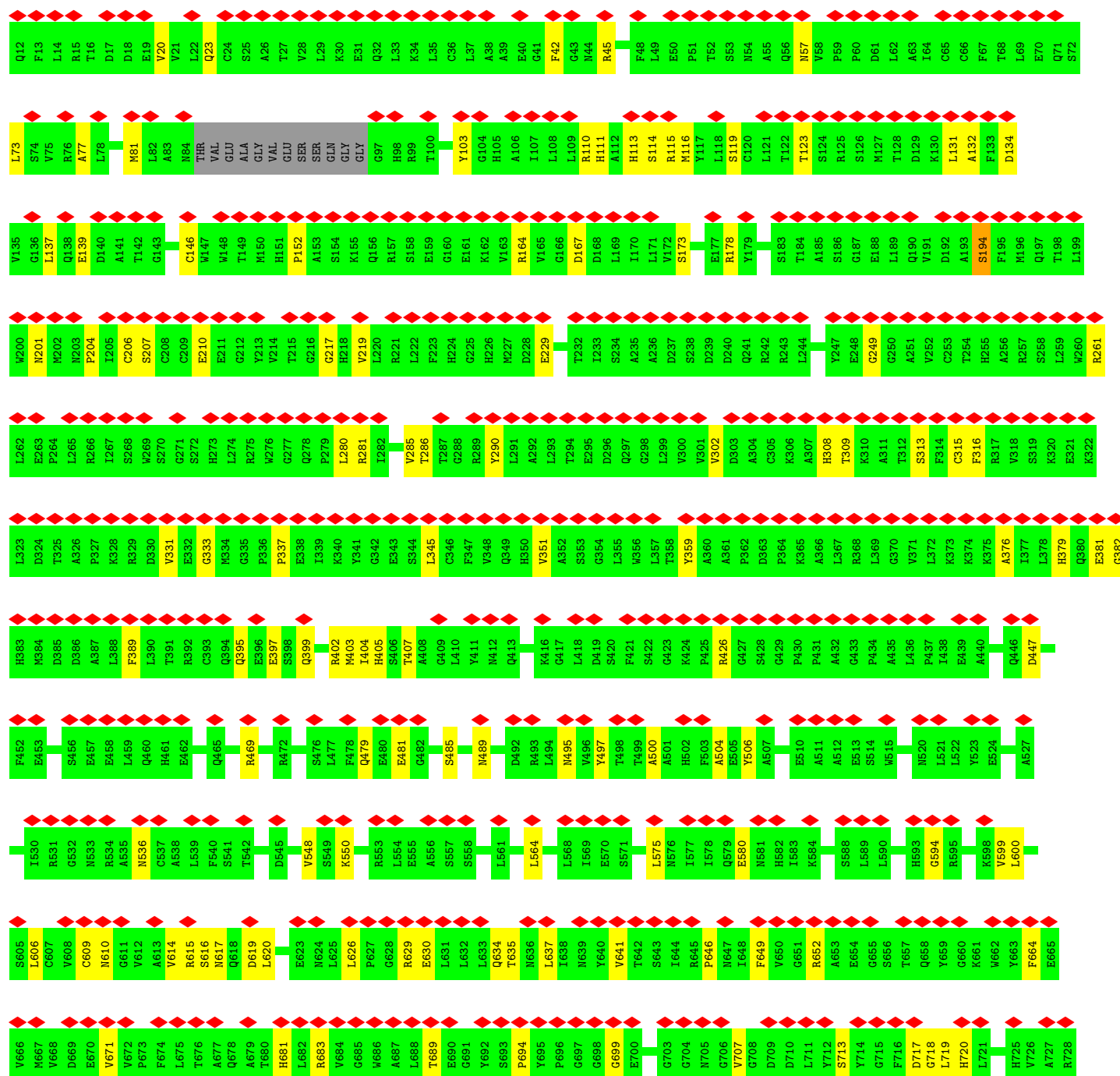
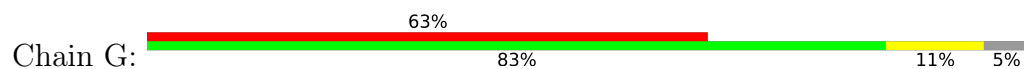


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X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518																			
X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414																		
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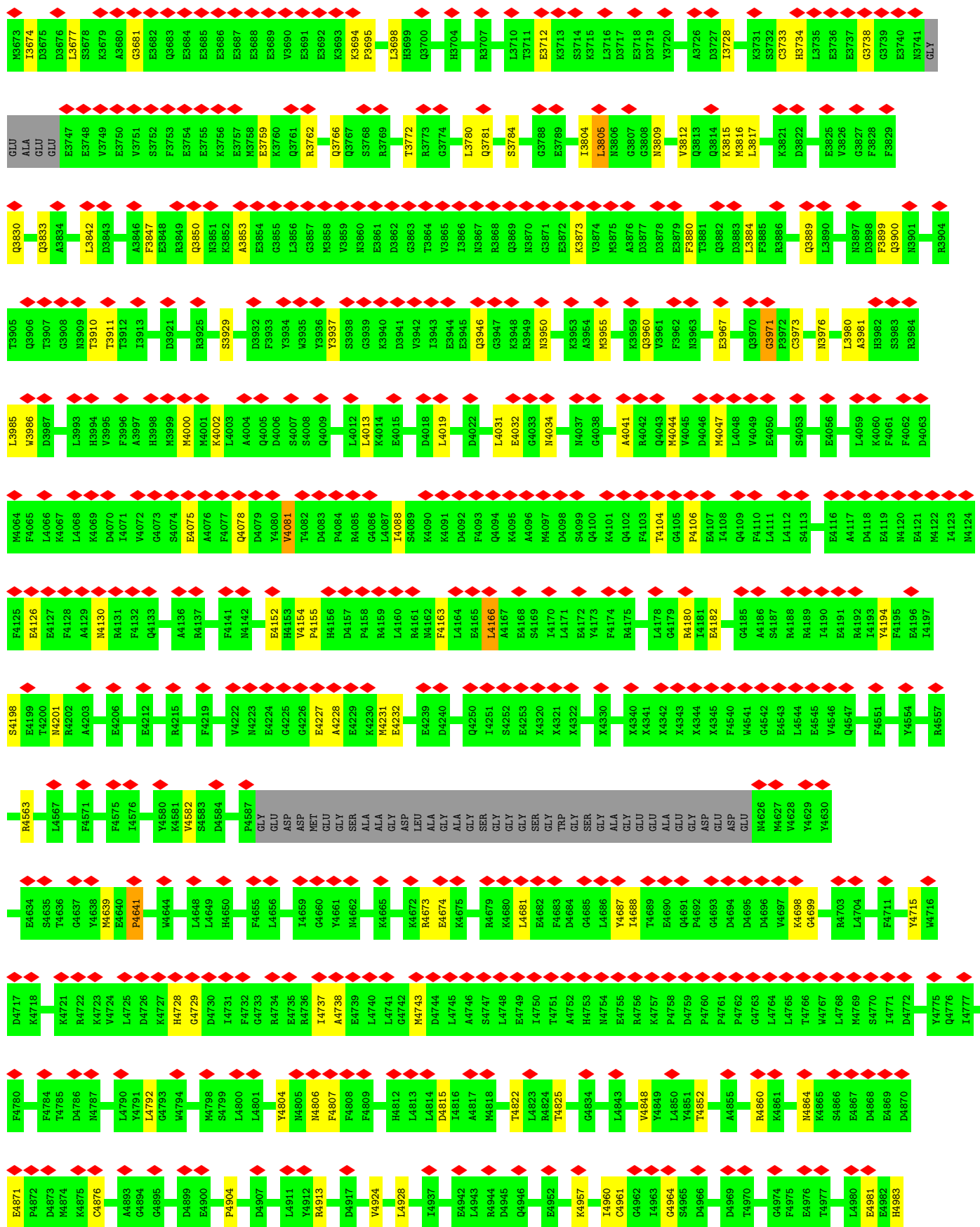
• Molecule 2: Ryanodine receptor 1

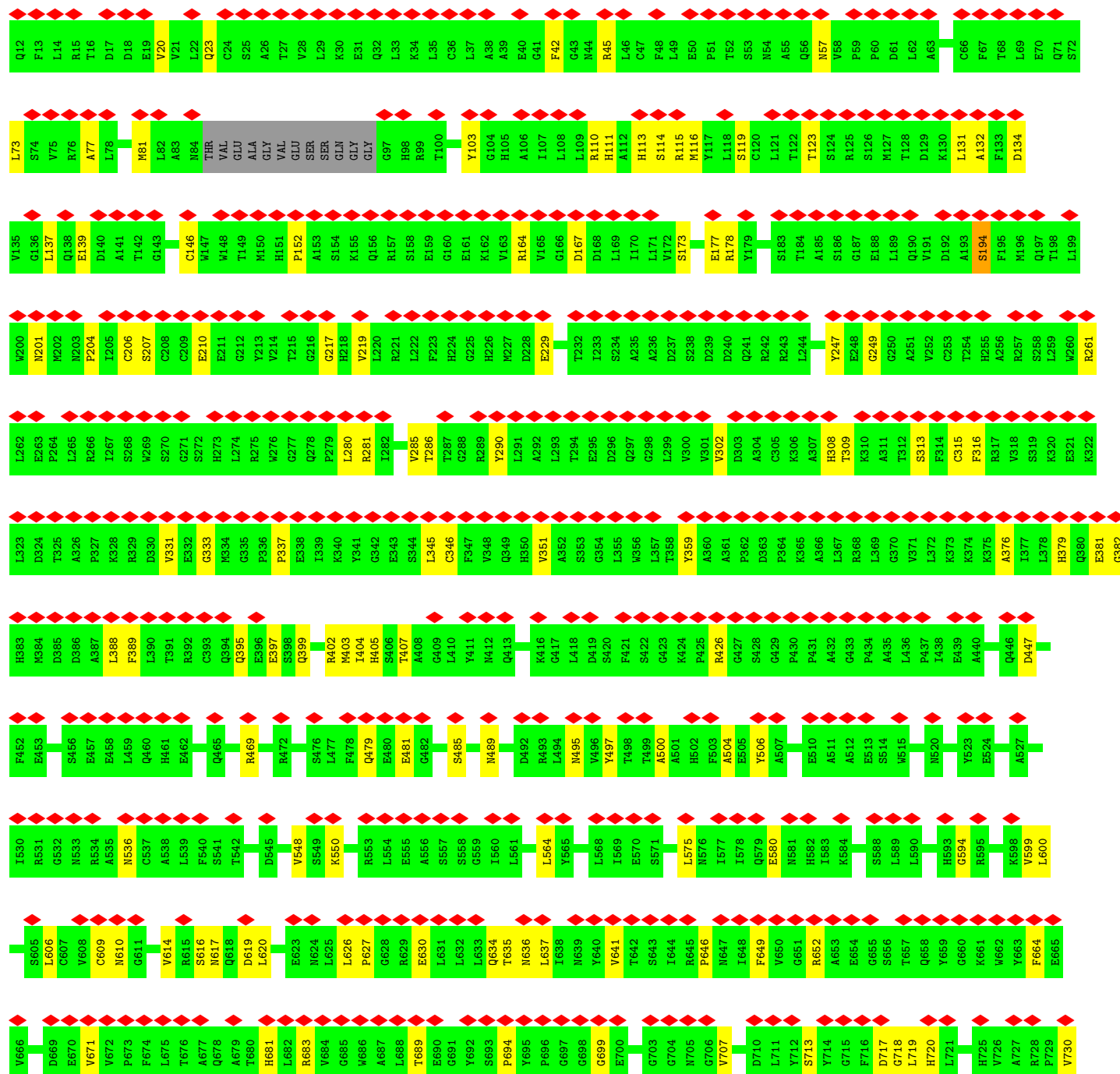


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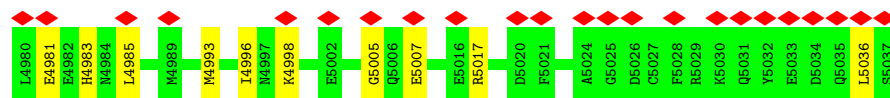




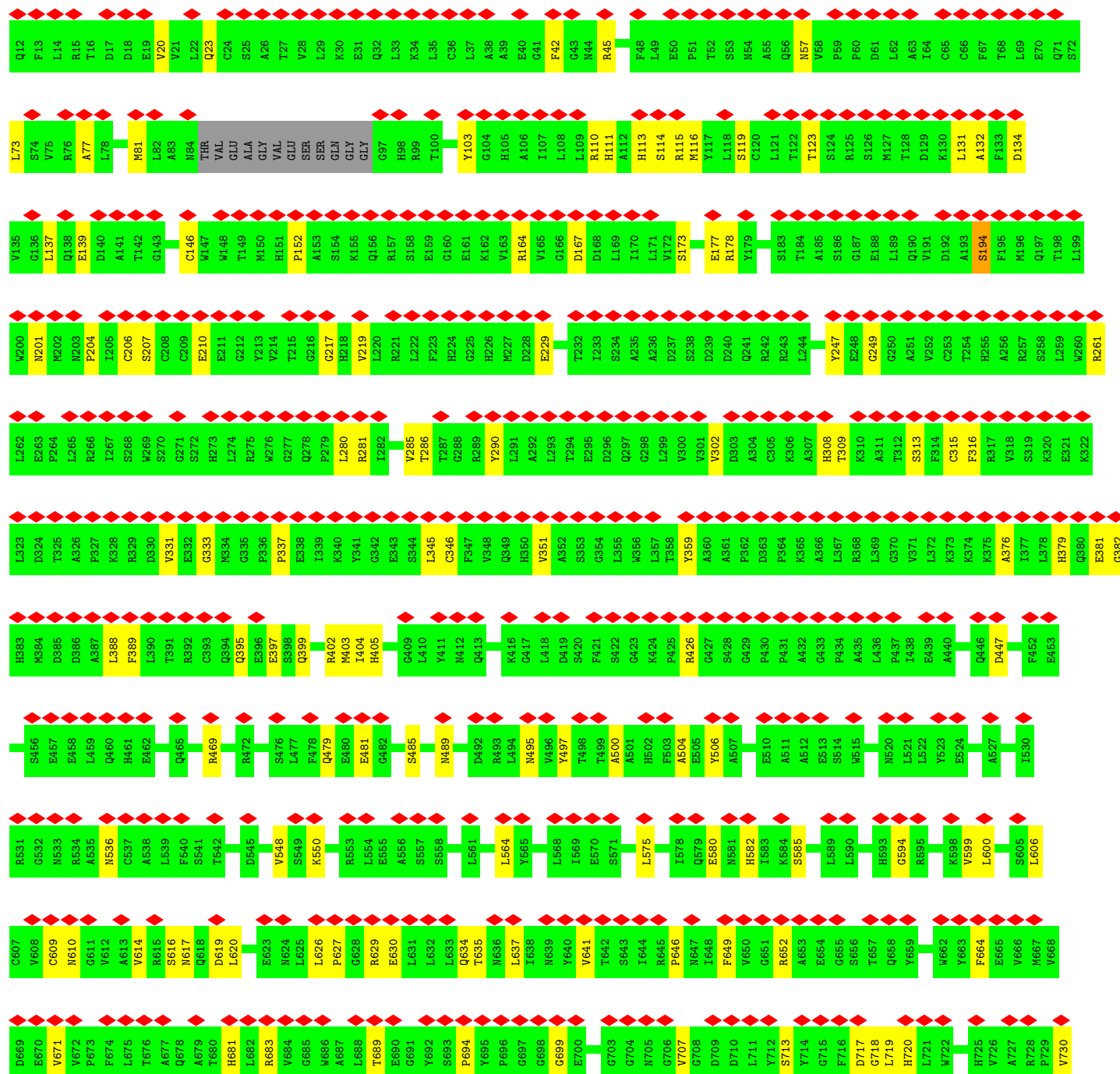
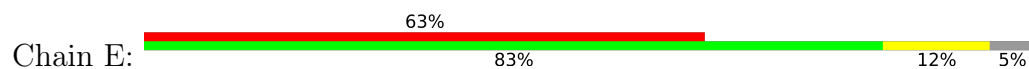


WORLDWIDE
PDB
PROTEIN DATA BANK

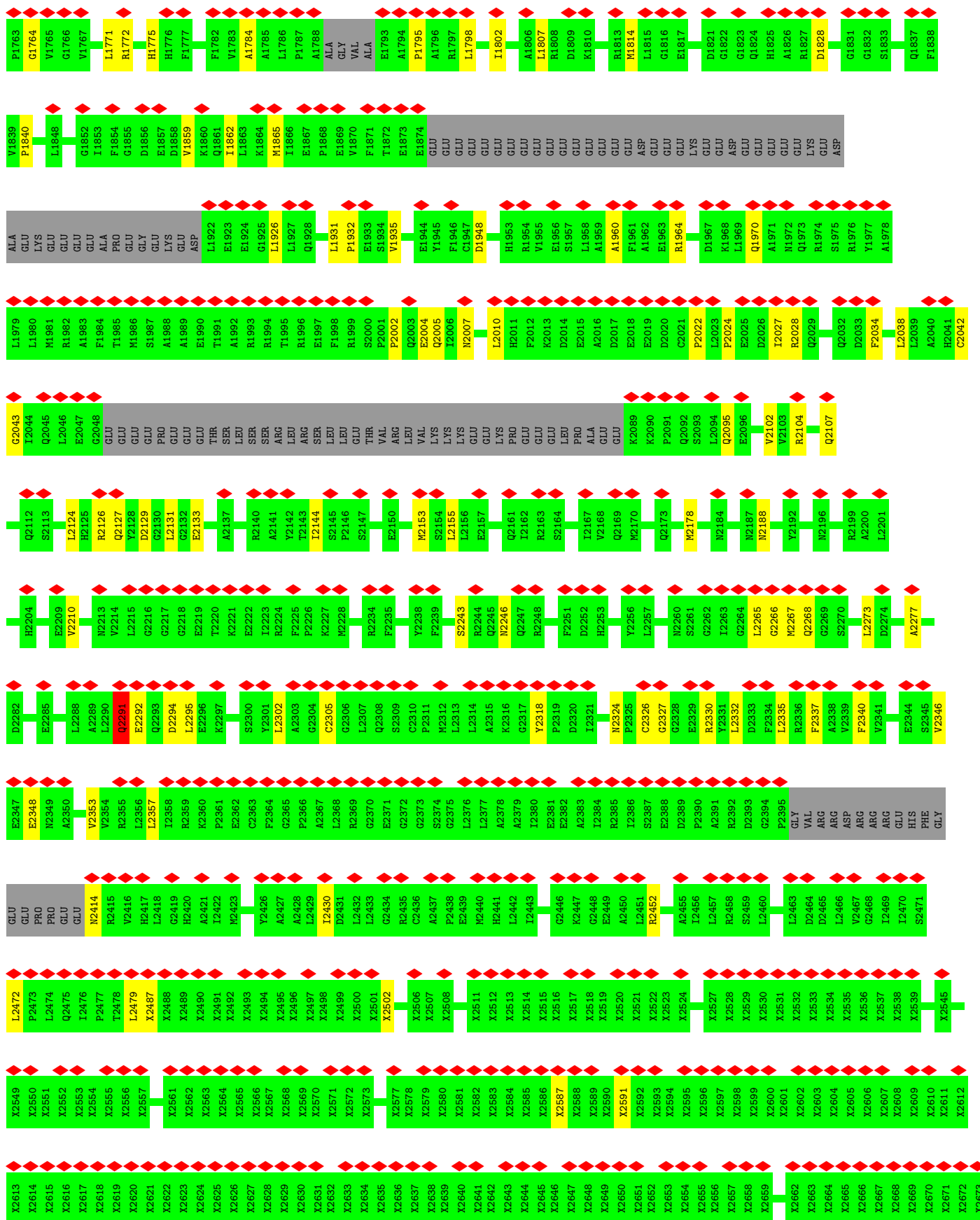




• Molecule 2: Ryanodine receptor 1

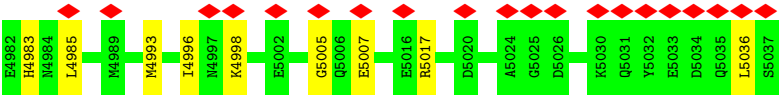


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X1447	X1448	X1449	X1450	X1451	X1452	X1457	X1458	X1459	X1460	X1464	X1473	X1474	X1475	X1476	X1479	X1480	X1486	X1487	X1488	X1489	X1492	X1497	X1502	X1503	X1504	X1505	X1506	X1507	X1510	X1511	X1512	X1513	X1514	X1515	X1516	X1519	X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532																																				
K1240	S1241	L1242	Q1243	Q1244	F1245	E1251	H1254	Y1255	E1256	V1257	A1258	R1259	M1260	D1261	G1262	T1263	V1264	D1265	T1266	P1267	C1268	C1269	L1270	R1271	L1272	A1273	R1274	R1275	X1276	X1277	X1278	X1279	X1280	X1281	X1282	X1283	X1284	X1285	X1286	X1287	X1297	X1430	X1434	X1435	X1436	X1437	X1438	X1439	X1442	X1443	X1444	X1445	X1446																																
D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	I1182	E1183	I1184	G1185	D1186	G1187	F1188	V1191	C1192	S1193	L1194	G1195	Q1198	V1199	G1200	H1201	L1202	M1203	L1204	G1205	Q1206	D1207	V1208	S1209	S1210	L1211	R1212	F1213	F1214	A1215	I1216	C1217	G1218	L1219	Q1220	E1221	G1222	F1223	F1226	A1227	I1228	M1229	M1230	Q1231	R1232	T1236																														
R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	A1118	E1119	L1120	A1121	Y1122	V1123	F1124	M1125	G1126	H1127	R1128	G1129	Q1130	R1131	W1132	H1133	L1134	G1135	S1136	E1137	P1138	F1139	G1140	R1141	P1142	W1143	Q1144	S1145	G1146	D1147	V1148	G1150	C1151	M1152	I1153	D1154	L1155	T1156	E1157	M1158	T1159	I1160	I1161	F1162	T1163	M1164	M1165	L1169	M1170	S1171																												
L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	ASN	SER	GLN	ARG	THR	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	Q1084	S1085	G1086	R1087	W1088	Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109																												
T978	P979	A980	Q981	T982	T983	L984	V985	D986	L988	A989	E990	N991	G992	D999	R1000	V1001	A1002	Q1003	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	T9953	K954	L955	P956	K957	T9958	Y959	N9960	N961	S962	N963	G964	Y965	K966	A968	P969	L970	H911	S912	L913	E915	P916	E917																												
R918	N919	Y920	N921	L922	Q923	M924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	N941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	N9960	N961	S962	N963	G964	Y965	K966	A968	P969	L970	H911	S912	L913	E915	P916	E917																												
THR	VAL	GLN	I961	V962	L963	P964	P965	H966	L967	E968	R969	I970	R971	E972	K973	L974	A975	E976	N977	I978	H979	E980	L981	W982	A983	L984	T985	R986	I987	E988	Q989	G990	W991	T992	Y993	G994	P995	V996	R997	D998	D999	N900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	E915	P916	E917																											
G794	G795	R796	H797	G798	E799	F800	K901	F802	L803	P804	P805	P806	G807	Y808	A809	H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	E824	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	S843	R844	C845	L846	S847	H848	T849	D850	F851	V852	P853	C854	P855	V856	D857																													





E4871	E4872	D4873	M4874	K4875	C4876	Y4888	A4893	G4894	G4895	D4899	E4900	P4904	D4907	L4911	M4912	R4913	F4907	F4908	F4909	H4812	L4813	L4814	D4815	L4816	G4742	M4743	D4744	L4745	A4746	S4747	L4748	E4749	L4750	T4751	A4752	H4753	V4848	Y4849	L4850	Y4851	T4852	A4855	R4860	K4861	M4864	K4865	F4975	E4976	T4977	L4980	E4981																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
Q4776	I4777	F4780	F4784	T4785	D4786	M4787	L4790	Y4791	L4792	G4793	M4794	L4800	L4801	Y4804	M4805	M4806	F4807	F4808	F4809	H4812	L4813	L4814	D4815	L4816	G4742	M4743	D4744	L4745	A4746	S4747	L4748	E4749	L4750	T4751	A4752	H4753	V4848	Y4849	L4850	Y4851	T4852	A4855	R4860	K4861	M4864	K4865	F4975	E4976	T4977	L4980	E4981																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
Y4715	M4716	D4717	K4718	K4721	R4722	K4723	V4724	L4725	D4726	K4727	H4728	G4729	D4730	I4731	F4732	G4733	R4734	E4735	R4736	I4737	A4738	E4739	L4740	L4741	G4742	M4743	D4744	L4745	A4746	S4747	L4748	E4749	L4750	T4751	A4752	H4753	V4848	Y4849	L4850	Y4851	T4852	A4855	R4860	K4861	M4864	K4865	F4975	E4976	T4977	L4980	E4981																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
Y4629	Y4630	E4634	S4635	T4636	G4637	M4638	E4639	E4640	P4641	M4644	L4648	L4649	M4650	F4655	L4656	C4657	I4658	I4659	G4660	Y4661	M4662	K4665	R4673	E4674	K4675	E4676	R4679	K4680	L4681	E4682	F4683	D4684	G4685	L4686	Y4687	T4688	G4690	Q4691	P4692	G4693	D4694	D4695	D4696	V4697	K4698	G4699	R4703	L4704	F4711																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
R4557	R4558	L4559	F4560	F4561	F4562	F4563	F4564	F4565	F4566	F4567	F4568	F4569	F4570	F4571	F4572	F4573	F4574	F4575	F4576	F4577	F4578	F4579	F4580	F4581	F4582	F4583	F4584	F4585	F4586	F4587	F4588	F4589	F4590	F4591	F4592	F4593	F4594	F4595	F4596	F4597	F4598	F4599	F4600	F4601	F4602	F4603	F4604	F4605	F4606	F4607	F4608	F4609	F4610	F4611	F4612	F4613	F4614	F4615	F4616	F4617	F4618	F4619	F4620	F4621	F4622	F4623	F4624	F4625	F4626	F4627	F4628	F4629	F4630	F4631	F4632	F4633	F4634	F4635	F4636	F4637	F4638	F4639	F4640	F4641	F4642	F4643	F4644	F4645	F4646	F4647	F4648	F4649	F4650	F4651	F4652	F4653	F4654	F4655	F4656	F4657	F4658	F4659	F4660	F4661	F4662	F4663	F4664	F4665	F4666	F4667	F4668	F4669	F4670	F4671	F4672	F4673	F4674	F4675	F4676	F4677	F4678	F4679	F4680	F4681	F4682	F4683	F4684	F4685	F4686	F4687	F4688	F4689	F4690	F4691	F4692	F4693	F4694	F4695	F4696	F4697	F4698	F4699	F4700	F4701	F4702	F4703	F4704	F4705	F4706	F4707	F4708	F4709	F4710	F4711	F4712	F4713	F4714	F4715	F4716	F4717	F4718	F4719	F4720	F4721	F4722	F4723	F4724	F4725	F4726	F4727	F4728	F4729	F4730	F4731	F4732	F4733	F4734	F4735	F4736	F4737	F4738	F4739	F4740	F4741	F4742	F4743	F4744	F4745	F4746	F4747	F4748	F4749	F4750	F4751	F4752	F4753	F4754	F4755	F4756	F4757	F4758	F4759	F4760	F4761	F4762	F4763	F4764	F4765	F4766	F4767	F4768	F4769	F4770	F4771	F4772	F4773	F4774	F4775	F4776	F4777	F4778	F4779	F4780	F4781	F4782	F4783	F4784	F4785	F4786	F4787	F4788	F4789	F4790	F4791	F4792	F4793	F4794	F4795	F4796	F4797	F4798	F4799	F4800	F4801	F4802	F4803	F4804	F4805	F4806	F4807	F4808	F4809	F4810	F4811	F4812	F4813	F4814	F4815	F4816	F4817	F4818	F4819	F4820	F4821	F4822	F4823	F4824	F4825	F4826	F4827	F4828	F4829	F4830	F4831	F4832	F4833	F4834	F4835	F4836	F4837	F4838	F4839	F4840	F4841	F4842	F4843	F4844	F4845	F4846	F4847	F4848	F4849	F4850	F4851	F4852	F4853	F4854	F4855	F4856	F4857	F4858	F4859	F4860	F4861	F4862	F4863	F4864	F4865	F4866	F4867	F4868	F4869	F4870	F4871	F4872	F4873	F4874	F4875	F4876	F4877	F4878	F4879	F4880	F4881	F4882	F4883	F4884	F4885	F4886	F4887	F4888	F4889	F4890	F4891	F4892	F4893	F4894	F4895	F4896	F4897	F4898	F4899	F4900	F4901	F4902	F4903	F4904	F4905	F4906	F4907	F4908	F4909	F4910	F4911	F4912	F4913	F4914	F4915	F4916	F4917	F4918	F4919	F4920	F4921	F4922	F4923	F4924	F4925	F4926	F4927	F4928	F4929	F4930	F4931	F4932	F4933	F4934	F4935	F4936	F4937	F4938	F4939	F4940	F4941	F4942	F4943	F4944	F4945	F4946	F4947	F4948	F4949	F4950	F4951	F4952	F4953	F4954	F4955	F4956	F4957	F4958	F4959	F4960	F4961	F4962	F4963	F4964	F4965	F4966	F4967	F4968	F4969	F4970	F4971	F4972	F4973	F4974	F4975	F4976	F4977	F4978	F4979	F4980	F4981	F4982	F4983	F4984	F4985	F4986	F4987	F4988	F4989	F4990	F4991	F4992	F4993	F4994	F4995	F4996	F4997	F4998	F4999	F5000	F5001	F5002	F5003	F5004	F5005	F5006	F5007	F5008	F5009	F5010	F5011	F5012	F5013	F5014	F5015	F5016	F5017	F5018	F5019	F5020	F5021	F5022	F5023	F5024	F5025	F5026	F5027	F5028	F5029	F5030	F5031	F5032	F5033	F5034	F5035	F5036	F5037	F5038	F5039	F5040	F5041	F5042	F5043	F5044	F5045	F5046	F5047	F5048	F5049	F5050	F5051	F5052	F5053	F5054	F5055	F5056	F5057	F5058	F5059	F5060	F5061	F5062	F5063	F5064	F5065	F5066	F5067	F5068	F5069	F5070	F5071	F5072	F5073	F5074	F5075	F5076	F5077	F5078	F5079	F5080	F5081	F5082	F5083	F5084	F5085	F5086	F5087	F5088	F5089	F5090	F5091	F5092	F5093	F5094	F5095	F5096	F5097	F5098	F5099	F5100	F5101	F5102	F5103	F5104	F5105	F5106	F5107	F5108	F5109	F5110	F5111	F5112	F5113	F5114	F5115	F5116	F5117	F5118	F5119	F5120	F5121	F5122	F5123	F5124	F5125	F5126	F5127	F5128	F5129	F5130	F5131	F5132	F5133	F5134	F5135	F5136	F5137	F5138	F5139	F5140	F5141	F5142	F5143	F5144	F5145	F5146	F5147	F5148	F5149	F5150	F5151	F5152	F5153	F5154	F5155	F5156	F5157	F5158	F5159	F5160	F5161	F5162	F5163	F5164	F5165	F5166	F5167	F5168	F5169	F5170	F5171	F5172	F5173	F5174	F5175	F5176	F5177	F5178	F5179	F5180	F5181	F5182	F5183	F5184	F5185	F5186	F5187	F5188	F5189	F5190	F5191	F5192	F5193	F5194	F5195	F5196	F5197	F5198	F5199	F5200	F5201	F5202	F5203	F5204	F5205	F5206	F5207	F5208	F5209	F5210	F5211	F5212	F5213	F5214	F5215	F5216	F5217	F5218	F5219	F5220	F5221	F5222	F5223	F5224	F5225	F5226	F5227	F5228	F5229	F5230	F5231	F5232	F5233	F5234	F5235	F5236	F5237	F5238	F5239	F5240	F5241	F5242	F5243	F5244	F5245	F5246	F5247	F5248	F5249	F5250	F5251	F5252	F5253	F5254	F5255	F5256	F5257	F5258	F5259	F5260	F5261	F5262	F5263	F5264	F5265	F5266	F5267	F5268	F5269	F5270	F5271	F5272	F5273	F5274	F5275	F5276	F5277	F5278	F5279	F5280	F5281	F5282	F5283	F5284	F5285	F5286	F5287	F5288	F5289	F5290	F5291	F5292	F5293	F5294	F5295	F5296	F5297	F5298	F5299	F5300	F5301	F5302	F5303	F5304	F5305	F5306	F5307	F5308	F5309	F5310	F5311	F5312	F5313	F5314	F5315	F5316	F5317	F5318	F5319	F5320	F5321	F5322	F5323	F5324	F5325	F5326	F5327	F5328	F5329	F5330	F5331	F5332	F5333	F5334	F5335	F5336	F5337	F5338	F5339	F5340	F5341	F5342	F5343	F5344	F5345	F5346	F5347	F5348	F5349	F5350	F5351	F5352	F5353	F5354	F5355	F5356	F5357	F5358	F5359	F5360	F5361	F5362	F5363	F5364	F5365	F5366	F5367	F5368	F5369	F5370	F5371	F5372	F5373	F5374	F5375	F5376	F5377	F5378	F5379	F5380	F5381	F5382	F5383	F5384	F5385	F5386	F5387	F5388	F5389	F5390	F5391	F5392	F5393	F5394	F5395	F5396	F5397	F5398	F5399	F5400	F5401	F5402	F5403	F5404	F5405	F5406	F5407	F5408	F5409	F5410	F5411	F5412	F5413	F5414	F5415	F5416	F5417	F5418	F5419	F5420	F5421	F5422	F5423	F5424	F5425	F5426	F5427	F5428	F5429	F5430	F5431	F5432	F5433	F5434	F5435	F5436	F5437	F5438	F5439	F5440	F5441	F5442	F5443	F5444	F5445	F5446	F5447	F5448	F5449	F5450	F5451	F5452	F5453	F5454	F5455	F5456	F5457	F5458	F5459	F5460	F5461	F5462	F5463	F5464	F5465	F5466	F5467	F5468	F5469	F5470	F5471	F5472	F5473	F5474	F5475	F5476	F5477	F5478	F5479	F5480	F5481	F5482	F5483	F5484	F5485	F5486	F5487	F5488	F5489	F5490	F5491	F5492	F5493	F5494	F5495	F5496	F5497	F5498	F5499	F5500	F5501	F5502	F5503	F5504	F5505	F5506	F5507	F5508	F5509	F5510	F5511	F5512	F5513	F5514	F5515	F5516	F5517	F5518	F5519	F5520	F5521	F5522	F5523	F5524	F5525	F5526	F5527	F5528	F5529	F5530	F5531	F5532	F5533	F5534	F5535	F5536	F5537	F5538	F5539	F5540	F5541	F5542	F5543	F5544	F5545	F5546	F5547	F5548	F5549	F5550	F5551	F5552	F5553	F5554	F5555	F5556	F5557	F5558	F5559	F5560	F5561	F5562	F5563	F5564	F5565	F5566	F5567	F5568	F5569	F5570	F5571	F5572	F5573	F5574	F5575	F5576	F5577	F5578	F5579	F5580	F5581	F5582	F5583	F5584	F5585	F5586	F5587	F5588	F5589	F5590	F5591	F5592	F5593	F5594	F5595	F5596	F5597	F5598	F5599	F5600	F5601	F5602	F5603	F5604	F5605	F5606	F5607	F5608	F5609	F5610	F5611	F5612	F5613	F5614	F5615	F5616	F5617	F5618	F5619	F5620	F5621	F5622	F5623	F5624	F5625	F5626	F5627	F5628	F5629	F5630	F5631	F5632	F5633	F5634	F5635	F5636	F5637	F5638	F5639	F5640	F5641	F5642	F5643	F5644	F5645	F5646	F5647	F5648	F5649	F5650	F5651	F5652	F5653	F5654	F5655	F5656	F5657	F5658	F5659	F5660	F5661	F5662	F5663	F5664	F5665	F5666	F5667	F5668	F5669	F5670	F5671	F5672	F5673	F5674	F5675	F5676	F5677	F5678	F5679	F5680	F5681	F5682	F5683	F5684	F5685	F5686	F5687	F5688	F5689	F5690	F5691	F5692	F5693	F5694	F5695	F5696	F5697	F5698	F5699	F5700	F5701	F5702	F5703	F5704	F5705	F5706	F5707	F



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	0.064	Depositor
Minimum map value	-0.029	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/834	0.47	0/1123
1	F	0.20	0/834	0.47	0/1123
1	H	0.20	0/834	0.47	0/1123
1	J	0.20	0/834	0.46	0/1123
2	B	0.21	0/25428	0.53	8/34534 (0.0%)
2	E	0.21	0/25428	0.53	6/34534 (0.0%)
2	G	0.21	0/25428	0.53	6/34534 (0.0%)
2	I	0.21	0/25428	0.53	6/34534 (0.0%)
All	All	0.21	0/105048	0.53	26/142628 (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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2807	TRP	CA-C-N	-7.95	111.88	120.94
2	G	2807	TRP	C-N-CA	-7.95	111.88	120.94
2	B	2807	TRP	CA-C-N	-7.93	111.90	120.94
2	B	2807	TRP	C-N-CA	-7.93	111.90	120.94
2	I	2807	TRP	CA-C-N	-7.92	111.91	120.94
2	I	2807	TRP	C-N-CA	-7.92	111.91	120.94
2	E	2807	TRP	CA-C-N	-7.91	111.92	120.94
2	E	2807	TRP	C-N-CA	-7.91	111.92	120.94
2	G	4639	MET	CA-C-N	5.44	135.07	121.80
2	G	4639	MET	C-N-CA	5.44	135.07	121.80
2	B	4639	MET	CA-C-N	5.43	135.04	121.80
2	B	4639	MET	C-N-CA	5.43	135.04	121.80
2	E	4639	MET	CA-C-N	5.42	135.02	121.80
2	E	4639	MET	C-N-CA	5.42	135.02	121.80
2	I	4639	MET	CA-C-N	5.41	135.01	121.80
2	I	4639	MET	C-N-CA	5.41	135.01	121.80
2	B	2291	GLN	CA-C-N	5.09	131.27	121.54
2	B	2291	GLN	C-N-CA	5.09	131.27	121.54
2	G	2291	GLN	CA-C-N	5.09	131.27	121.54
2	G	2291	GLN	C-N-CA	5.09	131.27	121.54
2	E	2291	GLN	CA-C-N	5.08	131.24	121.54
2	E	2291	GLN	C-N-CA	5.08	131.24	121.54
2	I	2291	GLN	CA-C-N	5.07	131.22	121.54
2	I	2291	GLN	C-N-CA	5.07	131.22	121.54
2	B	1828	ASP	CA-C-N	5.00	124.99	119.89
2	B	1828	ASP	C-N-CA	5.00	124.99	119.89

There are no chirality outliers.

All (60) 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	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	194	SER	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1720	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	194	SER	Peptide
2	E	2291	GLN	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4807	PHE	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	1720	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	194	SER	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4807	PHE	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	1720	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	194	SER	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide

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Mol	Chain	Res	Type	Group
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	13	0
1	F	818	0	824	18	0
1	H	818	0	824	17	0
1	J	818	0	824	19	0
2	B	29499	0	24746	288	0
2	E	29499	0	24745	291	0
2	G	29499	0	24745	281	0
2	I	29499	0	24745	290	0
3	B	31	0	12	2	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	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	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	102365	1191	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 (1191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.52	0.74
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.51	0.74
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.51	0.73
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.71	0.73
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.52	0.73
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.56	0.71
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.56	0.70
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.56	0.69
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.92	0.68
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.56	0.68
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.59	0.67
2:G:173:SER:HB3	2:G:178:ARG:H	1.60	0.67
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.77	0.67
2:E:173:SER:HB3	2:E:178:ARG:H	1.60	0.67
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.92	0.67
2:B:173:SER:HB3	2:B:178:ARG:H	1.60	0.66
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.93	0.66
2:I:173:SER:HB3	2:I:178:ARG:H	1.60	0.66
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.77	0.66
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.77	0.66
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.92	0.66
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.29	0.66
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.77	0.66
2:B:379:HIS:HD2	2:B:382:GLY:H	1.44	0.66
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.29	0.65
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.61	0.65
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.29	0.65
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.62	0.65
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.29	0.65
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.62	0.65
2:G:379:HIS:HD2	2:G:382:GLY:H	1.44	0.65
2:I:379:HIS:HD2	2:I:382:GLY:H	1.44	0.64
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.62	0.64
2:E:379:HIS:HD2	2:E:382:GLY:H	1.44	0.64
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.61	0.64
2:G:4904:PRO:HB3	2:G:4913:ARG:HD3	1.80	0.64
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.31	0.64
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.61	0.63
2:I:4904:PRO:HB3	2:I:4913:ARG:HD3	1.80	0.63
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.63	0.63
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.62	0.63
2:E:4904:PRO:HB3	2:E:4913:ARG:HD3	1.80	0.63
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.31	0.63
2:B:4904:PRO:HB3	2:B:4913:ARG:HD3	1.80	0.63
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.62	0.63
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.62	0.63
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.63	0.63
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.64	0.63
2:B:132:ALA:HA	2:B:194:SER:HB2	1.81	0.63
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.64	0.62
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.64	0.62
2:E:132:ALA:HA	2:E:194:SER:HB2	1.81	0.62
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.32	0.62
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.31	0.62
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.64	0.62
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.62
2:I:111:HIS:HD2	2:I:114:SER:H	1.47	0.62
2:I:641:VAL:HG11	2:I:681:HIS:HD1	1.64	0.62
2:I:132:ALA:HA	2:I:194:SER:HB2	1.81	0.62
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.65	0.62
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.64	0.62
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.65	0.62
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.32	0.62
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.32	0.62
2:B:111:HIS:HD2	2:B:114:SER:H	1.47	0.62
2:G:132:ALA:HA	2:G:194:SER:HB2	1.81	0.62
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.62
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.33	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.32	0.62
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.33	0.62
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.64	0.62
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.33	0.62
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.82	0.62
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.64	0.61
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.82	0.61
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.82	0.61
2:G:111:HIS:HD2	2:G:114:SER:H	1.47	0.61
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.33	0.61
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.65	0.61
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.64	0.61
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.83	0.61
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.64	0.61
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.33	0.61
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.65	0.61
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.64	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.31	0.61
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.33	0.61
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.64	0.61
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.82	0.61
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.61
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.33	0.61
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.82	0.60
2:E:111:HIS:HD2	2:E:114:SER:H	1.47	0.60
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.82	0.60
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.83	0.60
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.84	0.60
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.33	0.60
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.84	0.60
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.84	0.60
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.82	0.60
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.84	0.59
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.84	0.59
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.84	0.59
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.85	0.59
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.85	0.59
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.85	0.59
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.84	0.59
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.85	0.59
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.59
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.85	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.58
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.85	0.58
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.85	0.58
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.36	0.58
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.36	0.58
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.85	0.58
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.85	0.58
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.36	0.58
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.85	0.58
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.58
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.84	0.58
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.85	0.58
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.85	0.58
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.36	0.58
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.86	0.58
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.86	0.58
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.37	0.58
2:I:2107:GLN:HG3	2:I:3681:GLY:HA2	1.86	0.58
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.85	0.58
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.84	0.58
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.86	0.58
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.85	0.58
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.37	0.58
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.86	0.58
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.69	0.58
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.86	0.58
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.86	0.58
2:G:2107:GLN:HG3	2:G:3681:GLY:HA2	1.86	0.58
2:E:2107:GLN:HG3	2:E:3681:GLY:HA2	1.86	0.58
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.58
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.69	0.57
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.86	0.57
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.86	0.57
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.86	0.57
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.86	0.57
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.85	0.57
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.36	0.57
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.86	0.57
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.86	0.57
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.86	0.57
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.86	0.57
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.57
2:B:2107:GLN:HG3	2:B:3681:GLY:HA2	1.86	0.57
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.87	0.57
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.87	0.57
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.87	0.56
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.86	0.56
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:313:SER:HB3	2:G:351:VAL:HB	1.87	0.56
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.86	0.56
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.31	0.56
2:E:606:LEU:O	2:E:617:ASN:ND2	2.39	0.56
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.31	0.56
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.86	0.56
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.69	0.56
2:I:606:LEU:O	2:I:617:ASN:ND2	2.39	0.56
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.87	0.56
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.69	0.56
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.88	0.56
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.56
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.87	0.56
2:G:606:LEU:O	2:G:617:ASN:ND2	2.39	0.56
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.88	0.56
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.37	0.56
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.56
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.88	0.56
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.86	0.56
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.88	0.56
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.88	0.56
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.71	0.56
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.87	0.56
2:E:45:ARG:NH2	2:E:447:ASP:OD1	2.39	0.56
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.88	0.55
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.40	0.55
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.40	0.55
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.88	0.55
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.87	0.55
2:B:217:GLY:O	2:B:261:ARG:NH1	2.40	0.55
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.55
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.86	0.55
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.80	0.55
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.80	0.55
2:B:606:LEU:O	2:B:617:ASN:ND2	2.39	0.55
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.71	0.55
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.88	0.55
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.39	0.55
2:B:626:LEU:HD23	2:B:630:GLU:H	1.72	0.55
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.39	0.55
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.89	0.55
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.87	0.55
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.39	0.55
2:B:313:SER:HB3	2:B:351:VAL:HB	1.87	0.55
2:B:3733:CYS:HA	2:B:3766:GLN:HG2	1.89	0.55
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.87	0.55
2:I:217:GLY:O	2:I:261:ARG:NH1	2.39	0.55
2:E:313:SER:HB3	2:E:351:VAL:HB	1.88	0.55
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.40	0.55
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.89	0.55
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.39	0.55
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.89	0.55
2:E:217:GLY:O	2:E:261:ARG:NH1	2.39	0.55
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.89	0.55
2:G:3733:CYS:HA	2:G:3766:GLN:HG2	1.89	0.55
2:I:626:LEU:HD23	2:I:630:GLU:H	1.71	0.55
2:E:626:LEU:HD23	2:E:630:GLU:H	1.71	0.55
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.71	0.55
2:G:217:GLY:O	2:G:261:ARG:NH1	2.39	0.55
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.88	0.55
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.39	0.55
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.31	0.55
2:G:626:LEU:HD23	2:G:630:GLU:H	1.72	0.55
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.89	0.55
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.89	0.54
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.89	0.54
2:G:315:CYS:SG	2:G:316:PHE:N	2.81	0.54
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.80	0.54
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.89	0.54
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.89	0.54
2:G:652:ARG:HB2	2:G:750:LEU:HD13	1.88	0.54
2:E:111:HIS:CD2	2:E:114:SER:H	2.25	0.54
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.88	0.54
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.90	0.54
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.80	0.54
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.73	0.54
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.90	0.54
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.90	0.54
2:I:3733:CYS:HA	2:I:3766:GLN:HG2	1.89	0.54
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.89	0.54
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:614:VAL:HG22	2:B:616:SER:H	1.72	0.54
2:I:313:SER:HB3	2:I:351:VAL:HB	1.88	0.54
2:I:315:CYS:SG	2:I:316:PHE:N	2.81	0.54
2:E:614:VAL:HG22	2:E:616:SER:H	1.72	0.54
1:F:87:HIS:H	1:F:91:ILE:HB	1.73	0.54
1:H:87:HIS:H	1:H:91:ILE:HB	1.73	0.54
2:B:111:HIS:CD2	2:B:114:SER:H	2.25	0.54
2:B:2479:LEU:O	2:B:2487:UNK:N	2.41	0.54
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.89	0.54
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.73	0.54
2:G:614:VAL:HG22	2:G:616:SER:H	1.72	0.54
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.73	0.54
2:E:1948:ASP:OD1	2:E:2126:ARG:NH2	2.39	0.54
2:E:3733:CYS:HA	2:E:3766:GLN:HG2	1.89	0.54
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.89	0.54
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.73	0.54
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.88	0.54
2:B:4198:SER:HB3	2:B:4201:ASN:HB2	1.90	0.54
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.90	0.54
1:J:87:HIS:H	1:J:91:ILE:HB	1.73	0.54
2:B:45:ARG:NH2	2:B:447:ASP:OD1	2.39	0.54
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.89	0.54
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.73	0.54
1:A:87:HIS:H	1:A:91:ILE:HB	1.73	0.53
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.73	0.53
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.90	0.53
2:B:315:CYS:SG	2:B:316:PHE:N	2.81	0.53
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.53
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.81	0.53
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.89	0.53
2:G:4198:SER:HB3	2:G:4201:ASN:HB2	1.90	0.53
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.90	0.53
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.73	0.53
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.71	0.53
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.89	0.53
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.53
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.73	0.53
2:I:111:HIS:CD2	2:I:114:SER:H	2.25	0.53
2:E:315:CYS:SG	2:E:316:PHE:N	2.81	0.53
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.90	0.53
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.91	0.53
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.42	0.53
2:E:730:VAL:O	2:E:735:GLN:NE2	2.42	0.53
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.89	0.53
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.91	0.53
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.91	0.53
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.89	0.53
2:I:730:VAL:O	2:I:735:GLN:NE2	2.42	0.53
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.91	0.53
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.73	0.53
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.53
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.81	0.53
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.91	0.53
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.91	0.53
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.91	0.53
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.73	0.53
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.42	0.53
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.73	0.53
2:G:730:VAL:O	2:G:735:GLN:NE2	2.42	0.53
2:I:614:VAL:HG22	2:I:616:SER:H	1.72	0.53
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.91	0.53
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.90	0.53
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.42	0.53
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.42	0.53
2:I:2479:LEU:O	2:I:2487:UNK:N	2.42	0.53
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.91	0.53
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.91	0.53
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.91	0.53
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.42	0.53
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.91	0.53
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.90	0.53
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.91	0.53
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.91	0.52
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.91	0.52
2:G:331:VAL:HG12	2:G:333:GLY:H	1.74	0.52
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.31	0.52
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.42	0.52
2:G:111:HIS:CD2	2:G:114:SER:H	2.25	0.52
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.52
2:E:331:VAL:HG12	2:E:333:GLY:H	1.74	0.52
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:730:VAL:O	2:B:735:GLN:NE2	2.42	0.52
2:G:116:MET:HB2	2:G:137:LEU:HD12	1.92	0.52
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.81	0.52
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.73	0.52
2:E:4198:SER:HB3	2:E:4201:ASN:HB2	1.90	0.52
2:G:2479:LEU:O	2:G:2487:UNK:N	2.42	0.52
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.91	0.52
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.42	0.52
2:G:4961:CYS:HB3	2:G:4983:HIS:HE1	1.74	0.52
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.42	0.52
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.91	0.52
2:B:331:VAL:HG12	2:B:333:GLY:H	1.74	0.52
2:B:116:MET:HB2	2:B:137:LEU:HD12	1.92	0.52
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.43	0.52
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.91	0.52
2:I:4198:SER:HB3	2:I:4201:ASN:HB2	1.90	0.52
2:E:1771:LEU:HD12	2:E:2153:MET:HE3	1.92	0.52
2:E:4961:CYS:HB3	2:E:4983:HIS:HE1	1.75	0.52
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.92	0.52
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.43	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.92	0.52
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.73	0.52
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.92	0.52
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.52
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.43	0.52
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.91	0.52
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.92	0.51
2:I:45:ARG:NH2	2:I:447:ASP:OD1	2.39	0.51
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.91	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.92	0.51
2:E:2479:LEU:O	2:E:2487:UNK:N	2.42	0.51
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.43	0.51
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.92	0.51
2:I:1771:LEU:HD12	2:I:2153:MET:HE3	1.92	0.51
2:E:309:THR:O	2:E:313:SER:OG	2.29	0.51
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.91	0.51
2:B:485:SER:O	2:B:489:ASN:N	2.38	0.51
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.51
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.76	0.51
2:I:4961:CYS:HB3	2:I:4983:HIS:HE1	1.74	0.51
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.92	0.51
2:B:4914:VAL:HG23	2:E:4888:TYR:HD1	1.75	0.51
2:G:309:THR:O	2:G:313:SER:OG	2.29	0.51
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.44	0.51
2:I:331:VAL:HG12	2:I:333:GLY:H	1.74	0.51
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.44	0.51
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.43	0.51
2:G:1771:LEU:HD12	2:G:2153:MET:HE3	1.92	0.51
2:G:4182:GLU:OE2	2:G:4983:HIS:NE2	2.43	0.51
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.93	0.51
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.39	0.51
2:B:1457:UNK:N	2:B:1497:UNK:O	2.44	0.51
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.75	0.51
2:I:1457:UNK:N	2:I:1497:UNK:O	2.44	0.51
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.43	0.51
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.75	0.51
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.43	0.51
2:E:4044:MET:HA	2:E:4047:MET:HG2	1.92	0.51
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.44	0.51
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.92	0.51
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.39	0.51
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.92	0.51
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.76	0.51
2:B:309:THR:O	2:B:313:SER:OG	2.29	0.51
2:B:4961:CYS:HB3	2:B:4983:HIS:HE1	1.75	0.51
2:G:45:ARG:NH2	2:G:447:ASP:OD1	2.39	0.51
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.76	0.51
2:I:116:MET:HB2	2:I:137:LEU:HD12	1.92	0.51
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.76	0.51
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.44	0.51
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.51
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.92	0.51
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.93	0.51
2:G:4044:MET:HA	2:G:4047:MET:HG2	1.92	0.51
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.92	0.51
2:I:309:THR:O	2:I:313:SER:OG	2.29	0.51
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.76	0.50
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.75	0.50
2:G:2178:MET:HE1	2:G:2210:VAL:HG11	1.93	0.50
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.93	0.50
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.76	0.50
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.93	0.50
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.93	0.50
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.44	0.50
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.93	0.50
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.44	0.50
2:I:2178:MET:HE1	2:I:2210:VAL:HG11	1.93	0.50
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.50
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.93	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.45	0.50
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.81	0.50
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.43	0.50
2:I:594:GLY:H	2:I:1594:ARG:HD3	1.76	0.50
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.93	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.50
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.38	0.50
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.44	0.50
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.76	0.50
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.93	0.50
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.39	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.45	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.44	0.50
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.92	0.50
2:B:1771:LEU:HD12	2:B:2153:MET:HE3	1.92	0.50
2:B:4044:MET:HA	2:B:4047:MET:HG2	1.92	0.50
2:E:116:MET:HB2	2:E:137:LEU:HD12	1.92	0.50
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.85	0.50
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.75	0.50
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.42	0.50
2:I:4044:MET:HA	2:I:4047:MET:HG2	1.92	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.50
2:B:594:GLY:H	2:B:1594:ARG:HD3	1.76	0.50
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.94	0.50
2:B:3759:GLU:HA	2:B:3762:ARG:HE	1.77	0.50
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.92	0.50
2:B:4231:MET:HE1	2:B:4960:ILE:HA	1.94	0.50
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.94	0.50
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.94	0.50
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.93	0.50
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.50
2:G:594:GLY:H	2:G:1594:ARG:HD3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2178:MET:HE1	2:E:2210:VAL:HG11	1.93	0.50
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.76	0.49
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.85	0.49
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.45	0.49
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.94	0.49
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.49
2:E:594:GLY:H	2:E:1594:ARG:HD3	1.76	0.49
2:G:1457:UNK:N	2:G:1497:UNK:O	2.44	0.49
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.29	0.49
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.49
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.85	0.49
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.92	0.49
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.76	0.49
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.94	0.49
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.94	0.49
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.94	0.49
2:B:2178:MET:HE1	2:B:2210:VAL:HG11	1.93	0.49
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.49
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.85	0.49
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.93	0.49
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.92	0.49
2:E:4182:GLU:OE2	2:E:4983:HIS:NE2	2.43	0.49
2:G:3759:GLU:HA	2:G:3762:ARG:HE	1.77	0.49
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.95	0.49
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.49
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.94	0.49
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.94	0.49
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.93	0.49
1:H:21:THR:HA	1:H:49:ARG:HA	1.95	0.49
1:J:25:HIS:HB3	1:J:40:ARG:HD3	1.95	0.49
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.94	0.49
2:G:1636:MET:HE2	2:G:1638:ALA:HB2	1.95	0.49
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.93	0.49
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.38	0.49
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.95	0.49
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.94	0.49
2:G:4231:MET:HE1	2:G:4960:ILE:HA	1.94	0.49
1:A:25:HIS:HB3	1:A:40:ARG:HD3	1.95	0.49
1:J:21:THR:HA	1:J:49:ARG:HA	1.95	0.49
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.95	0.49
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:485:SER:O	2:I:489:ASN:N	2.38	0.49
2:I:4182:GLU:OE2	2:I:4983:HIS:NE2	2.43	0.49
2:I:4231:MET:HE1	2:I:4960:ILE:HA	1.94	0.49
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.95	0.48
2:I:1636:MET:HE2	2:I:1638:ALA:HB2	1.95	0.48
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.95	0.48
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.94	0.48
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	1.95	0.48
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.96	0.48
1:H:25:HIS:HB3	1:H:40:ARG:HD3	1.95	0.48
1:J:35:LYS:HD3	2:I:636:ASN:HD21	1.77	0.48
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	1.95	0.48
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.49	0.48
2:I:3759:GLU:HA	2:I:3762:ARG:HE	1.77	0.48
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.94	0.48
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.49	0.48
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	1.95	0.48
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	1.95	0.48
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.49	0.48
2:B:3734:HIS:O	2:B:3738:GLY:N	2.40	0.48
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.29	0.48
2:G:485:SER:O	2:G:489:ASN:N	2.38	0.48
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.95	0.48
2:E:73:LEU:HB3	2:E:77:ALA:HB3	1.96	0.48
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.79	0.48
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.94	0.48
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.96	0.48
2:E:3759:GLU:HA	2:E:3762:ARG:HE	1.77	0.48
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.95	0.48
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.95	0.48
2:G:395:GLN:HG3	2:G:397:GLU:H	1.79	0.48
2:G:2004:GLU:HA	2:G:2007:ASN:HB2	1.96	0.48
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.95	0.48
2:E:4231:MET:HE1	2:E:4960:ILE:HA	1.94	0.48
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.29	0.48
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.96	0.48
2:B:164:ARG:N	2:B:167:ASP:OD2	2.45	0.48
2:B:395:GLN:HG3	2:B:397:GLU:H	1.79	0.48
2:I:73:LEU:HB3	2:I:77:ALA:HB3	1.96	0.48
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.48
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:THR:HA	1:F:49:ARG:HA	1.95	0.48
1:A:21:THR:HA	1:A:49:ARG:HA	1.95	0.48
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.48
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.96	0.48
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.96	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.79	0.48
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.47	0.48
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.47	0.48
1:F:25:HIS:HB3	1:F:40:ARG:HD3	1.95	0.47
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.96	0.47
2:G:123:THR:OG1	2:G:134:ASP:OD1	2.32	0.47
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.79	0.47
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.47	0.47
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.29	0.47
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.96	0.47
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.95	0.47
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	1.97	0.47
1:J:34:LYS:HE3	2:I:634:GLN:HB3	1.96	0.47
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	1.96	0.47
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	1.96	0.47
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.96	0.47
2:I:395:GLN:HG3	2:I:397:GLU:H	1.79	0.47
2:E:1636:MET:HE2	2:E:1638:ALA:HB2	1.95	0.47
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.96	0.47
2:B:1636:MET:HE2	2:B:1638:ALA:HB2	1.95	0.47
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.96	0.47
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.47
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.48	0.47
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.96	0.47
2:I:123:THR:OG1	2:I:134:ASP:OD1	2.32	0.47
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.47
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.96	0.47
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.96	0.47
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.48	0.47
2:E:2004:GLU:HA	2:E:2007:ASN:HB2	1.96	0.47
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.95	0.47
2:G:73:LEU:HB3	2:G:77:ALA:HB3	1.96	0.47
2:G:1698:LEU:HG	2:G:1814:MET:HE3	1.97	0.47
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.97	0.47
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.97	0.47
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1698:LEU:HG	2:B:1814:MET:HE3	1.97	0.47
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.95	0.47
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.95	0.47
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.80	0.47
1:A:57:LYS:HB2	1:A:80:VAL:HB	1.97	0.47
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.97	0.47
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	1.97	0.47
2:B:2004:GLU:HA	2:B:2007:ASN:HB2	1.96	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.97	0.47
2:B:4182:GLU:OE2	2:B:4983:HIS:NE2	2.43	0.47
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.80	0.47
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.97	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.49	0.47
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.96	0.47
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	1.96	0.47
2:I:1698:LEU:HG	2:I:1814:MET:HE3	1.97	0.47
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.80	0.47
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	1.96	0.47
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.96	0.47
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.43	0.47
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.48	0.47
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.80	0.47
2:I:2353:VAL:O	2:I:2357:LEU:N	2.48	0.47
2:E:123:THR:OG1	2:E:134:ASP:OD1	2.32	0.47
2:E:1970:GLN:HB3	2:E:3641:LEU:HG	1.97	0.47
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.80	0.47
1:A:7:ILE:N	1:A:71:ARG:O	2.45	0.47
1:J:57:LYS:HB2	1:J:80:VAL:HB	1.97	0.47
2:B:206:CYS:SG	2:B:207:SER:N	2.88	0.47
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.47	0.47
2:G:164:ARG:N	2:G:167:ASP:OD2	2.45	0.47
2:G:3847:PHE:HD1	2:G:3850:GLN:HE21	1.63	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.79	0.47
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.96	0.47
2:E:1698:LEU:HG	2:E:1814:MET:HE3	1.97	0.47
2:B:73:LEU:HB3	2:B:77:ALA:HB3	1.96	0.47
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.97	0.47
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.48	0.47
2:B:1970:GLN:HB3	2:B:3641:LEU:HG	1.97	0.47
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.97	0.47
2:I:4848:VAL:O	2:I:4852:THR:OG1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:164:ARG:N	2:E:167:ASP:OD2	2.45	0.47
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.97	0.47
2:E:2129:ASP:O	2:E:2133:GLU:N	2.44	0.47
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.96	0.47
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.80	0.46
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.96	0.46
2:G:2353:VAL:O	2:G:2357:LEU:N	2.48	0.46
2:G:4822:THR:O	2:G:4825:THR:OG1	2.29	0.46
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.96	0.46
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.48	0.46
2:E:206:CYS:SG	2:E:207:SER:N	2.88	0.46
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.97	0.46
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.97	0.46
2:G:866:HIS:O	2:G:1051:TYR:OH	2.32	0.46
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.96	0.46
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.96	0.46
2:I:206:CYS:SG	2:I:207:SER:N	2.88	0.46
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.97	0.46
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.43	0.46
2:B:123:THR:OG1	2:B:134:ASP:OD1	2.32	0.46
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.80	0.46
2:I:699:GLY:H	2:I:1647:CYS:HB3	1.81	0.46
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	1.97	0.46
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.97	0.46
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.96	0.46
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.96	0.46
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.97	0.46
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.97	0.46
2:I:1970:GLN:HB3	2:I:3641:LEU:HG	1.97	0.46
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.97	0.46
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.97	0.46
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.97	0.46
2:B:2129:ASP:O	2:B:2133:GLU:N	2.45	0.46
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.81	0.46
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.97	0.46
2:I:776:LEU:HG	2:I:848:HIS:HA	1.98	0.46
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.48	0.46
2:I:2004:GLU:HA	2:I:2007:ASN:HB2	1.96	0.46
2:I:3734:HIS:O	2:I:3738:GLY:N	2.40	0.46
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.49	0.46
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:LEU:HD21	2:B:316:PHE:HE2	1.81	0.46
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.49	0.46
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.97	0.46
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.48	0.46
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.80	0.46
2:E:280:LEU:HD21	2:E:316:PHE:HE2	1.81	0.46
2:E:485:SER:O	2:E:489:ASN:N	2.38	0.46
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.48	0.46
2:G:206:CYS:SG	2:G:207:SER:N	2.88	0.46
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.81	0.46
2:I:164:ARG:N	2:I:167:ASP:OD2	2.45	0.46
2:I:280:LEU:HD21	2:I:316:PHE:HE2	1.81	0.46
2:I:866:HIS:O	2:I:1051:TYR:OH	2.32	0.46
2:I:2129:ASP:O	2:I:2133:GLU:N	2.44	0.46
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.49	0.46
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.98	0.46
2:B:2353:VAL:O	2:B:2357:LEU:N	2.48	0.46
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.49	0.46
2:I:3847:PHE:HD1	2:I:3850:GLN:HE21	1.63	0.46
1:H:57:LYS:HB2	1:H:80:VAL:HB	1.97	0.46
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.96	0.46
2:G:359:TYR:HA	2:G:376:ALA:HA	1.98	0.46
2:G:776:LEU:HG	2:G:848:HIS:HA	1.98	0.46
2:E:699:GLY:H	2:E:1647:CYS:HB3	1.81	0.46
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.97	0.46
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.50	0.45
2:G:1970:GLN:HB3	2:G:3641:LEU:HG	1.97	0.45
2:G:4000:MET:HG3	2:G:4013:LEU:HD11	1.99	0.45
2:I:77:ALA:O	2:I:81:MET:N	2.49	0.45
2:E:359:TYR:HA	2:E:376:ALA:HA	1.98	0.45
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.50	0.45
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	1.98	0.45
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.82	0.45
2:B:2034:PHE:O	2:B:2038:LEU:N	2.50	0.45
2:G:699:GLY:H	2:G:1647:CYS:HB3	1.81	0.45
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.47	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:B:699:GLY:H	2:B:1647:CYS:HB3	1.81	0.45
2:B:1269:CYS:HA	2:B:1473:UNK:HA	1.98	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.99	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.45
2:E:776:LEU:HG	2:E:848:HIS:HA	1.97	0.45
2:E:892:THR:N	2:E:902:ARG:O	2.49	0.45
2:E:2353:VAL:O	2:E:2357:LEU:N	2.48	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.97	0.45
2:G:870:ILE:HD12	2:G:873:LYS:HB2	1.99	0.45
2:G:2034:PHE:O	2:G:2038:LEU:N	2.50	0.45
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.98	0.45
1:F:57:LYS:HB2	1:F:80:VAL:HB	1.97	0.45
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.98	0.45
2:B:889:GLN:O	2:B:902:ARG:NH1	2.50	0.45
2:G:280:LEU:HD21	2:G:316:PHE:HE2	1.81	0.45
2:G:2874:MET:O	2:G:2878:LEU:N	2.45	0.45
2:I:4000:MET:HG3	2:I:4013:LEU:HD11	1.99	0.45
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.75	0.45
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	1.99	0.45
2:E:2950:UNK:O	2:E:2954:UNK:N	2.50	0.45
2:E:3847:PHE:HD1	2:E:3850:GLN:HE21	1.63	0.45
2:B:870:ILE:HD12	2:B:873:LYS:HB2	1.99	0.45
2:G:134:ASP:OD1	2:G:134:ASP:N	2.50	0.45
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	1.97	0.45
2:I:870:ILE:HD12	2:I:873:LYS:HB2	1.99	0.45
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.82	0.45
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.97	0.45
2:I:2243:SER:HB3	2:I:2246:ASN:H	1.82	0.45
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.98	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.45
2:E:889:GLN:O	2:E:902:ARG:NH1	2.50	0.45
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.98	0.45
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.97	0.45
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	1.99	0.45
2:I:2950:UNK:O	2:I:2954:UNK:N	2.50	0.45
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.81	0.45
2:E:4000:MET:HG3	2:E:4013:LEU:HD11	1.99	0.45
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.49	0.45
2:B:77:ALA:O	2:B:81:MET:N	2.49	0.45
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.99	0.45
2:B:3847:PHE:HD1	2:B:3850:GLN:HE21	1.63	0.45
2:G:548:VAL:HG12	2:G:564:LEU:HD22	1.99	0.45
2:G:1707:LEU:O	2:G:1710:GLY:N	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2243:SER:HB3	2:G:2246:ASN:H	1.82	0.45
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.50	0.45
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.33	0.45
2:E:548:VAL:HG12	2:E:564:LEU:HD22	1.99	0.45
2:E:870:ILE:HD12	2:E:873:LYS:HB2	1.99	0.45
2:E:894:GLY:HA3	2:E:903:LEU:HD22	1.99	0.45
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.52	0.45
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.98	0.45
2:B:776:LEU:HG	2:B:848:HIS:HA	1.98	0.45
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.99	0.45
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.75	0.45
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.49	0.45
2:I:359:TYR:HA	2:I:376:ALA:HA	1.98	0.45
2:E:1269:CYS:HA	2:E:1473:UNK:HA	1.98	0.45
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.98	0.45
2:E:3361:UNK:O	2:E:3365:UNK:N	2.50	0.45
2:E:4957:LYS:HA	2:E:4964:GLY:HA2	1.99	0.45
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.98	0.45
2:G:983:THR:O	2:G:987:ARG:N	2.48	0.45
2:E:134:ASP:OD1	2:E:134:ASP:N	2.50	0.45
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.99	0.44
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.99	0.44
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.82	0.44
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	1.99	0.44
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	1.98	0.44
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.99	0.44
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.99	0.44
2:I:4729:GLY:HA2	2:I:4737:ILE:HG13	1.99	0.44
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.83	0.44
2:G:894:GLY:HA3	2:G:903:LEU:HD22	1.99	0.44
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.99	0.44
2:G:4957:LYS:HA	2:G:4964:GLY:HA2	1.99	0.44
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.98	0.44
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.75	0.44
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	1.98	0.44
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.82	0.44
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.81	0.44
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.99	0.44
2:B:4957:LYS:HA	2:B:4964:GLY:HA2	1.99	0.44
2:I:983:THR:O	2:I:987:ARG:N	2.48	0.44
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.99	0.44
2:E:4729:GLY:HA2	2:E:4737:ILE:HG13	1.99	0.44
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.98	0.44
2:G:2950:UNK:O	2:G:2954:UNK:N	2.50	0.44
2:G:3361:UNK:O	2:G:3365:UNK:N	2.50	0.44
2:I:889:GLN:O	2:I:902:ARG:NH1	2.50	0.44
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.98	0.44
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.44
2:E:582:HIS:O	2:E:585:SER:OG	2.30	0.44
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.98	0.44
2:B:359:TYR:HA	2:B:376:ALA:HA	1.98	0.44
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	1.98	0.44
2:B:3361:UNK:O	2:B:3365:UNK:N	2.50	0.44
2:B:4000:MET:HG3	2:B:4013:LEU:HD11	1.99	0.44
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.49	0.44
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.75	0.44
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.83	0.44
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.49	0.44
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.99	0.44
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.52	0.44
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.82	0.44
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.99	0.44
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.83	0.44
2:B:548:VAL:HG12	2:B:564:LEU:HD22	1.99	0.44
2:B:2950:UNK:O	2:B:2954:UNK:N	2.51	0.44
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.99	0.44
2:G:892:THR:N	2:G:902:ARG:O	2.49	0.44
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.98	0.44
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.99	0.44
2:G:4031:LEU:HB3	2:G:4034:ASN:HB2	1.99	0.44
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.52	0.44
2:I:548:VAL:HG12	2:I:564:LEU:HD22	1.99	0.44
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	1.99	0.44
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.99	0.44
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.99	0.44
2:G:77:ALA:O	2:G:81:MET:N	2.49	0.44
2:G:889:GLN:O	2:G:902:ARG:NH1	2.50	0.44
2:I:794:GLY:H	2:I:798:GLY:HA3	1.83	0.44
2:E:2243:SER:HB3	2:E:2246:ASN:H	1.82	0.44
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	2.00	0.44
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.99	0.44
2:G:3900:GLN:NE2	2:G:3967:GLU:O	2.51	0.44
2:I:1716:ILE:HG23	2:I:1720:LEU:HD13	2.00	0.44
2:I:3361:UNK:O	2:I:3365:UNK:N	2.50	0.44
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.83	0.44
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.99	0.44
2:E:983:THR:O	2:E:987:ARG:N	2.48	0.44
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	2.00	0.44
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.99	0.44
2:B:1716:ILE:HG23	2:B:1720:LEU:HD13	2.00	0.44
2:B:4928:LEU:HD13	2:B:4928:LEU:HA	1.84	0.44
2:G:4729:GLY:HA2	2:G:4737:ILE:HG13	1.99	0.44
2:I:134:ASP:OD1	2:I:134:ASP:N	2.50	0.44
2:I:4031:LEU:HB3	2:I:4034:ASN:HB2	1.99	0.44
2:E:866:HIS:O	2:E:1051:TYR:OH	2.32	0.44
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.44
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.99	0.43
2:B:894:GLY:HA3	2:B:903:LEU:HD22	1.99	0.43
2:B:1865:MET:SD	2:B:1865:MET:N	2.91	0.43
2:B:2243:SER:HB3	2:B:2246:ASN:H	1.82	0.43
2:B:3552:UNK:O	2:B:3556:UNK:N	2.52	0.43
2:B:3900:GLN:NE2	2:B:3967:GLU:O	2.51	0.43
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.99	0.43
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.99	0.43
2:I:4957:LYS:HA	2:I:4964:GLY:HA2	1.99	0.43
2:E:1707:LEU:O	2:E:1710:GLY:N	2.35	0.43
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	2.00	0.43
2:E:3900:GLN:NE2	2:E:3967:GLU:O	2.51	0.43
2:B:23:GLN:HB3	2:B:201:ASN:HB2	2.00	0.43
2:B:866:HIS:O	2:B:1051:TYR:OH	2.32	0.43
2:B:1707:LEU:O	2:B:1710:GLY:N	2.36	0.43
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.52	0.43
2:G:23:GLN:HB3	2:G:201:ASN:HB2	2.00	0.43
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.00	0.43
2:I:23:GLN:HB3	2:I:201:ASN:HB2	2.00	0.43
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.50	0.43
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.00	0.43
2:B:286:THR:HA	2:B:405:HIS:HB2	2.01	0.43
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.33	0.43
2:I:286:THR:HA	2:I:405:HIS:HB2	2.01	0.43
2:I:894:GLY:HA3	2:I:903:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	2.00	0.43
2:E:495:ASN:HD21	2:E:550:LYS:HG3	1.84	0.43
2:E:1865:MET:SD	2:E:1865:MET:N	2.92	0.43
1:J:82:TYR:HB3	1:J:86:GLY:HA2	2.01	0.43
2:B:892:THR:N	2:B:902:ARG:O	2.49	0.43
2:B:4031:LEU:HB3	2:B:4034:ASN:HB2	1.99	0.43
2:B:4729:GLY:HA2	2:B:4737:ILE:HG13	1.99	0.43
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.17	0.43
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.01	0.43
2:E:23:GLN:HB3	2:E:201:ASN:HB2	2.00	0.43
2:E:3734:HIS:O	2:E:3738:GLY:N	2.40	0.43
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.99	0.43
2:B:794:GLY:H	2:B:798:GLY:HA3	1.83	0.43
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.51	0.43
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	2.00	0.43
2:G:794:GLY:H	2:G:798:GLY:HA3	1.83	0.43
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.99	0.43
2:I:1269:CYS:HA	2:I:1473:UNK:HA	1.99	0.43
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.00	0.43
1:F:30:LEU:HD23	1:F:33:GLY:HA3	2.01	0.43
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.36	0.43
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.43
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.83	0.43
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.99	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.01	0.43
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.01	0.43
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.01	0.43
2:G:1154:ASP:O	2:G:1158:ASN:N	2.52	0.43
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.00	0.43
2:G:1675:ALA:HB1	2:G:1676:LEU:HD13	2.01	0.43
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.43
2:I:1771:LEU:HD13	2:I:1771:LEU:HA	1.93	0.43
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.01	0.43
2:E:794:GLY:H	2:E:798:GLY:HA3	1.83	0.43
2:E:924:MET:O	2:E:928:THR:OG1	2.34	0.43
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.99	0.43
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.92	0.43
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.99	0.43
1:H:30:LEU:HD23	1:H:33:GLY:HA3	2.01	0.43
1:H:82:TYR:HB3	1:H:86:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4822:THR:O	2:B:4825:THR:OG1	2.29	0.43
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.01	0.43
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.00	0.43
2:I:1154:ASP:O	2:I:1158:ASN:N	2.52	0.43
2:I:1865:MET:SD	2:I:1865:MET:N	2.92	0.43
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.51	0.43
2:E:4031:LEU:HB3	2:E:4034:ASN:HB2	1.99	0.43
1:J:7:ILE:N	1:J:71:ARG:O	2.45	0.43
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.47	0.43
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	2.01	0.43
2:G:286:THR:HA	2:G:405:HIS:HB2	2.01	0.43
2:G:1716:ILE:HG23	2:G:1720:LEU:HD13	2.00	0.43
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.51	0.43
2:G:2129:ASP:O	2:G:2133:GLU:N	2.45	0.43
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.29	0.43
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.92	0.43
2:I:2959:UNK:O	2:I:2963:UNK:N	2.52	0.43
2:I:3900:GLN:NE2	2:I:3967:GLU:O	2.51	0.43
2:I:4998:LYS:NZ	2:I:5007:GLU:OE1	2.52	0.43
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.54	0.43
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.17	0.43
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.99	0.43
2:B:495:ASN:HD21	2:B:550:LYS:HG3	1.84	0.43
2:B:2305:CYS:HA	2:B:2324:ASN:HD22	1.84	0.43
2:G:2265:LEU:HD21	2:G:2273:LEU:HD13	2.01	0.43
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.01	0.43
2:I:2305:CYS:HA	2:I:2324:ASN:HD22	1.84	0.43
2:E:286:THR:HA	2:E:405:HIS:HB2	2.01	0.43
2:E:1716:ILE:HG23	2:E:1720:LEU:HD13	2.00	0.43
2:E:2305:CYS:HA	2:E:2324:ASN:HD22	1.84	0.43
1:J:30:LEU:HD23	1:J:33:GLY:HA3	2.01	0.42
2:B:119:SER:HA	2:B:146:CYS:HA	2.01	0.42
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.92	0.42
2:I:2034:PHE:O	2:I:2038:LEU:N	2.50	0.42
2:E:1675:ALA:HB1	2:E:1676:LEU:HD13	2.01	0.42
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.47	0.42
1:H:34:LYS:HE3	2:G:634:GLN:HB3	2.00	0.42
2:G:345:LEU:HD23	2:G:389:PHE:HB3	2.01	0.42
2:G:1865:MET:SD	2:G:1865:MET:N	2.92	0.42
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.92	0.42
2:I:495:ASN:HD21	2:I:550:LYS:HG3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.01	0.42
2:B:3842:LEU:O	2:B:3929:SER:OG	2.37	0.42
2:G:290:TYR:O	2:G:302:VAL:N	2.52	0.42
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	2.01	0.42
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.01	0.42
2:I:1675:ALA:HB1	2:I:1676:LEU:HD13	2.01	0.42
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.47	0.42
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	2.00	0.42
2:E:345:LEU:HD23	2:E:389:PHE:HB3	2.01	0.42
2:E:1154:ASP:O	2:E:1158:ASN:N	2.52	0.42
2:E:2034:PHE:O	2:E:2038:LEU:N	2.50	0.42
2:B:290:TYR:O	2:B:302:VAL:N	2.52	0.42
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.01	0.42
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.02	0.42
2:G:119:SER:HA	2:G:146:CYS:HA	2.01	0.42
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	2.01	0.42
2:G:2959:UNK:O	2:G:2963:UNK:N	2.53	0.42
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.00	0.42
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	2.01	0.42
1:A:30:LEU:HD23	1:A:33:GLY:HA3	2.01	0.42
2:B:2265:LEU:HD21	2:B:2273:LEU:HD13	2.01	0.42
2:G:495:ASN:HD21	2:G:550:LYS:HG3	1.84	0.42
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.42
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	2.01	0.42
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.51	0.42
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.02	0.42
2:E:4848:VAL:O	2:E:4852:THR:OG1	2.29	0.42
1:F:82:TYR:HB3	1:F:86:GLY:HA2	2.01	0.42
2:B:3365:UNK:O	2:B:3369:UNK:N	2.52	0.42
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.54	0.42
2:G:2452:ARG:HH12	2:E:177:GLU:HG3	1.84	0.42
2:G:3677:LEU:O	2:G:3698:LEU:N	2.52	0.42
2:I:1707:LEU:O	2:I:1710:GLY:N	2.35	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.01	0.42
2:E:2265:LEU:HD21	2:E:2273:LEU:HD13	2.01	0.42
2:E:3771:HIS:O	2:E:3774:GLY:N	2.48	0.42
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.91	0.42
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.01	0.42
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.01	0.42
2:G:3734:HIS:O	2:G:3738:GLY:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.17	0.42
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	2.01	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.54	0.42
2:B:346:CYS:N	2:B:388:LEU:O	2.52	0.42
2:B:924:MET:O	2:B:928:THR:OG1	2.34	0.42
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.85	0.42
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.52	0.42
2:I:113:HIS:CE1	2:I:402:ARG:HB3	2.54	0.42
2:I:892:THR:N	2:I:902:ARG:O	2.49	0.42
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.02	0.42
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.85	0.42
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.02	0.42
2:I:2874:MET:O	2:I:2878:LEU:N	2.45	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:E:290:TYR:O	2:E:302:VAL:N	2.52	0.42
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	2.02	0.42
2:E:3842:LEU:O	2:E:3929:SER:OG	2.37	0.42
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.01	0.42
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	2.01	0.42
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	2.02	0.42
2:B:4582:VAL:HG12	2:I:4877:ASP:HA	2.02	0.42
2:G:403:MET:O	2:G:407:THR:OG1	2.34	0.42
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.51	0.42
2:G:3842:LEU:O	2:G:3929:SER:OG	2.37	0.42
2:I:290:TYR:O	2:I:302:VAL:N	2.52	0.42
2:I:2265:LEU:HD21	2:I:2273:LEU:HD13	2.01	0.42
2:E:2959:UNK:O	2:E:2963:UNK:N	2.52	0.42
1:A:6:THR:HA	1:A:72:ALA:HA	2.02	0.42
1:A:82:TYR:HB3	1:A:86:GLY:HA2	2.01	0.42
2:B:134:ASP:OD1	2:B:134:ASP:N	2.50	0.42
2:B:689:THR:H	2:B:778:PHE:HE2	1.67	0.42
2:B:1154:ASP:O	2:B:1158:ASN:N	2.52	0.42
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.51	0.42
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.38	0.42
2:I:345:LEU:HD23	2:I:389:PHE:HB3	2.01	0.42
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	2.02	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:E:580:GLU:HG3	2:E:620:LEU:HD22	2.02	0.42
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	2.01	0.42
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
1:F:6:THR:HA	1:F:72:ALA:HA	2.02	0.41
1:J:6:THR:HA	1:J:72:ALA:HA	2.02	0.41
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.55	0.41
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	2.02	0.41
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.38	0.41
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.41
2:B:4804:TYR:HB3	2:B:4806:ASN:HD22	1.86	0.41
2:I:3771:HIS:O	2:I:3774:GLY:N	2.48	0.41
2:I:4928:LEU:HD13	2:I:4928:LEU:HA	1.84	0.41
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.51	0.41
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.53	0.41
2:B:247:TYR:HE2	2:B:359:TYR:HB3	1.85	0.41
2:B:580:GLU:HG3	2:B:620:LEU:HD22	2.02	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.54	0.41
2:B:4998:LYS:NZ	2:B:5007:GLU:OE1	2.52	0.41
2:G:1674:CYS:HB2	2:G:1685:LEU:HD13	2.03	0.41
2:I:119:SER:HA	2:I:146:CYS:HA	2.01	0.41
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.38	0.41
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.01	0.41
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.38	0.41
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.85	0.41
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.38	0.41
2:B:582:HIS:O	2:B:585:SER:OG	2.30	0.41
2:B:1675:ALA:HB1	2:B:1676:LEU:HD13	2.01	0.41
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.53	0.41
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.41	0.41
2:G:689:THR:H	2:G:778:PHE:HE2	1.67	0.41
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.38	0.41
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	2.02	0.41
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	2.02	0.41
2:I:3842:LEU:O	2:I:3929:SER:OG	2.37	0.41
2:E:119:SER:HA	2:E:146:CYS:HA	2.01	0.41
2:E:1674:CYS:HB2	2:E:1685:LEU:HD13	2.03	0.41
2:E:4804:TYR:HB3	2:E:4806:ASN:HD22	1.85	0.41
1:H:7:ILE:N	1:H:71:ARG:O	2.45	0.41
1:J:23:VAL:H	1:J:105:ASN:HB3	1.85	0.41
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.17	0.41
2:B:3793:MET:O	2:B:3797:THR:OG1	2.34	0.41
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.52	0.41
2:I:346:CYS:N	2:I:388:LEU:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:689:THR:H	2:I:778:PHE:HE2	1.67	0.41
2:I:1674:CYS:HB2	2:I:1685:LEU:HD13	2.03	0.41
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.03	0.41
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.54	0.41
1:F:23:VAL:H	1:F:105:ASN:HB3	1.85	0.41
1:J:35:LYS:HD3	2:I:636:ASN:ND2	2.35	0.41
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.02	0.41
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.38	0.41
2:B:3729:MET:O	2:B:3732:SER:OG	2.35	0.41
2:B:4163:PHE:HA	2:B:4166:LEU:HB2	2.03	0.41
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.03	0.41
2:I:247:TYR:HE2	2:I:359:TYR:HB3	1.86	0.41
2:E:3880:PHE:O	2:E:3884:LEU:N	2.54	0.41
1:F:92:PRO:HD3	2:E:627:PRO:HB2	2.03	0.41
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	2.02	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.95	0.41
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.03	0.41
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.03	0.41
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.41
1:H:6:THR:HA	1:H:72:ALA:HA	2.02	0.41
1:H:23:VAL:H	1:H:105:ASN:HB3	1.85	0.41
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.91	0.41
2:B:4914:VAL:HG23	2:E:4888:TYR:CD1	2.54	0.41
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.03	0.41
2:G:4163:PHE:HA	2:G:4166:LEU:HB2	2.03	0.41
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.01	0.41
2:E:346:CYS:N	2:E:388:LEU:O	2.52	0.41
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.54	0.41
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.03	0.41
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.54	0.41
2:G:1725:ARG:HH21	2:G:1725:ARG:HD2	1.71	0.41
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.38	0.41
2:I:4163:PHE:HA	2:I:4166:LEU:HB2	2.03	0.41
2:I:4804:TYR:HB3	2:I:4806:ASN:HD22	1.86	0.41
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.03	0.41
2:B:345:LEU:HD23	2:B:389:PHE:HB3	2.01	0.41
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.54	0.41
2:B:2144:ILE:H	2:B:2144:ILE:HG13	1.79	0.41
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	2.03	0.41
2:B:4685:GLY:HA3	2:B:4689:THR:HB	2.03	0.41
2:G:580:GLU:HG3	2:G:620:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.41
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.55	0.41
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.85	0.41
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.03	0.41
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.41
2:G:3880:PHE:O	2:G:3884:LEU:N	2.54	0.41
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.54	0.41
2:I:403:MET:O	2:I:407:THR:OG1	2.33	0.41
2:I:1141:ARG:HD2	2:I:1141:ARG:H	1.86	0.41
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.54	0.41
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.55	0.41
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	2.02	0.41
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.54	0.41
2:I:4886:HIS:O	2:I:4890:GLY:N	2.46	0.41
2:E:77:ALA:O	2:E:81:MET:N	2.49	0.41
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.01	0.41
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.54	0.41
2:E:2810:LYS:HE2	2:E:2814:LYS:HE3	2.03	0.41
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	2.02	0.41
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.52	0.41
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.54	0.41
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.91	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.01	0.41
2:G:1720:LEU:HD23	2:G:1721:GLU:HA	2.03	0.41
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.01	0.41
2:I:580:GLU:HG3	2:I:620:LEU:HD22	2.02	0.41
2:I:2288:LEU:O	2:I:3849:ARG:NH1	2.49	0.41
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.03	0.41
2:E:1720:LEU:HD23	2:E:1721:GLU:HA	2.03	0.41
2:E:4998:LYS:NZ	2:E:5007:GLU:OE1	2.52	0.41
1:F:34:LYS:HE3	2:E:634:GLN:HB3	2.01	0.40
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.87	0.40
2:B:1674:CYS:HB2	2:B:1685:LEU:HD13	2.03	0.40
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.38	0.40
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.03	0.40
2:I:2302:LEU:HD12	2:I:2305:CYS:HB3	2.03	0.40
2:E:689:THR:H	2:E:778:PHE:HE2	1.67	0.40
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.01	0.40
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.56	0.40
2:E:4822:THR:O	2:E:4825:THR:OG1	2.29	0.40
2:E:4913:ARG:O	2:E:4917:ASP:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:H	1:A:105:ASN:HB3	1.85	0.40
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.91	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.55	0.40
2:B:4041:ALA:HA	2:B:4044:MET:HB2	2.04	0.40
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.54	0.40
2:G:2305:CYS:HA	2:G:2324:ASN:HD22	1.84	0.40
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	2.03	0.40
2:G:4041:ALA:HA	2:G:4044:MET:HB2	2.04	0.40
2:I:875:ALA:HB2	2:I:925:SER:HB2	2.03	0.40
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.87	0.40
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.54	0.40
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.51	0.40
2:I:2587:UNK:O	2:I:2591:UNK:N	2.54	0.40
2:I:3677:LEU:O	2:I:3698:LEU:N	2.52	0.40
2:E:2587:UNK:O	2:E:2591:UNK:N	2.54	0.40
2:E:4163:PHE:HA	2:E:4166:LEU:HB2	2.03	0.40
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.03	0.40
2:B:2302:LEU:HD12	2:B:2305:CYS:HB3	2.03	0.40
2:B:2456:ILE:O	2:B:2459:SER:OG	2.32	0.40
2:G:913:LEU:O	2:G:918:ARG:NH2	2.55	0.40
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.54	0.40
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.40
2:E:2302:LEU:HD12	2:E:2305:CYS:HB3	2.03	0.40
2:E:3677:LEU:O	2:E:3698:LEU:N	2.52	0.40
2:E:4156:HIS:CE1	2:E:5036:LEU:HD11	2.56	0.40
1:F:15:PHE:HA	1:F:16:PRO:HD3	1.97	0.40
2:B:472:ARG:HA	2:B:475:GLN:HB2	2.04	0.40
2:B:2959:UNK:O	2:B:2963:UNK:N	2.54	0.40
2:B:3880:PHE:O	2:B:3884:LEU:N	2.54	0.40
2:B:4215:ARG:NH2	3:B:5101:ATP:O2A	2.55	0.40
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.04	0.40
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	2.03	0.40
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.56	0.40
2:I:4041:ALA:HA	2:I:4044:MET:HB2	2.04	0.40
2:I:4685:GLY:HA3	2:I:4689:THR:HB	2.04	0.40
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.04	0.40
2:B:803:LEU:HA	2:B:804:PRO:HD3	1.98	0.40
2:B:2587:UNK:O	2:B:2591:UNK:N	2.55	0.40
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	2.03	0.40
2:G:2810:LYS:O	2:G:2814:LYS:N	2.45	0.40
2:G:4804:TYR:HB3	2:G:4806:ASN:HD22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:913:LEU:O	2:I:918:ARG:NH2	2.55	0.40
2:I:3880:PHE:O	2:I:3884:LEU:N	2.54	0.40
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.03	0.40
2:E:247:TYR:HE2	2:E:359:TYR:HB3	1.85	0.40
2:E:2674:UNK:O	2:E:2676:UNK:N	2.54	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%)	2882 (89%)	348 (11%)	5 (0%)	43	77
2	E	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	43	77
2	G	3235/4416 (73%)	2881 (89%)	349 (11%)	5 (0%)	43	77
2	I	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	43	77
All	All	13360/18096 (74%)	11903 (89%)	1437 (11%)	20 (0%)	49	83

All (20) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
2	G	4641	PRO
2	I	4641	PRO
2	E	4641	PRO
2	B	1840	PRO
2	B	1932	PRO
2	B	2292	GLU
2	G	1840	PRO
2	G	1932	PRO
2	G	2292	GLU
2	I	1840	PRO
2	I	1932	PRO
2	I	2292	GLU
2	E	1840	PRO
2	E	1932	PRO
2	E	2292	GLU

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%)	2479 (99%)	14 (1%)	78	80
2	E	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	G	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	I	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
All	All	10324/12444 (83%)	10268 (100%)	56 (0%)	78	81

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	719	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1657	LEU
2	B	1676	LEU
2	B	2010	LEU
2	B	2144	ILE
2	B	3663	LEU
2	B	3805	LEU
2	B	4081	VAL
2	B	4154	VAL
2	B	4166	LEU
2	B	4792	LEU
2	G	131	LEU
2	G	719	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1657	LEU
2	G	1676	LEU
2	G	2010	LEU
2	G	2144	ILE
2	G	3663	LEU
2	G	3805	LEU
2	G	4081	VAL
2	G	4154	VAL
2	G	4166	LEU
2	G	4792	LEU
2	I	131	LEU
2	I	719	LEU
2	I	978	THR
2	I	1600	LEU
2	I	1657	LEU
2	I	1676	LEU
2	I	2010	LEU
2	I	2144	ILE
2	I	3663	LEU
2	I	3805	LEU
2	I	4081	VAL
2	I	4154	VAL
2	I	4166	LEU
2	I	4792	LEU
2	E	131	LEU

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Mol	Chain	Res	Type
2	E	719	LEU
2	E	978	THR
2	E	1600	LEU
2	E	1657	LEU
2	E	1676	LEU
2	E	2010	LEU
2	E	2144	ILE
2	E	3663	LEU
2	E	3805	LEU
2	E	4081	VAL
2	E	4154	VAL
2	E	4166	LEU
2	E	4792	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (216) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	113	HIS
2	B	151	HIS
2	B	156	GLN
2	B	201	ASN
2	B	273	HIS
2	B	379	HIS
2	B	395	GLN
2	B	461	HIS
2	B	465	GLN
2	B	479	GLN
2	B	520	ASN
2	B	582	HIS
2	B	725	HIS
2	B	797	HIS
2	B	838	HIS
2	B	949	ASN
2	B	1598	GLN
2	B	1611	HIS
2	B	1678	ASN
2	B	1679	ASN

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Mol	Chain	Res	Type
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1928	GLN
2	B	1949	GLN
2	B	2041	HIS
2	B	2127	GLN
2	B	2260	ASN
2	B	2349	ASN
2	B	2772	GLN
2	B	2788	HIS
2	B	2856	ASN
2	B	3809	ASN
2	B	3814	GLN
2	B	3830	GLN
2	B	3850	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3900	GLN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4109	GLN
2	B	4201	ASN
2	B	4209	GLN
2	B	4246	GLN
2	B	4700	GLN
2	B	4776	GLN
2	B	4806	ASN
2	B	4836	GLN
2	B	4946	GLN
2	B	5031	GLN
2	G	57	ASN
2	G	113	HIS
2	G	151	HIS
2	G	201	ASN
2	G	273	HIS
2	G	379	HIS
2	G	395	GLN
2	G	461	HIS

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Mol	Chain	Res	Type
2	G	465	GLN
2	G	479	GLN
2	G	520	ASN
2	G	582	HIS
2	G	725	HIS
2	G	797	HIS
2	G	838	HIS
2	G	949	ASN
2	G	1133	HIS
2	G	1598	GLN
2	G	1678	ASN
2	G	1679	ASN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	1928	GLN
2	G	2041	HIS
2	G	2260	ASN
2	G	2772	GLN
2	G	2788	HIS
2	G	2856	ASN
2	G	3809	ASN
2	G	3814	GLN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3900	GLN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4109	GLN
2	G	4201	ASN
2	G	4209	GLN
2	G	4246	GLN
2	G	4700	GLN
2	G	4776	GLN
2	G	4806	ASN
2	G	4836	GLN
2	G	4946	GLN
2	G	5031	GLN

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Mol	Chain	Res	Type
2	I	57	ASN
2	I	113	HIS
2	I	151	HIS
2	I	201	ASN
2	I	273	HIS
2	I	379	HIS
2	I	395	GLN
2	I	461	HIS
2	I	465	GLN
2	I	479	GLN
2	I	520	ASN
2	I	582	HIS
2	I	725	HIS
2	I	797	HIS
2	I	838	HIS
2	I	949	ASN
2	I	1598	GLN
2	I	1678	ASN
2	I	1679	ASN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1928	GLN
2	I	1949	GLN
2	I	2041	HIS
2	I	2260	ASN
2	I	2349	ASN
2	I	2772	GLN
2	I	2788	HIS
2	I	2856	ASN
2	I	3809	ASN
2	I	3814	GLN
2	I	3830	GLN
2	I	3850	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3900	GLN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN

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Mol	Chain	Res	Type
2	I	4109	GLN
2	I	4201	ASN
2	I	4209	GLN
2	I	4246	GLN
2	I	4700	GLN
2	I	4776	GLN
2	I	4806	ASN
2	I	4946	GLN
2	I	5031	GLN
2	E	57	ASN
2	E	113	HIS
2	E	151	HIS
2	E	156	GLN
2	E	201	ASN
2	E	273	HIS
2	E	379	HIS
2	E	395	GLN
2	E	461	HIS
2	E	465	GLN
2	E	479	GLN
2	E	520	ASN
2	E	582	HIS
2	E	725	HIS
2	E	797	HIS
2	E	838	HIS
2	E	949	ASN
2	E	1598	GLN
2	E	1611	HIS
2	E	1678	ASN
2	E	1679	ASN
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	1928	GLN
2	E	1949	GLN
2	E	2041	HIS
2	E	2127	GLN
2	E	2260	ASN
2	E	2349	ASN
2	E	2772	GLN
2	E	2788	HIS

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Mol	Chain	Res	Type
2	E	2856	ASN
2	E	3809	ASN
2	E	3814	GLN
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3900	GLN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	4109	GLN
2	E	4201	ASN
2	E	4209	GLN
2	E	4246	GLN
2	E	4553	ASN
2	E	4700	GLN
2	E	4776	GLN
2	E	4806	ASN
2	E	4836	GLN
2	E	4946	GLN
2	E	4973	HIS
2	E	5031	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
4	CFF	I	5102	-	15,15,15	1.95	7 (46%)	23,23,23	2.78	11 (47%)
4	CFF	E	5102	-	15,15,15	1.94	7 (46%)	23,23,23	2.78	11 (47%)
3	ATP	B	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.74	12 (25%)
4	CFF	B	5102	-	15,15,15	1.92	7 (46%)	23,23,23	2.78	11 (47%)
3	ATP	I	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.73	12 (25%)
4	CFF	G	5102	-	15,15,15	1.94	7 (46%)	23,23,23	2.78	11 (47%)
3	ATP	G	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.73	12 (25%)
3	ATP	E	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.74	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	E	5101	-	-	5/22/38/38	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5101	ATP	C5-C4	4.45	1.47	1.39
3	I	5101	ATP	C5-C4	4.43	1.47	1.39
3	B	5101	ATP	C5-C4	4.42	1.47	1.39
3	G	5101	ATP	C5-C4	4.42	1.47	1.39
4	I	5102	CFF	C6-N1	-3.92	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C6-N1	-3.92	1.32	1.40
4	B	5102	CFF	C6-N1	-3.89	1.32	1.40
4	G	5102	CFF	C6-N1	-3.88	1.32	1.40
4	G	5102	CFF	C4-N3	-2.75	1.33	1.38
4	I	5102	CFF	C4-N3	-2.75	1.33	1.38
4	E	5102	CFF	C4-N3	-2.65	1.33	1.38
4	B	5102	CFF	C4-N3	-2.62	1.33	1.38
3	I	5101	ATP	C5-N7	-2.60	1.34	1.39
3	E	5101	ATP	C5-N7	-2.59	1.34	1.39
3	G	5101	ATP	C5-N7	-2.57	1.34	1.39
3	B	5101	ATP	C5-N7	-2.56	1.34	1.39
3	B	5101	ATP	C5-C6	2.45	1.47	1.41
4	I	5102	CFF	C5-N7	-2.44	1.34	1.38
3	G	5101	ATP	C4-N9	-2.44	1.32	1.37
4	G	5102	CFF	C5-N7	-2.42	1.34	1.38
3	E	5101	ATP	C5-C6	2.42	1.47	1.41
3	G	5101	ATP	C5-C6	2.42	1.47	1.41
4	E	5102	CFF	C5-N7	-2.42	1.34	1.38
3	I	5101	ATP	C5-C6	2.41	1.47	1.41
4	B	5102	CFF	C5-N7	-2.41	1.34	1.38
3	I	5101	ATP	C4-N9	-2.41	1.32	1.37
3	B	5101	ATP	C4-N9	-2.40	1.32	1.37
3	E	5101	ATP	C4-N9	-2.39	1.32	1.37
3	G	5101	ATP	C8-N7	2.24	1.36	1.31
4	I	5102	CFF	O11-C2	-2.23	1.18	1.22
4	E	5102	CFF	O11-C2	-2.22	1.18	1.22
4	B	5102	CFF	O11-C2	-2.20	1.18	1.22
4	G	5102	CFF	O11-C2	-2.19	1.18	1.22
3	I	5101	ATP	C8-N7	2.18	1.35	1.31
3	B	5101	ATP	C8-N7	2.17	1.35	1.31
3	E	5101	ATP	C8-N7	2.17	1.35	1.31
4	E	5102	CFF	C2-N3	-2.14	1.34	1.39
4	B	5102	CFF	O13-C6	-2.12	1.18	1.23
4	E	5102	CFF	O13-C6	-2.11	1.18	1.23
4	I	5102	CFF	C2-N3	-2.11	1.34	1.39
4	G	5102	CFF	O13-C6	-2.10	1.18	1.23
4	B	5102	CFF	C2-N3	-2.09	1.34	1.39
4	G	5102	CFF	C2-N3	-2.07	1.35	1.39
4	I	5102	CFF	O13-C6	-2.07	1.18	1.23
4	B	5102	CFF	C2-N1	-2.05	1.35	1.39
4	I	5102	CFF	C2-N1	-2.04	1.35	1.39
4	E	5102	CFF	C2-N1	-2.04	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5102	CFF	C2-N1	-2.03	1.35	1.39

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C14-N7-C8	-7.87	111.56	126.28
4	I	5102	CFF	C14-N7-C8	-7.86	111.57	126.28
4	E	5102	CFF	C14-N7-C8	-7.84	111.61	126.28
4	B	5102	CFF	C14-N7-C8	-7.83	111.62	126.28
3	E	5101	ATP	C5-C4-N3	-5.28	119.45	126.72
3	B	5101	ATP	C5-C4-N3	-5.23	119.51	126.72
4	G	5102	CFF	C14-N7-C5	5.21	140.17	127.77
4	E	5102	CFF	C14-N7-C5	5.21	140.16	127.77
4	B	5102	CFF	C14-N7-C5	5.21	140.16	127.77
4	I	5102	CFF	C14-N7-C5	5.20	140.14	127.77
3	I	5101	ATP	C5-C4-N3	-5.16	119.61	126.72
3	G	5101	ATP	C5-C4-N3	-5.10	119.70	126.72
3	E	5101	ATP	N3-C4-N9	4.25	134.39	127.17
3	B	5101	ATP	N3-C4-N9	4.17	134.25	127.17
3	I	5101	ATP	N3-C4-N9	4.15	134.22	127.17
3	G	5101	ATP	N3-C4-N9	4.13	134.19	127.17
4	B	5102	CFF	C5-C6-N1	4.11	119.59	112.06
4	E	5102	CFF	C5-C6-N1	4.10	119.57	112.06
4	I	5102	CFF	C5-C6-N1	4.08	119.54	112.06
4	G	5102	CFF	C5-C6-N1	4.07	119.52	112.06
3	B	5101	ATP	C2-N3-C4	3.51	120.41	111.83
3	E	5101	ATP	C2-N3-C4	3.50	120.37	111.83
3	I	5101	ATP	C2-N3-C4	3.45	120.26	111.83
3	B	5101	ATP	N3-C2-N1	-3.44	123.38	128.58
3	G	5101	ATP	C2-N3-C4	3.43	120.22	111.83
3	G	5101	ATP	N3-C2-N1	-3.43	123.40	128.58
3	I	5101	ATP	N3-C2-N1	-3.41	123.42	128.58
3	E	5101	ATP	N3-C2-N1	-3.38	123.46	128.58
4	G	5102	CFF	C6-N1-C2	-3.36	120.20	125.66
3	B	5101	ATP	C4-C5-N7	-3.34	106.77	110.58
4	E	5102	CFF	C6-N1-C2	-3.31	120.27	125.66
4	B	5102	CFF	C6-N1-C2	-3.31	120.28	125.66
4	I	5102	CFF	C6-N1-C2	-3.31	120.28	125.66
3	I	5101	ATP	C4-C5-N7	-3.26	106.85	110.58
3	E	5101	ATP	C4-C5-N7	-3.24	106.87	110.58
3	G	5101	ATP	C4-C5-N7	-3.21	106.91	110.58
3	G	5101	ATP	C4-N9-C8	3.02	108.91	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5102	CFF	N3-C4-N9	3.00	130.99	126.27
4	B	5102	CFF	N3-C4-N9	2.97	130.93	126.27
3	I	5101	ATP	C4-N9-C8	2.91	108.79	105.74
4	I	5102	CFF	N3-C4-N9	2.91	130.84	126.27
4	I	5102	CFF	N7-C8-N9	-2.90	108.22	113.48
4	G	5102	CFF	N7-C8-N9	-2.89	108.24	113.48
3	B	5101	ATP	C4-N9-C8	2.89	108.77	105.74
4	E	5102	CFF	N7-C8-N9	-2.89	108.24	113.48
4	B	5102	CFF	N7-C8-N9	-2.88	108.27	113.48
3	E	5101	ATP	C4-N9-C8	2.87	108.75	105.74
4	G	5102	CFF	N3-C4-N9	2.85	130.74	126.27
4	B	5102	CFF	C6-C5-C4	-2.62	119.62	122.92
4	I	5102	CFF	C6-C5-C4	-2.61	119.63	122.92
4	I	5102	CFF	O13-C6-C5	-2.60	121.04	126.38
4	B	5102	CFF	O13-C6-C5	-2.60	121.05	126.38
4	E	5102	CFF	O13-C6-C5	-2.60	121.05	126.38
4	E	5102	CFF	C6-C5-C4	-2.59	119.66	122.92
4	G	5102	CFF	C6-C5-C4	-2.55	119.70	122.92
4	G	5102	CFF	O13-C6-C5	-2.55	121.16	126.38
4	G	5102	CFF	N3-C2-N1	2.51	120.28	117.14
4	E	5102	CFF	N3-C2-N1	2.47	120.22	117.14
4	I	5102	CFF	N3-C2-N1	2.44	120.19	117.14
4	B	5102	CFF	N3-C2-N1	2.44	120.19	117.14
3	B	5101	ATP	C5-N7-C8	2.39	107.20	103.45
3	I	5101	ATP	C5-N7-C8	2.36	107.15	103.45
3	E	5101	ATP	C3'-C2'-C1'	2.35	105.91	101.46
3	B	5101	ATP	C3'-C2'-C1'	2.33	105.87	101.46
3	I	5101	ATP	C3'-C2'-C1'	2.33	105.86	101.46
3	G	5101	ATP	C2-N1-C6	2.32	122.54	118.73
3	G	5101	ATP	C5-N7-C8	2.32	107.09	103.45
3	E	5101	ATP	C5-N7-C8	2.31	107.08	103.45
3	I	5101	ATP	C2-N1-C6	2.30	122.51	118.73
3	G	5101	ATP	C3'-C2'-C1'	2.29	105.80	101.46
3	B	5101	ATP	C6-C5-N7	2.29	136.51	132.09
4	G	5102	CFF	C12-N3-C2	2.26	121.28	117.33
3	B	5101	ATP	C2-N1-C6	2.25	122.42	118.73
3	G	5101	ATP	C6-C5-N7	2.24	136.41	132.09
3	E	5101	ATP	C2-N1-C6	2.24	122.41	118.73
3	I	5101	ATP	C6-C5-N7	2.23	136.39	132.09
3	G	5101	ATP	C2'-C1'-N9	-2.21	107.83	113.30
3	E	5101	ATP	C6-C5-N7	2.20	136.32	132.09
4	I	5102	CFF	C12-N3-C2	2.19	121.15	117.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	C2'-C1'-N9	-2.17	107.90	113.30
3	E	5101	ATP	C2'-C1'-N9	-2.14	107.99	113.30
4	B	5102	CFF	C12-N3-C2	2.13	121.04	117.33
4	G	5102	CFF	C10-N1-C6	2.10	120.90	117.64
4	I	5102	CFF	C10-N1-C6	2.09	120.88	117.64
3	G	5101	ATP	N9-C8-N7	-2.09	110.97	113.94
3	B	5101	ATP	C2'-C1'-N9	-2.07	108.16	113.30
4	B	5102	CFF	C10-N1-C6	2.05	120.82	117.64
3	B	5101	ATP	N9-C8-N7	-2.05	111.03	113.94
3	I	5101	ATP	N9-C8-N7	-2.05	111.03	113.94
4	E	5102	CFF	C12-N3-C2	2.04	120.88	117.33
4	E	5102	CFF	C10-N1-C6	2.03	120.79	117.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

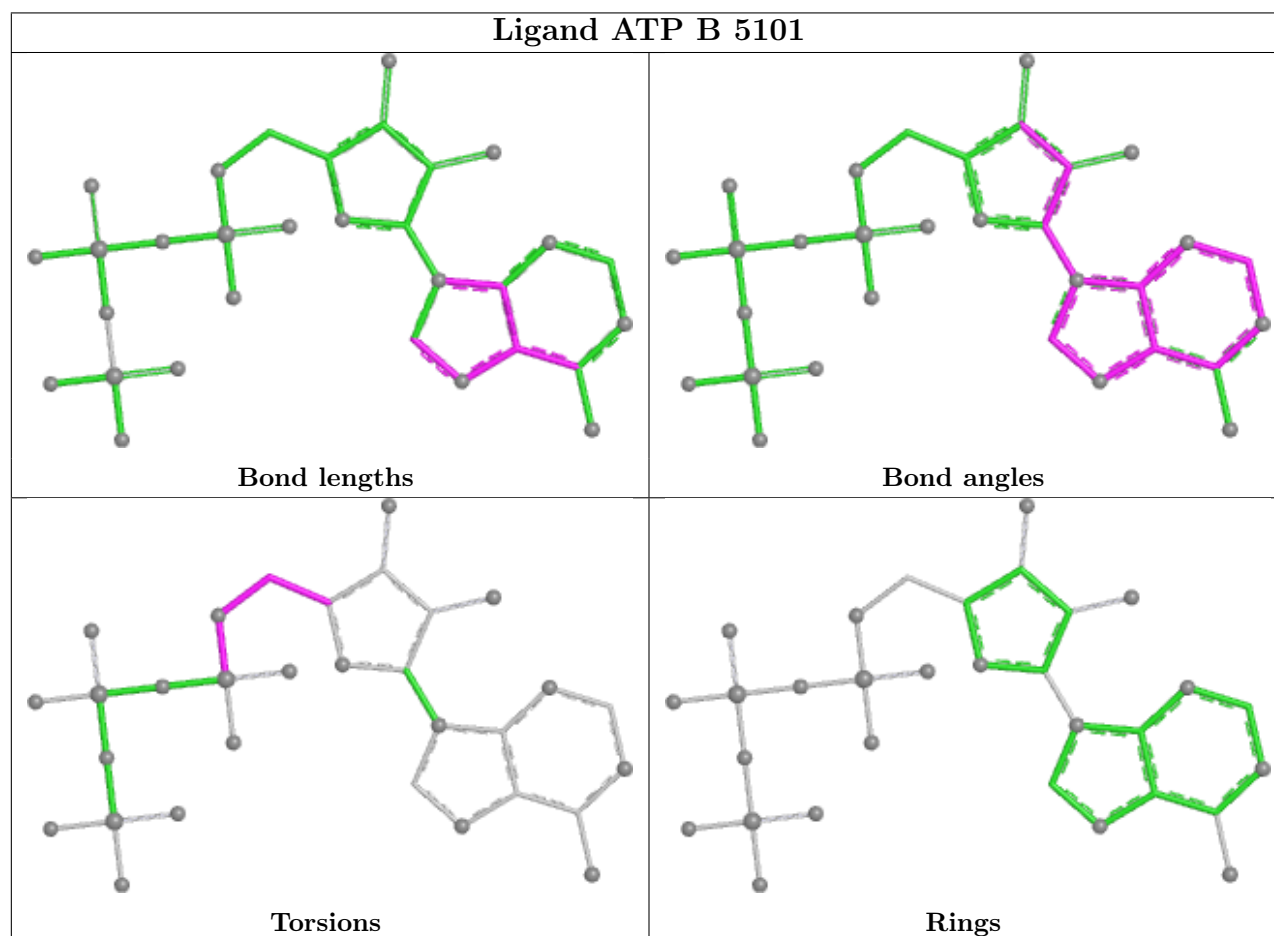
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	C5'-O5'-PA-O2A
3	G	5101	ATP	C5'-O5'-PA-O2A
3	I	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C4'-C5'-O5'-PA
3	G	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA
3	E	5101	ATP	C4'-C5'-O5'-PA

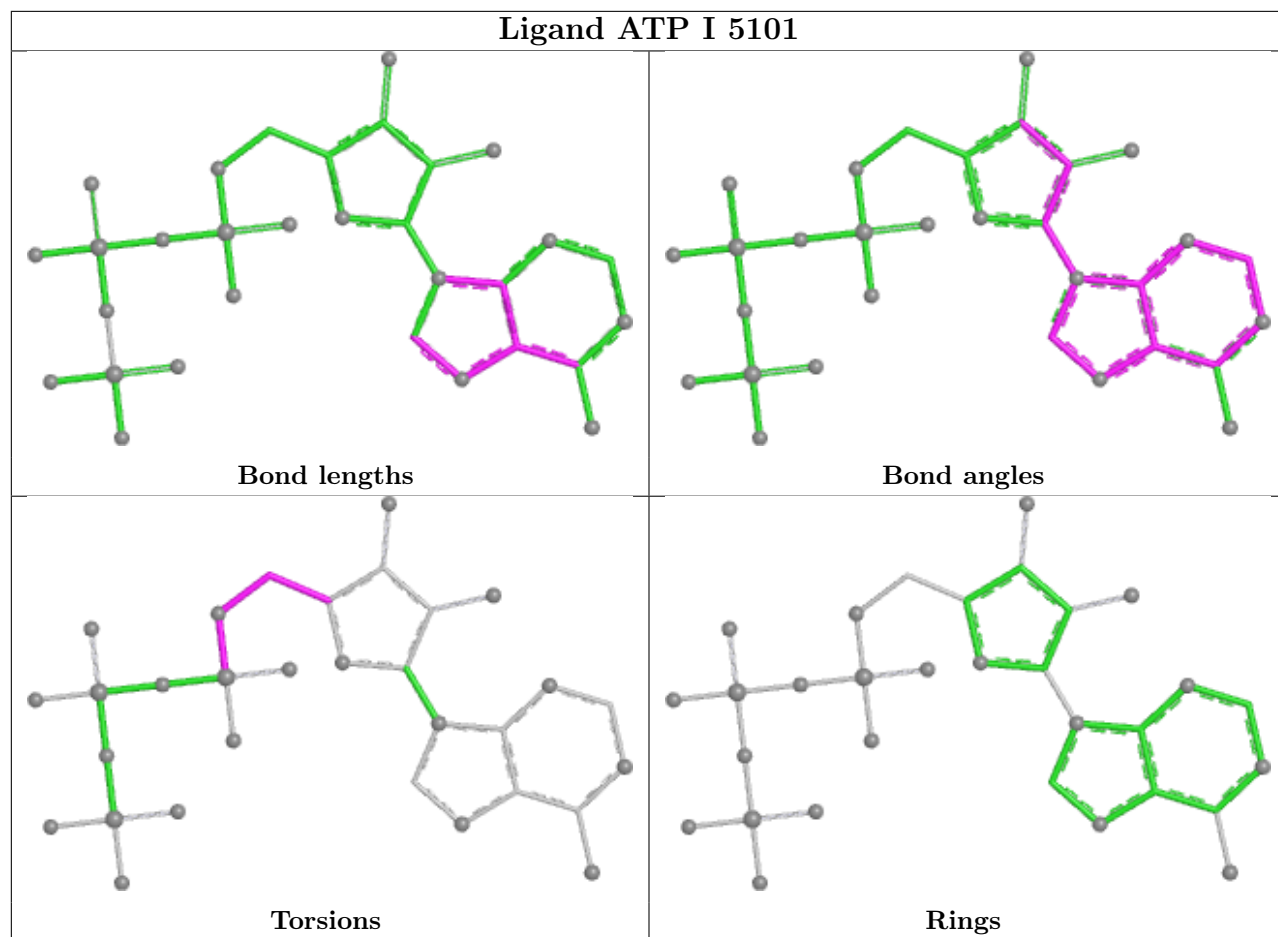
There are no ring outliers.

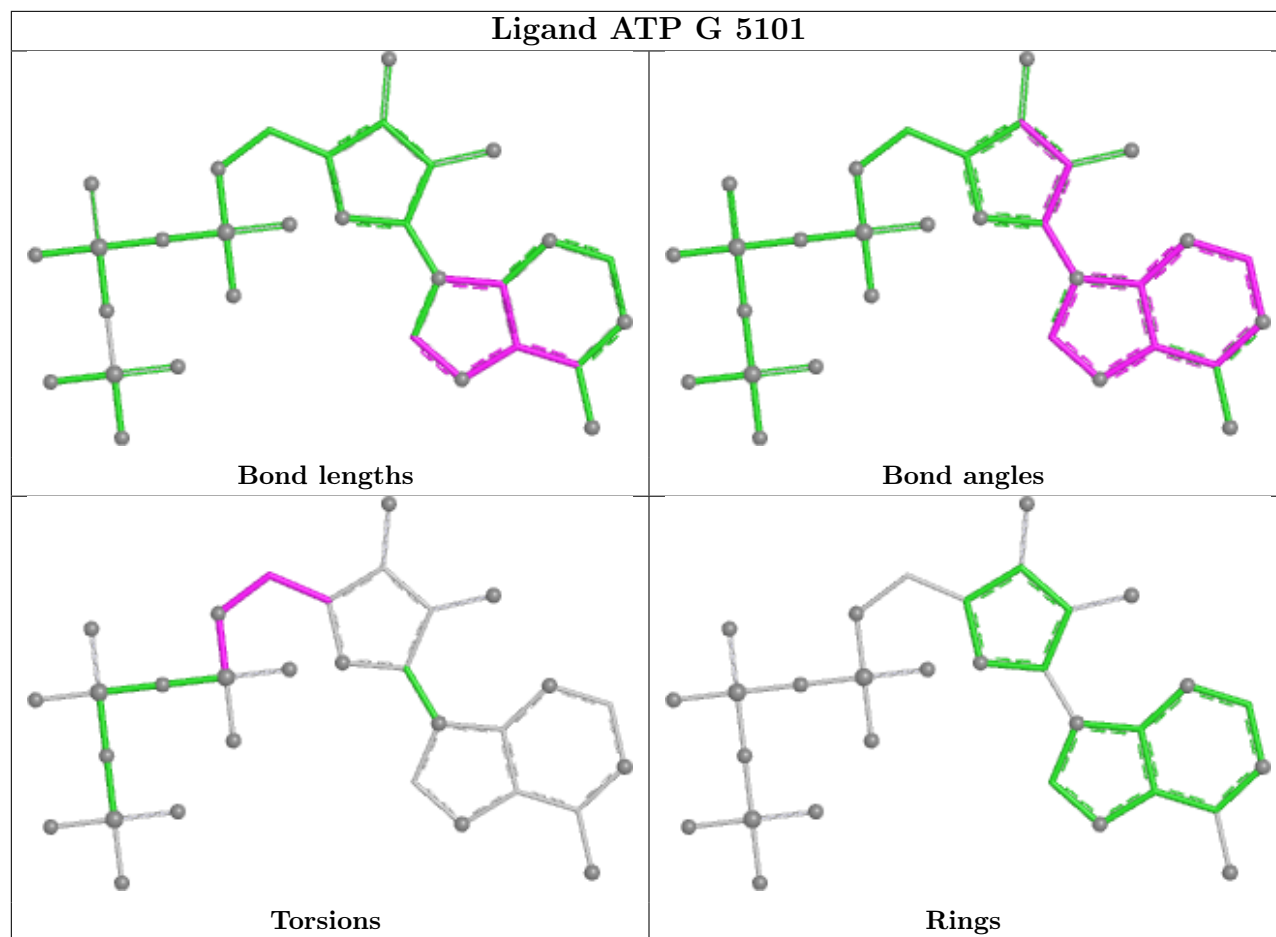
4 monomers are involved in 5 short contacts:

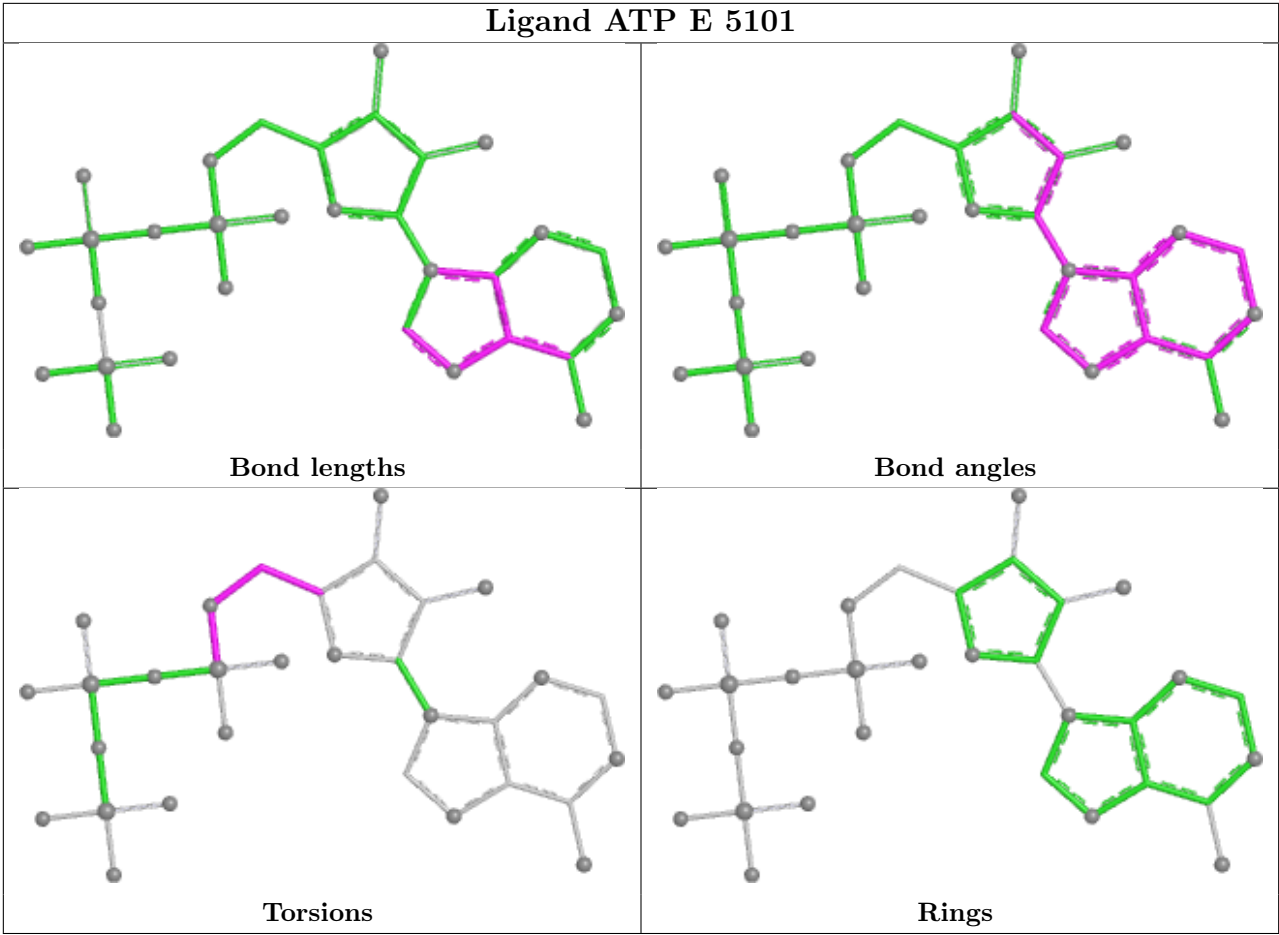
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
3	I	5101	ATP	1	0
3	G	5101	ATP	1	0
3	E	5101	ATP	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	14
2	B	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	E	4345:UNK	C	4540:PHE	N	73.04
1	B	4345:UNK	C	4540:PHE	N	73.02

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	73.01
1	G	4345:UNK	C	4540:PHE	N	73.00
1	E	3613:UNK	C	3639:THR	N	45.97
1	B	3613:UNK	C	3639:THR	N	45.94
1	G	3613:UNK	C	3639:THR	N	45.92
1	I	3613:UNK	C	3639:THR	N	45.92
1	E	4253:GLU	C	4320:UNK	N	28.30
1	B	4253:GLU	C	4320:UNK	N	28.29
1	I	4253:GLU	C	4320:UNK	N	28.27
1	G	4253:GLU	C	4320:UNK	N	28.26
1	B	3163:UNK	C	3170:UNK	N	16.28
1	G	3163:UNK	C	3170:UNK	N	16.26
1	I	3163:UNK	C	3170:UNK	N	16.26
1	E	3163:UNK	C	3170:UNK	N	16.25
1	E	3063:UNK	C	3134:UNK	N	14.92
1	G	3063:UNK	C	3134:UNK	N	14.91
1	I	3063:UNK	C	3134:UNK	N	14.91
1	B	3063:UNK	C	3134:UNK	N	14.90
1	B	3468:UNK	C	3511:UNK	N	14.45
1	G	3468:UNK	C	3511:UNK	N	14.45
1	I	3468:UNK	C	3511:UNK	N	14.45
1	E	3468:UNK	C	3511:UNK	N	14.44
1	B	2703:UNK	C	2734:ASN	N	13.67
1	E	2703:UNK	C	2734:ASN	N	13.63
1	I	2703:UNK	C	2734:ASN	N	13.61
1	G	2703:UNK	C	2734:ASN	N	13.60
1	I	3236:UNK	C	3241:UNK	N	12.64
1	E	3236:UNK	C	3241:UNK	N	12.64
1	B	3236:UNK	C	3241:UNK	N	12.63
1	G	3236:UNK	C	3241:UNK	N	12.63
1	B	1564:UNK	C	1573:MET	N	12.50
1	E	1564:UNK	C	1573:MET	N	12.50
1	G	1564:UNK	C	1573:MET	N	12.48
1	I	1564:UNK	C	1573:MET	N	12.48
1	E	2976:UNK	C	2995:UNK	N	11.98
1	I	2976:UNK	C	2995:UNK	N	11.97
1	G	2976:UNK	C	2995:UNK	N	11.96
1	B	2976:UNK	C	2995:UNK	N	11.94
1	B	3254:UNK	C	3261:UNK	N	8.41
1	G	3254:UNK	C	3261:UNK	N	8.40
1	I	3254:UNK	C	3261:UNK	N	8.40
1	E	3254:UNK	C	3261:UNK	N	8.40

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	1297:UNK	C	1430:UNK	N	6.01
1	B	1297:UNK	C	1430:UNK	N	6.00
1	E	1297:UNK	C	1430:UNK	N	5.99
1	G	1297:UNK	C	1430:UNK	N	5.97
1	G	2479:LEU	C	2487:UNK	N	3.26
1	I	2479:LEU	C	2487:UNK	N	3.26
1	B	2479:LEU	C	2487:UNK	N	3.25
1	E	2479:LEU	C	2487:UNK	N	3.25
1	E	2939:ARG	C	2942:UNK	N	3.23
1	B	2939:ARG	C	2942:UNK	N	3.22
1	G	2939:ARG	C	2942:UNK	N	3.21
1	I	2939:ARG	C	2942:UNK	N	3.21

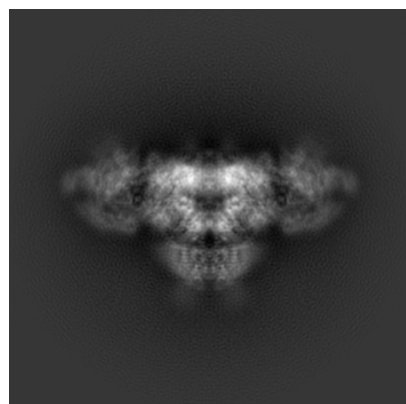
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8377. These allow visual inspection of the internal detail of the map and identification of artifacts.

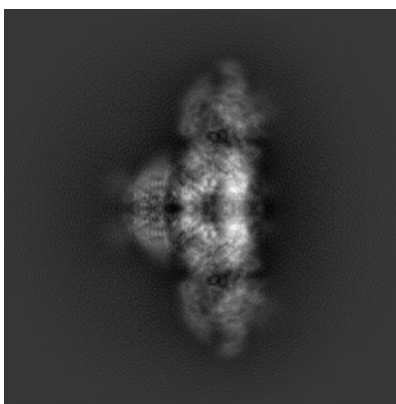
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

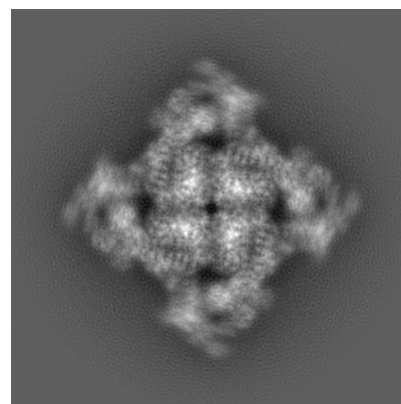
6.1.1 Primary map



X

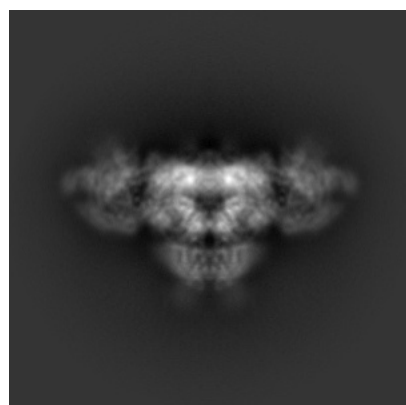


Y

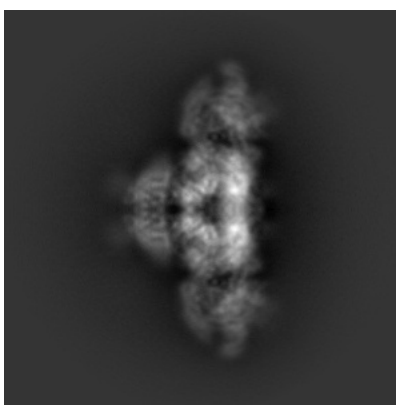


Z

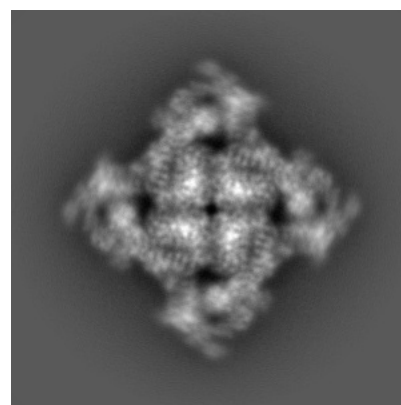
6.1.2 Raw map



X



Y

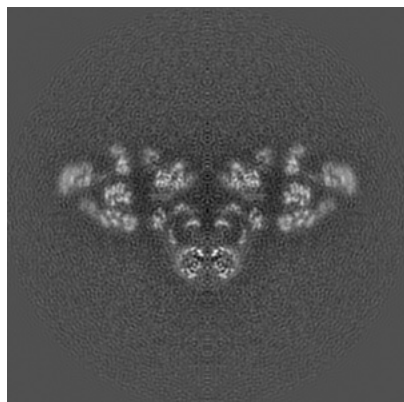


Z

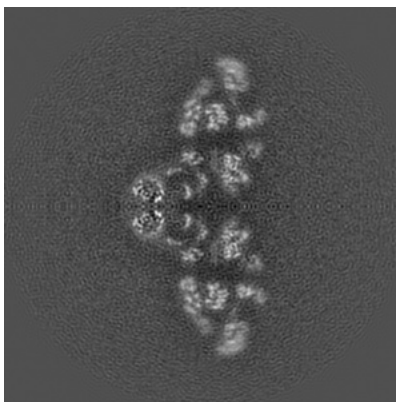
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

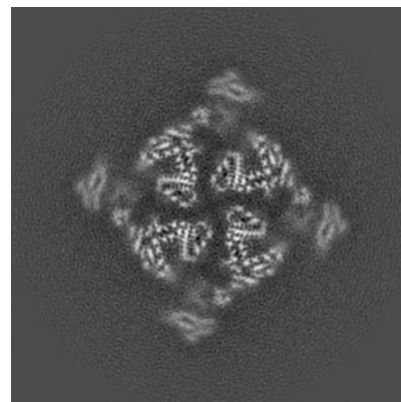
6.2.1 Primary map



X Index: 200

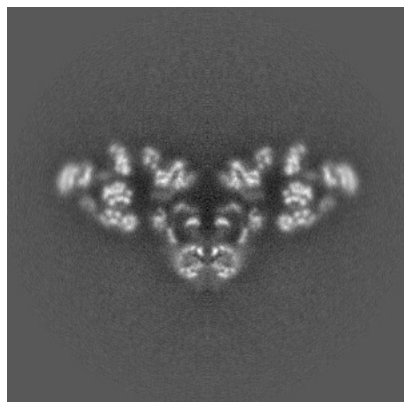


Y Index: 200

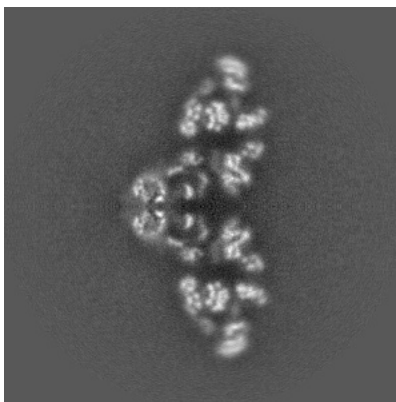


Z Index: 200

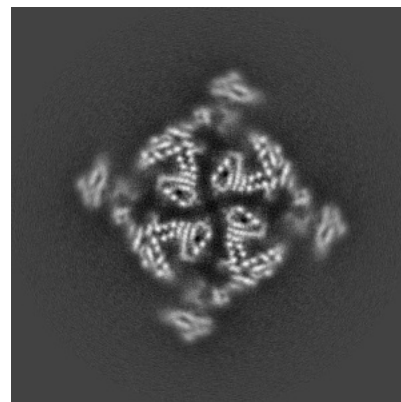
6.2.2 Raw map



X Index: 200



Y Index: 200

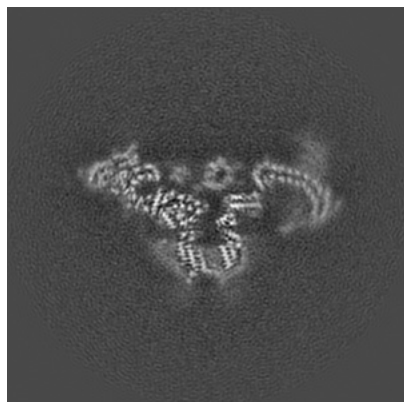


Z Index: 200

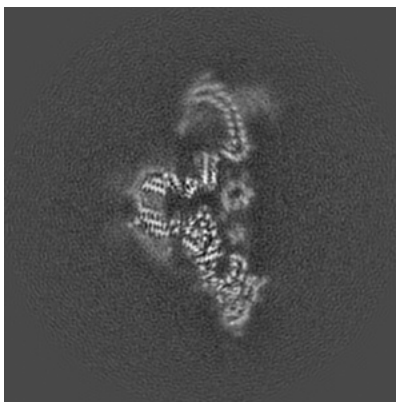
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

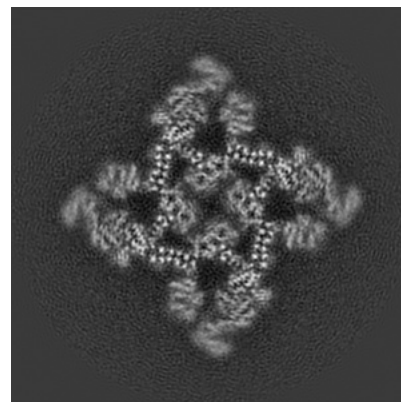
6.3.1 Primary map



X Index: 225

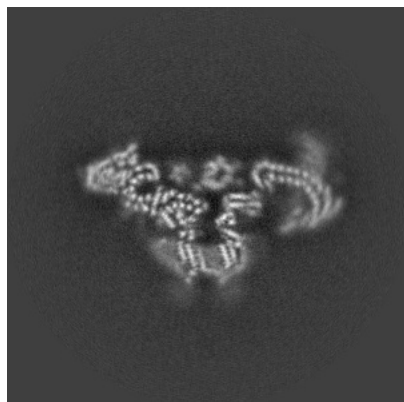


Y Index: 175

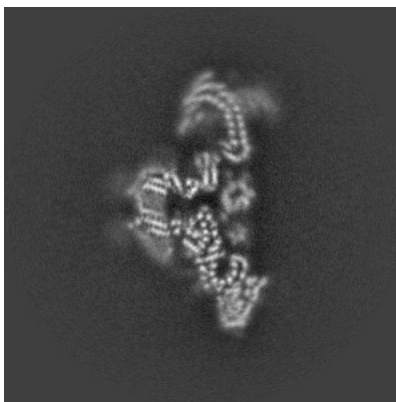


Z Index: 226

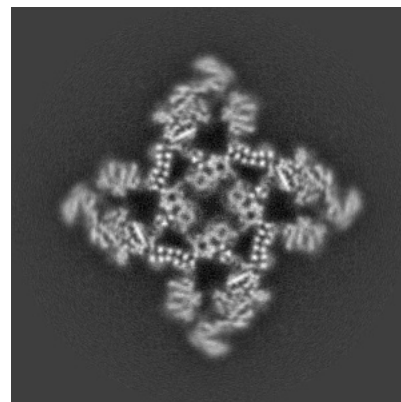
6.3.2 Raw map



X Index: 225



Y Index: 175

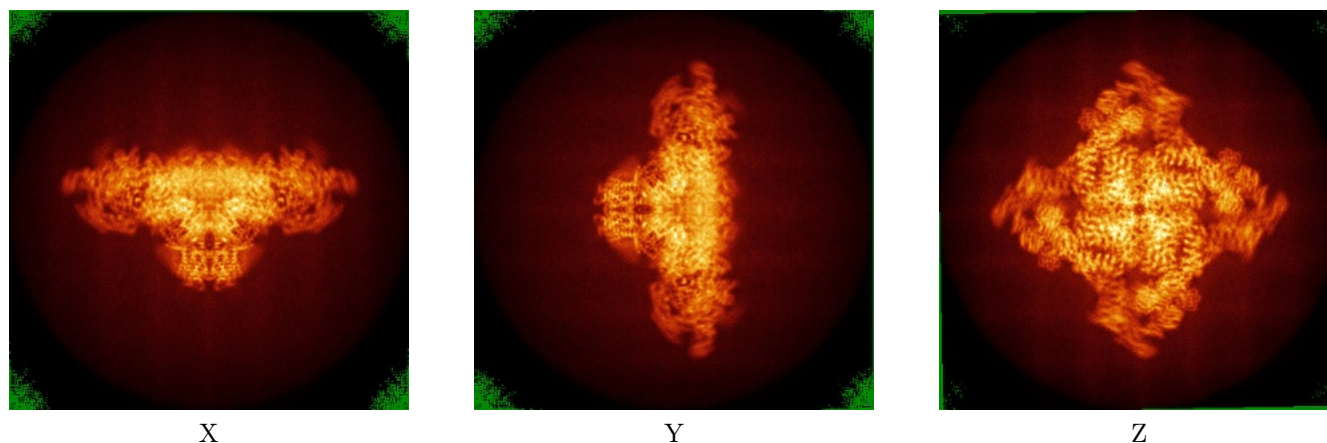


Z Index: 226

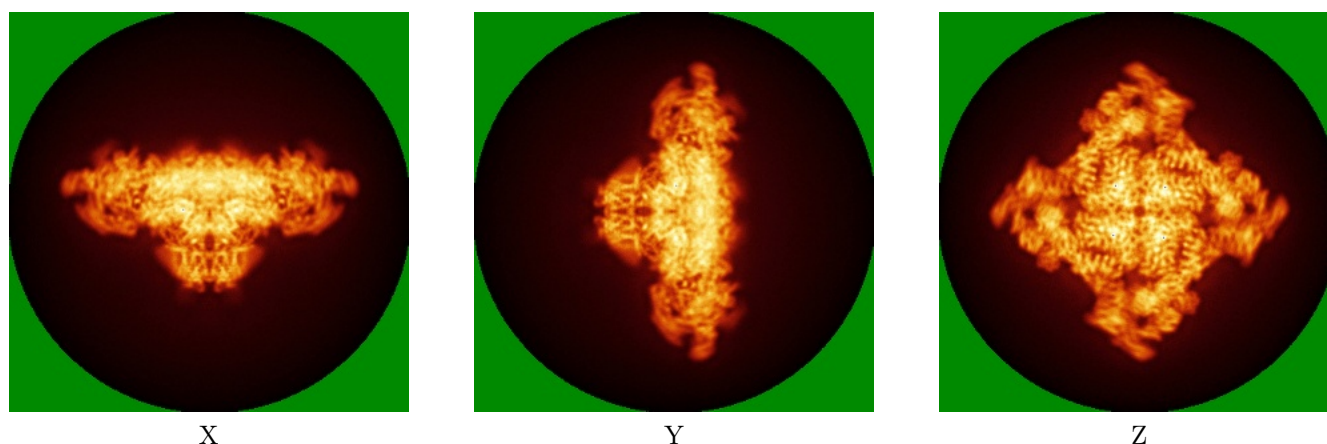
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

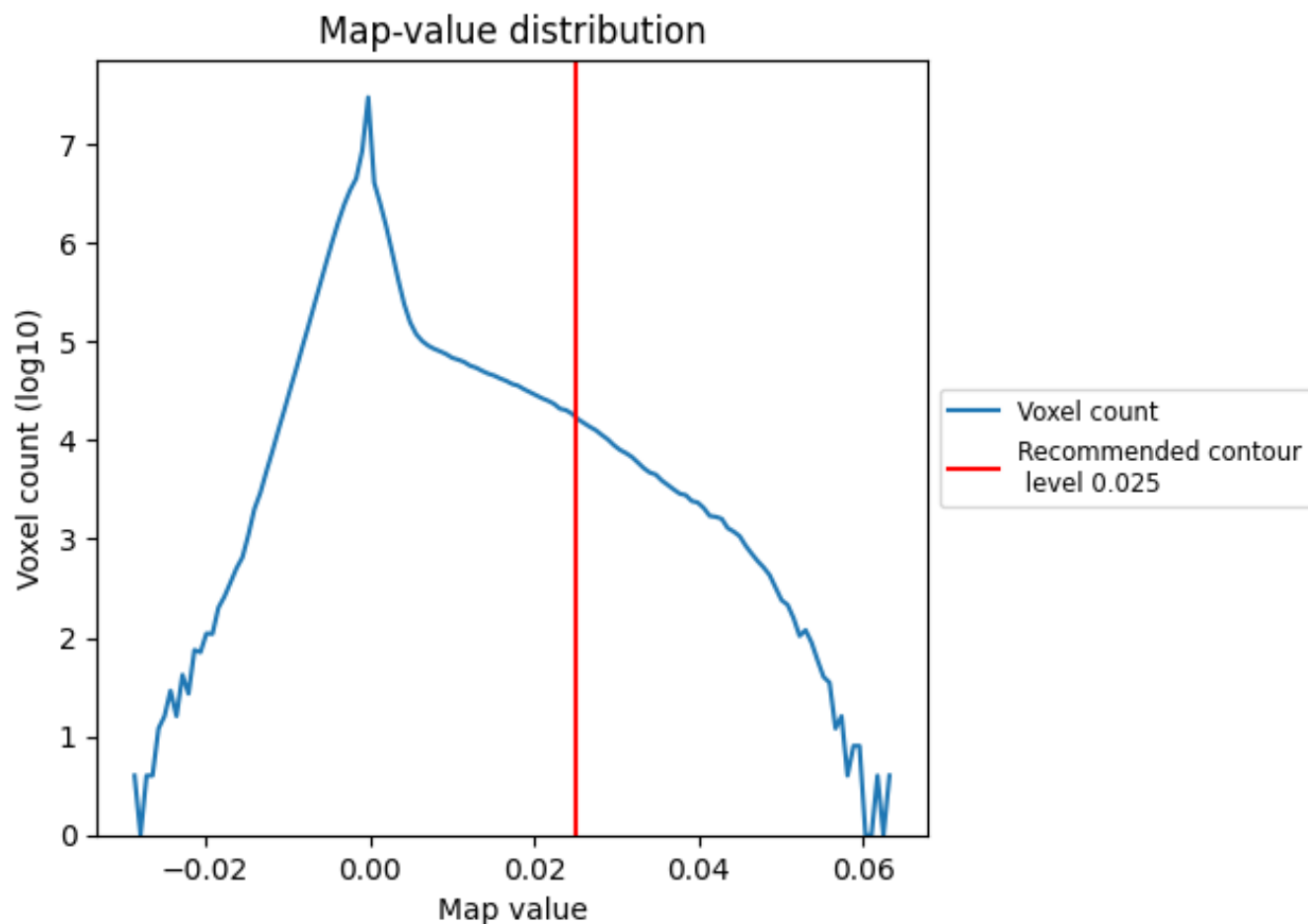
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

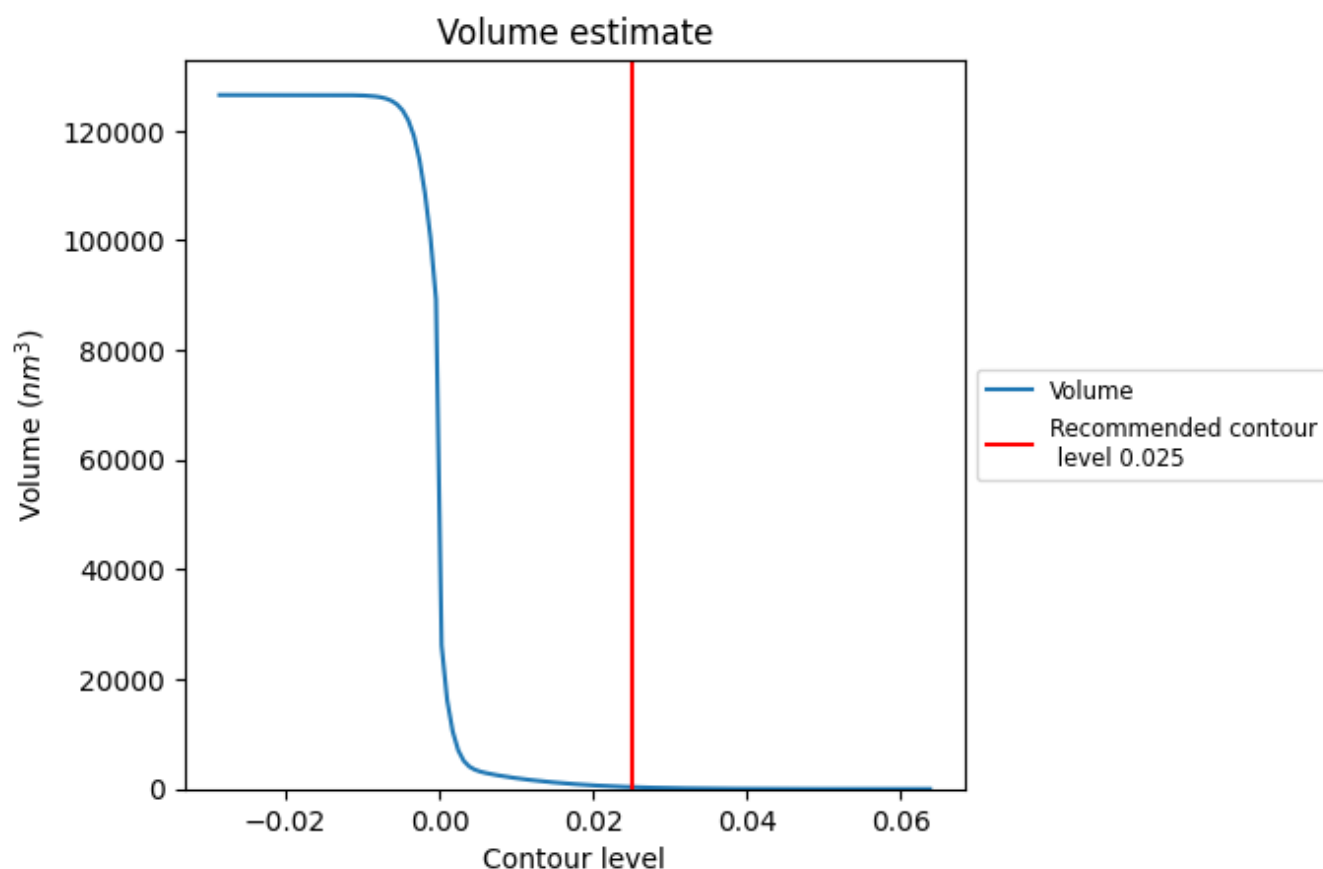
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

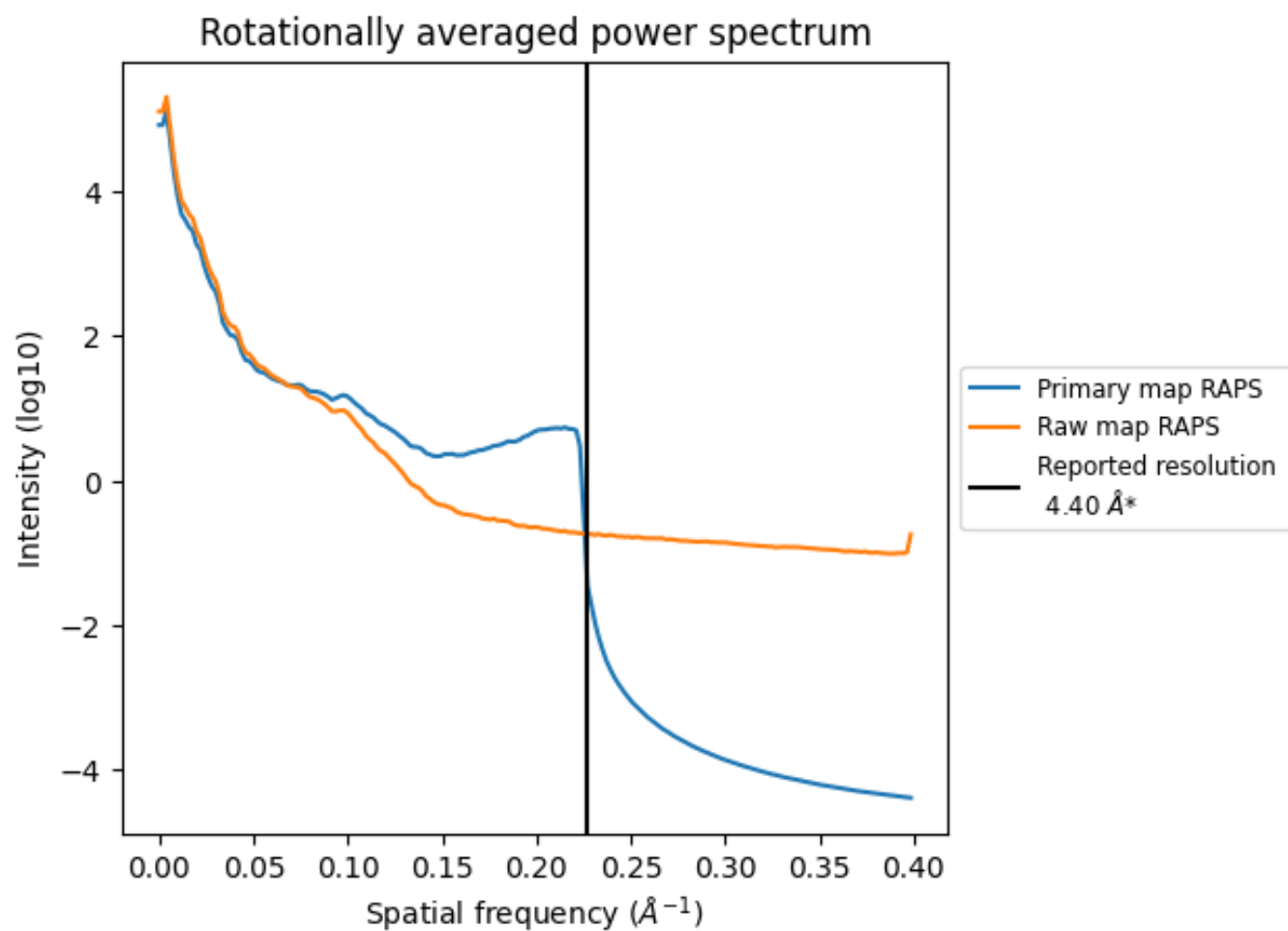
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm³; this corresponds to an approximate mass of 311 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 ⓘ

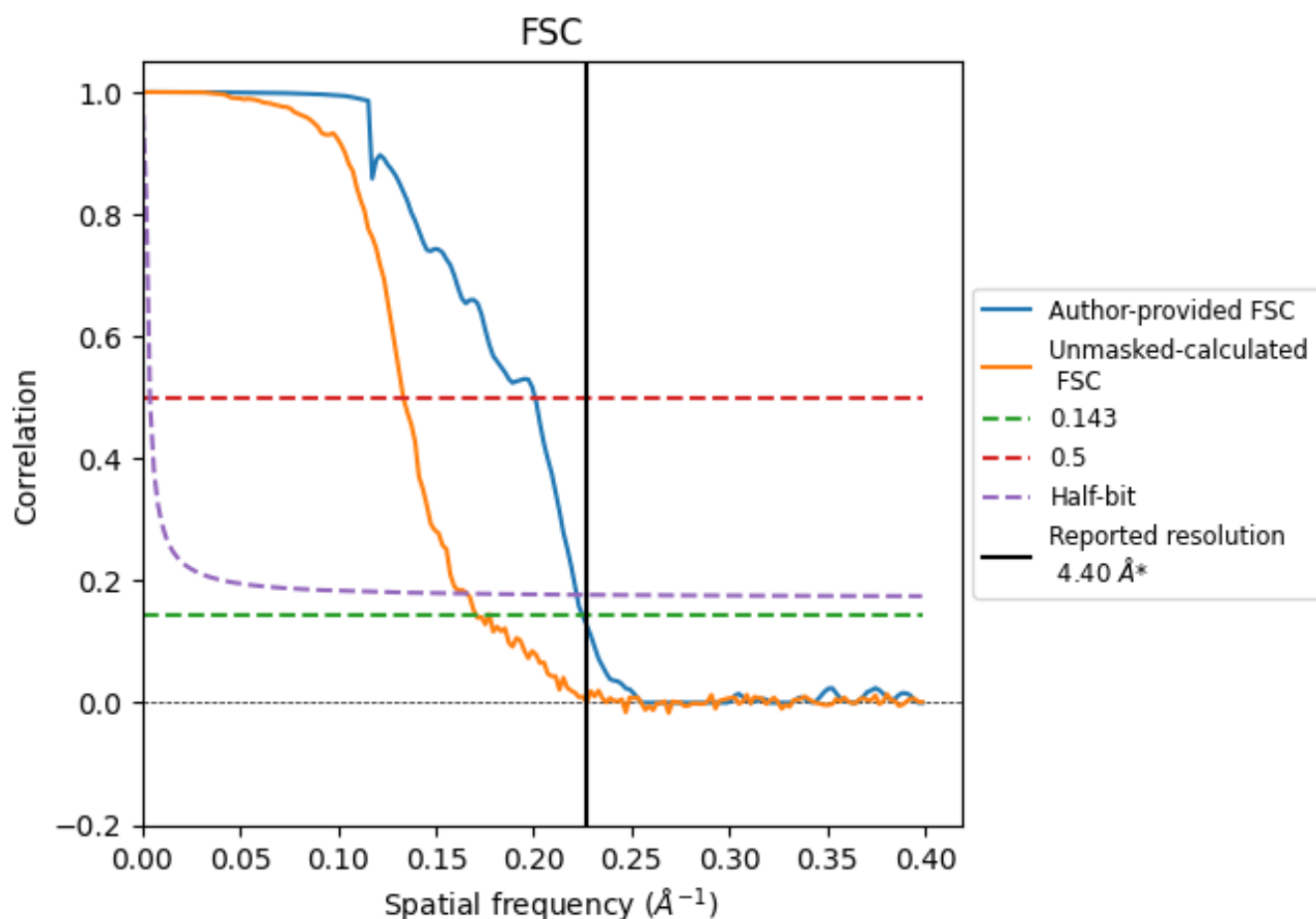


*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.45	4.99	4.50
Unmasked-calculated*	5.86	7.50	6.03

*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 5.86 differs from the reported value 4.4 by more than 10 %

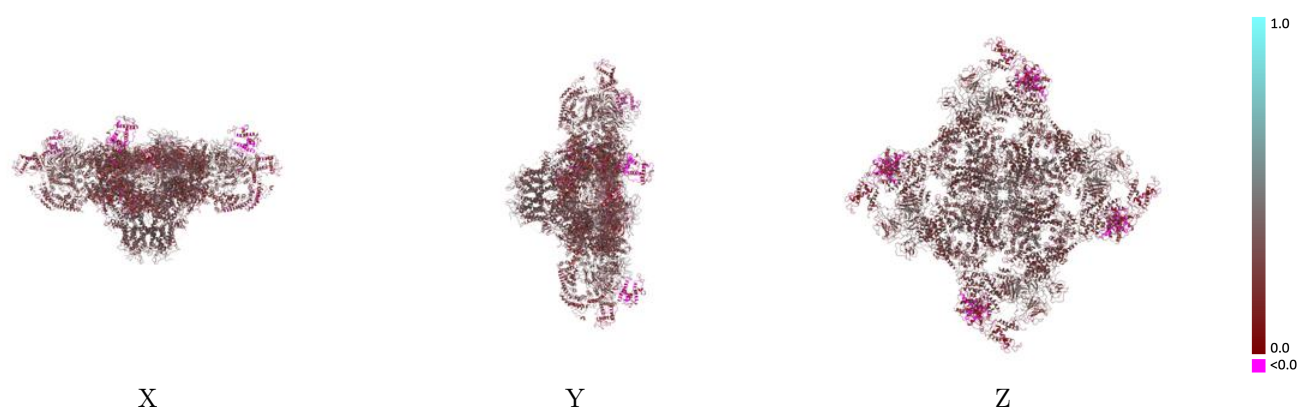
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8377 and PDB model 5TA3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

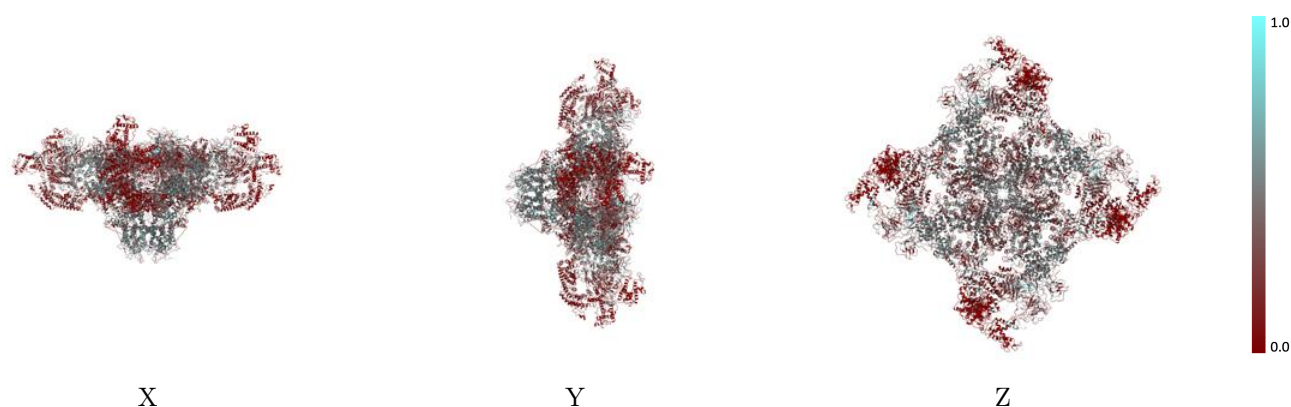
This section was not generated.

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



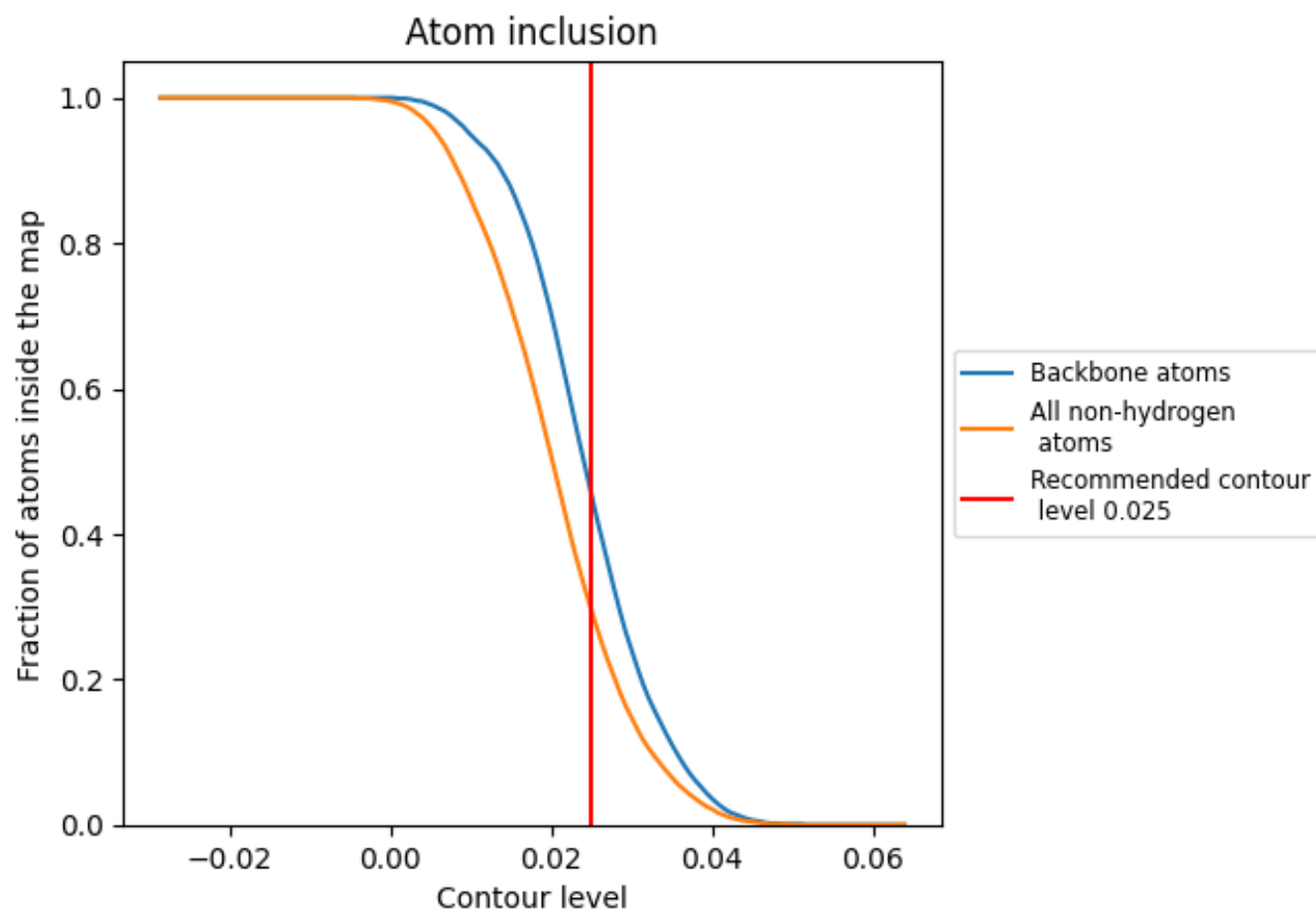
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 45% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2940	0.2750
A	0.3000	0.3110
B	0.2950	0.2780
E	0.2940	0.2720
F	0.2960	0.3140
G	0.2940	0.2750
H	0.3010	0.3150
I	0.2930	0.2730
J	0.3030	0.3120

1.0

0.0

<0.0