



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 19, 2018 – 08:02 pm GMT

PDB ID : 6B5B
EMDB ID: : EMD-7055
Title : Cryo-EM structure of the NAIP5-NLRC4-flagellin inflammasome
Authors : Tenthorey, J.L.; Haloupek, N.; Lopez-Blanco, J.R.; Grob, P.; Adamson, E.; Hartenian, E.; Lind, N.A.; Bourgeois, N.M.; Chacon, P.; Nogales, E.; Vance, R.E.
Deposited on : 2017-09-29
Resolution : 5.20 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

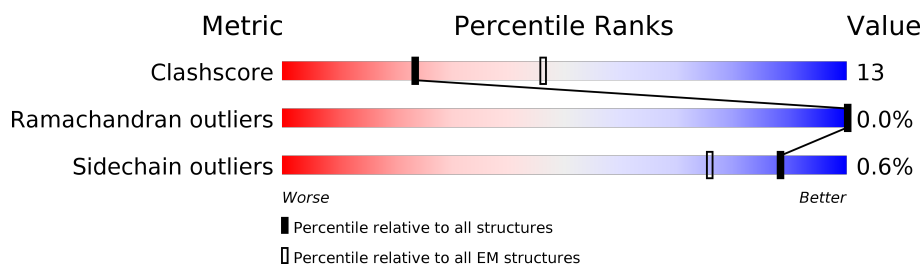
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1403	
2	B	1024	
2	C	1024	
3	F	566	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24555 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 Baculoviral IAP repeat-containing protein 1e.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1199	Total	C	N	O	S	0	0
			9583	6128	1608	1790	57		

- Molecule 2 is a protein called NLR family CARD domain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	903	Total	C	N	O	S	0	0
			7237	4622	1224	1351	40		
2	C	903	Total	C	N	O	S	0	0
			7237	4622	1224	1351	40		

- Molecule 3 is a protein called Flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	68	Total	C	N	O	S	0	0
			498	302	93	98	5		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-90	MET	-	initiating methionine	UNP G8U UW9
F	-89	GLU	-	expression tag	UNP G8U UW9
F	-88	GLN	-	expression tag	UNP G8U UW9
F	-87	LYS	-	expression tag	UNP G8U UW9
F	-86	LEU	-	expression tag	UNP G8U UW9
F	-85	ILE	-	expression tag	UNP G8U UW9
F	-84	SER	-	expression tag	UNP G8U UW9
F	-83	GLU	-	expression tag	UNP G8U UW9
F	-82	GLU	-	expression tag	UNP G8U UW9
F	-81	ASP	-	expression tag	UNP G8U UW9
F	-80	LEU	-	expression tag	UNP G8U UW9
F	-79	ASN	-	expression tag	UNP G8U UW9
F	-78	GLU	-	expression tag	UNP G8U UW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-77	MET	-	expression tag	UNP G8U UW9
F	-76	GLU	-	expression tag	UNP G8U UW9
F	-75	GLN	-	expression tag	UNP G8U UW9
F	-74	LYS	-	expression tag	UNP G8U UW9
F	-73	LEU	-	expression tag	UNP G8U UW9
F	-72	ILE	-	expression tag	UNP G8U UW9
F	-71	SER	-	expression tag	UNP G8U UW9
F	-70	GLU	-	expression tag	UNP G8U UW9
F	-69	GLU	-	expression tag	UNP G8U UW9
F	-68	ASP	-	expression tag	UNP G8U UW9
F	-67	LEU	-	expression tag	UNP G8U UW9
F	-66	ASN	-	expression tag	UNP G8U UW9
F	-65	GLU	-	expression tag	UNP G8U UW9
F	-64	MET	-	expression tag	UNP G8U UW9
F	-63	GLU	-	expression tag	UNP G8U UW9
F	-62	GLN	-	expression tag	UNP G8U UW9
F	-61	LYS	-	expression tag	UNP G8U UW9
F	-60	LEU	-	expression tag	UNP G8U UW9
F	-59	ILE	-	expression tag	UNP G8U UW9
F	-58	SER	-	expression tag	UNP G8U UW9
F	-57	GLU	-	expression tag	UNP G8U UW9
F	-56	GLU	-	expression tag	UNP G8U UW9
F	-55	ASP	-	expression tag	UNP G8U UW9
F	-54	LEU	-	expression tag	UNP G8U UW9
F	-53	ASN	-	expression tag	UNP G8U UW9
F	-52	GLU	-	expression tag	UNP G8U UW9
F	-51	MET	-	expression tag	UNP G8U UW9
F	-50	GLU	-	expression tag	UNP G8U UW9
F	-49	GLN	-	expression tag	UNP G8U UW9
F	-48	LYS	-	expression tag	UNP G8U UW9
F	-47	LEU	-	expression tag	UNP G8U UW9
F	-46	ILE	-	expression tag	UNP G8U UW9
F	-45	SER	-	expression tag	UNP G8U UW9
F	-44	GLU	-	expression tag	UNP G8U UW9
F	-43	GLU	-	expression tag	UNP G8U UW9
F	-42	ASP	-	expression tag	UNP G8U UW9
F	-41	LEU	-	expression tag	UNP G8U UW9
F	-40	ASN	-	expression tag	UNP G8U UW9
F	-39	GLU	-	expression tag	UNP G8U UW9
F	-38	MET	-	expression tag	UNP G8U UW9
F	-37	GLU	-	expression tag	UNP G8U UW9
F	-36	GLN	-	expression tag	UNP G8U UW9

Continued on next page...

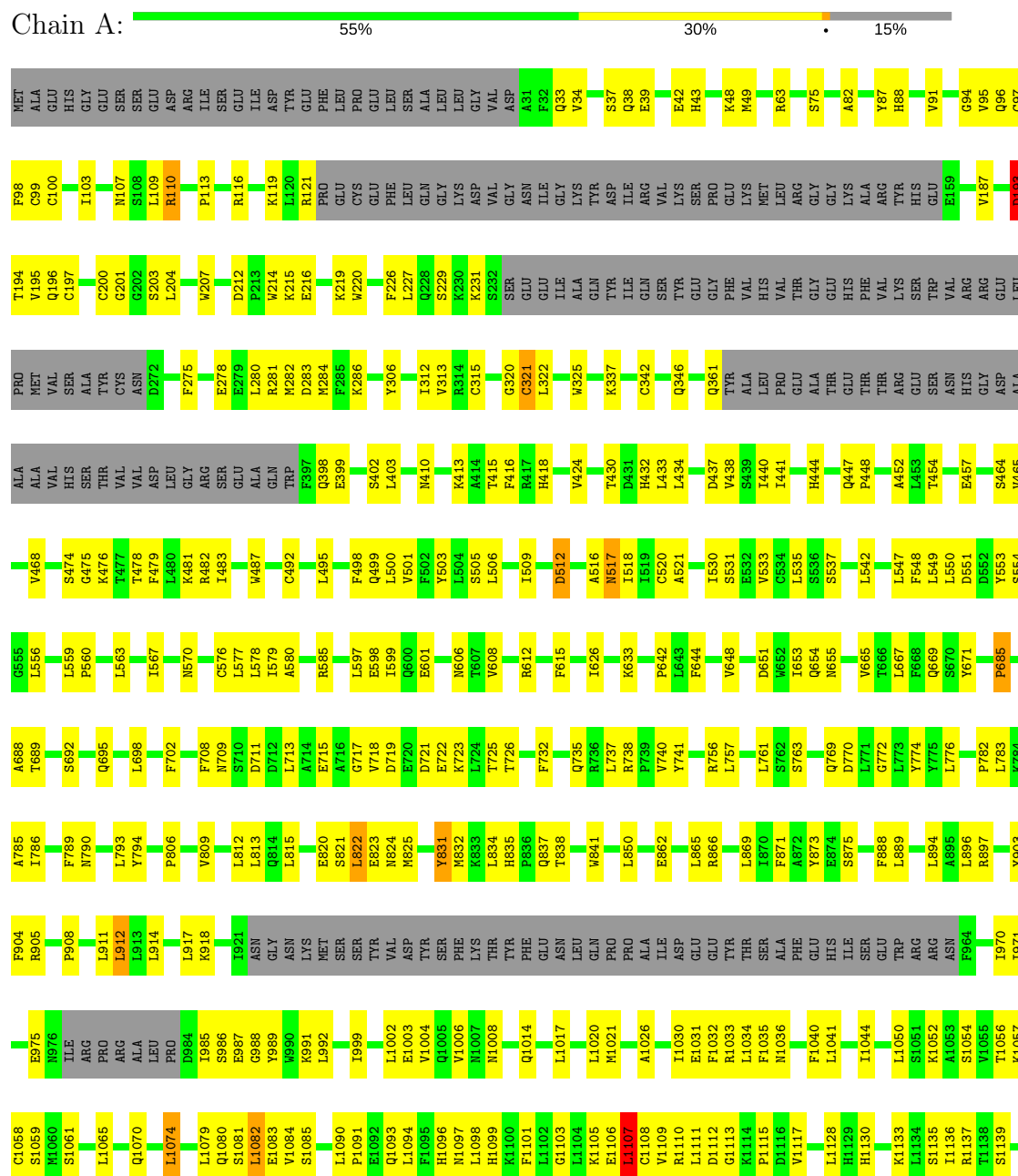
Continued from previous page...

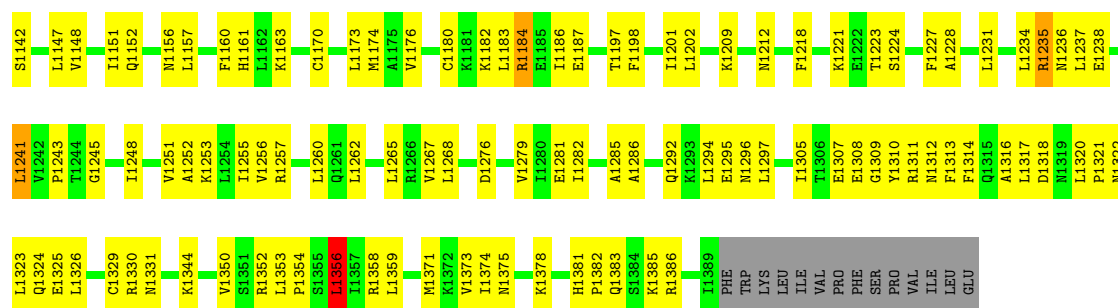
Chain	Residue	Modelled	Actual	Comment	Reference
F	-35	LYS	-	expression tag	UNP G8U UW9
F	-34	LEU	-	expression tag	UNP G8U UW9
F	-33	ILE	-	expression tag	UNP G8U UW9
F	-32	SER	-	expression tag	UNP G8U UW9
F	-31	GLU	-	expression tag	UNP G8U UW9
F	-30	GLU	-	expression tag	UNP G8U UW9
F	-29	ASP	-	expression tag	UNP G8U UW9
F	-28	LEU	-	expression tag	UNP G8U UW9
F	-27	ASN	-	expression tag	UNP G8U UW9
F	-26	GLU	-	expression tag	UNP G8U UW9
F	-25	MET	-	expression tag	UNP G8U UW9
F	-24	GLU	-	expression tag	UNP G8U UW9
F	-23	SER	-	expression tag	UNP G8U UW9
F	-22	LEU	-	expression tag	UNP G8U UW9
F	-21	GLY	-	expression tag	UNP G8U UW9
F	-20	ASP	-	expression tag	UNP G8U UW9
F	-19	LEU	-	expression tag	UNP G8U UW9
F	-18	THR	-	expression tag	UNP G8U UW9
F	-17	MET	-	expression tag	UNP G8U UW9
F	-16	GLU	-	expression tag	UNP G8U UW9
F	-15	GLN	-	expression tag	UNP G8U UW9
F	-14	LYS	-	expression tag	UNP G8U UW9
F	-13	LEU	-	expression tag	UNP G8U UW9
F	-12	ILE	-	expression tag	UNP G8U UW9
F	-11	SER	-	expression tag	UNP G8U UW9
F	-10	GLU	-	expression tag	UNP G8U UW9
F	-9	GLU	-	expression tag	UNP G8U UW9
F	-8	ASP	-	expression tag	UNP G8U UW9
F	-7	LEU	-	expression tag	UNP G8U UW9
F	-6	ASN	-	expression tag	UNP G8U UW9
F	-5	SER	-	expression tag	UNP G8U UW9
F	-4	GLY	-	expression tag	UNP G8U UW9
F	-3	ARG	-	expression tag	UNP G8U UW9
F	-2	PRO	-	expression tag	UNP G8U UW9
F	-1	ALA	-	expression tag	UNP G8U UW9
F	0	ALA	-	expression tag	UNP G8U UW9
F	1	MET	-	expression tag	UNP G8U UW9

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

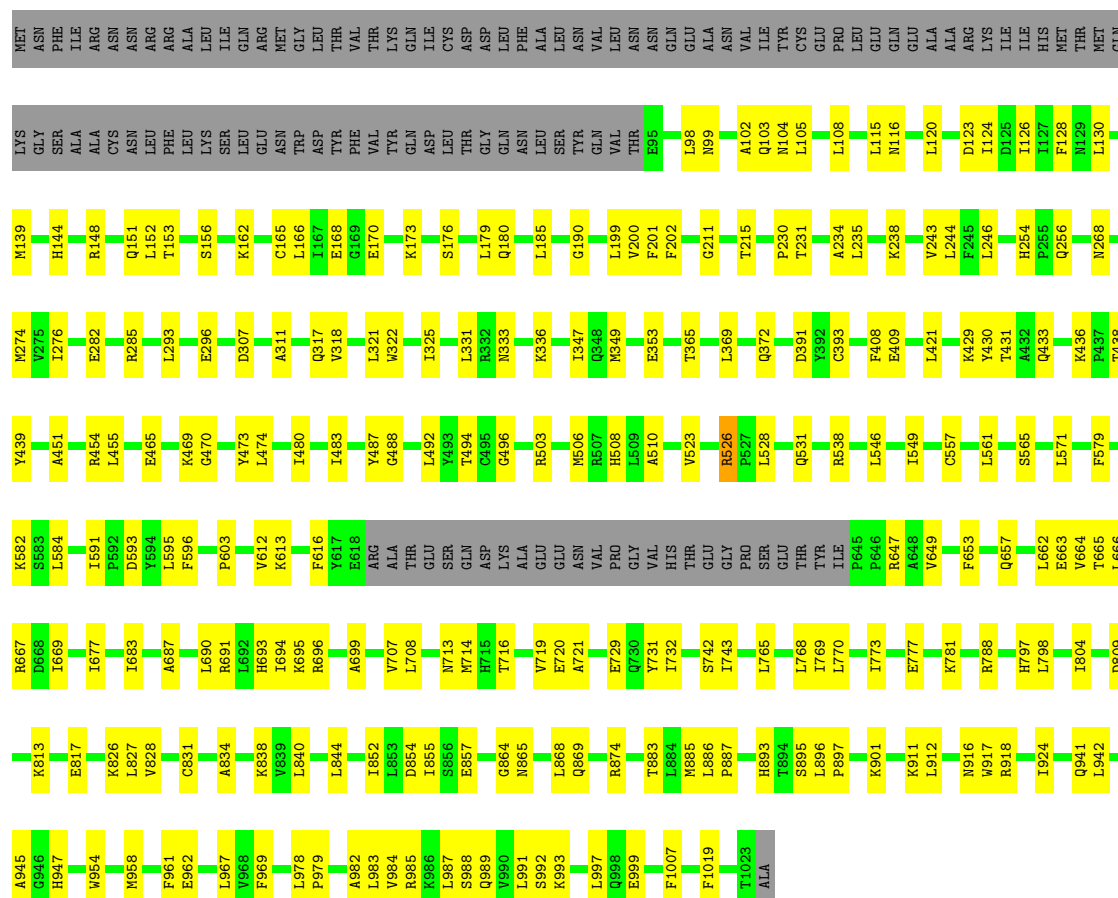
- Molecule 1: Baculoviral IAP repeat-containing protein 1e





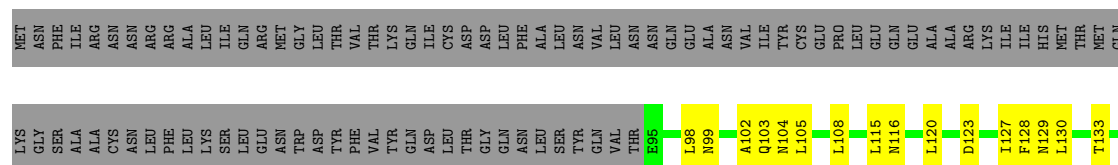
• Molecule 2: NLR family CARD domain-containing protein 4

Chain B: 66% 22% 12%



• Molecule 2: NLR family CARD domain-containing protein 4

Chain C: 66% 22% 12%



L595	F596	L599	F599	L600	F603	L603	F603	L604	F604	L605	F605	L606	F606	L607	F607	L608	F608	L609	F609	L610	F610	L611	F611	L612	F612	L613	F613	L614	F614	L615	F615	L616	F616	L617	F617	L618	F618	L619	F619	L620	F620	L621	F621	L622	F622	L623	F623	L624	F624	L625	F625	L626	F626	L627	F627	L628	F628	L629	F629	L630	F630	L631	F631	L632	F632	L633	F633	L634	F634	L635	F635	L636	F636	L637	F637	L638	F638	L639	F639	L640	F640	L641	F641	L642	F642	L643	F643	L644	F644	L645	F645	L646	F646	L647	F647	L648	F648	L649	F649	L650	F650	L651	F651	L652	F652	L653	F653	L654	F654	L655	F655	L656	F656	L657	F657	L658	F658	L659	F659	L660	F660	L661	F661	L662	F662	L663	F663	L664	F664	L665	F665	L666	F666	L667	F667	L668	F668	L669	F669	L670	F670	L671	F671	L672	F672	L673	F673	L674	F674	L675	F675	L676	F676	L677	F677	L678	F678	L679	F679	L680	F680	L681	F681	L682	F682	L683	F683	L684	F684	L685	F685	L686	F686	L687	F687	L688	F688	L689	F689	L690	F690	L691	F691	L692	F692	L693	F693	L694	F694	L695	F695	L696	F696	L697	F697	L698	F698	L699	F699	L700	F700	L701	F701	L702	F702	L703	F703	L704	F704	L705	F705	L706	F706	L707	F707	L708	F708	L709	F709	L710	F710	L711	F711	L712	F712	L713	F713	L714	F714	L715	F715	L716	F716	L717	F717	L718	F718	L719	F719	L720	F720	L721	F721	L722	F722	L723	F723	L724	F724	L725	F725	L726	F726	L727	F727	L728	F728	L729	F729	L730	F730	L731	F731	L732	F732	L733	F733	L734	F734	L735	F735	L736	F736	L737	F737	L738	F738	L739	F739	L740	F740	L741	F741	L742	F742	L743	F743	L744	F744	L745	F745	L746	F746	L747	F747	L748	F748	L749	F749	L750	F750	L751	F751	L752	F752	L753	F753	L754	F754	L755	F755	L756	F756	L757	F757	L758	F758	L759	F759	L760	F760	L761	F761	L762	F762	L763	F763	L764	F764	L765	F765	L766	F766	L767	F767	L768	F768	L769	F769	L770	F770	L771	F771	L772	F772	L773	F773	L774	F774	L775	F775	L776	F776	L777	F777	L778	F778	L779	F779	L780	F780	L781	F781	L782	F782	L783	F783	L784	F784	L785	F785	L786	F786	L787	F787	L788	F788	L789	F789	L790	F790	L791	F791	L792	F792	L793	F793	L794	F794	L795	F795	L796	F796	L797	F797	L798	F798	L799	F799	L800	F800	L801	F801	L802	F802	L803	F803	L804	F804	L805	F805	L806	F806	L807	F807	L808	F808	L809	F809	L810	F810	L811	F811	L812	F812	L813	F813	L814	F814	L815	F815	L816	F816	L817	F817	L818	F818	L819	F819	L820	F820	L821	F821	L822	F822	L823	F823	L824	F824	L825	F825	L826	F826	L827	F827	L828	F828	L829	F829	L830	F830	L831	F831	L832	F832	L833	F833	L834	F834	L835	F835	L836	F836	L837	F837	L838	F838	L839	F839	L840	F840	L841	F841	L842	F842	L843	F843	L844	F844	L845	F845	L846	F846	L847	F847	L848	F848	L849	F849	L850	F850	L851	F851	L852	F852	L853	F853	L854	F854	L855	F855	L856	F856	L857	F857	L858	F858	L859	F859	L860	F860	L861	F861	L862	F862	L863	F863	L864	F864	L865	F865	L866	F866	L867	F867	L868	F868	L869	F869	L870	F870	L871	F871	L872	F872	L873	F873	L874	F874	L875	F875	L876	F876	L877	F877	L878	F878	L879	F879	L880	F880	L881	F881	L882	F882	L883	F883	L884	F884	L885	F885	L886	F886	L887	F887	L888	F888	L889	F889	L890	F890	L891	F891	L892	F892	L893	F893	L894	F894	L895	F895	L896	F896	L897	F897	L898	F898	L899	F899	L900	F900	L901	F901	L902	F902	L903	F903	L904	F904	L905	F905	L906	F906	L907	F907	L908	F908	L909	F909	L910	F910	L911	F911	L912	F912	L913	F913	L914	F914	L915	F915	L916	F916	L917	F917	L918	F918	L919	F919	L920	F920	L921	F921	L922	F922	L923	F923	L924	F924	L925	F925	L926	F926	L927	F927	L928	F928	L929	F929	L930	F930	L931	F931	L932	F932	L933	F933	L934	F934	L935	F935	L936	F936	L937	F937	L938	F938	L939	F939	L940	F940	L941	F941	L942	F942	L943	F943	L944	F944	L945	F945	L946	F946	L947	F947	L948	F948	L949	F949	L950	F950	L951	F951	L952	F952	L953	F953	L954	F954	L955	F955	L956	F956	L957	F957	L958	F958	L959	F959	L960	F960	L961	F961	L962	F962	L963	F963	L964	F964	L965	F965	L966	F966	L967	F967	L968	F968	L969	F969	L970	F970	L971	F971	L972	F972	L973	F973	L974	F974	L975	F975	L976	F976	L977	F977	L978	F978	L979	F979	L980	F980	L981	F981	L982	F982	L983	F983	L984	F984	L985	F985	L986	F986	L987	F987	L988	F988	L989	F989	L990	F990	L991	F991	L992	F992	L993	F993	L994	F994	L995	F995	L996	F996	L997	F997	L998	F998	L999	F999	L1000	F1000	L1001	F1001	L1002	F1002	L1003	F1003	L1004	F1004	L1005	F1005	L1006	F1006	L1007	F1007	L1008	F1008	L1009	F1009	L1010	F1010	L1011	F1011	L1012	F1012	L1013	F1013	L1014	F1014	L1015	F1015	L1016	F1016	L1017	F1017	L1018	F1018	L1019	F1019	L1020	F1020	L1021	F1021	L1022	F1022	L1023	F1023	L1024	F1024	L1025	F1025	L1026	F1026	L1027	F1027	L1028	F1028	L1029	F1029	L1030	F1030	L1031	F1031	L1032	F1032	L1033	F1033	L1034	F1034	L1035	F1035	L1036	F1036	L1037	F1037	L1038	F1038	L1039	F1039	L1040	F1040	L1041	F1041	L1042	F1042	L1043	F1043	L1044	F1044	L1045	F1045	L1046	F1046	L1047	F1047	L1048	F1048	L1049	F1049	L1050	F1050	L1051	F1051	L1052	F1052	L1053	F1053	L1054	F1054	L1055	F1055	L1056	F1056	L1057	F1057	L1058	F1058	L1059	F1059	L1060	F1060	L1061	F1061	L1062	F1062	L1063	F1063	L1064	F1064	L1065	F1065	L1066	F1066	L1067	F1067	L1068	F1068	L1069	F1069	L1070	F1070	L1071	F1071	L1072	F1072	L1073	F1073	L1074	F1074	L1075	F1075	L1076	F1076	L1077	F1077	L1078	F1078	L1079	F1079	L1080	F1080	L1081	F1081	L1082	F1082	L1083	F1083	L1084	F1084	L1085	F1085	L1086	F1086	L1087	F1087	L1088	F1088	L1089	F1089	L1090	F1090	L1091	F1091	L1092	F1092	L1093	F1093	L1094	F1094	L1095	F1095	L1096	F1096	L1097	F1097	L1098	F1098	L1099	F1099	L1100	F1100	L1101	F1101	L1102	F1102	L1103	F1103	L1104	F1104	L1105	F1105	L1106	F1106	L1107	F1107	L1108	F1108	L1109	F1109	L1110	F1110	L1111	F1111	L1112	F1112	L1113	F1113	L1114	F1114	L1115	F1115	L1116	F1116	L1117	F1117	L1118	F1118	L1119	F1119	L1120	F1120	L1121	F1121	L1122	F1122	L1123	F1123	L1124	F1124	L1125	F1125	L1126	F1126	L1127	F1127	L1128	F1128	L1129	F1129	L1130	F1130	L1131	F1131	L1132	F1132	L1133	F1133	L1134	F1134	L1135	F1135	L1136	F1136	L1137	F1137	L1138	F1138	L1139	F1139	L1140	F1140	L1141	F1141	L1142	F1142	L1143	F1143	L1144	F1144	L1145	F1145	L1146	F1146	L1147	F1147	L1148	F1148	L1149	F1149	L1150	F1150	L1151	F1151	L1152	F1152	L1153	F1153	L1154	F1154	L1155	F1155	L1156	F1156	L1157	F1157	L1158	F1158	L1159	F1159	L1160	F1160	L1161	F1161	L1162	F1162	L1163	F1163	L1164	F1164	L1165	F1165	L1166	F1166	L1167	F1167	L1168	F1168	L1169	F1169	L1170	F1170	L1171	F1171	L1172	F1172	L1173	F1173	L1174	F1174	L1175	F1175	L1176	F1176	L1177	F1177	L1178	F1178	L1179	F1179	L1180	F1180	L1181	F1181	L1182	F1182	L1183	F1183	L1184	F1184	L1185	F1185	L1186	F1186	L1187	F1187	L1188	F1188	L1189	F1189	L1190	F1190	L1191	F1191	L1192	F1192	L1193	F1193	L1194	F1194	L1195	F1195	L1196	F1196	L1197	F1197	L1198	F1198	L1199	F1199	L1200	F1200	L1201	F1201	L1202	F1202	L1203	F1203	L1204	F1204	L1205	F1205	L1206	F1206	L1207	F1207	L1208	F1208	L1209	F1209	L1210	F1210	L1211	F1211	L1212	F1212	L1213	F1213	L1214	F1214	L1215	F1215	L1216	F1216	L1217	F1217	L1218	F1218	L1219	F1219	L1220	F1220	L1221	F1221	L1222	F1222	L1223	F1223	L1224	F1224	L1225	F1225	L1226	F1226	L1227	F1227	L1228	F1228	L1229	F1229	L1230	F1230	L1231	F1231	L1232	F1232	L1233	F1233	L1234	F1234	L1235	F1235	L1236	F1236	L1237	F1237	L1238	F1238	L1239	F1239	L1240	F1240	L1241	F1241	L1242	F1242	L1243	F1243	L1244	F1244	L1245	F1245	L1246	F1246	L1247	F1247	L1248	F1248	L1249	F1249	L1250	F1250	L1251	F1251	L1252	F1252	L1253	F1253	L1254	F1254	L1255	F1255	L1256	F1256	L1257	F1257	L1258	F1258	L1259	F1259	L1260	F1260	L1261	F1261	L1262	F1262	L1263	F1263	L1264	F1264	L1265	F1265	L1266	F1266	L1267	F1267	L1268	F1268	L1269	F1269	L1270	F1270	L1271	F1271	L1272	F1272	L1273	F1273	L1274	F1274	L1275	F1275	L1276	F1276	L1277	F1277	L1278	F1278	L1279	F1279	L1280	F1280	L1281	F1281	L1282	F1282	L1283	F1283	L1284	F1284	L1285	F1285	L1286	F1286	L1287	F1287	L1288	F1288	L1289	F1289	L1290	F1290	L1291	F1291	L1292	F1292	L1293	F1293	L1294	F1294	L1295	F1295	L1296	F1296	L1297	F1297	L1298	F1298	L1299	F1299	L1300	F1300	L1301	F1301	L1302	F1302	L1303	F1303	L1304	F1304	L1305	F1305	L1306	F1306	L1307	F1307	L1308	F1308	L1309	F1309	L1310	F1310	L1311	F1311	L1312	F1312	L1313	F1313	L1314	F1314	L1315	F1315	L1316	F1316	L1317	F1317	L1318	F1318	L1319	F1319	L1320	F1320	L1321	F1321	L1322	F1322	L1323	F1323	L1324	F1324	L1325	F1325	L1326	F1326	L1327</
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	---------

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	252214	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 ($e^-/\text{\AA}^2$)	45.8	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.31	0/9782	0.63	11/13218 (0.1%)
2	B	0.27	0/7376	0.50	0/9957
2	C	0.27	0/7376	0.50	0/9957
3	F	0.26	0/497	0.63	1/668 (0.1%)
All	All	0.29	0/25031	0.55	12/33800 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	822	LEU	CA-CB-CG	6.98	131.36	115.30
1	A	1241	LEU	CA-CB-CG	6.70	130.70	115.30
3	F	472	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	719	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	1356	LEU	CA-CB-CG	6.52	130.29	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1107	LEU	Peptide
1	A	321	CYS	Peptide
1	A	447	GLN	Peptide
1	A	685	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	831	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	9583	0	9567	310	0
2	B	7237	0	7285	165	0
2	C	7237	0	7285	164	0
3	F	498	0	525	18	0
All	All	24555	0	24662	648	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 13.

The worst 5 of 648 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:313:VAL:O	1:A:321:CYS:HA	1.10	1.25
1:A:313:VAL:O	1:A:321:CYS:CA	2.01	1.07
1:A:785:ALA:O	1:A:789:PHE:HB2	1.58	1.03
1:A:1252:ALA:O	1:A:1256:VAL:HB	1.62	0.98
3:F:459:LEU:O	3:F:463:ASN:HB2	1.64	0.97

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	1187/1403 (85%)	1011 (85%)	175 (15%)	1 (0%)	53	88
2	B	899/1024 (88%)	839 (93%)	60 (7%)	0	100	100
2	C	899/1024 (88%)	839 (93%)	60 (7%)	0	100	100
3	F	64/566 (11%)	60 (94%)	4 (6%)	0	100	100
All	All	3049/4017 (76%)	2749 (90%)	299 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ASP

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	1080/1258 (86%)	1069 (99%)	11 (1%)	78	89
2	B	807/913 (88%)	805 (100%)	2 (0%)	94	96
2	C	807/913 (88%)	805 (100%)	2 (0%)	94	96
3	F	56/437 (13%)	54 (96%)	2 (4%)	38	65
All	All	2750/3521 (78%)	2733 (99%)	17 (1%)	88	93

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1234	LEU
1	A	1235	ARG
2	C	268	ASN
1	A	1221	LYS
2	C	526	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1327	ASN
2	B	147	HIS
2	C	916	ASN
1	A	1381	HIS
2	B	144	HIS

5.3.3 RNA [i](#)

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 carbohydrates 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.