



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:11 AM UTC

PDB ID : 7XR3 / pdb_00007xr3
EMDB ID : EMD-33404
Title : 3.4 Angstrom cryoEM D5 reconstruction of mud crab reovirus
Authors : Zhang, Q.F.; Gao, Y.Z.
Deposited on : 2022-05-09
Resolution : 3.70 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:

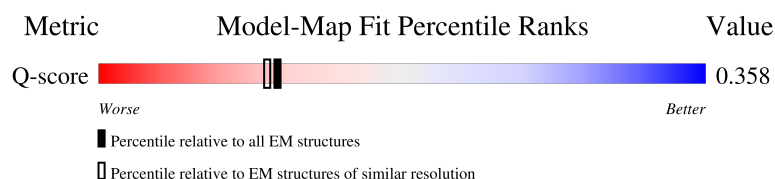
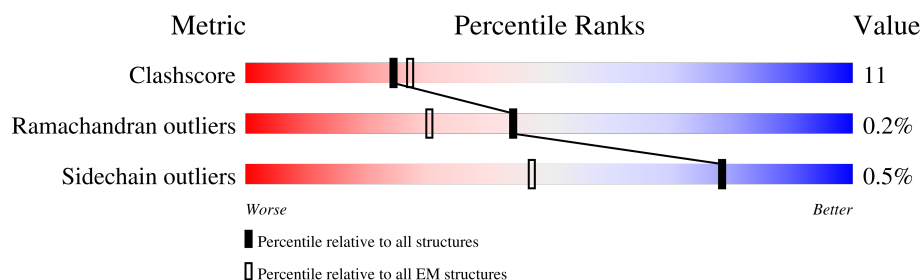
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	854	26% 77% 18% 5%
1	B	854	22% 75% 23% .
1	C	854	22% 72% 21% 7%
1	D	854	20% 79% 20% .

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Mol	Chain	Length	Quality of chain
1	E	854	
1	F	854	
1	G	854	
1	H	854	
1	I	854	
1	J	854	
2	Z	1425	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 76250 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 VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	815	Total	C	N	O	S	0	0
			6516	4128	1128	1232	28		
1	B	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	C	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	D	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	E	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	F	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	G	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	H	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		
1	I	794	Total	C	N	O	S	0	0
			6372	4043	1100	1201	28		
1	J	846	Total	C	N	O	S	0	0
			6746	4260	1175	1283	28		

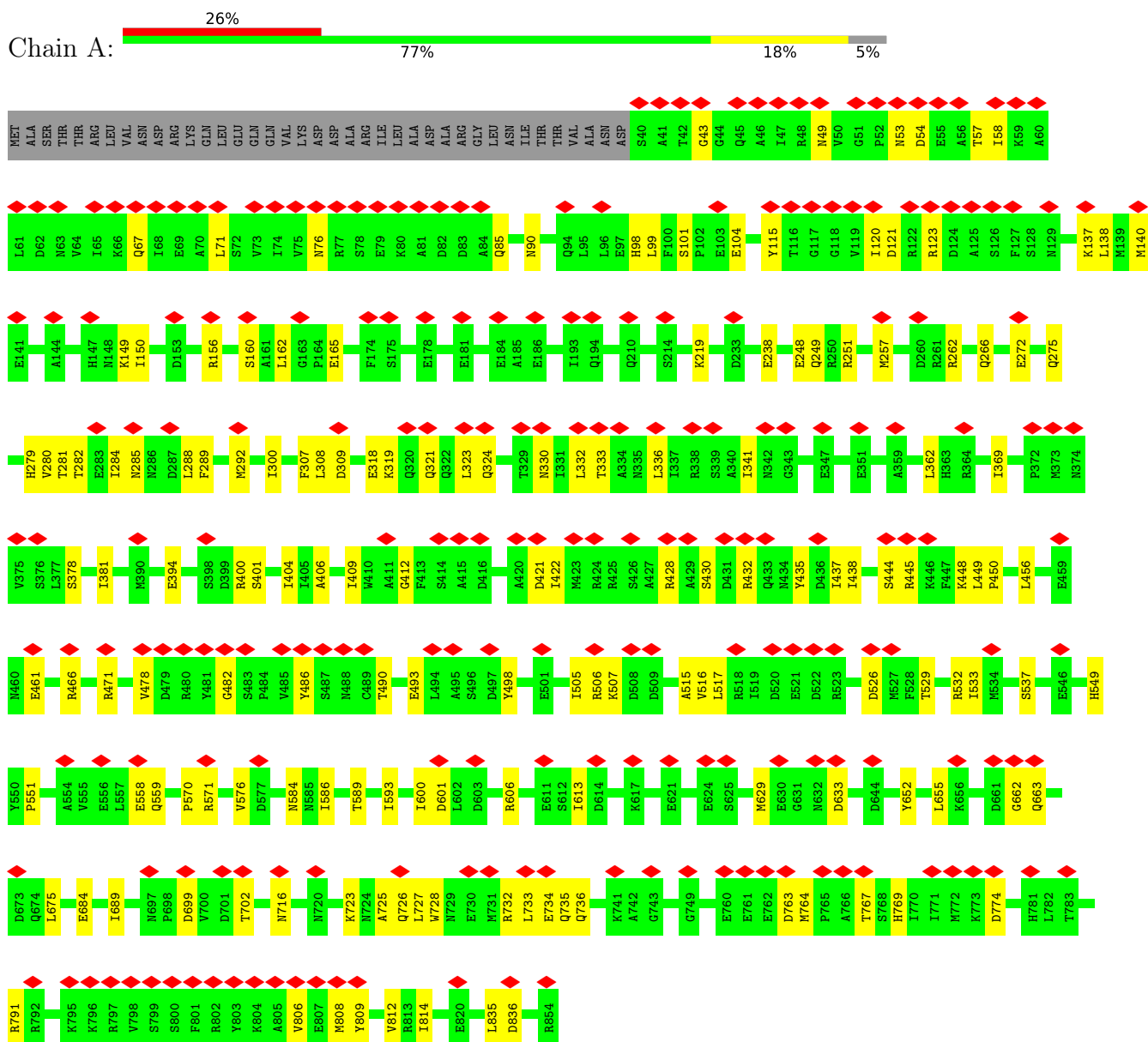
- Molecule 2 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	1320	Total	C	N	O	S	0	0
			10516	6661	1799	2000	56		

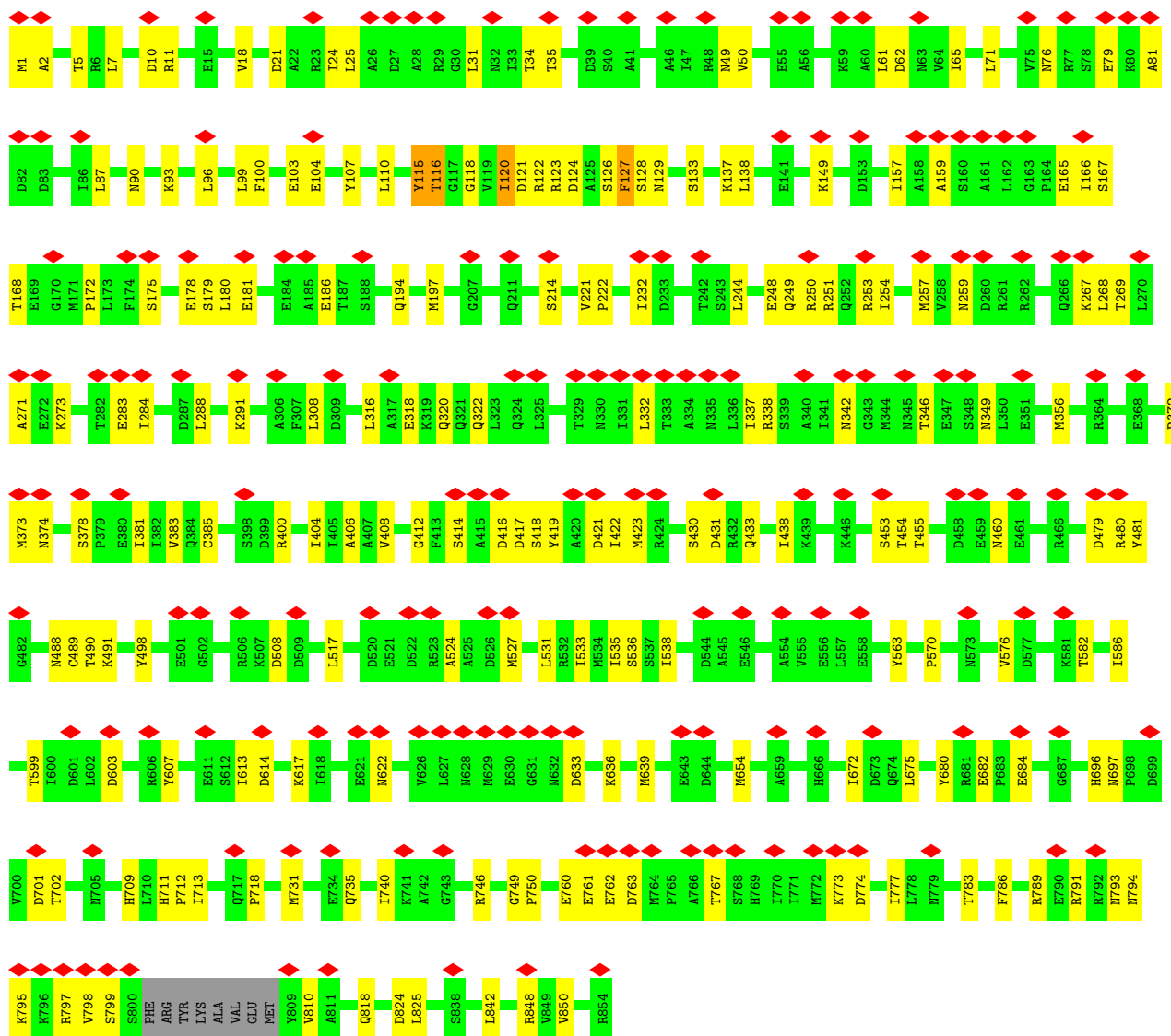
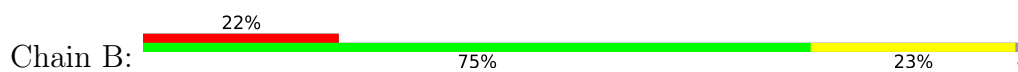
3 Residue-property plots

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.

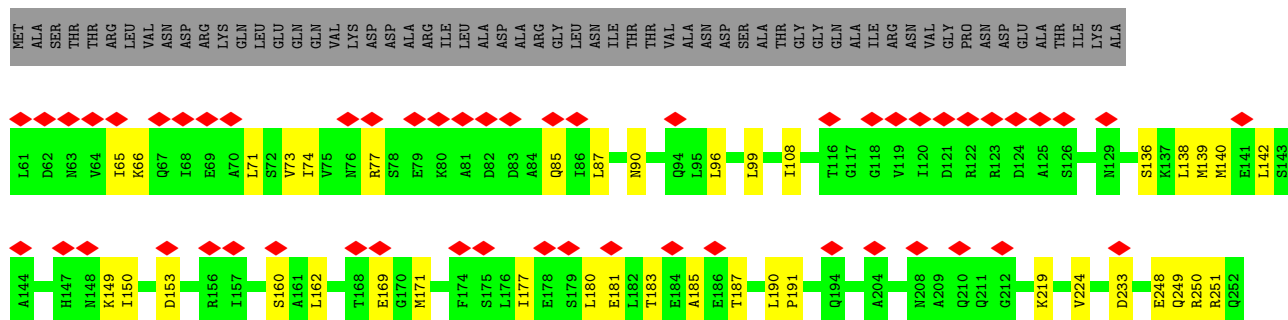
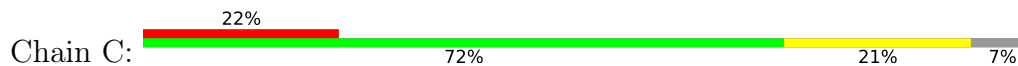
• Molecule 1: VP3

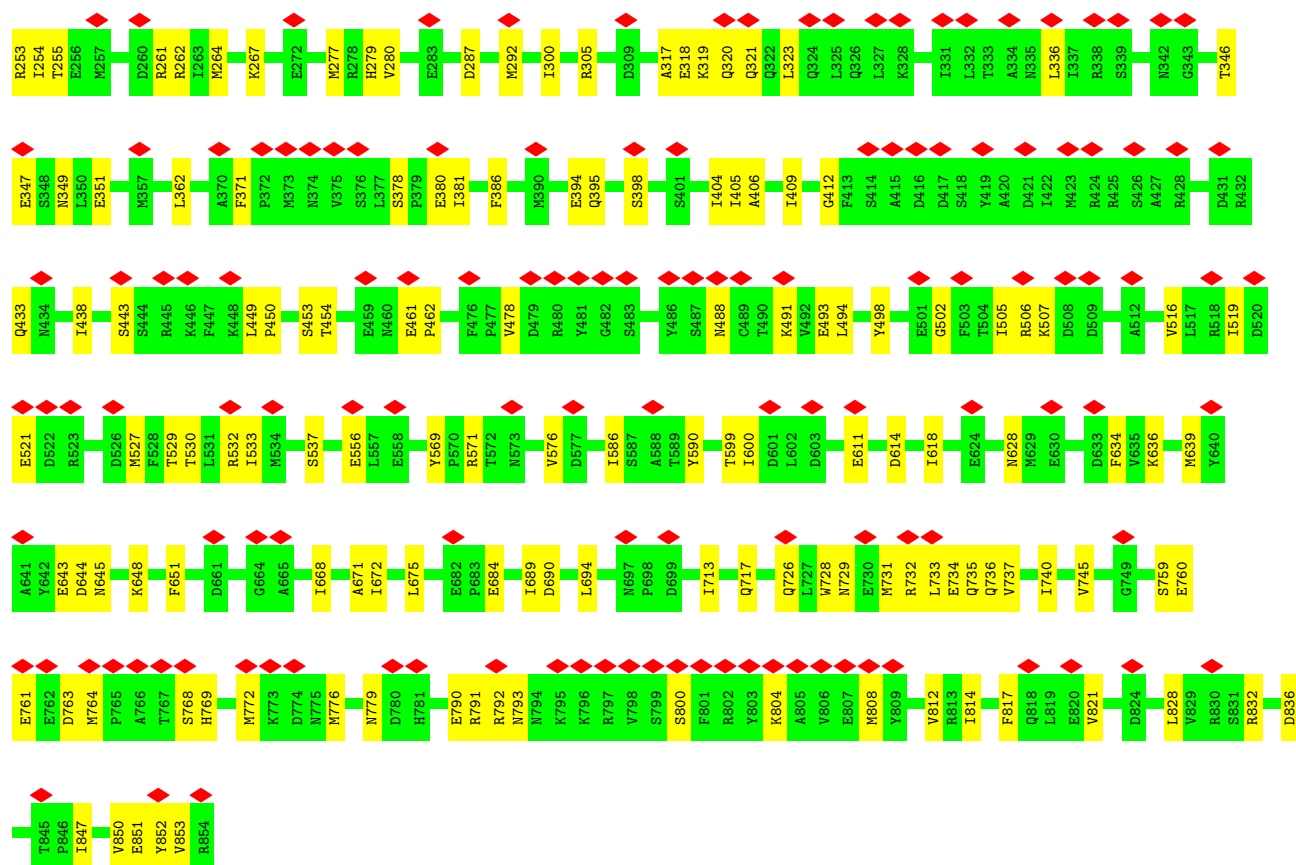


• Molecule 1: VP3

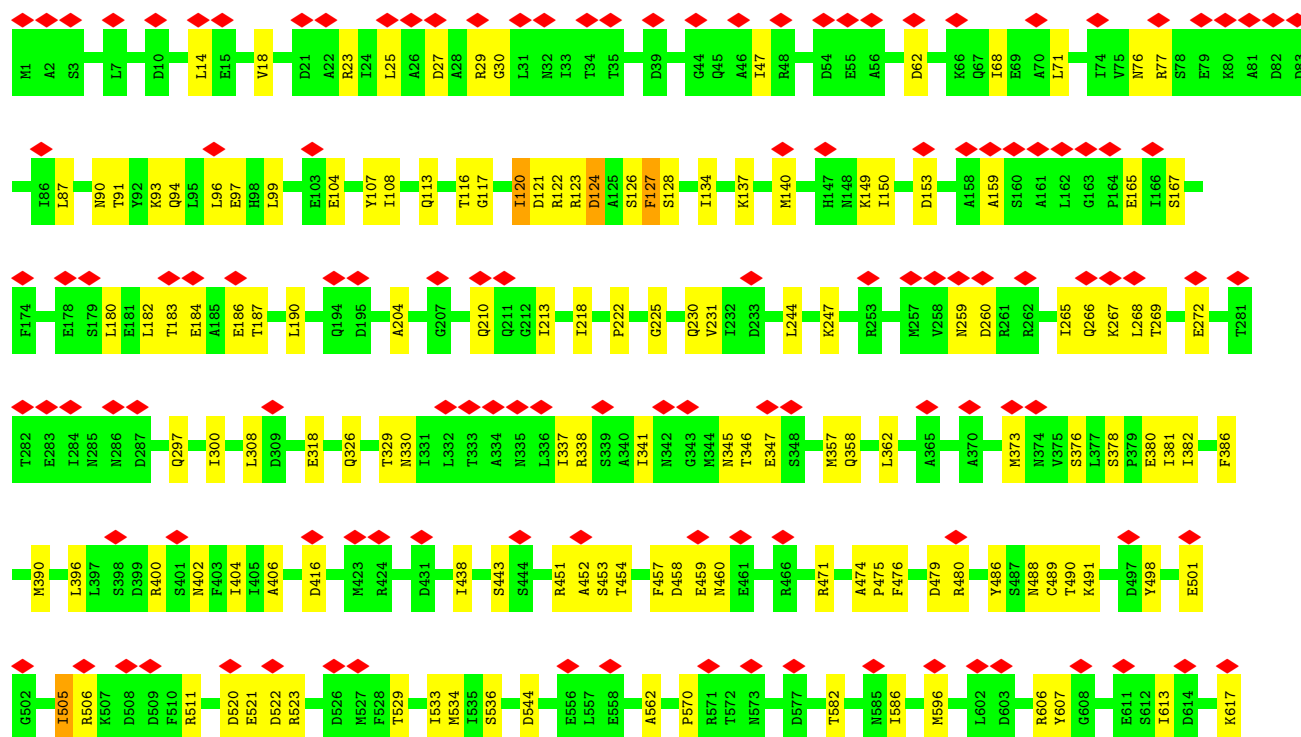
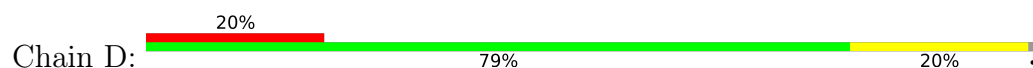


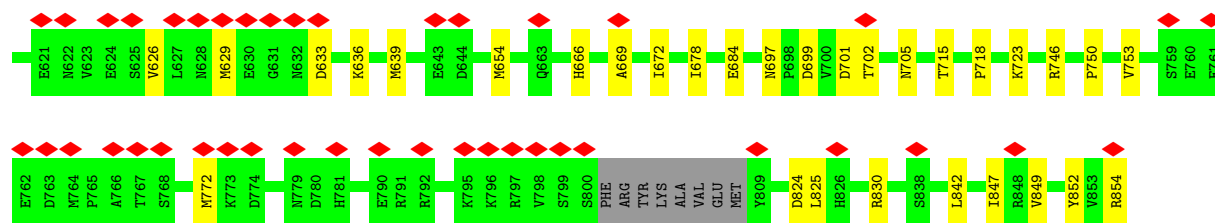
• Molecule 1: VP3



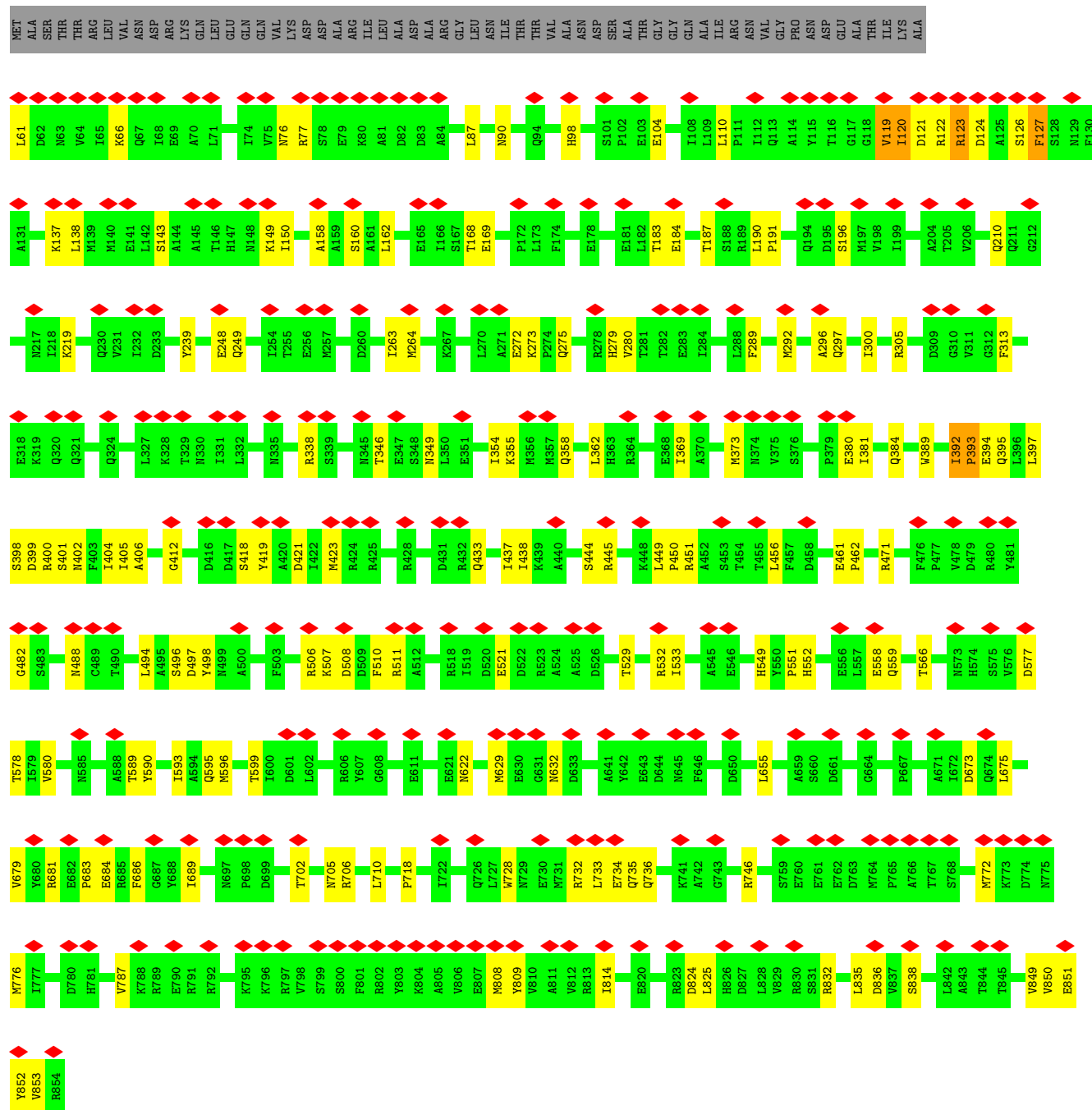
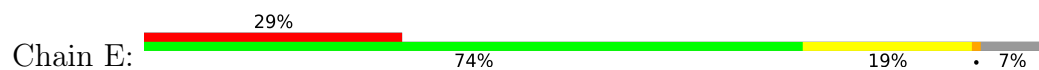


• Molecule 1: VP3



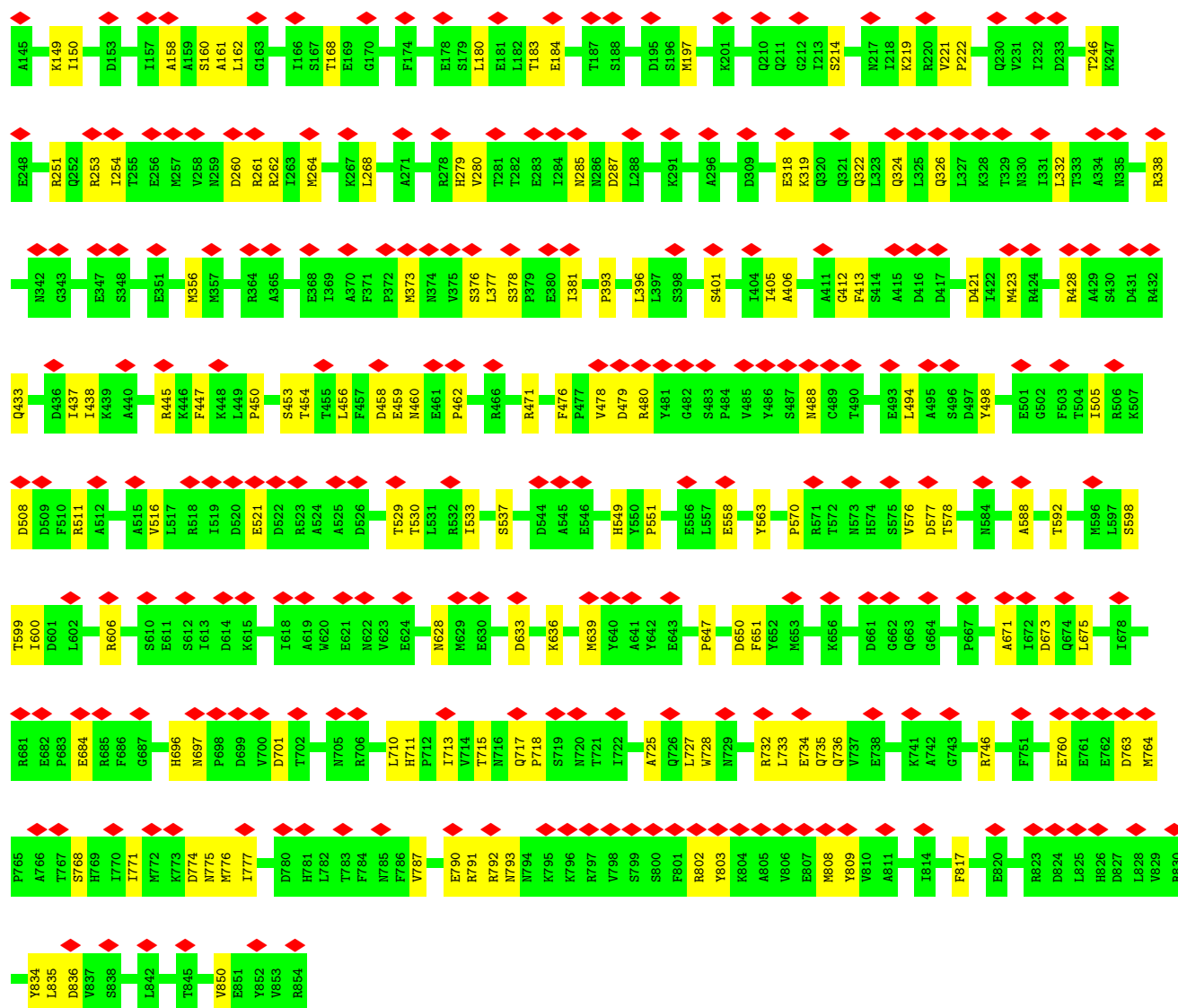


• Molecule 1: VP3

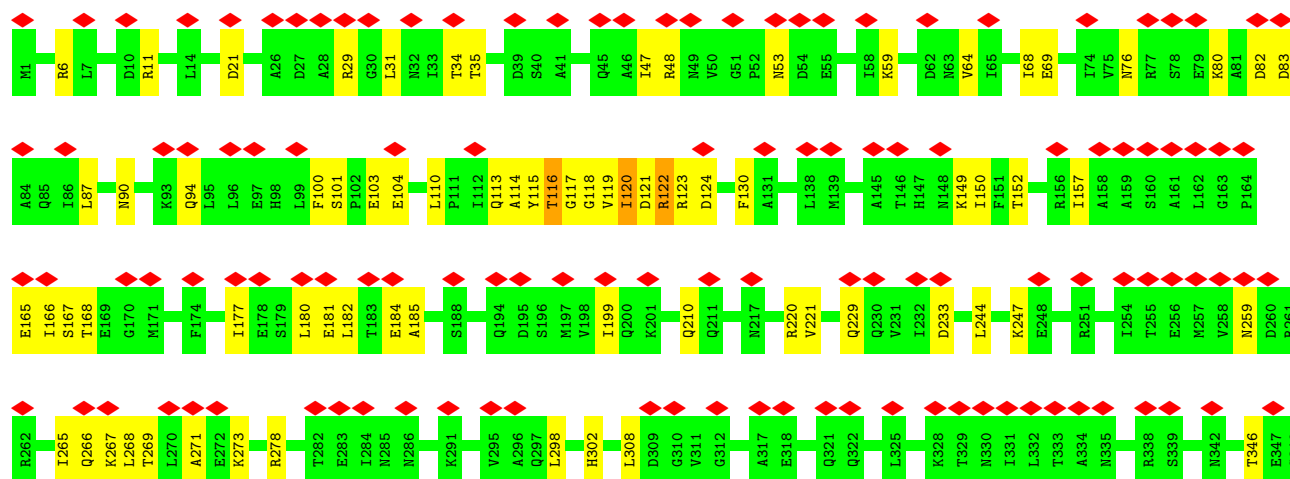
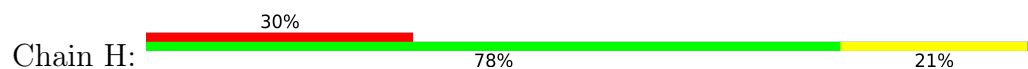


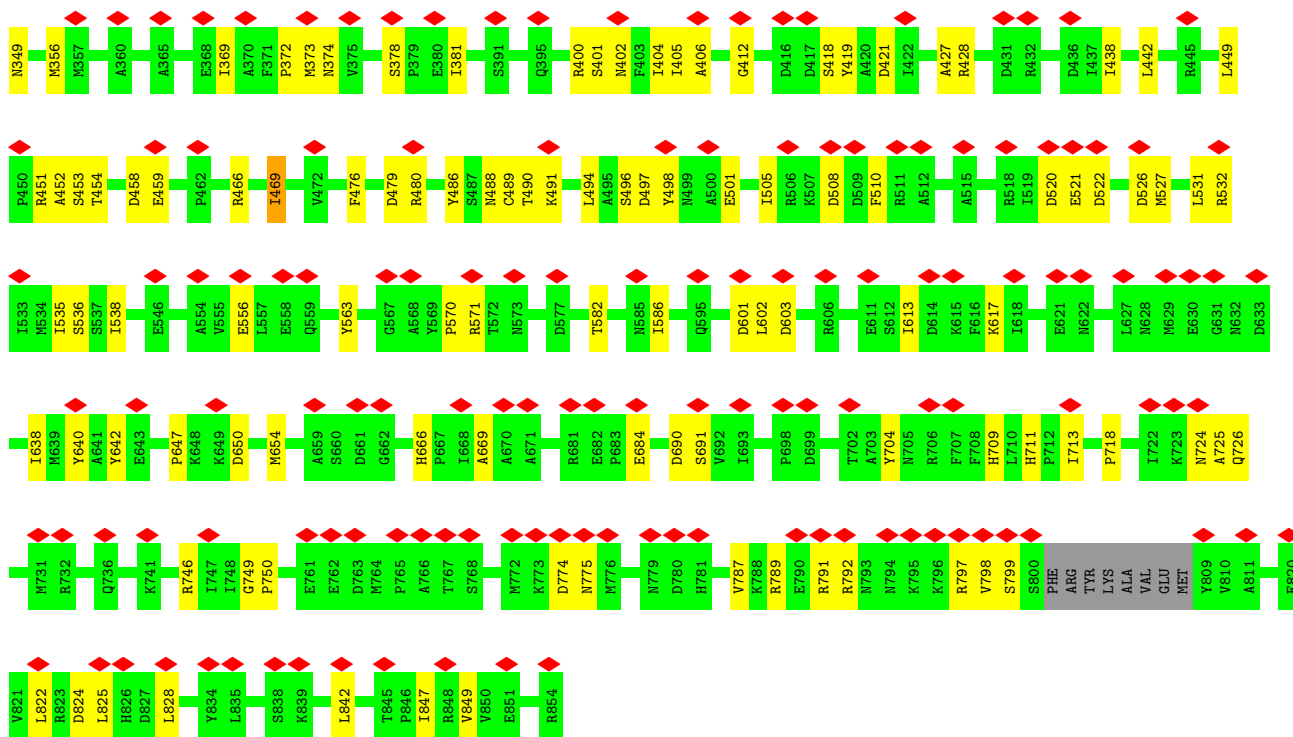
K839	S768	V679	M527	K448	N342	M264	D153	N76	M1
L842	I771	T680	L531	R451	N345	I285	R156	R77	A2
A843	M772	P681	R532	A452	T346	Q286	I157	S78	S3
T844	K773	E682	I533	S453	E347	K287	A158	E79	T4
	D774	E684	M534	T454		L268	A159	K80	R6
		R685	I535	T455	K356	T269	S160	A81	T5
R848	I777	F686	D544	L456	K357	L270	A161	D82	N9
V849	L778	G687	A545		Q358	A271	L162	D83	D10
V850	N779	Y688	Y550	E459	R363	E272	G163	K85	Q17
E851	T780	R689	Y550	E461	R364			I86	V18
Y852	L781	S691	Y556	R466	A365	V276		N90	K19
V853	T783	V692	E556				I166	T91	D20
R854	F784	T695	L557	I469	A370	T281	E169		D21
	N785	H696	E558	G470	F371	T282	G170		A22
	F786	G470	P570	R471	P372	E283		Q94	
A843	K788	D699	R571	D479	K373	I284	F174	L96	L25
R789	V700	R769	T572	R480	E380	N286	S175	E97	A26
E790	D701	N573	N573	Y481	I381	D287	L176	H98	D27
R791	T702	Q595	Q595	G482	V383	L288	I177		A28
N792	F707	T599	T599	Y486	N389	K291	E178	P102	R29
N793	H708	R606	R606	S487	L396	N292	S179	E103	
K795	H710	E511	E511	N488	L397	E181	L180	E104	N32
R797	P712	D614	D614	C489	S398	E182	N105	V106	I33
V798	I713	Y492	Y492	T490	D399	A296	T183	Y107	T36
S799	N716	E931	E931	K491	R400	Q297	E184	I108	V36
S800	Q717	L494	L494	V493	A406	L298	A185	L109	A37
PHE	Q718	A495	A495	E494		R305	E186	L110	
ARG	P718	S496	S496	D497	G412	L308	T187	P111	N38
LYS	A725	D497	D497	F413	F413	D309	S188	I112	D39
ALA	N729	M629	M629	S414	S414	F315	M197	Q113	S40
VAL	I740	E630	E630	A415	A415	L316		A114	A41
MET		G631	G631	D416	D416	A317	N208	Y115	T42
Y809	R746	N632	N632	D417	D417	E318	A209	T116	G43
V810	P750	I505	I505	S418	S418	K319	Q210	G117	G44
A811	F751	R506	R506	Y419	Y419	E318	Q211	G118	G45
V812	F752	K507	K507	D422	D422	Q320	T215	V119	A46
R813	V753	D508	D508	M423	M423	Q321	I216	I120	I47
I814	T754	D509	D509	S426	S426	Q322	F228	D121	R48
	Y755	F510	F510	R428	R428	L323		R122	R48
L819	H756	A512	A512	D431	D431	Q324	D233	A125	N49
E820	V757	D650	D650	R432	R432	L325	E248	S126	V50
V821	L758	D661	D661	A515	A515	K328	R251		G51
R823	S759	G562	G562	R518	R518	T329	I254	S133	D54
L822	D824	L675	L675	I519	I519	N330	T255	K137	E55
L825	E761	T676	T676	D520	D520	I331	E141	M140	I68
	E762	A671	A671	E521	E521	L332	A144	E141	K59
L828	D763	Q674	Q674	D522	D522	T333	M257	M140	D62
	A766	L676	L676	R523	R523	A394	V258	K148	I65
L835	D836	T677	T677	D526	D526	N335	L336	N148	K66
V837	T767	L678	L678			L337	I337	I149	E69
S838						R338	R261	I150	A70

Met	ALA	SER	THR	THR	ARG	LEU	VAL	ASP	ASP	ARG	LYS	GLN	LEU	GLU	GLN	GLN	VAL	LYS	ASP	ASP	ALA	ARG	ILE	LEU	ALA	ASP	ALA	ARG	GLY	LEU	ASN	THR	THR	VAL	ALA	ASN	ASP	SER	ALA	THR	GLY	GLY	GLN	ILE	ARG	ASN	VAL	GLY	PRO	ASN	ASP	GLU	ALA	THR	ILE	LYS	ALA
L61	D62	N63	V64	I65	K66	Q67	I68	L71	S72	V73	I74	V75	M76	R77	S78	E79	K80	A81	D82	D83	A84	N90	Q94	L95	L96	L99	E103	E104	L110	Q113	A114	Y115	T116	G118	V119	I120	D121	R122	R123	D124	A125	S126	A131	K137	L138	M139	M140	E141									

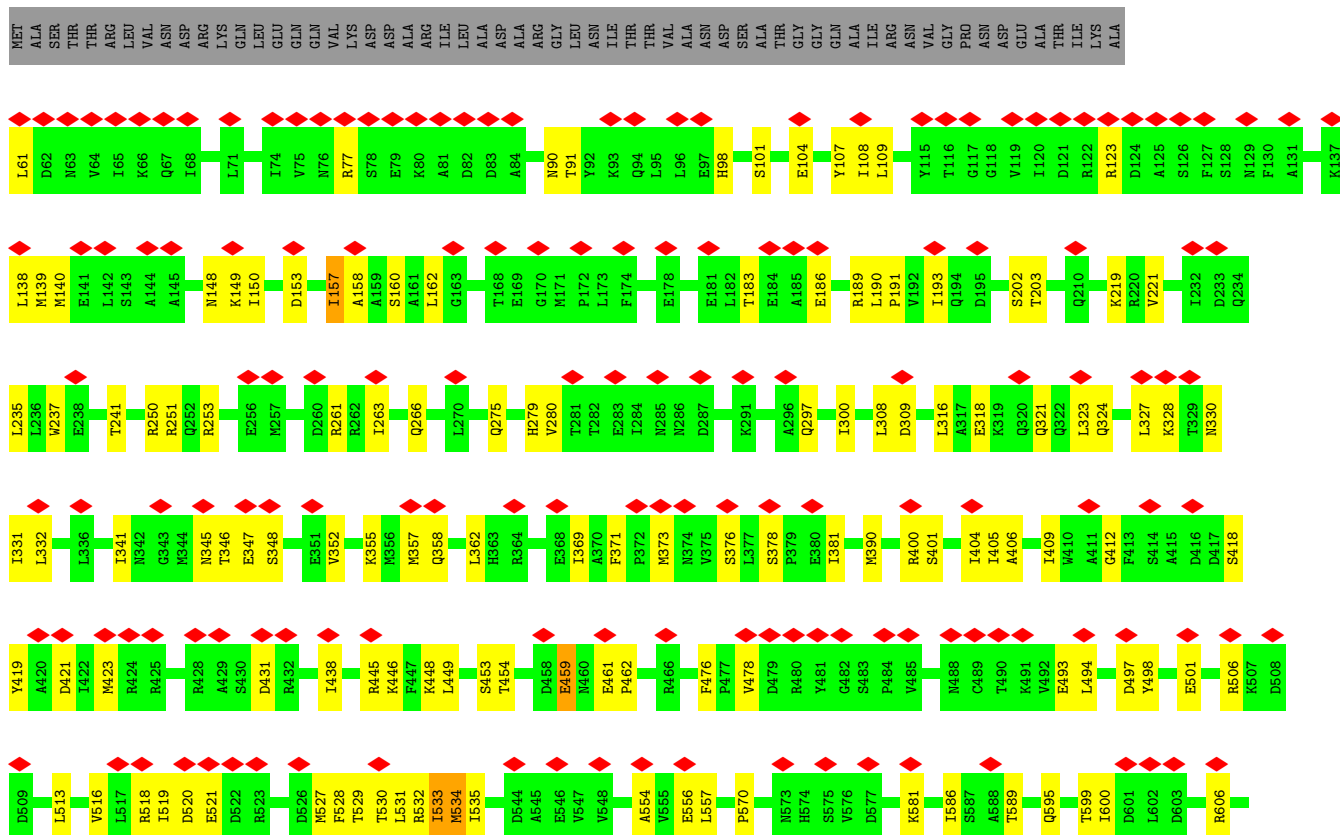


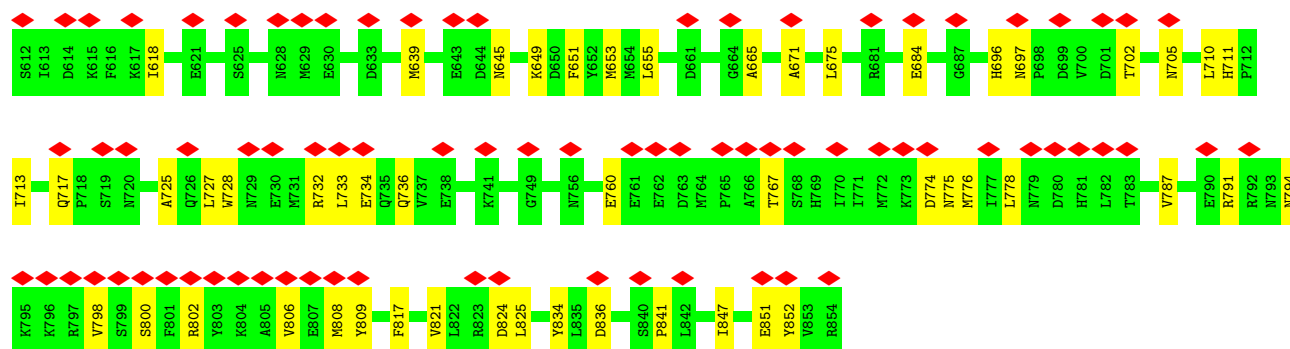
• Molecule 1: VP3



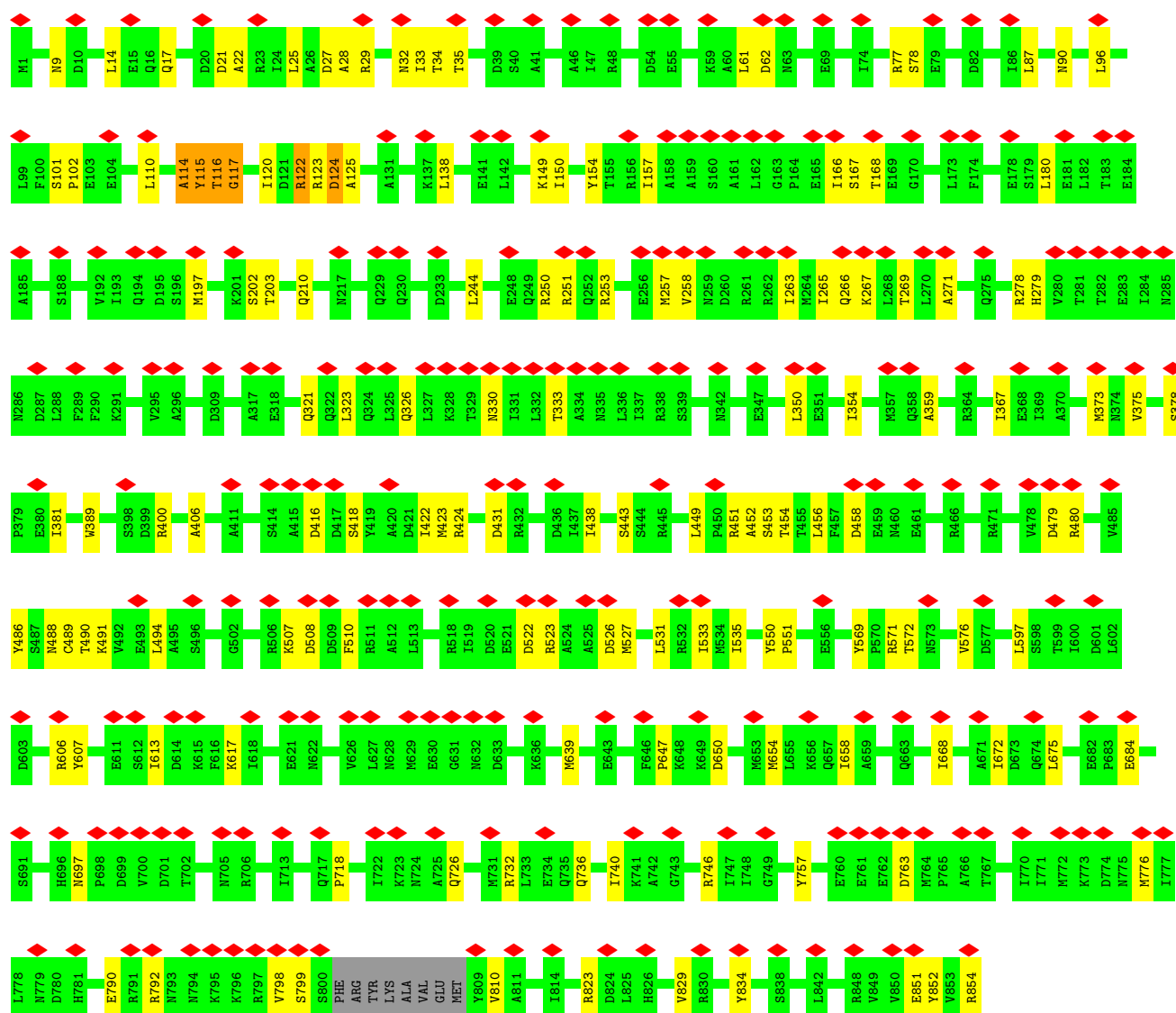
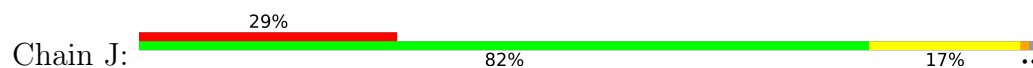


• Molecule 1: VP3





• Molecule 1: VP3



• Molecule 2: VP1



MET	ARG	ILE	MET	ALA	GLN	ARG	LEU	LYS	GLU	LEU	GLN	ARG	GLU	ILE	ASP	LYS	LYS	LYS	GLU	ARG	ILE	ALA	GLU	ALA	TYR	LEU	SER	SER	VAL	GLU	VAL	THR	ASN	SER	SER	PRO	SER	LEU	SER	ILE	LYS	GLN	ASP	ASP	ALA	LEU	THR	LEU	PRO	LYS	V52	SS3	P54	F55	L56	D57	SS8	T59	P60						
F61	T62	T63	L64	H65	H66	S67	G70	Q71	F72	L73	H74	S75	L76	D77	D78	E79	L80	A81	THR	ASP	GLY	THR	ALA	GLY	L83	C84	PHE	ARG	SER	THR	E87	Y88	E89	L90	VAL	ASP	ASP	ILE	HIS	SER	ILE	E97	Q98	Q99	T100	A101	L102	K103	K104	F105	L106	T107	T110	G111	S112	P113	Q114	E115	I116	Q117	V119	D120	K121	E122	W123
M124	K125	S126	H129	V130	P131	S132	F133	L134	G135	D136	V137	K138	L139	M140	F141	ASP	THR	ALA	GLY	THR	ALA	GLY	L206	PHE	ARG	SER	THR	E87	Y88	E89	L90	VAL	ASP	ASP	ILE	HIS	SER	ILE	THR	THR	SER	ASP	VAL	GLN	THR	ARG	SER	LYS	LYS	ASN	S180	Y181	V182	V183	Q184										
K185	K186	H187	K188	V189	Q190	Q191	P192	L193	K194	P195	N196	T197	L198	Y199	D200	Y201	K202	Y203	K204	G205	L206	P207	R208	V209	V210	L211	R212	F213	V214	P215	K216	V217	D218	T219	T220	S221	ASN	SER	ASN	ASN	SER	SER	ALA	SER	ASP	ASP	THR	ARG	SER	LYS	LYS	ASP	ALA	F238	S239	C240	D241	D242	L243	S244					
P245	T246	W247	K248	Y249	T252	E253	A254	K255	E256	A257	F258	P259	D260	R261	S262	Y263	S264	D265	C266	L267	H268	P269	W270	T271	W272	E273	E274	W275	L276	E277	E278	W279	Q280	L286	T287	Q288	Y289	A290	H291	Q292	L293	V296	T297	L298	L299	Q300	D301	F302	N303	L304	G309	A310	S311	R312	V313										
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T440	F441	D442	Y443	N444	M445	K446	R447	S448	E449	M450	L451	V452	V453	T454	R455	G456	H457	L458	A459	A460	H461	K462	V463	L464	E465	C466	A467	L468	R469	I470	V471	E472	Y475	T476	D478	I479	Q480	D481	E482	T483	F484	K485	D486	I487	L488	I489	D490	L491	G492	L494	I495	M496	R497	D498	P499	I500									
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K831	Y832	T833	E834	E838	N841	R842	D843	G844	S848	E849	L850	G855	E856	T857	V858	L859	E860	R861	M862	N863	P864	A865	D866	L867	N870	N874	T875	P876	P877	R878	Y879	Q882	T883	A884	L885	G886	D887	T888	T889	N890	L891	Q892	H893	D894	N895	R896	S897	G898	V899	P900	N901	T902													

R1362	R1363	G1364	P1365	P1366	L1367	P1368	I1369	I1370	D1371	R1372	T1373	L1374	N1375	R1376	L1377	L1378	M1383	L1384	M1385	F1386	M1389	G1390	K1391	S1392	I1393	D1394	S1395	T1396	K1397	I1398	D1399	P1400	T1401	L1402	S1403	W1404	R1405	A1406	I1407	L1408	E1409	S1410	N1411	D1412	Q1413	S1433	Q1344	A1345	I1348	R1349	I1350	N1351	D1352	A1353	L1354	M1355	D1356	S1357	I1358	T1359	Q1360	H1361
S1229	D1230	L1231	K1232	Q1233	D1234	D1235	Y1236	Y1239	Q1245	R1248	N1256	D1257	S1258	R1259	I1260	T1261	S1262	F1263	D1264	P1265	K1266	G1267	K1268	L1269	Q1270	H1271	L1272	L1273	A1274	K1275	N1276	S1277	Q1278	I1279	L1280	P1281	I1282	H1283	F1284	D1285	I1286	E1287	F1288	Y1289	R1290	R1291	L1292	Y1293	L1294	Q1295	A1296	G1297	T1298	M1299	G1300							
F1301	L1302	Q1303	V1304	M1305	S1306	V1307	Y1308	Q1309	L1310	P1311	D1312	T1313	L1314	T1315	H1316	E1317	M1318	L1319	A1320	A1321	V1322	V1323	A1324	I1325	E1326	L1327	Q1328	L1329	G1330	N1331	D1332	K1333	L1334	A1335	V1336	D1337	M1338	G1339	V1340	Y1341	L1342	S1343	Q1344	A1345	I1348	R1349	I1350	N1351	D1352	A1353	L1354	M1355	D1356	S1357	I1358	T1359	Q1360	H1361				
H1107	G1108	S1109	S1110	F1111	G1112	W1113	M1114	F1115	D1116	D1117	M1118	L1119	I1120	K1121	T1122	A1123	M1124	S1125	I1126	G1127	A1128	I1129	S1130	D1131	S1132	S1133	Y1134	D1135	A1136	I1137	S1138	T1139	K1140	I1141	T1142	M1143	L1144	A1145	D1146	M1147	K1148	D1149	S1150	Q1151	Q1152	R1153	I1154	T1155	R1156	D1157	I1158	I1159	T1160	S1161	G1162	R1163	L1164	P1165	Q1166			
H1167	L1168	M1169	R1170	Y1171	G1172	K1173	S1174	M1175	I1176	L1177	R1178	H1179	I1180	L1181	A1182	S1183	A1184	A1185	M1186	G1187	P1188	L1189	S1190	Q1191	I1192	E1193	K1194	M1195	V1196	N1197	A1198	Y1199	M1200	V1201	V1202	M1203	G1204	I1205	L1206	N1207	G1208	K1209	L1210	E1211	T1214	V1215	L1216	E1217	R1218	L1219	N1220	M1221	G1222	F1223	K1224	V1227	M1228					
I1041	R1042	D1043	I1044	T1045	D1046	W1047	L1049	D1054	E1055	T1056	R1057	K1058	W1059	K1060	Y1061	N1062	L1063	M1064	M1065	L1066	P1067	V1068	D1069	T1070	T1071	T1072	R1073	A1074	G1075	A1076	F1077	R1078	M1079	H1080	N1081	L1082	C1083	S1084	I1085	M1086	T1087	G1088	V1089	G1090	K1091	M1092	Y1093	L1094	L1098	N1099	N1100	K1101	G1033	V1034	I1103	A1104						
E976	Q979	D980	T981	A982	G983	T984	L985	G986	F987	A988	T989	N990	A991	R992	K993	G994	M995	I996	G997	R998	S1001	E1002	Y1003	L1004	K1005	M1006	S1007	A1008	I1009	Y1010	G1011	N1012	I1013	K1014	M1017	Q1018	V1019	T953	F954	I955	M956	D959	E960	S963	A964	E965	E966	V967	H968	L969	N970	C971	A972									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	128440	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	33.537	Depositor
Minimum map value	-21.310	Depositor
Average map value	0.081	Depositor
Map value standard deviation	1.814	Depositor
Recommended contour level	6	Depositor
Map size ($\text{\AA}$)	872.0, 872.0, 872.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.09, 1.09, 1.09	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	0.25	0/6644	0.43	0/9015
1	B	0.27	0/6871	0.45	1/9322 (0.0%)
1	C	0.23	0/6499	0.40	0/8818
1	D	0.33	0/6871	0.50	3/9322 (0.0%)
1	E	0.27	0/6499	0.43	3/8818 (0.0%)
1	F	0.36	0/6871	0.54	8/9322 (0.1%)
1	G	0.21	0/6499	0.37	0/8818
1	H	0.25	0/6871	0.42	1/9322 (0.0%)
1	I	0.24	0/6499	0.42	3/8818 (0.0%)
1	J	0.27	0/6871	0.44	3/9322 (0.0%)
2	Z	0.51	0/10724	0.72	3/14518 (0.0%)
All	All	0.31	0/77719	0.49	25/105415 (0.0%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	THR	CB-CA-C	-7.23	97.49	110.36
1	F	780	ASP	N-CA-C	-7.03	103.81	112.88
1	E	392	ILE	O-C-N	-6.70	115.52	121.61
1	E	123	ARG	N-CA-C	-6.47	105.49	113.19
1	H	114	ALA	O-C-N	-6.16	115.16	123.10

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	6516	0	6517	110	0
1	B	6746	0	6755	164	0
1	C	6372	0	6375	132	0
1	D	6746	0	6755	130	0
1	E	6372	0	6375	133	0
1	F	6746	0	6755	192	0
1	G	6372	0	6375	123	0
1	H	6746	0	6755	146	0
1	I	6372	0	6375	144	0
1	J	6746	0	6755	115	0
2	Z	10516	0	10497	347	0
All	All	76250	0	76289	1637	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 11.

The worst 5 of 1637 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:I:357:MET:HE2	1:I:534:MET:HG2	1.26	1.07
2:Z:895:ASN:HB3	2:Z:905:GLN:OE1	1.66	0.96
1:F:98:HIS:HB2	1:F:112:ILE:HD11	1.44	0.96
2:Z:686:PRO:HG3	2:Z:717:LYS:HA	1.48	0.94
1:B:126:SER:HB3	1:B:129:ASN:OD1	1.68	0.93

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	813/854 (95%)	741 (91%)	72 (9%)	0	100	100
1	B	842/854 (99%)	775 (92%)	65 (8%)	2 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	792/854 (93%)	721 (91%)	71 (9%)	0	100	100
1	D	842/854 (99%)	785 (93%)	56 (7%)	1 (0%)	48	78
1	E	792/854 (93%)	719 (91%)	70 (9%)	3 (0%)	30	60
1	F	842/854 (99%)	761 (90%)	76 (9%)	5 (1%)	21	52
1	G	792/854 (93%)	726 (92%)	66 (8%)	0	100	100
1	H	842/854 (99%)	786 (93%)	55 (6%)	1 (0%)	48	78
1	I	792/854 (93%)	733 (93%)	58 (7%)	1 (0%)	48	78
1	J	842/854 (99%)	777 (92%)	64 (8%)	1 (0%)	48	78
2	Z	1314/1425 (92%)	1162 (88%)	144 (11%)	8 (1%)	21	52
All	All	9505/9965 (95%)	8686 (91%)	797 (8%)	22 (0%)	44	72

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	127	PHE
1	F	689	ILE
1	J	115	TYR
2	Z	894	ASP
2	Z	901	TRP

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	718/751 (96%)	718 (100%)	0	100	100
1	B	744/751 (99%)	743 (100%)	1 (0%)	88	88
1	C	704/751 (94%)	703 (100%)	1 (0%)	88	88
1	D	744/751 (99%)	739 (99%)	5 (1%)	76	77
1	E	704/751 (94%)	703 (100%)	1 (0%)	88	88
1	F	744/751 (99%)	737 (99%)	7 (1%)	70	75
1	G	704/751 (94%)	703 (100%)	1 (0%)	88	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	744/751 (99%)	738 (99%)	6 (1%)	73	76
1	I	704/751 (94%)	701 (100%)	3 (0%)	84	81
1	J	744/751 (99%)	742 (100%)	2 (0%)	86	83
2	Z	1167/1263 (92%)	1149 (98%)	18 (2%)	57	68
All	All	8421/8773 (96%)	8376 (100%)	45 (0%)	78	80

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Z	330	HIS
2	Z	804	VAL
2	Z	333	LEU
2	Z	537	PHE
2	Z	807	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	595	GLN
1	I	361	GLN
2	Z	1316	HIS
1	G	697	ASN
1	H	663	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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.

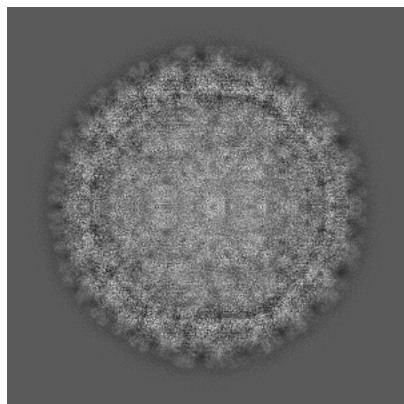
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33404. These allow visual inspection of the internal detail of the map and identification of artifacts.

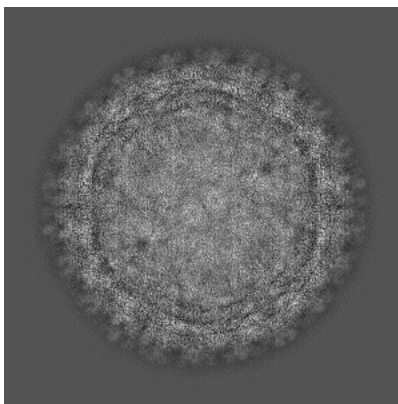
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

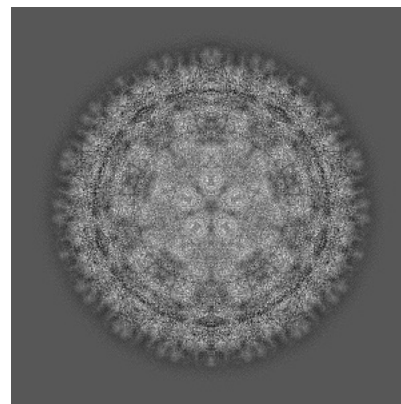
6.1.1 Primary map



X

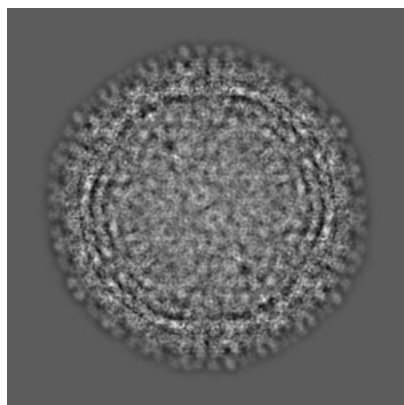


Y

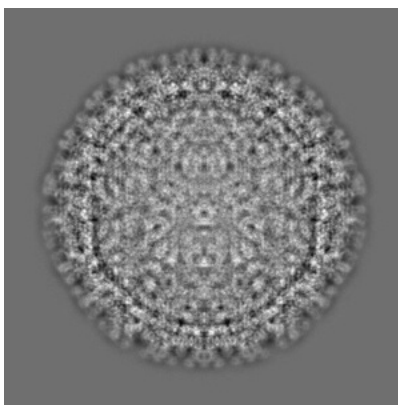


Z

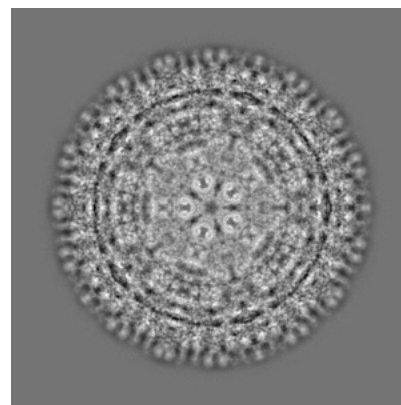
6.1.2 Raw map



X



Y

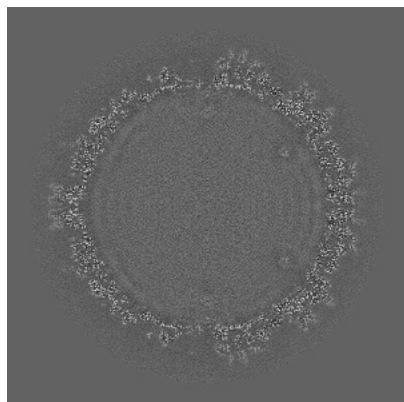


Z

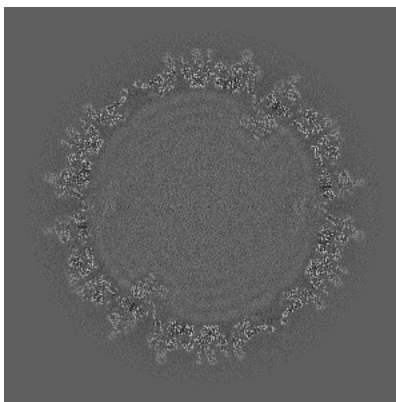
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

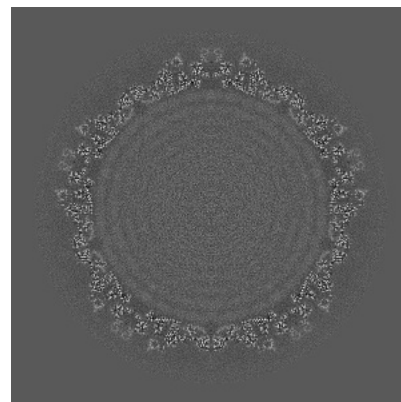
6.2.1 Primary map



X Index: 400

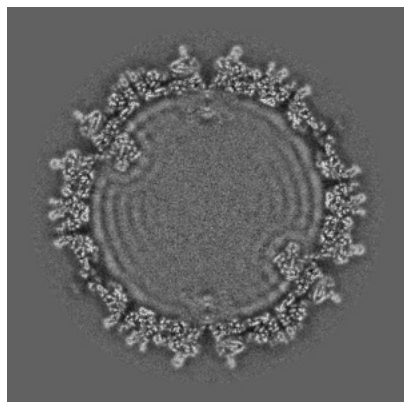


Y Index: 400

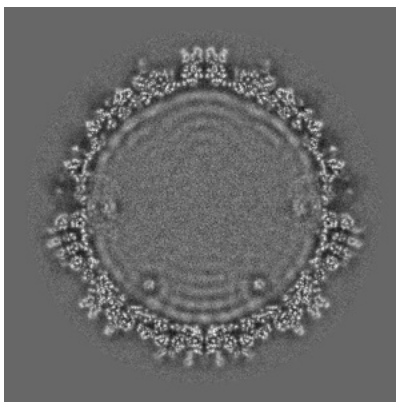


Z Index: 400

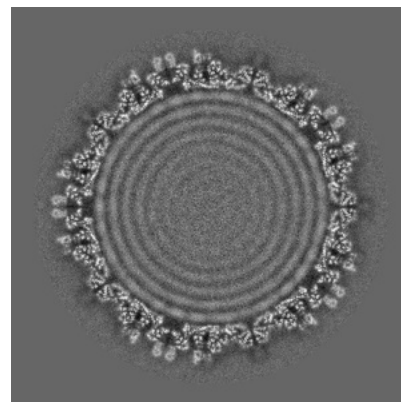
6.2.2 Raw map



X Index: 400



Y Index: 400

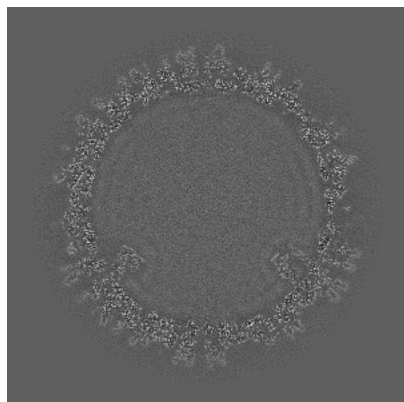


Z Index: 400

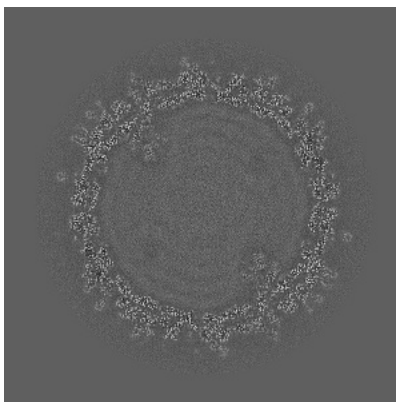
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

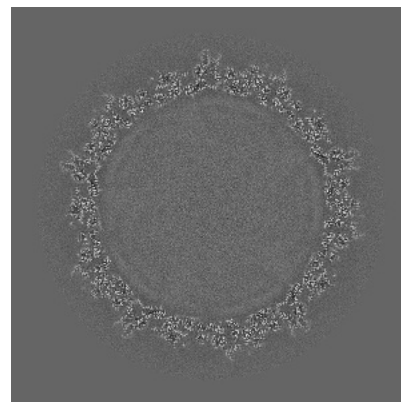
6.3.1 Primary map



X Index: 358

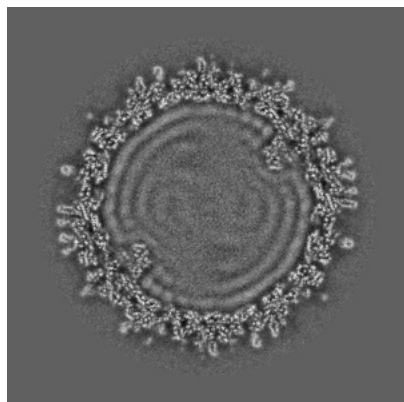


Y Index: 292

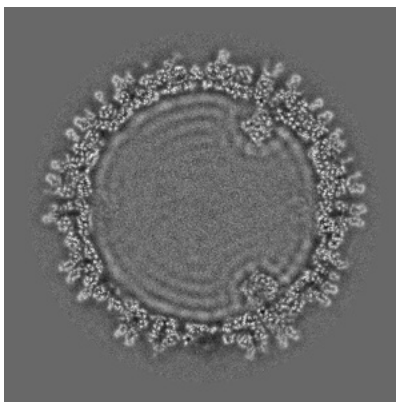


Z Index: 336

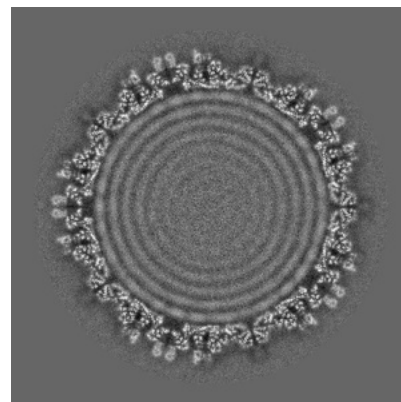
6.3.2 Raw map



X Index: 293



Y Index: 354

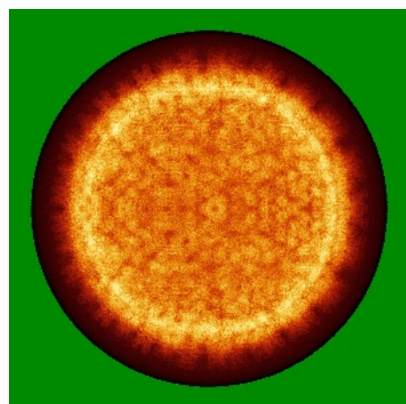


Z Index: 400

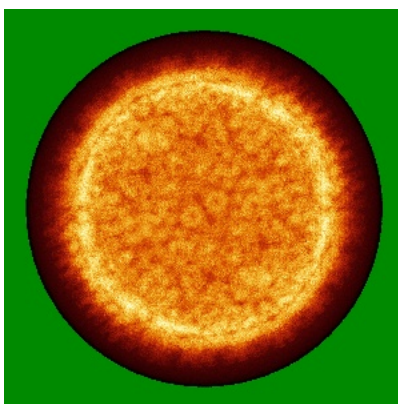
The images above show the largest variance slices of the map in three orthogonal directions.

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

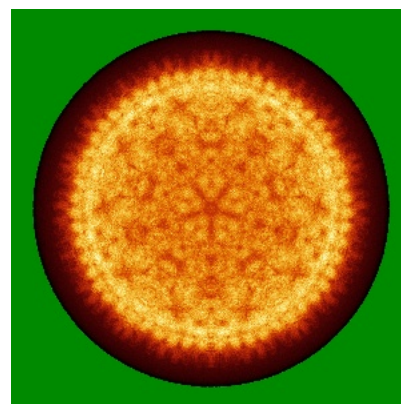
6.4.1 Primary map



X

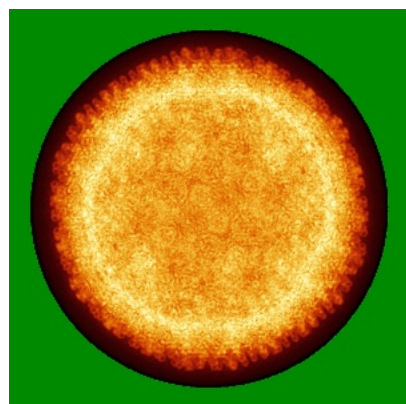


Y

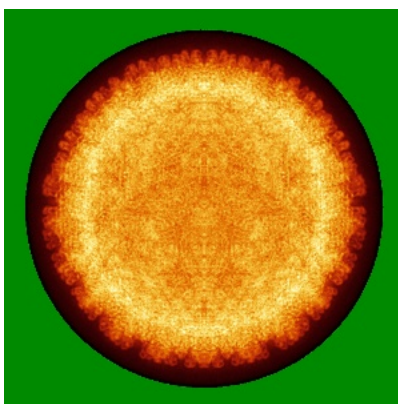


Z

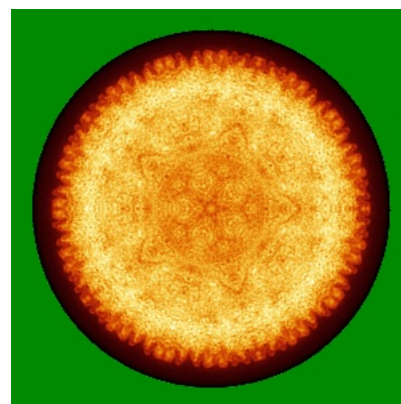
6.4.2 Raw map



X



Y

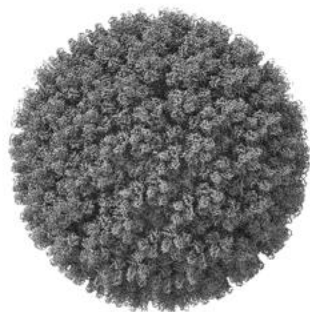


Z

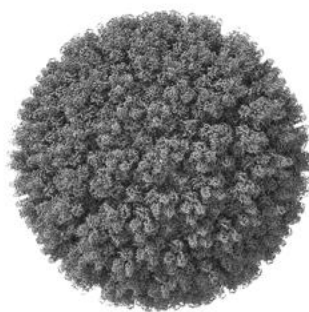
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

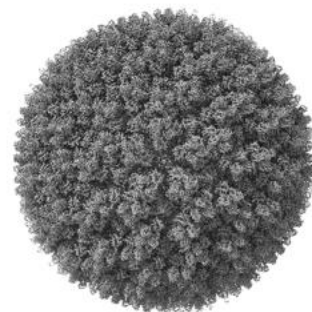
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

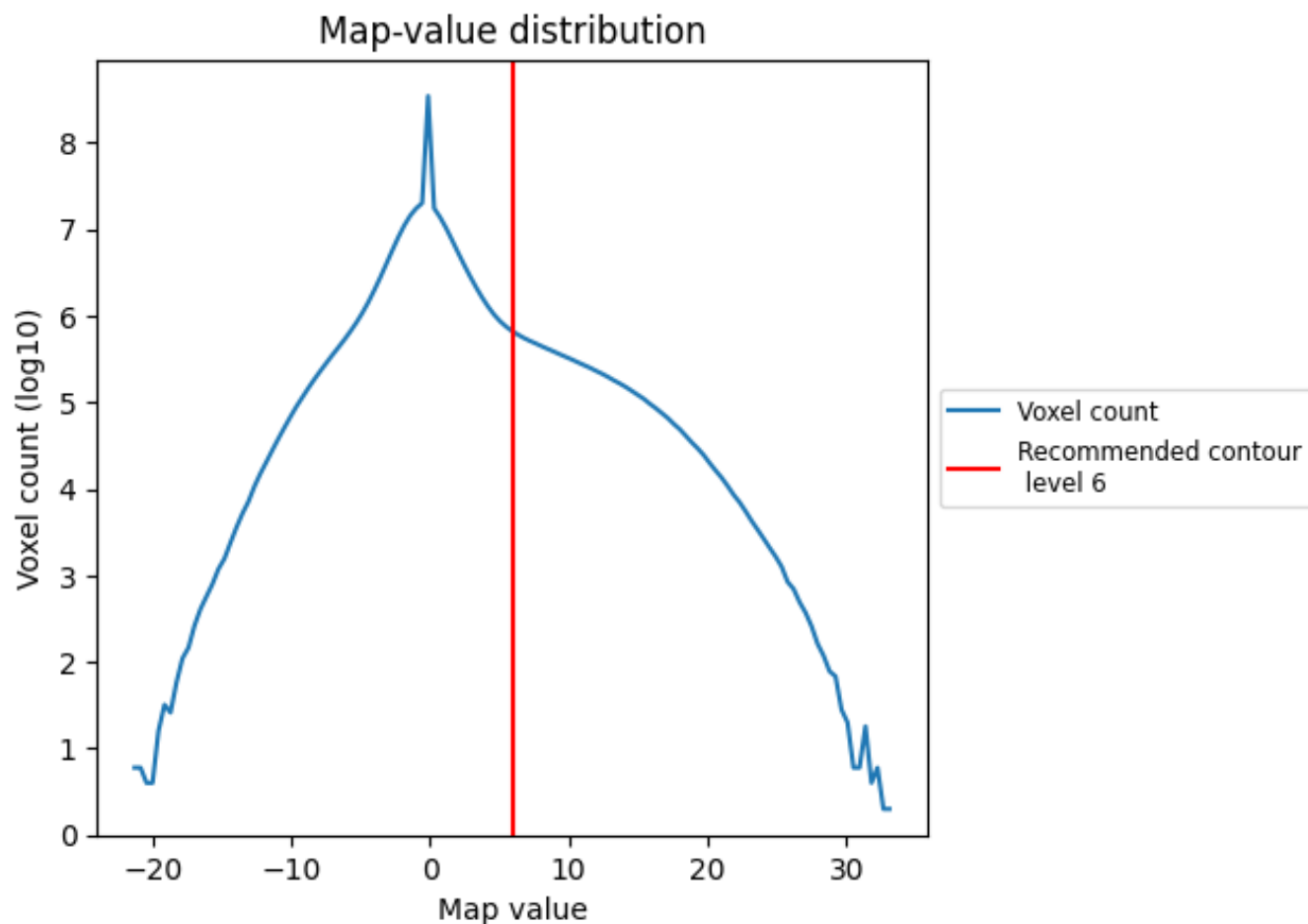
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

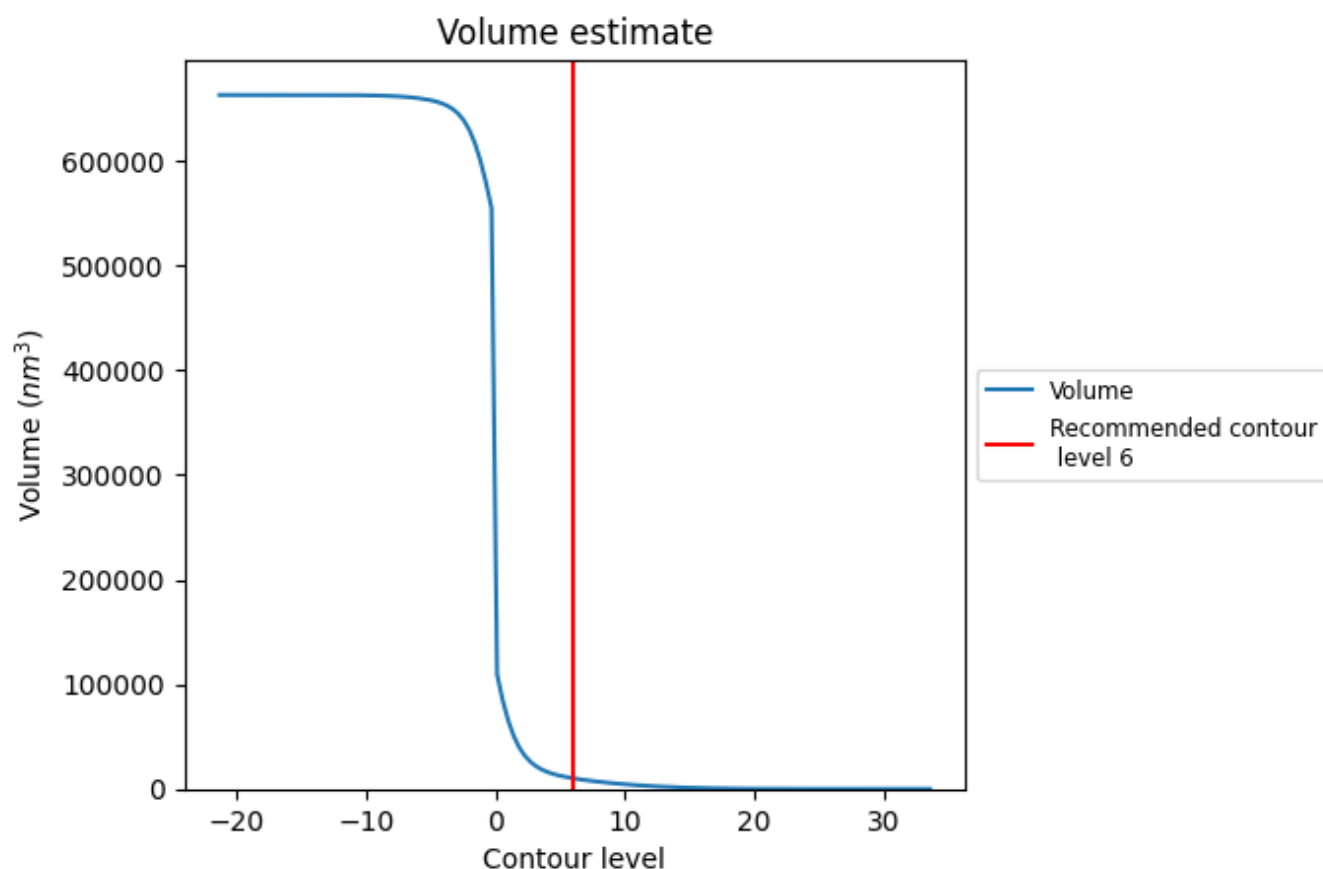
This section contains the results of statistical analysis of the map.

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.

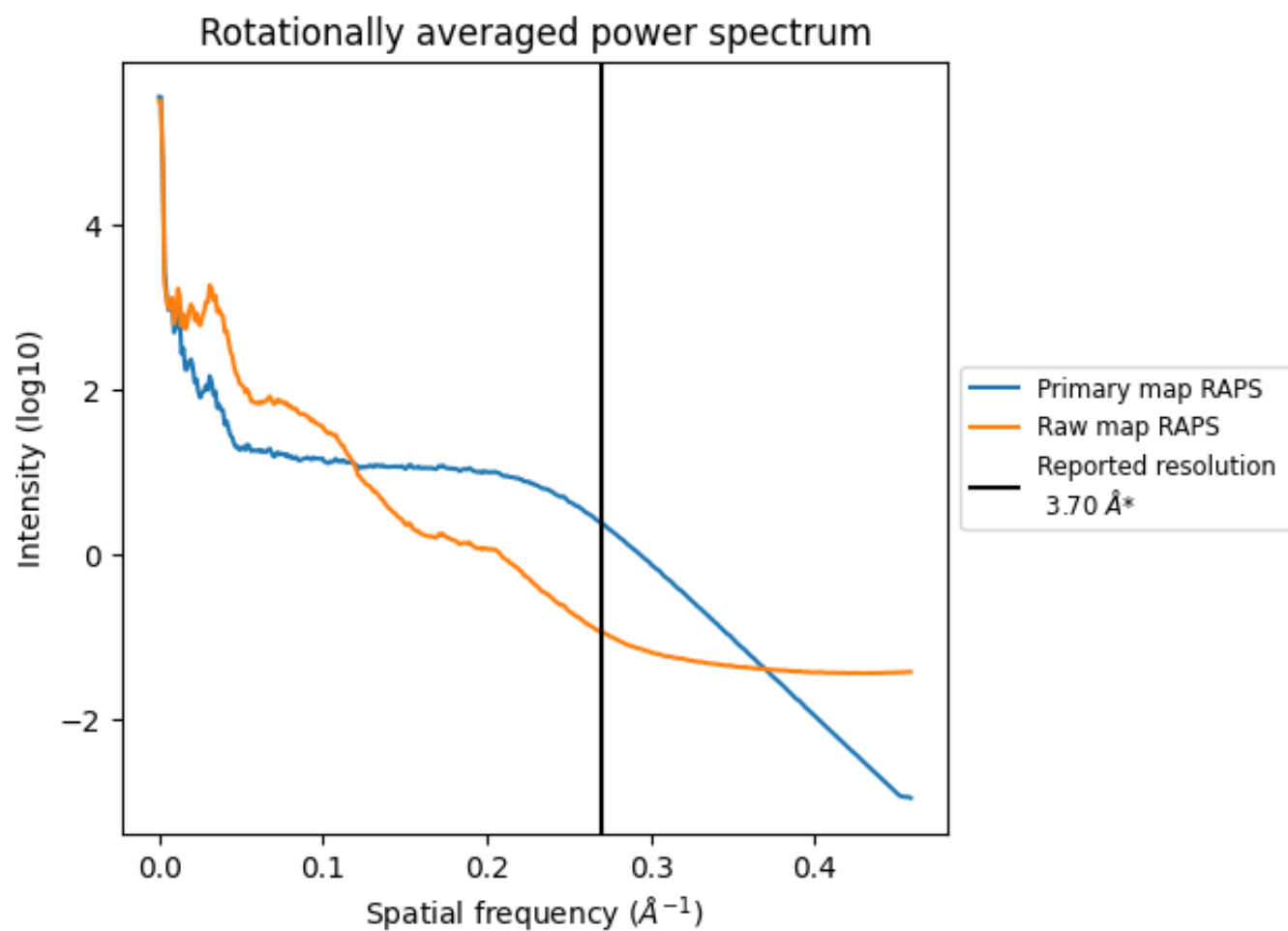
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10162 nm^3 ; this corresponds to an approximate mass of 9180 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 ⓘ

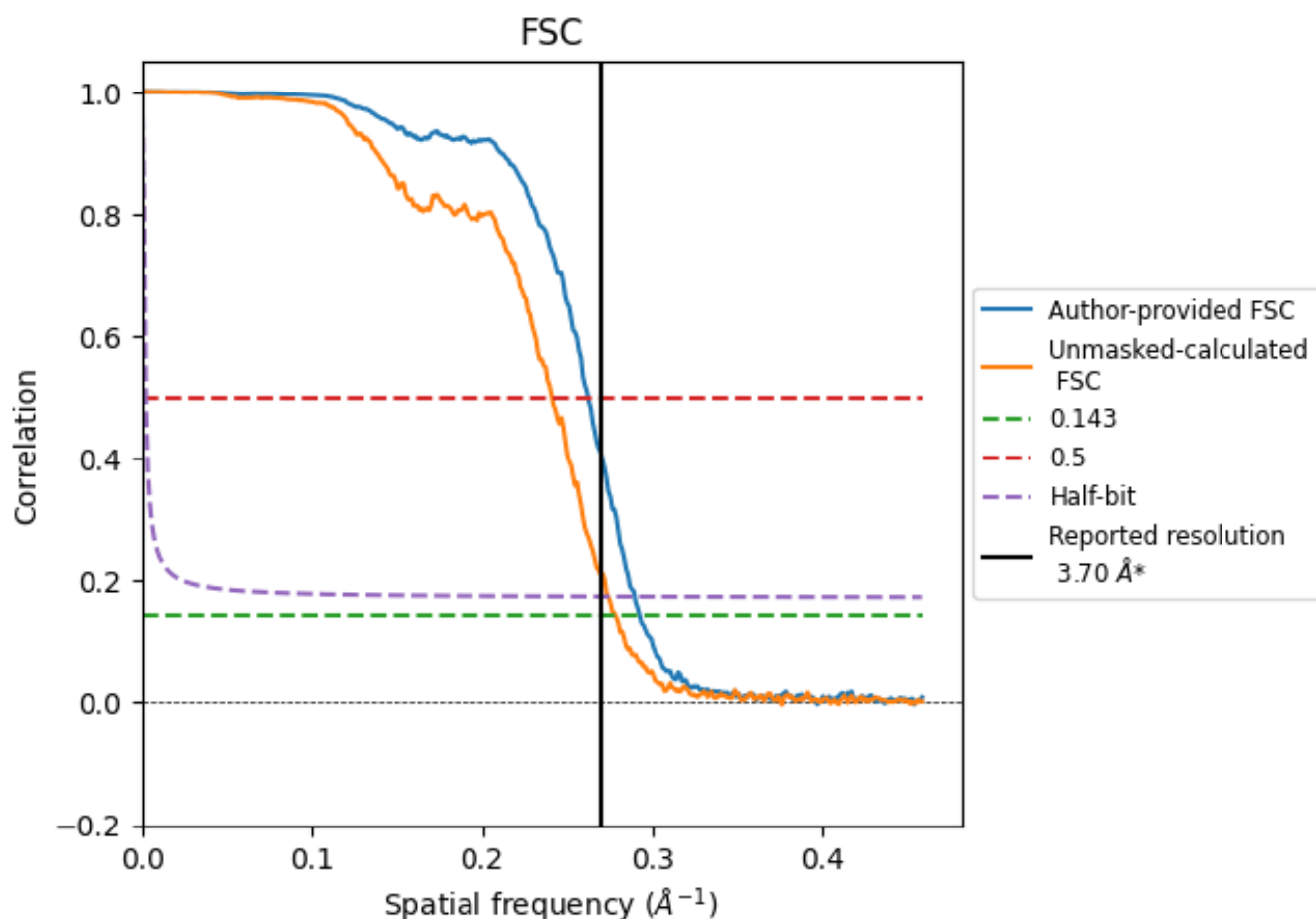


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.42	3.82	3.45
Unmasked-calculated*	3.59	4.15	3.65

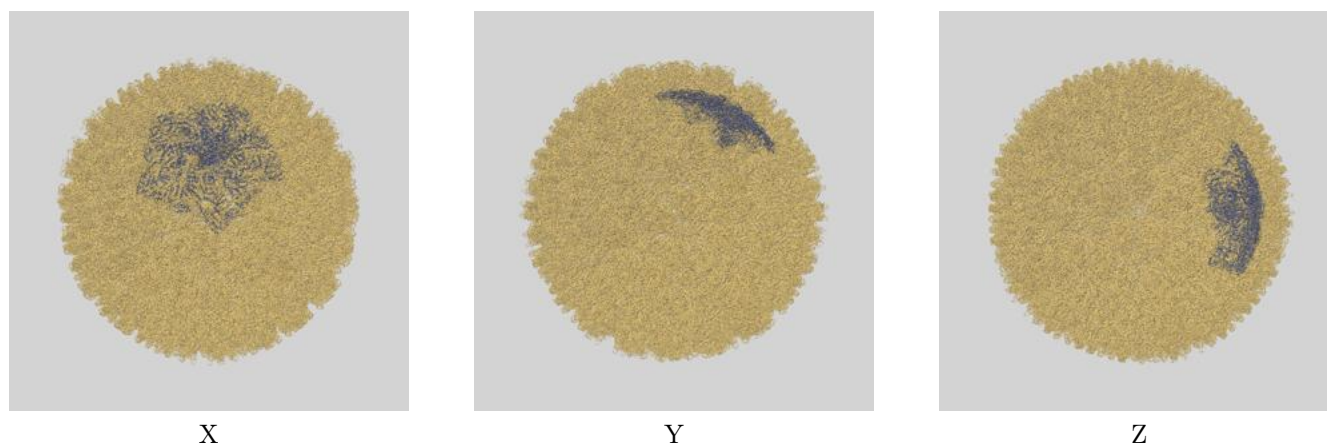
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

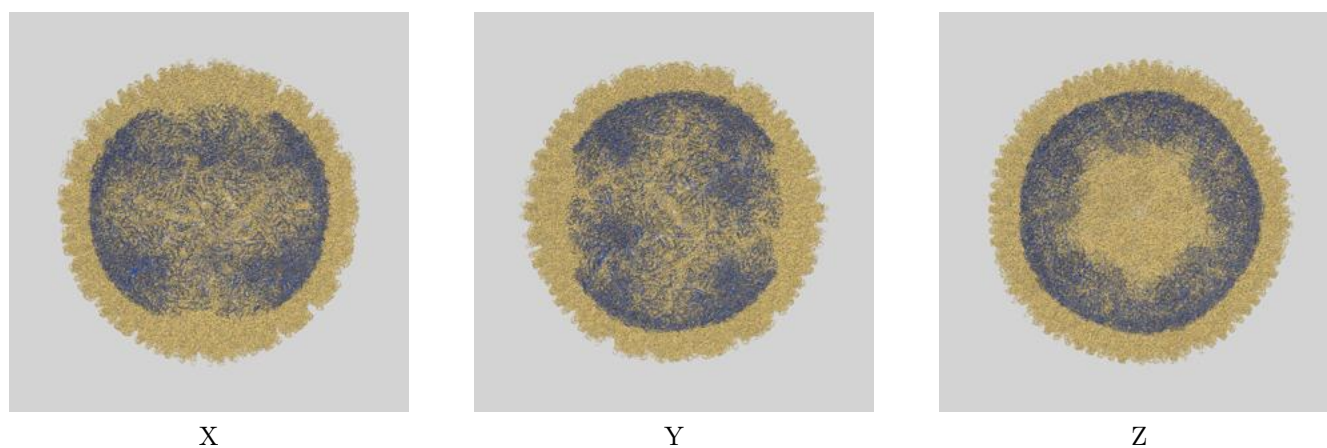
This section contains information regarding the fit between EMDB map EMD-33404 and PDB model 7XR3. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

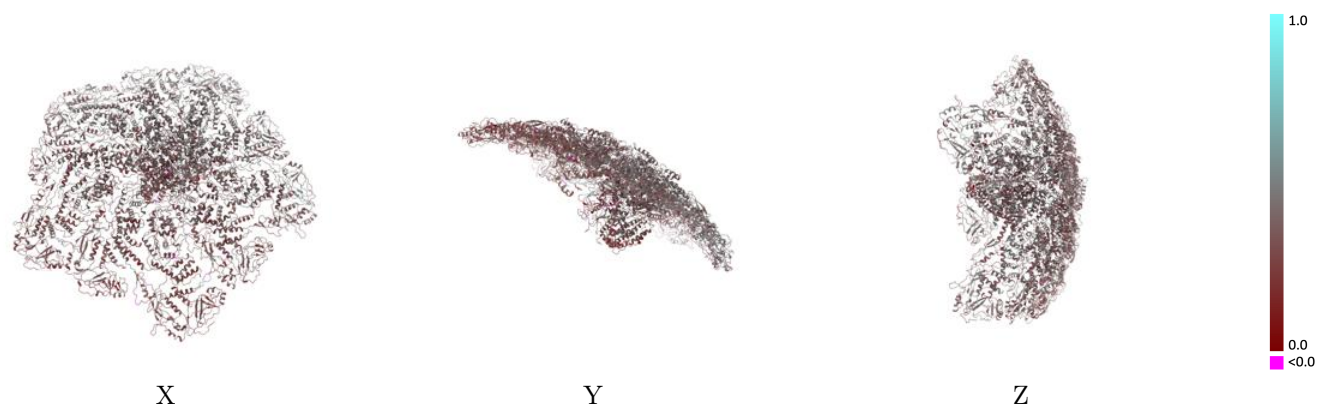


9.1.2 Map-model assembly overlay [i](#)



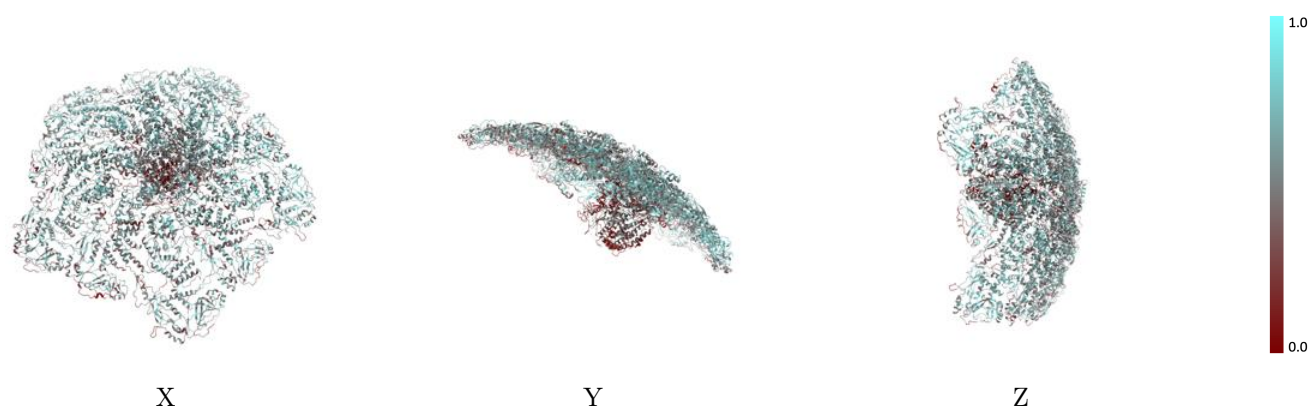
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



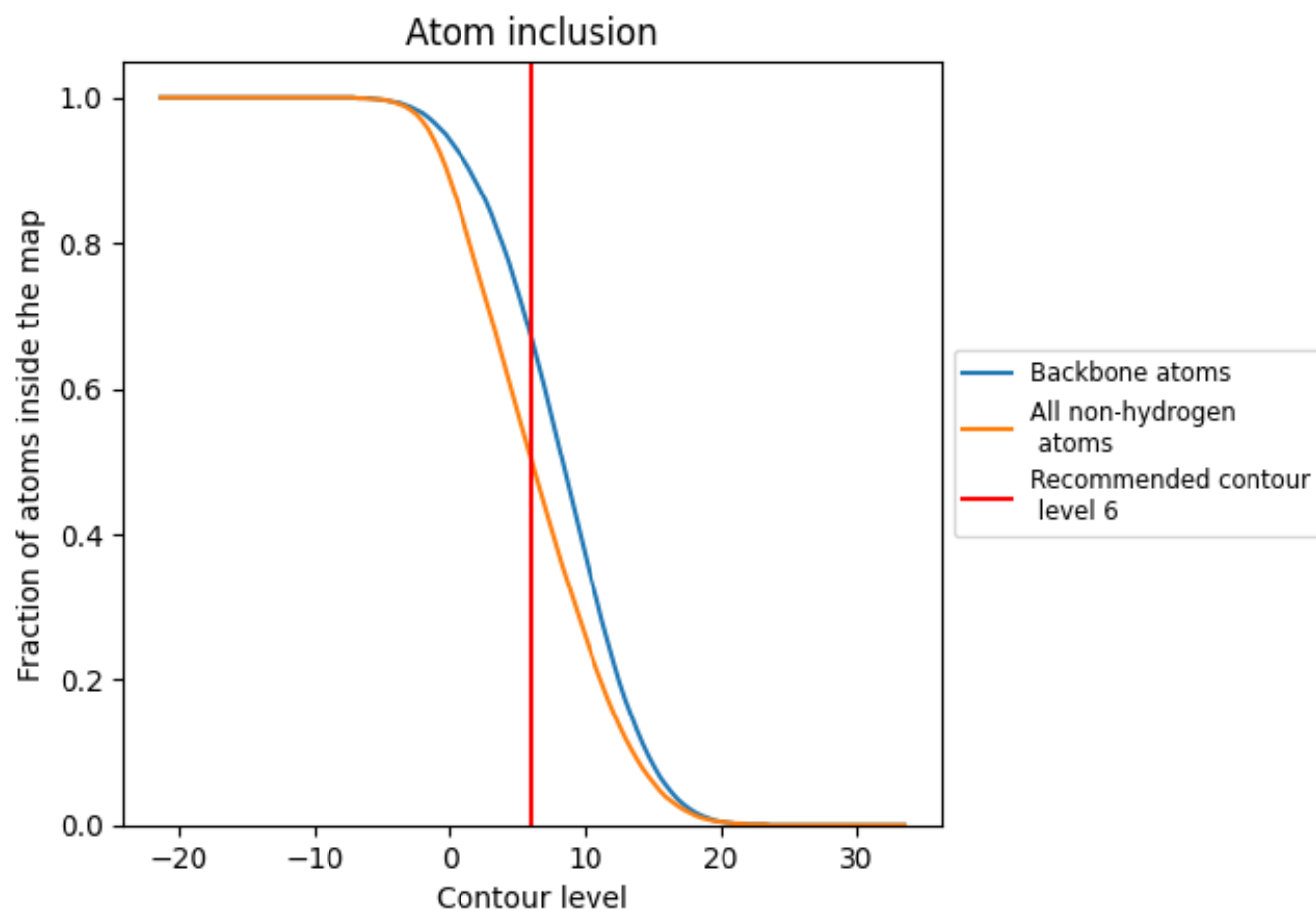
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 50% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5040	0.3580
A	0.5410	0.3990
B	0.5700	0.3920
C	0.5580	0.3950
D	0.5790	0.4090
E	0.5080	0.3430
F	0.5540	0.3670
G	0.4850	0.3300
H	0.5060	0.3160
I	0.5160	0.3590
J	0.5180	0.3340
Z	0.3130	0.3130

1.0

0.0

<0.0