



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 03:04 PM JST

PDB ID : 5ZVT
EMDB ID : EMD-6969
Title : Structure of RNA polymerase complex and genome within a dsRNA virus provides insights into the mechanisms of transcription and assembly
Authors : Liu, H.; Fang, Q.; Cheng, L.
Deposited on : 2018-05-12
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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

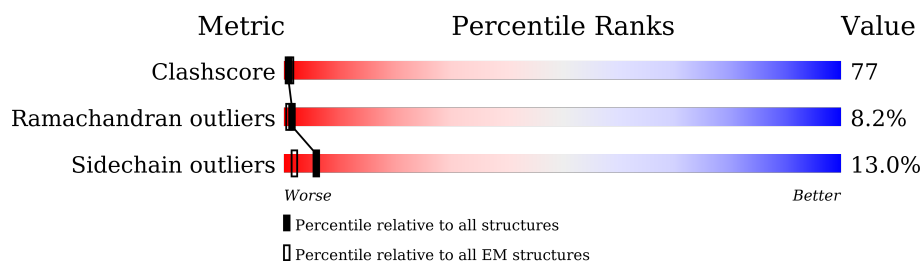
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	b	276	
1	d	276	
1	f	276	
1	h	276	
1	j	276	
1	l	276	
1	n	276	
1	p	276	

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Mol	Chain	Length	Quality of chain
1	r	276	
1	t	276	
2	A	42	
2	C	42	
2	E	42	
2	G	42	
2	I	42	
2	K	42	
2	M	42	
2	O	42	
2	Q	42	
2	S	42	
3	B	606	
3	D	606	
3	F	606	
3	H	606	
3	J	606	
3	L	606	
3	N	606	
3	P	606	
3	R	606	
3	T	606	
4	U	412	
4	V	412	
5	W	1299	

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Mol	Chain	Length	Quality of chain
6	X	1214	
6	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
7	MYR	A	101	-	-	X	-
7	MYR	C	101	-	-	X	-
7	MYR	E	101	-	-	X	-
7	MYR	G	101	-	-	X	-
7	MYR	I	101	-	-	X	-
7	MYR	K	101	-	-	X	-
7	MYR	M	101	-	-	X	-
7	MYR	O	101	-	-	X	-
7	MYR	Q	101	-	-	X	-
7	MYR	S	101	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 87645 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 VP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	l	86	Total 666	C 411	N 125	O 124	S 6	0	0
1	b	86	Total 666	C 411	N 125	O 124	S 6	0	0
1	f	86	Total 666	C 411	N 125	O 124	S 6	0	0
1	d	86	Total 666	C 411	N 125	O 124	S 6	0	0
1	h	86	Total 666	C 411	N 125	O 124	S 6	0	0
1	j	86	Total 666	C 411	N 125	O 124	S 6	0	0
1	n	86	Total 666	C 411	N 125	O 124	S 6	0	0
1	p	86	Total 666	C 411	N 125	O 124	S 6	0	0
1	r	86	Total 666	C 411	N 125	O 124	S 6	0	0
1	t	86	Total 666	C 411	N 125	O 124	S 6	0	0

- Molecule 2 is a protein called N-terminus of outer capsid protein VP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	41	Total 291	C 177	N 48	O 65	S 1	0	0
2	C	41	Total 291	C 177	N 48	O 65	S 1	0	0
2	E	41	Total 291	C 177	N 48	O 65	S 1	0	0
2	G	41	Total 284	C 174	N 46	O 63	S 1	0	0
2	I	41	Total 291	C 177	N 48	O 65	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
2	M	41	Total	C	N	O	S	0	0
			284	174	46	63	1		
2	O	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
2	Q	41	Total	C	N	O	S	0	0
			291	177	48	65	1		
2	S	41	Total	C	N	O	S	0	0
			284	174	46	63	1		

- Molecule 3 is a protein called C-terminus of outer capsid protein VP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
3	D	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
3	F	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
3	H	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
3	J	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
3	L	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
3	N	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
3	P	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
3	R	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		
3	T	604	Total	C	N	O	S	0	0
			4508	2858	761	872	17		

- Molecule 4 is a protein called Core protein VP6.

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

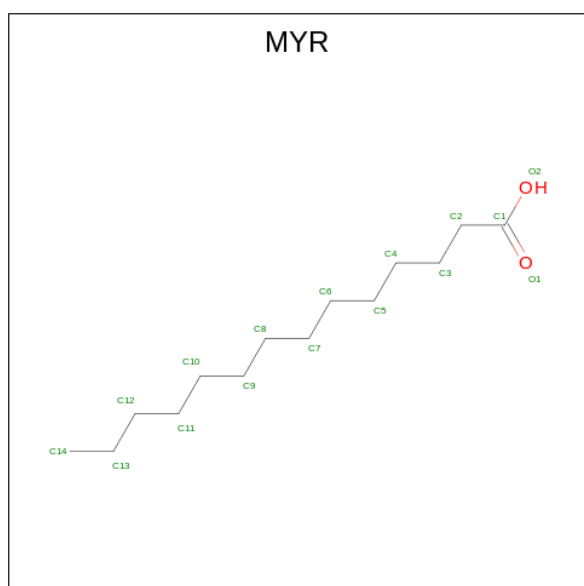
- Molecule 5 is a protein called VP1.

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

- Molecule 6 is a protein called VP3.

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

- Molecule 7 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			15	14	1	
7	C	1	Total	C	O	0
			15	14	1	
7	E	1	Total	C	O	0
			15	14	1	
7	G	1	Total	C	O	0
			15	14	1	
7	I	1	Total	C	O	0
			15	14	1	
7	K	1	Total	C	O	0
			15	14	1	

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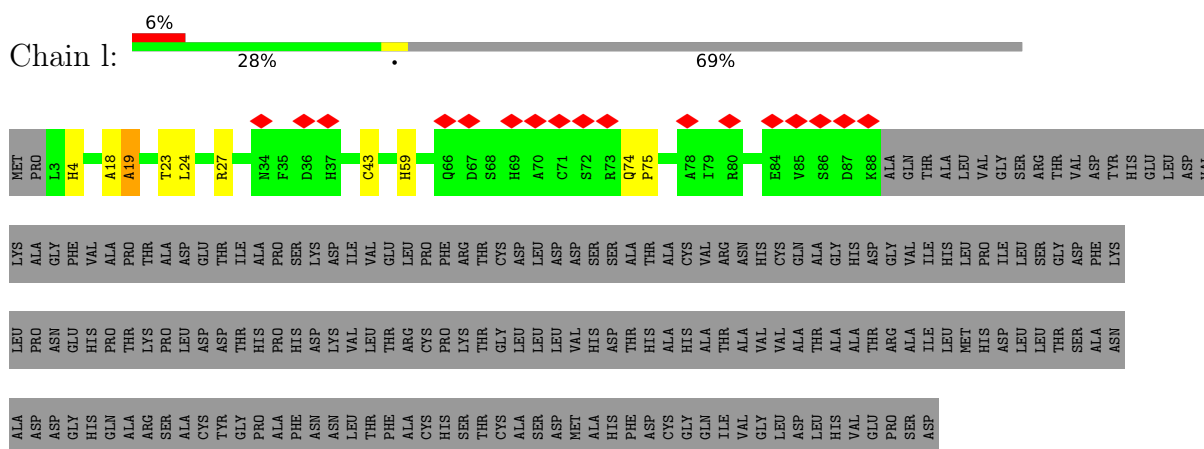
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Mol	Chain	Residues	Atoms			AltConf
7	M	1	Total	C	O	0
			15	14	1	
7	O	1	Total	C	O	0
			15	14	1	
7	Q	1	Total	C	O	0
			15	14	1	
7	S	1	Total	C	O	0
			15	14	1	

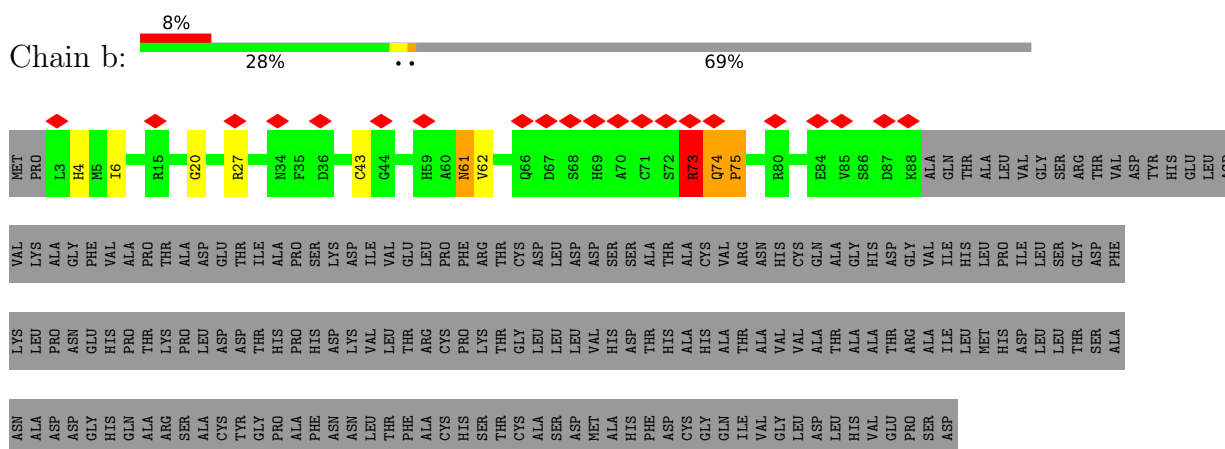
3 Residue-property plots

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.

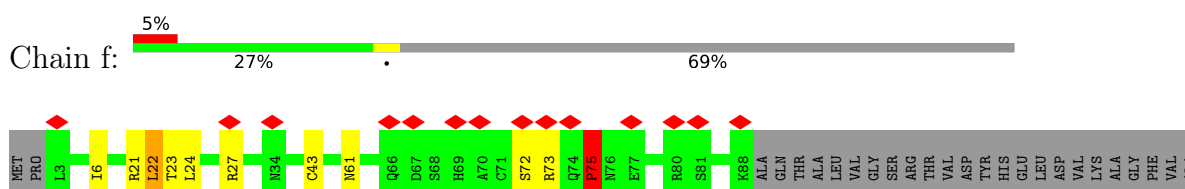
• Molecule 1: Outer capsid VP7



• Molecule 1: Outer capsid VP7



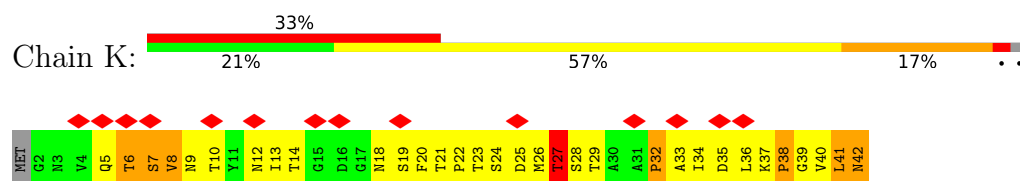
• Molecule 1: Outer capsid VP7



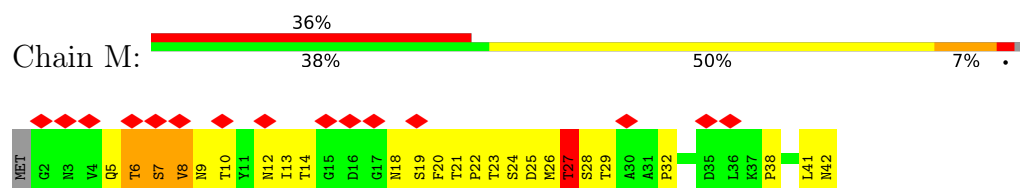




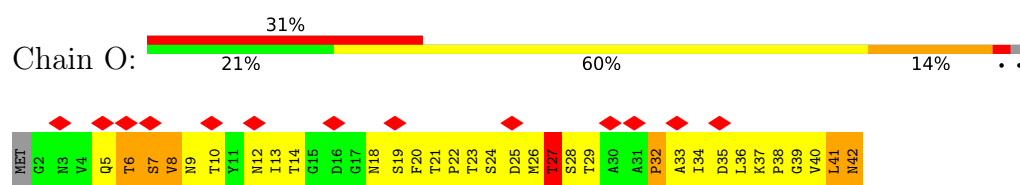
- Molecule 2: N-terminus of outer capsid protein VP5



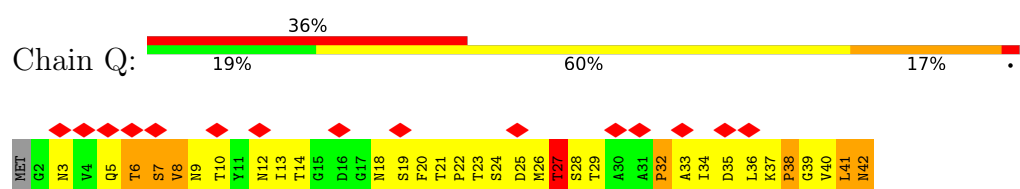
- Molecule 2: N-terminus of outer capsid protein VP5



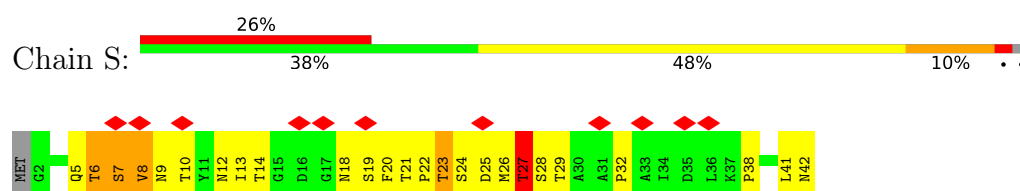
- Molecule 2: N-terminus of outer capsid protein VP5



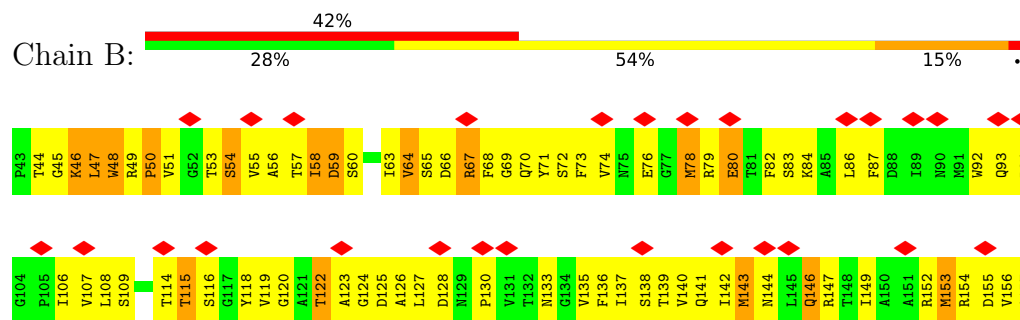
- Molecule 2: N-terminus of outer capsid protein VP5



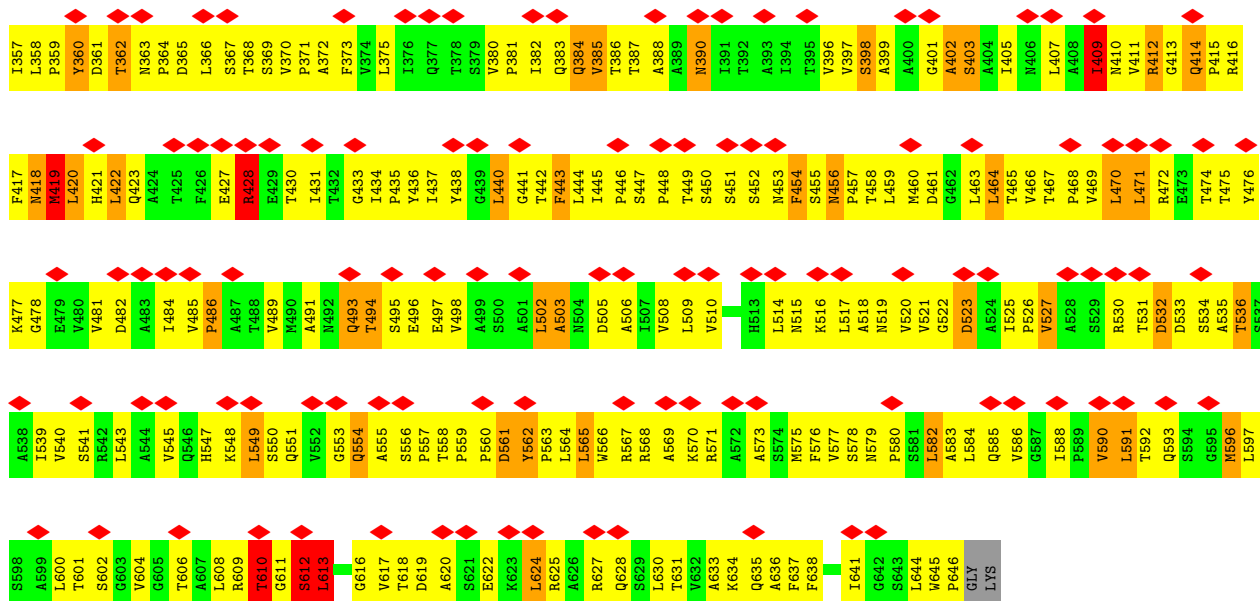
- Molecule 2: N-terminus of outer capsid protein VP5



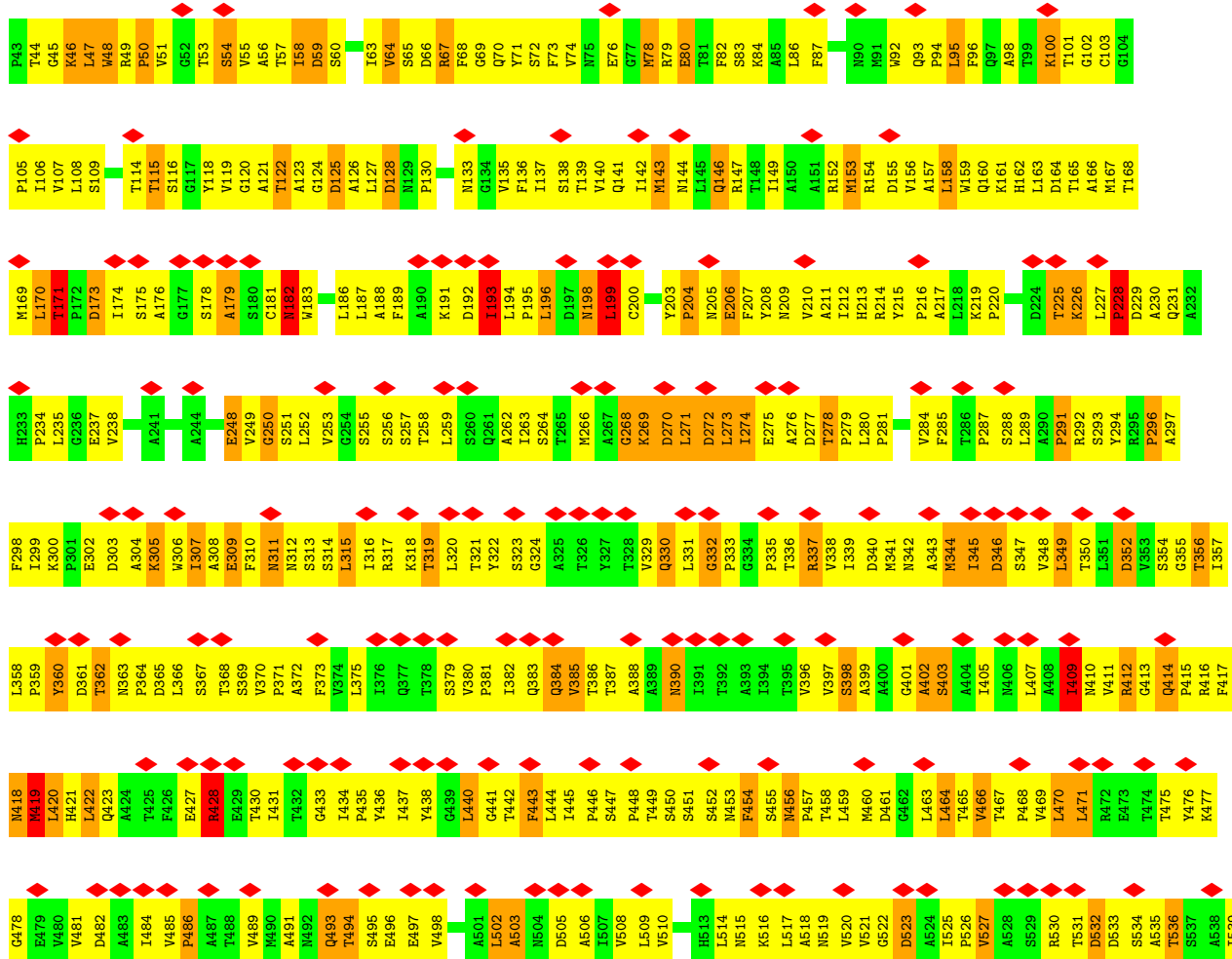
- Molecule 3: C-terminus of outer capsid protein VP5

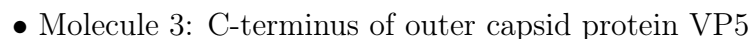


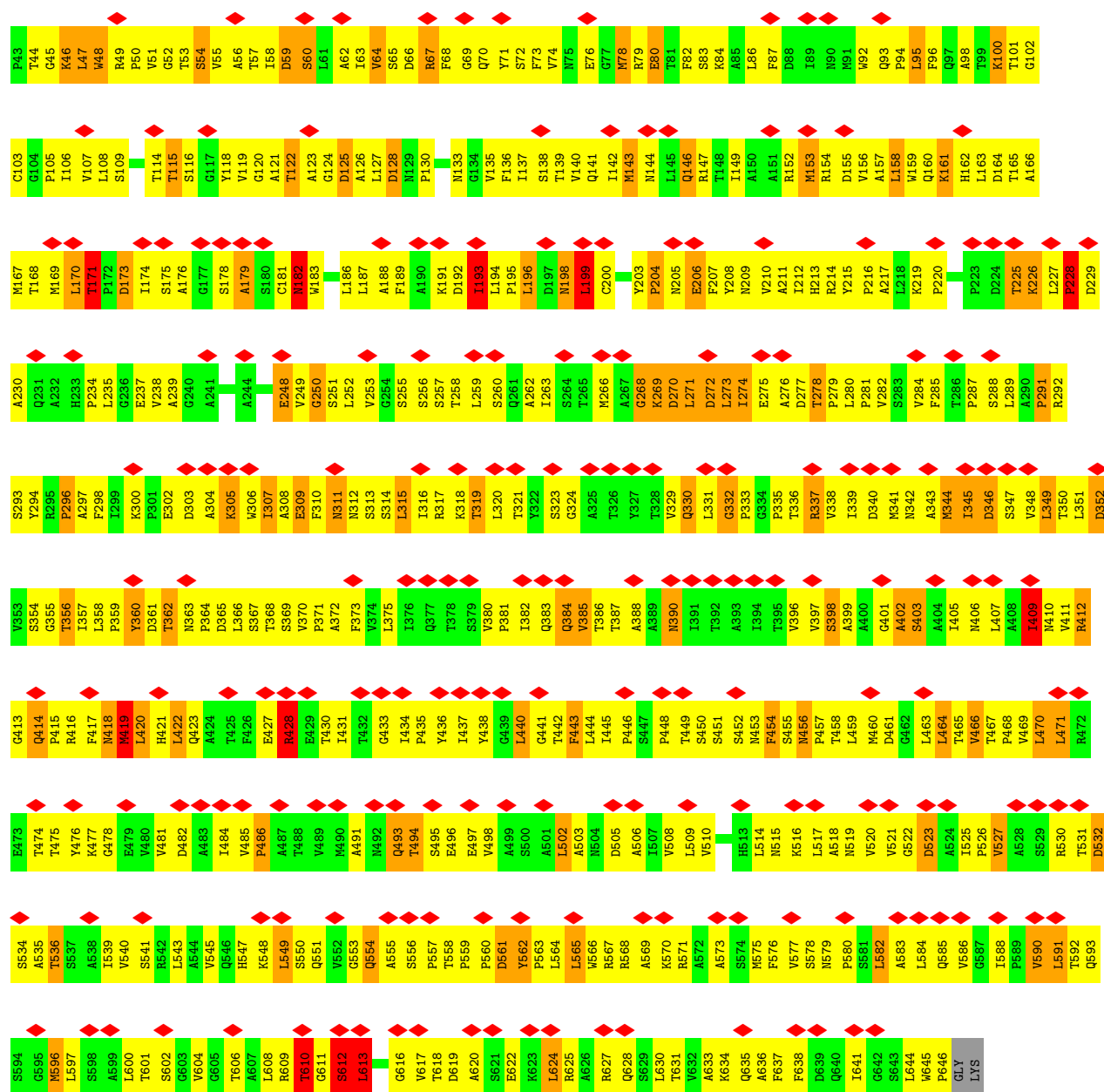




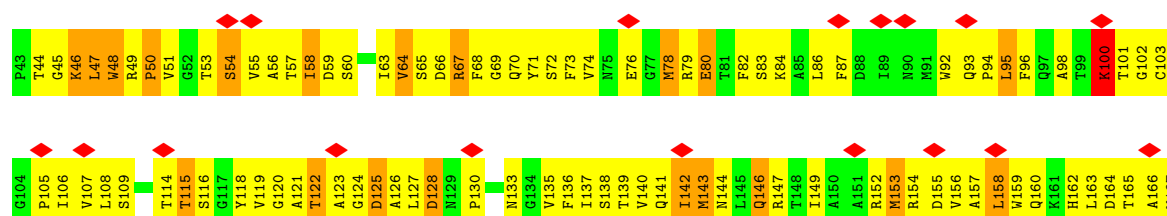
• Molecule 3: C-terminus of outer capsid protein VP5

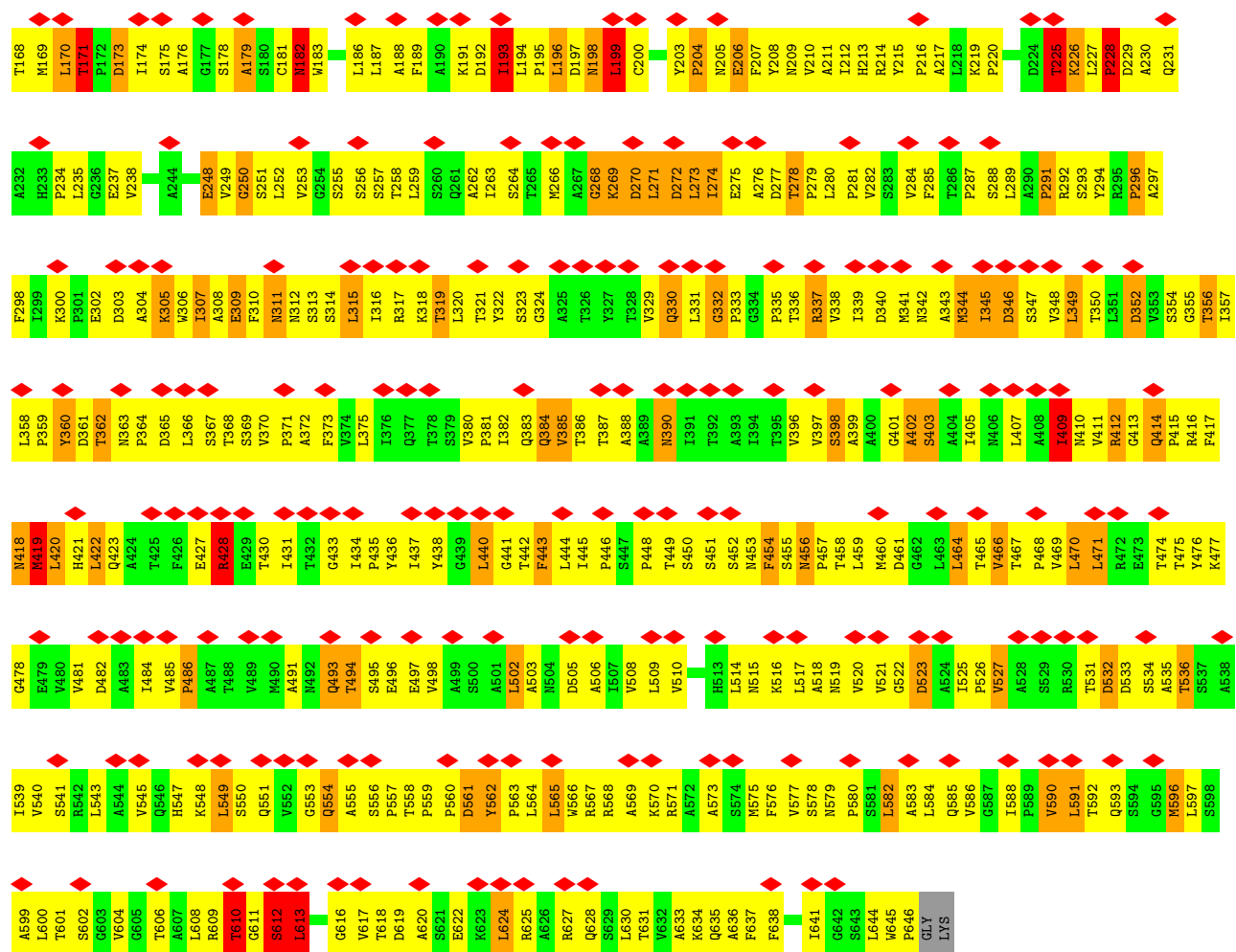




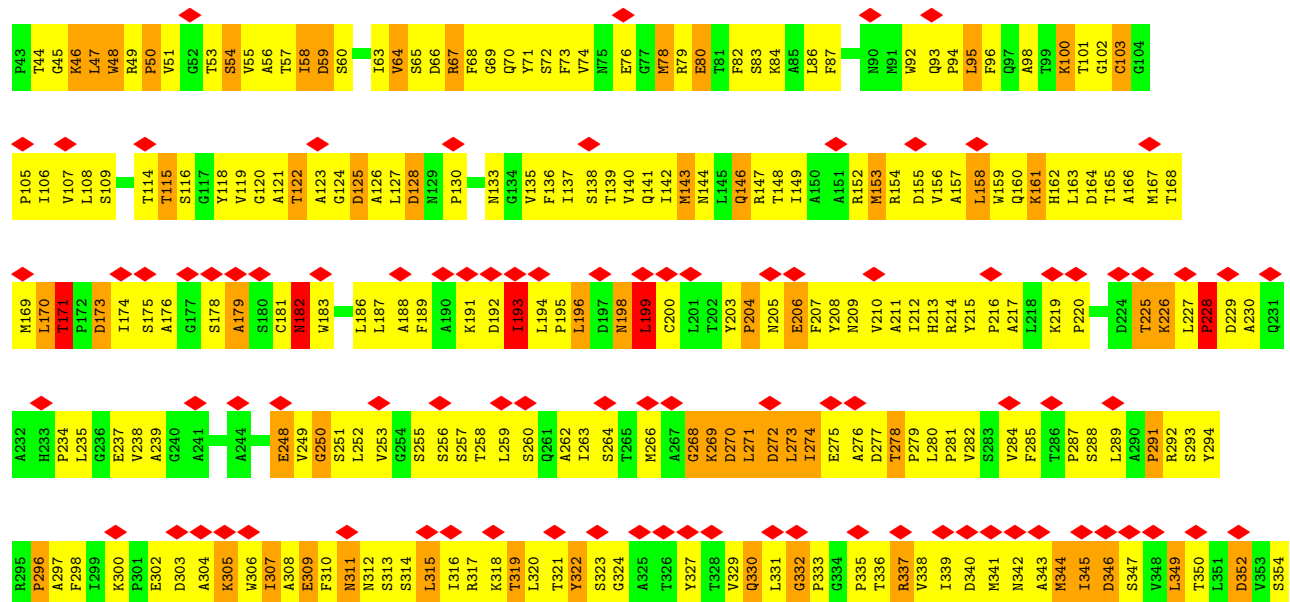


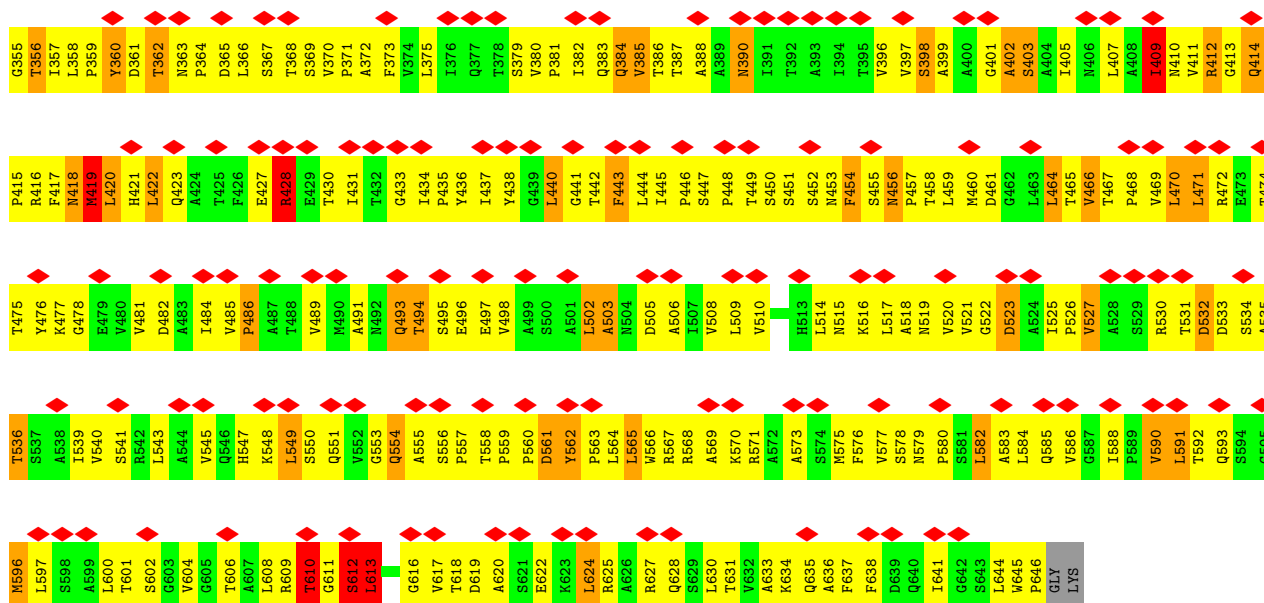
• Molecule 3: C-terminus of outer capsid protein VP5



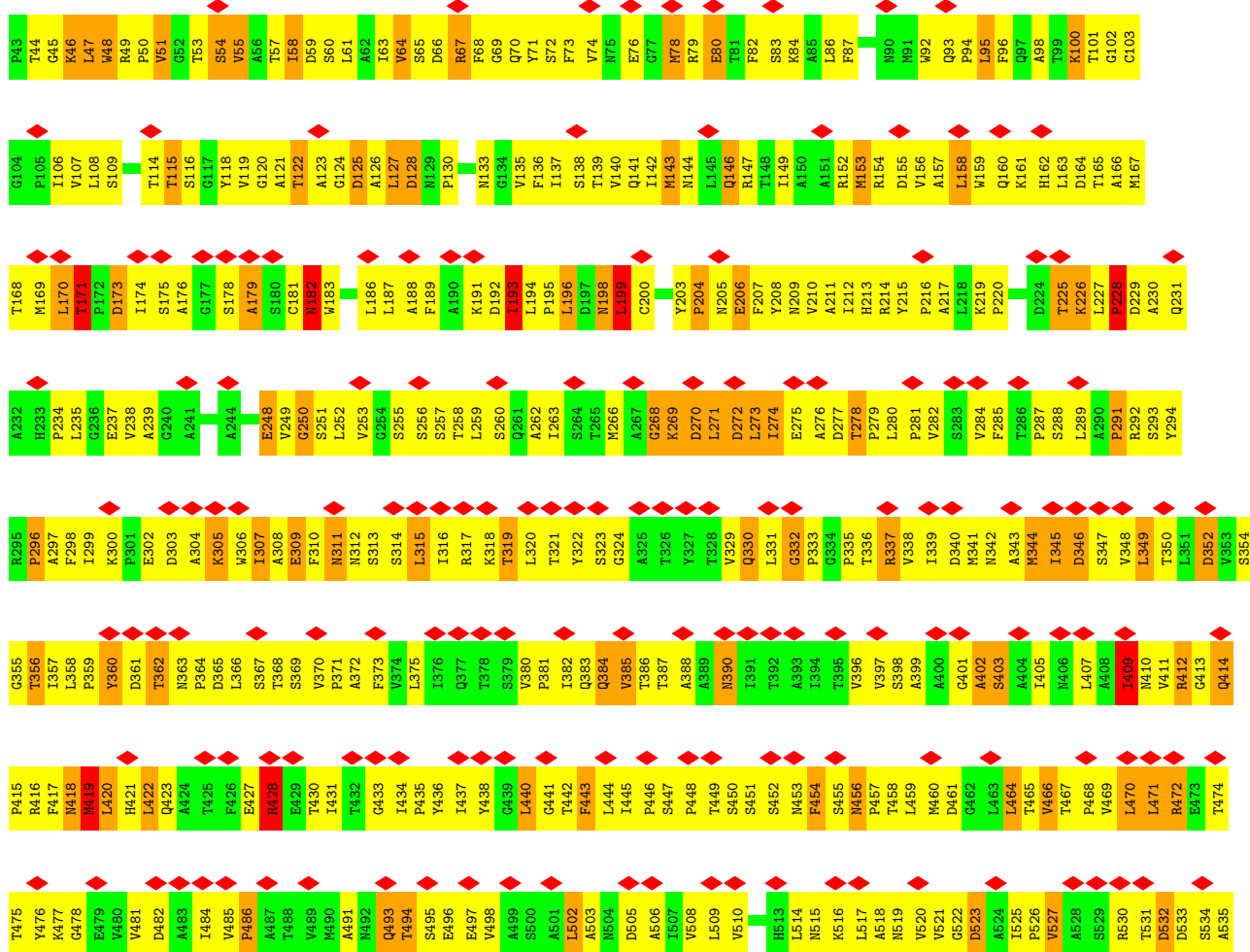


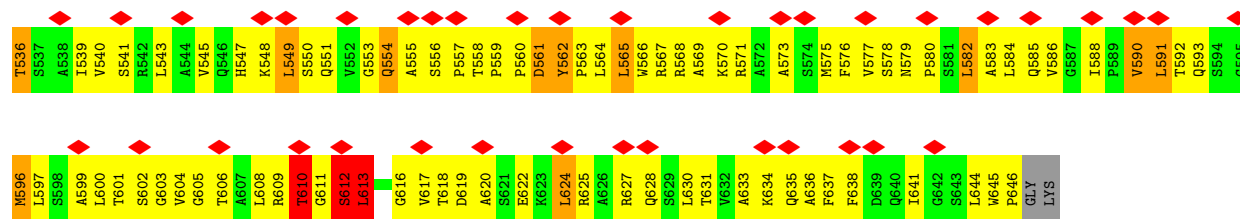
• Molecule 3: C-terminus of outer capsid protein VP5



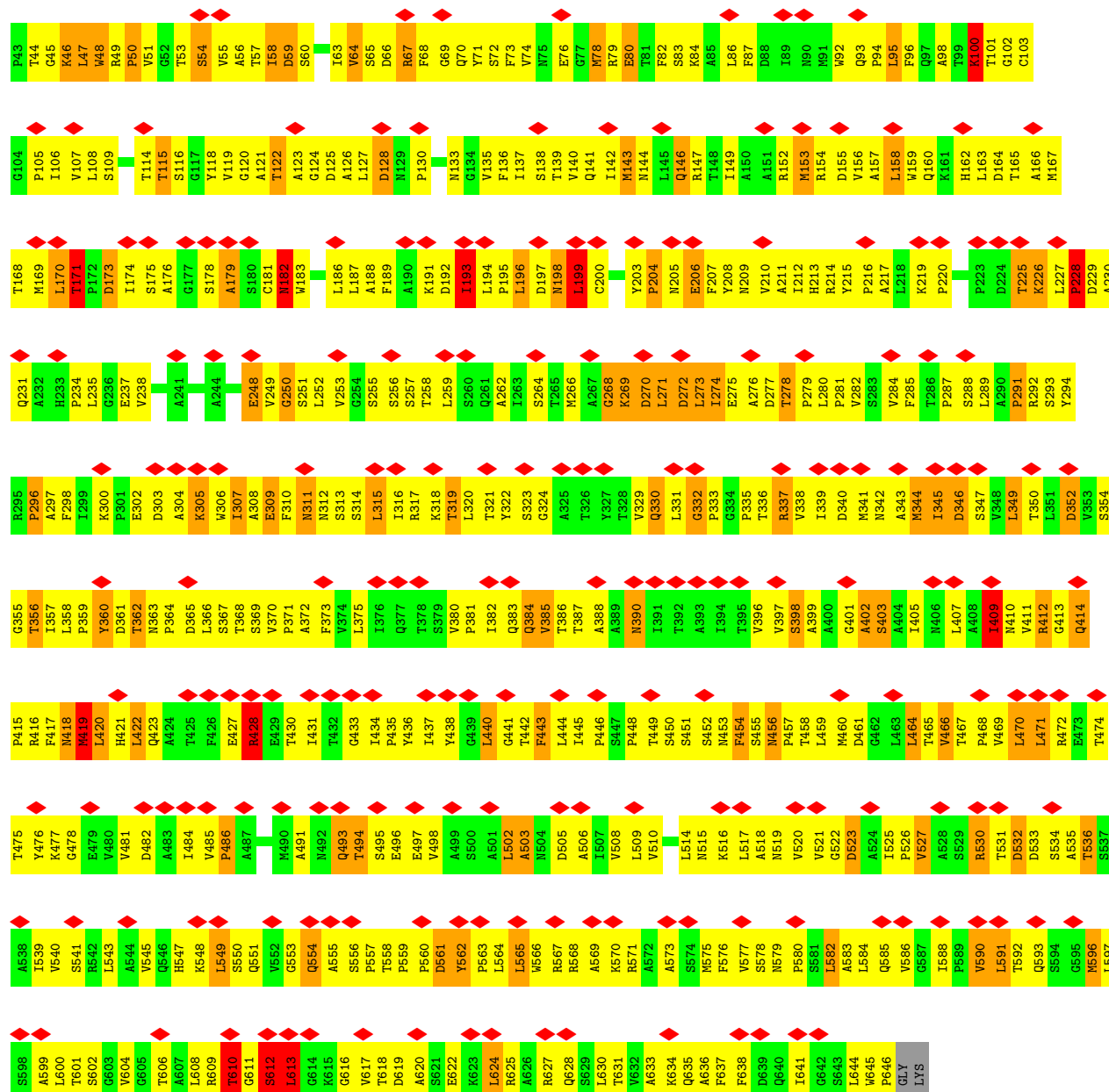


• Molecule 3: C-terminus of outer capsid protein VP5

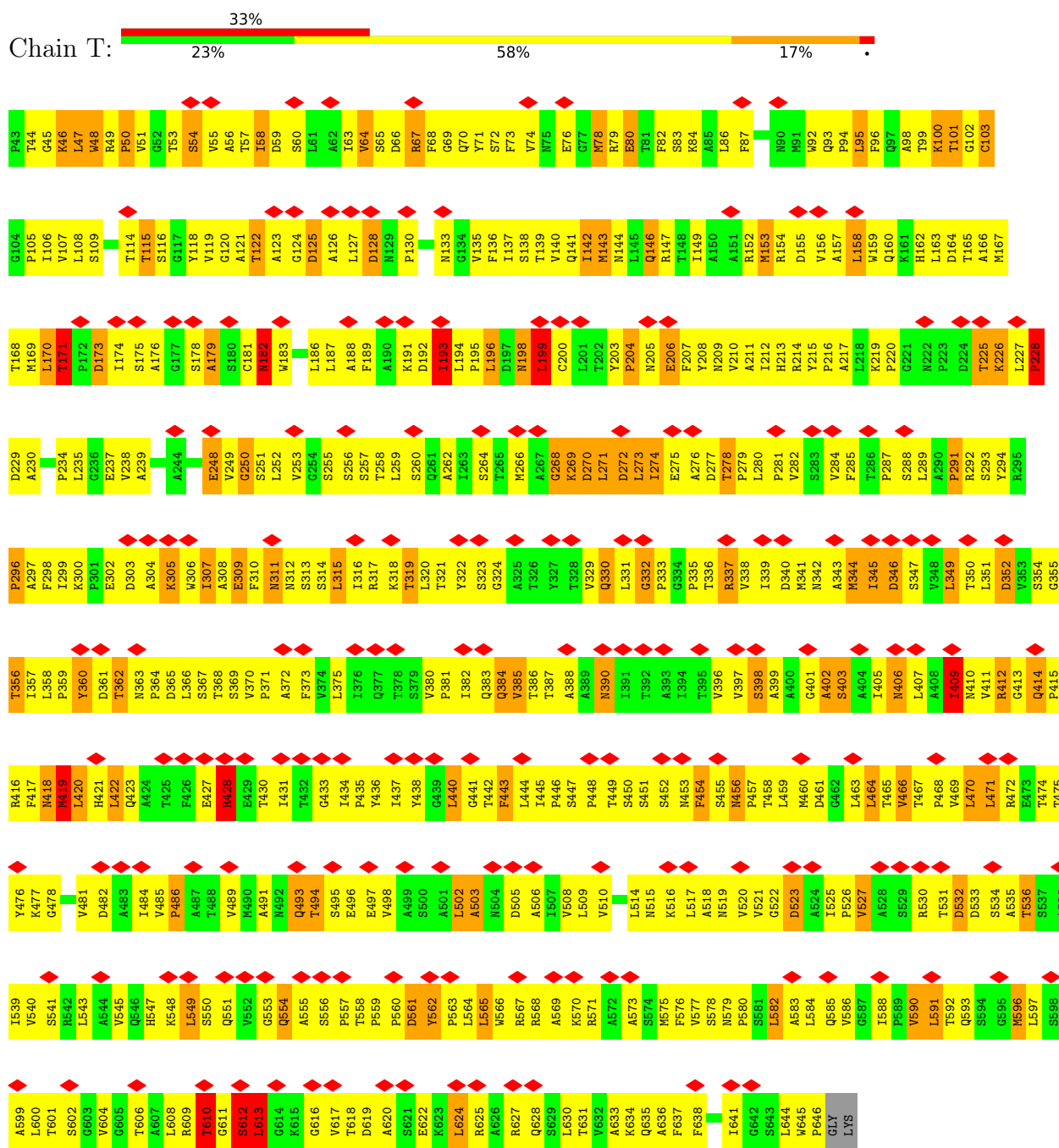




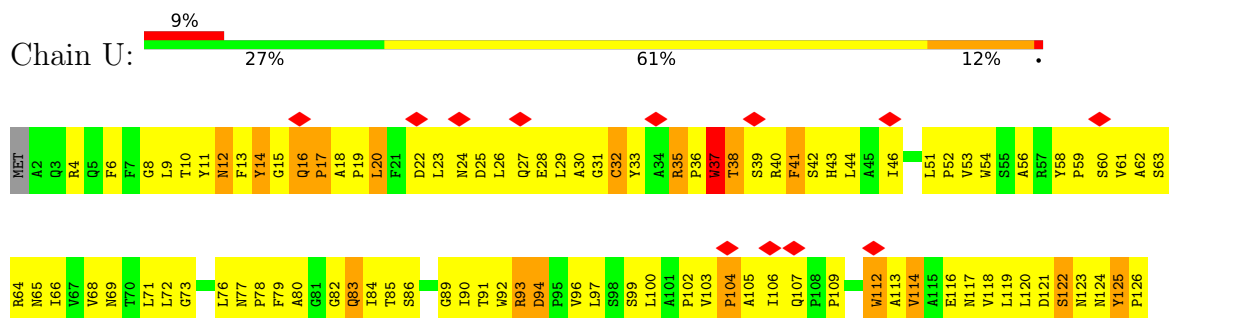
• Molecule 3: C-terminus of outer capsid protein VP5

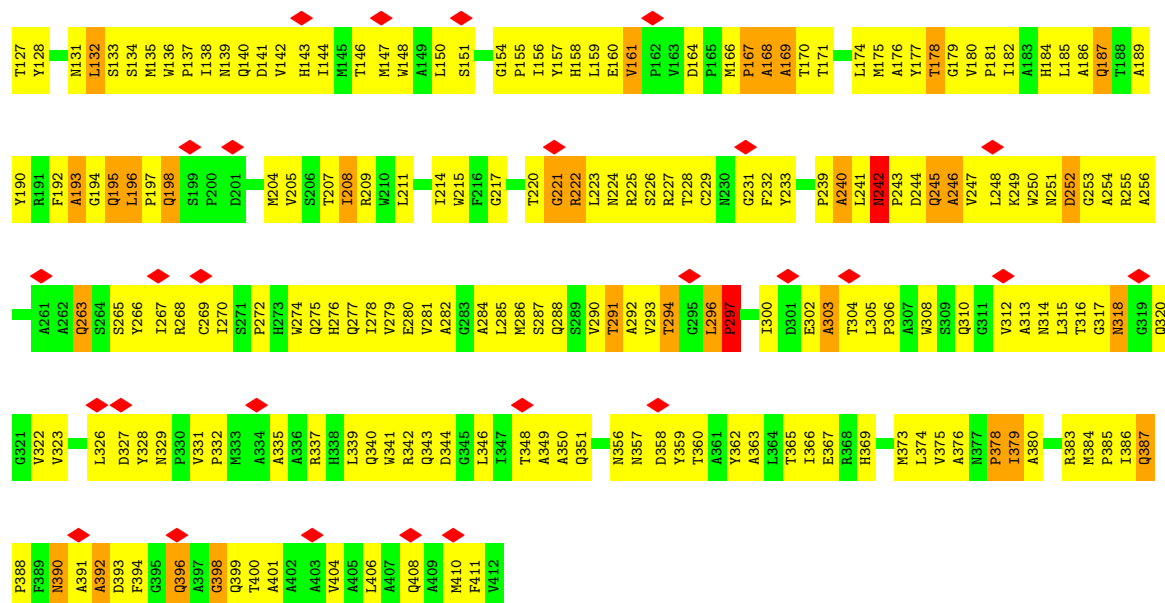


• Molecule 3: C-terminus of outer capsid protein VP5

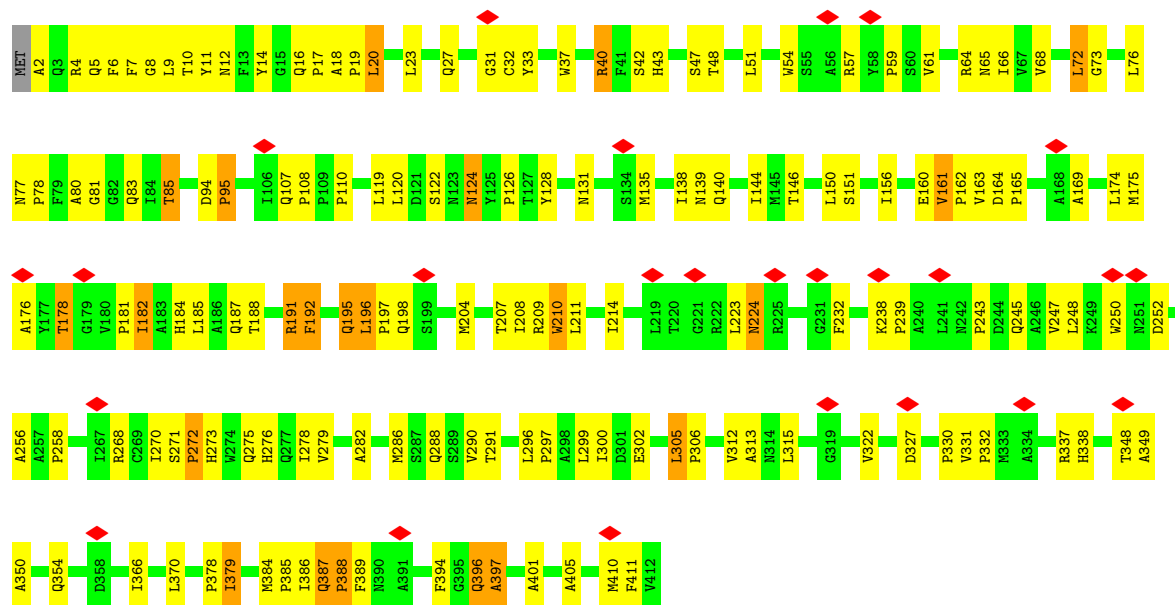


• Molecule 4: Core protein VP6

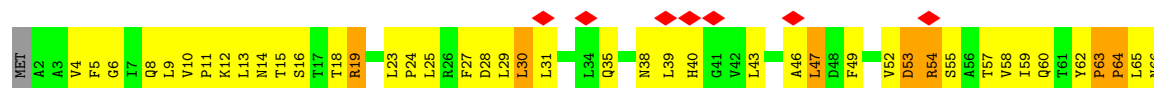




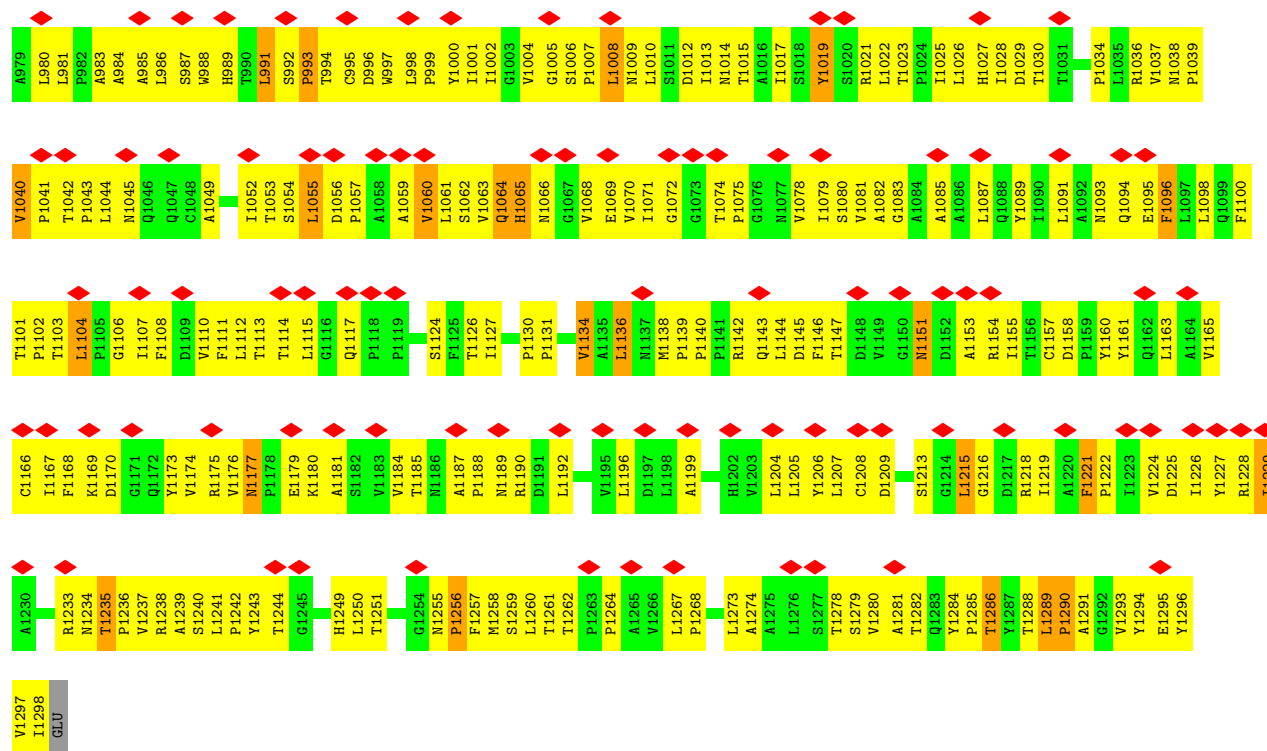
• Molecule 4: Core protein VP6



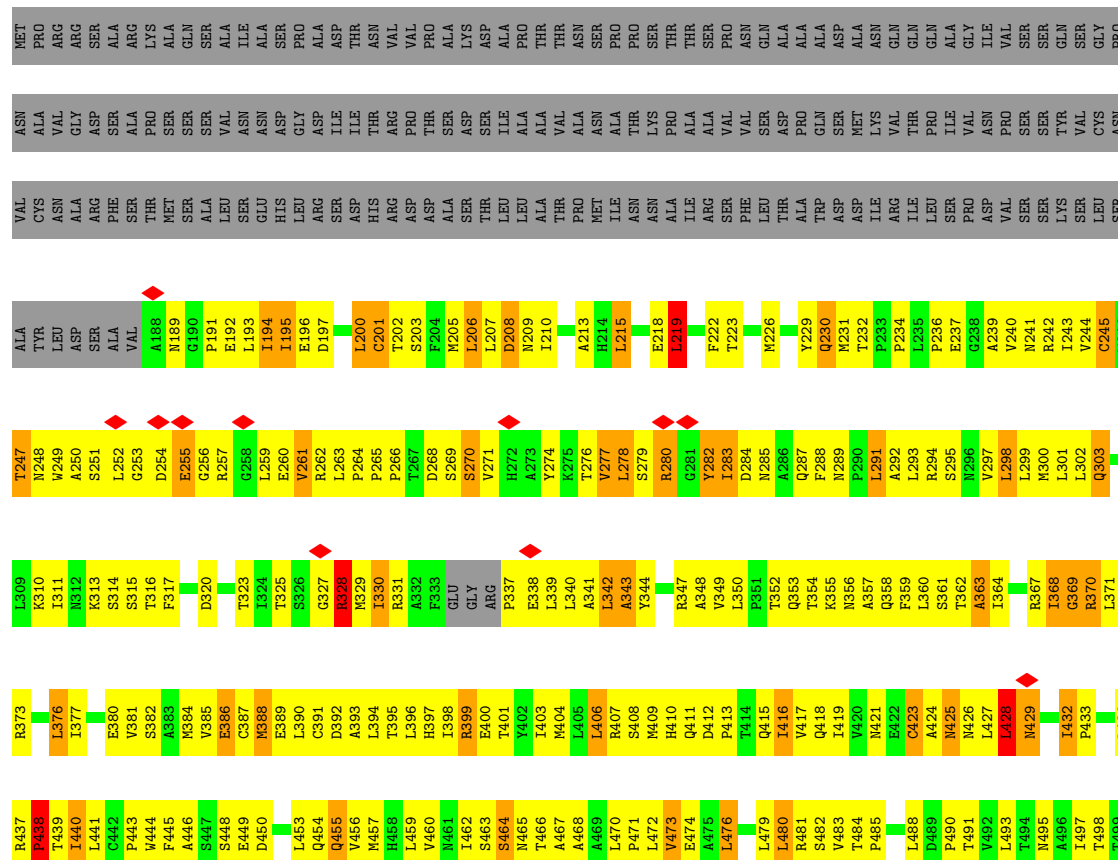
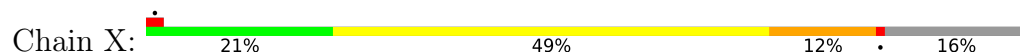
• Molecule 5: VP1



L917	T853	R789	L727	Q663	A601	ALA	Y464	R399	S335	P199	F134	A67
I918	M854	R790	F728	S664	ASN	ALA	F465	L400	F336	T200	L135	W68
P919	S855	F791	S729	N602	D529	ALA	R466	Y404	V337	Y201	D136	S89
R920	D856	T792	N730	L603	P530	ALA	R467	R405	A338	A202	R137	H71
I921	S857	T793	A731	G604	F531	ALA	E468	R406	R339	T203	L138	H72
V922	R858	P794	L732	T605	P532	ALA	R469	A407	L340	F205	F139	A73
A923	P859	F797	A733	T606	V533	ALA	R470	A408	M341	T206	Y140	A74
A924	C860	T798	S734	A606	I533	ALA	A471	L409	G344	Y207	P142	I75
G925	A861	L798	L735	T610	L534	ALA	R472	T410	D345	S208	D141	E76
G926	E862	F800	R736	A673	A535	ALA	R473	Y411	P346	T209	P142	I77
T927	L863	S801	S737	T611	D536	ALA	D474	Q412	Q347	L210	T143	E78
A928	M864	S802	R738	L674	I537	ALA	L475	Q413	Q348	P211	Q144	P78
M929	E803	R804	V739	Q675	I542	ALA	F476	A414	F350	A212	S146	L79
V930	S866	V805	V740	R676	P543	ALA	R477	A415	P351	R213	S147	D80
L931	F867	V805	V741	A677	P543	ALA	R478	D416	G352	R214	I147	Y81
Q932	T868	T809	S742	V617	I554	ALA	L479	A417	Y352	S214	T149	R82
L933	P869	L810	R743	L618	V552	ALA	R480	Y418	R353	R215	A150	R83
N934	A870	V811	T744	K619	Q553	ALA	A481	E419	P352	L216	T151	W84
T935	L871	A812	M745	V620	F554	ALA	P482	D420	Q356	A218	T152	T85
P936	T872	R813	T746	N621	D557	ALA	ASP	L423	I357	N219	K153	I88
L937	R873	G814	T747	R622	V558	ALA	R485	P425	L358	L220	P155	H89
Y938	Y874	Y815	V749	P623	V559	ALA	R486	L426	Y359	A221	Y156	D90
F939	V875	N816	P750	R624	H560	ALA	A487	L427	W360	A222	Q157	R91
V940	Q876	S817	S751	R625	C561	ALA	L488	L427	P363	G223	W158	A94
S941	G877	F818	G752	A626	S562	ALA	K489	T428	F365	T225	T159	F95
R942	R878	I819	G753	V628	L563	ALA	D490	T429	V366	V226	I160	V96
L943	Y879	A691	T576	V629	L564	ALA	R491	Q431	P367	P233	S162	L99
P944	S880	E821	T577	D630	D565	ALA	A492	Q432	N301	T234	N163	L99
D945	T881	Q822	T578	V631	L566	ALA	V493	Q433	T302	Y235	Q101	Q101
L946	A882	T823	V760	F632	V570	ALA	F494	V434	L303	G236	R102	R102
I947	A883	R824	T579	V632	P571	ALA	D495	T435	Q304	P237	Y103	Y103
E948	F884	N825	T580	V633	I572	ALA	F496	T436	L304	P371	P104	P104
I949	W885	P826	T581	V634	T573	ALA	L497	Q437	P371	L240	L105	L105
D950	N886	P826	T582	V635	T574	ALA	A498	V438	F372	L241	T171	T171
L951	G887	V827	T583	V636	F575	ALA	S499	F439	Y373	P242	S172	S172
R952	I888	A829	T584	V637	G576	ALA	L500	T440	N309	Q243	A173	A173
Q953	L889	H830	T585	V638	L577	ALA	V501	S441	L310	T244	G174	G174
H954	R890	L831	T586	V639	V578	ALA	T504	D444	A311	T245	C175	C175
V955	C891	R832	T587	V640	V579	ALA	T505	D445	L312	G246	K176	K176
S956	D891	L833	T588	V641	A580	ALA	T506	I445	L313	D246	Y177	Y177
Y957	R892	L834	T589	V642	D581	ALA	A506	D446	L314	L246	L178	L178
F958	F893	G835	T590	V643	L582	ALA	P507	D447	L315	G249	T179	T179
N959	T894	R836	T591	V644	D583	ALA	P508	D448	L316	Y250	L180	L180
G960	A895	G837	T592	V645	Q584	ALA	V509	D449	Q317	S251	Y183	Y183
P961	I896	P838	T593	V646	Q585	ALA	V510	P449	G317	L255	L184	L184
E962	F897	E839	T594	V647	V586	ALA	L510	Y450	T384	S256	P185	P185
R963	T898	C840	T595	V648	ASP	ALA	D511	Y451	Y388	Q257	S186	S186
V964	A901	R841	T596	V649	ALA	ALA	T512	Y452	V391	L254	G119	G119
E965	G901	L842	T597	V650	GLY	ALA	T513	Y453	P392	L255	A120	A120
P966	P966	L843	T598	V651	THR	ALA	T514	Y454	S393	S256	F122	F122
Y967	A904	S844	T599	V652	D591	ALA	A517	Q455	R393	A258	G123	G123
A968	A905	T845	T600	V653	M592	ALA	Y518	Q456	P328	L259	D124	D124
P969	A906	L846	T601	V654	P593	ALA	L519	L457	T329	L260	T193	T193
R970	G907	P847	T602	V655	P594	ALA	L520	L458	S395	L261	Y194	Y194
V971	T908	P848	T603	V656	N596	ALA	G520	D459	R396	L262	G195	G195
P972	D909	T849	T604	V657	R597	ALA	A521	A460	D332	M262	N127	N127
L973	L910	L850	T605	V658	A598	ALA	S522	A461	V333	V263	K196	K196
Q974	V914	Q915	T606	V659	A599	ALA	S523	A462	R334	E264	H197	H197
A978	Q916	V852	T607	V660	A599	ALA	S524	A463	L398		D132	D132
			T608	V661	A599	ALA	S525	A464			I133	I133

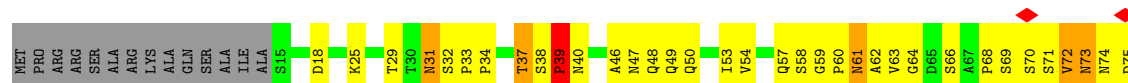


• Molecule 6: VP3



- Molecule 6: VP3

Chain Y:







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	134.413	Depositor
Minimum map value	-88.945	Depositor
Average map value	0.680	Depositor
Map value standard deviation	8.761	Depositor
Recommended contour level	9	Depositor
Map size (Å)	838.8, 838.8, 838.8	wwPDB
Map dimensions	900, 900, 900	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	b	0.83	2/678 (0.3%)	1.10	3/922 (0.3%)
1	d	0.43	0/678	0.78	0/922
1	f	0.42	0/678	0.92	4/922 (0.4%)
1	h	0.43	0/678	0.76	0/922
1	j	0.43	0/678	0.76	0/922
1	l	0.40	0/678	0.83	2/922 (0.2%)
1	n	0.41	0/678	0.75	0/922
1	p	0.42	0/678	0.74	0/922
1	r	0.41	0/678	0.76	0/922
1	t	0.42	0/678	0.71	0/922
2	A	0.60	0/295	1.00	0/405
2	C	0.60	0/295	1.00	0/405
2	E	0.60	0/295	0.99	0/405
2	G	0.60	0/286	0.95	0/391
2	I	0.60	0/295	1.00	0/405
2	K	0.60	0/295	0.99	0/405
2	M	0.60	0/286	0.95	0/391
2	O	0.60	0/295	0.99	0/405
2	Q	0.60	0/295	0.99	0/405
2	S	0.60	0/286	0.95	0/391
3	B	0.52	0/4601	0.80	0/6295
3	D	0.51	0/4601	0.80	1/6295 (0.0%)
3	F	0.52	0/4601	0.80	0/6295
3	H	0.52	0/4601	0.80	0/6295
3	J	0.51	0/4601	0.80	0/6295
3	L	0.52	0/4601	0.80	0/6295
3	N	0.52	0/4601	0.80	0/6295
3	P	0.51	0/4601	0.80	0/6295
3	R	0.52	0/4601	0.80	0/6295
3	T	0.52	0/4601	0.80	0/6295
4	U	0.33	0/3233	0.55	0/4443
4	V	0.31	0/3233	0.49	0/4443

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	W	0.32	0/10148	0.60	0/13935
6	X	0.53	0/8078	0.75	2/11071 (0.0%)
6	Y	0.38	0/9056	0.66	2/12412 (0.0%)
All	All	0.47	2/89461 (0.0%)	0.75	14/122482 (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	b	0	4
1	d	0	3
1	f	0	2
1	h	0	2
1	j	0	2
1	l	0	2
1	n	0	3
1	p	0	3
1	r	0	2
1	t	0	2
3	B	0	1
3	D	0	1
3	F	0	1
3	H	0	1
3	J	0	1
3	L	0	1
3	N	0	1
3	P	0	1
3	R	0	1
3	T	0	1
6	X	0	3
6	Y	0	2
All	All	0	40

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	74	GLN	C-N	17.97	1.68	1.34
1	b	73	ARG	C-N	5.02	1.45	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	73	ARG	O-C-N	-19.95	90.78	122.70
1	b	73	ARG	CA-C-N	10.04	139.28	117.20
1	f	75	PRO	N-CA-CB	-6.70	95.23	102.60
1	b	74	GLN	O-C-N	-6.47	108.81	121.10
1	l	18	ALA	C-N-CA	6.35	137.58	121.70

There are no chirality outliers.

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	b	43	CYS	Peptide
1	b	73	ARG	Peptide,Mainchain
1	b	75	PRO	Peptide
1	l	43	CYS	Peptide
1	l	75	PRO	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	b	666	0	660	0	0
1	d	666	0	660	0	0
1	f	666	0	657	0	0
1	h	666	0	655	0	0
1	j	666	0	659	0	0
1	l	666	0	656	0	0
1	n	666	0	658	0	0
1	p	666	0	659	0	0
1	r	666	0	657	0	0
1	t	666	0	659	0	0
2	A	291	0	277	54	0
2	C	291	0	277	78	0
2	E	291	0	277	77	0
2	G	284	0	267	56	0
2	I	291	0	277	81	0
2	K	291	0	277	78	0
2	M	284	0	267	57	0
2	O	291	0	277	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	291	0	277	85	0
2	S	284	0	267	58	0
3	B	4508	0	4555	645	0
3	D	4508	0	4554	904	0
3	F	4508	0	4554	874	0
3	H	4508	0	4554	865	0
3	J	4508	0	4553	890	0
3	L	4508	0	4555	874	0
3	N	4508	0	4555	889	0
3	P	4508	0	4555	899	0
3	R	4508	0	4554	883	0
3	T	4508	0	4555	883	0
4	U	3138	0	3061	444	0
4	V	3138	0	3061	174	0
5	W	9882	0	9821	1051	0
6	X	7873	0	7851	1242	0
6	Y	8835	0	8748	1054	0
7	A	15	0	27	27	0
7	C	15	0	27	33	0
7	E	15	0	27	27	0
7	G	15	0	27	29	0
7	I	15	0	27	29	0
7	K	15	0	27	27	0
7	M	15	0	27	26	0
7	O	15	0	27	28	0
7	Q	15	0	27	27	0
7	S	15	0	27	30	0
All	All	87645	0	87676	11633	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 77.

The worst 5 of 11633 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)
4:U:32:CYS:HB3	6:X:958:HIS:CE1	1.55	1.38
6:X:464:SER:HB2	6:Y:500:ILE:CG2	1.52	1.38
3:R:628:GLN:NE2	5:W:870:ALA:HA	1.41	1.35
3:D:469:VAL:HG21	3:F:575:MET:CE	1.59	1.33
3:F:469:VAL:HG21	3:H:575:MET:CE	1.59	1.33

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	b	84/276 (30%)	70 (83%)	9 (11%)	5 (6%)	1	9
1	d	84/276 (30%)	70 (83%)	11 (13%)	3 (4%)	3	18
1	f	84/276 (30%)	68 (81%)	12 (14%)	4 (5%)	2	12
1	h	84/276 (30%)	71 (84%)	10 (12%)	3 (4%)	3	18
1	j	84/276 (30%)	72 (86%)	9 (11%)	3 (4%)	3	18
1	l	84/276 (30%)	70 (83%)	13 (16%)	1 (1%)	11	38
1	n	84/276 (30%)	69 (82%)	12 (14%)	3 (4%)	3	18
1	p	84/276 (30%)	74 (88%)	7 (8%)	3 (4%)	3	18
1	r	84/276 (30%)	71 (84%)	11 (13%)	2 (2%)	5	25
1	t	84/276 (30%)	72 (86%)	10 (12%)	2 (2%)	5	25
2	A	39/42 (93%)	25 (64%)	9 (23%)	5 (13%)	0	1
2	C	39/42 (93%)	25 (64%)	9 (23%)	5 (13%)	0	1
2	E	39/42 (93%)	25 (64%)	9 (23%)	5 (13%)	0	1
2	G	37/42 (88%)	24 (65%)	8 (22%)	5 (14%)	0	1
2	I	39/42 (93%)	25 (64%)	9 (23%)	5 (13%)	0	1
2	K	39/42 (93%)	25 (64%)	9 (23%)	5 (13%)	0	1
2	M	37/42 (88%)	24 (65%)	8 (22%)	5 (14%)	0	1
2	O	39/42 (93%)	25 (64%)	9 (23%)	5 (13%)	0	1
2	Q	39/42 (93%)	25 (64%)	9 (23%)	5 (13%)	0	1
2	S	37/42 (88%)	24 (65%)	8 (22%)	5 (14%)	0	1
3	B	602/606 (99%)	407 (68%)	134 (22%)	61 (10%)	0	3
3	D	602/606 (99%)	416 (69%)	129 (21%)	57 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	602/606 (99%)	408 (68%)	133 (22%)	61 (10%)	0	3
3	H	602/606 (99%)	409 (68%)	132 (22%)	61 (10%)	0	3
3	J	602/606 (99%)	411 (68%)	132 (22%)	59 (10%)	0	3
3	L	602/606 (99%)	409 (68%)	132 (22%)	61 (10%)	0	3
3	N	602/606 (99%)	408 (68%)	133 (22%)	61 (10%)	0	3
3	P	602/606 (99%)	410 (68%)	132 (22%)	60 (10%)	0	3
3	R	602/606 (99%)	406 (67%)	135 (22%)	61 (10%)	0	3
3	T	602/606 (99%)	406 (67%)	135 (22%)	61 (10%)	0	3
4	U	409/412 (99%)	283 (69%)	81 (20%)	45 (11%)	0	2
4	V	409/412 (99%)	330 (81%)	60 (15%)	19 (5%)	2	13
5	W	1276/1299 (98%)	1063 (83%)	173 (14%)	40 (3%)	3	21
6	X	1012/1214 (83%)	714 (71%)	219 (22%)	79 (8%)	1	5
6	Y	1146/1214 (94%)	860 (75%)	204 (18%)	82 (7%)	1	6
All	All	11496/13791 (83%)	8294 (72%)	2255 (20%)	947 (8%)	1	5

5 of 947 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	l	19	ALA
1	b	62	VAL
1	b	75	PRO
1	f	75	PRO
1	d	22	LEU

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	b	72/228 (32%)	67 (93%)	5 (7%)	13	38
1	d	72/228 (32%)	68 (94%)	4 (6%)	17	45
1	f	72/228 (32%)	67 (93%)	5 (7%)	13	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	h	72/228 (32%)	66 (92%)	6 (8%)	9	31
1	j	72/228 (32%)	67 (93%)	5 (7%)	13	38
1	l	72/228 (32%)	66 (92%)	6 (8%)	9	31
1	n	72/228 (32%)	68 (94%)	4 (6%)	17	45
1	p	72/228 (32%)	68 (94%)	4 (6%)	17	45
1	r	72/228 (32%)	66 (92%)	6 (8%)	9	31
1	t	72/228 (32%)	68 (94%)	4 (6%)	17	45
2	A	34/35 (97%)	27 (79%)	7 (21%)	1	4
2	C	34/35 (97%)	27 (79%)	7 (21%)	1	4
2	E	34/35 (97%)	27 (79%)	7 (21%)	1	4
2	G	32/35 (91%)	25 (78%)	7 (22%)	1	3
2	I	34/35 (97%)	27 (79%)	7 (21%)	1	4
2	K	34/35 (97%)	27 (79%)	7 (21%)	1	4
2	M	32/35 (91%)	25 (78%)	7 (22%)	1	3
2	O	34/35 (97%)	27 (79%)	7 (21%)	1	4
2	Q	34/35 (97%)	27 (79%)	7 (21%)	1	4
2	S	32/35 (91%)	25 (78%)	7 (22%)	1	3
3	B	499/501 (100%)	425 (85%)	74 (15%)	2	11
3	D	499/501 (100%)	425 (85%)	74 (15%)	2	11
3	F	499/501 (100%)	426 (85%)	73 (15%)	2	12
3	H	499/501 (100%)	426 (85%)	73 (15%)	2	12
3	J	499/501 (100%)	423 (85%)	76 (15%)	2	10
3	L	499/501 (100%)	425 (85%)	74 (15%)	2	11
3	N	499/501 (100%)	423 (85%)	76 (15%)	2	10
3	P	499/501 (100%)	423 (85%)	76 (15%)	2	10
3	R	499/501 (100%)	425 (85%)	74 (15%)	2	11
3	T	499/501 (100%)	423 (85%)	76 (15%)	2	10
4	U	325/326 (100%)	305 (94%)	20 (6%)	15	41
4	V	325/326 (100%)	305 (94%)	20 (6%)	15	41
5	W	1082/1092 (99%)	977 (90%)	105 (10%)	6	25
6	X	869/1030 (84%)	736 (85%)	133 (15%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Y	976/1030 (95%)	864 (88%)	112 (12%)	4	18
All	All	9621/11444 (84%)	8366 (87%)	1255 (13%)	6	14

5 of 1255 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	W	264	GLU
6	Y	39	PRO
5	W	519	LEU
5	W	262	MET
6	X	376	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 375 such sidechains are listed below:

Mol	Chain	Res	Type
4	U	3	GLN
5	W	596	ASN
4	U	124	ASN
4	V	88	GLN
5	W	1151	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	$\# Z > 2$
7	MYR	S	101	2	14,14,15	0.46	0	13,13,15	0.56	0
7	MYR	E	101	2	14,14,15	0.46	0	13,13,15	0.56	0
7	MYR	K	101	2	14,14,15	0.46	0	13,13,15	0.56	0
7	MYR	Q	101	2	14,14,15	0.46	0	13,13,15	0.56	0
7	MYR	A	101	2	14,14,15	0.46	0	13,13,15	0.56	0
7	MYR	I	101	2	14,14,15	0.46	0	13,13,15	0.55	0
7	MYR	C	101	2	14,14,15	0.46	0	13,13,15	0.55	0
7	MYR	G	101	2	14,14,15	0.46	0	13,13,15	0.55	0
7	MYR	O	101	2	14,14,15	0.46	0	13,13,15	0.56	0
7	MYR	M	101	2	14,14,15	0.46	0	13,13,15	0.56	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
7	MYR	S	101	2	-	8/11/12/13	-
7	MYR	E	101	2	-	8/11/12/13	-
7	MYR	K	101	2	-	8/11/12/13	-
7	MYR	Q	101	2	-	8/11/12/13	-
7	MYR	A	101	2	-	8/11/12/13	-
7	MYR	I	101	2	-	8/11/12/13	-
7	MYR	C	101	2	-	8/11/12/13	-
7	MYR	G	101	2	-	8/11/12/13	-
7	MYR	O	101	2	-	8/11/12/13	-
7	MYR	M	101	2	-	8/11/12/13	-

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
7	C	101	MYR	C3-C4-C5-C6
7	G	101	MYR	C3-C4-C5-C6
7	O	101	MYR	C3-C4-C5-C6
7	A	101	MYR	C3-C4-C5-C6
7	E	101	MYR	C3-C4-C5-C6

There are no ring outliers.

10 monomers are involved in 283 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	S	101	MYR	30	0
7	E	101	MYR	27	0
7	K	101	MYR	27	0
7	Q	101	MYR	27	0
7	A	101	MYR	27	0
7	I	101	MYR	29	0
7	C	101	MYR	33	0
7	G	101	MYR	29	0
7	O	101	MYR	28	0
7	M	101	MYR	26	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	b	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	74:GLN	C	75:PRO	N	1.68

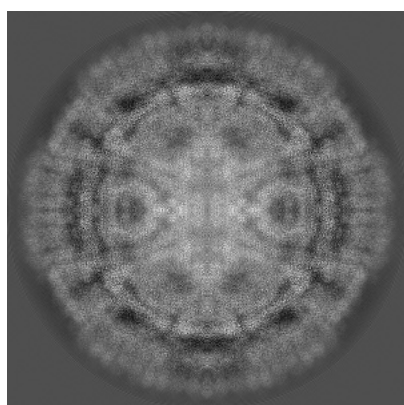
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6969. These allow visual inspection of the internal detail of the map and identification of artifacts.

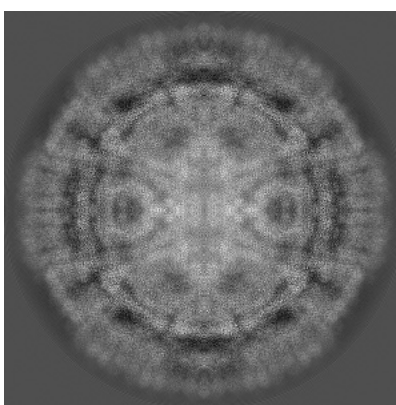
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

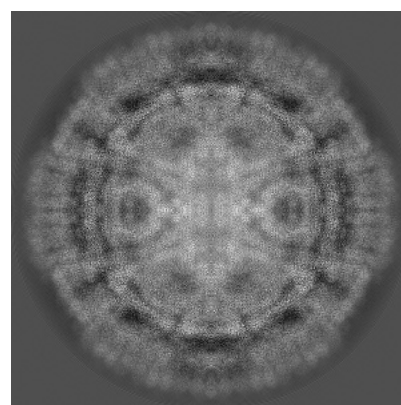
6.1.1 Primary map



X



Y

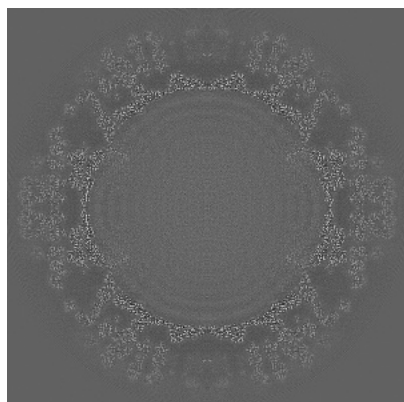


Z

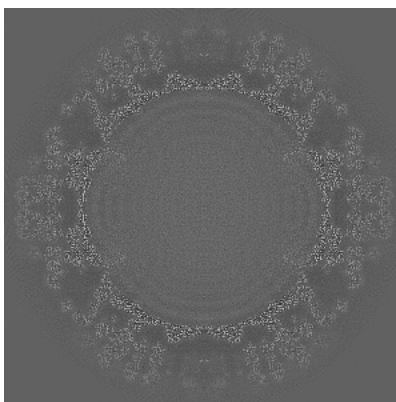
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

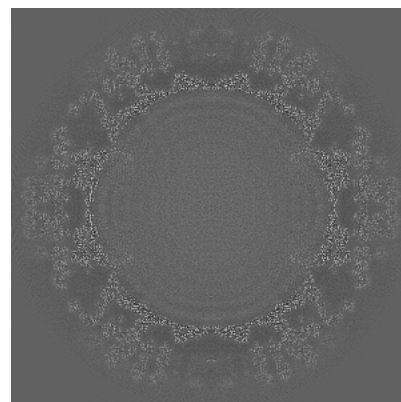
6.2.1 Primary map



X Index: 450



Y Index: 450

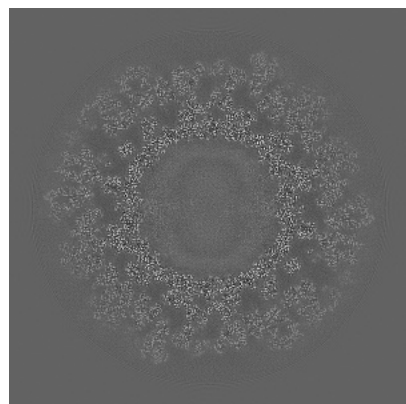


Z Index: 450

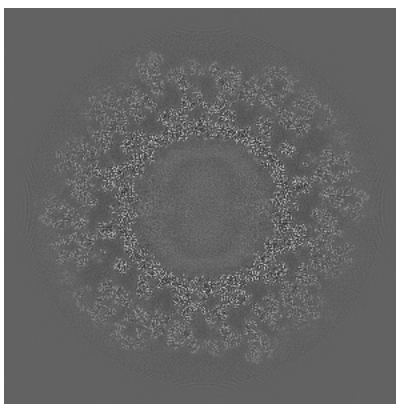
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

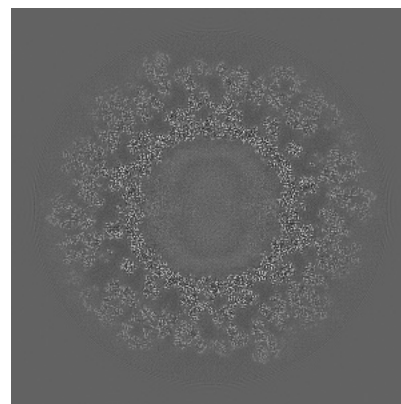
6.3.1 Primary map



X Index: 241



Y Index: 659

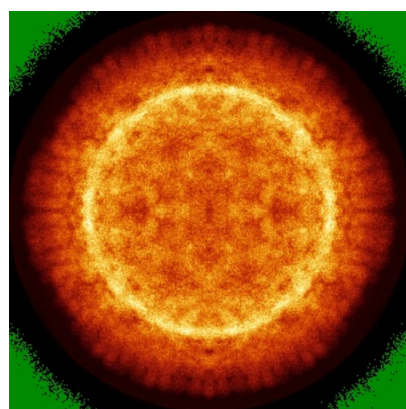


Z Index: 659

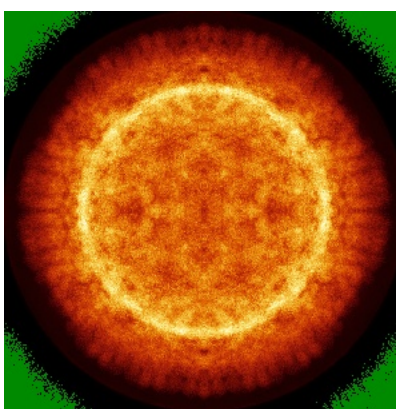
The images above show the largest variance slices of the map in three orthogonal directions.

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

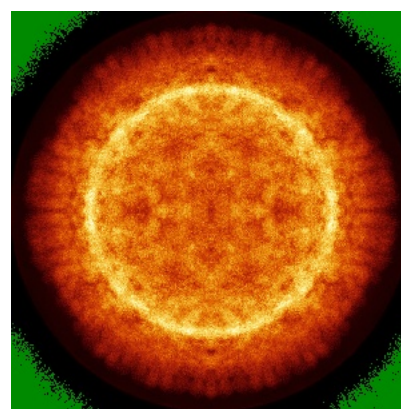
6.4.1 Primary map



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 9.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

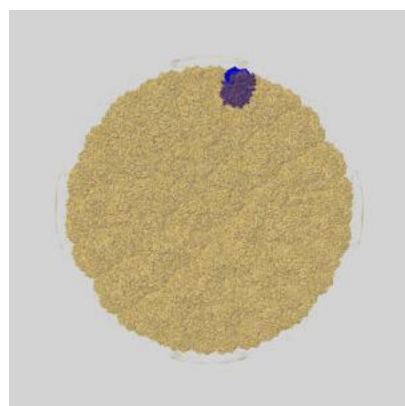
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

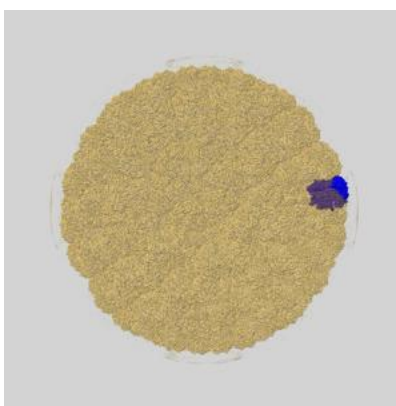
A mask typically either:

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

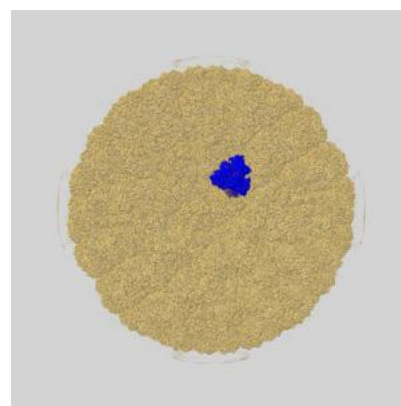
6.6.1 emd_6969_msk_1.map [i](#)



X



Y

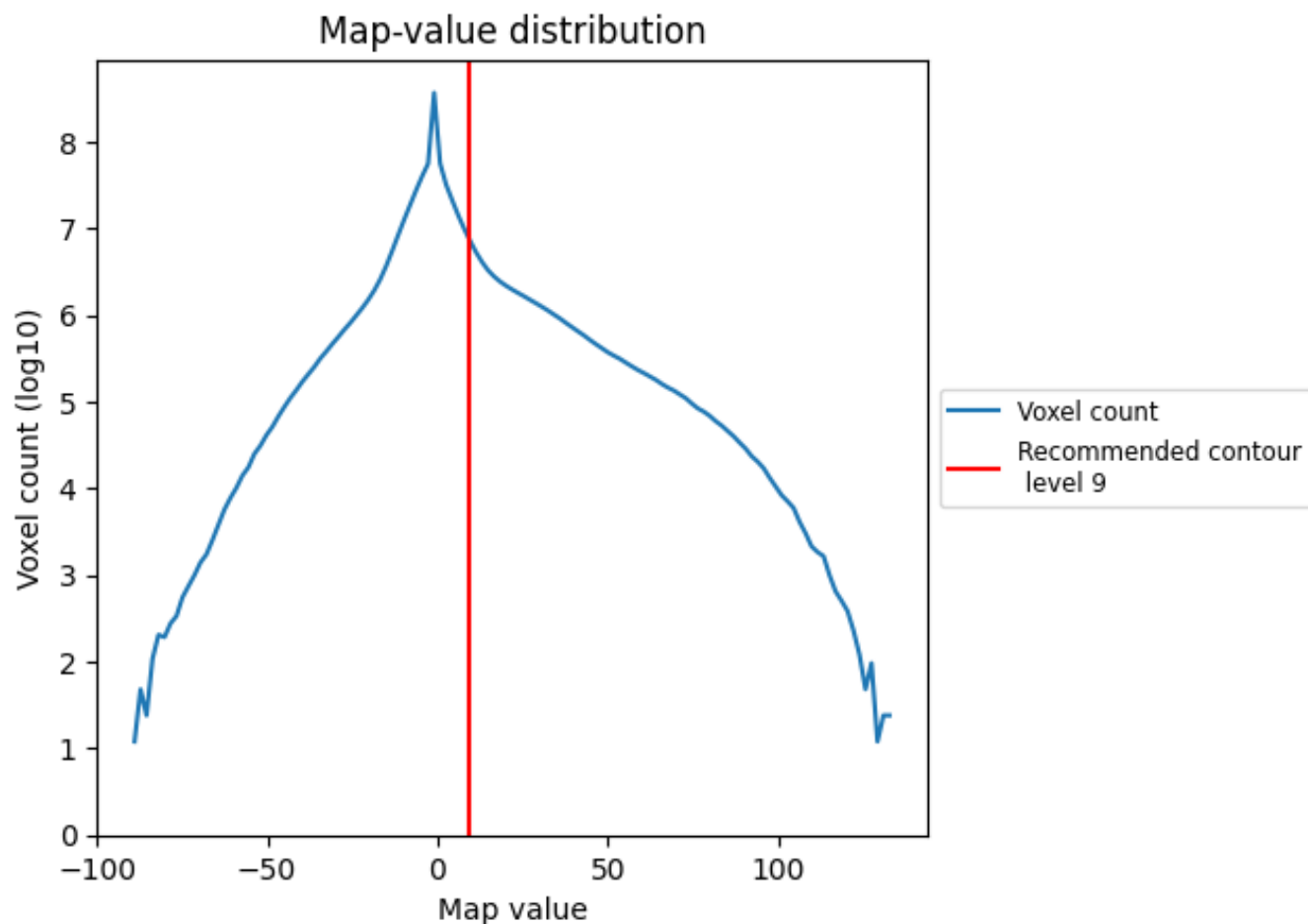


Z

7 Map analysis [i](#)

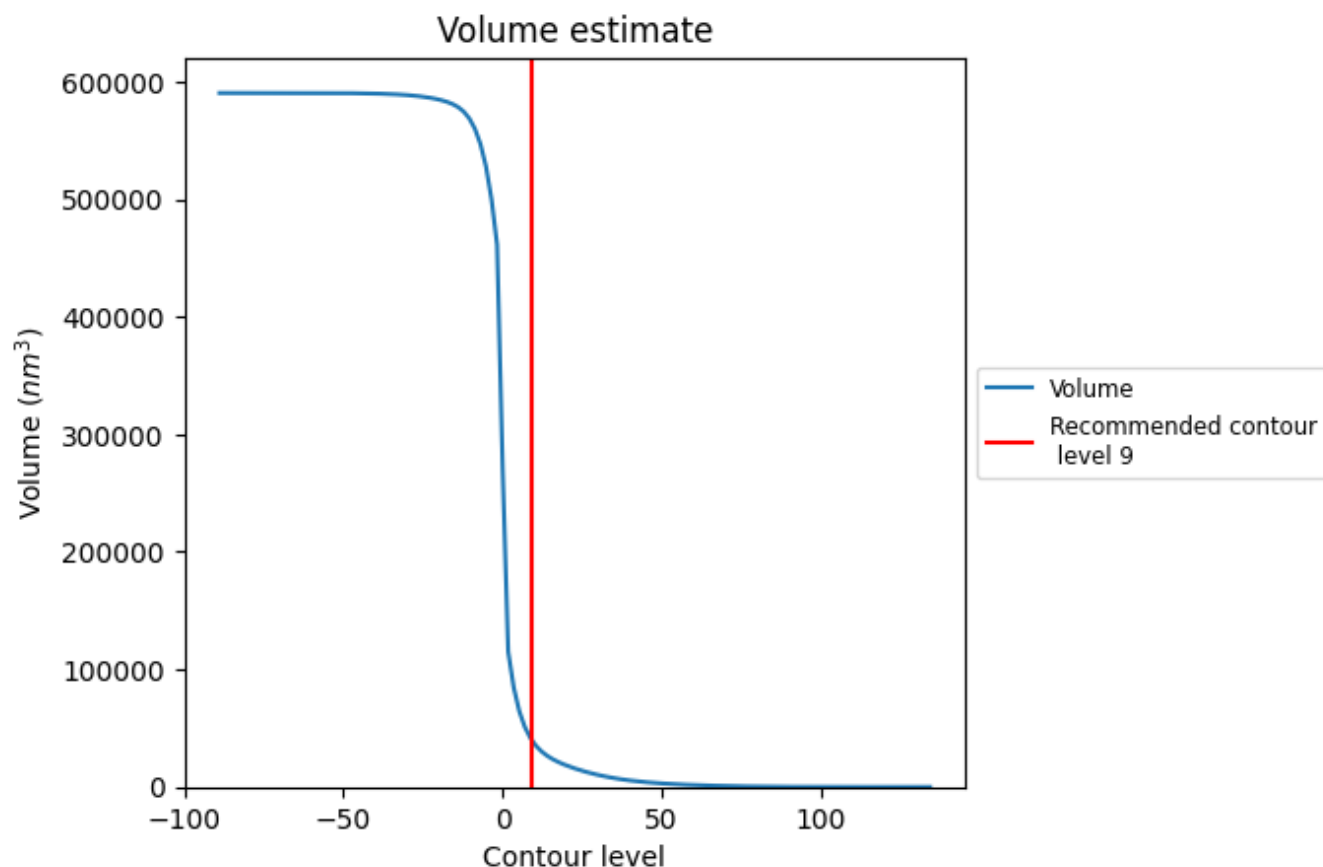
This section contains the results of statistical analysis of the map.

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.

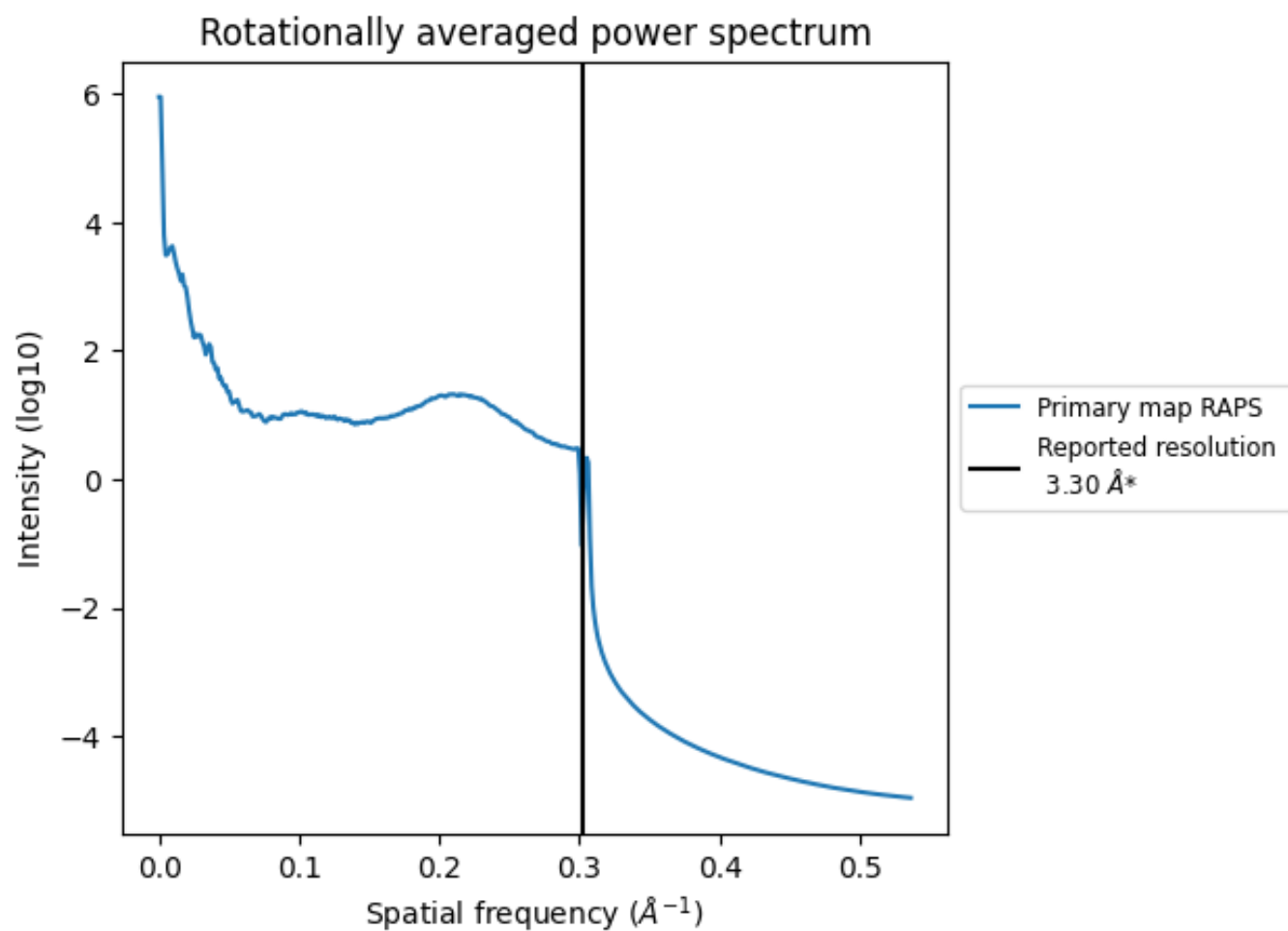
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40818 nm^3 ; this corresponds to an approximate mass of 36872 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

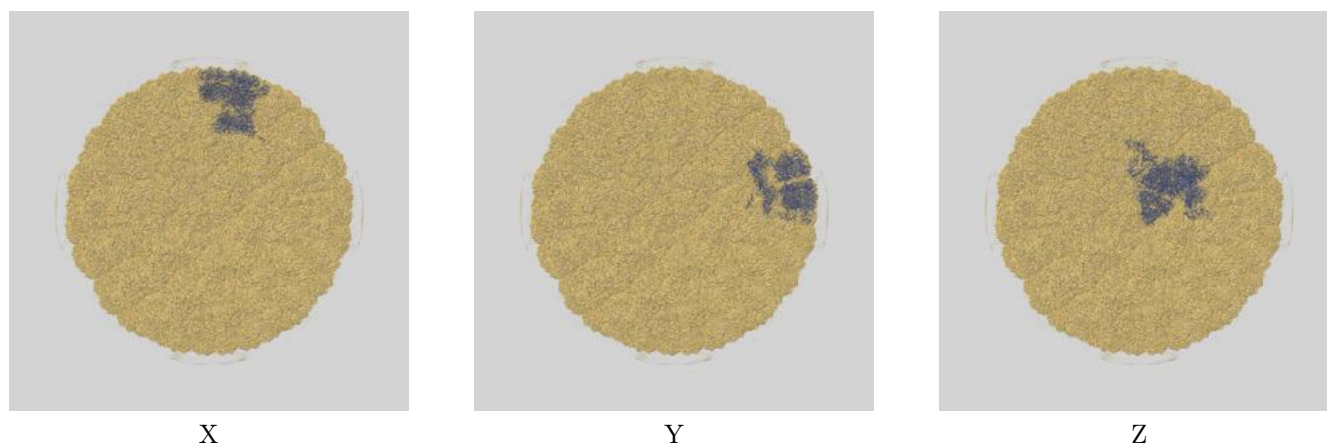
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

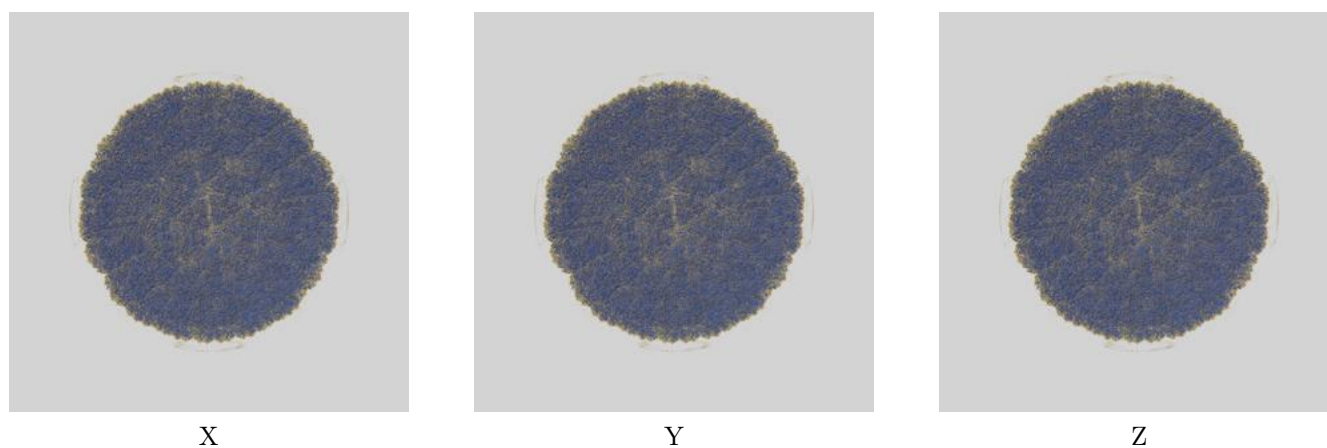
This section contains information regarding the fit between EMDB map EMD-6969 and PDB model 5ZVT. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

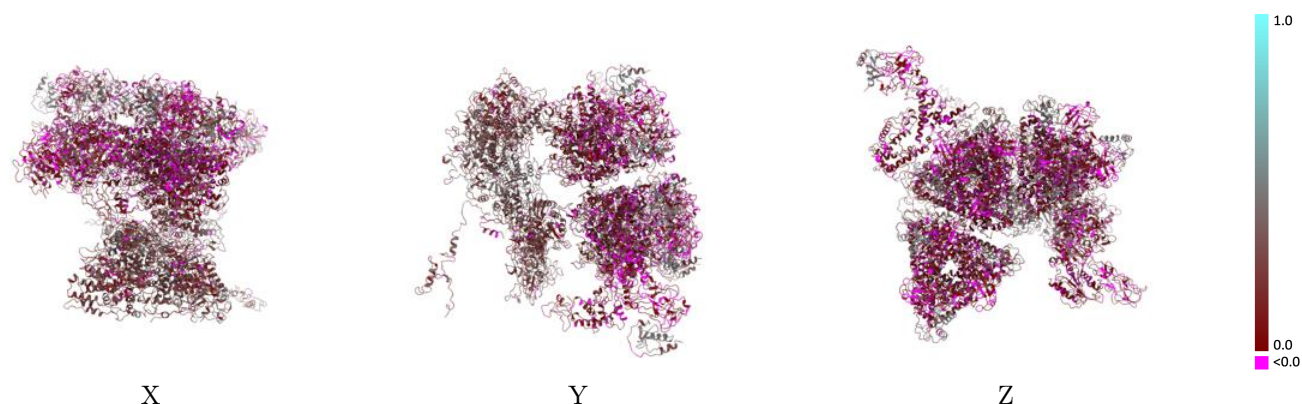


9.1.2 Map-model assembly overlay [i](#)



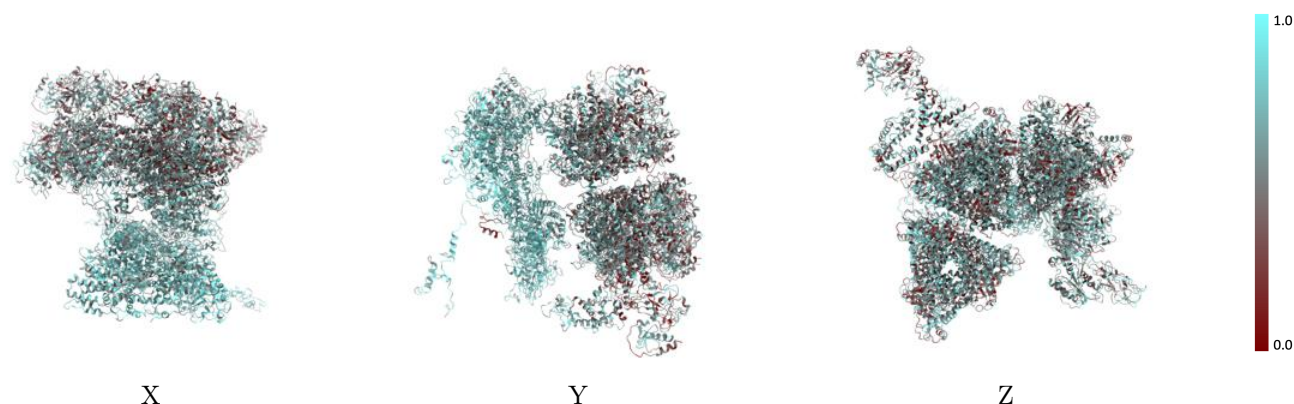
The images above show the 3D surface view of the map at the recommended contour level 9.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



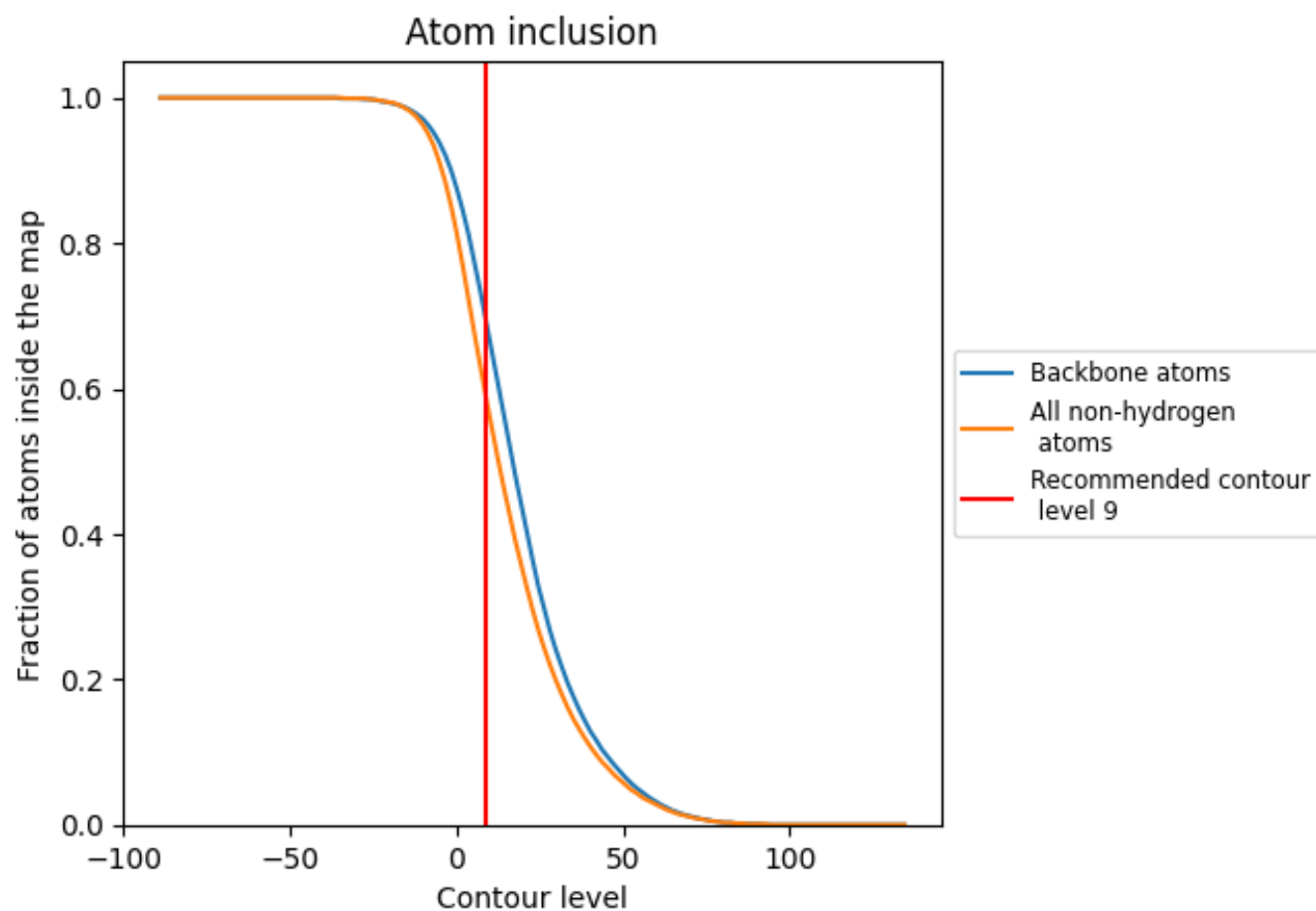
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 58% 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 (9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5820	 0.1950
A	 0.5020	 0.1370
B	 0.4820	 0.1040
C	 0.5180	 0.1540
D	 0.5200	 0.1290
E	 0.5180	 0.1500
F	 0.5270	 0.1390
G	 0.5300	 0.1670
H	 0.5220	 0.1340
I	 0.5050	 0.1360
J	 0.5110	 0.1220
K	 0.5280	 0.1550
L	 0.5070	 0.1240
M	 0.4800	 0.1230
N	 0.5110	 0.1200
O	 0.5340	 0.1600
P	 0.5200	 0.1270
Q	 0.5210	 0.1220
R	 0.5070	 0.1210
S	 0.5600	 0.1760
T	 0.5240	 0.1310
U	 0.6810	 0.2370
V	 0.7020	 0.2490
W	 0.5820	 0.1600
X	 0.7510	 0.3170
Y	 0.7450	 0.3150
b	 0.5450	 0.3850
d	 0.6160	 0.3980
f	 0.5960	 0.4170
h	 0.5810	 0.4070
j	 0.5810	 0.4010
l	 0.5640	 0.3930
n	 0.6380	 0.4120
p	 0.5380	 0.4020
r	 0.5670	 0.4080
t	 0.4410	 0.3620

