



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:56 PM UTC

PDB ID : 3IYL / pdb_00003iyl
EMDB ID : EMD-5160
Title : Atomic CryoEM Structure of a Nonenveloped Virus Suggests How Membrane Penetration Protein is Primed for Cell Entry
Authors : Zhang, X.; Jin, L.; Fang, Q.; Hui, W.; Zhou, Z.H.
Deposited on : 2010-02-02
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

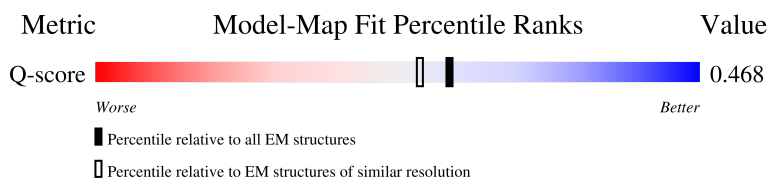
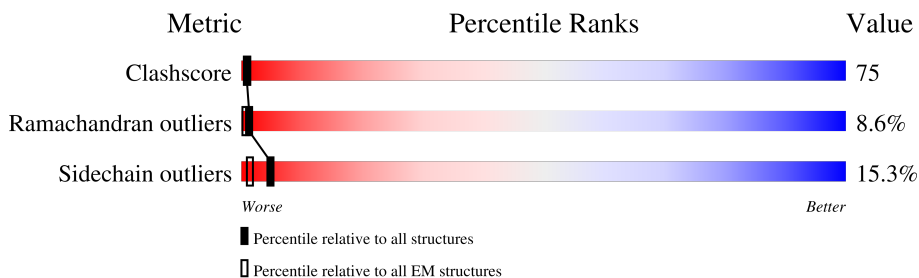
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



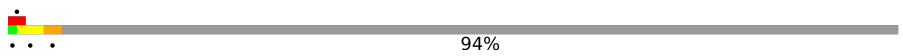
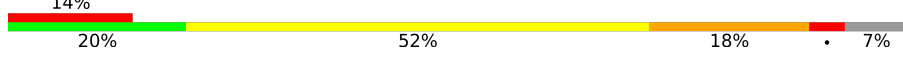
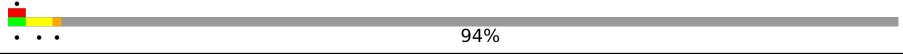
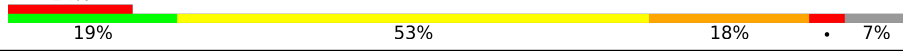
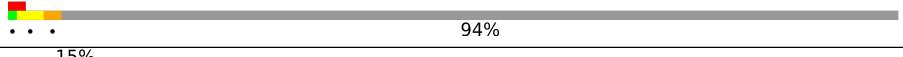
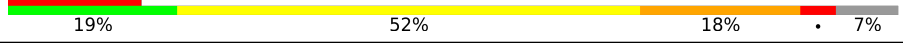
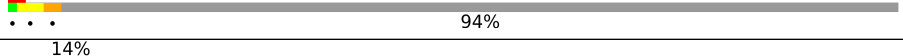
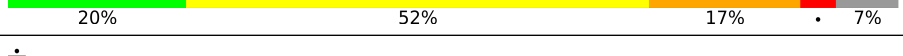
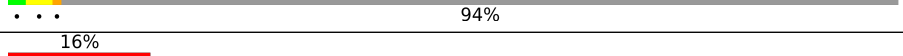
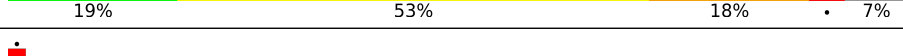
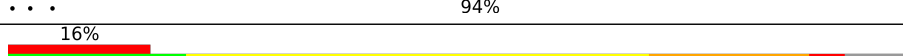
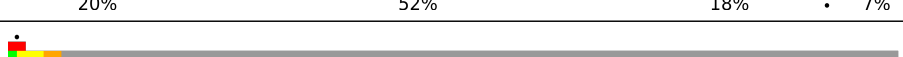
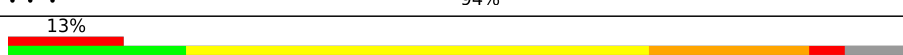
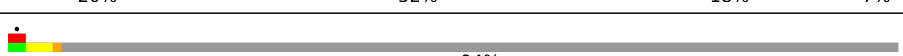
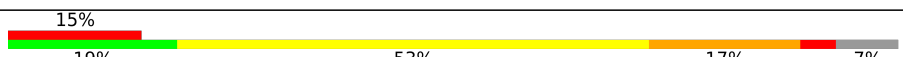
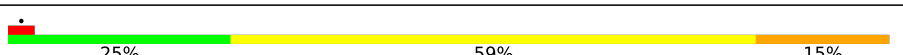
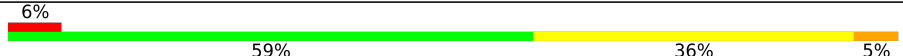
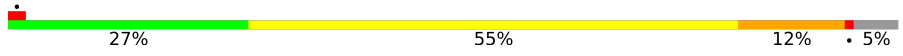
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	648	
1	B	648	
1	C	648	
1	D	648	

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Mol	Chain	Length	Quality of chain
1	E	648	
1	F	648	
1	G	648	
1	H	648	
1	I	648	
1	J	648	
1	K	648	
1	L	648	
1	M	648	
1	N	648	
1	O	648	
1	P	648	
1	Q	648	
1	R	648	
1	S	648	
1	T	648	
2	U	412	
2	V	412	
3	W	1299	
4	X	1214	
4	Y	1214	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MYR	A	649	-	-	X	-
5	MYR	C	649	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MYR	E	649	-	-	X	-
5	MYR	G	649	-	-	X	-
5	MYR	I	649	-	-	X	-
5	MYR	K	649	-	-	X	-
5	MYR	M	649	-	-	X	-
5	MYR	O	649	-	-	X	-
5	MYR	Q	649	-	-	X	-
5	MYR	S	649	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 80985 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 Outer capsid VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	B	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	C	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	D	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	E	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	F	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	G	41	Total	C	N	O	S	0	0
			284	174	46	63	1		
1	H	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	I	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	J	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	K	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	L	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	M	41	Total	C	N	O	S	0	0
			284	174	46	63	1		
1	N	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	O	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
1	P	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	Q	41	Total	C	N	O	S	0	0
			291	177	48	65	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
1	S	41	Total	C	N	O	S	0	0
			284	174	46	63	1		
1	T	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		

- Molecule 2 is a protein called Core protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	411	Total	C	N	O	S	0	0
			3138	2008	544	571	15		
2	V	411	Total	C	N	O	S	0	0
			3138	2008	544	571	15		

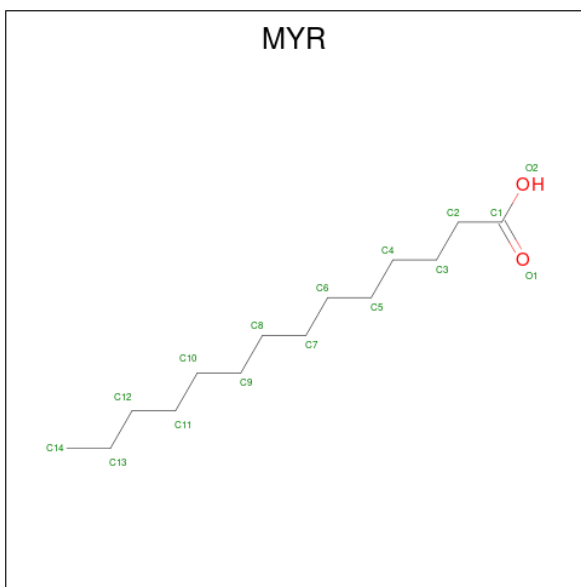
- Molecule 3 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	1284	Total	C	N	O	S	0	0
			9882	6335	1681	1839	27		

- Molecule 4 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	1018	Total	C	N	O	S	0	0
			7873	5033	1347	1447	46		
4	Y	1154	Total	C	N	O	S	0	0
			8835	5604	1525	1656	50		

- Molecule 5 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



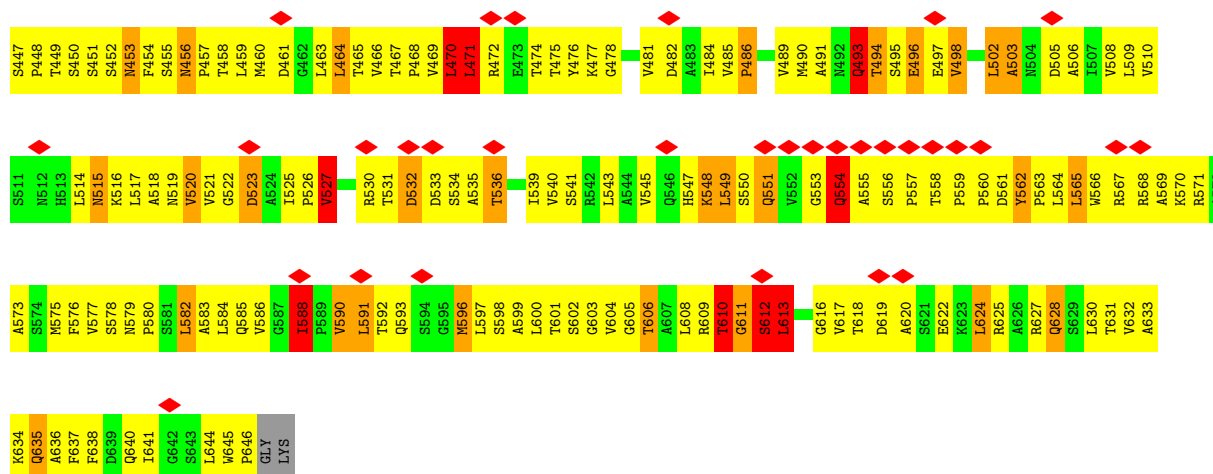
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			15	14	1	
5	C	1	Total	C	O	0
			15	14	1	
5	E	1	Total	C	O	0
			15	14	1	
5	G	1	Total	C	O	0
			15	14	1	
5	I	1	Total	C	O	0
			15	14	1	
5	K	1	Total	C	O	0
			15	14	1	
5	M	1	Total	C	O	0
			15	14	1	
5	O	1	Total	C	O	0
			15	14	1	
5	Q	1	Total	C	O	0
			15	14	1	
5	S	1	Total	C	O	0
			15	14	1	

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.

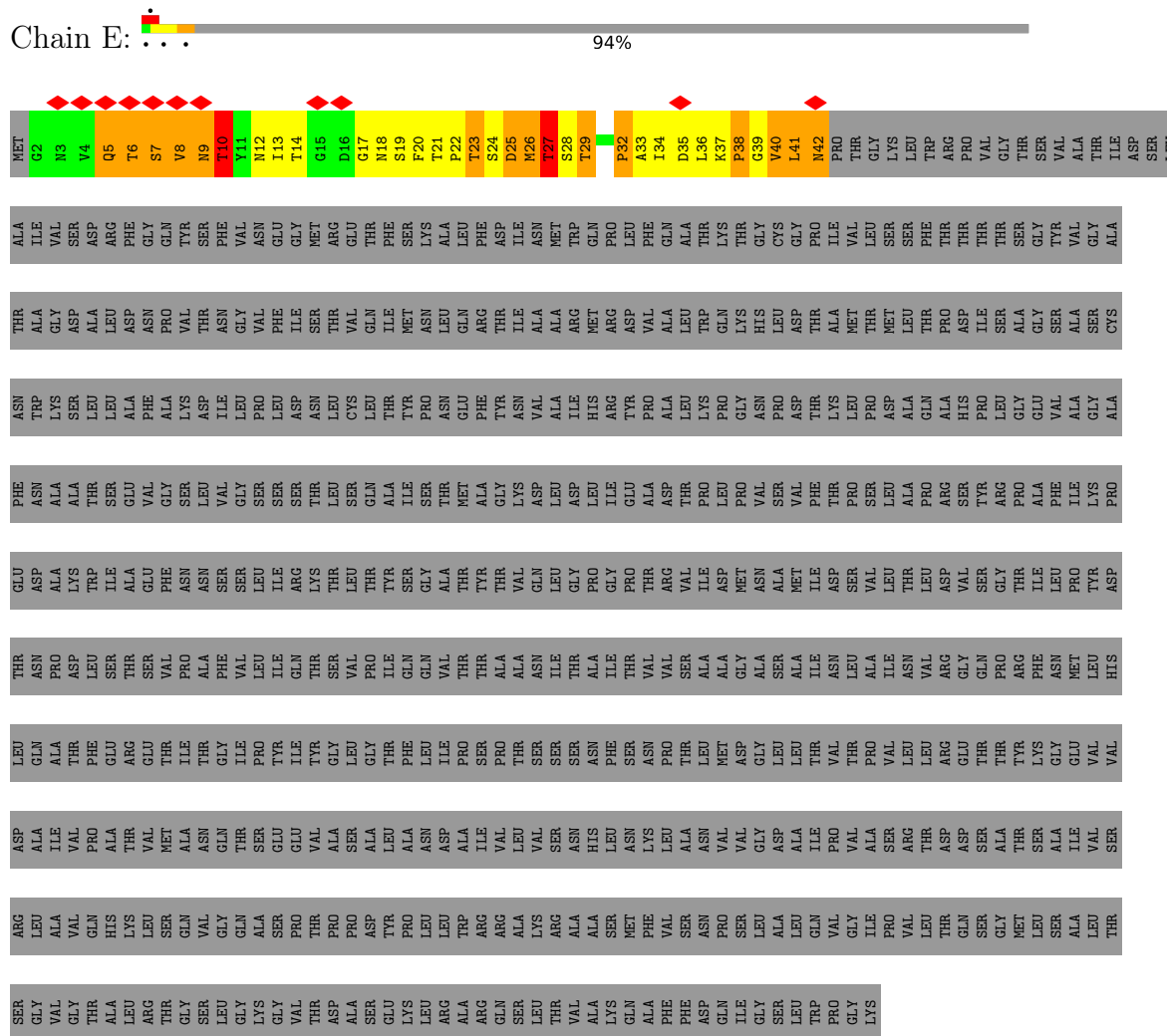
[illegible]

Chain B: 14% 23% 50% 17% 7%

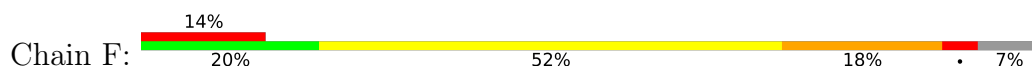




• Molecule 1: Outer capsid VP4

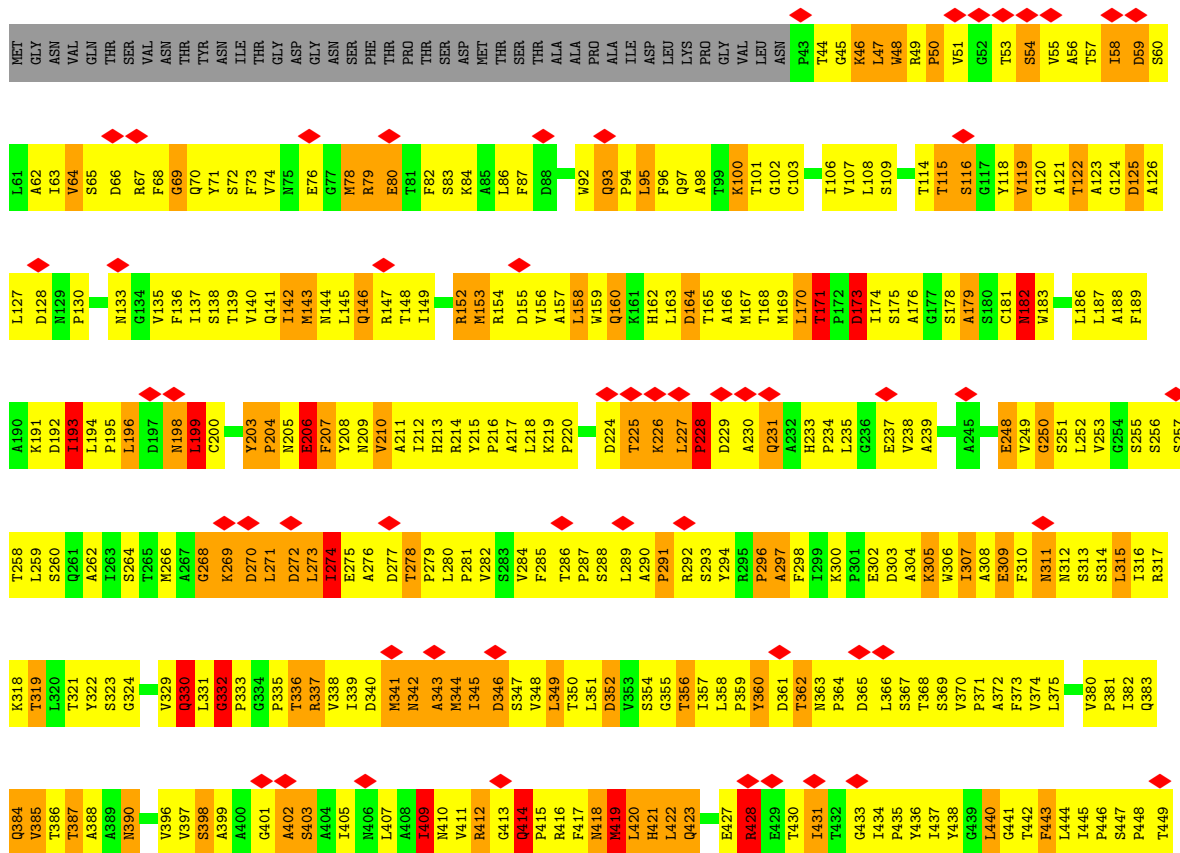
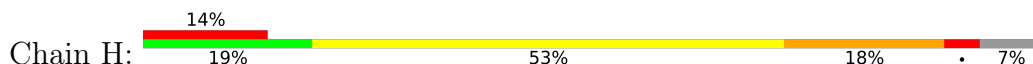


• Molecule 1: Outer capsid VP4



[illegible]

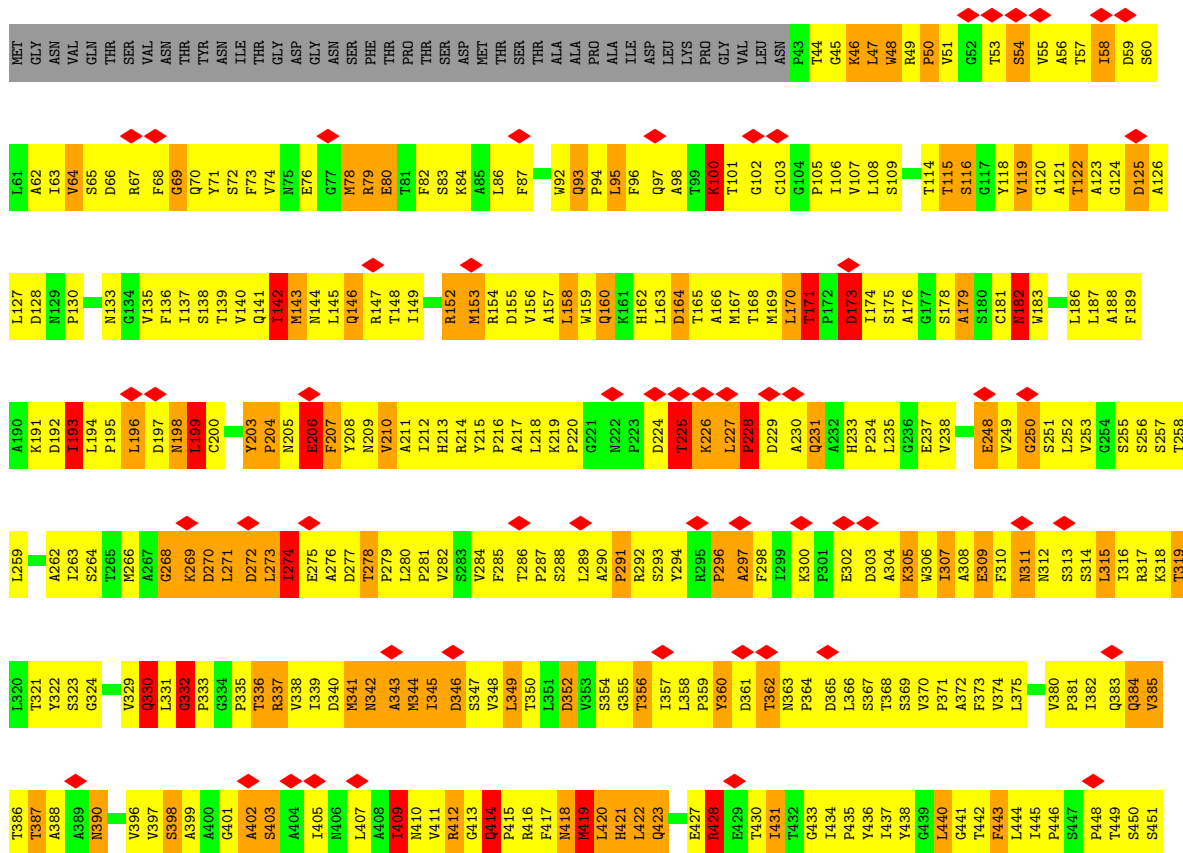
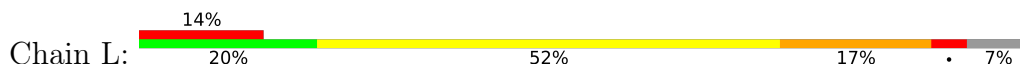
- Molecule 1: Outer capsid VP4





[illegible]

- Molecule 1: Outer capsid VP4



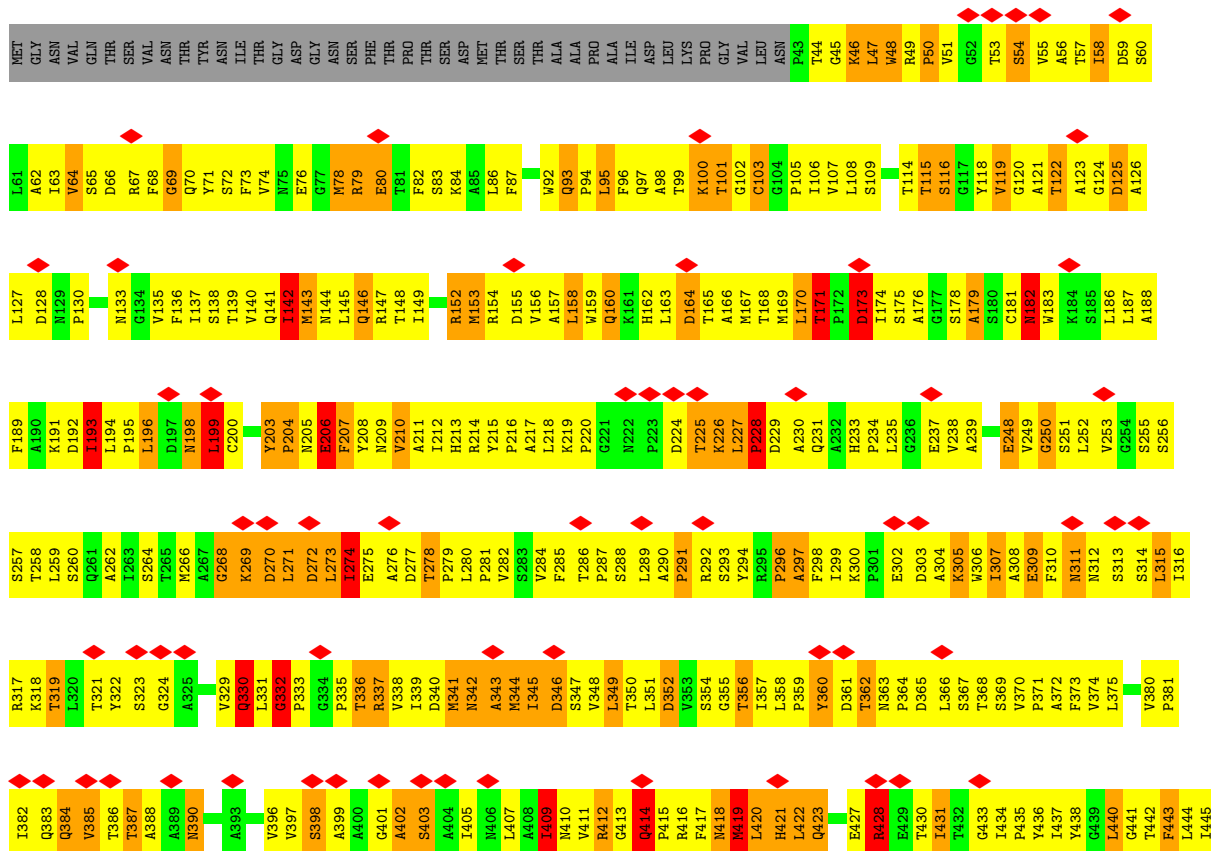
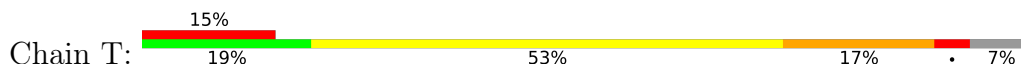


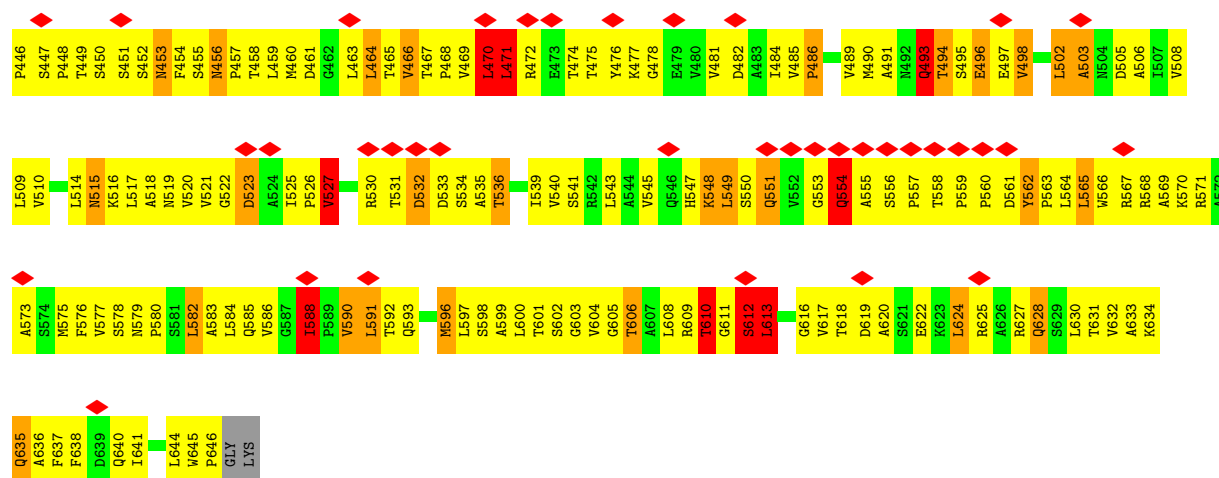




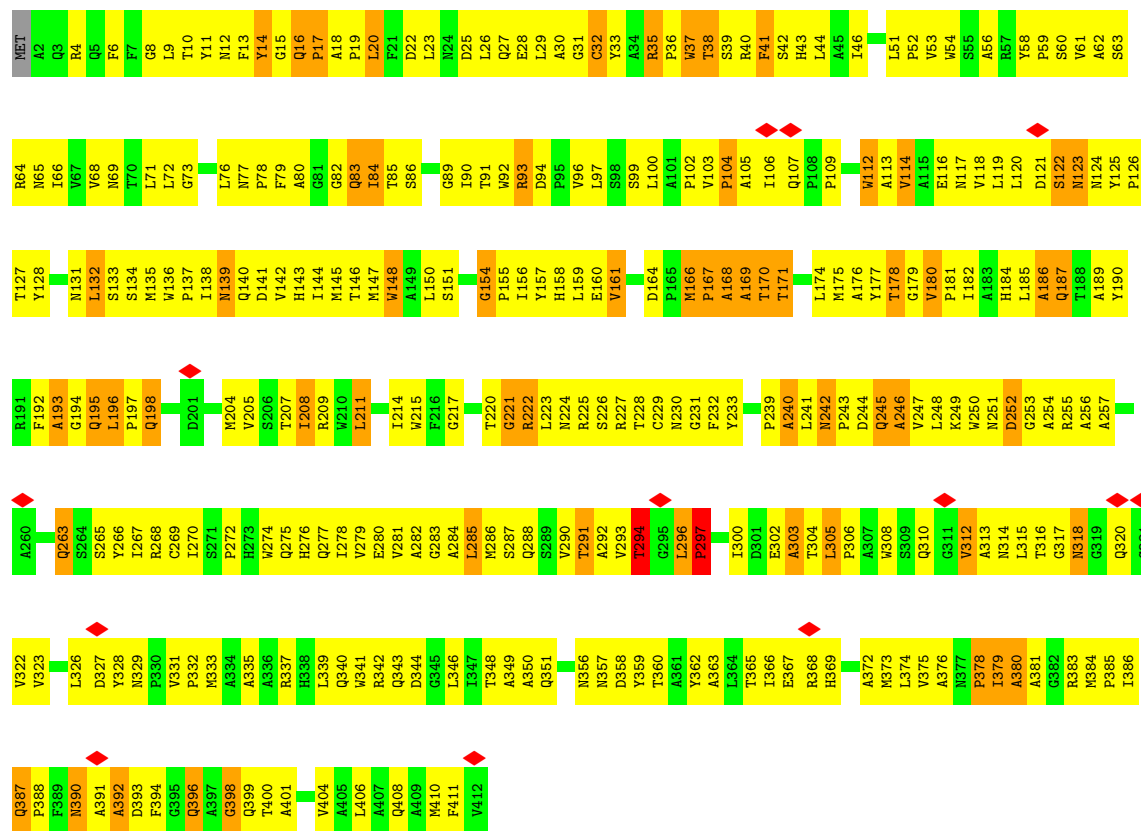
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- Molecule 1: Outer capsid VP4



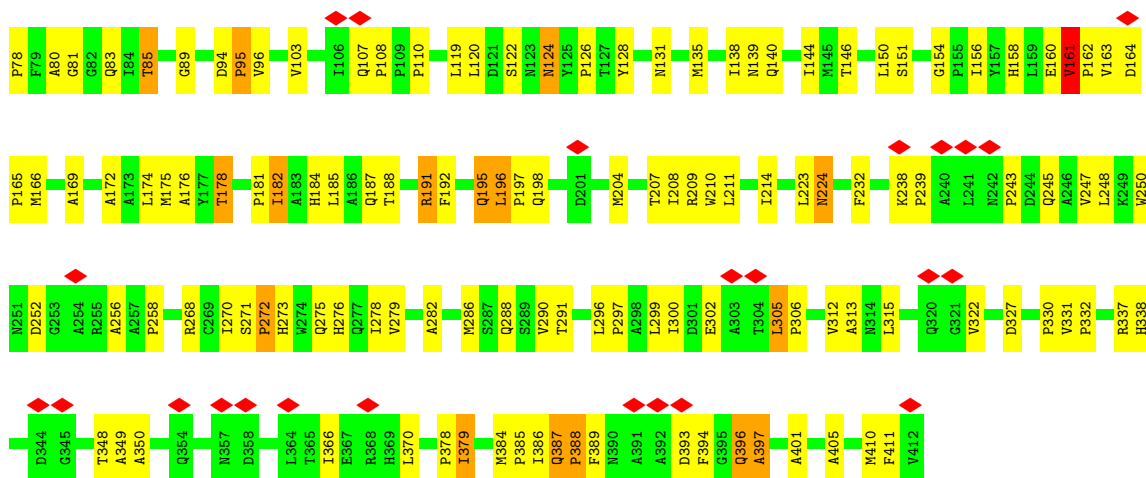


• Molecule 2: Core protein VP6

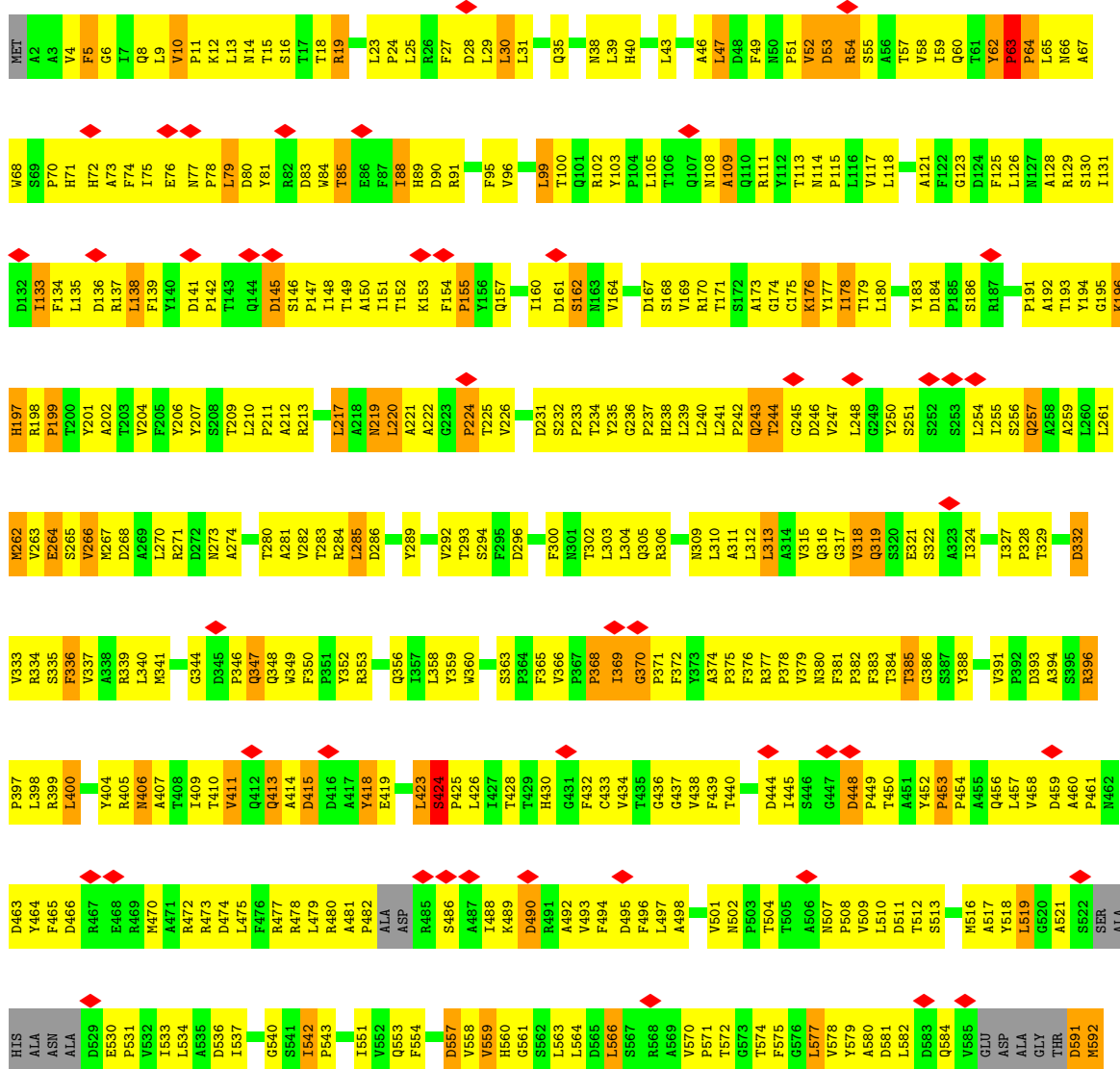


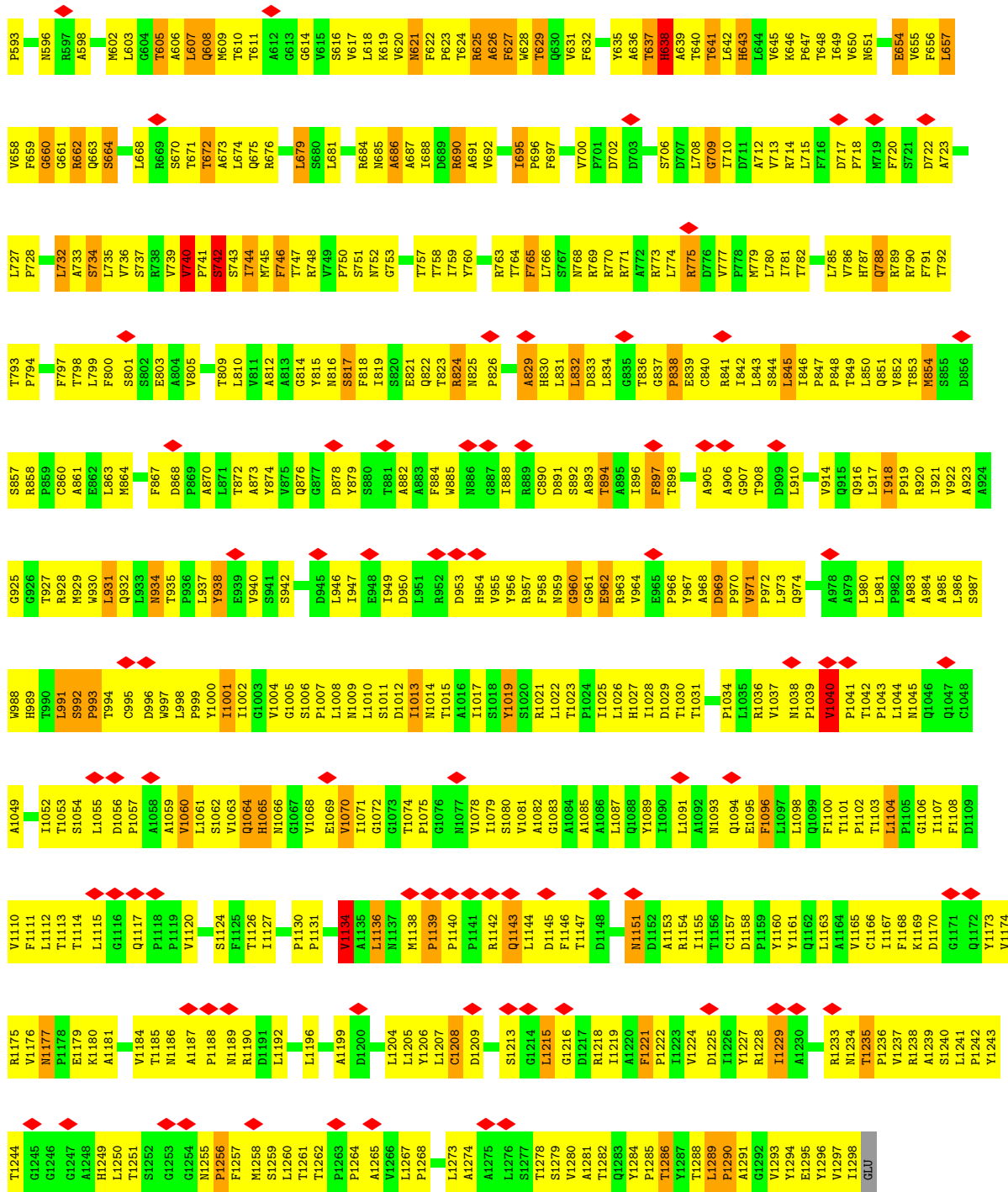
• Molecule 2: Core protein VP6



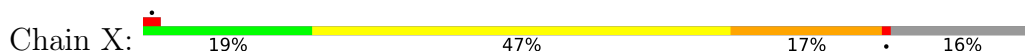


• Molecule 3: VP1





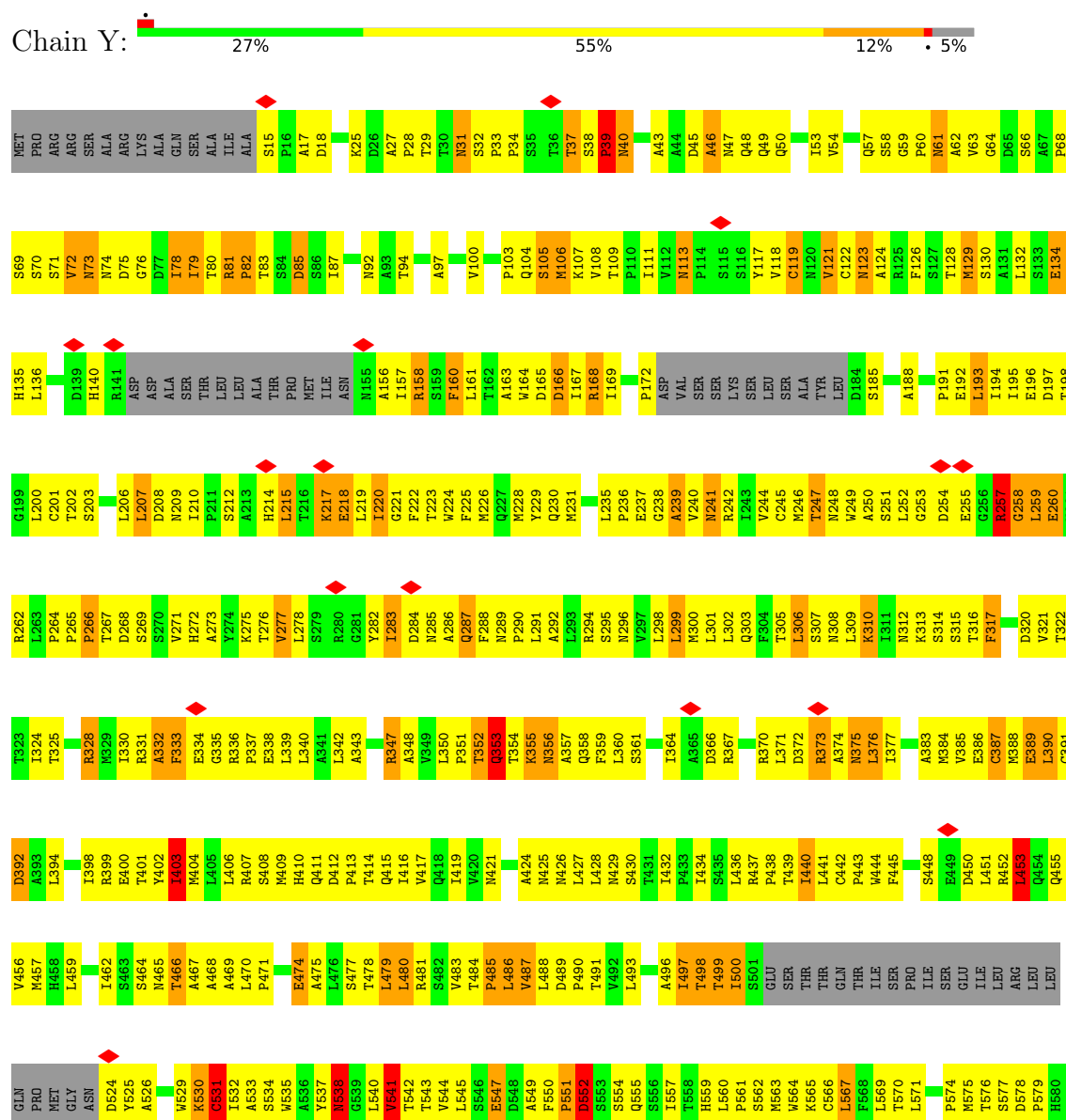
• Molecule 4: VP3



MET	ASN
PRO	ALA
ARG	VAL
GLY	GLY
ASP	ASP
SER	SER
ALA	ALA
ARG	ALA
LYS	PRO
ALA	SER
GLN	SER
SER	SER
ILE	VAL
ALA	ASN
ASN	ASN
ASP	ASP
PRO	GLY
ASP	ASP
ALA	ILE
ASP	ILE
THR	THR
ASN	ARG
VAL	VAL
PRO	PRO
PRO	THR
ALA	SER
ALA	ALA
LYS	ASP
THR	SER
THR	ILE
ALA	ALA
ALA	ALA
THR	VAL
SER	VAL
PRO	ASN
GLN	ASN
ALA	ILE
ALA	SER
ASP	SER
ALA	TTR
ALA	VAL
THR	CYS
GLN	ASN
GLY	
PRO	



- Molecule 4: VP3



L1172	L1173	D1174	P1175	N1176	Y1177	R1178	V1179	N1182	N1183	D1184	P1185	N1186	T1189	L1190	Y1191	N1192	S1193	L1194	Y1195	R1196	Y1197	N1198	Y1201	P1202	T1203	L1204	D1205	G1206	N1207	M1208	Y1209	V1210	R1211	S1212	A1213	T1214	S581	P582	F586	M587	A588	L589	A590	N591	L592	L593	A594	Q595	G596	E597	P598	T601	I599	A600	I601	Q602	V603	M606	H607	Q608	F609	I670	P671	P611	A612	S613	Q614	F615	S616	H617	P618	G619	V620	W621	P622	P623	L626	N627	P628	Q629	L630	I631	N632	P633	Q634	Q635	A636	P637	L638	L639	R640	A641	F642	A643	E644	H645	I646	R647	A648	N649	W650	P651	Q652	P653	S654	G655	F656	G657	Y658	G659	S660	T661	I599	L662	Q663	G664	A666	N667	L668	F669	I670	P671	S672	N673	K674	S613	T741	M675	V676	Y677	P683	L684	R685	R686	L687	T688	V689	A690	P691	T692	Y693	A696	M697	S698	N699	L705	A706	F707	F708	T709	T710	V711	T712	N713	S714	V715	N716	M717	T718	A719	T720	V721	N722	D723	L724	T725	R726	R727	T728	T729	T730	G731	M732	M733	T734	Q737	Q738	V739	K740	I800	A867	R868	H804	F807	A808	A809	A810	L811	P812	V813	D814	P815	A816	A817	I818	A821	C824	G825	Q826	T827	E828	T829	N830	L831	I832	P833	S834	H835	H836	Y837	G838	K839	N840	F841	A842	P843	L844	S847	N848	A849	M850	F851	R853	R856	A857	V858	I859	T860	R861	E862	A863	F864	V865	C866	L839	Q867	Y941	G942	G943	N944	V945	V946	R947	V950	P951	G952	G953	P954	S955	H956	I957	A960	V964	E965	F968	M969	M972	N973	L974	I901	M902	H903	V977	A978	G979	G980	N981	L982	V985	Q986	T987	A988	T989	R990	W993	S994	P995	A996	A997	P998	A1001	P1002	P1003	F1004	V1005	R1006	G1007	L1008	P1009	M1010	V1011	R1012	G1015	R1016	F1017	G1018	T1019	I1020	V1021	P1022	R1023	P1024	N1025	G1026	L1027	E1028	P1029	Q1030	L1031	I1032	D1033	D1034	G1035	N1036	V1037	P1038	R1039	D1040	I1041	A1042	G1043	Y1047	P1048	S1049	D1050	V1051	V1054	S1055	V1056	F1059	R1060	V1063	V1064	P1065	M1066	A1069	G1070	R1071	T1072	R1073	V1074	L1075	V1076	E1077	L1078	G1079	H1080	Y1081	V1082	Y1083	T1084	L1085	H1086	Y1087	Y1088	D1089	P1090	Q1091	I1092	S1093	L1094	D1095	E1096	A1097	P1098	Y1099	L1100	E1101	E1102	W1103	W1169	P1170	S1105	K1106	I1107	M1108	P1109	A1110	G1111	I1112	P1113	P1114	V1115	P1116	F1117	G1118	I1119	P1120	I1121	P1122	Q1123	G1127	L1128	T1129	A1130	R1131	R1132	V1133	H1134	Y1135	A1136	F1137	T1138	S1139	E1140	N1141	N1142	N1143	D1144	S1145	L1146	F1147	S1148	T1149	N1150	A1151	A1152	S1153	I1154	D1155	T1156	A1157	P1158	G1159	E1160	N1161	A1162	L1167	R1168	W1169	P1170	S1171	G1172	N1176	Y1177	R1178	V1179	N1182	N1183	D1184	P1185	N1186	T1189	L1190	Y1191	N1192	S1193	L1194	Y1195	R1196	Y1197	N1198	Y1201	P1202	T1203	L1204	D1205	G1206	N1207	M1208	Y1209	V1210	R1211	S1212	A1213	T1214	S581	P582	F586	M587	A588	L589	A590	N591	L592	L593	A594	Q595	G596	E597	P598	T601	I599	A600	I601	Q602	V603	M606	H607	Q608	F609	I670	P671	P611	A612	S613	Q614	F615	S616	H617	P618	G619	V620	W621	P622	P623	L626	N627	P628	Q629	L630	I631	N632	P633	Q634	Q635	A636	P637	L638	L639	R640	A641	F642	A643	E644	H645	I646	R647	A648	N649	W650	P651	Q652	P653	S654	G655	F656	G657	Y658	G659	S660	T661	I599	L662	Q663	G664	A666	N667	L668	F669	I670	P671	S672	N673	K674	S613	T741	M675	V676	Y677	P683	L684	R685	R686	L687	T688	V689	A690	P691	T692	Y693	A696	M697	S698	N699	L705	A706	F707	F708	T709	T710	V711	T712	N713	S714	V715	N716	M717	T718	A719	T720	V721	N722	D723	L724	T725	R726	R727	T728	T729	T730	G731	M732	M733	T734	Q737	Q738	V739	K740	I800	A867	R868	H804	F807	A808	A809	A810	L811	P812	V813	D814	P815	A816	A817	I818	A821	C824	G825	Q826	T827	E828	T829	N830	L831	I832	P833	S834	H835	H836	Y837	G838	K839	N840	F841	A842	P843	L844	S847	N848	A849	M850	F851	R853	R856	A857	V858	I859	T860	R861	E862	A863	F864	V865	C866	L839	Q867	Y941	G942	G943	N944	V945	V946	R947	V950	P951	G952	G953	P954	S955	H956	I957	A960	V964	E965	F968	M969	M972	N973	L974	I901	M902	H903	V977	A978	G979	G980	N981	L982	V985	Q986	T987	A988	T989	R990	W993	S994	P995	A996	A997	P998	A1001	P1002	P1003	F1004	V1005	R1006	G1007	L1008	P1009	M1010	V1011	R1012	G1015	R1016	F1017	G1018	T1019	I1020	V1021	P1022	R1023	P1024	N1025	G1026	L1027	E1028	P1029	Q1030	L1031	I1032	D1033	D1034	G1035	N1036	V1037	P1038	R1039	D1040	I1041	A1042	G1043	Y1047	P1048	S1049	D1050	V1051	V1054	S1055	V1056	F1059	R1060	V1063	V1064	P1065	M1066	A1069	G1070	R1071	T1072	R1073	V1074	L1075	V1076	E1077	L1078	G1079	H1080	Y1081	V1082	Y1083	T1084	L1085	H1086	Y1087	Y1088	D1089	P1090	Q1091	I1092	S1093	L1094	D1095	E1096	A1097	P1098	Y1099	L1100	E1101	E1102	W1103	W1169	P1170	S1105	K1106	I1107	M1108	P1109	A1110	G1111	I1112	P1113	P1114	V1115	P1116	F1117	G1118	I1119	P1120	I1121	P1122	Q1123	G1127	L1128	T1129	A1130	R1131	R1132	V1133	H1134	Y1135	A1136	F1137	T1138	S1139	E1140	N1141	N1142	N1143	D1144	S1145	L1146	F1147	S1148	T1149	N1150	A1151	A1152	S1153	I1154	D1155	T1156	A1157	P1158	G1159	E1160	N1161	A1162	L1167	R1168	W1169	P1170	S1171	G1172	N1176	Y1177	R1178	V1179	N1182	N1183	D1184	P1185	N1186	T1189	L1190	Y1191	N1192	S1193	L1194	Y1195	R1196	Y1197	N1198	Y1201	P1202	T1203	L1204	D1205	G1206	N1207	M1208	Y1209	V1210	R1211	S1212	A1213	T1214	S581	P582	F586	M587	A588	L589	A590	N591	L592	L593	A594	Q595	G596	E597	P598	T601	I599	A600	I601	Q602	V603	M606	H607	Q608	F609	I670	P671	P611	A612	S613	Q614	F615	S616	H617	P618	G619	V620	W621	P622	P623	L626	N627	P628	Q629	L630	I631	N632	P633	Q634	Q635	A636	P637	L638	L639	R640	A641	F642	A643	E644	H645	I646	R647	A648	N649	W650	P651	Q652	P653	S654	G655	F656	G657	Y658	G659	S660	T661	I599	L662	Q663	G664	A666	N667	L668	F669	I670	P671	S672	N673	K674	S613	T741	M675	V676	Y677	P683	L684	R685	R686	L687	T688	V689	A690	P691	T692	Y693	A696	M697	S698	N699	L705	A706	F707	F708	T709	T710	V711	T712	N713	S714	V715	N716	M717	T718	A719	T720	V721	N722	D723	L724	T725	R726	R727	T728	T729	T730	G731	M732	M733	T734	Q737	Q738	V739	K740	I800	A867	R868	H804	F807	A808	A809	A810	L811	P812	V813	D814	P815	A816	A817	I818	A821	C824	G825	Q826	T827	E828	T829	N830	L831	I832	P833	S834	H835	H836	Y837	G838	K839	N840	F841	A842	P843	L844	S847	N848	A849	M850	F851	R853	R856	A857	V858	I859	T860	R861	E862	A863	F864	V865	C866	L839	Q867	Y941	G942	G943	N944	V945	V946	R947	V950	P951	G952	G953	P954	S955	H956	I957	A960	V964	E965	F968	M969	M972	N973	L974	I901	M902	H903	V977	A978	G979	G980	N981	L982	V985	Q986	T987	A988	T989	R990	W993	S994	P995	A996	A997	P998	A1001	P1002	P1003	F1004	V1005	R1006	G1007	L1008	P1009	M1010	V1011	R1012	G1015	R1016	F1017	G1018	T1019	I1020	V1021	P1022	R1023	P1024	N1025	G1026	L1027	E1028	P1029	Q1030	L1031	I1032	D1033	D1034	G1035	N1036	V1037	P1038	R1039	D1040	I1041	A1042	G1043	Y1047	P1048	S1049	D1050	V1051	V1054	S1055	V1056	F1059	R1060	V1063	V1064	P1065	M1066	A1069	G1070	R1071	T1072	R1073	V1074	L1075	V1076	E1077	L1078	G1079	H1080	Y1081	V1082	Y1083	T1084	L1085	H1086	Y1087	Y1088	D1089	P1090	Q1091	I1092	S1093	L1094	D1095	E1096	A1097	P1098	Y1099	L1100	E1101	E1102	W1103	W1169	P1170	S1105	K1106	I1107	M1108	P1109	A1110	G1111	I1112	P1113	P1114	V1115	P1116	F1117	G1118	I1119	P1120	I1121	P1122	Q1123	G1127	L1128	T1129	A1130	R1131	R1132	V1133	H1134	Y1135	A1136	F1137	T1138	S1139	E1140	N1141	N1142	N1143	D1144	S1145	L1146	F1147	S1148	T1149	N1150	A1151	A1152	S1153	I1154	D1155	T1156	A1157	P1158	G1159	E1160	N1161	A1162	L1167	R1168	W1169	P1170	S1171	G1172	N1176	Y1177	R1178	V1179	N1182	N1183	D1184	P1185	N1186	T1189	L1190	Y1191	N1192	S1193	L1194	Y1195	R1196	Y1197	N1198	Y1201	P1202	T1203	L1204	D1205	G1206	N1207	M1208	Y1209	V1210	R1211	S1212	A1213	T1214	S581	P582	F586	M587	A588	L589	A590	N591	L592	L593	A594	Q595	G596	E597	P598	T601	I599	A600	I601	Q602	V603	M606	H607	Q608	F609	I670	P671	P611	A612	S613	Q614	F615	S616	H617	P618	G619	V620	W621	P622	P623	L626	N627	P628	Q629	L630	I631	N632	P633	Q634	Q635	A636	P637	L638	L639	R640	A641	F642	A643	E644	H645	I646	R647	A648	N649	W650	P651	Q652	P653	S654	G655	F656	G657	Y658	G659	S660	T661	I599	L662	Q663	G664	A666	N667	L668	F669	I670	P671	S672	N673	K674	S613	T741	M675	V676	Y677	P683	L684	R685	R686	L687	T688	V689	A690	P691	T692	Y693	A696	M697	S698	N699	L705	A706
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	18464	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	57700	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.305	Depositor
Minimum map value	-0.193	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	814.0, 814.0, 814.0	wwPDB
Map dimensions	740, 740, 740	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.90	2/295 (0.7%)	1.53	6/405 (1.5%)
1	B	0.70	1/4601 (0.0%)	1.28	52/6295 (0.8%)
1	C	0.90	2/295 (0.7%)	1.53	6/405 (1.5%)
1	D	0.70	1/4601 (0.0%)	1.30	54/6295 (0.9%)
1	E	0.90	2/295 (0.7%)	1.53	6/405 (1.5%)
1	F	0.70	1/4601 (0.0%)	1.28	52/6295 (0.8%)
1	G	0.89	2/286 (0.7%)	1.38	3/391 (0.8%)
1	H	0.70	1/4601 (0.0%)	1.28	53/6295 (0.8%)
1	I	0.90	2/295 (0.7%)	1.53	6/405 (1.5%)
1	J	0.69	1/4601 (0.0%)	1.28	53/6295 (0.8%)
1	K	0.90	2/295 (0.7%)	1.53	6/405 (1.5%)
1	L	0.70	1/4601 (0.0%)	1.28	52/6295 (0.8%)
1	M	0.89	2/286 (0.7%)	1.38	3/391 (0.8%)
1	N	0.70	1/4601 (0.0%)	1.28	52/6295 (0.8%)
1	O	0.90	2/295 (0.7%)	1.53	6/405 (1.5%)
1	P	0.70	1/4601 (0.0%)	1.28	52/6295 (0.8%)
1	Q	0.90	2/295 (0.7%)	1.53	6/405 (1.5%)
1	R	0.70	1/4601 (0.0%)	1.28	52/6295 (0.8%)
1	S	0.89	2/286 (0.7%)	1.38	3/391 (0.8%)
1	T	0.70	1/4601 (0.0%)	1.28	51/6295 (0.8%)
2	U	0.38	0/3233	0.93	16/4443 (0.4%)
2	V	0.41	0/3233	0.88	5/4443 (0.1%)
3	W	0.38	0/10148	1.00	52/13935 (0.4%)
4	X	0.65	5/8078 (0.1%)	1.16	69/11071 (0.6%)
4	Y	0.45	1/9056 (0.0%)	1.04	52/12412 (0.4%)
All	All	0.63	36/82681 (0.0%)	1.19	768/113262 (0.7%)

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	B	0	1
1	D	0	1
1	F	0	1
1	H	0	1
1	J	0	1
1	L	0	1
1	N	0	1
1	P	0	1
1	R	0	1
1	T	0	1
4	X	0	3
4	Y	0	2
All	All	0	15

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	227	LEU	N-CA	7.64	1.52	1.45
1	H	227	LEU	N-CA	7.64	1.52	1.45
1	R	227	LEU	N-CA	7.63	1.52	1.45
1	F	227	LEU	N-CA	7.60	1.52	1.45
1	D	227	LEU	N-CA	7.60	1.52	1.45

The worst 5 of 768 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	51	VAL	N-CA-C	17.02	126.53	110.53
4	X	526	ALA	N-CA-C	-11.80	98.50	111.36
3	W	63	PRO	N-CA-C	11.78	125.07	110.70
1	F	551	GLN	OE1-CD-NE2	-10.57	112.03	122.60
1	D	551	GLN	OE1-CD-NE2	-10.56	112.04	122.60

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	337	ARG	Sidechain
1	D	337	ARG	Sidechain
1	F	337	ARG	Sidechain
1	H	337	ARG	Sidechain
1	J	337	ARG	Sidechain

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	291	0	277	57	0
1	B	4508	0	4555	671	0
1	C	291	0	277	81	0
1	D	4508	0	4555	931	0
1	E	291	0	277	80	0
1	F	4508	0	4555	902	0
1	G	284	0	267	58	0
1	H	4508	0	4555	890	0
1	I	291	0	277	84	0
1	J	4508	0	4555	916	0
1	K	291	0	277	81	0
1	L	4508	0	4555	904	0
1	M	284	0	267	60	0
1	N	4508	0	4555	908	0
1	O	291	0	277	78	0
1	P	4508	0	4555	927	0
1	Q	291	0	277	88	0
1	R	4508	0	4555	912	0
1	S	284	0	267	60	0
1	T	4508	0	4555	904	0
2	U	3138	0	3061	471	0
2	V	3138	0	3061	181	0
3	W	9882	0	9821	1088	0
4	X	7873	0	7851	1319	0
4	Y	8835	0	8748	1111	0
5	A	15	0	27	27	0
5	C	15	0	27	31	0
5	E	15	0	27	27	0
5	G	15	0	27	28	0
5	I	15	0	27	29	0
5	K	15	0	27	27	0
5	M	15	0	27	26	0
5	O	15	0	27	28	0
5	Q	15	0	27	27	0
5	S	15	0	27	30	0
All	All	80985	0	81102	12113	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 75.

The worst 5 of 12113 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:32:CYS:HB3	4:X:958:HIS:CE1	1.55	1.38
4:X:464:SER:HB2	4:Y:500:ILE:CG2	1.52	1.38
1:R:628:GLN:NE2	3:W:870:ALA:HA	1.41	1.35
1:D:469:VAL:HG21	1:F:575:MET:CE	1.59	1.33
1:F:469:VAL:HG21	1:H:575:MET:CE	1.59	1.33

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	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	B	602/648 (93%)	407 (68%)	134 (22%)	61 (10%)	0	3
1	C	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	D	602/648 (93%)	416 (69%)	129 (21%)	57 (10%)	0	3
1	E	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	F	602/648 (93%)	408 (68%)	133 (22%)	61 (10%)	0	3
1	G	37/648 (6%)	24 (65%)	8 (22%)	5 (14%)	0	1
1	H	602/648 (93%)	409 (68%)	132 (22%)	61 (10%)	0	3
1	I	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	J	602/648 (93%)	411 (68%)	132 (22%)	59 (10%)	0	3
1	K	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	L	602/648 (93%)	409 (68%)	132 (22%)	61 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	37/648 (6%)	24 (65%)	8 (22%)	5 (14%)	0	1
1	N	602/648 (93%)	408 (68%)	133 (22%)	61 (10%)	0	3
1	O	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	P	602/648 (93%)	410 (68%)	132 (22%)	60 (10%)	0	3
1	Q	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	1
1	R	602/648 (93%)	406 (67%)	135 (22%)	61 (10%)	0	3
1	S	37/648 (6%)	24 (65%)	8 (22%)	5 (14%)	0	1
1	T	602/648 (93%)	406 (67%)	135 (22%)	61 (10%)	0	3
2	U	409/412 (99%)	283 (69%)	81 (20%)	45 (11%)	0	2
2	V	409/412 (99%)	330 (81%)	60 (15%)	19 (5%)	2	13
3	W	1276/1299 (98%)	1063 (83%)	173 (14%)	40 (3%)	3	20
4	X	1012/1214 (83%)	714 (71%)	219 (22%)	79 (8%)	1	5
4	Y	1146/1214 (94%)	860 (75%)	204 (18%)	82 (7%)	1	6
All	All	10656/17511 (61%)	7587 (71%)	2151 (20%)	918 (9%)	1	4

5 of 918 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	ASP
1	B	103	CYS
1	B	179	ALA
1	B	225	THR
1	B	228	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	34/536 (6%)	25 (74%)	9 (26%)	0	2
1	B	499/536 (93%)	413 (83%)	86 (17%)	2	10
1	C	34/536 (6%)	25 (74%)	9 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	499/536 (93%)	410 (82%)	89 (18%)	2	8
1	E	34/536 (6%)	25 (74%)	9 (26%)	0	2
1	F	499/536 (93%)	413 (83%)	86 (17%)	2	10
1	G	32/536 (6%)	23 (72%)	9 (28%)	0	2
1	H	499/536 (93%)	413 (83%)	86 (17%)	2	10
1	I	34/536 (6%)	25 (74%)	9 (26%)	0	2
1	J	499/536 (93%)	412 (83%)	87 (17%)	2	9
1	K	34/536 (6%)	25 (74%)	9 (26%)	0	2
1	L	499/536 (93%)	412 (83%)	87 (17%)	2	9
1	M	32/536 (6%)	23 (72%)	9 (28%)	0	2
1	N	499/536 (93%)	411 (82%)	88 (18%)	2	9
1	O	34/536 (6%)	25 (74%)	9 (26%)	0	2
1	P	499/536 (93%)	410 (82%)	89 (18%)	2	8
1	Q	34/536 (6%)	25 (74%)	9 (26%)	0	2
1	R	499/536 (93%)	412 (83%)	87 (17%)	2	9
1	S	32/536 (6%)	23 (72%)	9 (28%)	0	2
1	T	499/536 (93%)	411 (82%)	88 (18%)	2	9
2	U	325/326 (100%)	305 (94%)	20 (6%)	16	45
2	V	325/326 (100%)	306 (94%)	19 (6%)	18	47
3	W	1082/1092 (99%)	979 (90%)	103 (10%)	8	29
4	X	869/1030 (84%)	726 (84%)	143 (16%)	2	11
4	Y	976/1030 (95%)	865 (89%)	111 (11%)	5	21
All	All	8901/14524 (61%)	7542 (85%)	1359 (15%)	5	13

5 of 1359 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	360	TYR
4	X	432	ILE
1	T	548	LYS
1	T	356	THR
3	W	418	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 416 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	144	ASN
2	V	158	HIS
4	Y	835	HIS
1	T	330	GLN
2	U	69	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	MYR	K	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	I	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	M	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	S	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	Q	649	1	13,14,15	0.45	0	12,13,15	0.49	0
5	MYR	G	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	A	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	E	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	C	649	1	13,14,15	0.44	0	12,13,15	0.49	0
5	MYR	O	649	1	13,14,15	0.44	0	12,13,15	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MYR	K	649	1	-	8/12/12/13	-
5	MYR	I	649	1	-	8/12/12/13	-
5	MYR	M	649	1	-	8/12/12/13	-
5	MYR	S	649	1	-	8/12/12/13	-
5	MYR	Q	649	1	-	8/12/12/13	-
5	MYR	G	649	1	-	8/12/12/13	-
5	MYR	A	649	1	-	8/12/12/13	-
5	MYR	E	649	1	-	8/12/12/13	-
5	MYR	C	649	1	-	8/12/12/13	-
5	MYR	O	649	1	-	8/12/12/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	649	MYR	C3-C4-C5-C6
5	K	649	MYR	C3-C4-C5-C6
5	Q	649	MYR	C3-C4-C5-C6
5	A	649	MYR	C3-C4-C5-C6
5	C	649	MYR	C3-C4-C5-C6

There are no ring outliers.

10 monomers are involved in 280 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	649	MYR	27	0
5	I	649	MYR	29	0
5	M	649	MYR	26	0
5	S	649	MYR	30	0
5	Q	649	MYR	27	0
5	G	649	MYR	28	0
5	A	649	MYR	27	0
5	E	649	MYR	27	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	649	MYR	31	0
5	O	649	MYR	28	0

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.

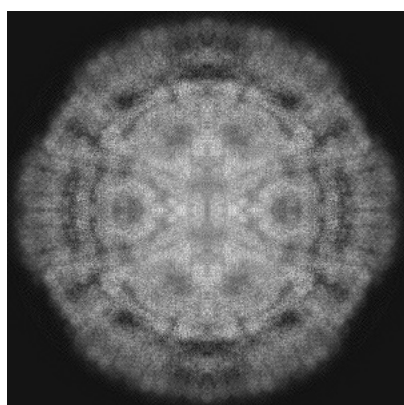
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5160. These allow visual inspection of the internal detail of the map and identification of artifacts.

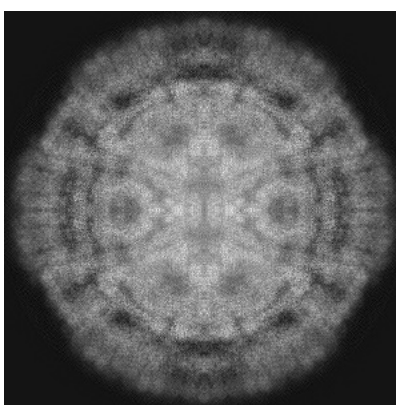
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

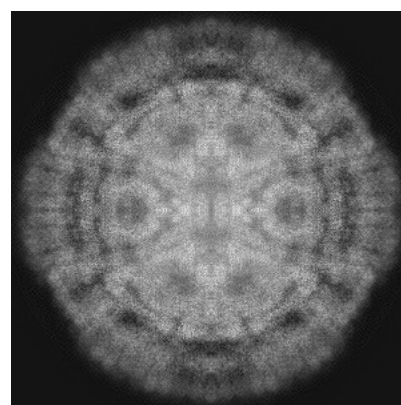
6.1.1 Primary map



X



Y

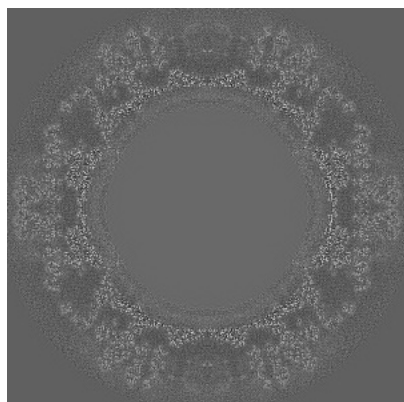


Z

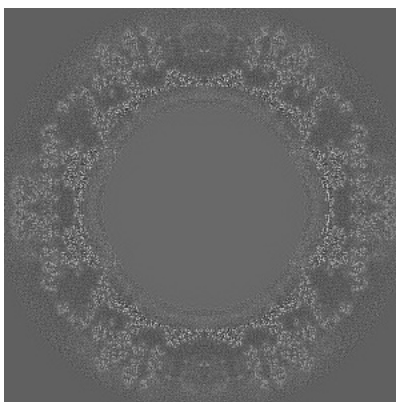
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

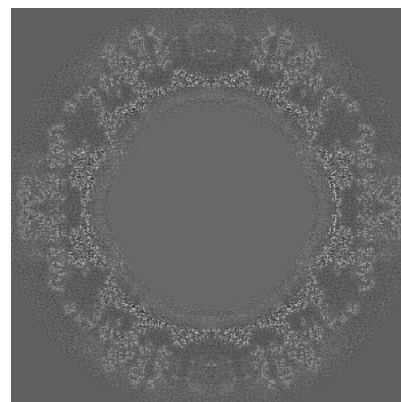
6.2.1 Primary map



X Index: 370



Y Index: 370

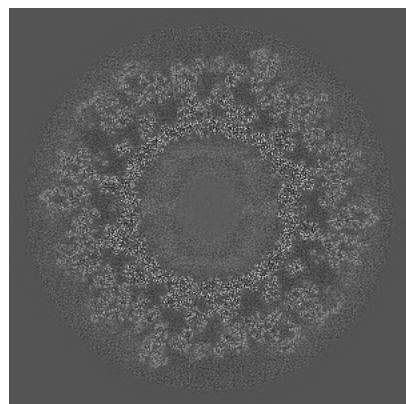


Z Index: 370

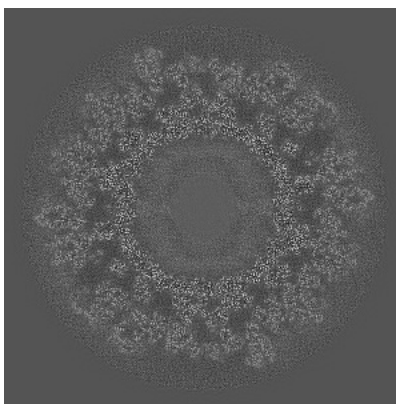
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

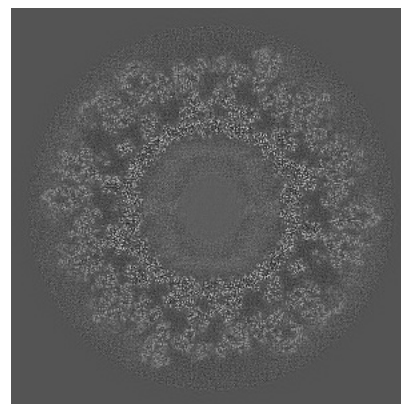
6.3.1 Primary map



X Index: 194



Y Index: 546

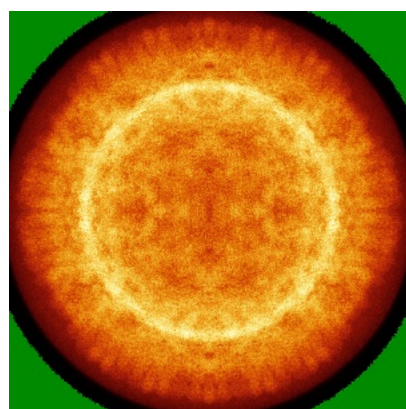


Z Index: 194

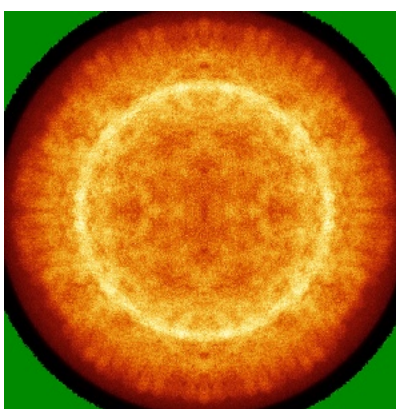
The images above show the largest variance slices of the map in three orthogonal directions.

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

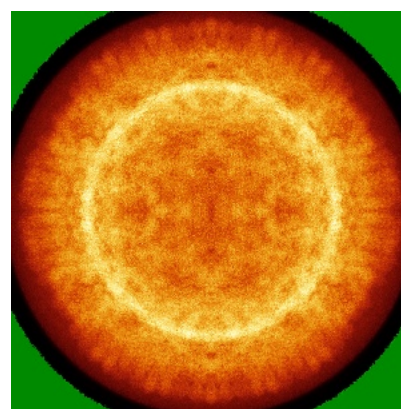
6.4.1 Primary map



X



Y

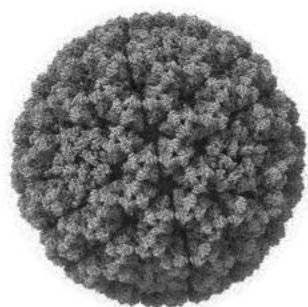


Z

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](#)

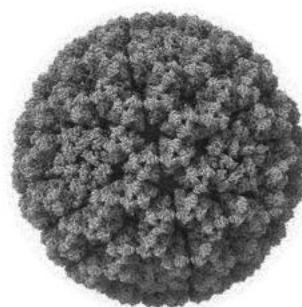
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. 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 shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

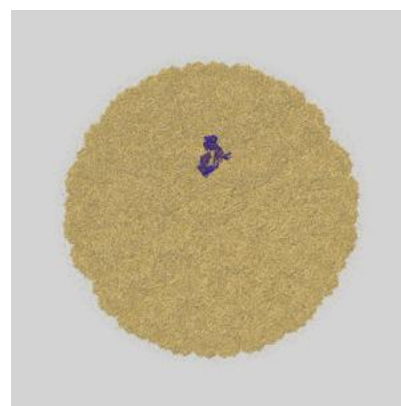
6.6.1 emd_5160_msk_1.map [i](#)



X



Y

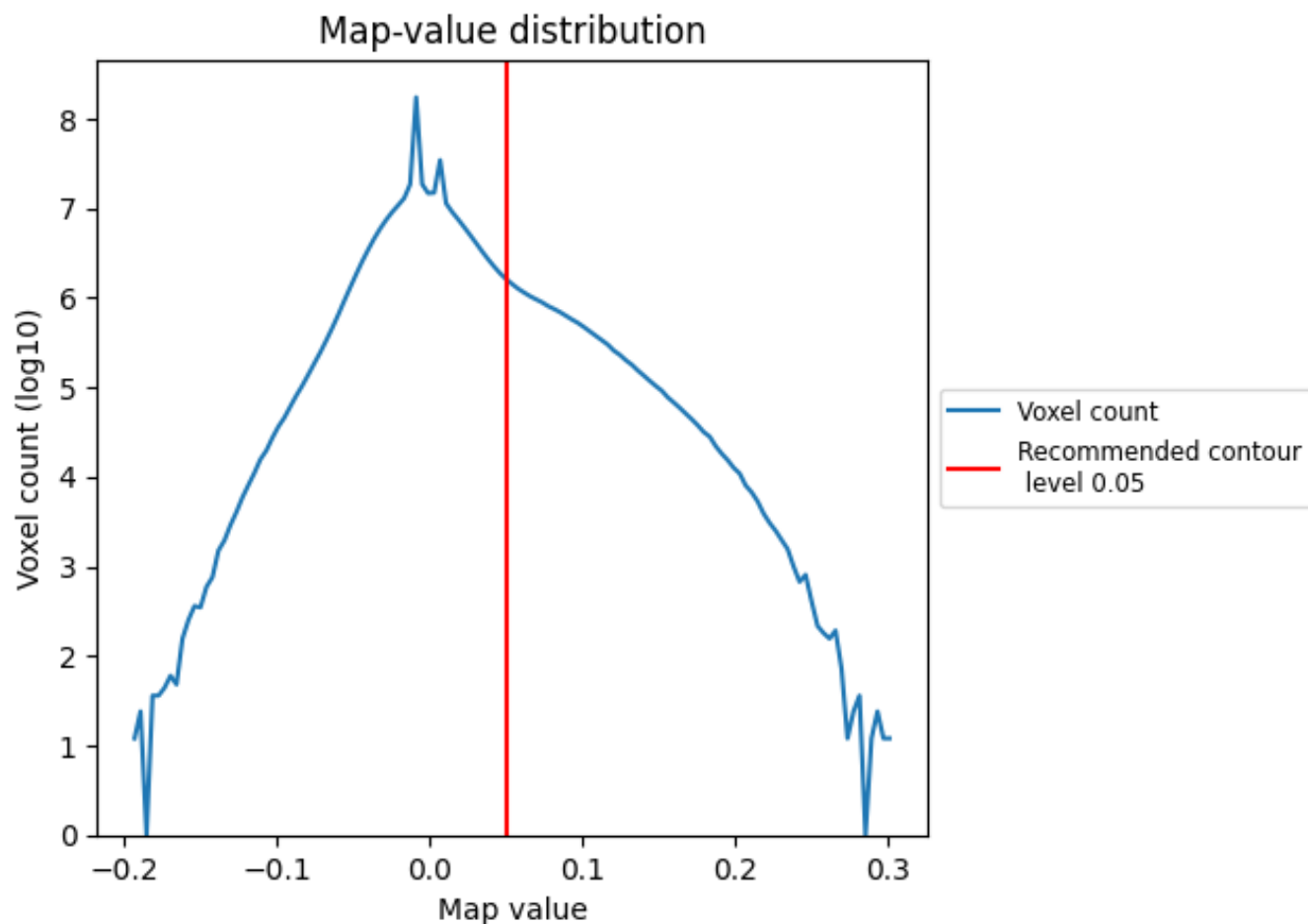


Z

7 Map analysis [i](#)

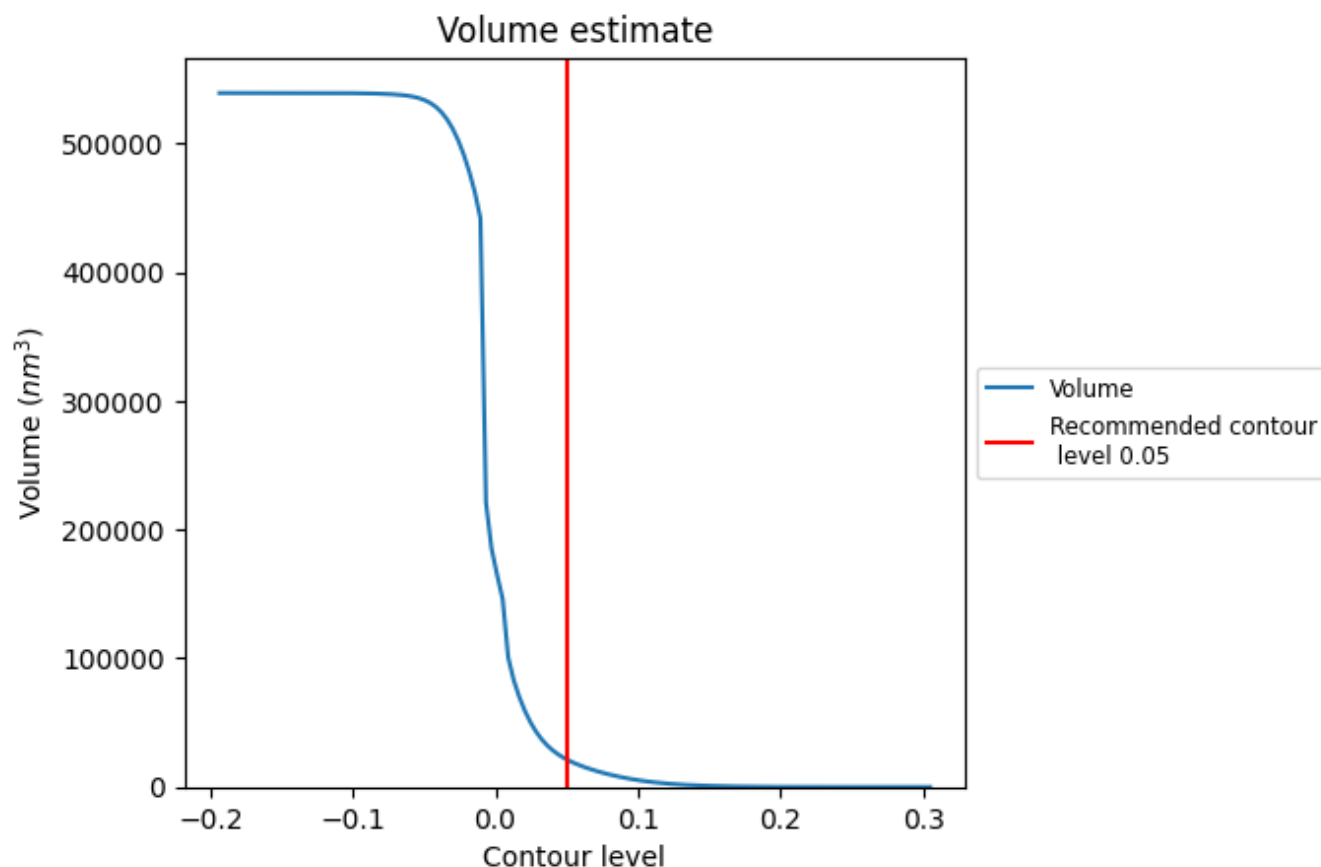
This section contains the results of statistical analysis of the map.

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.

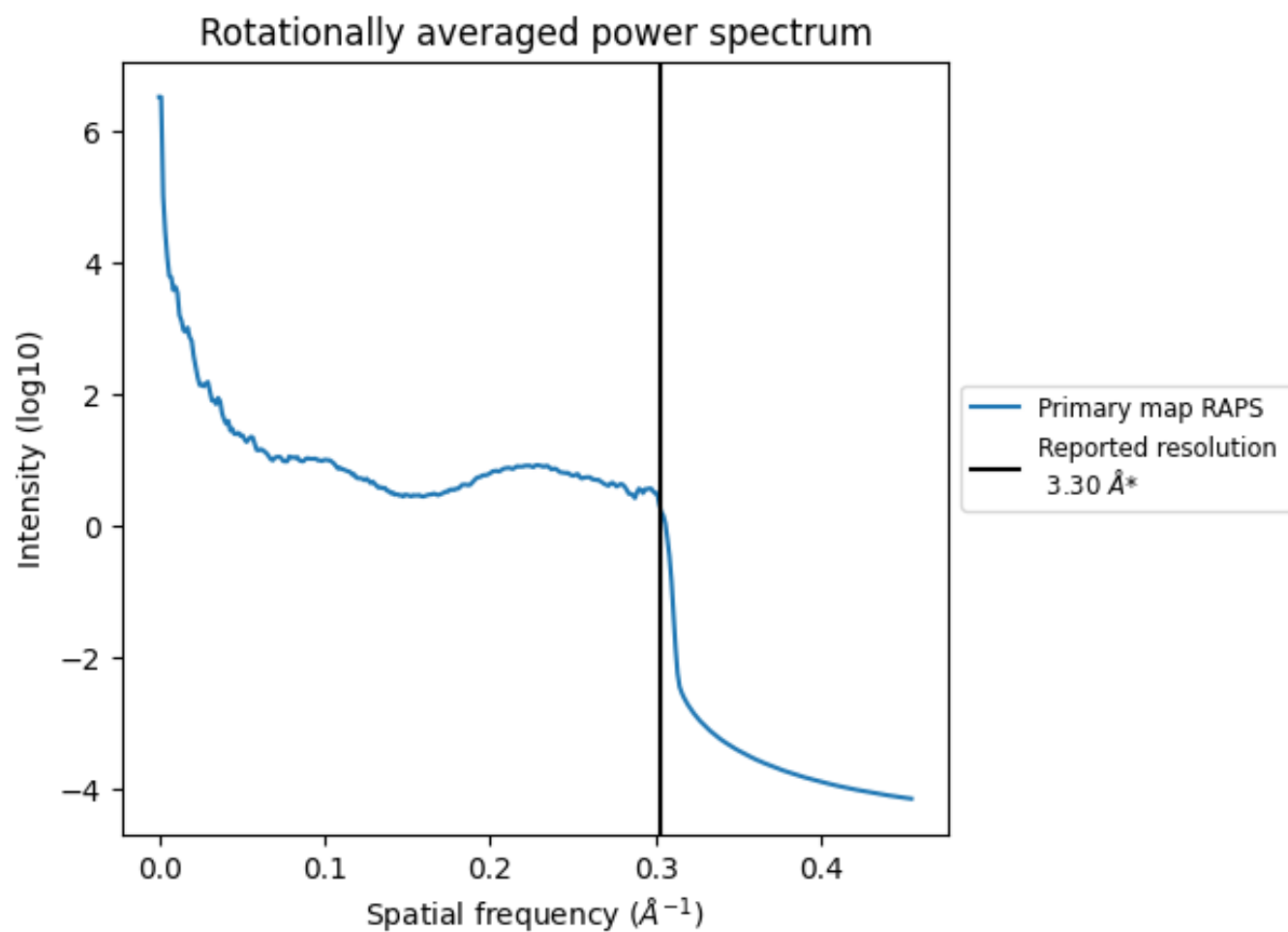
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 21462 nm^3 ; this corresponds to an approximate mass of 19387 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 0.303 Å⁻¹

8 Fourier-Shell correlation

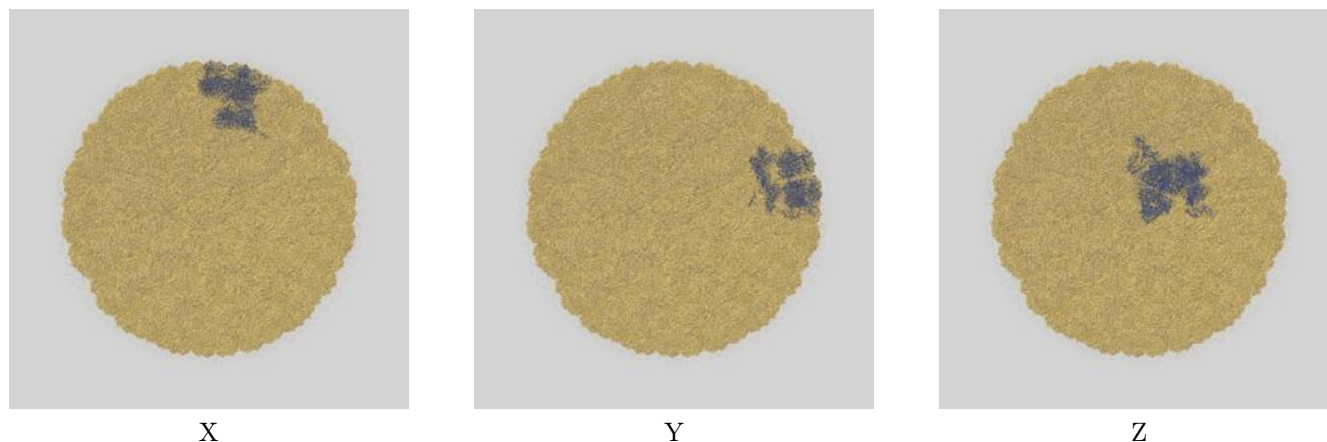
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5160 and PDB model 3IYL. Per-residue inclusion information can be found in section [3](#) on page [8](#).

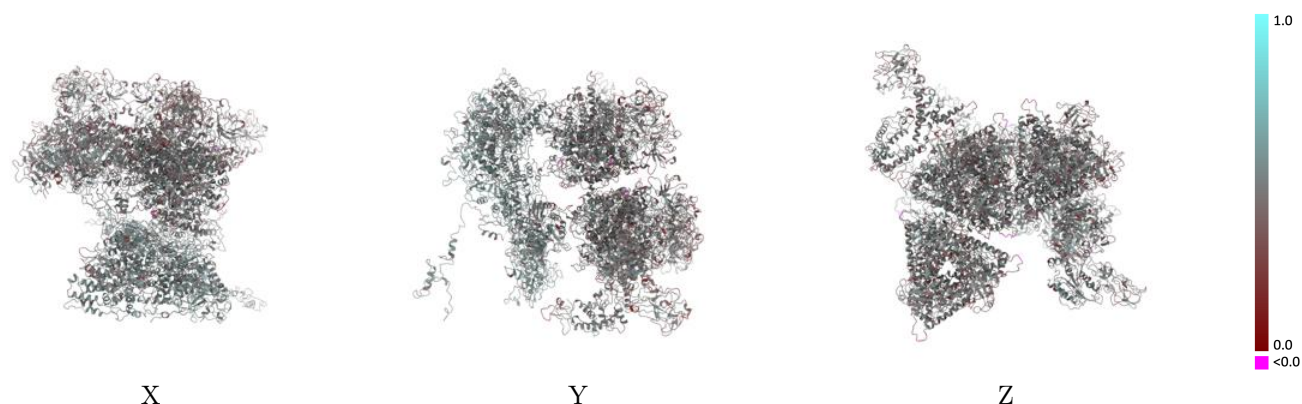
9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



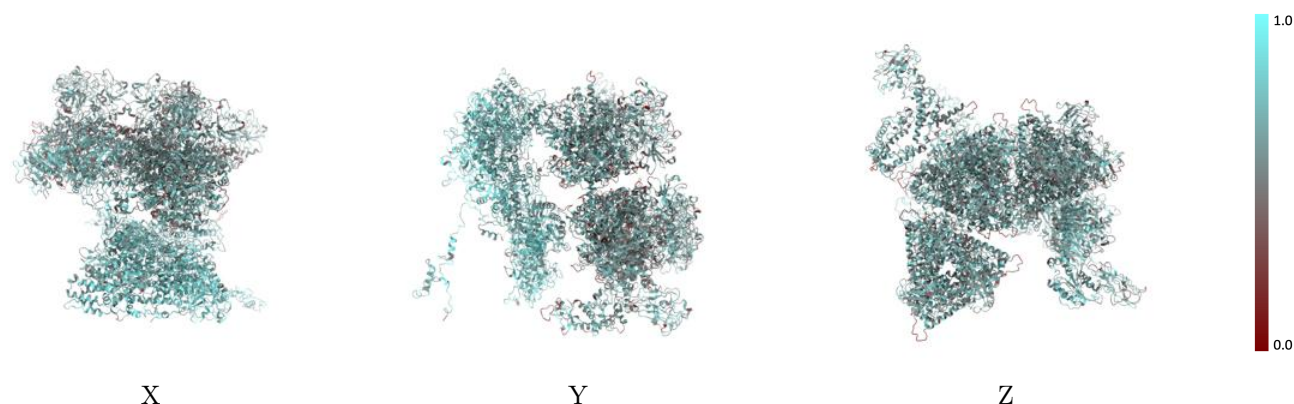
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



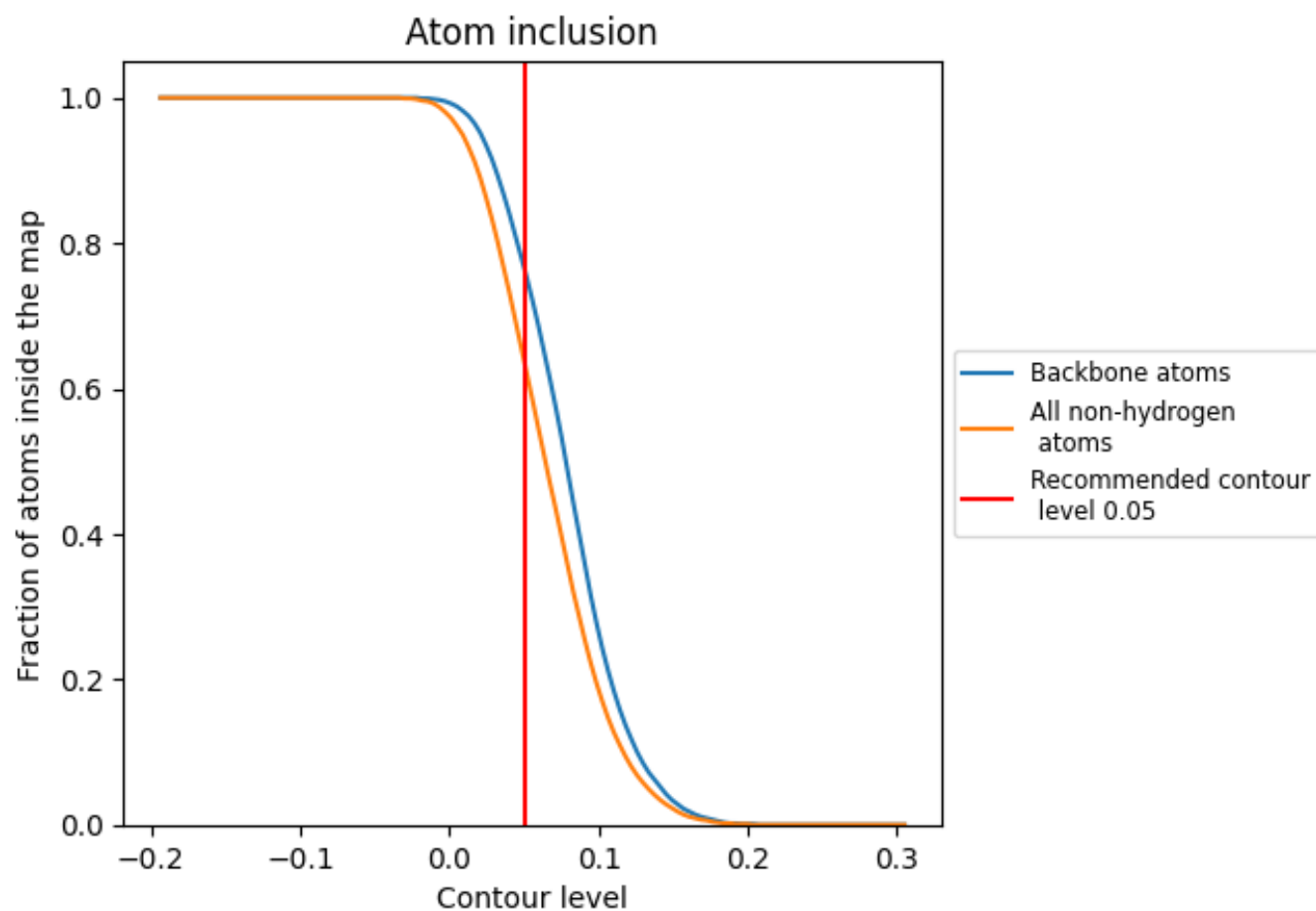
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 64% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6400	 0.4680
A	 0.4850	 0.4200
B	 0.5820	 0.4440
C	 0.5180	 0.4100
D	 0.5980	 0.4510
E	 0.4980	 0.4050
F	 0.5930	 0.4470
G	 0.5000	 0.4020
H	 0.5930	 0.4490
I	 0.4980	 0.4310
J	 0.5920	 0.4490
K	 0.4850	 0.3870
L	 0.5890	 0.4460
M	 0.5100	 0.4070
N	 0.5900	 0.4550
O	 0.5210	 0.3990
P	 0.5880	 0.4440
Q	 0.4880	 0.4090
R	 0.5920	 0.4530
S	 0.4660	 0.3980
T	 0.5860	 0.4460
U	 0.7550	 0.5140
V	 0.7040	 0.4740
W	 0.6610	 0.4690
X	 0.7580	 0.5230
Y	 0.7530	 0.5230

