



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 07:33 PM EST

PDB ID : 7JMF
EMDB ID : EMD-22392
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots
- Frame 42 - State 6 (S6)
Authors : Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.
Deposited on : 2020-07-31
Resolution : 4.50 Å(reported)
Based on initial model : 5TB4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

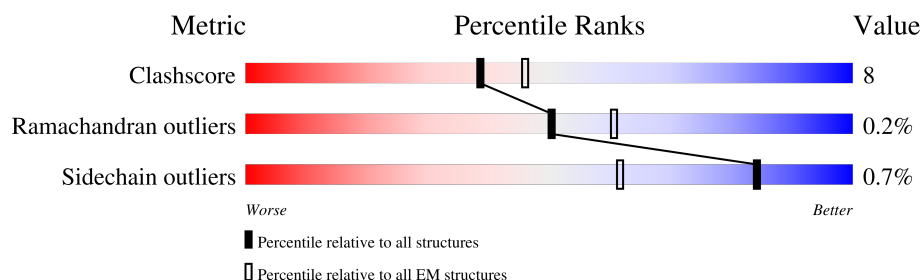
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	
1	F	108	
1	H	108	
1	J	108	
2	B	4687	
2	E	4687	
2	G	4687	
2	I	4687	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

- Molecule 2 is a protein called ryanodine receptor 1.

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

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

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

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

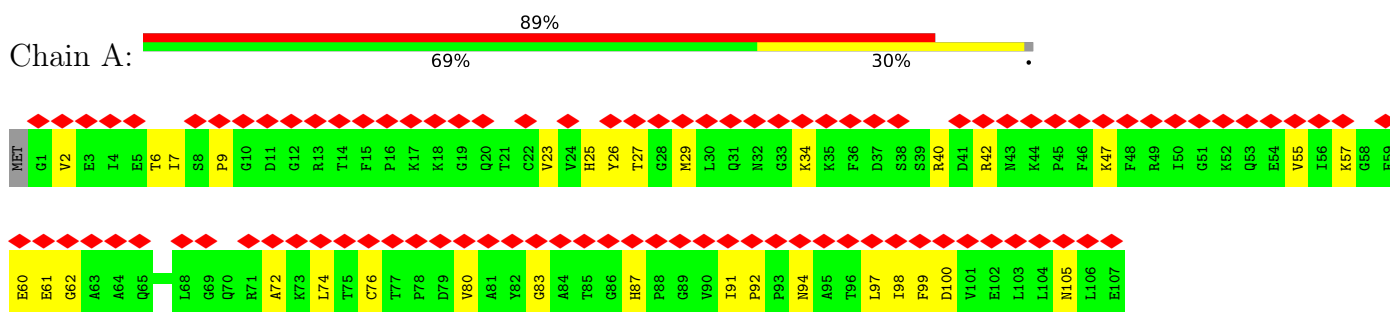
Interest" by depositor).

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

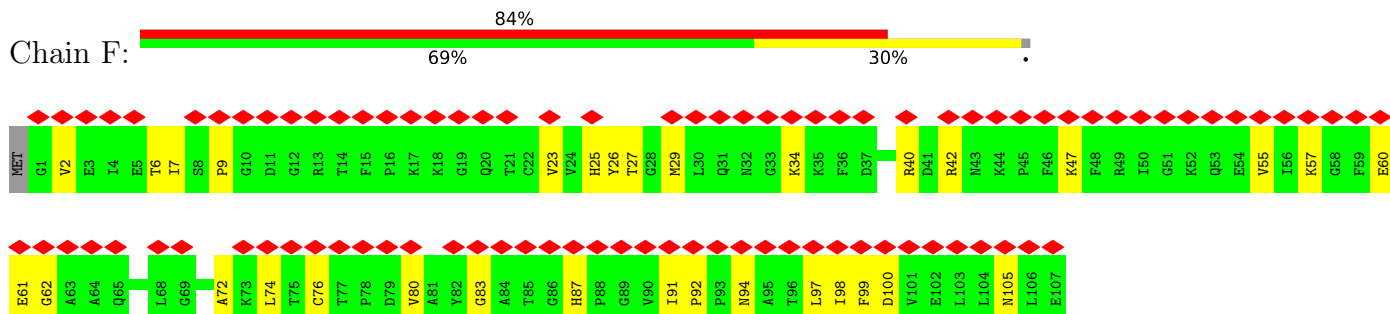
3 Residue-property plots [i](#)

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

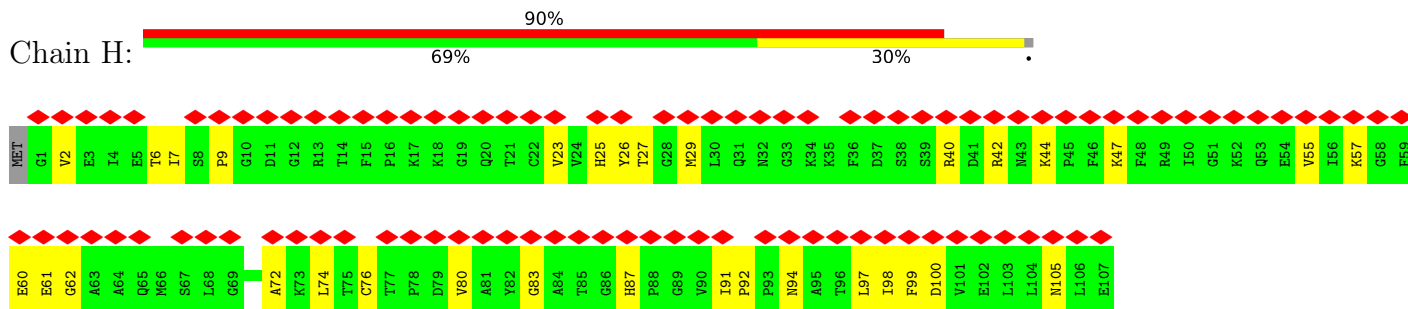
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



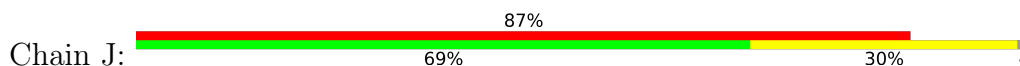
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

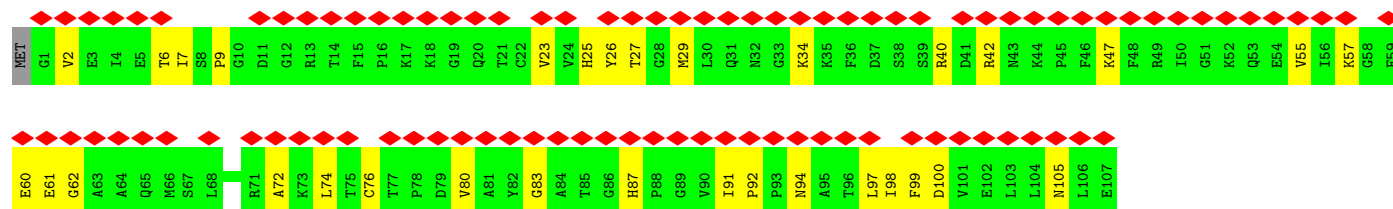


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

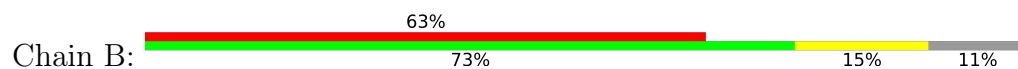


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 2: ryanodine receptor 1



M1648	D1649	I1650	L1651	E1652	L1653	R1656	L1657	D1658	L1659	Q1660	R1661	F1662	H1663	S1664	H1665	T1666	L1667	R1668	L1669	Y1670	R1671	A1672	A1675	L1676	G1677	M1678	N1679	L1680	V1681	A1682	H1683	A1684	S1687	H1688	L1689	D1690	Q1691	Q1692	L1693	L1694	L1695	H1696	A1697	L1698	E1699	D1700	A1701	H1702	L1703	P1704	G1705	P1706	L1707	A1708	R1709	G1710																																																																
P1587	A1588	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	E1596	V1597	Q1598	M1599	L1600	V1603	S1604	W1605	S1606	R1607	M1608	P1609	M1610	H1611	F1612	L1613	Q1614	GLU	THR	ARG	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	Q1629	C1630	Q1631	D1632	L1633	L1634	T1635	M1636	M1637	A1638	L1639	H1640	I1641	P1642	E1643	E1644	M1645	R1646	C1647																																																																
Q1244	F1245	E1246	P1247	V1248	P1249	P1250	E1251	H1252	P1253	H1254	Y1255	E1256	V1257	A1258	R1259	M1260	D1261	G1262	T1263	D1264	D1265	T1266	P1267	C1268	L1270	R1271	L1272	A1273	H1274	R1275	X1276	X1277	X1278	X1279	X1280	X1281	X1282	X1283	X1284	X1285	X1286	X1287	X1288	X1289	X1290	X1291	X1292	X1293	X1294	X1295	X1296	X1297	X1298	X1299	X1300	X1301	X1302	X1303	X1304	X1305	X1306	X1307	X1308	X1309	C1040	Q1041	A1042	V1043	W1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	L1120	E1181	L1182	E1183	P1243																															
X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1459	X1460	X1467	X1468	X1469	X1470	X1471	X1472	X1475	X1476	X1485	X1486	X1487	X1488	X1489	X1490	X1491	X1492	X1493	X1494	X1497	X1498	X1499	X1500	X1501	X1502	X1503	X1504	X1505	X1506	X1507	X1508	X1509	X1510	X1511	X1512	X1513	X1514	X1515	X1516	X1517	X1518	X1519	X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1535	X1536	X1537	X1538	X1539	X1540	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1563	X1564	X1565	X1566	X1567	X1568	X1569	X1570	X1571	X1572	X1573	X1574	A1577	A1578	M1579	F1580	L1581	S1582	E1583	R1584	X1585	N1586
L1184	G1185	D1186	G1187	F1188	L1189	P1190	V1191	C1192	S1193	L1194	G1195	P1196	G1197	Q1198	V1199	G1200	H1201	L1202	M1203	L1204	G1205	Q1206	D1207	V1208	S1209	S1210	L1211	R1212	F1213	F1214	A1215	I1216	G1217	G1218	L1219	Q1220	E1221	G1222	F1223	P1224	P1225	F1226	A1227	I1228	N1229	M1230	Q1231	R1232	P1233	V1234	T1235	W1236	W1237	F1238	S1239	K1240	S1241	L1242	X1434	X1436																																																												
A1121	Y1122	V1123	F1124	N1125	G1126	H1127	R1128	G1129	Q1130	R1131	W1132	H1133	L1134	G1135	S1136	F1139	G1140	R1141	P1142	W1143	Q1144	S1145	G1146	D1147	V1148	Y1149	G1150	C1151	M1152	L1155	T1156	E1157	N1158	I1161	F1162	L1163	L1164	M1165	G1166	E1167	V1168	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	L1179	R1180	E1181	L1182	E1183	P1243																																																															
PRO	SER	GLN	VAL	GLU	ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	I1073	L1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	T1082	V1083	Q1084	S1085	G1086	R1087	W1088	Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096	T1097	M1100	R1101	V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120																																																														
G992	V1001	A1002	Q1003	G1004	W1005	S1006	Y1007	S1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R1020	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	L1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	W1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	L1182	E1183	P1243																																																													
T928	L929	K930	T931	L932	L933	A934	L935	G936	N937	E938	L939	G940	M941	A942	D943	T944	R945	A946	E947	D948	N949	L950	K951	K952	T953	G954	P955	V956	R957	D958	D959	N960	K961	L962	S962	N963	G964	A968	P969	L970	D971	L972	S973	H974	V975	R976	T978	P979	A980	Q981	T982	T983	L984	V985	D986	L988	A989																																																															
E968	R969	I970	R971	E972	K973	L974	A975	E976	N977	I978	H979	E980	L981	Q982	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	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	S925	G926	E927																																																													
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P740	E741	D742	S745	C746	D749	L750	S751	V752	P753	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	S784	A785	G786	V787	K788	V789	R790	F791	L792	L793	H797	G798	E799	F800	K801	F802	L803	P804	P805	P806																																																																		



X3432	X3433	X3434	X3435	X3436	X3437	X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3448	X3451	X3452	X3453	X3454	X3455	X3456	X3459	X3460	X3461	X3462	X3463	X3464	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535																				
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X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2973	X2974	X2975	X2976	X2977	X2978	X2979	X2980	X2981	X2982	X2983	X2984	X2985	X2986	X2987	X2988	X2989	X2990	X2991	X2992	X2993	X2994	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3030	X3031	X3034	X3035	X3036		
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THR	GLU	LYS	THR	ARG	LYS	SER	GLN	THR	ALA	GLN	THR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893																					
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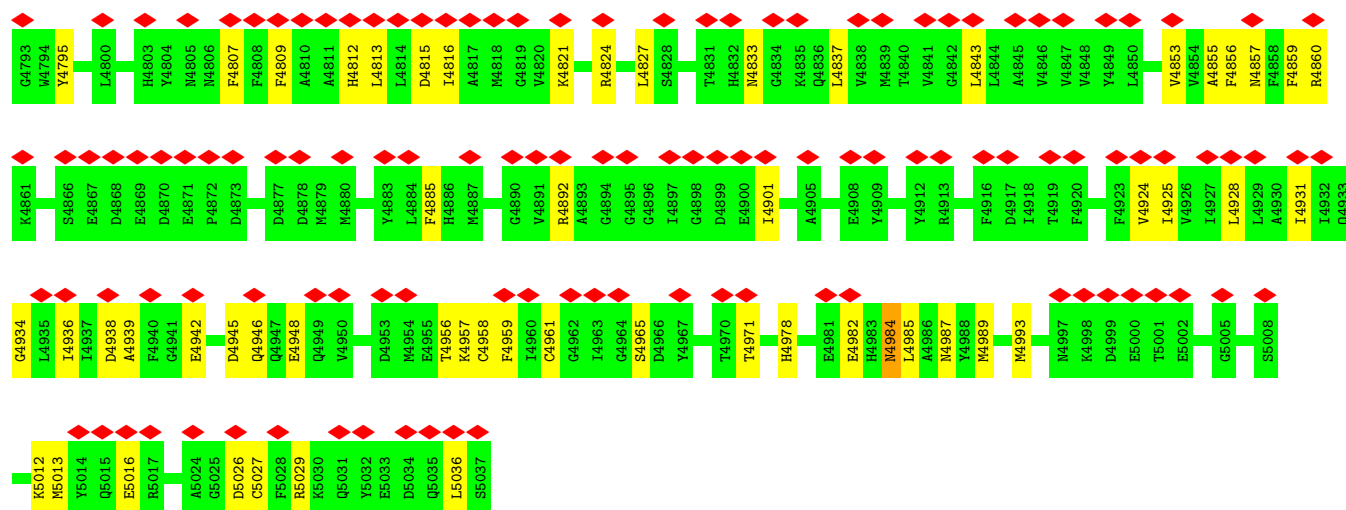
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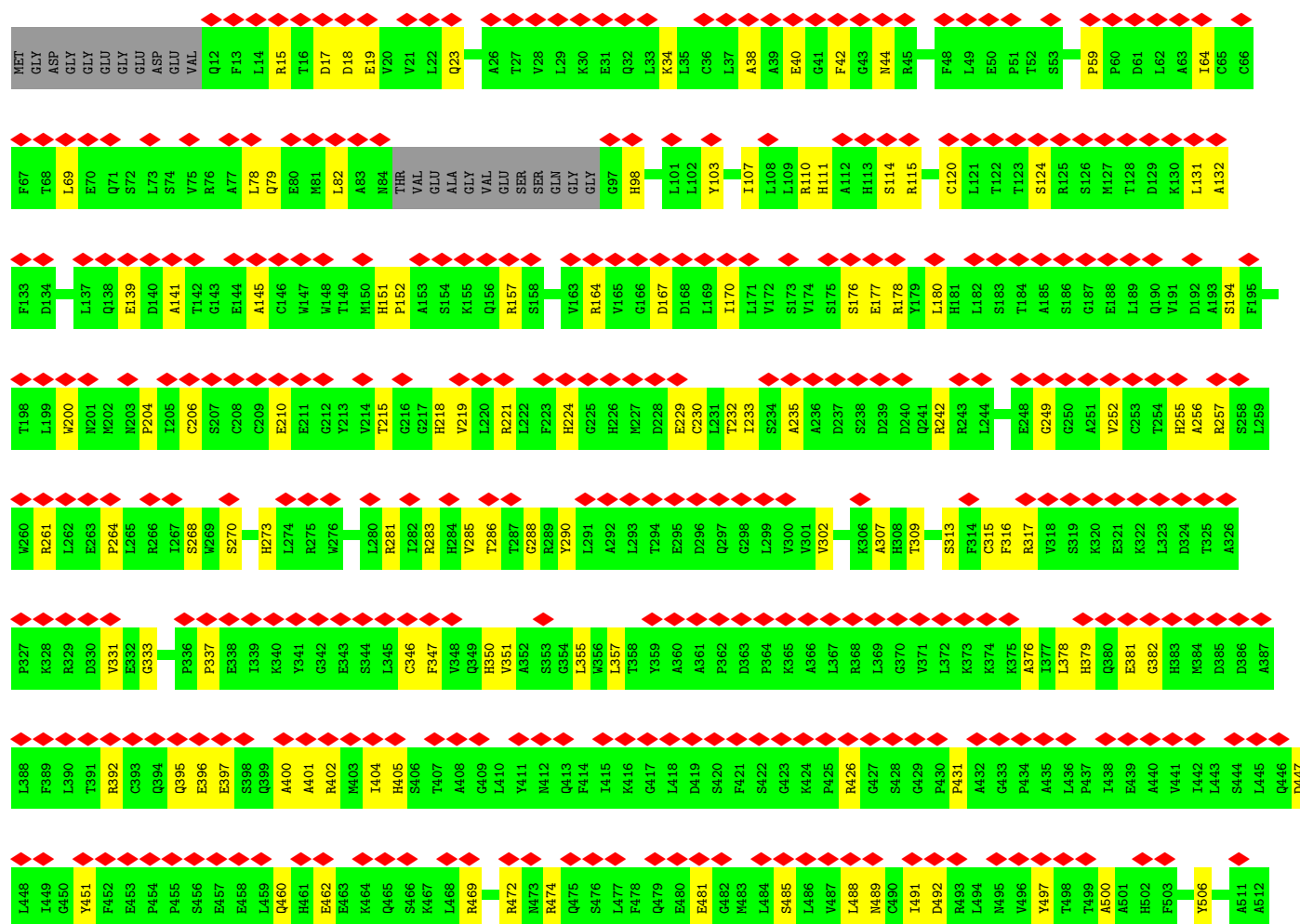
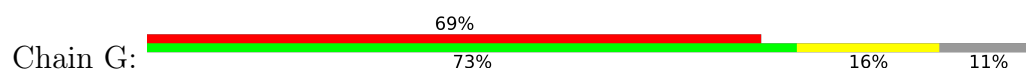
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• Molecule 2: ryanodine receptor 1



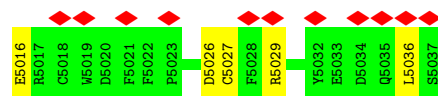
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X1447	Y1255	P1196									
X1448	E1256										



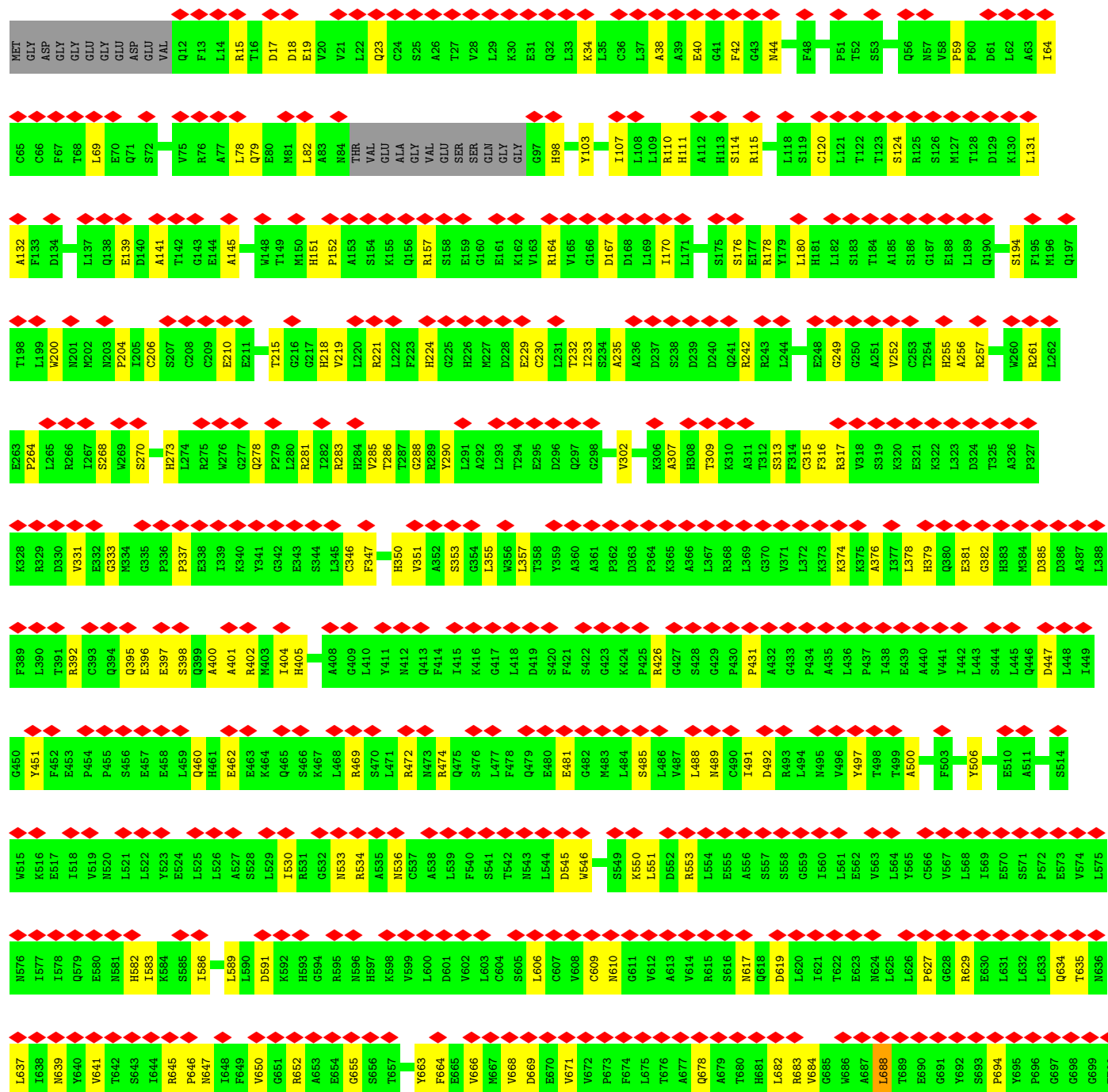
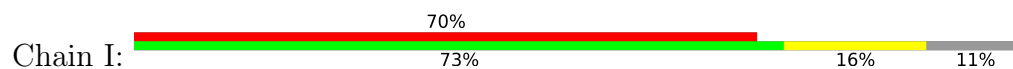
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W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	THR	THR	LYS	LYS	LYS	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	N2860	D2861	L2862	S2863	R2864	Z2865	T2866	L2867	S2868	R2869	E2870	L2871	K2872	A2873	M2874	E2875	Q2876	Q2877	L2878	A2879	E2880																			
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A2350	N2351	V2352	V2353	V2354	L2355	L2356	L2357	L2358	R2359	E2361	E2362	C2363	F2364	G2365	P2366	A2367	L2368	R2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378	A2379	I2380	E2381	E2382	A2383	I2384	R2385	I2386	S2387	G2388	E2389	P2390	A2391	G2394	P2395	GLY	VAL	ARG	ASP	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO																		
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N2283	N2284	E2285	L2286	A2287	L2288	A2289	L2290	Q2291	E2292	Q2293	D2294	L2295	E2296	K2297	V2298	V2299	S2300	Y2301	L2302	A2303	E2371	G2372	G2373	S2374	L2307	Q2308	S2309	C2310	P2311	L2312	L2313	L2314	P2319	D2320	I2321	G2322	G2327	E2328	E2329	R2330	Y2331	L2332	D2333	F2334	L2335	R2336	F2337	F2340	V2341	N2342	G2343	E2344	S2345	V2346	E2347	E2348	N2349																		



E4948	D4877	A4811	A4746	K4680	GLY	E4554	GLU	GLY	LYS	SER	E4182	C4114
Q4949	D4878	H4812	S4747	L4681	ALA	Y4554	PRO	GLY	LYS	LEU	S4115	S4115
V4950	M4879	L4813	L4748	E4682	GLY	R4557	GLU	GLU	VAL	ARG	E4116	E4116
K4951	M4880	L4814	E4749	F4683	GLU	N4558	PRO	VAL	THR	ARG	A4117	A4117
E4952	Y4883	D4815	T4750	D4684	ALA	F4559	PRO	VAL	THR	ARG	D4118	D4118
D4953	Y4884	L4816	T4751	G4685	GLY	Y4560	GLU	VAL	GLU	ARG	E4119	E4119
M4954	A4752	A4817	A4752	L4686	ASP	T4561	PRO	VAL	LEU	ARG	M4120	M4120
E4955	H4753	A4818	H4753	Y4687	GLU	L4562	LYS	VAL	LEU	ALA	E4121	E4121
T4956	M4754	G4819	M4754	I4688	ASP	R4563	ALA	VAL	ALA	ALA	M4122	M4122
C4957	E4755	G4820	E4755	T4689	GLU	F4564	ASP	GLY	MET	ASP	E4191	E4191
F4959	R4756	K4821	R4756	P4692	M4627	Y4564	GLY	GLY	PRO	THR	R4123	R4123
I4960	K4757	L4822	K4757	G4693	Y4630	L4565	GLU	PRO	ASP	ALA	M4124	M4124
G4962	D4758	L4823	D4758	D4694	F4631	A4566	ASN	PHE	PRO	GLU	F4125	F4125
L4963	P4759	T4826	P4759	L4695	F4631	L4567	GLY	ARG	THR	GLU	E4126	E4126
G4964	P4760	L4827	P4760	D4696	E4633	F4668	LYS	PRO	ASP	ALA	E4127	E4127
S4965	P4761	L4827	P4761	V4697	E4634	A4569	GLU	GLY	THR	GLU	F4128	F4128
P4966	P4762	S4828	P4762	K4698	S4635	A4570	GLU	ALA	VAL	ALA	M4129	M4129
Y4967	G4763	S4829	G4763	Y4701	Y4636	A4572	VAL	HIS	VAL	ALA	E4199	E4199
G4968	L4764	V4830	L4764	D4702	G4637	I4573	PRO	GLY	ALA	ALA	T4200	T4200
D4969	L4765	T4831	L4765	L4704	Y4638	N4574	ALA	GLY	GLU	ALA	R4131	R4131
T4970	L4766	H4832	L4766	V4705	P4641	F4575	PRO	GLY	GLN	GLY	E4134	E4134
T4971	L4767	Q4833	L4767	L4706	A4642	I4576	PRO	GLY	LEU	ALA	P4135	P4135
T4977	L4768	K4835	L4768	P4709	C4645	L4578	ALA	ASP	LEU	LEU	A4136	A4136
A4905	M4769	Q4836	M4769	S4710	L4646	F4579	PRO	GLY	TRP	ALA	R4137	R4137
E4908	I4770	L4837	I4770	F4711	L4647	Y4580	PRO	GLY	ALA	ALA	D4138	D4138
Y4909	D4772	M4838	D4772	P4712	S4647	K4581	PRO	GLY	ALA	ALA	E4203	E4203
Y4912	V4773	T4840	V4773	S4713	L4648	V4582	SER	PRO	GLY	ALA	Q4204	Q4204
F4916	K4774	V4841	K4774	M4714	L4649	S4583	PRO	THR	GLY	ALA	W4205	W4205
F4920	Y4775	G4842	Y4775	Y4715	L4650	P4586	PRO	GLY	GLY	GLY	E4206	E4206
F4924	L4776	L4843	L4776	D4716	L4652	P4587	ALA	GLY	THR	ALA	M4207	M4207
I4925	G4781	L4844	G4781	K4717	V4653	GLY	LYS	GLY	GLY	VAL	P4208	P4208
V4926	V4782	A4845	V4782	F4718	C4657	GLU	ALA	ALA	ALA	ALA	K4211	K4211
I4928	L4783	Y4846	L4783	Y4719	P4655	A4584	GLY	ILE	GLY	GLY	R4215	R4215
L4928	T4785	Y4853	T4785	L4725	L4656	S4585	ALA	LYS	ASP	ALA	I4218	I4218
L4929	D4786	V4854	D4786	D4726	L4657	P4586	GLY	ASP	ALA	ALA	F4219	F4219
M4997	I4931	A4855	I4931	K4727	M4662	GLY	GLY	ASP	GLY	ALA	S4151	S4151
K4998	I4932	F4856	K4998	H4728	C4663	LEU	GLY	LEU	GLY	GLY	V4154	V4154
D4999	Q4933	M4857	D4999	G4729	L4664	ALA	GLY	GLY	ALA	ARG	P4155	P4155
E5000	G4934	F4858	E5000	D4730	K4665	ALA	GLY	LEU	GLY	LEU	H4156	H4156
T5001	L4935	F4859	T5001	I4731	Y4666	ALA	GLY	TRP	ASP	ALA	D4157	D4157
E5002	I4936	R4860	E5002	F4732	P4667	S4546	GLY	GLY	ALA	ALA	G4226	G4226
H5003	I4937	K4865	H5003	G4733	L4668	GLY	VAL	GLY	GLY	ALA	E4227	E4227
T5004	D4938	S4866	T5004	R4734	F4671	GLY	ASP	ASP	ALA	ALA	L4160	L4160
E5007	F4940	E4867	E5007	E4735	K4672	GLY	GLY	GLY	GLY	ALA	R4161	R4161
H5011	G4941	D4868	H5011	R4736	R4673	LEU	GLY	GLY	GLY	ALA	M4162	M4162
K5012	E4942	E4869	K5012	I4737	E4674	ALA	GLY	GLY	VAL	ARG	E4165	E4165
M5013	L4943	D4870	M5013	A4738	K4675	GLY	GLY	GLY	GLY	LEU	L4166	L4166
Y5014	E4871	P4872	Y5014	L4741	A4678	GLY	GLY	GLY	HIS	ARG	A4167	A4167
Q5015	R4944	E4872	Q5015	G4742	R4679	GLY	GLY	GLY	GLY	VAL	E4168	E4168
	D4945	P4872		M4743		GLY	GLY	GLY	GLY	ALA	S4235	S4235
	Q4946	D4873		L4744		GLY	GLY	GLY	GLY	GLY	S4236	S4236
	Q4947			L4745		GLY	GLY	GLY	GLY	GLY	F4237	F4237
						GLY	GLY	GLY	GLY	GLY	C4238	C4238
						GLY	GLY	GLY	GLY	GLY	E4239	E4239
						GLY	GLY	GLY	GLY	GLY	D4240	D4240
						GLY	GLY	GLY	GLY	GLY	T4241	T4241
						GLY	GLY	GLY	GLY	GLY	I4242	I4242
						GLY	GLY	GLY	GLY	GLY	M4245	M4245
						GLY	GLY	GLY	GLY	GLY	Q4246	Q4246
						GLY	GLY	GLY	GLY	GLY	I4247	I4247
						GLY	GLY	GLY	GLY	GLY	A4248	A4248
						GLY	GLY	GLY	GLY	GLY	A4249	A4249
						GLY	GLY	GLY	GLY	GLY	Q4250	Q4250



• Molecule 2: ryanodine receptor 1



R1584	K1585	N1586	P1587	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	E1596	V1597	Q1598	N1599	L1600	M1601	P1602	V1603	S1604	W1605	S1606	R1607	M1608	P1609	M1610	H1611	F1612	L1613	Q1614	V1615	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	C1629	C1630	Q1631	D1632	P1633	L1634	T1635	M1636	M1637	A1638	L1639	H1640	I1641	P1642	E1643																																																																																																																																					
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GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	T1053	E1054	PRO	PRO	GLN	GLU	PRO	GLN	SER	GLN	VAL	ASN	GLN	SER	ARG	THR	D1070																																																																																																																																					
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A4203	Q4204	W4205	E4206	W4207	P4208	K4211	K4214	R4215	I4218	F4219	D4220	V4221	N4223	E4224	G4225	G4226	E4227	A4228	E4229	K4230	N4231	F4234	F4237	C4238	E4239	D4240	T4241	I4242	F4243	E4244	M4245	L4247	A4248	A4249	Q4250	I4251	S4252	E4253	PRD	GLU	GLY	PRD	ALA	ASP	GLU	ASP	GLY	GLY	NET	GLY																																																																																																																			
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X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3469	X3470	X3471	X3472	X3473	X3474	X3475	X3476	X3477	X3478	X3479	X3480	X3481	X3482	X3483	X3484	X3485	X3486	X3487	X3488	X3489	X3490	X3491	X3492	X3493	X3494	X3495	X3496	X3497	X3498	X3499	X3500	X3501	X3502	X3503	X3504	X3505	X3506	X3507	X3508	X3509	X3510	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3572	X3573	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3594	X3595	X3596	X3597	X3598	X3599	X3600	X3601	X3602	X3603	X3604	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	T3639	F3640	X3641	X3642
X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3469	X3470	X3471	X3472	X3473	X3474	X3475	X3476	X3477	X3478	X3479	X3480	X3481	X3482	X3483	X3484	X3485	X3486	X3487	X3488	X3489	X3490	X3491	X3492	X3493	X3494	X3495	X3496	X3497	X3498	X3499	X3500	X3501	X3502	X3503	X3504	X3505	X3506	X3507	X3508	X3509	X3510	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3572	X3573	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3594	X3595	X3596	X3597	X3598	X3599	X3600	X3601	X3602	X3603	X3604	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	T3639	F3640	X3641	X3642
X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3469	X3470	X3471	X3472	X3473	X3474	X3475	X3476	X3477	X3478	X3479	X3480	X3481	X3482	X3483	X3484	X3485	X3486	X3487	X3488	X3489	X3490	X3491	X3492	X3493	X3494	X3495	X3496	X3497	X3498	X3499	X3500	X3501	X3502	X3503	X3504	X3505	X3506	X3507	X3508	X3509	X3510	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3572	X3573	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3594	X3595	X3596	X3597	X3598	X3599	X3600	X3601	X3602	X3603	X3604	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	T3639	F3640	X3641	X3642
X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3469	X3470	X3471	X3472	X3473	X3474	X3475	X3476	X3477	X3478	X3479	X3480	X3481	X3482	X3483	X3484	X3485	X3486	X3487	X3488	X3489	X3490	X3491	X3492	X3493	X3494	X3																																																																																																																										



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/834	0.58	0/1123
1	F	0.32	0/834	0.57	0/1123
1	H	0.32	0/834	0.58	0/1123
1	J	0.32	0/834	0.57	0/1123
2	B	0.32	0/25428	0.57	5/34534 (0.0%)
2	E	0.33	0/25428	0.57	5/34534 (0.0%)
2	G	0.33	0/25428	0.57	5/34534 (0.0%)
2	I	0.33	0/25428	0.57	5/34534 (0.0%)
All	All	0.33	0/105048	0.57	20/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	17
2	E	0	18
2	G	0	17
2	I	0	17
All	All	0	69

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	719	LEU	CA-CB-CG	6.48	130.21	115.30
2	E	719	LEU	CA-CB-CG	6.45	130.14	115.30
2	G	719	LEU	CA-CB-CG	6.45	130.13	115.30
2	B	719	LEU	CA-CB-CG	6.44	130.11	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	I	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	G	977	LEU	CA-CB-CG	6.04	129.19	115.30
2	E	977	LEU	CA-CB-CG	6.03	129.17	115.30
2	B	1667	LEU	CA-CB-CG	5.27	127.41	115.30
2	I	1667	LEU	CA-CB-CG	5.26	127.40	115.30
2	G	1667	LEU	CA-CB-CG	5.25	127.37	115.30
2	E	1667	LEU	CA-CB-CG	5.24	127.36	115.30
2	B	4985	LEU	CA-CB-CG	5.13	127.10	115.30
2	E	4985	LEU	CA-CB-CG	5.12	127.07	115.30
2	I	4985	LEU	CA-CB-CG	5.10	127.04	115.30
2	G	4985	LEU	CA-CB-CG	5.10	127.02	115.30
2	I	2463	LEU	CA-CB-CG	5.09	127.01	115.30
2	E	2463	LEU	CA-CB-CG	5.07	126.97	115.30
2	G	2463	LEU	CA-CB-CG	5.06	126.93	115.30
2	B	2463	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (69) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3786	CYS	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4696	ASP	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1828	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	E	1840	PRO	Peptide
2	E	194	SER	Peptide
2	E	2291	GLN	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3786	CYS	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4696	ASP	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3786	CYS	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4696	ASP	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3786	CYS	Peptide

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Mol	Chain	Res	Type	Group
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4696	ASP	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	19	0
1	F	818	0	824	19	0
1	H	818	0	824	19	0
1	J	818	0	824	21	0
2	B	29369	0	24710	415	0
2	E	29369	0	24708	425	0
2	G	29369	0	24708	429	0
2	I	29369	0	24711	430	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102133	1756	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 8.

All (1756) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:177:GLU:HG3	2:I:2452:ARG:HH12	1.54	0.70
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.72	0.70
2:G:111:HIS:HD2	2:G:114:SER:H	1.38	0.70
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.72	0.70
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.72	0.70
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.57	0.70
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.57	0.70
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.72	0.70
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.57	0.70
2:B:111:HIS:HD2	2:B:114:SER:H	1.38	0.69
2:E:111:HIS:HD2	2:E:114:SER:H	1.38	0.69
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.57	0.69
2:I:111:HIS:HD2	2:I:114:SER:H	1.38	0.69
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.27	0.68
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.27	0.68
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.27	0.68
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.75	0.68
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.75	0.68
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.27	0.67
2:E:4855:ALA:HA	2:E:4859:PHE:HB2	1.76	0.67
2:I:4855:ALA:HA	2:I:4859:PHE:HB2	1.76	0.67
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.75	0.67
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.60	0.67
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.75	0.67
2:G:4855:ALA:HA	2:G:4859:PHE:HB2	1.76	0.67
2:B:4855:ALA:HA	2:B:4859:PHE:HB2	1.76	0.66
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.60	0.66
2:I:224:HIS:H	2:I:230:CYS:HA	1.61	0.66
2:G:224:HIS:H	2:G:230:CYS:HA	1.61	0.66
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.78	0.65
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.60	0.65
2:E:224:HIS:H	2:E:230:CYS:HA	1.61	0.65
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.78	0.65
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.78	0.65
2:B:224:HIS:H	2:B:230:CYS:HA	1.61	0.65
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.79	0.65
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.79	0.64
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.78	0.64
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.79	0.64
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.79	0.64
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.30	0.64
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.60	0.64
2:B:3767:GLN:HB3	2:B:3772:THR:HG22	1.80	0.64
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.30	0.64
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.80	0.64
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.64
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.78	0.64
2:I:4821:LYS:HA	2:I:4824:ARG:HE	1.64	0.64
2:B:4821:LYS:HA	2:B:4824:ARG:HE	1.63	0.63
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.78	0.63
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.79	0.63
2:I:3767:GLN:HB3	2:I:3772:THR:HG22	1.80	0.63
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.81	0.63
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.32	0.63
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.32	0.63
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.80	0.63
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.32	0.63
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.63	0.63
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.32	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.63
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.63	0.63
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.30	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:G:4821:LYS:HA	2:G:4824:ARG:HE	1.63	0.63
2:G:3767:GLN:HB3	2:G:3772:THR:HG22	1.80	0.63
2:B:606:LEU:O	2:B:617:ASN:ND2	2.32	0.63
2:E:4821:LYS:HA	2:E:4824:ARG:HE	1.63	0.63
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.30	0.63
2:E:3767:GLN:HB3	2:E:3772:THR:HG22	1.80	0.62
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.80	0.62
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.63	0.62
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.82	0.62
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.81	0.62
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.64	0.62
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.80	0.62
2:G:606:LEU:O	2:G:617:ASN:ND2	2.32	0.62
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.82	0.62
2:B:1830:VAL:HB	2:B:1837:GLN:HA	1.82	0.62
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.33	0.62
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.33	0.62
2:E:606:LEU:O	2:E:617:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.81	0.62
2:I:606:LEU:O	2:I:617:ASN:ND2	2.32	0.62
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.81	0.61
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.33	0.61
2:G:853:PRO:HB3	2:G:1024:TYR:H	1.65	0.61
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.82	0.61
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.33	0.61
2:E:1830:VAL:HB	2:E:1837:GLN:HA	1.82	0.61
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.61
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.66	0.61
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.33	0.61
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.33	0.61
2:I:728:ARG:NH2	2:I:1527:UNK:O	2.33	0.61
2:I:1830:VAL:HB	2:I:1837:GLN:HA	1.82	0.61
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.82	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.33	0.61
2:G:1830:VAL:HB	2:G:1837:GLN:HA	1.81	0.61
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.81	0.61
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.33	0.61
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.81	0.61
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.83	0.60
2:I:1091:GLU:HB3	2:I:1203:ASN:HB3	1.83	0.60
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.83	0.60
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.83	0.60
2:E:395:GLN:HG3	2:E:397:GLU:H	1.67	0.60
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.83	0.60
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.83	0.60
2:G:1101:ARG:HE	2:G:1115:LEU:HB3	1.67	0.60
2:B:853:PRO:HB3	2:B:1024:TYR:H	1.66	0.60
2:I:1101:ARG:HE	2:I:1115:LEU:HB3	1.67	0.60
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.84	0.60
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.66	0.60
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.83	0.60
2:G:221:ARG:NH2	2:G:255:HIS:O	2.34	0.60
2:E:4083:ASP:HA	2:E:4085:ARG:HH11	1.66	0.60
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.83	0.60
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.83	0.60
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.84	0.60
2:E:4809:PHE:HA	2:E:4812:HIS:HD1	1.67	0.60
1:J:27:THR:HB	1:J:100:ASP:HB3	1.84	0.60
2:B:395:GLN:HG3	2:B:397:GLU:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4809:PHE:HA	2:B:4812:HIS:HD1	1.67	0.59
2:E:1241:SER:HA	2:E:1603:VAL:HA	1.84	0.59
2:G:1241:SER:HA	2:G:1603:VAL:HA	1.84	0.59
2:I:1241:SER:HA	2:I:1603:VAL:HA	1.84	0.59
2:B:1241:SER:HA	2:B:1603:VAL:HA	1.84	0.59
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.84	0.59
2:E:1091:GLU:HB3	2:E:1203:ASN:HB3	1.83	0.59
1:F:27:THR:HB	1:F:100:ASP:HB3	1.84	0.59
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.84	0.59
1:H:27:THR:HB	1:H:100:ASP:HB3	1.84	0.59
2:I:395:GLN:HG3	2:I:397:GLU:H	1.67	0.59
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.34	0.59
2:G:1973:GLN:O	2:G:1977:TYR:N	2.36	0.59
2:G:2281:ILE:HG23	2:G:2341:VAL:HG11	1.85	0.59
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.34	0.59
2:B:1091:GLU:HB3	2:B:1203:ASN:HB3	1.83	0.59
2:B:221:ARG:NH2	2:B:255:HIS:O	2.34	0.59
2:B:1218:GLY:HA2	2:B:1223:PHE:HB2	1.84	0.59
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.84	0.59
2:G:395:GLN:HG3	2:G:397:GLU:H	1.67	0.59
1:A:6:THR:HA	1:A:72:ALA:HA	1.85	0.59
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.84	0.59
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.34	0.59
2:G:4809:PHE:HA	2:G:4812:HIS:HD1	1.67	0.59
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.83	0.59
2:B:4083:ASP:HA	2:B:4085:ARG:HH11	1.66	0.59
2:E:18:ASP:HB2	2:E:69:LEU:HD12	1.84	0.59
2:E:1973:GLN:O	2:E:1977:TYR:N	2.36	0.59
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.36	0.59
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.84	0.59
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.84	0.59
1:A:27:THR:HB	1:A:100:ASP:HB3	1.84	0.59
2:G:1091:GLU:HB3	2:G:1203:ASN:HB3	1.83	0.59
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	1.84	0.59
2:I:2281:ILE:HG23	2:I:2341:VAL:HG11	1.84	0.59
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.34	0.59
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.36	0.59
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.36	0.59
2:I:1973:GLN:O	2:I:1977:TYR:N	2.36	0.59
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.84	0.59
2:E:1101:ARG:HE	2:E:1115:LEU:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.36	0.59
2:I:4083:ASP:HA	2:I:4085:ARG:HH11	1.67	0.59
2:I:4809:PHE:HA	2:I:4812:HIS:HD1	1.67	0.59
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.85	0.58
2:B:1101:ARG:HE	2:B:1115:LEU:HB3	1.66	0.58
2:E:1218:GLY:HA2	2:E:1223:PHE:HB2	1.84	0.58
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.68	0.58
2:G:4061:PHE:HA	2:G:4065:PHE:HB3	1.85	0.58
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.36	0.58
2:B:18:ASP:HB2	2:B:69:LEU:HD12	1.85	0.58
2:B:4892:ARG:NH2	2:I:4895:GLY:O	2.33	0.58
2:E:2281:ILE:HG23	2:E:2341:VAL:HG11	1.85	0.58
2:E:4061:PHE:HA	2:E:4065:PHE:HB3	1.85	0.58
2:G:18:ASP:HB2	2:G:69:LEU:HD12	1.84	0.58
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.84	0.58
2:G:1218:GLY:HA2	2:G:1223:PHE:HB2	1.84	0.58
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.84	0.58
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.36	0.58
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.86	0.58
2:G:4083:ASP:HA	2:G:4085:ARG:HH11	1.66	0.58
2:B:650:VAL:HB	2:B:777:PHE:HB2	1.86	0.58
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.86	0.58
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.36	0.58
2:I:18:ASP:HB2	2:I:69:LEU:HD12	1.84	0.58
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.36	0.58
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.84	0.58
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.37	0.58
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.36	0.58
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.85	0.58
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.36	0.58
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.76	0.58
1:F:6:THR:HA	1:F:72:ALA:HA	1.85	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.58
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.84	0.58
2:E:650:VAL:HB	2:E:777:PHE:HB2	1.86	0.58
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	1.84	0.58
2:G:1271:ARG:HA	2:G:1471:UNK:HA	1.85	0.58
2:I:379:HIS:HD2	2:I:382:GLY:H	1.52	0.58
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.86	0.58
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	1.84	0.58
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.36	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.58
2:B:2281:ILE:HG23	2:B:2341:VAL:HG11	1.84	0.58
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.58
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	1.84	0.58
2:B:1973:GLN:O	2:B:1977:TYR:N	2.36	0.58
2:E:221:ARG:NH2	2:E:255:HIS:O	2.34	0.58
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.76	0.58
2:I:650:VAL:HB	2:I:777:PHE:HB2	1.86	0.58
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.69	0.58
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.36	0.58
2:B:2440:MET:O	2:B:2444:GLN:N	2.37	0.58
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.68	0.58
2:E:827:LYS:O	2:E:1073:ARG:NH2	2.37	0.58
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.36	0.58
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.68	0.58
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.84	0.57
2:B:827:LYS:O	2:B:1073:ARG:NH2	2.37	0.57
2:E:177:GLU:HG3	2:G:2452:ARG:HH12	1.69	0.57
2:I:1218:GLY:HA2	2:I:1223:PHE:HB2	1.84	0.57
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.69	0.57
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.70	0.57
2:G:650:VAL:HB	2:G:777:PHE:HB2	1.86	0.57
2:I:827:LYS:O	2:I:1073:ARG:NH2	2.37	0.57
2:B:379:HIS:HD2	2:B:382:GLY:H	1.51	0.57
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.84	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.57
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.84	0.57
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.86	0.57
2:B:4061:PHE:HA	2:B:4065:PHE:HB3	1.85	0.57
2:E:1271:ARG:HA	2:E:1471:UNK:HA	1.85	0.57
2:I:1232:ARG:HH21	2:I:1701:ALA:HB1	1.70	0.57
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.76	0.57
2:I:4061:PHE:HA	2:I:4065:PHE:HB3	1.85	0.57
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.69	0.57
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.86	0.57
2:G:2440:MET:O	2:G:2444:GLN:N	2.37	0.57
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.36	0.57
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.85	0.57
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.87	0.57
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:639:ASN:H	2:G:678:GLN:HE22	1.53	0.57
2:G:2205:GLU:HG2	2:G:2253:HIS:HE1	1.70	0.57
1:H:6:THR:HA	1:H:72:ALA:HA	1.85	0.57
2:I:2205:GLU:HG2	2:I:2253:HIS:HE1	1.70	0.57
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.87	0.57
1:J:6:THR:HA	1:J:72:ALA:HA	1.85	0.57
2:E:2440:MET:O	2:E:2444:GLN:N	2.37	0.57
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.70	0.57
2:G:827:LYS:O	2:G:1073:ARG:NH2	2.37	0.57
2:G:3904:ARG:NH2	2:G:3973:CYS:SG	2.78	0.57
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.86	0.57
2:I:3904:ARG:NH2	2:I:3973:CYS:SG	2.78	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.57
2:E:639:ASN:H	2:E:678:GLN:HE22	1.53	0.57
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.86	0.57
2:G:379:HIS:HD2	2:G:382:GLY:H	1.51	0.57
2:G:1232:ARG:HH21	2:G:1701:ALA:HB1	1.69	0.57
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.69	0.57
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.57
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.70	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.68	0.56
2:B:451:TYR:O	2:B:474:ARG:NH1	2.38	0.56
2:B:813:GLU:OE2	2:B:1020:ARG:N	2.38	0.56
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.87	0.56
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.87	0.56
2:I:221:ARG:NH2	2:I:255:HIS:O	2.34	0.56
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.70	0.56
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.87	0.56
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.88	0.56
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.87	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.85	0.56
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.86	0.56
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.37	0.56
2:B:1232:ARG:HH21	2:B:1701:ALA:HB1	1.70	0.56
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.38	0.56
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.38	0.56
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.87	0.56
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.56
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.85	0.56
2:I:4581:LYS:HB2	2:I:4632:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:639:ASN:H	2:B:678:GLN:HE22	1.53	0.56
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.87	0.56
2:E:3904:ARG:NH2	2:E:3973:CYS:SG	2.78	0.56
2:E:4581:LYS:HB2	2:E:4632:LEU:HB2	1.87	0.56
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.87	0.56
2:I:2440:MET:O	2:I:2444:GLN:N	2.37	0.56
2:B:3904:ARG:NH2	2:B:3973:CYS:SG	2.78	0.56
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.88	0.56
2:B:2205:GLU:HG2	2:B:2253:HIS:HE1	1.70	0.56
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.86	0.56
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.69	0.56
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.87	0.56
2:E:2205:GLU:HG2	2:E:2253:HIS:HE1	1.70	0.56
2:E:4843:LEU:HD12	2:G:4823:LEU:HD21	1.86	0.56
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.39	0.56
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.69	0.56
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.39	0.56
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.39	0.56
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.88	0.56
2:E:157:ARG:NH2	2:E:167:ASP:OD1	2.38	0.56
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.88	0.56
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.69	0.56
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.38	0.56
2:G:4581:LYS:HB2	2:G:4632:LEU:HB2	1.87	0.56
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.88	0.56
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.38	0.56
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.38	0.56
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.88	0.56
2:B:4918:ILE:HG23	2:E:4892:ARG:HD3	1.88	0.56
2:E:379:HIS:HD2	2:E:382:GLY:H	1.52	0.56
2:I:639:ASN:H	2:I:678:GLN:HE22	1.53	0.56
2:I:1271:ARG:HA	2:I:1471:UNK:HA	1.87	0.56
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.86	0.56
2:B:157:ARG:NH2	2:B:167:ASP:OD1	2.38	0.56
2:B:1211:LEU:HD11	2:B:1225:PRO:HB3	1.88	0.56
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.70	0.56
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.39	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.38	0.56
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.88	0.56
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.88	0.56
2:E:1232:ARG:HH21	2:E:1701:ALA:HB1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.39	0.56
2:E:4984:ASN:OD1	2:E:4987:ASN:ND2	2.39	0.55
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.88	0.55
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.39	0.55
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.39	0.55
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.89	0.55
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.89	0.55
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.87	0.55
2:B:331:VAL:HG12	2:B:333:GLY:H	1.71	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.87	0.55
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.88	0.55
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.87	0.55
2:E:1211:LEU:HD11	2:E:1225:PRO:HB3	1.88	0.55
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.88	0.55
2:G:451:TYR:O	2:G:474:ARG:NH1	2.38	0.55
2:I:331:VAL:HG12	2:I:333:GLY:H	1.71	0.55
2:I:451:TYR:O	2:I:474:ARG:NH1	2.38	0.55
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.88	0.55
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.88	0.55
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.88	0.55
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.88	0.55
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.39	0.55
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.88	0.55
2:B:4984:ASN:OD1	2:B:4987:ASN:ND2	2.40	0.55
2:G:132:ALA:HA	2:G:194:SER:HB2	1.89	0.55
2:I:132:ALA:HA	2:I:194:SER:HB2	1.89	0.55
2:B:283:ARG:HH21	2:B:402:ARG:HH12	1.54	0.55
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.39	0.55
2:E:627:PRO:HB2	1:F:92:PRO:HD3	1.89	0.55
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.89	0.55
2:B:4581:LYS:HB2	2:B:4632:LEU:HB2	1.87	0.55
2:E:451:TYR:O	2:E:474:ARG:NH1	2.38	0.55
2:G:1211:LEU:HD11	2:G:1225:PRO:HB3	1.88	0.55
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.89	0.55
2:I:1211:LEU:HD11	2:I:1225:PRO:HB3	1.88	0.55
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.89	0.55
2:I:4984:ASN:OD1	2:I:4987:ASN:ND2	2.39	0.55
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.89	0.55
2:B:3767:GLN:NE2	2:B:3804:ILE:O	2.40	0.55
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.76	0.54
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.88	0.54
2:G:23:GLN:HE21	2:G:34:LYS:HB3	1.73	0.54
2:G:3767:GLN:NE2	2:G:3804:ILE:O	2.40	0.54
2:G:4984:ASN:OD1	2:G:4987:ASN:ND2	2.40	0.54
2:I:283:ARG:HH21	2:I:402:ARG:HH12	1.54	0.54
2:I:3767:GLN:NE2	2:I:3804:ILE:O	2.40	0.54
2:B:23:GLN:HE21	2:B:34:LYS:HB3	1.73	0.54
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.89	0.54
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.89	0.54
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.90	0.54
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.89	0.54
2:E:331:VAL:HG12	2:E:333:GLY:H	1.71	0.54
2:E:647:ASN:ND2	2:E:820:ARG:O	2.39	0.54
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.90	0.54
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.90	0.54
2:I:157:ARG:NH2	2:I:167:ASP:OD1	2.38	0.54
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.88	0.54
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.54
1:A:25:HIS:HB3	1:A:40:ARG:HD3	1.90	0.54
2:E:3767:GLN:NE2	2:E:3804:ILE:O	2.40	0.54
2:G:157:ARG:NH2	2:G:167:ASP:OD1	2.38	0.54
2:G:1667:LEU:O	2:G:1671:ARG:NH1	2.41	0.54
2:B:1667:LEU:O	2:B:1671:ARG:NH1	2.41	0.54
2:E:3843:ASP:H	2:E:3874:VAL:HG13	1.73	0.54
2:G:283:ARG:HH21	2:G:402:ARG:HH12	1.54	0.54
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.41	0.54
2:B:2248:ARG:NH2	2:B:2285:GLU:OE1	2.41	0.54
2:G:331:VAL:HG12	2:G:333:GLY:H	1.71	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.89	0.54
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.88	0.54
2:E:283:ARG:HH21	2:E:402:ARG:HH12	1.54	0.54
2:I:2248:ARG:NH2	2:I:2285:GLU:OE1	2.41	0.54
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.36	0.54
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.90	0.54
2:E:132:ALA:HA	2:E:194:SER:HB2	1.89	0.54
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.89	0.54
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.41	0.54
2:B:396:GLU:O	2:B:400:ALA:N	2.40	0.53
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.88	0.53
2:I:655:GLY:HA2	2:I:1002:ALA:HB2	1.90	0.53
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:25:HIS:HB3	1:J:40:ARG:HD3	1.90	0.53
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.39	0.53
2:E:1667:LEU:O	2:E:1671:ARG:NH1	2.41	0.53
2:I:1667:LEU:O	2:I:1671:ARG:NH1	2.41	0.53
2:E:655:GLY:HA2	2:E:1002:ALA:HB2	1.90	0.53
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.53
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.89	0.53
1:F:25:HIS:HB3	1:F:40:ARG:HD3	1.90	0.53
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.41	0.53
2:I:23:GLN:HE21	2:I:34:LYS:HB3	1.73	0.53
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.90	0.53
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.38	0.53
2:E:2248:ARG:NH2	2:E:2285:GLU:OE1	2.41	0.53
2:G:17:ASP:HB2	2:G:98:HIS:HE1	1.73	0.53
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.41	0.53
2:B:3843:ASP:H	2:B:3874:VAL:HG13	1.73	0.53
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.91	0.53
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.91	0.53
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.90	0.53
2:G:2248:ARG:NH2	2:G:2285:GLU:OE1	2.41	0.53
2:G:3843:ASP:H	2:G:3874:VAL:HG13	1.73	0.53
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.91	0.53
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.41	0.53
2:E:23:GLN:HE21	2:E:34:LYS:HB3	1.73	0.53
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.89	0.53
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.91	0.53
1:H:25:HIS:HB3	1:H:40:ARG:HD3	1.90	0.53
2:I:17:ASP:HB2	2:I:98:HIS:HE1	1.73	0.53
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.91	0.53
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.53
2:E:3992:PHE:O	2:E:3996:PHE:N	2.37	0.53
2:G:261:ARG:HB3	2:G:283:ARG:HB3	1.91	0.53
2:G:647:ASN:ND2	2:G:820:ARG:O	2.40	0.53
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.36	0.53
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.90	0.53
2:I:4958:CYS:SG	2:I:4959:PHE:N	2.82	0.53
2:B:647:ASN:ND2	2:B:820:ARG:O	2.40	0.53
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.91	0.53
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.90	0.53
2:G:3992:PHE:O	2:G:3996:PHE:N	2.38	0.53
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ASP:HB2	2:B:98:HIS:HE1	1.73	0.53
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.90	0.53
2:E:645:ARG:N	2:E:824:GLU:O	2.39	0.53
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	1.90	0.53
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.91	0.53
2:G:4843:LEU:HD12	2:I:4823:LEU:HD21	1.91	0.53
2:B:655:GLY:HA2	2:B:1002:ALA:HB2	1.90	0.52
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.90	0.52
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.91	0.52
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.90	0.52
2:G:655:GLY:HA2	2:G:1002:ALA:HB2	1.90	0.52
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.90	0.52
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	1.92	0.52
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.41	0.52
2:G:4958:CYS:SG	2:G:4959:PHE:N	2.82	0.52
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.91	0.52
2:E:1196:PRO:O	2:E:1198:GLN:NE2	2.41	0.52
2:E:4958:CYS:SG	2:E:4959:PHE:N	2.82	0.52
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.41	0.52
2:I:914:PRO:O	2:I:918:ARG:N	2.42	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.52
2:I:3843:ASP:H	2:I:3874:VAL:HG13	1.73	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.52
2:E:261:ARG:HB3	2:E:283:ARG:HB3	1.91	0.52
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.41	0.52
2:I:627:PRO:HB2	1:J:92:PRO:HD3	1.92	0.52
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.38	0.52
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.91	0.52
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.36	0.52
2:B:4958:CYS:SG	2:B:4959:PHE:N	2.82	0.52
2:E:17:ASP:HB2	2:E:98:HIS:HE1	1.73	0.52
2:E:4012:LEU:O	2:E:4016:LEU:N	2.43	0.52
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.39	0.52
2:I:2128:TYR:OH	2:I:3676:ASP:OD2	2.28	0.52
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	1.90	0.52
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.91	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.52
2:I:261:ARG:HB3	2:I:283:ARG:HB3	1.91	0.52
2:I:488:LEU:O	2:I:492:ASP:N	2.41	0.52
2:E:396:GLU:O	2:E:400:ALA:N	2.40	0.52
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4704:LEU:HD22	2:E:4778:TRP:HB2	1.92	0.52
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.92	0.52
2:G:4704:LEU:HD22	2:G:4778:TRP:HB2	1.92	0.52
2:I:396:GLU:O	2:I:400:ALA:N	2.40	0.52
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	1.92	0.52
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.91	0.52
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	1.90	0.52
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.43	0.52
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.92	0.52
2:B:1032:LYS:O	2:B:1036:ARG:N	2.40	0.51
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.92	0.51
2:G:1676:LEU:HD22	2:G:2167:ILE:HG13	1.93	0.51
2:G:1965:TYR:OH	2:G:2027:ILE:O	2.26	0.51
2:I:1865:MET:N	2:I:1865:MET:SD	2.83	0.51
2:I:2185:ILE:HA	2:I:2188:ASN:HD21	1.75	0.51
2:B:2128:TYR:OH	2:B:3676:ASP:OD2	2.28	0.51
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.43	0.51
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	1.92	0.51
2:G:4201:ASN:O	2:G:4205:TRP:N	2.43	0.51
2:I:647:ASN:ND2	2:I:820:ARG:O	2.39	0.51
2:B:3905:THR:HA	2:B:3912:THR:HG23	1.93	0.51
2:E:2128:TYR:OH	2:E:3676:ASP:OD2	2.28	0.51
2:G:264:PRO:HG2	2:G:270:SER:HB2	1.92	0.51
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.92	0.51
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.75	0.51
2:I:4704:LEU:HD22	2:I:4778:TRP:HB2	1.92	0.51
2:B:261:ARG:HB3	2:B:283:ARG:HB3	1.91	0.51
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.93	0.51
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.93	0.51
2:G:3905:THR:HA	2:G:3912:THR:HG23	1.93	0.51
2:I:1196:PRO:O	2:I:1198:GLN:NE2	2.41	0.51
2:I:4201:ASN:O	2:I:4205:TRP:N	2.43	0.51
2:B:1865:MET:N	2:B:1865:MET:SD	2.84	0.51
2:B:2185:ILE:HA	2:B:2188:ASN:HD21	1.75	0.51
2:B:3990:VAL:HG13	2:B:4051:SER:HB2	1.92	0.51
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.93	0.51
2:E:2950:UNK:O	2:E:2954:UNK:N	2.43	0.51
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.44	0.51
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.93	0.51
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.44	0.51
2:I:3990:VAL:HG13	2:I:4051:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.76	0.51
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.92	0.51
2:B:4237:PHE:O	2:B:4241:THR:OG1	2.22	0.51
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	1.92	0.51
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.92	0.51
2:I:666:VAL:HG21	2:I:684:VAL:HG21	1.93	0.51
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.76	0.51
2:I:1240:LYS:O	2:I:1604:SER:N	2.43	0.51
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.92	0.51
2:E:666:VAL:HG21	2:E:684:VAL:HG21	1.93	0.51
2:E:831:ARG:HD2	2:E:1199:VAL:HG12	1.93	0.51
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.44	0.51
2:G:488:LEU:O	2:G:492:ASP:N	2.41	0.51
2:G:831:ARG:HD2	2:G:1199:VAL:HG12	1.93	0.51
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.92	0.51
2:G:2128:TYR:OH	2:G:3676:ASP:OD2	2.28	0.51
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	1.92	0.51
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.44	0.51
2:B:3552:UNK:O	2:B:3556:UNK:N	2.44	0.51
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	1.92	0.51
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.76	0.51
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.92	0.51
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.44	0.51
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.51
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	1.92	0.51
2:E:264:PRO:HG2	2:E:270:SER:HB2	1.92	0.51
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.93	0.51
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.93	0.51
2:G:666:VAL:HG21	2:G:684:VAL:HG21	1.93	0.51
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.44	0.51
2:G:1231:GLN:NE2	2:G:1821:ASP:O	2.44	0.51
2:G:1258:ALA:HB3	2:G:1271:ARG:HB3	1.93	0.51
2:G:4012:LEU:O	2:G:4016:LEU:N	2.43	0.51
2:I:1676:LEU:HD22	2:I:2167:ILE:HG13	1.92	0.51
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.44	0.51
2:I:3992:PHE:O	2:I:3996:PHE:N	2.37	0.51
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.75	0.51
2:B:645:ARG:N	2:B:824:GLU:O	2.39	0.51
2:B:1231:GLN:NE2	2:B:1821:ASP:O	2.44	0.51
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.44	0.51
2:B:4704:LEU:HD22	2:B:4778:TRP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1865:MET:N	2:E:1865:MET:SD	2.84	0.51
2:E:2185:ILE:HA	2:E:2188:ASN:HD21	1.75	0.51
2:E:4024:VAL:HG23	2:E:4027:LEU:HD12	1.92	0.51
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	1.92	0.51
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.93	0.51
2:B:666:VAL:HG21	2:B:684:VAL:HG21	1.93	0.50
2:B:1258:ALA:HB3	2:B:1271:ARG:HB3	1.93	0.50
2:B:4012:LEU:O	2:B:4016:LEU:N	2.42	0.50
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.44	0.50
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.92	0.50
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.92	0.50
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.75	0.50
2:G:2185:ILE:HA	2:G:2188:ASN:HD21	1.75	0.50
2:G:3552:UNK:O	2:G:3556:UNK:N	2.44	0.50
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	1.93	0.50
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.93	0.50
2:I:1258:ALA:HB3	2:I:1271:ARG:HB3	1.93	0.50
2:B:4201:ASN:O	2:B:4205:TRP:N	2.43	0.50
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.75	0.50
2:E:1235:THR:OG1	2:E:1607:ARG:NE	2.45	0.50
2:E:1240:LYS:O	2:E:1604:SER:N	2.43	0.50
2:G:1865:MET:N	2:G:1865:MET:SD	2.84	0.50
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.44	0.50
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.93	0.50
2:I:4813:LEU:HD12	2:I:4816:ILE:HD11	1.93	0.50
2:B:15:ARG:HD3	2:B:98:HIS:HB3	1.93	0.50
2:B:831:ARG:HD2	2:B:1199:VAL:HG12	1.93	0.50
2:B:1240:LYS:O	2:B:1604:SER:N	2.43	0.50
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.93	0.50
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.93	0.50
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.44	0.50
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.76	0.50
2:I:3905:THR:HA	2:I:3912:THR:HG23	1.93	0.50
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.44	0.50
2:E:488:LEU:O	2:E:492:ASP:N	2.41	0.50
2:I:831:ARG:HD2	2:I:1199:VAL:HG12	1.93	0.50
2:B:313:SER:HB3	2:B:351:VAL:HB	1.94	0.50
2:B:1676:LEU:HD22	2:B:2167:ILE:HG13	1.93	0.50
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.93	0.50
2:E:1258:ALA:HB3	2:E:1271:ARG:HB3	1.94	0.50
2:G:1203:ASN:ND2	2:G:1210:SER:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.93	0.50
2:I:1032:LYS:O	2:I:1036:ARG:N	2.40	0.50
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.92	0.50
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.92	0.50
2:B:914:PRO:O	2:B:918:ARG:N	2.42	0.50
2:B:1721:GLU:HG2	2:B:1725:ARG:HH12	1.77	0.50
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.92	0.50
2:E:313:SER:HB3	2:E:351:VAL:HB	1.94	0.50
2:E:3552:UNK:O	2:E:3556:UNK:N	2.44	0.50
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.43	0.50
2:G:15:ARG:HD3	2:G:98:HIS:HB3	1.93	0.50
2:G:396:GLU:O	2:G:400:ALA:N	2.40	0.50
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.50
2:I:1231:GLN:NE2	2:I:1821:ASP:O	2.44	0.50
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	1.93	0.50
1:A:7:ILE:HG22	1:A:9:PRO:HD2	1.94	0.50
2:B:355:LEU:HB3	2:B:378:LEU:HB3	1.94	0.50
2:B:460:GLN:HG2	2:B:462:GLU:H	1.77	0.50
2:B:1235:THR:OG1	2:B:1607:ARG:NE	2.45	0.50
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.94	0.50
2:E:4088:ILE:HG23	2:E:4123:ILE:HB	1.94	0.50
2:G:645:ARG:N	2:G:824:GLU:O	2.39	0.50
2:G:4088:ILE:HG23	2:G:4123:ILE:HB	1.94	0.50
1:H:7:ILE:HG22	1:H:9:PRO:HD2	1.94	0.50
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.94	0.50
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.94	0.50
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.93	0.50
2:I:4956:THR:O	2:I:4965:SER:N	2.42	0.50
1:J:7:ILE:HG22	1:J:9:PRO:HD2	1.94	0.50
2:E:838:HIS:HB3	2:E:1200:GLY:H	1.77	0.50
2:E:3990:VAL:HG13	2:E:4051:SER:HB2	1.93	0.50
1:F:7:ILE:HG22	1:F:9:PRO:HD2	1.94	0.50
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.45	0.50
2:G:1235:THR:OG1	2:G:1607:ARG:NE	2.44	0.50
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.93	0.50
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.93	0.50
2:B:4813:LEU:HD12	2:B:4816:ILE:HD11	1.93	0.50
2:E:914:PRO:O	2:E:918:ARG:N	2.42	0.50
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.94	0.50
2:E:4044:MET:HA	2:E:4047:MET:HG2	1.94	0.50
2:G:3674:ILE:HG13	2:G:3732:SER:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.94	0.50
2:G:4813:LEU:HD12	2:G:4816:ILE:HD11	1.93	0.50
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.43	0.50
2:I:4024:VAL:HG23	2:I:4027:LEU:HD12	1.93	0.50
2:B:264:PRO:HG2	2:B:270:SER:HB2	1.92	0.49
2:B:485:SER:O	2:B:489:ASN:N	2.44	0.49
2:B:1196:PRO:O	2:B:1198:GLN:NE2	2.41	0.49
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.93	0.49
2:G:728:ARG:NH2	2:G:1527:UNK:O	2.45	0.49
2:G:1196:PRO:O	2:G:1198:GLN:NE2	2.41	0.49
2:I:355:LEU:HB3	2:I:378:LEU:HB3	1.94	0.49
2:I:3552:UNK:O	2:I:3556:UNK:N	2.44	0.49
2:I:4012:LEU:O	2:I:4016:LEU:N	2.43	0.49
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.94	0.49
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.93	0.49
2:B:4088:ILE:HG23	2:B:4123:ILE:HB	1.94	0.49
2:E:355:LEU:HB3	2:E:378:LEU:HB3	1.94	0.49
2:E:1721:GLU:HG2	2:E:1725:ARG:HH12	1.77	0.49
2:E:3905:THR:HA	2:E:3912:THR:HG23	1.93	0.49
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.93	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.94	0.49
2:I:229:GLU:OE2	2:I:374:LYS:NZ	2.35	0.49
2:I:264:PRO:HG2	2:I:270:SER:HB2	1.92	0.49
2:I:1235:THR:OG1	2:I:1607:ARG:NE	2.44	0.49
2:I:1691:GLN:HG2	1:J:42:ARG:HG2	1.93	0.49
2:I:3674:ILE:HG13	2:I:3732:SER:HB3	1.94	0.49
2:I:4088:ILE:HG23	2:I:4123:ILE:HB	1.94	0.49
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.93	0.49
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.94	0.49
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.49
2:E:15:ARG:HD3	2:E:98:HIS:HB3	1.93	0.49
2:E:139:GLU:O	2:E:141:ALA:N	2.45	0.49
2:E:1231:GLN:NE2	2:E:1821:ASP:O	2.44	0.49
2:E:1676:LEU:HD22	2:E:2167:ILE:HG13	1.92	0.49
2:E:3674:ILE:HG13	2:E:3732:SER:HB3	1.94	0.49
2:G:139:GLU:O	2:G:141:ALA:N	2.45	0.49
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.94	0.49
2:G:4024:VAL:HG23	2:G:4027:LEU:HD12	1.92	0.49
2:I:1269:CYS:HA	2:I:1473:UNK:HA	1.95	0.49
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.95	0.49
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1271:ARG:HA	2:B:1471:UNK:HA	1.94	0.49
2:E:913:LEU:HD13	2:E:918:ARG:HA	1.94	0.49
2:G:838:HIS:HB3	2:G:1200:GLY:H	1.77	0.49
2:G:2336:ARG:HD3	2:G:2435:ARG:HD2	1.94	0.49
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.45	0.49
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.95	0.49
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.95	0.49
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.95	0.49
2:B:2336:ARG:HD3	2:B:2435:ARG:HD2	1.94	0.49
2:B:4024:VAL:HG23	2:B:4027:LEU:HD12	1.93	0.49
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.95	0.49
2:E:682:LEU:HD13	2:E:787:VAL:HG11	1.94	0.49
2:E:2235:PHE:HA	2:E:2238:TYR:HD2	1.78	0.49
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	1.93	0.49
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.45	0.49
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.94	0.49
2:I:15:ARG:HD3	2:I:98:HIS:HB3	1.93	0.49
2:I:682:LEU:HD13	2:I:787:VAL:HG11	1.94	0.49
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.94	0.49
2:I:2336:ARG:HD3	2:I:2435:ARG:HD2	1.94	0.49
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.94	0.49
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	1.93	0.49
2:E:4813:LEU:HD12	2:E:4816:ILE:HD11	1.93	0.49
2:G:913:LEU:HD13	2:G:918:ARG:HA	1.94	0.49
2:G:914:PRO:O	2:G:918:ARG:N	2.42	0.49
2:G:3990:VAL:HG13	2:G:4051:SER:HB2	1.92	0.49
2:B:838:HIS:HB3	2:B:1200:GLY:H	1.77	0.49
2:B:3674:ILE:HG13	2:B:3732:SER:HB3	1.94	0.49
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.95	0.49
2:E:460:GLN:HG2	2:E:462:GLU:H	1.77	0.49
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.36	0.49
2:G:355:LEU:HB3	2:G:378:LEU:HB3	1.94	0.49
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.49
2:G:4044:MET:HA	2:G:4047:MET:HG2	1.94	0.49
2:I:313:SER:HB3	2:I:351:VAL:HB	1.93	0.49
2:I:4044:MET:HA	2:I:4047:MET:HG2	1.94	0.49
2:B:229:GLU:OE2	2:B:374:LYS:NZ	2.35	0.49
2:B:1203:ASN:ND2	2:B:1210:SER:O	2.44	0.49
2:B:3882:GLN:HB2	2:B:3957:VAL:HG22	1.95	0.49
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.49
2:E:4560:TYR:O	2:E:4564:PHE:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:232:THR:HB	2:I:252:VAL:HG11	1.95	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.95	0.49
2:I:1684:ALA:HA	2:I:1782:PHE:HZ	1.77	0.49
2:G:1240:LYS:O	2:G:1604:SER:N	2.43	0.49
2:G:1979:LEU:HA	2:G:1983:ALA:HB3	1.95	0.49
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.95	0.49
2:I:1721:GLU:HG2	2:I:1725:ARG:HH12	1.77	0.49
1:A:62:GLY:HA3	1:A:74:LEU:HD21	1.93	0.49
2:B:139:GLU:O	2:B:141:ALA:N	2.45	0.49
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.95	0.49
2:B:2257:LEU:O	2:B:2261:SER:N	2.46	0.49
2:E:1203:ASN:ND2	2:E:1210:SER:O	2.44	0.49
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.94	0.49
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.95	0.49
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.94	0.49
2:E:4201:ASN:O	2:E:4205:TRP:N	2.43	0.49
2:G:1684:ALA:HA	2:G:1782:PHE:HZ	1.77	0.49
2:G:2235:PHE:HA	2:G:2238:TYR:HD2	1.78	0.49
2:I:139:GLU:O	2:I:141:ALA:N	2.45	0.49
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.95	0.49
2:B:4044:MET:HA	2:B:4047:MET:HG2	1.94	0.48
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.94	0.48
1:F:62:GLY:HA3	1:F:74:LEU:HD21	1.94	0.48
2:G:313:SER:HB3	2:G:351:VAL:HB	1.93	0.48
2:G:1721:GLU:HG2	2:G:1725:ARG:HH12	1.77	0.48
2:I:793:LEU:HD12	2:I:797:HIS:HB2	1.95	0.48
2:B:682:LEU:HD13	2:B:787:VAL:HG11	1.94	0.48
2:E:1684:ALA:HA	2:E:1782:PHE:HZ	1.77	0.48
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.95	0.48
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.95	0.48
1:H:62:GLY:HA3	1:H:74:LEU:HD21	1.94	0.48
1:J:62:GLY:HA3	1:J:74:LEU:HD21	1.94	0.48
2:E:652:ARG:HB3	2:E:773:LEU:HD13	1.95	0.48
2:E:2013:LYS:HA	2:E:2028:ARG:HB2	1.95	0.48
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.95	0.48
2:G:4795:TYR:HE1	2:G:4812:HIS:HA	1.79	0.48
2:I:460:GLN:HG2	2:I:462:GLU:H	1.77	0.48
2:I:838:HIS:HB3	2:I:1200:GLY:H	1.77	0.48
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.95	0.48
2:I:3882:GLN:HB2	2:I:3957:VAL:HG22	1.95	0.48
2:B:652:ARG:HB3	2:B:773:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:793:LEU:HD12	2:B:797:HIS:HB2	1.95	0.48
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.95	0.48
2:B:1931:LEU:HD22	2:B:1935:VAL:HG11	1.96	0.48
2:B:4795:TYR:HE1	2:B:4812:HIS:HA	1.79	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.48
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.45	0.48
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.95	0.48
2:G:232:THR:HB	2:G:252:VAL:HG11	1.95	0.48
2:G:460:GLN:HG2	2:G:462:GLU:H	1.77	0.48
2:G:652:ARG:HB3	2:G:773:LEU:HD13	1.96	0.48
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.94	0.48
2:G:2257:LEU:O	2:G:2261:SER:N	2.46	0.48
2:G:4837:LEU:HD11	2:G:4936:ILE:HD11	1.96	0.48
2:G:4849:TYR:OH	2:I:4574:ASN:O	2.29	0.48
2:I:652:ARG:HB3	2:I:773:LEU:HD13	1.96	0.48
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.95	0.48
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.95	0.48
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.48
2:B:1778:SER:N	2:B:1799:SER:O	2.46	0.48
2:E:3994:HIS:O	2:E:3998:HIS:ND1	2.39	0.48
2:E:4837:LEU:HD11	2:E:4936:ILE:HD11	1.96	0.48
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.48
2:I:4105:GLY:HA2	2:I:4108:ILE:HD12	1.95	0.48
2:I:4837:LEU:HD11	2:I:4936:ILE:HD11	1.96	0.48
2:B:1684:ALA:HA	2:B:1782:PHE:HZ	1.77	0.48
2:E:880:GLU:OE1	2:E:968:ALA:N	2.47	0.48
2:G:682:LEU:HD13	2:G:787:VAL:HG11	1.94	0.48
2:G:793:LEU:HD12	2:G:797:HIS:HB2	1.95	0.48
2:G:1032:LYS:O	2:G:1036:ARG:N	2.40	0.48
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.95	0.48
2:I:1713:ASP:O	2:I:1717:SER:N	2.46	0.48
2:I:1931:LEU:HD22	2:I:1935:VAL:HG11	1.96	0.48
2:I:2235:PHE:HA	2:I:2238:TYR:HD2	1.78	0.48
1:A:57:LYS:HB2	1:A:80:VAL:HB	1.96	0.48
2:B:215:THR:HG22	2:B:273:HIS:HA	1.95	0.48
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.95	0.48
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.48
2:B:1979:LEU:HA	2:B:1983:ALA:HB3	1.95	0.48
2:B:2235:PHE:HA	2:B:2238:TYR:HD2	1.78	0.48
2:E:2336:ARG:HD3	2:E:2435:ARG:HD2	1.94	0.48
2:G:1075:PHE:HB2	2:G:1192:CYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1647:CYS:SG	2:G:1648:MET:N	2.87	0.48
2:I:3729:MET:HB3	2:I:3770:LEU:HD21	1.96	0.48
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.94	0.48
2:B:1659:LEU:O	2:B:1663:HIS:N	2.44	0.48
2:B:1952:GLN:HA	2:B:1955:VAL:HG12	1.96	0.48
2:B:4956:THR:O	2:B:4965:SER:N	2.42	0.48
2:E:3882:GLN:HB2	2:E:3957:VAL:HG22	1.95	0.48
2:G:215:THR:HG22	2:G:273:HIS:HA	1.95	0.48
1:H:57:LYS:HB2	1:H:80:VAL:HB	1.96	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
1:J:57:LYS:HB2	1:J:80:VAL:HB	1.96	0.48
1:J:87:HIS:N	1:J:91:ILE:O	2.47	0.48
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.94	0.48
2:E:1647:CYS:SG	2:E:1648:MET:N	2.87	0.48
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	1.95	0.48
2:E:1979:LEU:HA	2:E:1983:ALA:HB3	1.95	0.48
2:E:4795:TYR:HE1	2:E:4812:HIS:HA	1.79	0.48
2:G:988:LEU:O	2:G:992:GLY:N	2.46	0.48
2:G:1931:LEU:HD22	2:G:1935:VAL:HG11	1.96	0.48
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.79	0.48
2:B:913:LEU:HD13	2:B:918:ARG:HA	1.95	0.48
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.95	0.48
2:B:1854:PHE:HD1	2:B:1858:ASP:HB3	1.79	0.48
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.79	0.48
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.95	0.48
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.95	0.48
2:E:2257:LEU:O	2:E:2261:SER:N	2.46	0.48
1:F:57:LYS:HB2	1:F:80:VAL:HB	1.96	0.48
2:G:731:THR:OG1	2:G:1519:UNK:O	2.27	0.48
2:G:4105:GLY:HA2	2:G:4108:ILE:HD12	1.95	0.48
2:G:4956:THR:O	2:G:4965:SER:N	2.42	0.48
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.94	0.48
1:H:87:HIS:N	1:H:91:ILE:O	2.47	0.48
2:I:1952:GLN:HA	2:I:1955:VAL:HG12	1.96	0.48
2:I:2257:LEU:O	2:I:2261:SER:N	2.46	0.48
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.94	0.48
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.95	0.47
2:B:2950:UNK:O	2:B:2954:UNK:N	2.47	0.47
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.47
2:E:4105:GLY:HA2	2:E:4108:ILE:HD12	1.95	0.47
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3806:ASN:HA	2:G:3890:LEU:HD13	1.96	0.47
2:G:3882:GLN:HB2	2:G:3957:VAL:HG22	1.95	0.47
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.79	0.47
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.45	0.47
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.96	0.47
2:I:645:ARG:N	2:I:824:GLU:O	2.39	0.47
2:I:913:LEU:HD13	2:I:918:ARG:HA	1.95	0.47
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.79	0.47
2:I:4795:TYR:HE1	2:I:4812:HIS:HA	1.79	0.47
2:B:488:LEU:O	2:B:492:ASP:N	2.41	0.47
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.96	0.47
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.95	0.47
2:B:2013:LYS:HA	2:B:2028:ARG:HB2	1.95	0.47
2:E:1931:LEU:HD22	2:E:1935:VAL:HG11	1.96	0.47
1:F:87:HIS:N	1:F:91:ILE:O	2.47	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.47
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.95	0.47
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.47
2:I:1647:CYS:SG	2:I:1648:MET:N	2.87	0.47
2:B:1647:CYS:SG	2:B:1648:MET:N	2.87	0.47
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.96	0.47
2:E:1232:ARG:HD3	2:E:1702:HIS:HB3	1.96	0.47
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.95	0.47
2:E:3806:ASN:HA	2:E:3890:LEU:HD13	1.96	0.47
2:G:3729:MET:HB3	2:G:3770:LEU:HD21	1.96	0.47
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	1.96	0.47
2:B:3992:PHE:O	2:B:3996:PHE:N	2.38	0.47
2:B:4571:PHE:O	2:B:4575:PHE:N	2.48	0.47
2:B:4837:LEU:HD11	2:B:4936:ILE:HD11	1.96	0.47
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.95	0.47
2:E:4571:PHE:O	2:E:4575:PHE:N	2.48	0.47
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.96	0.47
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.95	0.47
2:G:1232:ARG:HD3	2:G:1702:HIS:HB3	1.96	0.47
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.95	0.47
2:I:1232:ARG:HD3	2:I:1702:HIS:HB3	1.96	0.47
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.95	0.47
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.48	0.47
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.96	0.47
2:B:1516:UNK:N	2:B:1529:UNK:O	2.47	0.47
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	1.96	0.47
2:E:232:THR:HB	2:E:252:VAL:HG11	1.95	0.47
2:E:1075:PHE:HB2	2:E:1192:CYS:HB2	1.95	0.47
2:E:1713:ASP:O	2:E:1717:SER:N	2.46	0.47
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.47
2:E:4116:GLU:H	2:E:4128:PHE:HZ	1.63	0.47
2:G:637:LEU:HG	2:G:1693:GLN:HB3	1.96	0.47
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.95	0.47
2:G:2347:GLU:O	2:G:2351:ASN:N	2.43	0.47
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.80	0.47
2:B:3806:ASN:HA	2:B:3890:LEU:HD13	1.96	0.47
2:E:215:THR:HG22	2:E:273:HIS:HA	1.95	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.47
2:E:3920:VAL:O	2:E:3924:LEU:N	2.44	0.47
2:I:215:THR:HG22	2:I:273:HIS:HA	1.95	0.47
2:I:637:LEU:HG	2:I:1693:GLN:HB3	1.96	0.47
2:I:2013:LYS:HA	2:I:2028:ARG:HB2	1.96	0.47
2:I:2950:UNK:O	2:I:2954:UNK:N	2.48	0.47
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.45	0.47
2:B:988:LEU:O	2:B:992:GLY:N	2.46	0.47
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.97	0.47
2:B:3729:MET:HB3	2:B:3770:LEU:HD21	1.96	0.47
2:E:793:LEU:HD12	2:E:797:HIS:HB2	1.95	0.47
2:E:988:LEU:O	2:E:992:GLY:N	2.46	0.47
2:E:1032:LYS:O	2:E:1036:ARG:N	2.40	0.47
2:E:1778:SER:N	2:E:1799:SER:O	2.46	0.47
2:E:1854:PHE:HD1	2:E:1858:ASP:HB3	1.79	0.47
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.97	0.47
2:G:2013:LYS:HA	2:G:2028:ARG:HB2	1.95	0.47
2:G:4116:GLU:H	2:G:4128:PHE:HZ	1.63	0.47
2:I:379:HIS:CD2	2:I:382:GLY:H	2.33	0.47
2:I:880:GLU:OE1	2:I:968:ALA:N	2.47	0.47
2:I:1075:PHE:HB2	2:I:1192:CYS:HB2	1.95	0.47
2:I:1659:LEU:O	2:I:1663:HIS:N	2.44	0.47
2:I:1854:PHE:HD1	2:I:1858:ASP:HB3	1.79	0.47
2:I:1979:LEU:HA	2:I:1983:ALA:HB3	1.95	0.47
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.79	0.47
2:I:3994:HIS:O	2:I:3998:HIS:ND1	2.39	0.47
2:I:4824:ARG:HA	2:I:4827:LEU:HB3	1.97	0.47
1:A:87:HIS:N	1:A:91:ILE:O	2.47	0.47
2:B:1075:PHE:HB2	2:B:1192:CYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.97	0.47
2:E:2347:GLU:O	2:E:2351:ASN:N	2.43	0.47
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.96	0.47
2:G:120:CYS:H	2:G:145:ALA:HB1	1.80	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.44	0.47
2:G:880:GLU:OE1	2:G:968:ALA:N	2.47	0.47
2:G:2950:UNK:O	2:G:2954:UNK:N	2.48	0.47
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.97	0.47
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.79	0.47
1:A:34:LYS:NZ	2:B:635:THR:O	2.47	0.47
2:B:232:THR:HB	2:B:252:VAL:HG11	1.95	0.47
2:B:4105:GLY:HA2	2:B:4108:ILE:HD12	1.95	0.47
2:E:1952:GLN:HA	2:E:1955:VAL:HG12	1.96	0.47
2:G:1713:ASP:O	2:G:1717:SER:N	2.46	0.47
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.95	0.47
2:E:120:CYS:H	2:E:145:ALA:HB1	1.80	0.47
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	1.97	0.47
2:I:485:SER:O	2:I:489:ASN:N	2.44	0.47
2:I:1286:UNK:HA	2:I:1461:UNK:HA	1.96	0.47
2:B:4560:TYR:O	2:B:4564:PHE:N	2.43	0.46
2:B:4824:ARG:HA	2:B:4827:LEU:HB3	1.97	0.46
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.81	0.46
2:I:5012:LYS:O	2:I:5016:GLU:N	2.43	0.46
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.96	0.46
2:B:379:HIS:CD2	2:B:382:GLY:H	2.33	0.46
2:B:1232:ARG:HD3	2:B:1702:HIS:HB3	1.97	0.46
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.98	0.46
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.80	0.46
2:B:5012:LYS:O	2:B:5016:GLU:N	2.43	0.46
2:E:3729:MET:HB3	2:E:3770:LEU:HD21	1.96	0.46
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.79	0.46
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.80	0.46
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.79	0.46
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	1.96	0.46
2:G:733:PRO:HD2	2:G:763:PRO:HD2	1.97	0.46
2:G:1854:PHE:HD1	2:G:1858:ASP:HB3	1.79	0.46
2:G:1952:GLN:HA	2:G:1955:VAL:HG12	1.96	0.46
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	1.97	0.46
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	1.96	0.46
2:I:1778:SER:N	2:I:1799:SER:O	2.46	0.46
2:I:4571:PHE:O	2:I:4575:PHE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4116:GLU:H	2:B:4128:PHE:HZ	1.63	0.46
2:E:733:PRO:HD2	2:E:763:PRO:HD2	1.97	0.46
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.96	0.46
2:G:4560:TYR:O	2:G:4564:PHE:N	2.43	0.46
2:G:4571:PHE:O	2:G:4575:PHE:N	2.48	0.46
2:I:865:PRO:O	2:I:869:ARG:N	2.49	0.46
2:I:1855:GLY:O	2:I:1859:VAL:N	2.45	0.46
2:B:637:LEU:HG	2:B:1693:GLN:HB3	1.96	0.46
2:E:164:ARG:N	2:E:167:ASP:OD2	2.48	0.46
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.96	0.46
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.98	0.46
2:G:164:ARG:N	2:G:167:ASP:OD2	2.48	0.46
2:G:1778:SER:N	2:G:1799:SER:O	2.46	0.46
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.96	0.46
2:I:120:CYS:H	2:I:145:ALA:HB1	1.80	0.46
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.98	0.46
2:I:3806:ASN:HA	2:I:3890:LEU:HD13	1.96	0.46
2:B:120:CYS:H	2:B:145:ALA:HB1	1.80	0.46
2:B:731:THR:OG1	2:B:1519:UNK:O	2.27	0.46
2:E:637:LEU:HG	2:E:1693:GLN:HB3	1.96	0.46
2:E:1229:ASN:O	2:E:1827:ARG:N	2.43	0.46
2:E:1729:SER:O	2:E:2163:ARG:NH1	2.49	0.46
2:G:1779:PRO:HG2	1:H:44:LYS:HE3	1.98	0.46
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.98	0.46
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.81	0.46
2:I:69:LEU:HD22	2:I:107:ILE:HD11	1.98	0.46
2:B:38:ALA:HB1	2:B:64:ILE:HG13	1.97	0.46
2:B:880:GLU:OE1	2:B:968:ALA:N	2.47	0.46
2:E:731:THR:OG1	2:E:1519:UNK:O	2.34	0.46
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.97	0.46
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.48	0.46
2:G:1229:ASN:O	2:G:1827:ARG:N	2.43	0.46
2:G:4824:ARG:HA	2:G:4827:LEU:HB3	1.97	0.46
2:B:69:LEU:HD22	2:B:107:ILE:HD11	1.98	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.98	0.46
2:B:1713:ASP:O	2:B:1717:SER:N	2.46	0.46
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.79	0.46
2:E:379:HIS:CD2	2:E:382:GLY:H	2.33	0.46
2:E:4824:ARG:HA	2:E:4827:LEU:HB3	1.97	0.46
2:G:1729:SER:O	2:G:2163:ARG:NH1	2.49	0.46
2:I:838:HIS:CE1	2:I:1201:HIS:HD2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.97	0.46
2:B:838:HIS:CE1	2:B:1201:HIS:HD2	2.34	0.46
2:B:3758:MET:O	2:B:3762:ARG:NE	2.46	0.46
2:B:4051:SER:HG	2:B:4054:ASN:HB2	1.80	0.46
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.98	0.46
2:I:733:PRO:HD2	2:I:763:PRO:HD2	1.97	0.46
1:A:83:GLY:O	1:A:94:ASN:N	2.48	0.46
2:E:3927:GLN:O	2:E:3931:SER:N	2.45	0.46
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.81	0.46
2:I:4942:GLU:O	2:I:4946:GLN:N	2.44	0.46
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.32	0.45
2:B:733:PRO:HD2	2:B:763:PRO:HD2	1.97	0.45
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.80	0.45
2:B:4697:VAL:O	2:B:4701:TRP:N	2.49	0.45
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.32	0.45
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.42	0.45
2:I:1203:ASN:ND2	2:I:1210:SER:O	2.44	0.45
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	1.97	0.45
2:I:4116:GLU:H	2:I:4128:PHE:HZ	1.63	0.45
1:J:83:GLY:O	1:J:94:ASN:N	2.48	0.45
2:B:1729:SER:O	2:B:2163:ARG:NH1	2.49	0.45
2:B:2336:ARG:NH2	2:B:2428:ALA:O	2.49	0.45
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.51	0.45
2:E:4934:GLY:O	2:E:4938:ASP:N	2.47	0.45
1:F:23:VAL:HB	1:F:105:ASN:HA	1.99	0.45
2:I:38:ALA:HB1	2:I:64:ILE:HG13	1.97	0.45
2:I:1729:SER:O	2:I:2163:ARG:NH1	2.49	0.45
1:A:23:VAL:HB	1:A:105:ASN:HA	1.99	0.45
2:B:4942:GLU:O	2:B:4946:GLN:N	2.43	0.45
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.98	0.45
2:G:38:ALA:HB1	2:G:64:ILE:HG13	1.97	0.45
2:G:865:PRO:O	2:G:869:ARG:N	2.49	0.45
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.97	0.45
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.45
2:I:2880:GLU:O	2:I:2884:ASN:N	2.45	0.45
2:B:124:SER:HA	2:B:132:ALA:HB3	1.99	0.45
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.52	0.45
2:E:38:ALA:HB1	2:E:64:ILE:HG13	1.97	0.45
2:E:2286:LEU:HA	2:E:2289:ALA:HB3	1.99	0.45
2:E:4697:VAL:O	2:E:4701:TRP:N	2.49	0.45
2:G:838:HIS:CE1	2:G:1201:HIS:HD2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4791:TYR:HD2	2:G:4792:LEU:HD22	1.82	0.45
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.52	0.45
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.98	0.45
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.97	0.45
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	1.97	0.45
2:B:2880:GLU:O	2:B:2884:ASN:N	2.45	0.45
2:E:124:SER:HA	2:E:132:ALA:HB3	1.99	0.45
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.32	0.45
2:E:838:HIS:CE1	2:E:1201:HIS:HD2	2.34	0.45
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.52	0.45
1:H:23:VAL:HB	1:H:105:ASN:HA	1.99	0.45
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.98	0.45
2:I:2347:GLU:O	2:I:2351:ASN:N	2.43	0.45
1:J:23:VAL:HB	1:J:105:ASN:HA	1.99	0.45
2:B:546:TRP:O	2:B:550:LYS:NZ	2.38	0.45
2:B:2132:GLY:O	2:B:2136:ARG:N	2.50	0.45
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.99	0.45
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.98	0.45
2:E:1659:LEU:O	2:E:1663:HIS:N	2.44	0.45
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.98	0.45
2:G:124:SER:HA	2:G:132:ALA:HB3	1.99	0.45
2:G:4109:GLN:O	2:G:4113:SER:N	2.45	0.45
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.99	0.45
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.99	0.45
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.98	0.45
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.45	0.45
2:B:4961:CYS:SG	2:B:4978:HIS:NE2	2.90	0.45
2:E:1577:ALA:HB1	2:E:1584:ARG:HA	1.99	0.45
2:G:69:LEU:HD22	2:G:107:ILE:HD11	1.98	0.45
2:G:2286:LEU:HA	2:G:2289:ALA:HB3	1.99	0.45
2:G:4705:VAL:HB	2:G:4778:TRP:CG	2.52	0.45
1:H:83:GLY:O	1:H:94:ASN:N	2.48	0.45
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.99	0.45
2:I:124:SER:HA	2:I:132:ALA:HB3	1.99	0.45
2:B:2286:LEU:HA	2:B:2289:ALA:HB3	1.99	0.45
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.98	0.45
2:B:4853:VAL:HA	2:B:4856:PHE:HB3	1.98	0.45
2:E:69:LEU:HD22	2:E:107:ILE:HD11	1.98	0.45
2:E:485:SER:O	2:E:489:ASN:N	2.44	0.45
2:E:1041:GLN:O	2:E:1045:THR:OG1	2.29	0.45
1:F:83:GLY:O	1:F:94:ASN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.97	0.45
2:I:629:ARG:HB3	2:I:634:GLN:NE2	2.31	0.45
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.99	0.45
2:I:3920:VAL:O	2:I:3924:LEU:N	2.44	0.45
2:I:4961:CYS:SG	2:I:4978:HIS:NE2	2.90	0.45
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.99	0.45
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.48	0.45
2:E:732:SER:HB3	2:E:764:VAL:HA	1.99	0.45
2:G:732:SER:HB3	2:G:764:VAL:HA	1.99	0.45
2:G:2132:GLY:O	2:G:2136:ARG:N	2.50	0.45
2:G:2758:PHE:O	2:G:2762:THR:N	2.47	0.45
2:G:4853:VAL:HA	2:G:4856:PHE:HB3	1.98	0.45
2:I:180:LEU:HD22	2:I:200:TRP:NE1	2.32	0.45
2:I:233:ILE:HD12	2:I:242:ARG:HB3	1.99	0.45
2:I:2132:GLY:O	2:I:2136:ARG:N	2.50	0.45
2:I:3758:MET:O	2:I:3762:ARG:NE	2.46	0.45
1:J:29:MET:HB3	1:J:98:ILE:HB	1.99	0.45
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.99	0.45
2:B:865:PRO:O	2:B:869:ARG:N	2.49	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.50	0.45
2:E:4791:TYR:HD2	2:E:4792:LEU:HD22	1.81	0.45
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.99	0.45
2:G:233:ILE:HD12	2:G:242:ARG:HB3	1.99	0.45
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.99	0.45
2:G:1577:ALA:HB1	2:G:1584:ARG:HA	1.99	0.45
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.48	0.45
2:G:2869:ARG:HH12	2:G:2945:UNK:C	2.30	0.45
2:G:3773:ARG:HG2	2:G:3815:LYS:HD3	1.99	0.45
2:I:4560:TYR:O	2:I:4564:PHE:N	2.43	0.45
2:I:4791:TYR:HD2	2:I:4792:LEU:HD22	1.82	0.45
2:I:4989:MET:O	2:I:4993:MET:N	2.42	0.45
2:B:1294:UNK:HA	2:B:1455:UNK:HA	1.99	0.44
2:B:4791:TYR:HD2	2:B:4792:LEU:HD22	1.82	0.44
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.98	0.44
1:F:29:MET:HB3	1:F:98:ILE:HB	1.99	0.44
2:G:4885:PHE:HE2	2:G:4901:ILE:HD11	1.82	0.44
2:G:4961:CYS:SG	2:G:4978:HIS:NE2	2.90	0.44
2:I:2286:LEU:HA	2:I:2289:ALA:HB3	1.99	0.44
2:I:4853:VAL:HA	2:I:4856:PHE:HB3	1.98	0.44
2:B:3765:TYR:O	2:B:3769:ARG:N	2.48	0.44
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4705:VAL:HB	2:E:4778:TRP:CG	2.52	0.44
2:E:5012:LYS:O	2:E:5016:GLU:N	2.43	0.44
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.98	0.44
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.99	0.44
2:I:1497:UNK:HA	2:I:1535:UNK:HA	1.98	0.44
2:I:4885:PHE:HE2	2:I:4901:ILE:HD11	1.82	0.44
2:B:1229:ASN:O	2:B:1827:ARG:N	2.43	0.44
2:E:59:PRO:HG3	2:E:307:ALA:HB3	1.99	0.44
2:E:233:ILE:HD12	2:E:242:ARG:HB3	1.99	0.44
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.99	0.44
2:G:78:LEU:O	2:G:82:LEU:N	2.49	0.44
2:G:379:HIS:CD2	2:G:382:GLY:H	2.33	0.44
2:G:978:THR:HB	2:G:980:ALA:H	1.83	0.44
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.50	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.48	0.44
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.44
2:B:59:PRO:HG3	2:B:307:ALA:HB3	1.99	0.44
2:B:233:ILE:HD12	2:B:242:ARG:HB3	1.99	0.44
2:E:639:ASN:HD22	2:E:1635:THR:HA	1.83	0.44
2:G:1659:LEU:O	2:G:1663:HIS:N	2.44	0.44
2:G:2142:TYR:CG	2:G:2197:LEU:HD13	2.53	0.44
2:G:3649:ALA:O	2:G:3653:PHE:N	2.46	0.44
2:G:4237:PHE:O	2:G:4241:THR:OG1	2.22	0.44
2:I:59:PRO:HG3	2:I:307:ALA:HB3	2.00	0.44
2:I:4705:VAL:HB	2:I:4778:TRP:CG	2.52	0.44
1:A:29:MET:HB3	1:A:98:ILE:HB	1.99	0.44
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.44
2:B:3713:LYS:HG2	2:B:3715:LYS:H	1.83	0.44
2:B:4109:GLN:O	2:B:4113:SER:N	2.45	0.44
2:B:4885:PHE:HE2	2:B:4901:ILE:HD11	1.82	0.44
2:E:546:TRP:O	2:E:550:LYS:NZ	2.39	0.44
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.53	0.44
2:E:1817:GLU:O	2:E:1821:ASP:N	2.44	0.44
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.99	0.44
2:G:3927:GLN:O	2:G:3931:SER:N	2.45	0.44
2:G:5012:LYS:O	2:G:5016:GLU:N	2.43	0.44
2:I:357:LEU:HD21	2:I:376:ALA:HB1	1.99	0.44
2:I:1649:ASP:OD1	2:I:1650:ILE:N	2.51	0.44
2:I:3773:ARG:HG2	2:I:3815:LYS:HD3	2.00	0.44
2:B:639:ASN:HD22	2:B:1635:THR:HA	1.83	0.44
2:B:870:ILE:HD11	2:B:1049:TYR:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1577:ALA:HB1	2:B:1584:ARG:HA	1.99	0.44
2:B:4705:VAL:HB	2:B:4778:TRP:CG	2.52	0.44
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.99	0.44
2:E:3773:ARG:HG2	2:E:3815:LYS:HD3	1.99	0.44
2:E:4782:VAL:O	2:E:4785:THR:OG1	2.34	0.44
2:E:4885:PHE:HE2	2:E:4901:ILE:HD11	1.82	0.44
2:E:4961:CYS:SG	2:E:4978:HIS:NE2	2.90	0.44
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.45	0.44
2:G:1991:THR:O	2:G:1995:THR:OG1	2.30	0.44
2:I:1516:UNK:N	2:I:1529:UNK:O	2.51	0.44
2:I:1577:ALA:HB1	2:I:1584:ARG:HA	1.99	0.44
2:I:3927:GLN:NE2	2:I:3988:ALA:O	2.47	0.44
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.99	0.44
2:E:3998:HIS:CE1	2:E:4054:ASN:HD21	2.36	0.44
2:G:180:LEU:HD22	2:G:200:TRP:NE1	2.32	0.44
2:G:639:ASN:HD22	2:G:1635:THR:HA	1.83	0.44
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.98	0.44
2:G:3880:PHE:O	2:G:3884:LEU:N	2.51	0.44
2:G:4702:ASP:HA	2:G:4778:TRP:HE1	1.83	0.44
2:I:639:ASN:HD22	2:I:1635:THR:HA	1.83	0.44
2:I:978:THR:HB	2:I:980:ALA:H	1.83	0.44
2:I:2142:TYR:CG	2:I:2197:LEU:HD13	2.53	0.44
2:B:732:SER:HB3	2:B:764:VAL:HA	1.99	0.44
2:E:316:PHE:HB3	2:E:346:CYS:HB3	2.00	0.44
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.50	0.44
2:E:4853:VAL:HA	2:E:4856:PHE:HB3	1.98	0.44
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.99	0.44
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.98	0.44
2:G:546:TRP:O	2:G:550:LYS:NZ	2.38	0.44
2:G:867:LEU:HD22	2:G:929:LEU:HD22	2.00	0.44
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.98	0.44
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.44
2:B:17:ASP:HB2	2:B:98:HIS:CE1	2.53	0.44
2:B:180:LEU:HD22	2:B:200:TRP:NE1	2.32	0.44
2:B:2347:GLU:O	2:B:2351:ASN:N	2.43	0.44
2:E:865:PRO:O	2:E:869:ARG:N	2.49	0.44
2:E:1516:UNK:N	2:E:1529:UNK:O	2.51	0.44
2:G:663:TYR:HB2	2:G:808:TYR:HB3	2.00	0.44
2:G:1245:PHE:HE1	2:G:1600:LEU:HD23	1.83	0.44
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.83	0.44
1:H:29:MET:HB3	1:H:98:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:709:ASP:O	2:I:725:HIS:ND1	2.51	0.44
2:I:3713:LYS:HG2	2:I:3715:LYS:H	1.83	0.44
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.43
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.83	0.43
2:E:663:TYR:HB2	2:E:808:TYR:HB3	2.00	0.43
2:E:829:TYR:HB3	2:E:1073:ARG:HH11	1.83	0.43
2:E:3880:PHE:O	2:E:3884:LEU:N	2.51	0.43
2:E:4109:GLN:O	2:E:4113:SER:N	2.45	0.43
2:G:59:PRO:HG3	2:G:307:ALA:HB3	2.00	0.43
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.83	0.43
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.99	0.43
2:I:1663:HIS:O	2:I:1667:LEU:N	2.50	0.43
2:B:316:PHE:HB3	2:B:346:CYS:HB3	2.00	0.43
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.99	0.43
2:B:867:LEU:HD22	2:B:929:LEU:HD22	2.00	0.43
2:B:1965:TYR:OH	2:B:2027:ILE:O	2.26	0.43
2:B:3880:PHE:O	2:B:3884:LEU:N	2.51	0.43
2:E:357:LEU:HD21	2:E:376:ALA:HB1	2.00	0.43
2:E:709:ASP:O	2:E:725:HIS:ND1	2.51	0.43
2:E:1245:PHE:HE1	2:E:1600:LEU:HD23	1.83	0.43
2:E:1649:ASP:OD1	2:E:1650:ILE:N	2.51	0.43
2:E:2142:TYR:CG	2:E:2197:LEU:HD13	2.53	0.43
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	2.00	0.43
2:G:357:LEU:HD21	2:G:376:ALA:HB1	1.99	0.43
2:G:1817:GLU:O	2:G:1821:ASP:N	2.44	0.43
2:G:3974:THR:HA	2:G:3977:GLN:HB2	2.00	0.43
2:G:4782:VAL:O	2:G:4785:THR:OG1	2.34	0.43
2:I:78:LEU:O	2:I:82:LEU:N	2.49	0.43
2:B:709:ASP:O	2:B:725:HIS:ND1	2.51	0.43
2:B:1991:THR:O	2:B:1995:THR:OG1	2.30	0.43
2:B:2142:TYR:CG	2:B:2197:LEU:HD13	2.53	0.43
2:B:2758:PHE:O	2:B:2762:THR:N	2.47	0.43
2:E:3974:THR:HA	2:E:3977:GLN:HB2	2.00	0.43
2:E:4745:LEU:O	2:E:4749:GLU:N	2.50	0.43
2:G:1663:HIS:O	2:G:1667:LEU:N	2.50	0.43
2:G:3758:MET:O	2:G:3762:ARG:NE	2.46	0.43
2:G:4989:MET:O	2:G:4993:MET:N	2.42	0.43
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.53	0.43
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	2.01	0.43
2:I:2207:VAL:HG13	2:I:2232:CYS:HB2	2.00	0.43
2:I:4697:VAL:O	2:I:4701:TRP:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ARG:N	2:B:167:ASP:OD2	2.48	0.43
2:B:2361:PRO:HA	2:B:2364:PHE:HD2	1.83	0.43
2:E:978:THR:HB	2:E:980:ALA:H	1.83	0.43
2:G:1649:ASP:OD1	2:G:1650:ILE:N	2.51	0.43
2:G:2361:PRO:HA	2:G:2364:PHE:HD2	1.83	0.43
2:I:732:SER:HB3	2:I:764:VAL:HA	1.99	0.43
2:I:3676:ASP:N	2:I:3676:ASP:OD1	2.51	0.43
2:B:709:ASP:HA	2:B:725:HIS:H	1.84	0.43
2:B:1649:ASP:OD1	2:B:1650:ILE:N	2.51	0.43
2:B:1679:ASN:O	2:B:1683:HIS:ND1	2.38	0.43
2:B:2207:VAL:HG13	2:B:2232:CYS:HB2	2.00	0.43
2:B:3773:ARG:HG2	2:B:3815:LYS:HD3	1.99	0.43
2:B:3974:THR:HA	2:B:3977:GLN:HB2	2.00	0.43
2:B:3998:HIS:CE1	2:B:4054:ASN:HD21	2.36	0.43
2:E:180:LEU:HD22	2:E:200:TRP:NE1	2.32	0.43
2:E:867:LEU:HD22	2:E:929:LEU:HD22	2.00	0.43
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	2.01	0.43
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.99	0.43
2:I:709:ASP:HA	2:I:725:HIS:H	1.84	0.43
2:I:765:GLN:NE2	2:I:1522:UNK:O	2.51	0.43
2:I:1095:VAL:HA	2:I:1146:GLY:H	1.84	0.43
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.50	0.43
2:I:4957:LYS:HB3	2:I:4957:LYS:HE3	1.83	0.43
2:B:151:HIS:HB2	2:B:170:ILE:HB	2.01	0.43
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.01	0.43
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.51	0.43
2:B:4702:ASP:HA	2:B:4778:TRP:HE1	1.83	0.43
2:E:1092:PHE:O	2:E:1149:VAL:N	2.48	0.43
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.83	0.43
2:E:2144:ILE:H	2:E:2144:ILE:HG13	1.75	0.43
2:E:3713:LYS:HG2	2:E:3715:LYS:H	1.83	0.43
2:G:252:VAL:HA	2:G:255:HIS:CG	2.54	0.43
2:G:1095:VAL:HA	2:G:1146:GLY:H	1.84	0.43
2:G:4697:VAL:O	2:G:4701:TRP:N	2.49	0.43
2:I:634:GLN:HB3	1:J:34:LYS:HZ2	1.84	0.43
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.83	0.43
2:I:2361:PRO:HA	2:I:2364:PHE:HD2	1.83	0.43
2:I:3880:PHE:O	2:I:3884:LEU:N	2.51	0.43
2:I:4702:ASP:HA	2:I:4778:TRP:HE1	1.83	0.43
2:B:357:LEU:HD21	2:B:376:ALA:HB1	1.99	0.43
2:B:4745:LEU:O	2:B:4749:GLU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:809:ALA:O	2:E:811:CYS:N	2.50	0.43
2:E:2207:VAL:HG13	2:E:2232:CYS:HB2	2.00	0.43
2:E:4702:ASP:HA	2:E:4778:TRP:HE1	1.83	0.43
2:G:316:PHE:HB3	2:G:346:CYS:HB3	2.00	0.43
2:I:546:TRP:O	2:I:550:LYS:NZ	2.38	0.43
2:B:79:GLN:HA	2:B:82:LEU:HB2	2.01	0.43
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	2.01	0.43
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.84	0.43
2:B:2869:ARG:HH12	2:B:2945:UNK:C	2.32	0.43
2:B:4934:GLY:O	2:B:4938:ASP:N	2.47	0.43
2:E:79:GLN:HA	2:E:82:LEU:HB2	2.01	0.43
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.01	0.43
2:E:3765:TYR:O	2:E:3769:ARG:N	2.48	0.43
2:G:685:GLY:N	2:G:780:VAL:O	2.39	0.43
2:G:709:ASP:O	2:G:725:HIS:ND1	2.51	0.43
2:G:829:TYR:HB3	2:G:1073:ARG:HH11	1.84	0.43
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	2.01	0.43
2:G:1105:ALA:O	2:G:1189:LEU:N	2.52	0.43
2:G:1516:UNK:N	2:G:1529:UNK:O	2.51	0.43
2:G:3998:HIS:CE1	2:G:4054:ASN:HD21	2.36	0.43
2:I:401:ALA:HA	2:I:404:ILE:HD12	2.01	0.43
2:I:3974:THR:HA	2:I:3977:GLN:HB2	2.00	0.43
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.01	0.43
2:B:1497:UNK:HA	2:B:1535:UNK:HA	2.01	0.43
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	2.00	0.43
2:B:3927:GLN:O	2:B:3931:SER:N	2.45	0.43
2:E:151:HIS:HB2	2:E:170:ILE:HB	2.00	0.43
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.01	0.43
2:E:4857:ASN:HB2	2:G:4807:PHE:CE1	2.53	0.43
2:G:533:ASN:HB3	2:G:536:ASN:HB2	2.01	0.43
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.53	0.43
2:G:1866:ILE:HG13	2:G:1926:LEU:HB3	2.01	0.43
2:I:379:HIS:CD2	2:I:381:GLU:H	2.37	0.43
2:I:829:TYR:HB3	2:I:1073:ARG:HH11	1.84	0.43
2:I:867:LEU:HD22	2:I:929:LEU:HD22	2.00	0.43
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.84	0.43
2:I:1268:PRO:HB2	2:I:1591:CYS:HB2	2.01	0.43
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.00	0.43
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.84	0.43
2:B:663:TYR:HB2	2:B:808:TYR:HB3	2.00	0.43
2:B:1095:VAL:HA	2:B:1146:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3927:GLN:NE2	2:B:3988:ALA:O	2.48	0.43
2:E:2880:GLU:O	2:E:2884:ASN:N	2.45	0.43
2:G:709:ASP:HA	2:G:725:HIS:H	1.84	0.43
2:G:731:THR:OG1	2:G:1520:UNK:O	2.37	0.43
2:G:1149:VAL:HG22	2:G:1164:LEU:HD13	2.01	0.43
2:G:3713:LYS:HG2	2:G:3715:LYS:H	1.83	0.43
2:I:1046:LEU:HB3	2:I:1051:TYR:HB2	2.01	0.43
2:I:1092:PHE:O	2:I:1149:VAL:N	2.48	0.43
2:I:1777:PHE:HA	2:I:1799:SER:HB2	2.01	0.43
2:I:2021:CYS:HA	2:I:2022:PRO:HD3	1.91	0.43
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	2.00	0.43
2:E:2132:GLY:O	2:E:2136:ARG:N	2.50	0.42
2:E:4956:THR:O	2:E:4965:SER:N	2.42	0.42
2:E:5026:ASP:OD1	2:E:5027:CYS:N	2.52	0.42
2:G:176:SER:HB2	2:G:178:ARG:HH21	1.84	0.42
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.45	0.42
2:I:663:TYR:HB2	2:I:808:TYR:HB3	2.00	0.42
2:I:2185:ILE:HA	2:I:2188:ASN:ND2	2.34	0.42
2:I:3842:LEU:O	2:I:3929:SER:OG	2.37	0.42
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.01	0.42
2:I:4791:TYR:OH	2:I:4815:ASP:HB2	2.19	0.42
2:B:379:HIS:CD2	2:B:381:GLU:H	2.37	0.42
2:B:684:VAL:HA	2:B:781:VAL:HA	2.01	0.42
2:B:978:THR:HB	2:B:980:ALA:H	1.83	0.42
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.02	0.42
2:E:17:ASP:HB2	2:E:98:HIS:CE1	2.53	0.42
2:E:401:ALA:HA	2:E:404:ILE:HD12	2.01	0.42
2:G:809:ALA:O	2:G:811:CYS:N	2.50	0.42
2:G:932:LEU:HD23	2:G:935:LEU:HD12	2.02	0.42
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.01	0.42
2:G:3663:LEU:H	2:G:3663:LEU:HG	1.64	0.42
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.01	0.42
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.84	0.42
2:I:176:SER:HB2	2:I:178:ARG:HH21	1.84	0.42
2:I:731:THR:OG1	2:I:1519:UNK:O	2.28	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.01	0.42
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	2.01	0.42
2:B:1268:PRO:HB2	2:B:1591:CYS:HB2	2.01	0.42
2:E:932:LEU:HD23	2:E:935:LEU:HD12	2.02	0.42
2:E:1095:VAL:HA	2:E:1146:GLY:H	1.84	0.42
2:E:1663:HIS:O	2:E:1667:LEU:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1777:PHE:HA	2:G:1799:SER:HB2	2.01	0.42
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.51	0.42
2:I:316:PHE:HB3	2:I:346:CYS:HB3	2.00	0.42
2:I:684:VAL:HA	2:I:781:VAL:HA	2.01	0.42
2:I:4237:PHE:O	2:I:4241:THR:OG1	2.22	0.42
2:I:4934:GLY:O	2:I:4938:ASP:N	2.47	0.42
1:A:91:ILE:HD12	1:A:97:LEU:HD11	2.02	0.42
2:B:252:VAL:HA	2:B:255:HIS:CG	2.54	0.42
2:B:3842:LEU:O	2:B:3929:SER:OG	2.37	0.42
2:B:4791:TYR:OH	2:B:4815:ASP:HB2	2.19	0.42
2:E:252:VAL:HA	2:E:255:HIS:CG	2.54	0.42
2:E:315:CYS:SG	2:E:316:PHE:N	2.93	0.42
2:E:1149:VAL:HG22	2:E:1164:LEU:HD13	2.01	0.42
2:E:2361:PRO:HA	2:E:2364:PHE:HD2	1.83	0.42
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	2.01	0.42
2:G:79:GLN:HA	2:G:82:LEU:HB2	2.01	0.42
2:G:379:HIS:CD2	2:G:381:GLU:H	2.37	0.42
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.01	0.42
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	2.01	0.42
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	2.00	0.42
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.01	0.42
2:G:3927:GLN:NE2	2:G:3988:ALA:O	2.48	0.42
2:I:426:ARG:HG2	2:I:431:PRO:HA	2.02	0.42
2:I:3765:TYR:O	2:I:3769:ARG:N	2.48	0.42
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.01	0.42
2:I:4945:ASP:HA	2:I:4948:GLU:HB2	2.02	0.42
2:B:176:SER:HB2	2:B:178:ARG:HH21	1.84	0.42
2:B:876:GLU:O	2:B:880:GLU:N	2.48	0.42
2:B:1105:ALA:O	2:B:1189:LEU:N	2.52	0.42
2:B:4945:ASP:HA	2:B:4948:GLU:HB2	2.02	0.42
2:B:5026:ASP:OD1	2:B:5027:CYS:N	2.52	0.42
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.84	0.42
2:E:3840:SER:OG	2:E:3875:MET:O	2.30	0.42
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.84	0.42
2:G:627:PRO:HB2	1:H:92:PRO:HD3	2.02	0.42
2:G:684:VAL:HA	2:G:781:VAL:HA	2.01	0.42
2:G:1268:PRO:HB2	2:G:1591:CYS:HB2	2.01	0.42
2:G:2207:VAL:HG13	2:G:2232:CYS:HB2	2.00	0.42
2:G:3842:LEU:O	2:G:3929:SER:OG	2.38	0.42
2:G:4051:SER:HG	2:G:4054:ASN:HB2	1.83	0.42
2:G:4568:PHE:HA	2:G:4571:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:79:GLN:HA	2:I:82:LEU:HB2	2.01	0.42
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.84	0.42
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	2.01	0.42
2:I:3998:HIS:CE1	2:I:4054:ASN:HD21	2.36	0.42
2:B:1046:LEU:HB3	2:B:1051:TYR:HB2	2.01	0.42
2:B:1703:LEU:HD21	2:B:1830:VAL:HG13	2.01	0.42
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.01	0.42
2:B:1866:ILE:HG13	2:B:1926:LEU:HB3	2.01	0.42
2:E:426:ARG:HG2	2:E:431:PRO:HA	2.02	0.42
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.84	0.42
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.01	0.42
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.01	0.42
2:G:426:ARG:HG2	2:G:431:PRO:HA	2.02	0.42
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.84	0.42
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.01	0.42
2:G:4063:ASP:HB3	2:G:4170:ILE:HG13	2.02	0.42
2:G:5026:ASP:OD1	2:G:5027:CYS:N	2.52	0.42
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.55	0.42
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.01	0.42
2:I:3915:ILE:O	2:I:3919:THR:N	2.51	0.42
2:I:4051:SER:HG	2:I:4054:ASN:HB2	1.83	0.42
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.84	0.42
2:B:426:ARG:HG2	2:B:431:PRO:HA	2.02	0.42
2:B:533:ASN:HB3	2:B:536:ASN:HB2	2.01	0.42
2:B:1092:PHE:O	2:B:1149:VAL:N	2.48	0.42
2:B:2185:ILE:HA	2:B:2188:ASN:ND2	2.34	0.42
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	2.01	0.42
2:E:684:VAL:HA	2:E:781:VAL:HA	2.01	0.42
2:E:3842:LEU:O	2:E:3929:SER:OG	2.37	0.42
1:F:91:ILE:HD12	1:F:97:LEU:HD11	2.02	0.42
2:G:488:LEU:HA	2:G:491:ILE:HB	2.02	0.42
2:G:2185:ILE:HA	2:G:2188:ASN:ND2	2.34	0.42
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	2.01	0.42
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.02	0.42
2:I:533:ASN:HB3	2:I:536:ASN:HB2	2.01	0.42
2:I:1105:ALA:O	2:I:1189:LEU:N	2.52	0.42
2:I:1970:GLN:HB2	2:I:3642:TYR:HA	2.01	0.42
2:B:317:ARG:N	2:B:347:PHE:O	2.52	0.42
2:B:1149:VAL:HG22	2:B:1164:LEU:HD13	2.01	0.42
2:E:379:HIS:CD2	2:E:381:GLU:H	2.37	0.42
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3649:ALA:O	2:E:3653:PHE:N	2.46	0.42
2:E:3676:ASP:OD1	2:E:3676:ASP:N	2.51	0.42
2:E:4051:SER:HG	2:E:4054:ASN:HB2	1.83	0.42
2:G:315:CYS:SG	2:G:316:PHE:N	2.93	0.42
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	2.01	0.42
2:I:278:GLN:N	2:I:315:CYS:SG	2.90	0.42
2:I:932:LEU:HD23	2:I:935:LEU:HD12	2.02	0.42
2:I:1245:PHE:HE1	2:I:1600:LEU:HD23	1.83	0.42
2:I:1951:LEU:HD13	2:I:2126:ARG:HH21	1.85	0.42
2:B:932:LEU:HD23	2:B:935:LEU:HD12	2.02	0.42
2:B:1245:PHE:HE1	2:B:1600:LEU:HD23	1.83	0.42
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	2.01	0.42
2:E:709:ASP:HA	2:E:725:HIS:H	1.83	0.42
2:E:1777:PHE:HA	2:E:1799:SER:HB2	2.01	0.42
2:E:1970:GLN:HB2	2:E:3642:TYR:HA	2.01	0.42
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.02	0.42
2:G:401:ALA:HA	2:G:404:ILE:HD12	2.01	0.42
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.84	0.42
2:G:4942:GLU:O	2:G:4946:GLN:N	2.44	0.42
2:I:151:HIS:HB2	2:I:170:ILE:HB	2.01	0.42
2:I:634:GLN:HB3	1:J:34:LYS:NZ	2.35	0.42
2:I:809:ALA:O	2:I:811:CYS:N	2.50	0.42
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	2.01	0.42
2:I:4182:GLU:HA	2:I:4192:ARG:HA	2.02	0.42
2:I:4568:PHE:HA	2:I:4571:PHE:HD2	1.85	0.42
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.02	0.42
2:B:313:SER:HB2	2:B:350:HIS:CE1	2.55	0.42
2:B:315:CYS:SG	2:B:316:PHE:N	2.93	0.42
2:B:401:ALA:HA	2:B:404:ILE:HD12	2.01	0.42
2:E:176:SER:HB2	2:E:178:ARG:HH21	1.84	0.42
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.55	0.42
2:E:2185:ILE:HA	2:E:2188:ASN:ND2	2.34	0.42
2:G:151:HIS:HB2	2:G:170:ILE:HB	2.01	0.42
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.55	0.42
2:G:2829:GLY:HA3	2:G:2933:ASN:H	1.85	0.42
2:G:2880:GLU:O	2:G:2884:ASN:N	2.45	0.42
2:I:17:ASP:HB2	2:I:98:HIS:CE1	2.53	0.42
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.01	0.42
2:I:3927:GLN:O	2:I:3931:SER:N	2.45	0.42
2:B:204:PRO:HG2	2:B:268:SER:HB3	2.02	0.41
2:B:947:GLU:HG3	2:B:1049:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.02	0.41
2:E:317:ARG:N	2:E:347:PHE:O	2.52	0.41
2:E:1268:PRO:HB2	2:E:1591:CYS:HB2	2.01	0.41
2:E:1693:GLN:HA	2:E:1696:HIS:HB3	2.02	0.41
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	2.00	0.41
2:E:4945:ASP:HA	2:E:4948:GLU:HB2	2.02	0.41
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.02	0.41
2:G:3932:ASP:HA	2:G:3935:TRP:HD1	1.85	0.41
2:I:252:VAL:HA	2:I:255:HIS:CG	2.54	0.41
2:I:313:SER:HB2	2:I:350:HIS:CE1	2.55	0.41
2:I:947:GLU:HG3	2:I:1049:TYR:HD1	1.85	0.41
2:E:1866:ILE:HG13	2:E:1926:LEU:HB3	2.01	0.41
2:E:2869:ARG:HH12	2:E:2945:UNK:C	2.33	0.41
2:E:4942:GLU:O	2:E:4946:GLN:N	2.43	0.41
2:G:1046:LEU:HB3	2:G:1051:TYR:HB2	2.01	0.41
2:G:1693:GLN:HA	2:G:1696:HIS:HB3	2.02	0.41
2:G:4791:TYR:OH	2:G:4815:ASP:HB2	2.19	0.41
2:G:4945:ASP:HA	2:G:4948:GLU:HB2	2.02	0.41
2:I:204:PRO:HG2	2:I:268:SER:HB3	2.02	0.41
2:I:350:HIS:CG	2:I:353:SER:HG	2.38	0.41
2:I:1866:ILE:HG13	2:I:1926:LEU:HB3	2.01	0.41
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.03	0.41
2:B:288:GLY:HA3	2:B:405:HIS:CE1	2.55	0.41
2:B:4182:GLU:HA	2:B:4192:ARG:HA	2.02	0.41
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.84	0.41
2:E:1046:LEU:HB3	2:E:1051:TYR:HB2	2.01	0.41
2:E:1105:ALA:O	2:E:1189:LEU:N	2.52	0.41
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	2.02	0.41
2:E:4568:PHE:HA	2:E:4571:PHE:HD2	1.85	0.41
2:E:4989:MET:O	2:E:4993:MET:N	2.42	0.41
2:G:317:ARG:N	2:G:347:PHE:O	2.52	0.41
2:G:1703:LEU:HD21	2:G:1830:VAL:HG13	2.01	0.41
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.02	0.41
2:G:2336:ARG:NH2	2:G:2428:ALA:O	2.49	0.41
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.54	0.41
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.56	0.41
1:A:55:VAL:HG23	1:A:60:GLU:HB2	2.03	0.41
2:B:668:VAL:HG22	2:B:789:VAL:HG23	2.03	0.41
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.01	0.41
2:B:3662:ILE:H	2:B:3662:ILE:HG13	1.71	0.41
2:E:204:PRO:HG2	2:E:268:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2829:GLY:HA3	2:E:2933:ASN:H	1.85	0.41
2:E:3663:LEU:H	2:E:3663:LEU:HG	1.64	0.41
2:E:5013:MET:HA	2:E:5016:GLU:HB3	2.02	0.41
2:G:1951:LEU:HD13	2:G:2126:ARG:HH21	1.85	0.41
2:I:1149:VAL:HG22	2:I:1164:LEU:HD13	2.01	0.41
2:I:1679:ASN:O	2:I:1683:HIS:ND1	2.38	0.41
2:I:2874:MET:HA	2:I:2877:GLN:HB3	2.03	0.41
2:B:1951:LEU:HD13	2:B:2126:ARG:HH21	1.85	0.41
2:B:4568:PHE:HA	2:B:4571:PHE:HD2	1.85	0.41
2:B:4928:LEU:HA	2:B:4931:ILE:HD12	2.01	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.01	0.41
2:E:1703:LEU:HD21	2:E:1830:VAL:HG13	2.01	0.41
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.01	0.41
2:E:4791:TYR:OH	2:E:4815:ASP:HB2	2.19	0.41
2:G:17:ASP:HB2	2:G:98:HIS:CE1	2.53	0.41
2:G:204:PRO:HG2	2:G:268:SER:HB3	2.02	0.41
2:G:290:TYR:O	2:G:302:VAL:N	2.53	0.41
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.01	0.41
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.27	0.41
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.02	0.41
2:G:4182:GLU:HA	2:G:4192:ARG:HA	2.02	0.41
2:I:315:CYS:SG	2:I:316:PHE:N	2.93	0.41
2:I:488:LEU:HA	2:I:491:ILE:HB	2.02	0.41
2:I:668:VAL:HG22	2:I:789:VAL:HG23	2.03	0.41
2:I:1703:LEU:HD21	2:I:1830:VAL:HG13	2.01	0.41
2:I:4928:LEU:HA	2:I:4931:ILE:HD12	2.01	0.41
1:J:91:ILE:HD12	1:J:97:LEU:HD11	2.02	0.41
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.03	0.41
2:B:792:LEU:HD22	2:B:799:GLU:H	1.85	0.41
2:B:809:ALA:O	2:B:811:CYS:N	2.50	0.41
2:B:829:TYR:HB3	2:B:1073:ARG:HH11	1.84	0.41
2:B:1777:PHE:HA	2:B:1799:SER:HB2	2.01	0.41
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.02	0.41
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.01	0.41
2:E:385:ASP:N	2:E:385:ASP:OD1	2.54	0.41
2:E:3927:GLN:NE2	2:E:3988:ALA:O	2.47	0.41
2:E:4182:GLU:HA	2:E:4192:ARG:HA	2.02	0.41
2:G:530:ILE:HA	2:G:536:ASN:HB3	2.02	0.41
2:G:1970:GLN:HB2	2:G:3642:TYR:HA	2.01	0.41
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.03	0.41
1:J:55:VAL:HG23	1:J:60:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PRO:HD3	2:B:627:PRO:HB2	2.02	0.41
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.41
2:B:2874:MET:HA	2:B:2877:GLN:HB3	2.03	0.41
2:E:947:GLU:HG3	2:E:1049:TYR:HD1	1.85	0.41
2:E:3932:ASP:HA	2:E:3935:TRP:HD1	1.85	0.41
1:F:55:VAL:HG23	1:F:60:GLU:HB2	2.03	0.41
2:G:313:SER:HB2	2:G:350:HIS:CE1	2.55	0.41
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	2.02	0.41
2:I:3663:LEU:H	2:I:3663:LEU:HG	1.64	0.41
2:I:4745:LEU:O	2:I:4749:GLU:N	2.50	0.41
2:I:5026:ASP:OD1	2:I:5027:CYS:N	2.52	0.41
2:B:218:HIS:HB3	2:B:392:ARG:HD3	2.03	0.41
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.03	0.41
2:B:2032:GLN:O	2:B:2036:GLN:N	2.49	0.41
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.54	0.41
2:B:5013:MET:HA	2:B:5016:GLU:HB3	2.02	0.41
2:E:313:SER:HB2	2:E:350:HIS:CE1	2.55	0.41
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.45	0.41
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.56	0.41
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	2.02	0.41
2:E:3758:MET:O	2:E:3762:ARG:NE	2.46	0.41
2:E:4710:SER:OG	2:E:4772:ASP:OD2	2.31	0.41
2:G:4843:LEU:HA	2:G:4846:VAL:HG12	2.03	0.41
1:H:91:ILE:HD12	1:H:97:LEU:HD11	2.02	0.41
2:I:218:HIS:HB3	2:I:392:ARG:HD3	2.03	0.41
2:I:988:LEU:O	2:I:992:GLY:N	2.47	0.41
2:B:290:TYR:O	2:B:302:VAL:N	2.53	0.41
2:B:530:ILE:HA	2:B:536:ASN:HB3	2.02	0.41
2:B:688:LEU:HB3	2:B:777:PHE:CE1	2.56	0.41
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.03	0.41
2:B:1694:LEU:HD23	2:B:1715:LEU:HD13	2.03	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.56	0.41
2:B:1721:GLU:O	2:B:1725:ARG:NH2	2.54	0.41
2:B:2437:ALA:HA	2:B:2438:PRO:HD3	1.94	0.41
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.02	0.41
2:B:3932:ASP:HA	2:B:3935:TRP:HD1	1.85	0.41
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.86	0.41
2:E:290:TYR:O	2:E:302:VAL:N	2.53	0.41
2:E:379:HIS:NE2	2:E:381:GLU:OE1	2.54	0.41
2:E:392:ARG:HH12	2:E:398:SER:HB2	1.86	0.41
2:E:488:LEU:HA	2:E:491:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:533:ASN:HB3	2:E:536:ASN:HB2	2.01	0.41
2:E:1679:ASN:O	2:E:1683:HIS:ND1	2.38	0.41
2:E:1965:TYR:OH	2:E:2027:ILE:O	2.26	0.41
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.03	0.41
2:E:2255:SER:HA	2:E:2258:LEU:HB3	2.03	0.41
2:E:2874:MET:HA	2:E:2877:GLN:HB3	2.03	0.41
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.54	0.41
2:E:4833:ASN:HD22	2:E:4936:ILE:HD13	1.86	0.41
2:G:218:HIS:HB3	2:G:392:ARG:HD3	2.03	0.41
2:G:379:HIS:NE2	2:G:381:GLU:OE1	2.54	0.41
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.45	0.41
2:G:668:VAL:HG22	2:G:789:VAL:HG23	2.03	0.41
2:G:876:GLU:O	2:G:880:GLU:N	2.48	0.41
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.56	0.41
2:G:1721:GLU:O	2:G:1725:ARG:NH2	2.54	0.41
2:G:3920:VAL:O	2:G:3924:LEU:N	2.44	0.41
2:G:3994:HIS:O	2:G:3998:HIS:ND1	2.39	0.41
2:G:5013:MET:HA	2:G:5016:GLU:HB3	2.02	0.41
1:H:55:VAL:HG23	1:H:60:GLU:HB2	2.03	0.41
2:I:379:HIS:NE2	2:I:381:GLU:OE1	2.54	0.41
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.03	0.41
2:I:1739:THR:H	2:I:1742:THR:HB	1.86	0.41
2:I:3901:ASN:OD1	2:I:3904:ARG:NH1	2.43	0.41
2:I:3932:ASP:HA	2:I:3935:TRP:HD1	1.85	0.41
2:I:4558:ASN:OD1	2:I:4558:ASN:N	2.52	0.41
2:B:758:ARG:NH2	2:B:803:LEU:O	2.54	0.41
2:B:2318:TYR:HA	2:B:2319:PRO:HD3	1.89	0.41
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.54	0.41
2:E:792:LEU:HD22	2:E:799:GLU:H	1.85	0.41
2:E:3901:ASN:OD1	2:E:3904:ARG:NH1	2.43	0.41
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.54	0.41
2:G:792:LEU:HD22	2:G:799:GLU:H	1.85	0.41
2:G:3953:LYS:O	2:G:3956:SER:OG	2.32	0.41
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.54	0.41
2:G:4833:ASN:HD21	2:G:4939:ALA:HB2	1.86	0.41
2:G:4934:GLY:O	2:G:4938:ASP:N	2.48	0.41
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.41
2:I:758:ARG:NH2	2:I:803:LEU:O	2.54	0.41
2:I:2336:ARG:NH2	2:I:2428:ALA:O	2.49	0.41
2:I:2829:GLY:HA3	2:I:2933:ASN:H	1.85	0.41
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4971:THR:HG21	2:I:5029:ARG:HH12	1.86	0.41
2:I:5013:MET:HA	2:I:5016:GLU:HB3	2.02	0.41
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.03	0.40
2:B:4989:MET:O	2:B:4993:MET:N	2.42	0.40
2:E:241:GLN:O	2:E:289:ARG:NH1	2.49	0.40
2:E:758:ARG:NH2	2:E:803:LEU:O	2.54	0.40
2:E:1721:GLU:O	2:E:1725:ARG:NH2	2.54	0.40
2:E:1950:GLU:OE2	2:E:1954:ARG:NH2	2.54	0.40
2:E:1951:LEU:HD13	2:E:2126:ARG:HH21	1.85	0.40
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.86	0.40
2:G:1497:UNK:HA	2:G:1535:UNK:HA	2.03	0.40
2:I:290:TYR:O	2:I:302:VAL:N	2.53	0.40
2:I:545:ASP:HA	2:I:582:HIS:CE1	2.56	0.40
2:I:688:LEU:HB3	2:I:777:PHE:CE1	2.56	0.40
2:I:2039:LEU:HA	2:I:2042:CYS:HB3	2.03	0.40
2:I:4097:MET:HB3	2:I:4108:ILE:HG12	2.03	0.40
2:B:392:ARG:HH12	2:B:398:SER:HB2	1.86	0.40
2:E:218:HIS:HB3	2:E:392:ARG:HD3	2.03	0.40
2:E:688:LEU:HB3	2:E:777:PHE:CE1	2.56	0.40
2:E:2758:PHE:O	2:E:2762:THR:N	2.47	0.40
2:E:4833:ASN:HD21	2:E:4939:ALA:HB2	1.87	0.40
2:G:545:ASP:HA	2:G:582:HIS:CE1	2.56	0.40
2:G:758:ARG:NH2	2:G:803:LEU:O	2.54	0.40
2:G:1071:ARG:HD3	2:G:1241:SER:HB3	2.03	0.40
2:I:317:ARG:N	2:I:347:PHE:O	2.52	0.40
2:I:385:ASP:OD1	2:I:385:ASP:N	2.54	0.40
2:I:1694:LEU:HD23	2:I:1715:LEU:HD13	2.03	0.40
2:I:1950:GLU:OE2	2:I:1954:ARG:NH2	2.54	0.40
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.55	0.40
2:B:78:LEU:O	2:B:82:LEU:N	2.49	0.40
2:B:1663:HIS:O	2:B:1667:LEU:N	2.50	0.40
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.86	0.40
2:B:2587:UNK:O	2:B:2591:UNK:N	2.55	0.40
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.03	0.40
2:E:2336:ARG:NH2	2:E:2428:ALA:O	2.49	0.40
2:E:4971:THR:HG21	2:E:5029:ARG:HH12	1.86	0.40
2:G:688:LEU:HB3	2:G:777:PHE:CE1	2.56	0.40
2:G:947:GLU:HG3	2:G:1049:TYR:HD1	1.85	0.40
2:G:3765:TYR:O	2:G:3769:ARG:N	2.48	0.40
2:G:4826:ILE:O	2:G:4829:SER:OG	2.33	0.40
2:G:4833:ASN:HD22	2:G:4936:ILE:HD13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.02	0.40
2:I:2144:ILE:H	2:I:2144:ILE:HG13	1.76	0.40
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.54	0.40
2:I:4833:ASN:HD21	2:I:4939:ALA:HB2	1.86	0.40
2:B:379:HIS:NE2	2:B:381:GLU:OE1	2.54	0.40
2:B:1693:GLN:HA	2:B:1696:HIS:HB3	2.02	0.40
2:B:3229:UNK:HA	2:B:3302:UNK:HA	2.03	0.40
2:B:4192:ARG:HH12	2:B:4982:GLU:HG2	1.87	0.40
2:E:530:ILE:HA	2:E:536:ASN:HB3	2.02	0.40
2:E:668:VAL:HG22	2:E:789:VAL:HG23	2.03	0.40
2:E:2039:LEU:HA	2:E:2042:CYS:HB3	2.04	0.40
2:E:2212:VAL:O	2:E:2216:GLY:N	2.53	0.40
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.03	0.40
2:G:2255:SER:HA	2:G:2258:LEU:HB3	2.03	0.40
2:G:2874:MET:HA	2:G:2877:GLN:HB3	2.03	0.40
2:G:3361:UNK:O	2:G:3365:UNK:N	2.55	0.40
2:G:3915:ILE:O	2:G:3919:THR:N	2.51	0.40
2:G:4192:ARG:HH12	2:G:4982:GLU:HG2	1.87	0.40
2:I:530:ILE:HA	2:I:536:ASN:HB3	2.02	0.40
2:I:792:LEU:HD22	2:I:799:GLU:H	1.85	0.40
2:I:1693:GLN:HA	2:I:1696:HIS:HB3	2.02	0.40
2:I:4833:ASN:HD22	2:I:4936:ILE:HD13	1.86	0.40
2:B:1829:PRO:HB2	2:B:1837:GLN:HB2	2.04	0.40
2:B:1970:GLN:HB2	2:B:3642:TYR:HA	2.01	0.40
2:B:3649:ALA:O	2:B:3653:PHE:N	2.46	0.40
2:E:176:SER:HB2	2:E:178:ARG:HD3	2.04	0.40
2:E:635:THR:O	1:F:34:LYS:NZ	2.51	0.40
2:E:870:ILE:HD12	2:E:870:ILE:HA	1.89	0.40
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.04	0.40
2:E:4978:HIS:ND1	2:E:4982:GLU:OE1	2.43	0.40
2:G:4971:THR:HG21	2:G:5029:ARG:HH12	1.86	0.40
2:I:392:ARG:HH12	2:I:398:SER:HB2	1.86	0.40
2:I:4782:VAL:O	2:I:4785:THR:OG1	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4687 (69%)	2862 (88%)	367 (11%)	6 (0%)	47	81
2	E	3235/4687 (69%)	2861 (88%)	367 (11%)	7 (0%)	47	81
2	G	3235/4687 (69%)	2863 (88%)	365 (11%)	7 (0%)	47	81
2	I	3235/4687 (69%)	2863 (88%)	365 (11%)	7 (0%)	47	81
All	All	13360/19180 (70%)	11833 (89%)	1500 (11%)	27 (0%)	50	81

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1829	PRO
2	B	1932	PRO
2	E	1829	PRO
2	G	1829	PRO
2	I	1829	PRO
2	B	1708	ARG
2	B	4667	PRO
2	E	1708	ARG
2	E	1932	PRO
2	E	4667	PRO
2	G	1708	ARG
2	G	1932	PRO
2	G	4667	PRO
2	I	1708	ARG
2	I	1932	PRO
2	I	4667	PRO
2	B	2343	GLY

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Mol	Chain	Res	Type
2	E	2343	GLY
2	I	2343	GLY
2	G	2343	GLY
2	B	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	I	1840	PRO
2	I	4641	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (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	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
2	E	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
2	G	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
2	I	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
All	All	10324/13192 (78%)	10252 (99%)	72 (1%)	84	90

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	688	LEU
2	B	978	THR

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Continued from previous page...

Mol	Chain	Res	Type
2	B	1076	ARG
2	B	1141	ARG
2	B	1964	ARG
2	B	3663	LEU
2	B	3762	ARG
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4957	LYS
2	B	4984	ASN
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	688	LEU
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1964	ARG
2	E	3663	LEU
2	E	3762	ARG
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4957	LYS
2	E	4984	ASN
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	688	LEU
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1964	ARG
2	G	3663	LEU
2	G	3762	ARG
2	G	3787	LYS

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Mol	Chain	Res	Type
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4957	LYS
2	G	4984	ASN
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	688	LEU
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG
2	I	1964	ARG
2	I	3663	LEU
2	I	3762	ARG
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4957	LYS
2	I	4984	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	23	GLN
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	203	ASN
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	405	HIS
2	B	639	ASN
2	B	838	HIS

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Mol	Chain	Res	Type
2	B	1035	ASN
2	B	1158	ASN
2	B	1231	GLN
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2127	GLN
2	B	2858	GLN
2	B	3809	ASN
2	B	3882	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4142	ASN
2	B	4691	GLN
2	B	4833	ASN
2	B	4886	HIS
2	B	4984	ASN
2	B	4987	ASN
2	E	23	GLN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	203	ASN
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	405	HIS
2	E	639	ASN
2	E	838	HIS
2	E	1035	ASN
2	E	1158	ASN
2	E	1231	GLN
2	E	1598	GLN

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Mol	Chain	Res	Type
2	E	1679	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1973	GLN
2	E	2005	GLN
2	E	2127	GLN
2	E	2858	GLN
2	E	3809	ASN
2	E	3882	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3960	GLN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4142	ASN
2	E	4691	GLN
2	E	4833	ASN
2	E	4886	HIS
2	E	4984	ASN
2	E	4987	ASN
2	G	23	GLN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	203	ASN
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	405	HIS
2	G	639	ASN
2	G	838	HIS
2	G	1035	ASN
2	G	1158	ASN
2	G	1231	GLN
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN

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Mol	Chain	Res	Type
2	G	1719	HIS
2	G	1775	HIS
2	G	1973	GLN
2	G	2005	GLN
2	G	2127	GLN
2	G	2858	GLN
2	G	3809	ASN
2	G	3882	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4142	ASN
2	G	4691	GLN
2	G	4833	ASN
2	G	4886	HIS
2	G	4984	ASN
2	G	4987	ASN
2	I	23	GLN
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	203	ASN
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	405	HIS
2	I	639	ASN
2	I	765	GLN
2	I	838	HIS
2	I	1035	ASN
2	I	1158	ASN
2	I	1231	GLN
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1719	HIS

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Mol	Chain	Res	Type
2	I	1775	HIS
2	I	2127	GLN
2	I	2858	GLN
2	I	3809	ASN
2	I	3882	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4130	ASN
2	I	4142	ASN
2	I	4691	GLN
2	I	4833	ASN
2	I	4886	HIS
2	I	4984	ASN
2	I	4987	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3613:UNK	C	3639:THR	N	43.91
1	B	3613:UNK	C	3639:THR	N	43.68
1	G	3613:UNK	C	3639:THR	N	43.62
1	E	3613:UNK	C	3639:THR	N	43.61
1	I	3163:UNK	C	3170:UNK	N	16.30
1	B	3163:UNK	C	3170:UNK	N	16.29
1	E	3163:UNK	C	3170:UNK	N	16.26
1	G	3163:UNK	C	3170:UNK	N	16.24
1	G	3468:UNK	C	3511:UNK	N	15.09
1	I	3468:UNK	C	3511:UNK	N	15.04
1	E	3468:UNK	C	3511:UNK	N	15.02
1	B	3468:UNK	C	3511:UNK	N	15.00
1	I	2703:UNK	C	2734:ASN	N	14.81
1	E	2703:UNK	C	2734:ASN	N	14.71
1	B	2703:UNK	C	2734:ASN	N	14.67
1	G	2703:UNK	C	2734:ASN	N	14.61
1	I	3063:UNK	C	3134:UNK	N	14.51
1	G	3063:UNK	C	3134:UNK	N	14.50
1	E	3063:UNK	C	3134:UNK	N	14.48
1	B	3063:UNK	C	3134:UNK	N	14.47
1	I	3236:UNK	C	3241:UNK	N	13.17
1	G	3236:UNK	C	3241:UNK	N	13.16
1	E	3236:UNK	C	3241:UNK	N	13.07

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3236:UNK	C	3241:UNK	N	13.05
1	B	1564:UNK	C	1573:MET	N	12.84
1	E	1564:UNK	C	1573:MET	N	12.81
1	I	1564:UNK	C	1573:MET	N	12.73
1	G	1564:UNK	C	1573:MET	N	12.72
1	B	2976:UNK	C	2995:UNK	N	12.10
1	E	2976:UNK	C	2995:UNK	N	12.09
1	G	2976:UNK	C	2995:UNK	N	12.09
1	I	2976:UNK	C	2995:UNK	N	12.07
1	G	3254:UNK	C	3261:UNK	N	8.66
1	E	3254:UNK	C	3261:UNK	N	8.62
1	I	3254:UNK	C	3261:UNK	N	8.62
1	B	3254:UNK	C	3261:UNK	N	8.56
1	B	1297:UNK	C	1430:UNK	N	5.73
1	G	1297:UNK	C	1430:UNK	N	5.70
1	E	1297:UNK	C	1430:UNK	N	5.67
1	I	1297:UNK	C	1430:UNK	N	5.44
1	B	2939:ARG	C	2942:UNK	N	3.59
1	I	2939:ARG	C	2942:UNK	N	3.56
1	G	2479:LEU	C	2487:UNK	N	3.55
1	I	2479:LEU	C	2487:UNK	N	3.55
1	E	2479:LEU	C	2487:UNK	N	3.47
1	G	2939:ARG	C	2942:UNK	N	3.46
1	B	2479:LEU	C	2487:UNK	N	3.45
1	E	2939:ARG	C	2942:UNK	N	3.34

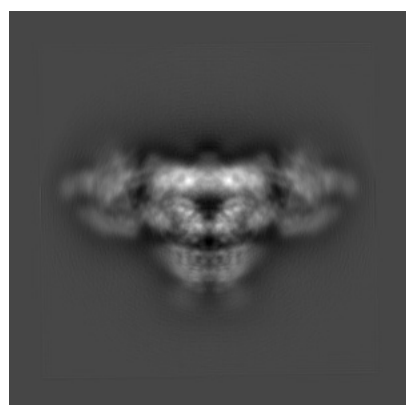
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22392. These allow visual inspection of the internal detail of the map and identification of artifacts.

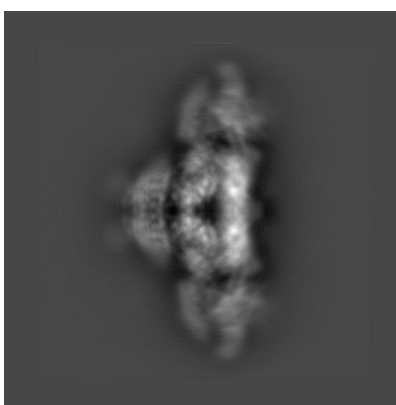
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

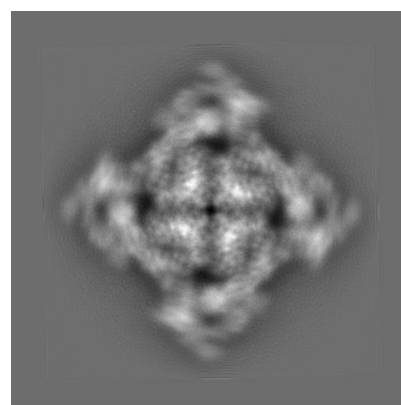
6.1.1 Primary map



X



Y

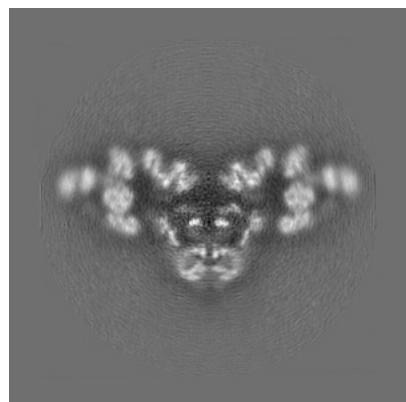


Z

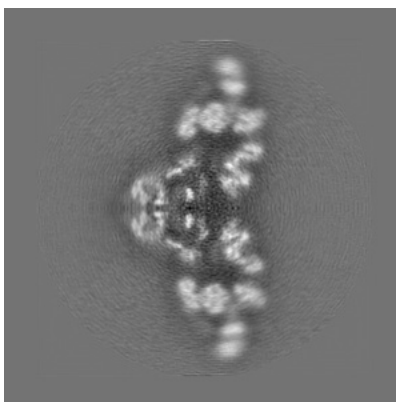
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

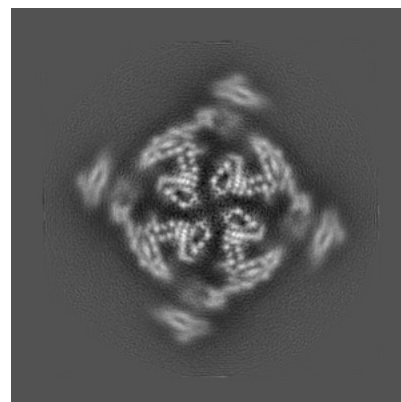
6.2.1 Primary map



X Index: 200



Y Index: 200

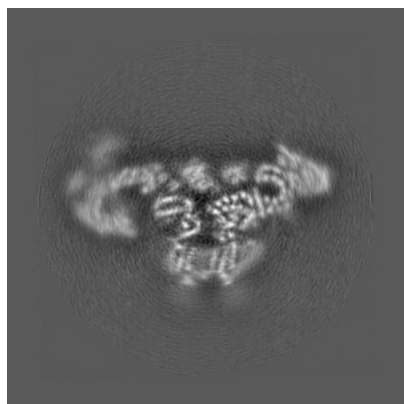


Z Index: 200

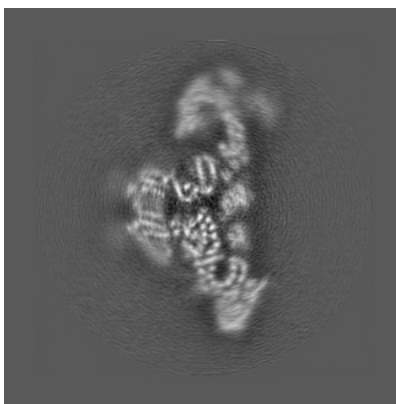
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

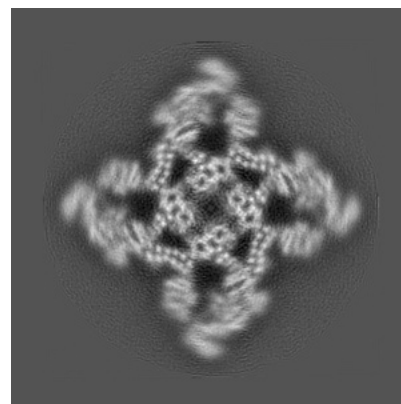
6.3.1 Primary map



X Index: 177



Y Index: 177



Z Index: 226

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

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

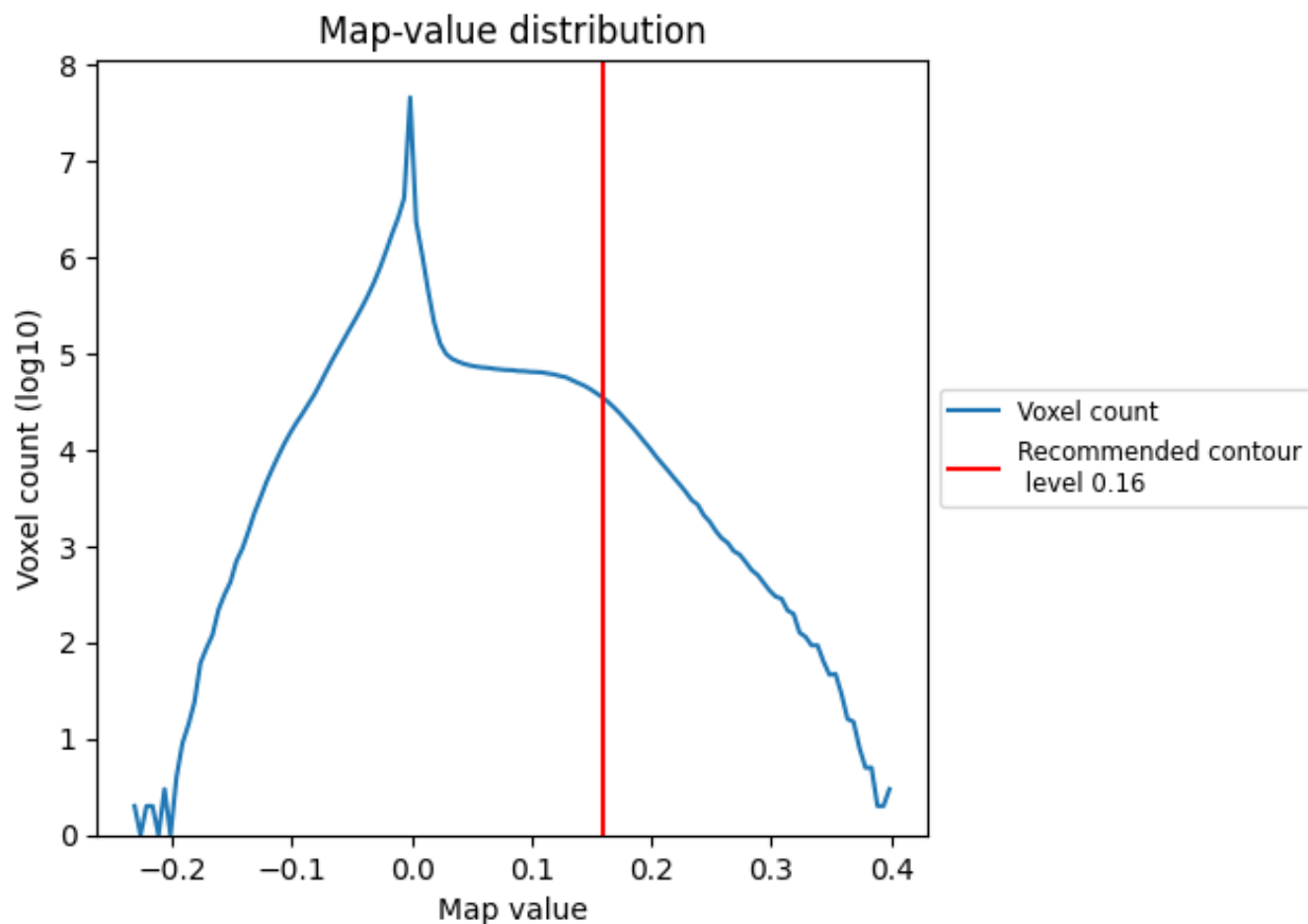
6.5 Mask visualisation

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

7 Map analysis [i](#)

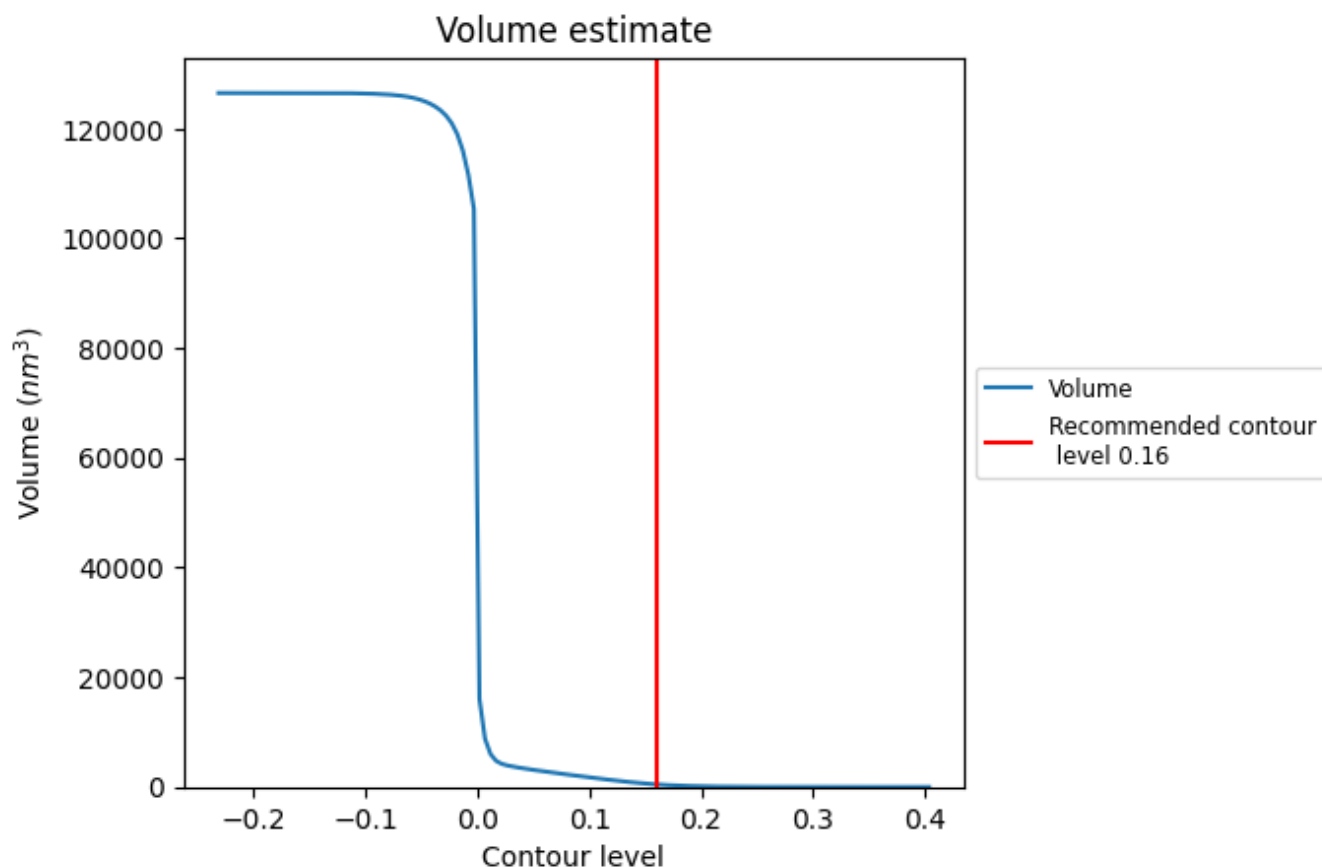
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

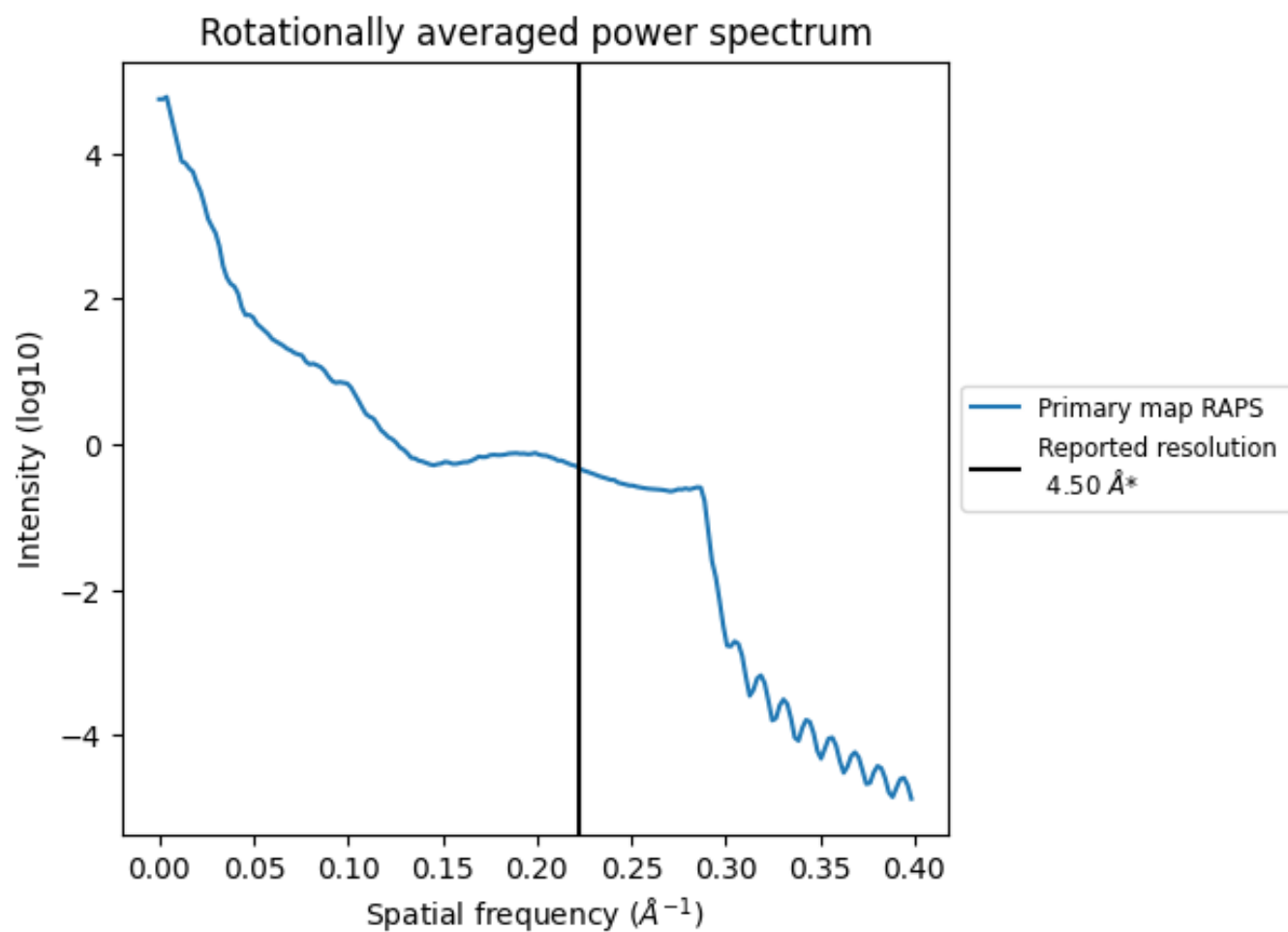
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 469 nm^3 ; this corresponds to an approximate mass of 423 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

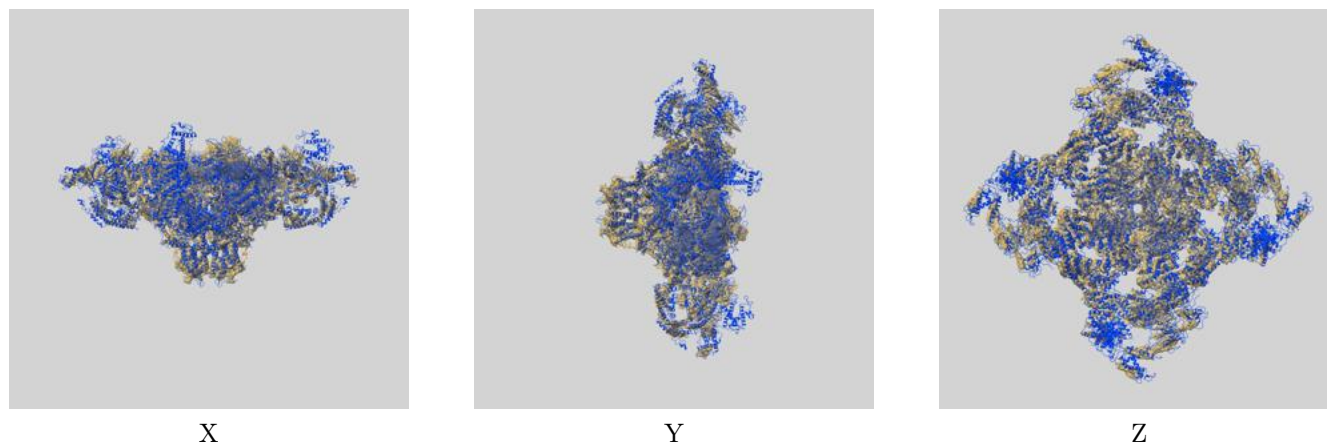
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

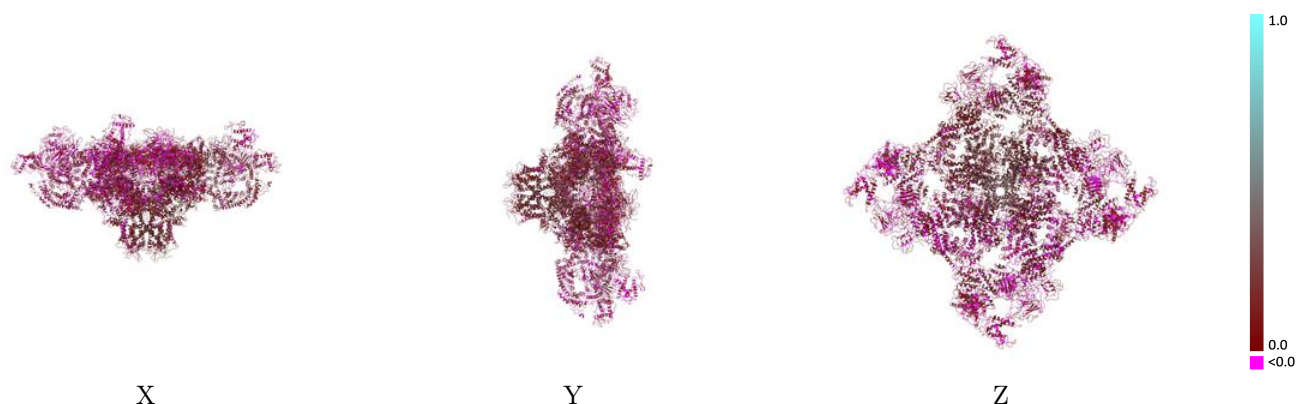
This section contains information regarding the fit between EMDB map EMD-22392 and PDB model 7JMF. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



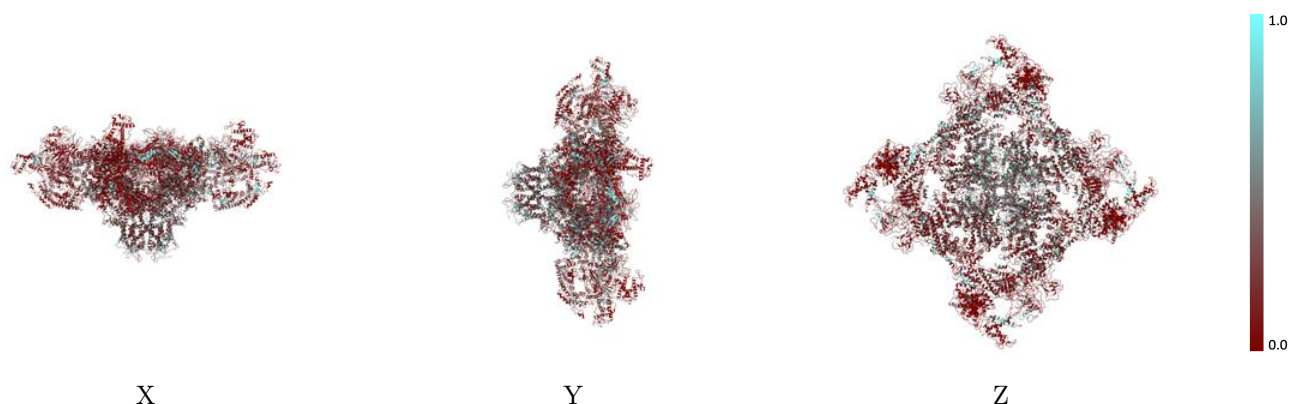
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



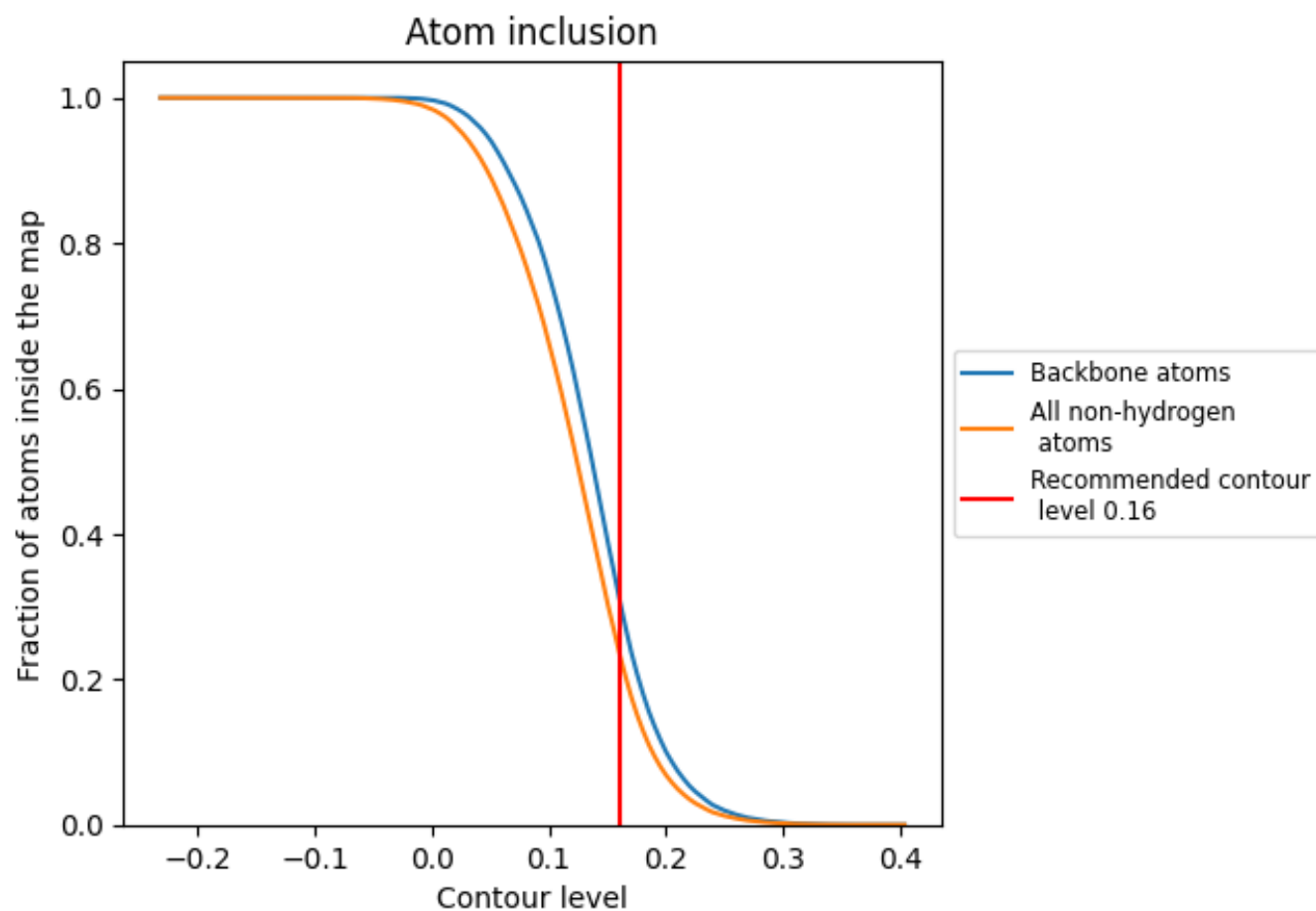
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 31% of all backbone atoms, 24% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2382	<div></div> 0.1100
A	<div></div> 0.1452	<div></div> 0.1330
B	<div></div> 0.2722	<div></div> 0.1490
E	<div></div> 0.2580	<div></div> 0.1200
F	<div></div> 0.1427	<div></div> 0.0750
G	<div></div> 0.2199	<div></div> 0.0820
H	<div></div> 0.1092	<div></div> 0.0850
I	<div></div> 0.2146	<div></div> 0.0890
J	<div></div> 0.1253	<div></div> 0.0820

