



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:21 PM UTC

PDB ID : 7PTY / pdb_00007pty
EMDB ID : EMD-13643
Title : Delta-latroinsectotoxin dimer
Authors : Chen, M.; Gatsogiannis, C.
Deposited on : 2021-09-27
Resolution : 4.63 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

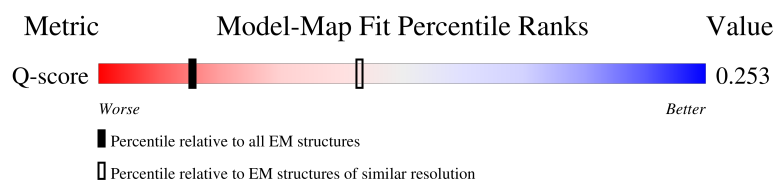
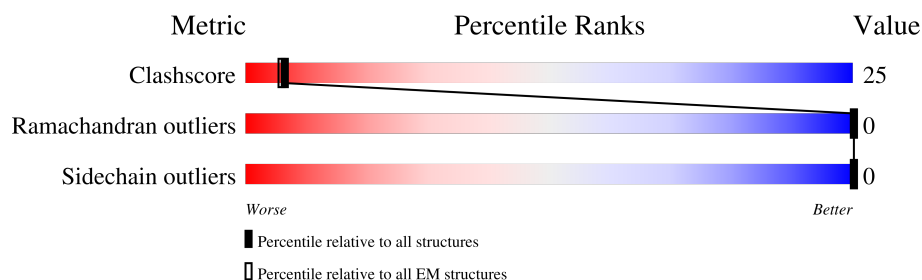
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.63 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2068 (4.13 - 5.13)

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	1296	
1	B	1296	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13433 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 Delta-latroinsectotoxin-Lt1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	850	Total	C	N	O	S	0	0
			6663	4229	1125	1293	16		
1	B	865	Total	C	N	O	S	0	0
			6770	4293	1142	1318	17		

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-62	MET	-	initiating methionine	UNP Q25338
A	-61	LYS	-	expression tag	UNP Q25338
A	-60	PHE	-	expression tag	UNP Q25338
A	-59	LEU	-	expression tag	UNP Q25338
A	-58	VAL	-	expression tag	UNP Q25338
A	-57	ASN	-	expression tag	UNP Q25338
A	-56	VAL	-	expression tag	UNP Q25338
A	-55	ALA	-	expression tag	UNP Q25338
A	-54	LEU	-	expression tag	UNP Q25338
A	-53	VAL	-	expression tag	UNP Q25338
A	-52	PHE	-	expression tag	UNP Q25338
A	-51	MET	-	expression tag	UNP Q25338
A	-50	VAL	-	expression tag	UNP Q25338
A	-49	VAL	-	expression tag	UNP Q25338
A	-48	TYR	-	expression tag	UNP Q25338
A	-47	ILE	-	expression tag	UNP Q25338
A	-46	SER	-	expression tag	UNP Q25338
A	-45	TYR	-	expression tag	UNP Q25338
A	-44	ILE	-	expression tag	UNP Q25338
A	-43	TYR	-	expression tag	UNP Q25338
A	-42	ALA	-	expression tag	UNP Q25338
A	-41	MET	-	expression tag	UNP Q25338
A	-40	TRP	-	expression tag	UNP Q25338
A	-39	SER	-	expression tag	UNP Q25338
A	-38	HIS	-	expression tag	UNP Q25338
A	-37	PRO	-	expression tag	UNP Q25338

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-36	GLN	-	expression tag	UNP Q25338
A	-35	PHE	-	expression tag	UNP Q25338
A	-34	GLU	-	expression tag	UNP Q25338
A	-33	LYS	-	expression tag	UNP Q25338
A	-32	GLY	-	expression tag	UNP Q25338
A	-31	SER	-	expression tag	UNP Q25338
A	-30	ALA	-	expression tag	UNP Q25338
A	-29	GLY	-	expression tag	UNP Q25338
A	-28	SER	-	expression tag	UNP Q25338
A	-27	ALA	-	expression tag	UNP Q25338
A	-26	ALA	-	expression tag	UNP Q25338
A	-25	GLY	-	expression tag	UNP Q25338
A	-24	SER	-	expression tag	UNP Q25338
A	-23	GLY	-	expression tag	UNP Q25338
A	-22	ALA	-	expression tag	UNP Q25338
A	-21	GLY	-	expression tag	UNP Q25338
A	-20	TRP	-	expression tag	UNP Q25338
A	-19	SER	-	expression tag	UNP Q25338
A	-18	HIS	-	expression tag	UNP Q25338
A	-17	PRO	-	expression tag	UNP Q25338
A	-16	GLN	-	expression tag	UNP Q25338
A	-15	PHE	-	expression tag	UNP Q25338
A	-14	GLU	-	expression tag	UNP Q25338
A	-13	LYS	-	expression tag	UNP Q25338
A	-12	GLY	-	expression tag	UNP Q25338
A	-11	ALA	-	expression tag	UNP Q25338
A	-10	GLY	-	expression tag	UNP Q25338
A	-9	LEU	-	expression tag	UNP Q25338
A	-8	GLU	-	expression tag	UNP Q25338
A	-7	VAL	-	expression tag	UNP Q25338
A	-6	LEU	-	expression tag	UNP Q25338
A	-5	PHE	-	expression tag	UNP Q25338
A	-4	GLN	-	expression tag	UNP Q25338
A	-3	GLY	-	expression tag	UNP Q25338
A	-2	PRO	-	expression tag	UNP Q25338
A	-1	PRO	-	expression tag	UNP Q25338
A	0	TRP	-	expression tag	UNP Q25338
A	1215	LEU	-	expression tag	UNP Q25338
A	1216	GLU	-	expression tag	UNP Q25338
A	1217	SER	-	expression tag	UNP Q25338
A	1218	SER	-	expression tag	UNP Q25338
A	1219	GLY	-	expression tag	UNP Q25338

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1220	LEU	-	expression tag	UNP Q25338
A	1221	VAL	-	expression tag	UNP Q25338
A	1222	PRO	-	expression tag	UNP Q25338
A	1223	ARG	-	expression tag	UNP Q25338
A	1224	GLY	-	expression tag	UNP Q25338
A	1225	SER	-	expression tag	UNP Q25338
A	1226	HIS	-	expression tag	UNP Q25338
A	1227	HIS	-	expression tag	UNP Q25338
A	1228	HIS	-	expression tag	UNP Q25338
A	1229	HIS	-	expression tag	UNP Q25338
A	1230	HIS	-	expression tag	UNP Q25338
A	1231	HIS	-	expression tag	UNP Q25338
A	1232	HIS	-	expression tag	UNP Q25338
A	1233	HIS	-	expression tag	UNP Q25338
B	-62	MET	-	initiating methionine	UNP Q25338
B	-61	LYS	-	expression tag	UNP Q25338
B	-60	PHE	-	expression tag	UNP Q25338
B	-59	LEU	-	expression tag	UNP Q25338
B	-58	VAL	-	expression tag	UNP Q25338
B	-57	ASN	-	expression tag	UNP Q25338
B	-56	VAL	-	expression tag	UNP Q25338
B	-55	ALA	-	expression tag	UNP Q25338
B	-54	LEU	-	expression tag	UNP Q25338
B	-53	VAL	-	expression tag	UNP Q25338
B	-52	PHE	-	expression tag	UNP Q25338
B	-51	MET	-	expression tag	UNP Q25338
B	-50	VAL	-	expression tag	UNP Q25338
B	-49	VAL	-	expression tag	UNP Q25338
B	-48	TYR	-	expression tag	UNP Q25338
B	-47	ILE	-	expression tag	UNP Q25338
B	-46	SER	-	expression tag	UNP Q25338
B	-45	TYR	-	expression tag	UNP Q25338
B	-44	ILE	-	expression tag	UNP Q25338
B	-43	TYR	-	expression tag	UNP Q25338
B	-42	ALA	-	expression tag	UNP Q25338
B	-41	MET	-	expression tag	UNP Q25338
B	-40	TRP	-	expression tag	UNP Q25338
B	-39	SER	-	expression tag	UNP Q25338
B	-38	HIS	-	expression tag	UNP Q25338
B	-37	PRO	-	expression tag	UNP Q25338
B	-36	GLN	-	expression tag	UNP Q25338
B	-35	PHE	-	expression tag	UNP Q25338

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-34	GLU	-	expression tag	UNP Q25338
B	-33	LYS	-	expression tag	UNP Q25338
B	-32	GLY	-	expression tag	UNP Q25338
B	-31	SER	-	expression tag	UNP Q25338
B	-30	ALA	-	expression tag	UNP Q25338
B	-29	GLY	-	expression tag	UNP Q25338
B	-28	SER	-	expression tag	UNP Q25338
B	-27	ALA	-	expression tag	UNP Q25338
B	-26	ALA	-	expression tag	UNP Q25338
B	-25	GLY	-	expression tag	UNP Q25338
B	-24	SER	-	expression tag	UNP Q25338
B	-23	GLY	-	expression tag	UNP Q25338
B	-22	ALA	-	expression tag	UNP Q25338
B	-21	GLY	-	expression tag	UNP Q25338
B	-20	TRP	-	expression tag	UNP Q25338
B	-19	SER	-	expression tag	UNP Q25338
B	-18	HIS	-	expression tag	UNP Q25338
B	-17	PRO	-	expression tag	UNP Q25338
B	-16	GLN	-	expression tag	UNP Q25338
B	-15	PHE	-	expression tag	UNP Q25338
B	-14	GLU	-	expression tag	UNP Q25338
B	-13	LYS	-	expression tag	UNP Q25338
B	-12	GLY	-	expression tag	UNP Q25338
B	-11	ALA	-	expression tag	UNP Q25338
B	-10	GLY	-	expression tag	UNP Q25338
B	-9	LEU	-	expression tag	UNP Q25338
B	-8	GLU	-	expression tag	UNP Q25338
B	-7	VAL	-	expression tag	UNP Q25338
B	-6	LEU	-	expression tag	UNP Q25338
B	-5	PHE	-	expression tag	UNP Q25338
B	-4	GLN	-	expression tag	UNP Q25338
B	-3	GLY	-	expression tag	UNP Q25338
B	-2	PRO	-	expression tag	UNP Q25338
B	-1	PRO	-	expression tag	UNP Q25338
B	0	TRP	-	expression tag	UNP Q25338
B	1215	LEU	-	expression tag	UNP Q25338
B	1216	GLU	-	expression tag	UNP Q25338
B	1217	SER	-	expression tag	UNP Q25338
B	1218	SER	-	expression tag	UNP Q25338
B	1219	GLY	-	expression tag	UNP Q25338
B	1220	LEU	-	expression tag	UNP Q25338
B	1221	VAL	-	expression tag	UNP Q25338

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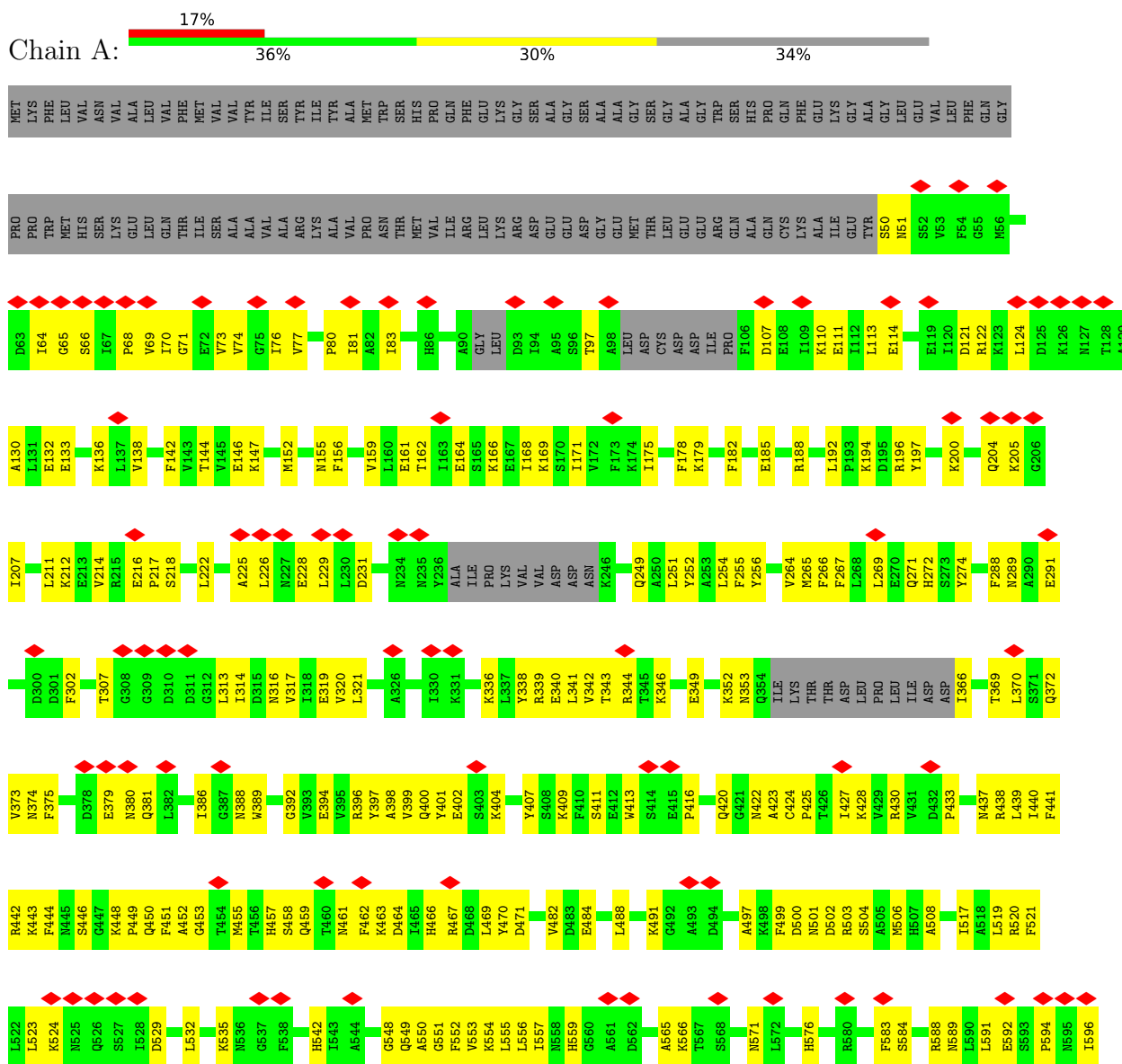
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1222	PRO	-	expression tag	UNP Q25338
B	1223	ARG	-	expression tag	UNP Q25338
B	1224	GLY	-	expression tag	UNP Q25338
B	1225	SER	-	expression tag	UNP Q25338
B	1226	HIS	-	expression tag	UNP Q25338
B	1227	HIS	-	expression tag	UNP Q25338
B	1228	HIS	-	expression tag	UNP Q25338
B	1229	HIS	-	expression tag	UNP Q25338
B	1230	HIS	-	expression tag	UNP Q25338
B	1231	HIS	-	expression tag	UNP Q25338
B	1232	HIS	-	expression tag	UNP Q25338
B	1233	HIS	-	expression tag	UNP Q25338

3 Residue-property plots

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: Delta-latroinsectotoxin-Lt1a



PRO	LYS	VAL	ASP	N245	K246	A247	F248	Q249	A250	L251	A253	L254	F255	Y256	G257	T258	Q259	T260	Y261	M265	F266	F267	L268	L269	E270	L275	Y279	K282	G283	D284	D285	V286	N287	F288	N289	A290	E291	V295	D301	S304	S305	L306	T307	G308	G309	L313	I314	D315																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
N316	E319	N322	T323	V324	K325	A326	L327	P328	F329	I330	K331	N332	A333	K336	L337	Y338	R339	T343	F344	L348	L351	Q354	I355	L356	T357	T358	T359	T360	T361	T362	T363	T364	T365	T366	T367	T368	T369	T370	T371	T372	T373	T374	T375	T376	T377	T378	T379	T380	T381	T382	T383	T384	T385	T386	T387	T388	T389	T390	T391	T392	T393	T394	T395	T396	T397	T398	T399	T400	T401	T402	T403	T404	T405	T406	T407	T408	T409	T410	T411	T412	T413	T414	T415	T416	T417	T418	T419	T420	T421	T422	T423	T424	T425	T426	T427	T428	T429	T430	T431	T432	T433	T434	T435	T436	T437	T438	T439	T440	T441	T442	T443	T444	T445	T446	T447	T448	T449	T450	T451	T452	T453	T454	T455	T456	T457	T458	T459	T460	T461	T462	T463	T464	T465	T466	T467	T468	T469	T470	T471	T472	T473	T474	T475	T476	T477	T478	T479	T480	T481	T482	T483	T484	T485	T486	T487	T488	T489	T490	T491	T492	T493	T494	T495	T496	T497	T498	T499	T500	T501	T502	T503	T504	T505	T506	T507	T508	T509	T510	T511	T512	T513	T514	T515	T516	T517	T518	T519	T520	T521	T522	T523	T524	T525	T526	T527	T528	T529	T530	T531	T532	T533	T534	T535	T536	T537	T538	T539	T540	T541	T542	T543	T544	T545	T546	T547	T548	T549	T550	T551	T552	T553	T554	T555	T556	T557	T558	T559	T560	T561	T562	T563	T564	T565	T566	T567	T568	T569	T570	T571	T572	T573	T574	T575	T576	T577	T578	T579	T580	T581	T582	T583	T584	T585	T586	T587	T588	T589	T590	T591	T592	T593	T594	T595	T596	T597	T598	T599	T600	T601	T602	T603	T604	T605	T606	T607	T608	T609	T610	T611	T612	T613	T614	T615	T616	T617	T618	T619	T620	T621	T622	T623	T624	T625	T626	T627	T628	T629	T630	T631	T632	T633	T634	T635	T636	T637	T638	T639	T640	T641	T642	T643	T644	T645	T646	T647	T648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	T712	T713	T714	T715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826	T827	T828	T829	T830	T831	T832	T833	T834	T835	T836	T837	T838	T839	T840	T841	T842	T843	T844	T845	T846	T847	T848	T849	T850	T851	T852	T853	T854	T855	T856	T857	T858	T859	T860	T861	T862	T863	T864	T865	T866	T867	T868	T869	T870	T871	T872	T873	T874	T875	T876	T877	T878	T879	T880	T881	T882	T883	T884	T885	T886	T887	T888	T889	T890	T891	T892	T893	T894	T895	T896	T897	T898	T899	T900	T901	T902	T903	T904	T905	T906	T907	T908	T909	T910	T911	T912	T913	T914	T915	T916	T917	T918	T919	T920	T921	T922	T923	T924	T925	T926	T927	T928	T929	T930	T931	T932	T933	T934	T935	T936	T937	T938	T939	T940	T941	T942	T943	T944	T945	T946	T947	T948	T949	T950	T951	T952	T953	T954	T955	T956	T957	T958	T959	T960	T961	T962	T963	T964	T965	T966	T967	T968	T969	T970	T971	T972	T973	T974	T975	T976	T977	T978	T979	T980	T981	T982	T983	T984	T985	T986	T987	T988	T989	T990	T991	T992	T993	T994	T995	T996	T997	T998	T999	T1000	T1001	T1002	T1003	T1004	T1005	T1006	T1007	T1008	T1009	T1010	T1011	T1012	T1013	T1014	T1015	T1016	T1017	T1018	T1019	T1020	T1021	T1022	T1023	T1024	T1025	T1026	T1027	T1028	T1029	T1030	T1031	T1032	T1033	T1034	T1035	T1036	T1037	T1038	T1039	T1040	T1041	T1042	T1043	T1044	T1045	T1046	T1047	T1048	T1049	T1050	T1051	T1052	T1053	T1054	T1055	T1056	T1057	T1058	T1059	T1060	T1061	T1062	T1063	T1064	T1065	T1066	T1067	T1068	T1069	T1070	T1071	T1072	T1073	T1074	T1075	T1076	T1077	T1078	T1079	T1080	T1081	T1082	T1083	T1084	T1085	T1086	T1087	T1088	T1089	T1090	T1091	T1092	T1093	T1094	T1095	T1096	T1097	T1098	T1099	T1100	T1101	T1102	T1103	T1104	T1105	T1106	T1107	T1108	T1109	T1110	T1111	T1112	T1113	T1114	T1115	T1116	T1117	T1118	T1119	T1120	T1121	T1122	T1123	T1124	T1125	T1126	T1127	T1128	T1129	T1130	T1131	T1132	T1133	T1134	T1135	T1136	T1137	T1138	T1139	T1140	T1141	T1142	T1143	T1144	T1145	T1146	T1147	T1148	T1149	T1150	T1151	T1152	T1153	T1154	T1155	T1156	T1157	T1158	T1159	T1160	T1161	T1162	T1163	T1164	T1165	T1166	T1167	T1168	T1169	T1170	T1171	T1172	T1173	T1174	T1175	T1176	T1177	T1178	T1179	T1180	T1181	T1182	T1183	T1184	T1185	T1186	T1187	T1188	T1189	T1190	T1191	T1192	T1193	T1194	T1195	T1196	T1197	T1198	T1199	T1200	T1201	T1202	T1203	T1204	T1205	T1206	T1207	T1208	T1209	T1210	T1211	T1212	T1213	T1214	T1215	T1216	T1217	T1218	T1219	T1220	T1221	T1222	T1223	T1224	T1225	T1226	T1227	T1228	T1229	T1230	T1231	T1232	T1233	T1234	T1235	T1236	T1237	T1238	T1239	T1240	T1241	T1242	T1243	T1244	T1245	T1246	T1247	T1248	T1249	T1250	T1251	T1252	T1253	T1254	T1255	T1256	T1257	T1258	T1259	T1260	T1261	T1262	T1263	T1264	T1265	T1266	T1267	T1268	T1269	T1270	T1271	T1272	T1273	T1274	T1275	T1276	T1277	T1278	T1279	T1280	T1281	T1282	T1283	T1284	T1285	T1286	T1287	T1288	T1289	T1290	T1291	T1292	T1293	T1294	T1295	T1296	T1297	T1298	T1299	T1300	T1301	T1302	T1303	T1304	T1305	T1306	T1307	T1308	T1309	T1310	T1311	T1312	T1313	T1314	T1315	T1316	T1317	T1318	T1319	T1320	T1321	T1322	T1323	T1324	T1325	T1326	T1327	T1328	T1329	T1330	T1331	T1332	T1333	T1334	T1335	T1336	T1337	T1338	T1339	T1340	T1341	T1342	T1343	T1344	T1345	T1346	T1347	T1348	T1349	T1350	T1351	T1352	T1353	T1354	T1355	T1356	T1357	T1358	T1359	T1360	T1361	T1362	T1363	T1364	T1365	T1366	T1367	T1368	T1369	T1370	T1371	T1372	T1373	T1374	T1375	T1376	T1377	T1378	T1379	T1380	T1381	T1382	T1383	T1384	T1385	T1386	T1387	T1388	T1389	T1390	T1391	T1392	T1393	T1394	T1395	T1396	T1397	T1398	T1399	T1400	T1401	T1402	T1403	T1404	T1405	T1406	T1407	T1408	T1409	T1410	T1411	T1412	T1413	T1414	T1415	T1416	T1417	T1418	T1419	T1420	T1421	T1422	T1423	T1424	T1425	T1426	T1427	T1428	T1429	T1430	T1431	T1432	T1433	T1434	T1435	T1436	T1437	T1438	T1439	T1440	T1441	T1442	T1443	T1444	T1445	T1446	T1447	T1448	T1449	T1450	T1451	T1452	T1453	T1454	T1455	T1456	T1457	T1458	T1459	T1460	T1461	T1462	T1463	T1464	T1465	T1466	T1467	T1468	T1469	T1470	T1471	T1472	T1473	T1474	T1475	T1476	T1477	T1478	T1479	T1480	T1481	T1482	T1483	T1484	T1485	T1486	T1487	T1488	T1489	T1490	T1491	T1492	T1493	T1494	T1495	T1496	T1497	T1498	T1499	T1500	T1501	T1502	T1503	T1504	T1505	T1506	T1507	T1508	T1509	T1510	T1511	T1512	T1513	T1514	T1515	T1516	T1517	T1518	T1519	T1520	T1521	T1522	T1523	T1524	T1525	T1526	T1527	T1528	T1529	T1530	T1531	T1532	T1533	T1534	T1535	T1536	T1537	T1538	T1539	T1540	T1541	T1542	T1543	T1544	T1545	T1546	T1547	T1548	T1549	T1550	T1551	T1552	T1553	T1554	T1555	T1556	T1557	T1558	T1559	T1560	T1561	T1562	T1563	T1564	T1565	T1566	T1567	T1568	T1569	T1570	T1571	T1572	T1573	T1574	T1575	T1576	T1577	T1578	T1579	T1580	T1581	T1582	T1583	T1584	T1585	T1586	T1587	T1588	T1589	T1590	T1591	T1592	T1593	T1594	T1595	T1596	T1597	T1598	T1599	T1600	T1601	T1602	T1603	T1604	T1605	T1606	T1607	T1608	T1609	T1610	T1611	T1612	T1613	T1614	T1615	T1616	T1617	T1618	T1619	T1620	T1621	T1622	T1623	T1624	T1625	T1626	T1627	T1628	T1629	T1630	T1631	T1632	T1633	T1634	T1635	T1636	T1637	T1638	T1639	T1640	T1641	T1642	T1643	T1644	T1645	T1646	T1647	T1648	T1649	T1650	T1651	T1652	T1653	T1654	T1655	T1656	T1657	T1658	T1659	T1660	T1661	T1662	T1663	T1664	T1665	T1666	T1667	T1668	T1669	T1670	T1671	T1672	T1673	T1674	T1675	T1676	T1677	T1678	T1679	T1680	T1681	T1682	T1683	T1684	T1685	T1686	T1687	T1688	T1689	T1690	T1691	T1692	T1693	T1694	T1695	T1696	T1697	T1698	T1699	T1700	T1701	T1702	T1703	T1704	T1705	T1706	T1707	T1708	T1709	T1710	T1711	T1712	T1713	T1714	T1715	T1716	T1717	T1718	T1719	T1720	T1721	T1722

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81192	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	78.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.010	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.003	Depositor
Map size ($\text{\AA}$)	324.0, 324.0, 324.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.9, 0.9, 0.9	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.17	0/6769	0.40	0/9147
1	B	0.16	0/6878	0.39	0/9300
All	All	0.17	0/13647	0.40	0/18447

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6663	0	6706	337	0
1	B	6770	0	6807	347	0
All	All	13433	0	13513	681	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 25.

All (681) 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)
1:A:288:PHE:CE1	1:A:409:LYS:HD2	1.37	1.58
1:A:288:PHE:CE1	1:A:409:LYS:CD	2.25	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:PHE:CD1	1:A:409:LYS:HD2	1.89	1.07
1:A:407:TYR:CE2	1:A:409:LYS:HE3	1.91	1.04
1:A:130:ALA:HB3	1:A:409:LYS:HZ1	1.27	0.98
1:A:130:ALA:HB3	1:A:409:LYS:NZ	1.86	0.91
1:A:640:THR:HG21	1:A:664:LEU:HB3	1.57	0.86
1:B:452:ALA:HA	1:B:467:ARG:HD2	1.56	0.85
1:A:430:ARG:HD3	1:A:458:SER:HB2	1.58	0.85
1:A:288:PHE:HE1	1:A:409:LYS:HD2	1.36	0.83
1:A:400:GLN:HG2	1:A:409:LYS:HA	1.62	0.82
1:A:407:TYR:HE2	1:A:409:LYS:HE3	1.41	0.82
1:A:444:PHE:H	1:A:448:LYS:HG3	1.46	0.80
1:A:549:GLN:HB3	1:A:552:PHE:HD2	1.46	0.79
1:A:80:PRO:HA	1:A:83:ILE:HG12	1.64	0.79
1:A:372:GLN:HB2	1:B:512:ARG:HA	1.65	0.79
1:B:245:ASN:HB3	1:B:248:PHE:HB2	1.63	0.78
1:B:94:ILE:HG12	1:B:783:MET:HE3	1.65	0.78
1:A:255:PHE:HB2	1:A:338:TYR:HE1	1.50	0.77
1:A:288:PHE:CD1	1:A:409:LYS:CD	2.62	0.76
1:A:748:ALA:HB1	1:A:757:ILE:HG12	1.67	0.76
1:B:587:VAL:HG11	1:B:619:VAL:HG23	1.66	0.76
1:B:441:PHE:HA	1:B:452:ALA:HB3	1.67	0.76
1:A:860:LEU:HA	1:A:864:ALA:HA	1.67	0.76
1:A:226:LEU:HD13	1:A:254:LEU:HD22	1.68	0.76
1:A:820:LYS:HD2	1:A:854:LYS:HB3	1.68	0.76
1:A:130:ALA:CB	1:A:409:LYS:HZ1	2.00	0.75
1:A:288:PHE:CZ	1:A:409:LYS:CE	2.70	0.75
1:B:474:LEU:HA	1:B:512:ARG:HG3	1.67	0.75
1:A:164:GLU:H	1:A:169:LYS:HD2	1.51	0.74
1:A:467:ARG:HA	1:A:470:TYR:CE1	2.21	0.74
1:A:715:ILE:HG21	1:A:747:LEU:HB3	1.70	0.74
1:B:511:TYR:O	1:B:549:GLN:NE2	2.20	0.74
1:B:741:ASN:HB3	1:B:772:GLY:H	1.54	0.72
1:A:891:LEU:HA	1:A:895:LYS:HB3	1.72	0.72
1:B:634:GLN:HG3	1:B:638:GLY:HA2	1.70	0.72
1:A:321:LEU:HD22	1:A:342:VAL:HG11	1.72	0.71
1:B:462:PHE:O	1:B:466:HIS:ND1	2.21	0.71
1:A:521:PHE:O	1:A:524:LYS:NZ	2.23	0.71
1:B:401:TYR:HB3	1:B:408:SER:HB3	1.72	0.70
1:A:640:THR:HG22	1:A:642:PHE:H	1.54	0.70
1:A:711:LEU:HD13	1:A:726:LEU:HD11	1.73	0.70
1:A:381:GLN:O	1:A:491:LYS:NZ	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ASP:OD1	1:A:503:ARG:N	2.25	0.70
1:A:152:MET:HE2	1:A:256:TYR:HD1	1.56	0.69
1:A:920:LEU:HB3	1:A:923:TYR:HB2	1.75	0.69
1:B:812:HIS:HB3	1:B:846:LEU:HD12	1.74	0.69
1:A:121:ASP:O	1:A:194:LYS:NZ	2.24	0.69
1:B:900:LYS:HD2	1:B:928:ASN:HB2	1.74	0.69
1:A:375:PHE:HB2	1:A:424:CYS:HB3	1.76	0.68
1:B:279:TYR:HA	1:B:283:GLY:HA3	1.74	0.68
1:B:598:VAL:HG11	1:B:629:ILE:HA	1.75	0.68
1:A:667:GLN:HE22	1:A:703:THR:HA	1.58	0.68
1:A:469:LEU:HD13	1:A:488:LEU:HD11	1.73	0.68
1:A:556:LEU:O	1:A:559:HIS:ND1	2.27	0.68
1:A:185:GLU:OE1	1:A:188:ARG:NH2	2.27	0.68
1:A:188:ARG:O	1:A:200:LYS:NZ	2.27	0.67
1:B:679:ALA:HB1	1:B:714:ALA:HB2	1.75	0.67
1:B:365:ASP:HA	1:B:438:ARG:HH12	1.59	0.67
1:A:638:GLY:HA3	1:A:668:ASP:HB2	1.77	0.66
1:A:693:ILE:HG22	1:A:695:ASP:H	1.59	0.66
1:A:803:ARG:NH1	1:A:804:SER:O	2.28	0.66
1:B:448:LYS:HG3	1:B:450:GLN:H	1.61	0.66
1:A:542:HIS:NE2	1:A:565:ALA:O	2.27	0.66
1:A:808:LEU:HA	1:A:812:HIS:HD1	1.60	0.66
1:B:322:ASN:OD1	1:B:325:LYS:NZ	2.28	0.66
1:A:695:ASP:OD1	1:A:696:LYS:NZ	2.28	0.66
1:B:910:SER:O	1:B:914:ILE:HD12	1.96	0.65
1:A:83:ILE:HG21	1:A:677:PHE:HE1	1.62	0.65
1:B:726:LEU:HA	1:B:729:GLN:HG2	1.78	0.65
1:B:601:LYS:NZ	1:B:634:GLN:O	2.30	0.65
1:B:370:LEU:HD22	1:B:442:ARG:HH12	1.61	0.65
1:A:849:SER:O	1:A:851:ARG:NH2	2.29	0.65
1:B:156:PHE:HA	1:B:159:VAL:HB	1.77	0.65
1:B:784:ARG:HG3	1:B:786:GLU:H	1.61	0.65
1:A:430:ARG:HE	1:B:583:PHE:HE1	1.45	0.65
1:A:601:LYS:NZ	1:A:605:GLY:O	2.29	0.65
1:A:159:VAL:HG13	1:A:249:GLN:HB3	1.78	0.64
1:A:482:VAL:HA	1:A:517:ILE:HD11	1.79	0.64
1:B:670:ASN:HB2	1:B:672:MET:HE1	1.77	0.64
1:A:803:ARG:NH1	1:A:807:ASN:OD1	2.29	0.64
1:B:787:PRO:HB2	1:B:825:TYR:HE2	1.63	0.64
1:A:640:THR:HG23	1:A:641:PRO:HD2	1.80	0.64
1:B:725:GLU:O	1:B:729:GLN:NE2	2.20	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:908:ARG:O	1:B:912:MET:N	2.27	0.64
1:B:503:ARG:NE	1:B:533:LYS:O	2.31	0.64
1:B:702:VAL:HB	1:B:707:ASN:HA	1.79	0.64
1:B:289:ASN:OD1	1:B:411:SER:N	2.31	0.64
1:B:266:PHE:HA	1:B:269:LEU:HD12	1.79	0.63
1:B:551:GLY:HA2	1:B:554:LYS:HE2	1.79	0.63
1:A:122:ARG:HA	1:A:194:LYS:HG2	1.80	0.63
1:A:396:ARG:HB3	1:A:413:TRP:CD1	2.34	0.63
1:B:776:THR:OG1	1:B:779:HIS:ND1	2.29	0.63
1:B:916:GLN:HE21	1:B:919:LEU:HD21	1.62	0.63
1:B:402:GLU:HB2	1:B:407:TYR:HD1	1.63	0.63
1:A:130:ALA:CB	1:A:409:LYS:NZ	2.61	0.63
1:A:107:ASP:OD1	1:A:110:LYS:NZ	2.31	0.62
1:B:163:ILE:HD12	1:B:169:LYS:HG2	1.81	0.62
1:B:478:LYS:HA	1:B:514:ASN:HD21	1.64	0.62
1:A:727:LEU:O	1:A:763:ARG:NH2	2.31	0.62
1:B:779:HIS:NE2	1:B:808:LEU:O	2.22	0.62
1:A:205:LYS:NZ	1:A:291:GLU:OE2	2.32	0.62
1:B:622:ALA:O	1:B:626:HIS:ND1	2.32	0.62
1:A:908:ARG:O	1:A:912:MET:N	2.30	0.62
1:B:576:HIS:O	1:B:580:ARG:NH1	2.32	0.62
1:A:902:ASP:HA	1:A:907:GLY:HA3	1.80	0.62
1:A:910:SER:O	1:A:914:ILE:HG12	2.00	0.62
1:A:920:LEU:HG	1:A:922:LEU:H	1.63	0.62
1:A:729:GLN:O	1:A:763:ARG:NH2	2.32	0.61
1:A:265:MET:SD	1:A:302:PHE:HB2	2.40	0.61
1:A:869:TYR:HB2	1:A:873:LYS:HA	1.82	0.61
1:B:737:VAL:HG13	1:B:741:ASN:HA	1.82	0.61
1:B:779:HIS:HE1	1:B:803:ARG:HA	1.65	0.61
1:B:887:ASP:OD1	1:B:888:MET:N	2.33	0.61
1:B:910:SER:HA	1:B:913:LEU:HD12	1.83	0.61
1:A:640:THR:CG2	1:A:641:PRO:HD2	2.30	0.61
1:B:143:VAL:O	1:B:146:GLU:HG2	1.99	0.61
1:A:677:PHE:HB3	1:A:681:MET:HE1	1.83	0.61
1:A:396:ARG:HD3	1:A:416:PRO:HB2	1.82	0.60
1:A:155:ASN:HB2	1:A:252:TYR:OH	2.00	0.60
1:A:427:ILE:HD11	1:A:459:GLN:HB3	1.83	0.60
1:A:138:VAL:HG13	1:A:266:PHE:HD1	1.66	0.60
1:A:288:PHE:CE1	1:A:409:LYS:CE	2.82	0.60
1:A:288:PHE:CZ	1:A:409:LYS:HE2	2.36	0.60
1:B:186:ARG:HA	1:B:189:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLN:OE1	1:A:372:GLN:N	2.34	0.60
1:A:785:LYS:HG2	1:A:819:ARG:HH21	1.66	0.60
1:B:178:PHE:HE1	1:B:211:LEU:HD22	1.66	0.60
1:A:852:LYS:HE3	1:A:854:LYS:HG3	1.82	0.60
1:A:381:GLN:O	1:A:422:ASN:ND2	2.35	0.60
1:A:640:THR:HG23	1:A:664:LEU:HD23	1.84	0.60
1:A:724:LYS:HG3	1:A:728:LYS:HZ2	1.66	0.60
1:B:685:LYS:HG3	1:B:686:MET:SD	2.42	0.60
1:A:255:PHE:CZ	1:A:341:LEU:HB3	2.37	0.60
1:A:924:ASN:OD1	1:A:925:TYR:N	2.34	0.60
1:B:874:TYR:O	1:B:879:LYS:NZ	2.35	0.60
1:A:50:SER:OG	1:A:51:ASN:N	2.32	0.59
1:A:806:ASP:HB3	1:A:808:LEU:HG	1.84	0.59
1:B:285:ASP:O	1:B:409:LYS:NZ	2.35	0.59
1:A:554:LYS:NZ	1:A:589:ASN:OD1	2.27	0.59
1:B:364:ASP:O	1:B:438:ARG:NH1	2.35	0.59
1:A:519:LEU:HD11	1:A:555:LEU:HB3	1.83	0.59
1:A:455:MET:SD	1:A:457:HIS:N	2.70	0.59
1:A:721:ASP:HA	1:A:724:LYS:HE3	1.85	0.59
1:B:267:PHE:HA	1:B:270:GLU:OE2	2.03	0.59
1:B:501:ASN:HB3	1:B:535:LYS:HD3	1.84	0.59
1:A:837:THR:HG22	1:A:841:SER:H	1.68	0.59
1:B:185:GLU:OE1	1:B:188:ARG:NH2	2.36	0.59
1:B:528:ILE:HG23	1:B:532:LEU:HD22	1.83	0.59
1:B:784:ARG:NE	1:B:786:GLU:OE1	2.35	0.59
1:A:440:ILE:HG23	1:A:452:ALA:HB3	1.85	0.58
1:B:571:ASN:N	1:B:603:ASP:OD2	2.36	0.58
1:A:302:PHE:HZ	1:A:352:LYS:HB2	1.67	0.58
1:A:375:PHE:N	1:A:424:CYS:O	2.28	0.58
1:A:778:LEU:HD13	1:A:793:LEU:HD22	1.86	0.58
1:B:533:LYS:HB3	1:B:537:GLY:HA2	1.85	0.58
1:B:684:ILE:HG22	1:B:688:ARG:HH21	1.67	0.58
1:B:228:GLU:HB3	1:B:232:LYS:HE3	1.85	0.58
1:A:341:LEU:HA	1:A:344:ARG:HE	1.68	0.58
1:A:906:GLU:HG3	1:A:908:ARG:HG2	1.86	0.58
1:A:64:ILE:HG22	1:A:66:SER:H	1.68	0.58
1:A:877:ILE:HD12	1:A:880:ALA:HB3	1.85	0.58
1:A:396:ARG:HA	1:A:416:PRO:HB3	1.86	0.58
1:A:617:TYR:HB3	1:A:619:VAL:HG12	1.86	0.58
1:B:407:TYR:CZ	1:B:409:LYS:HB2	2.39	0.57
1:A:288:PHE:CZ	1:A:409:LYS:NZ	2.71	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ASN:HB3	1:A:535:LYS:HD3	1.86	0.57
1:A:130:ALA:HB2	1:A:407:TYR:HD2	1.70	0.57
1:A:741:ASN:ND2	1:A:770:LYS:O	2.38	0.57
1:B:477:ASN:HB3	1:B:480:LYS:HB2	1.85	0.57
1:A:388:ASN:ND2	1:A:471:ASP:OD2	2.37	0.57
1:B:849:SER:O	1:B:851:ARG:NH1	2.37	0.57
1:B:706:ASN:HB2	1:B:708:TRP:NE1	2.20	0.57
1:A:254:LEU:HD21	1:A:317:VAL:HG12	1.86	0.57
1:A:462:PHE:HB3	1:A:466:HIS:CE1	2.40	0.57
1:A:422:ASN:OD1	1:A:423:ALA:N	2.37	0.57
1:A:725:GLU:HA	1:A:728:LYS:HD2	1.86	0.57
1:B:149:ARG:HD2	1:B:152:MET:HE3	1.87	0.57
1:B:904:THR:H	1:B:907:GLY:HA2	1.69	0.57
1:A:451:PHE:HB3	1:A:499:PHE:CE1	2.39	0.56
1:B:539:THR:OG1	1:B:542:HIS:ND1	2.27	0.56
1:A:836:LYS:HD3	1:A:840:GLY:HA2	1.88	0.56
1:B:114:GLU:O	1:B:118:ASN:ND2	2.38	0.56
1:B:469:LEU:HG	1:B:488:LEU:HD22	1.87	0.56
1:B:148:THR:HG22	1:B:152:MET:HE2	1.86	0.56
1:B:233:ASN:HD22	1:B:323:THR:HG21	1.70	0.56
1:A:441:PHE:HB2	1:A:450:GLN:C	2.29	0.56
1:A:923:TYR:HA	1:A:926:PHE:HD2	1.70	0.56
1:B:750:SER:O	1:B:784:ARG:NH1	2.37	0.56
1:A:138:VAL:HG21	1:A:269:LEU:HD22	1.88	0.56
1:A:594:PRO:HB2	1:A:596:ILE:HG22	1.87	0.56
1:B:578:ALA:O	1:B:581:SER:OG	2.24	0.56
1:A:316:ASN:O	1:A:319:GLU:HG3	2.05	0.56
1:B:839:ASP:O	1:B:871:ASN:ND2	2.38	0.56
1:B:875:LEU:HD12	1:B:877:ILE:HD11	1.88	0.56
1:A:255:PHE:HB2	1:A:338:TYR:CE1	2.36	0.55
1:A:754:ILE:HA	1:A:757:ILE:HD12	1.89	0.55
1:A:827:LEU:HD23	1:A:831:ALA:HB3	1.87	0.55
1:B:427:ILE:HD11	1:B:442:ARG:HH21	1.70	0.55
1:B:533:LYS:NZ	1:B:566:LYS:O	2.31	0.55
1:A:144:THR:HA	1:A:147:LYS:HD3	1.89	0.55
1:A:554:LYS:HA	1:A:557:ILE:HG22	1.88	0.55
1:B:114:GLU:HA	1:B:117:PHE:CD2	2.42	0.55
1:B:338:TYR:O	1:B:342:VAL:HG23	2.07	0.55
1:B:156:PHE:CZ	1:B:256:TYR:HB2	2.42	0.55
1:A:444:PHE:N	1:A:448:LYS:HG3	2.21	0.54
1:B:107:ASP:OD1	1:B:108:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:CYS:N	1:A:425:PRO:HD3	2.22	0.54
1:A:700:ASN:ND2	1:A:731:ASP:O	2.31	0.54
1:B:149:ARG:HH22	1:B:179:LYS:HD3	1.72	0.54
1:A:668:ASP:OD1	1:A:671:HIS:N	2.40	0.54
1:A:759:GLU:HA	1:A:762:LYS:HE3	1.89	0.54
1:A:401:TYR:OH	1:A:404:LYS:HB2	2.07	0.54
1:A:484:GLU:HG2	1:A:488:LEU:HD23	1.90	0.54
1:B:502:ASP:HB2	1:B:535:LYS:HZ3	1.73	0.54
1:B:859:LEU:O	1:B:863:GLY:N	2.40	0.54
1:B:255:PHE:O	1:B:258:THR:OG1	2.24	0.54
1:B:786:GLU:OE1	1:B:786:GLU:N	2.41	0.54
1:A:349:GLU:OE2	1:A:353:ASN:ND2	2.41	0.54
1:B:495:ILE:HB	1:B:506:MET:HE3	1.89	0.54
1:B:668:ASP:OD1	1:B:672:MET:N	2.29	0.53
1:B:547:ALA:HB1	1:B:549:GLN:HE22	1.74	0.53
1:B:577:LEU:HD12	1:B:580:ARG:HH22	1.73	0.53
1:A:162:THR:O	1:A:169:LYS:NZ	2.27	0.53
1:A:407:TYR:CD2	1:A:409:LYS:NZ	2.77	0.53
1:B:552:PHE:HA	1:B:555:LEU:HB2	1.89	0.53
1:B:875:LEU:HG	1:B:878:HIS:CE1	2.43	0.53
1:A:651:GLN:HB2	1:A:686:MET:HE1	1.88	0.53
1:B:482:VAL:HG22	1:B:517:ILE:HG21	1.89	0.53
1:A:640:THR:CG2	1:A:664:LEU:HB3	2.32	0.53
1:A:886:LEU:HD12	1:A:890:ARG:HH11	1.74	0.53
1:B:397:TYR:OH	1:B:414:SER:OG	2.26	0.53
1:B:721:ASP:OD1	1:B:722:ALA:N	2.40	0.53
1:B:226:LEU:O	1:B:230:LEU:HG	2.09	0.53
1:B:517:ILE:HA	1:B:520:ARG:HG2	1.90	0.53
1:B:683:SER:OG	1:B:686:MET:HE2	2.09	0.53
1:B:806:ASP:O	1:B:837:THR:OG1	2.24	0.53
1:B:401:TYR:CE1	1:B:403:SER:HB3	2.44	0.52
1:B:549:GLN:HB3	1:B:552:PHE:HD2	1.74	0.52
1:B:233:ASN:OD1	1:B:245:ASN:ND2	2.43	0.52
1:B:787:PRO:HB2	1:B:825:TYR:CE2	2.45	0.52
1:B:879:LYS:O	1:B:883:ASN:ND2	2.36	0.52
1:A:396:ARG:HB3	1:A:413:TRP:HD1	1.74	0.52
1:B:399:VAL:HA	1:B:440:ILE:HA	1.92	0.52
1:A:444:PHE:H	1:A:448:LYS:CG	2.19	0.52
1:B:847:ALA:O	1:B:851:ARG:N	2.35	0.52
1:A:576:HIS:HE2	1:A:608:PRO:HG3	1.74	0.52
1:B:706:ASN:HB2	1:B:708:TRP:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:O	1:A:222:LEU:HB2	2.10	0.52
1:A:401:TYR:O	1:A:407:TYR:HD1	1.93	0.51
1:A:402:GLU:HG3	1:A:407:TYR:HB2	1.92	0.51
1:B:80:PRO:HA	1:B:83:ILE:HG12	1.92	0.51
1:B:309:GLY:O	1:B:313:LEU:HG	2.10	0.51
1:A:746:HIS:NE2	1:A:769:GLU:O	2.42	0.51
1:A:911:ILE:HA	1:A:914:ILE:HG12	1.92	0.51
1:B:159:VAL:HG13	1:B:249:GLN:HE21	1.74	0.51
1:B:448:LYS:O	1:B:450:GLN:HG3	2.10	0.51
1:B:903:GLU:HG2	1:B:904:THR:HG23	1.93	0.51
1:A:179:LYS:HE2	1:A:256:TYR:HE2	1.76	0.51
1:A:413:TRP:NE1	1:A:443:LYS:HE3	2.25	0.51
1:B:366:ILE:N	1:B:367:PRO:HD3	2.26	0.51
1:B:600:GLU:O	1:B:608:PRO:HD3	2.10	0.51
1:B:701:SER:OG	1:B:702:VAL:N	2.40	0.51
1:A:556:LEU:HD12	1:A:557:ILE:N	2.25	0.51
1:A:702:VAL:HG12	1:A:709:THR:HG22	1.92	0.51
1:A:860:LEU:HD21	1:A:892:PHE:HE1	1.76	0.51
1:A:225:ALA:O	1:A:229:LEU:HD13	2.10	0.51
1:A:321:LEU:HD11	1:A:339:ARG:HD2	1.93	0.51
1:A:566:LYS:HD3	1:A:571:ASN:HB3	1.92	0.51
1:A:708:TRP:HE3	1:A:712:HIS:HB3	1.76	0.51
1:A:854:LYS:O	1:A:857:GLU:HG3	2.10	0.51
1:A:466:HIS:CD2	1:A:497:ALA:HB3	2.46	0.51
1:B:375:PHE:H	1:B:425:PRO:HG3	1.76	0.51
1:B:819:ARG:HH21	1:B:821:SER:H	1.58	0.50
1:A:786:GLU:HG2	1:A:789:ILE:HG12	1.94	0.50
1:A:588:ARG:O	1:A:592:GLU:HG3	2.11	0.50
1:B:207:ILE:O	1:B:211:LEU:HG	2.11	0.50
1:B:291:GLU:O	1:B:295:VAL:HG13	2.11	0.50
1:B:819:ARG:HE	1:B:821:SER:H	1.58	0.50
1:A:69:VAL:HG12	1:A:71:GLY:H	1.76	0.50
1:A:302:PHE:CZ	1:A:352:LYS:HB2	2.46	0.50
1:A:366:ILE:HG12	1:A:438:ARG:HH21	1.77	0.50
1:B:424:CYS:HA	1:B:461:ASN:HB2	1.93	0.50
1:B:534:ASP:H	1:B:538:PHE:H	1.56	0.50
1:A:370:LEU:HG	1:A:373:VAL:HG23	1.93	0.50
1:A:467:ARG:HA	1:A:470:TYR:HE1	1.71	0.50
1:B:365:ASP:HB3	1:B:400:GLN:HA	1.93	0.50
1:A:81:ILE:HG13	1:A:113:LEU:HG	1.93	0.50
1:B:818:GLY:HA2	1:B:855:THR:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:HIS:CE1	1:B:608:PRO:HG3	2.47	0.50
1:B:609:LEU:HD23	1:B:641:PRO:HG2	1.94	0.50
1:A:197:TYR:OH	1:A:271:GLN:NE2	2.35	0.49
1:A:251:LEU:O	1:A:254:LEU:HB3	2.12	0.49
1:A:179:LYS:HE2	1:A:256:TYR:CE2	2.47	0.49
1:A:552:PHE:HA	1:A:555:LEU:HB2	1.94	0.49
1:A:386:ILE:HG22	1:A:389:TRP:H	1.78	0.49
1:A:604:ASP:HB2	1:A:606:PHE:CE2	2.47	0.49
1:A:892:PHE:O	1:A:898:SER:N	2.45	0.49
1:B:201:LEU:HD21	1:B:275:LEU:HD22	1.94	0.49
1:B:370:LEU:HB2	1:B:442:ARG:HH22	1.78	0.49
1:B:426:THR:HG21	1:B:430:ARG:NH2	2.27	0.49
1:B:866:LEU:HB2	1:B:868:GLU:HG2	1.93	0.49
1:A:407:TYR:CD2	1:A:409:LYS:HE3	2.44	0.49
1:B:502:ASP:OD1	1:B:503:ARG:N	2.45	0.49
1:B:913:LEU:HB2	1:B:923:TYR:OH	2.13	0.49
1:B:109:ILE:O	1:B:113:LEU:HG	2.13	0.49
1:B:261:TYR:O	1:B:265:MET:HG3	2.13	0.49
1:A:424:CYS:HA	1:A:461:ASN:ND2	2.27	0.49
1:B:588:ARG:HA	1:B:591:LEU:HD12	1.95	0.49
1:B:486:THR:O	1:B:490:GLU:HG3	2.13	0.49
1:B:779:HIS:CE1	1:B:803:ARG:HA	2.45	0.49
1:A:500:ASP:C	1:A:502:ASP:H	2.21	0.49
1:B:507:HIS:HB3	1:B:543:ILE:HG13	1.94	0.49
1:A:178:PHE:HE1	1:A:211:LEU:HD11	1.78	0.48
1:A:379:GLU:OE2	1:A:380:ASN:ND2	2.46	0.48
1:A:503:ARG:HB3	1:A:506:MET:HE2	1.94	0.48
1:A:606:PHE:CD1	1:A:635:SER:OG	2.53	0.48
1:A:166:LYS:HE3	1:A:168:ILE:H	1.77	0.48
1:A:462:PHE:HB3	1:A:466:HIS:HE1	1.76	0.48
1:A:850:GLY:O	1:A:851:ARG:HG2	2.13	0.48
1:B:370:LEU:HD23	1:B:397:TYR:HB3	1.95	0.48
1:B:794:ILE:HG13	1:B:829:LYS:HE2	1.94	0.48
1:A:399:VAL:HG23	1:A:439:LEU:C	2.38	0.48
1:A:430:ARG:HH11	1:A:458:SER:HA	1.77	0.48
1:A:637:SER:HB2	1:A:639:LEU:HD13	1.94	0.48
1:B:365:ASP:HA	1:B:438:ARG:HH22	1.79	0.48
1:B:154:GLU:O	1:B:158:LEU:HG	2.14	0.48
1:B:229:LEU:HA	1:B:232:LYS:HB2	1.95	0.48
1:B:676:HIS:HA	1:B:710:PRO:HB3	1.95	0.48
1:B:218:SER:O	1:B:222:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:LEU:O	1:B:613:VAL:HG23	2.12	0.48
1:A:430:ARG:O	1:A:433:PRO:HD3	2.13	0.48
1:A:890:ARG:O	1:A:895:LYS:N	2.40	0.48
1:B:885:ASP:HB3	1:B:888:MET:HB2	1.95	0.48
1:A:428:LYS:HA	1:A:430:ARG:NH2	2.28	0.48
1:B:490:GLU:OE1	1:B:491:LYS:NZ	2.46	0.48
1:B:503:ARG:HB2	1:B:507:HIS:CE1	2.48	0.48
1:B:620:VAL:O	1:B:624:LEU:HG	2.13	0.48
1:B:869:TYR:HB2	1:B:873:LYS:HA	1.95	0.48
1:B:878:HIS:HA	1:B:881:ILE:HD12	1.95	0.48
1:A:517:ILE:HA	1:A:520:ARG:HB3	1.95	0.48
1:A:819:ARG:O	1:A:822:THR:OG1	2.31	0.48
1:B:667:GLN:HB3	1:B:671:HIS:HA	1.96	0.48
1:A:374:ASN:HB2	1:B:476:ILE:HD12	1.96	0.48
1:A:519:LEU:O	1:A:523:LEU:HB2	2.13	0.48
1:B:177:ASP:O	1:B:180:LYS:HG2	2.13	0.48
1:A:877:ILE:HA	1:A:880:ALA:HB3	1.96	0.47
1:A:443:LYS:HG2	1:A:448:LYS:HG2	1.97	0.47
1:A:548:GLY:HA3	1:A:583:PHE:CG	2.49	0.47
1:A:920:LEU:HG	1:A:922:LEU:N	2.29	0.47
1:B:443:LYS:HA	1:B:448:LYS:HD3	1.95	0.47
1:A:142:PHE:HE1	1:A:267:PHE:HB2	1.78	0.47
1:B:791:VAL:O	1:B:794:ILE:HB	2.15	0.47
1:A:97:THR:O	1:A:784:ARG:NH1	2.46	0.47
1:A:640:THR:HG22	1:A:641:PRO:N	2.30	0.47
1:A:689:TYR:CZ	1:A:693:ILE:HD11	2.50	0.47
1:A:698:SER:HB2	1:A:701:SER:HB2	1.96	0.47
1:B:376:PRO:O	1:B:422:ASN:ND2	2.45	0.47
1:B:397:TYR:OH	1:B:412:GLU:OE2	2.26	0.47
1:B:136:LYS:O	1:B:140:LYS:HG2	2.15	0.47
1:B:198:VAL:O	1:B:202:LEU:HG	2.15	0.47
1:B:706:ASN:HB2	1:B:708:TRP:CD1	2.50	0.47
1:A:550:ALA:HB1	1:A:589:ASN:OD1	2.14	0.47
1:A:684:ILE:HA	1:A:687:LEU:HB3	1.97	0.47
1:B:397:TYR:HA	1:B:442:ARG:HG2	1.96	0.47
1:B:519:LEU:HD22	1:B:523:LEU:HD13	1.96	0.47
1:B:588:ARG:HA	1:B:591:LEU:HB2	1.97	0.47
1:B:912:MET:HA	1:B:915:VAL:HG12	1.96	0.47
1:B:362:LEU:HD22	1:B:410:PHE:HD1	1.78	0.47
1:B:383:PRO:HG3	1:B:421:GLY:HA2	1.97	0.47
1:B:912:MET:HE3	1:B:912:MET:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:TYR:HA	1:A:341:LEU:HD12	1.97	0.47
1:A:453:GLY:HA3	1:A:463:LYS:NZ	2.29	0.47
1:B:251:LEU:O	1:B:254:LEU:HG	2.15	0.47
1:A:77:VAL:O	1:A:81:ILE:HG12	2.14	0.47
1:A:211:LEU:HA	1:A:214:VAL:HB	1.97	0.47
1:A:307:THR:HG22	1:A:352:LYS:HE3	1.97	0.47
1:A:632:ASN:HB3	1:A:664:LEU:HD13	1.97	0.47
1:B:370:LEU:HD21	1:B:415:GLU:O	2.15	0.47
1:B:426:THR:HG22	1:B:428:LYS:H	1.79	0.47
1:B:549:GLN:HB3	1:B:552:PHE:HB2	1.96	0.47
1:B:602:GLU:HG2	1:B:604:ASP:H	1.80	0.47
1:B:853:MET:SD	1:B:853:MET:N	2.88	0.47
1:A:640:THR:CG2	1:A:641:PRO:CD	2.93	0.46
1:B:186:ARG:HG3	1:B:267:PHE:CZ	2.49	0.46
1:B:475:ASN:OD1	1:B:476:ILE:N	2.48	0.46
1:B:502:ASP:HA	1:B:534:ASP:HB2	1.97	0.46
1:A:392:GLY:C	1:A:420:GLN:HE21	2.23	0.46
1:A:914:ILE:HD12	1:A:927:ILE:HG12	1.97	0.46
1:A:182:PHE:CE1	1:A:264:VAL:HG22	2.50	0.46
1:B:504:SER:O	1:B:508:ALA:HB3	2.15	0.46
1:B:824:LEU:O	1:B:828:GLU:OE1	2.34	0.46
1:A:369:THR:HG23	1:A:397:TYR:CE1	2.50	0.46
1:A:917:LYS:HG3	1:A:918:LEU:H	1.80	0.46
1:B:104:ILE:HB	1:B:105:PRO:HD3	1.96	0.46
1:B:482:VAL:HG22	1:B:517:ILE:HD13	1.96	0.46
1:A:152:MET:HE2	1:A:256:TYR:CD1	2.43	0.46
1:A:430:ARG:HD3	1:A:458:SER:CB	2.37	0.46
1:B:258:THR:OG1	1:B:259:GLN:NE2	2.48	0.46
1:B:284:ASP:HB3	1:B:287:ASN:HB2	1.98	0.46
1:A:720:GLU:HA	1:A:756:ILE:HD11	1.97	0.46
1:B:65:GLY:O	1:B:68:PRO:HD2	2.16	0.46
1:B:519:LEU:HD12	1:B:555:LEU:HD12	1.97	0.46
1:B:691:ILE:HG21	1:B:729:GLN:OE1	2.15	0.46
1:B:790:ALA:O	1:B:794:ILE:HG12	2.15	0.46
1:B:905:GLU:O	1:B:906:GLU:HG2	2.15	0.46
1:A:448:LYS:HB3	1:A:449:PRO:HD2	1.97	0.46
1:A:503:ARG:HG2	1:A:532:LEU:HD11	1.97	0.46
1:B:107:ASP:HB2	1:B:110:LYS:NZ	2.31	0.46
1:B:506:MET:HA	1:B:509:VAL:HG12	1.98	0.46
1:A:342:VAL:O	1:A:346:LYS:HG2	2.16	0.46
1:B:504:SER:O	1:B:508:ALA:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ASN:ND2	1:B:409:LYS:O	2.49	0.46
1:B:534:ASP:OD1	1:B:537:GLY:N	2.49	0.46
1:B:825:TYR:O	1:B:829:LYS:HD2	2.16	0.46
1:A:461:ASN:ND2	1:A:464:ASP:OD2	2.43	0.45
1:B:304:SER:O	1:B:307:THR:OG1	2.25	0.45
1:B:874:TYR:HB3	1:B:878:HIS:HB2	1.98	0.45
1:A:743:THR:HG21	1:A:769:GLU:HG2	1.97	0.45
1:B:201:LEU:HD11	1:B:275:LEU:HB2	1.97	0.45
1:A:708:TRP:CE3	1:A:712:HIS:HB3	2.52	0.45
1:B:374:ASN:HA	1:B:425:PRO:HB3	1.97	0.45
1:A:908:ARG:HB2	1:A:911:ILE:HB	1.99	0.45
1:B:288:PHE:CE1	1:B:409:LYS:HB3	2.51	0.45
1:B:391:ASP:HB3	1:B:420:GLN:HG3	1.97	0.45
1:B:636:THR:HG23	1:B:637:SER:N	2.32	0.45
1:A:249:GLN:OE1	1:A:249:GLN:N	2.37	0.45
1:A:879:LYS:HE2	1:A:882:ILE:HD12	1.97	0.45
1:B:115:GLU:HA	1:B:118:ASN:HD21	1.81	0.45
1:B:149:ARG:HA	1:B:152:MET:HE3	1.98	0.45
1:B:395:VAL:O	1:B:395:VAL:HG13	2.16	0.45
1:B:635:SER:H	1:B:639:LEU:H	1.64	0.45
1:B:451:PHE:CE2	1:B:499:PHE:HA	2.52	0.45
1:A:520:ARG:O	1:A:520:ARG:NH1	2.37	0.45
1:A:923:TYR:O	1:A:927:ILE:HG13	2.16	0.45
1:B:617:TYR:O	1:B:620:VAL:HG22	2.16	0.45
1:B:673:ALA:H	1:B:676:HIS:CE1	2.34	0.45
1:B:687:LEU:HD21	1:B:726:LEU:HG	1.98	0.45
1:A:313:LEU:O	1:A:317:VAL:HG13	2.16	0.45
1:A:709:THR:HG23	1:A:712:HIS:CE1	2.52	0.45
1:A:721:ASP:OD1	1:A:721:ASP:N	2.50	0.45
1:A:749:VAL:HG21	1:A:777:SER:HB3	1.99	0.45
1:B:643:HIS:CD2	1:B:674:PRO:HG3	2.51	0.45
1:B:780:ILE:O	1:B:784:ARG:N	2.48	0.45
1:A:668:ASP:OD1	1:A:672:MET:HG3	2.17	0.45
1:A:869:TYR:CD2	1:A:873:LYS:HD2	2.52	0.45
1:B:443:LYS:HD2	1:B:447:GLY:HA2	1.99	0.45
1:B:535:LYS:O	1:B:569:LYS:NZ	2.40	0.45
1:B:602:GLU:HG2	1:B:603:ASP:N	2.31	0.45
1:A:503:ARG:N	1:A:503:ARG:HD2	2.32	0.45
1:A:591:LEU:O	1:A:594:PRO:HD3	2.17	0.45
1:B:549:GLN:O	1:B:553:VAL:N	2.47	0.45
1:B:856:VAL:HA	1:B:859:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD11	1:A:320:VAL:HG21	1.99	0.44
1:A:343:THR:HA	1:A:346:LYS:HE2	1.99	0.44
1:A:837:THR:HG23	1:A:839:ASP:H	1.81	0.44
1:B:448:LYS:HZ1	1:B:452:ALA:N	2.15	0.44
1:B:823:VAL:O	1:B:827:LEU:HD23	2.17	0.44
1:A:407:TYR:CE2	1:A:409:LYS:CE	2.81	0.44
1:B:424:CYS:N	1:B:425:PRO:HD2	2.31	0.44
1:B:549:GLN:O	1:B:553:VAL:HG23	2.17	0.44
1:A:222:LEU:HD11	1:A:254:LEU:HA	1.99	0.44
1:A:366:ILE:HD13	1:A:438:ARG:HE	1.83	0.44
1:A:482:VAL:HG13	1:A:517:ILE:HD13	1.97	0.44
1:A:859:LEU:O	1:A:863:GLY:N	2.49	0.44
1:A:868:GLU:O	1:A:876:PRO:HD3	2.17	0.44
1:B:69:VAL:HG13	1:B:69:VAL:O	2.18	0.44
1:B:139:SER:O	1:B:143:VAL:HG23	2.17	0.44
1:B:152:MET:HA	1:B:155:ASN:HB3	1.98	0.44
1:B:333:ALA:HA	1:B:336:LYS:HD3	2.00	0.44
1:B:439:LEU:HG	1:B:454:THR:HA	1.99	0.44
1:A:50:SER:HG	1:A:51:ASN:H	1.62	0.44
1:A:551:GLY:O	1:A:555:LEU:HD23	2.17	0.44
1:A:745:LEU:HD13	1:A:760:LEU:HD22	1.99	0.44
1:B:600:GLU:OE1	1:B:601:LYS:N	2.51	0.44
1:A:166:LYS:HG3	1:A:168:ILE:HG22	1.99	0.44
1:A:446:SER:O	1:A:448:LYS:HG2	2.18	0.44
1:B:159:VAL:HG13	1:B:249:GLN:NE2	2.33	0.44
1:B:177:ASP:HA	1:B:180:LYS:HG2	1.99	0.44
1:B:683:SER:OG	1:B:686:MET:HB2	2.17	0.44
1:A:73:VAL:HG12	1:A:74:VAL:H	1.83	0.44
1:A:255:PHE:CE2	1:A:341:LEU:HB3	2.53	0.44
1:A:396:ARG:HA	1:A:416:PRO:CB	2.48	0.44
1:A:608:PRO:O	1:A:611:THR:OG1	2.29	0.44
1:B:222:LEU:O	1:B:226:LEU:HG	2.17	0.44
1:B:514:ASN:HB3	1:B:517:ILE:HG12	2.00	0.44
1:A:204:GLN:HA	1:A:207:ILE:HD13	2.00	0.44
1:A:373:VAL:HG21	1:A:428:LYS:HD3	2.00	0.44
1:B:365:ASP:O	1:B:438:ARG:NH2	2.48	0.44
1:B:461:ASN:O	1:B:465:ILE:HG12	2.17	0.44
1:B:819:ARG:NH2	1:B:821:SER:OG	2.51	0.44
1:A:166:LYS:HG3	1:A:168:ILE:H	1.83	0.44
1:A:389:TRP:CE2	1:A:423:ALA:HB2	2.53	0.44
1:A:820:LYS:HE3	1:A:858:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:PRO:HA	1:B:713:PHE:HD2	1.82	0.44
1:A:132:GLU:OE2	1:A:133:GLU:HG2	2.18	0.44
1:A:192:LEU:HB3	1:A:196:ARG:HB2	2.00	0.44
1:B:400:GLN:HB2	1:B:408:SER:O	2.18	0.43
1:B:466:HIS:NE2	1:B:494:ASP:HB3	2.32	0.43
1:B:889:VAL:O	1:B:893:LEU:HG	2.17	0.43
1:A:908:ARG:HA	1:A:911:ILE:HD13	2.00	0.43
1:B:577:LEU:HD12	1:B:580:ARG:NH2	2.33	0.43
1:A:289:ASN:OD1	1:A:411:SER:HB2	2.18	0.43
1:A:448:LYS:HD3	1:A:448:LYS:HA	1.73	0.43
1:A:754:ILE:HG22	1:A:758:LYS:HZ3	1.83	0.43
1:B:400:GLN:HB2	1:B:409:LYS:HA	2.00	0.43
1:B:593:SER:HB3	1:B:594:PRO:HD3	2.00	0.43
1:B:803:ARG:NE	1:B:807:ASN:OD1	2.35	0.43
1:B:892:PHE:O	1:B:896:ASP:HB3	2.18	0.43
1:B:908:ARG:HA	1:B:911:ILE:HD12	2.01	0.43
1:A:597:LYS:HD2	1:A:597:LYS:O	2.19	0.43
1:A:737:VAL:HG13	1:A:741:ASN:HA	1.99	0.43
1:B:327:LEU:HD12	1:B:328:PRO:HD2	2.00	0.43
1:B:396:ARG:HA	1:B:413:TRP:HB3	2.01	0.43
1:A:630:ASP:OD1	1:A:630:ASP:N	2.49	0.43
1:B:110:LYS:O	1:B:114:GLU:OE1	2.36	0.43
1:B:396:ARG:HB3	1:B:413:TRP:CD1	2.54	0.43
1:B:876:PRO:HA	1:B:879:LYS:HD3	2.00	0.43
1:B:894:GLU:HG2	1:B:895:LYS:N	2.33	0.43
1:A:443:LYS:HB2	1:A:450:GLN:HG2	2.01	0.43
1:A:699:ILE:HD11	1:A:731:ASP:HB3	2.01	0.43
1:A:900:LYS:HD2	1:A:900:LYS:HA	1.86	0.43
1:B:348:LEU:O	1:B:351:LEU:HB3	2.18	0.43
1:B:770:LYS:NZ	1:B:774:GLY:HA2	2.34	0.43
1:A:171:ILE:O	1:A:175:ILE:HG23	2.19	0.43
1:A:549:GLN:O	1:A:553:VAL:HG23	2.19	0.43
1:A:686:MET:O	1:A:690:LEU:HG	2.17	0.43
1:A:786:GLU:N	1:A:786:GLU:OE1	2.52	0.43
1:B:61:ALA:O	1:B:64:ILE:HB	2.18	0.43
1:B:903:GLU:HG2	1:B:904:THR:N	2.33	0.43
1:A:288:PHE:CD1	1:A:409:LYS:HD3	2.52	0.43
1:A:506:MET:HB3	1:A:529:ASP:CG	2.44	0.43
1:A:642:PHE:CE2	1:A:663:ASP:HA	2.53	0.43
1:A:676:HIS:HD2	1:A:710:PRO:HB3	1.84	0.43
1:B:316:ASN:O	1:B:319:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:ILE:HD11	1:B:442:ARG:NH2	2.32	0.43
1:B:534:ASP:OD1	1:B:538:PHE:N	2.52	0.43
1:B:556:LEU:HD12	1:B:557:ILE:N	2.34	0.43
1:B:137:LEU:O	1:B:141:THR:HG23	2.18	0.43
1:B:401:TYR:HE2	1:B:406:MET:HG3	1.83	0.43
1:B:667:GLN:HE22	1:B:703:THR:HA	1.83	0.43
1:A:124:LEU:HG	1:A:274:TYR:HE1	1.84	0.42
1:A:349:GLU:O	1:A:352:LYS:HG2	2.19	0.42
1:A:398:ALA:O	1:A:440:ILE:HG13	2.19	0.42
1:A:584:SER:OG	1:A:619:VAL:HB	2.19	0.42
1:B:168:ILE:HG12	1:B:225:ALA:HB2	2.01	0.42
1:B:400:GLN:HG3	1:B:409:LYS:HA	2.00	0.42
1:A:891:LEU:HD13	1:A:895:LYS:HD2	2.01	0.42
1:B:118:ASN:HA	1:B:121:ASP:OD2	2.18	0.42
1:B:703:THR:OG1	1:B:708:TRP:N	2.50	0.42
1:B:886:LEU:HD12	1:B:887:ASP:N	2.35	0.42
1:A:441:PHE:HB2	1:A:450:GLN:O	2.19	0.42
1:A:837:THR:HG23	1:A:839:ASP:N	2.35	0.42
1:B:693:ILE:C	1:B:695:ASP:H	2.27	0.42
1:A:341:LEU:N	1:A:344:ARG:HH21	2.17	0.42
1:A:401:TYR:HE1	1:A:437:ASN:H	1.68	0.42
1:B:255:PHE:O	1:B:259:GLN:HG2	2.19	0.42
1:B:669:VAL:HG23	1:B:670:ASN:ND2	2.35	0.42
1:B:687:LEU:HD23	1:B:725:GLU:CD	2.45	0.42
1:B:727:LEU:HD21	1:B:763:ARG:HG3	2.01	0.42
1:B:783:MET:HA	1:B:817:ILE:HD13	2.01	0.42
1:A:443:LYS:HG2	1:A:448:LYS:CG	2.50	0.42
1:A:504:SER:O	1:A:508:ALA:HB3	2.19	0.42
1:A:890:ARG:O	1:A:894:GLU:N	2.46	0.42
1:B:282:LYS:NZ	1:B:447:GLY:O	2.51	0.42
1:B:478:LYS:O	1:B:482:VAL:HG23	2.20	0.42
1:A:111:GLU:O	1:A:114:GLU:HG3	2.19	0.42
1:A:394:GLU:H	1:A:394:GLU:CD	2.27	0.42
1:A:599:ASN:OD1	1:A:629:ILE:HA	2.19	0.42
1:A:682:GLY:HA3	1:A:719:LYS:HZ2	1.85	0.42
1:B:441:PHE:HB2	1:B:448:LYS:NZ	2.35	0.42
1:B:516:LYS:HB2	1:B:520:ARG:HH22	1.84	0.42
1:B:685:LYS:HE3	1:B:686:MET:HE1	2.01	0.42
1:A:200:LYS:O	1:A:204:GLN:HG2	2.19	0.42
1:A:639:LEU:HD23	1:A:644:LEU:HD21	2.02	0.42
1:A:723:ALA:O	1:A:726:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:GLN:OE1	1:A:755:ASN:ND2	2.53	0.42
1:B:252:TYR:HA	1:B:338:TYR:CE1	2.55	0.42
1:B:377:ASN:OD1	1:B:378:ASP:N	2.53	0.42
1:B:441:PHE:HB2	1:B:448:LYS:HZ1	1.85	0.42
1:B:478:LYS:HG3	1:B:514:ASN:OD1	2.19	0.42
1:B:566:LYS:HB3	1:B:571:ASN:HB3	2.01	0.42
1:B:890:ARG:HA	1:B:893:LEU:HD12	2.01	0.42
1:A:142:PHE:O	1:A:146:GLU:HG2	2.19	0.42
1:A:754:ILE:HG22	1:A:758:LYS:NZ	2.35	0.42
1:A:760:LEU:HD21	1:A:765:SER:HB3	2.02	0.42
1:B:396:ARG:HB2	1:B:443:LYS:HB2	2.01	0.42
1:A:216:GLU:OE1	1:A:217:PRO:HD3	2.19	0.42
1:A:336:LYS:O	1:A:340:GLU:OE1	2.38	0.42
1:B:776:THR:O	1:B:780:ILE:HG13	2.20	0.42
1:B:852:LYS:HB2	1:B:855:THR:OG1	2.20	0.42
1:A:73:VAL:H	1:A:76:ILE:HB	1.85	0.42
1:A:212:LYS:HE3	1:A:212:LYS:HB3	1.86	0.42
1:A:775:TYR:HD2	1:A:780:ILE:HD11	1.84	0.42
1:B:179:LYS:HE2	1:B:256:TYR:CE2	2.54	0.42
1:B:525:ASN:OD1	1:B:527:SER:OG	2.23	0.42
1:B:587:VAL:O	1:B:590:LEU:HG	2.19	0.42
1:B:624:LEU:O	1:B:629:ILE:HG21	2.20	0.42
1:A:147:LYS:HB2	1:A:147:LYS:HE2	1.84	0.41
1:B:70:ILE:HD11	1:B:580:ARG:NE	2.35	0.41
1:B:98:ALA:N	1:B:783:MET:HE1	2.35	0.41
1:B:149:ARG:NH2	1:B:179:LYS:HD3	2.34	0.41
1:B:165:SER:OG	1:B:246:LYS:HE2	2.20	0.41
1:B:370:LEU:HD23	1:B:397:TYR:CD1	2.55	0.41
1:B:470:TYR:O	1:B:474:LEU:HG	2.20	0.41
1:B:487:THR:HA	1:B:490:GLU:CD	2.44	0.41
1:B:516:LYS:HB2	1:B:520:ARG:NH2	2.34	0.41
1:B:581:SER:HB2	1:B:583:PHE:CE2	2.55	0.41
1:A:155:ASN:O	1:A:159:VAL:HG23	2.19	0.41
1:A:349:GLU:HA	1:A:352:LYS:HG2	2.01	0.41
1:A:407:TYR:HD2	1:A:409:LYS:NZ	2.16	0.41
1:A:780:ILE:HA	1:A:783:MET:HG3	2.01	0.41
1:B:689:TYR:CD2	1:B:690:LEU:HD22	2.55	0.41
1:B:845:HIS:HA	1:B:848:VAL:HG22	2.02	0.41
1:A:845:HIS:O	1:A:849:SER:OG	2.30	0.41
1:B:689:TYR:CZ	1:B:693:ILE:HD11	2.55	0.41
1:A:255:PHE:CE1	1:A:341:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ARG:HH12	1:A:444:PHE:HD1	1.67	0.41
1:A:778:LEU:HA	1:A:781:ALA:HB3	2.01	0.41
1:B:819:ARG:O	1:B:823:VAL:HG23	2.21	0.41
1:A:205:LYS:HE3	1:A:272:HIS:NE2	2.36	0.41
1:A:407:TYR:CD2	1:A:409:LYS:CE	3.03	0.41
1:B:179:LYS:HE2	1:B:256:TYR:HE2	1.85	0.41
1:B:314:ILE:HD13	1:B:314:ILE:HA	1.89	0.41
1:B:742:LEU:HD21	1:B:773:GLU:HG3	2.01	0.41
1:B:894:GLU:N	1:B:894:GLU:OE1	2.54	0.41
1:B:515:ASN:HB3	1:B:552:PHE:CD1	2.56	0.41
1:B:581:SER:HB2	1:B:583:PHE:CD2	2.55	0.41
1:B:610:HIS:NE2	1:B:639:LEU:O	2.53	0.41
1:B:708:TRP:HE3	1:B:712:HIS:CG	2.38	0.41
1:B:855:THR:O	1:B:859:LEU:HD13	2.21	0.41
1:A:448:LYS:HB2	1:A:450:GLN:HG3	2.03	0.41
1:A:646:ILE:O	1:A:649:GLU:HG3	2.21	0.41
1:B:486:THR:HA	1:B:489:ILE:HG22	2.02	0.41
1:B:683:SER:O	1:B:687:LEU:HB2	2.21	0.41
1:A:413:TRP:HA	1:A:416:PRO:HD2	2.02	0.41
1:B:643:HIS:HD2	1:B:677:PHE:HE2	1.68	0.41
1:B:844:LEU:O	1:B:848:VAL:HG13	2.20	0.41
1:A:194:LYS:H	1:A:194:LYS:HG3	1.66	0.41
1:A:314:ILE:HA	1:A:317:VAL:HG22	2.02	0.41
1:A:676:HIS:CD2	1:A:676:HIS:N	2.89	0.41
1:A:842:THR:HG22	1:A:843:ALA:N	2.36	0.41
1:B:129:ALA:HB3	1:B:131:LEU:HD22	2.01	0.41
1:B:161:GLU:CD	1:B:162:THR:HG22	2.46	0.41
1:B:684:ILE:HG23	1:B:725:GLU:OE1	2.21	0.41
1:B:703:THR:HG21	1:B:713:PHE:HZ	1.85	0.41
1:A:136:LYS:HB3	1:A:136:LYS:HE2	1.80	0.41
1:A:727:LEU:HD23	1:A:732:ILE:HG21	2.03	0.41
1:B:60:VAL:O	1:B:64:ILE:HG12	2.21	0.41
1:B:166:LYS:HD2	1:B:166:LYS:HA	1.95	0.41
1:B:362:LEU:N	1:B:408:SER:HG	2.18	0.41
1:B:443:LYS:HG2	1:B:448:LYS:H	1.86	0.41
1:B:500:ASP:O	1:B:535:LYS:NZ	2.39	0.41
1:B:746:HIS:CD2	1:B:777:SER:HB3	2.56	0.41
1:B:112:ILE:HD12	1:B:112:ILE:H	1.86	0.40
1:B:115:GLU:O	1:B:116:ARG:C	2.64	0.40
1:B:324:VAL:HG22	1:B:339:ARG:HH21	1.86	0.40
1:B:375:PHE:H	1:B:425:PRO:CG	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:TYR:CZ	1:B:504:SER:HB2	2.56	0.40
1:B:724:LYS:HB3	1:B:728:LYS:NZ	2.36	0.40
1:A:70:ILE:HD12	1:A:70:ILE:HA	1.95	0.40
1:B:448:LYS:HE2	1:B:452:ALA:HB2	2.04	0.40
1:B:837:THR:OG1	1:B:838:ALA:N	2.54	0.40
1:A:65:GLY:C	1:A:68:PRO:HD2	2.47	0.40
1:A:867:LYS:HE2	1:A:876:PRO:HG2	2.03	0.40
1:B:51:ASN:N	1:B:51:ASN:OD1	2.53	0.40
1:B:301:ASP:O	1:B:305:SER:OG	2.32	0.40
1:B:575:LEU:CD2	1:B:608:PRO:HB3	2.51	0.40
1:B:676:HIS:CD2	1:B:710:PRO:HG3	2.57	0.40
1:B:758:LYS:O	1:B:762:LYS:HG2	2.21	0.40
1:A:156:PHE:N	1:A:252:TYR:HE2	2.20	0.40
1:A:228:GLU:O	1:A:231:ASP:HB2	2.22	0.40
1:A:640:THR:HB	1:A:643:HIS:ND1	2.37	0.40
1:A:712:HIS:O	1:A:715:ILE:HB	2.22	0.40
1:A:791:VAL:HG12	1:A:795:GLU:OE2	2.21	0.40
1:A:161:GLU:OE1	1:A:161:GLU:N	2.54	0.40
1:A:576:HIS:NE2	1:A:608:PRO:HG3	2.35	0.40
1:A:643:HIS:CE1	1:A:674:PRO:HG3	2.57	0.40
1:B:403:SER:OG	1:B:404:LYS:HG3	2.21	0.40
1:B:580:ARG:HG2	1:B:614:MET:HB2	2.02	0.40
1:B:861:ASN:O	1:B:862:LYS:HE2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	840/1296 (65%)	761 (91%)	79 (9%)	0	100	100
1	B	859/1296 (66%)	753 (88%)	106 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1699/2592 (66%)	1514 (89%)	185 (11%)	0	100	100

There are no Ramachandran outliers to report.

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	732/1127 (65%)	732 (100%)	0	100	100
1	B	745/1127 (66%)	745 (100%)	0	100	100
All	All	1477/2254 (66%)	1477 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	271	GLN
1	A	289	ASN
1	A	353	ASN
1	A	420	GLN
1	A	457	HIS
1	A	632	ASN
1	A	928	ASN
1	B	234	ASN
1	B	353	ASN
1	B	741	ASN
1	B	865	ASN
1	B	916	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

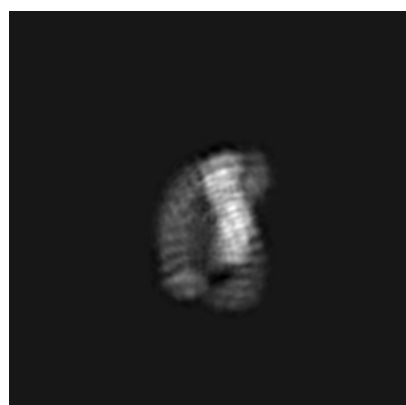
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13643. These allow visual inspection of the internal detail of the map and identification of artifacts.

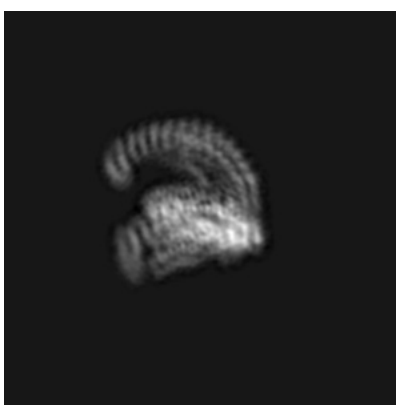
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

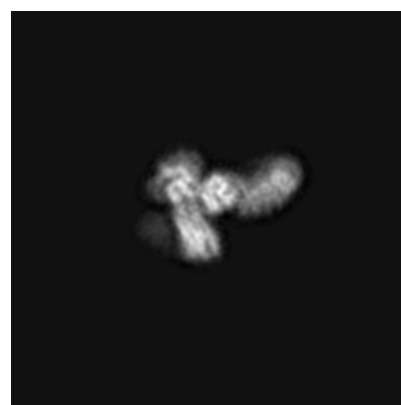
6.1.1 Primary map



X



Y

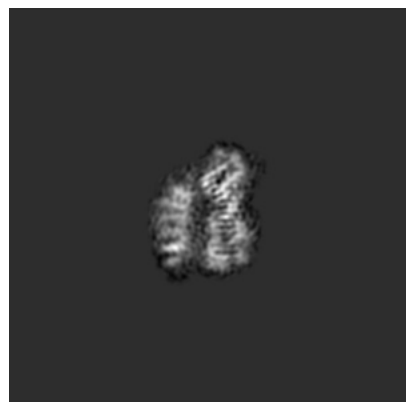


Z

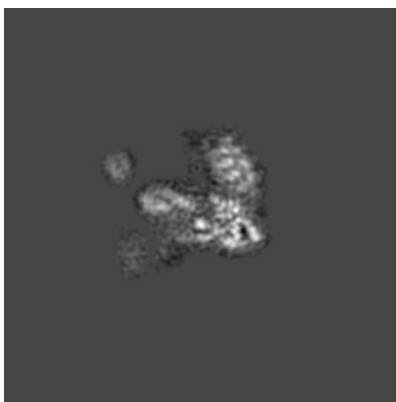
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

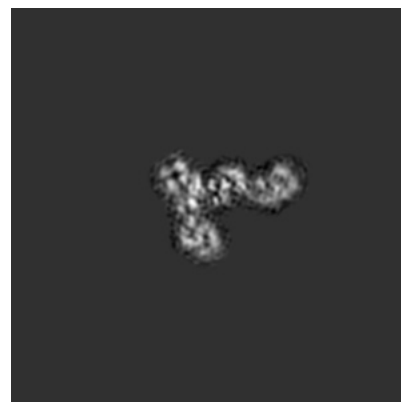
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

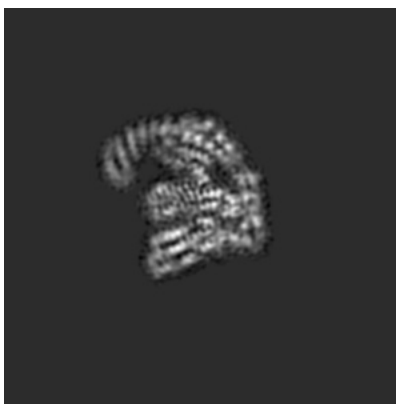
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

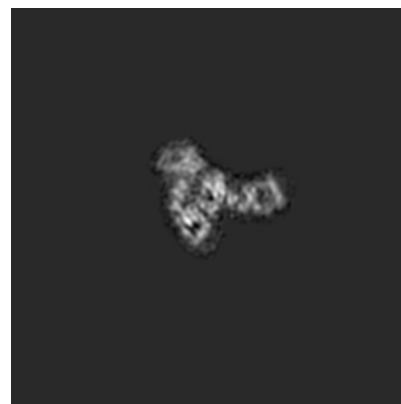
6.3.1 Primary map



X Index: 157



Y Index: 202

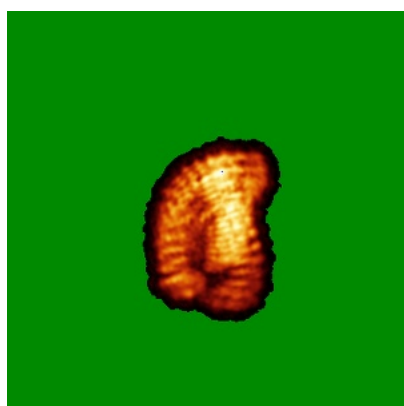


Z Index: 204

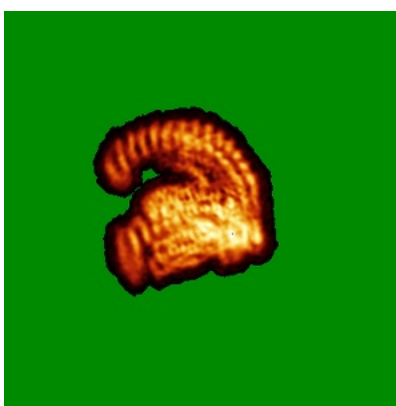
The images above show the largest variance slices of the map in three orthogonal directions.

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

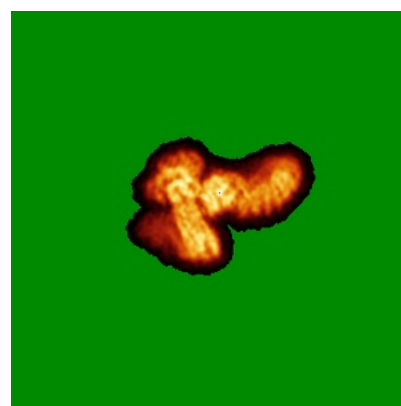
6.4.1 Primary map



X



Y

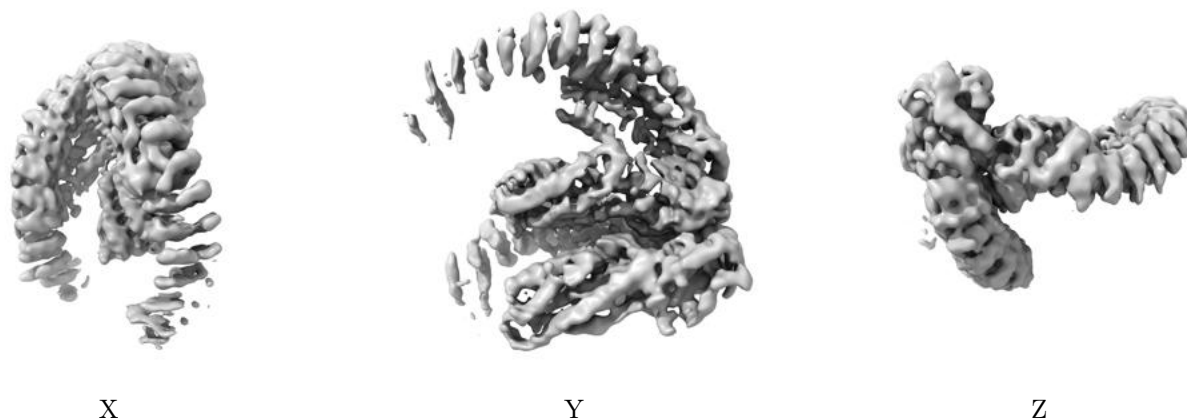


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

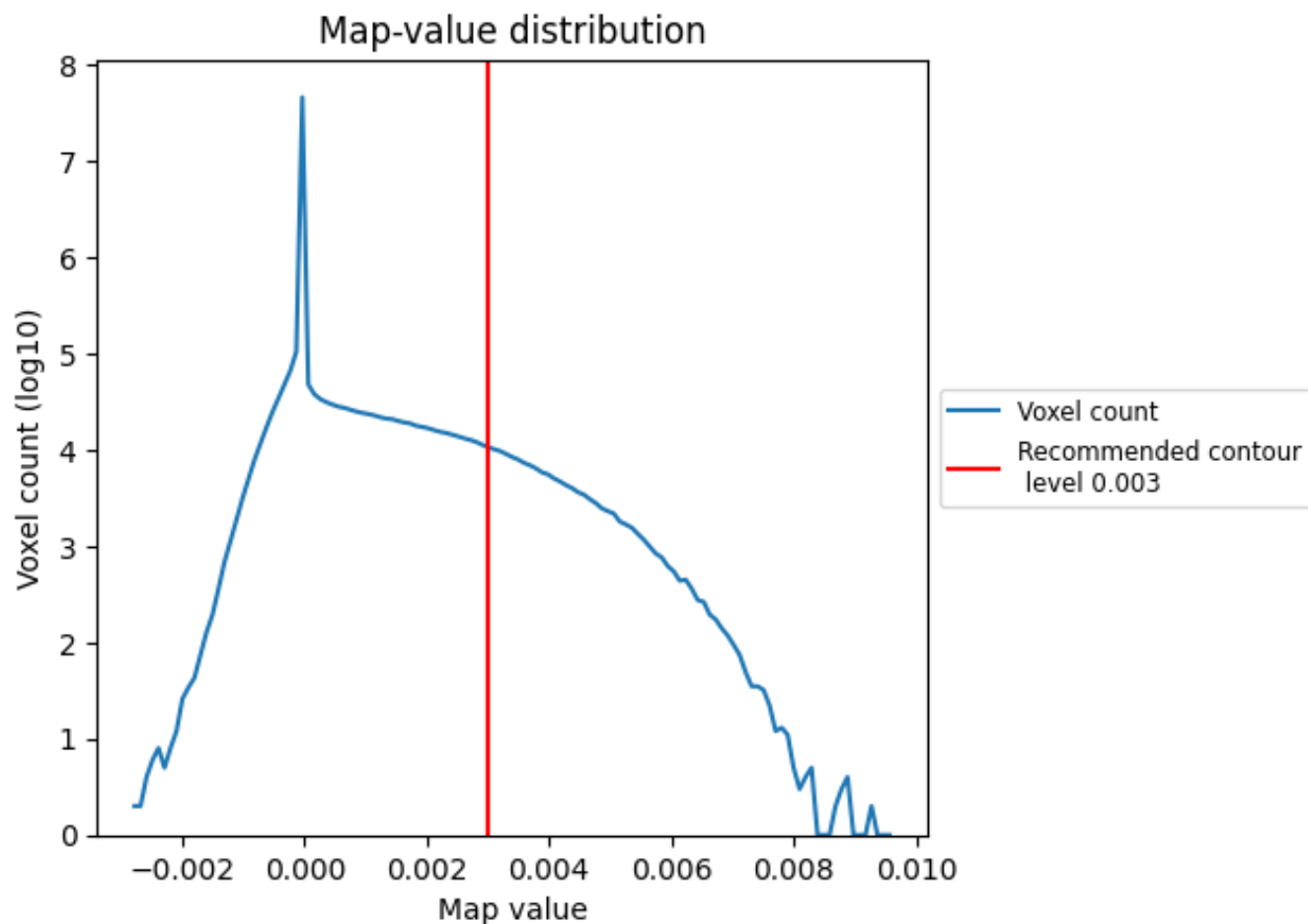
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

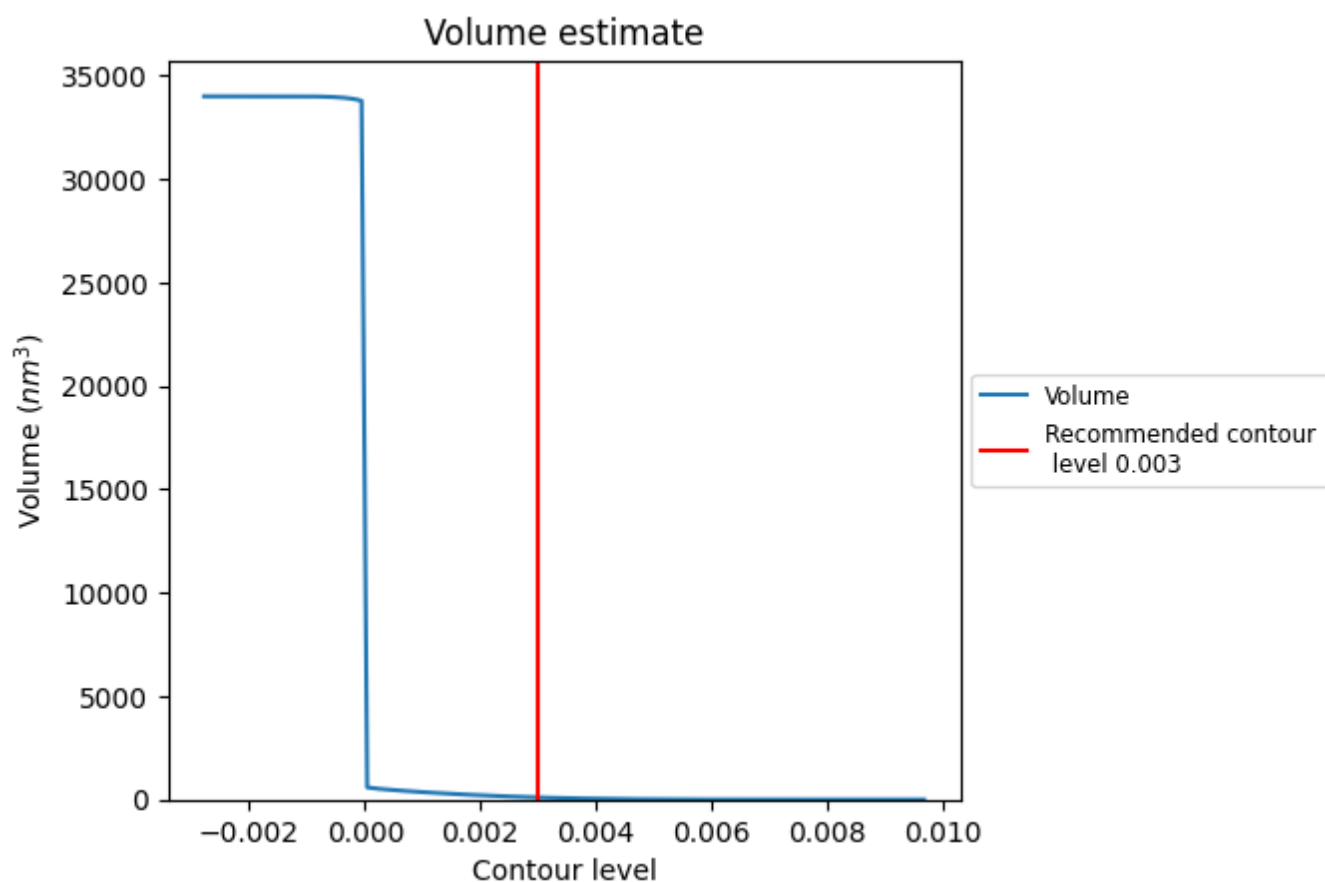
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

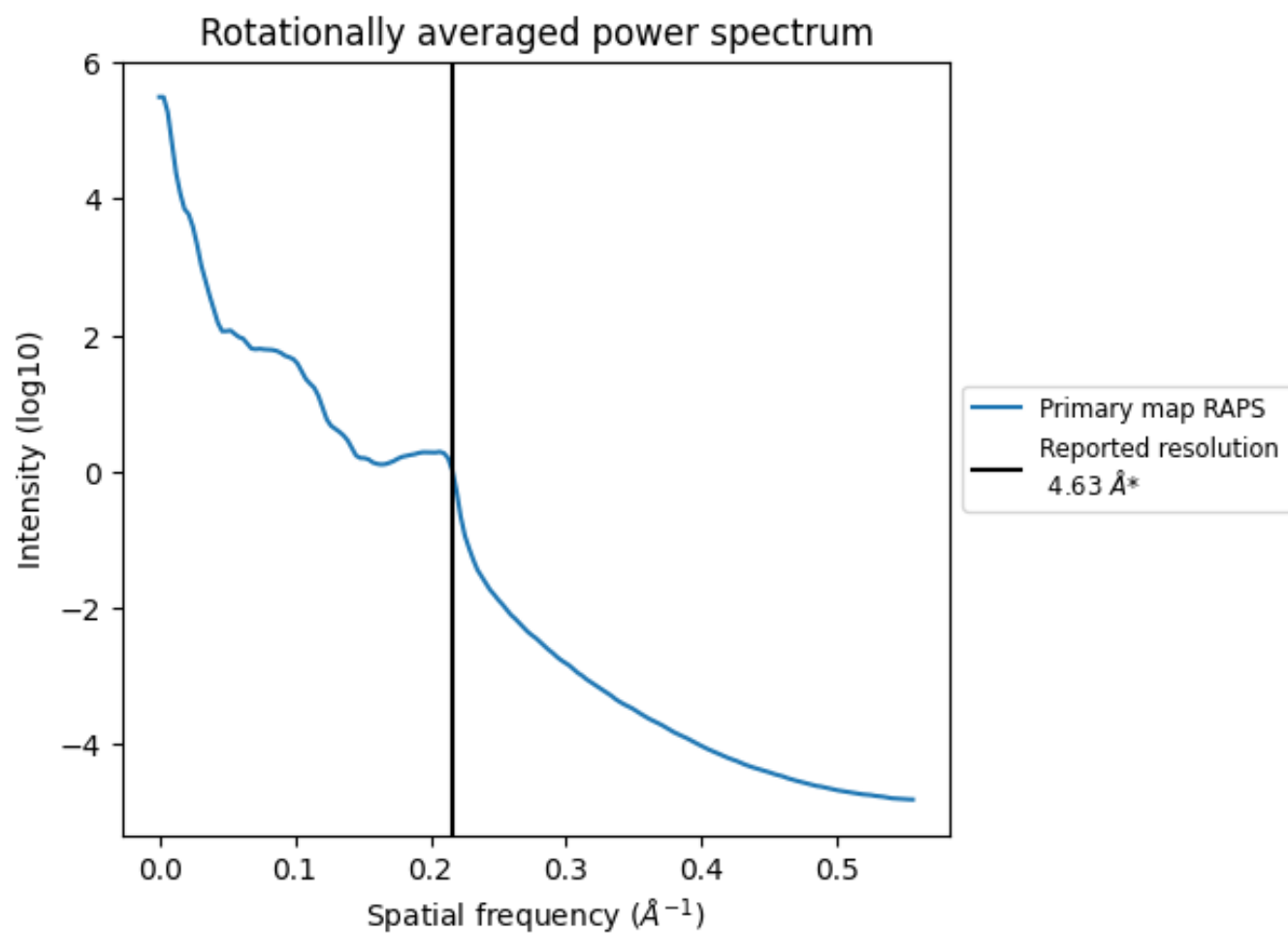
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm³; this corresponds to an approximate mass of 92 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 0.216 Å⁻¹

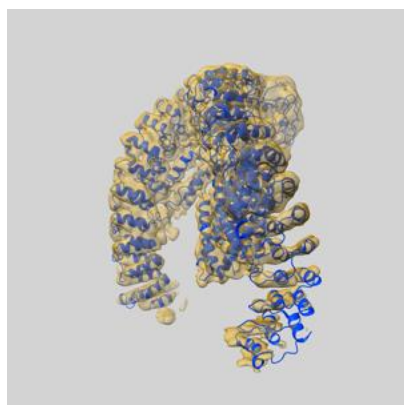
8 Fourier-Shell correlation

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

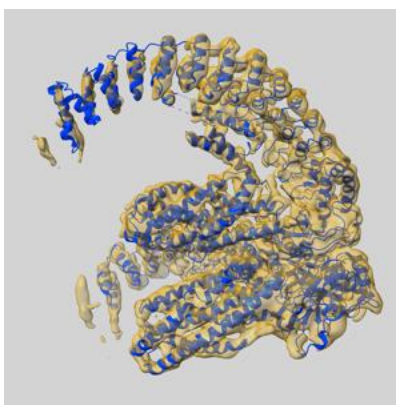
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13643 and PDB model 7PTY. Per-residue inclusion information can be found in section [3](#) on page [8](#).

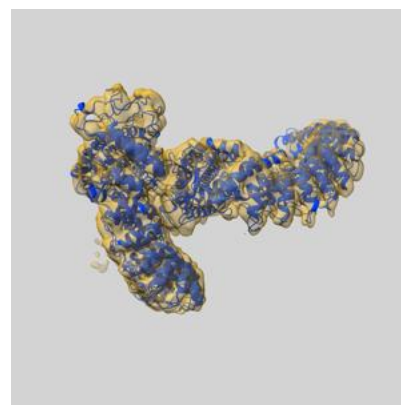
9.1 Map-model overlay [i](#)



X



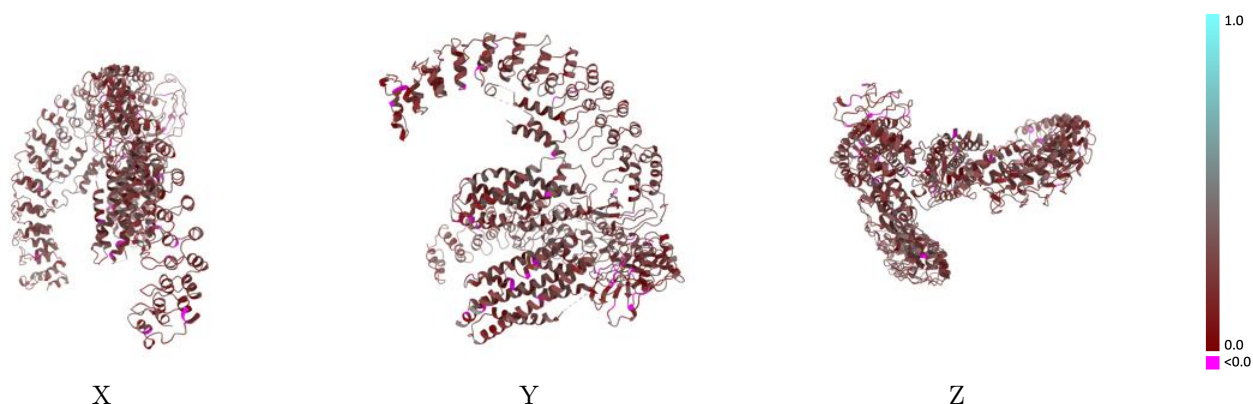
Y



Z

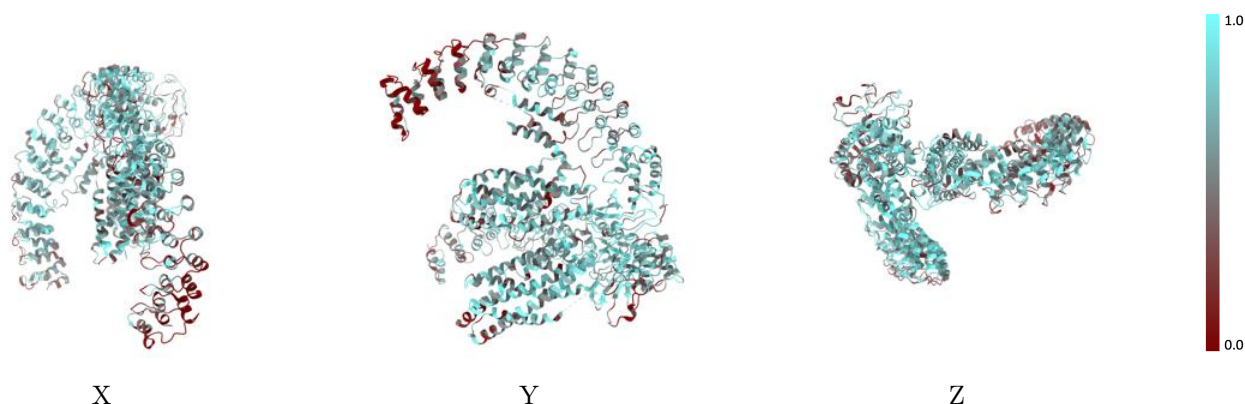
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



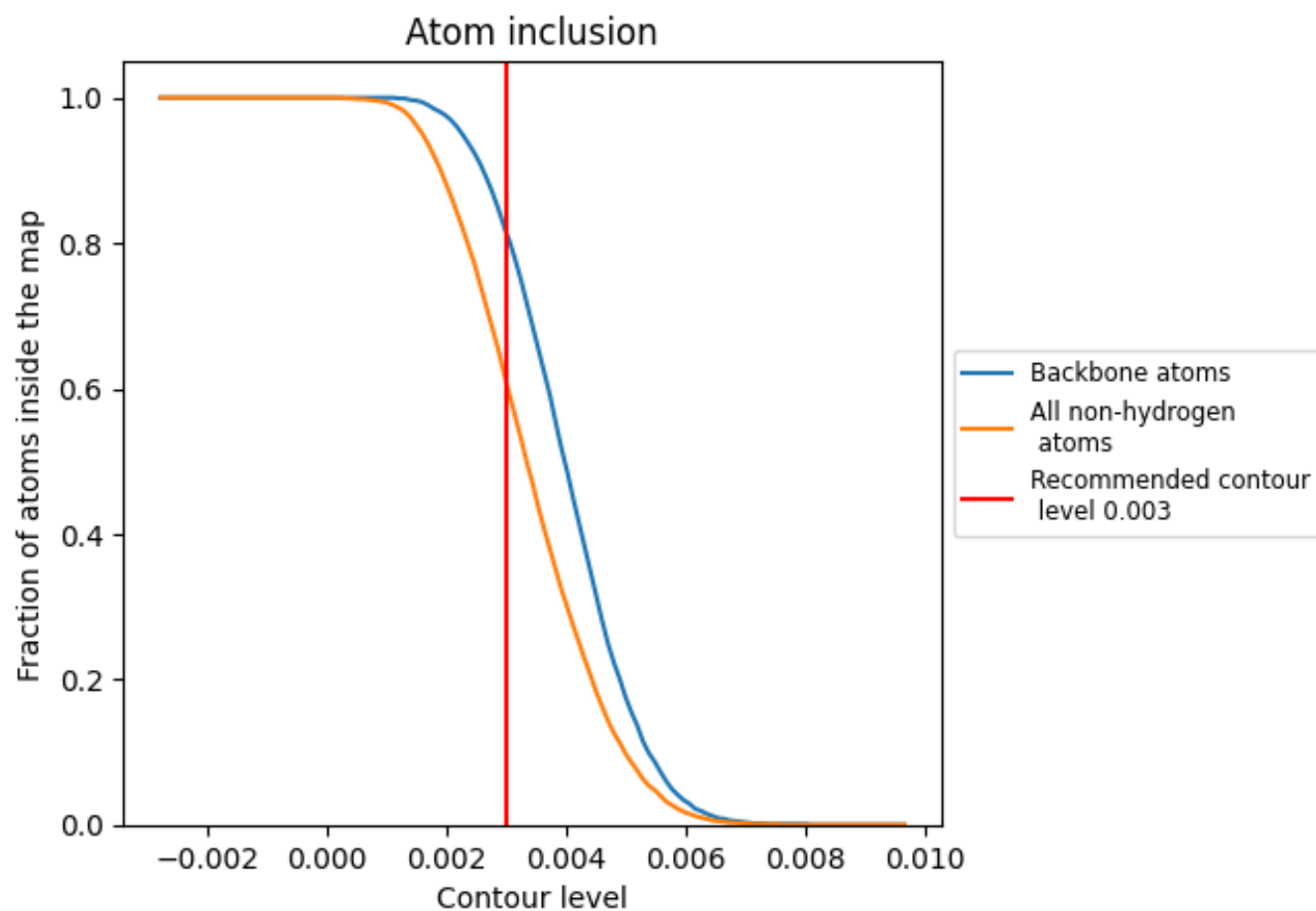
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 61% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6100	0.2530
A	0.5670	0.2540
B	0.6530	0.2520

