



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 17, 2018 – 06:53 PM EST

PDB ID : 6BX0
EMDB ID: : EMD-7301
Title : Atomic resolution structure of human bufavirus 2
Authors : Mietzsch, M.; Agbandje-McKenna, M.
Deposited on : 2017-12-15
Resolution : 3.79 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

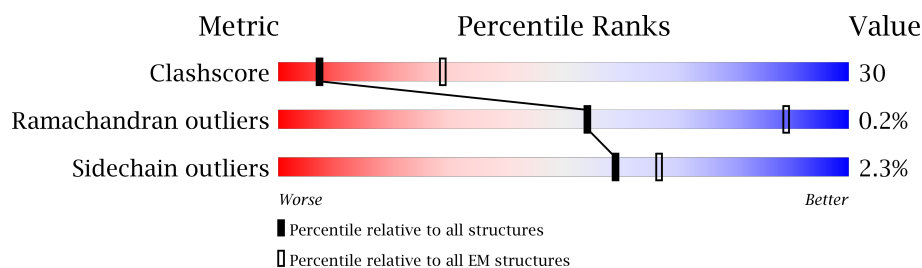
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.79 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.






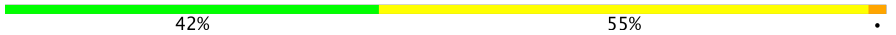
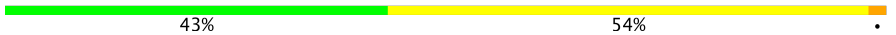
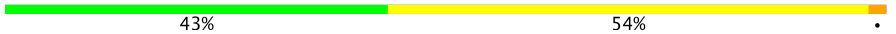
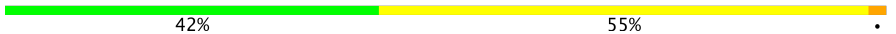
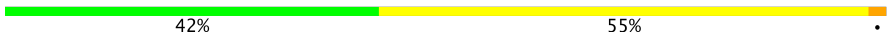
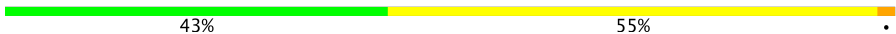
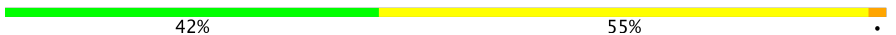
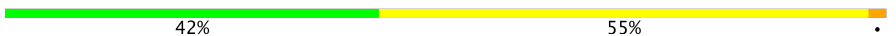
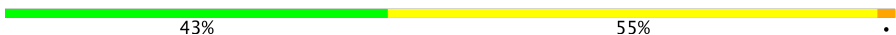
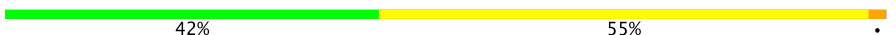
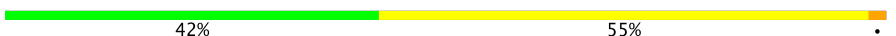











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	537	
1	1	537	
1	2	537	
1	3	537	
1	4	537	
1	5	537	
1	6	537	
1	7	537	
1	A	537	

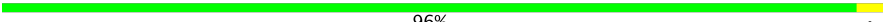
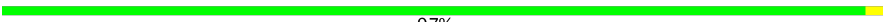
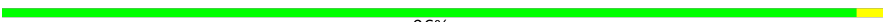












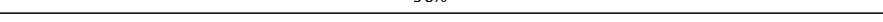
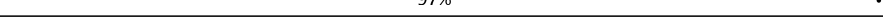
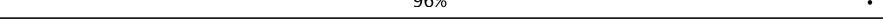
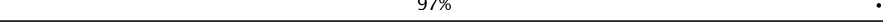
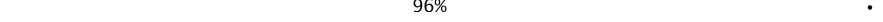
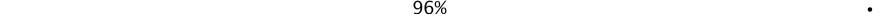
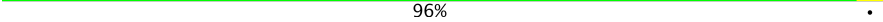
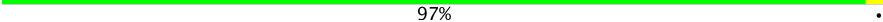
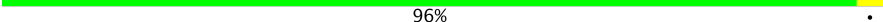
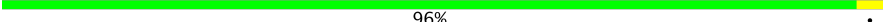
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Mol	Chain	Length	Quality of chain	
1	B	537		.
1	C	537		.
1	D	537		.
1	E	537		.
1	F	537		.
1	G	537		.
1	H	537		.
1	I	537		.
1	J	537		.
1	K	537		.
1	L	537		.
1	M	537		.
1	N	537		.
1	O	537		.
1	P	537		.
1	Q	537		.
1	R	537		.
1	S	537		.
1	T	537		.
1	U	537		.
1	V	537		.
1	W	537		.
1	X	537		.
1	Y	537		.
1	Z	537		.

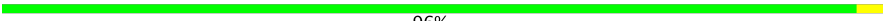
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Mol	Chain	Length	Quality of chain
1	a	537	 96% .
1	b	537	 97% .
1	c	537	 96% .
1	d	537	 96% .
1	e	537	 96% .
1	f	537	 96% .
1	g	537	 96% .
1	h	537	 97% .
1	i	537	 97% .
1	j	537	 97% .
1	k	537	 96% .
1	l	537	 96% .
1	m	537	 96% .
1	n	537	 97% .
1	o	537	 96% .
1	p	537	 97% .
1	q	537	 96% .
1	r	537	 97% .
1	s	537	 96% .
1	t	537	 96% .
1	u	537	 96% .
1	v	537	 97% .
1	w	537	 96% .
1	x	537	 96% .
1	y	537	 97% .

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Mol	Chain	Length	Quality of chain
1	z	537	 96%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 259560 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 VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	B	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	C	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	D	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	E	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	F	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	G	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	H	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	I	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	J	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	K	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	L	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	M	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	N	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	O	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	P	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	Q	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	S	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	T	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	U	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	V	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	W	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	X	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	Y	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	Z	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	0	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	1	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	2	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	3	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	4	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	5	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	a	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	b	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	c	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	d	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	e	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	f	535	Total 4326	C 2727	N 763	O 817	S 19	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	h	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	i	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	j	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	k	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	l	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	m	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	n	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	o	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	p	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	q	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	r	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	s	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	t	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	u	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	v	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	w	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	x	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	y	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	z	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	6	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	7	535	4326	2727	763	817	19	0	0

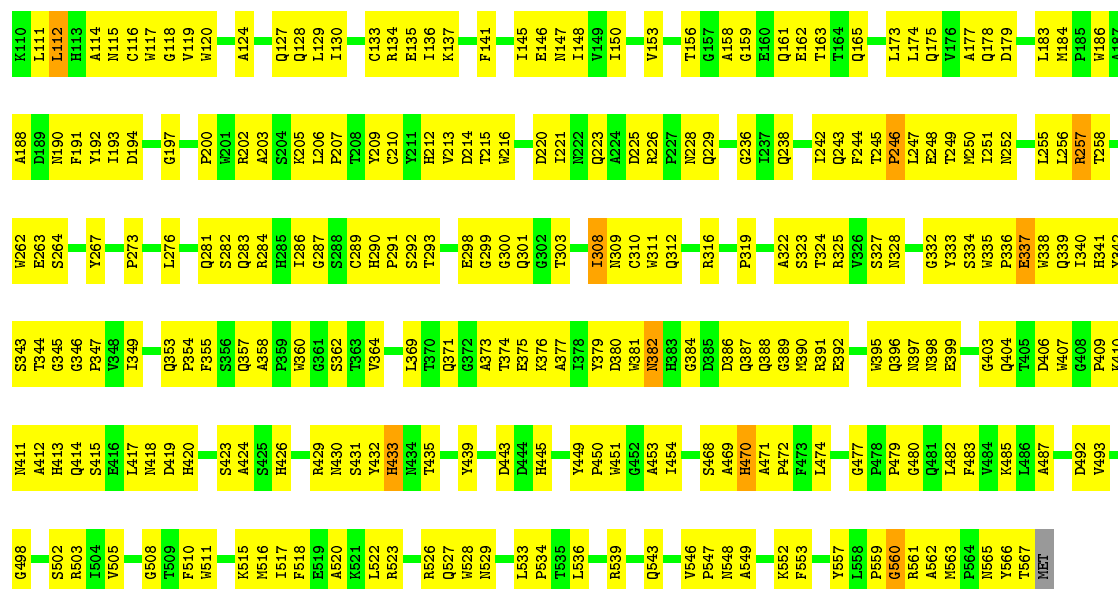
i

- Molecule 1: VP2



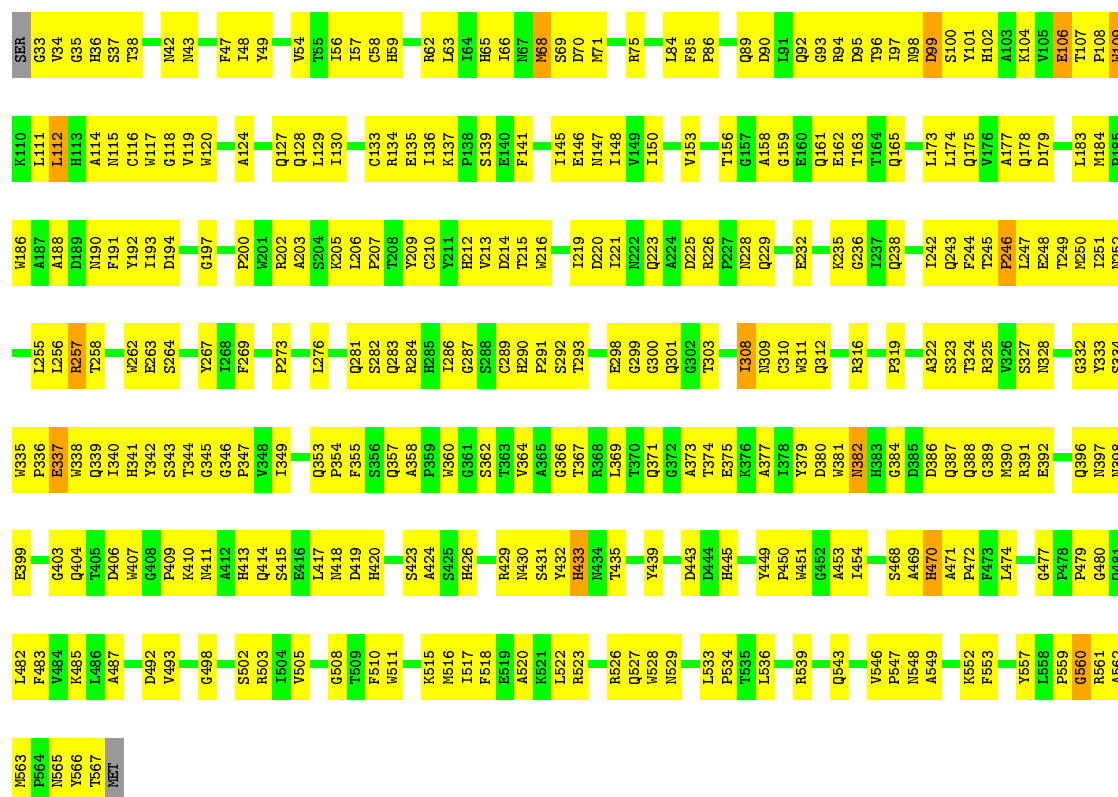






• Molecule 1: VP2

Chain G: 43% 54%



• Molecule 1: VP2

Chain H: 42% 55%



L482	F483	P484	L485	K485	Y566	Y567	ME1	E399	P336	E337	W338	Q339	I340	H341	Y342	S343	T344	G345	G346	P347	F269	P273	L276	Q281	S282	Q283	R284	Q357	Q358	A358	H360	G361	S362	T363	N364	M68	L522	S69	R523	R526	Q527	W528	N529	L533	P534	T535	L536	R539	Q543	V546	P547	N548	A549	K552	F553	Y557	I558	P559	G560	R561	A562	L486	T405	D406	H407	G408	P409	K410	N411	A412	H413	Q414	S415	L417	N418	D419	H420	S423	A424	G425	H426	R429	N430	S431	Y432	H433	N434	T435	Y439	D443	P444	H445	Y449	P450	N451	G452	A453	L454	S468	H470	A471	P472	F473	L474	G477	P476	P479	G480	Q481	L186	A187	D188	N190	F191	Y192	L193	D194	G197	P200	E201	R202	S204	K205	L206	P207	T208	Y209	C210	E211	H212	V213	D214	T215	W216	L219	D220	I221	N222	Q223	A224	D225	R226	P227	N228	Q229	E232	G236	I237	Q238	I242	Q243	F244	T245	P246	V326	L247	E248	T249	M250	N252	L173	L174	T246	L175	A176	V176	A177	Q178	D179	L183	L184	N185	L111	L112	H113	A114	N115	C116	W117	G118	W120	A124	Q127	Q128	L129	I130	C133	R134	E135	I136	K137	P138	S139	F141	I145	E146	N147	I148	V149	I150	V153	T156	G157	A158	G159	E160	Q161	E162	T163	Q165	L173	L174	T246	L175	A176	V176	A177	Q178	D179	L183	L184	N185
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• Molecule 1: VP2

Chain I:  42% 55%

SER	G33	V34	G35	H36	S37	T38	N42	N43	F47	I48	Y49	V54	T55	I56	I57	C58	H59	R62	L63	I64	H65	I66	N67	M68	S69	D70	N71	R75	L84	P86	Q89	L91	Q92	G93	R94	T96	I97	N98	D99	S100	Y101	H102	A103	K104	V105	E106	T107	P108	W109	L111	L112	H113	A114	N115	C116	W117	G118	W120	A124	Q127	Q128	L129	I130	C133	R134	E135	I136	K137	P138	S139	F141	I145	E146	N147	I148	V149	I150	V153	T156	G157	A158	G159	E160	Q161	E162	T163	Q165	L173	L174	T246	L175	A176	V176	A177	Q178	D179	L183	L184	N185	L111	L112	H113	A114	N115	C116	W117	G118	W120	A124	Q127	Q128	L129	I130	C133	R134	E135	I136	K137	P138	S139	F141	I145	E146	N147	I148	V149	I150	V153	T156	G157	A158	G159	E160	Q161	E162	T163	Q165	L173	L174	T246	L175	A176	V176	A177	Q178	D179	L183	L184	N185
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• Molecule 1: VP2

Chain J:  43% 55%

Chain K: 42% 55%

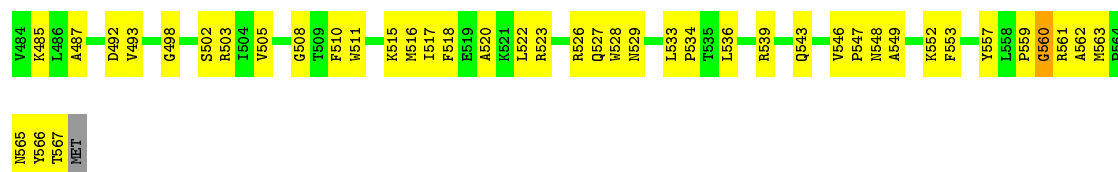
L482	E399	P336	L255	W186	K110	S8
P463	E337	E337	L256	A187	L111	G33
V484	G403	E338	R257	A188	L112	V34
V566	Q404	Q339	T258	D189	H113	G35
L486	W405	I240		N190	A114	H36
A487	D406	H341	W262	F191	M115	S37
	W407	V342	E263	I192	C116	T38
D492	G408	S343	S264	D194	M117	
V493	P409	T344			G118	M42
	K410	G345	Y267	G197	V119	M43
G498	M411	G346	T268		M120	
	A412	P347	F269			F47
S502	H413	V348		P200	A124	L48
R503	Q414	I349	P273	W201	G127	Y49
I504	A415			R202	Q128	
V505	E416		L276	A203	L129	V54
	L417	Q353		S204	I130	T55
	M418	F354	Q281	K205		I56
G508		F355	S282	L206		I57
T509	D419	S356	Q283	P207	C133	H59
F510	H420	Q357	R284	L208	R134	
W511		A358	E285	Y209	E135	
	S423	P359	R286	C210	I136	R62
K515	A424	H360	G287	G211	K137	L63
M516	S425	G361		H212	P138	I64
F518	H426	S362	C289	V213	S139	H65
E519	R429	T363	E290	D214	E140	I66
A520	M430	V364	P291	T215	F141	N67
F521	S431	A365	S292	W216		M68
L522	Y432	G366	T293		I145	S69
M523	H433	T367			E146	D70
	M434	R368	E298	D220	M147	M71
R526	T435	L369	G299	I221	I148	
Q527		Q371	G300	H222	V149	R75
W528	Y439	G372	Q301	Q223	I150	
M529		A373	G302	A224		
	D443	T374	T303	D225	V153	L34
L533	P444	E375		R226		F85
P534	H445	K376	I308	P227	T156	P86
T535		A377	N309	N228	G157	Q89
L536	Y449	I378	C310	Q229	A158	D90
	P450	Y379	W311	E232	G159	L91
R539	W451	D380	Q312		E160	Q92
	W452	W381			Q161	G93
Q543	A453	N382	R316	G236	E162	R94
	L454	H383		T237	T163	D95
V546		G384	P319	Q238	T164	T96
P547	S468	D385			Q165	N97
M548	A469	D386	A322	T242		N98
A549	H470	Q387	S323	Q243	L173	D99
	A471	Q388	T324	F244	L174	S100
K552	P472	G389	R325	T245	Q175	Y101
F553	F473	M390	W326	P246	V176	H102
	L474	R391	S327	L247	A177	A103
		E392	N328	E248	Q178	K104
				T249	D179	V105
	G477			M250		T107
P559	P478	W395	G332	T251	L183	O106
G560	F479	Q396	Y332	L252	M184	F108
R561	G480	N397	S334			S109
A562	S481	V398	V325		F185	



• Molecule 1: VP2

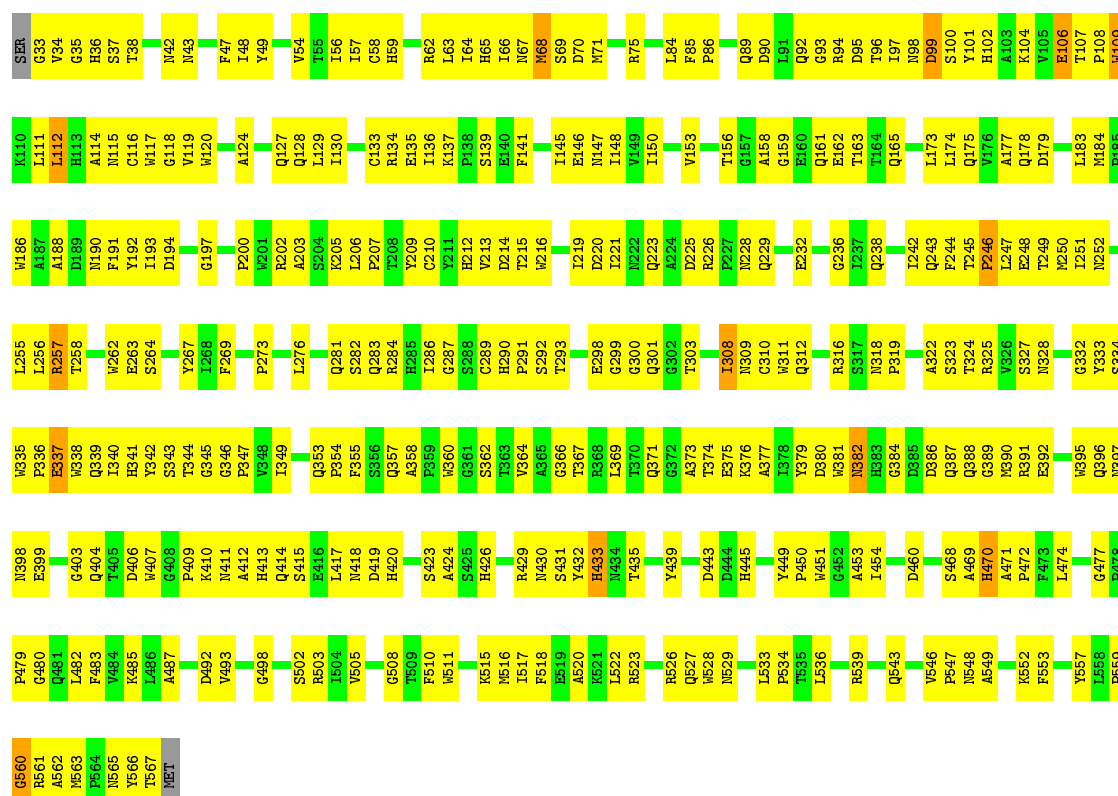
Chain N:  42% 55%

SER	G403	V484	N565	L111	H586	L255	W335	G403	V484	N565
	K485	K485	Y566	L111	A187	L256	P336	T405	T405	Y567
	L486	L486	T567	L112	A188	R257	E337	H406	H406	A487
	A487	A487		H113	D189	T258	N338	H407	H408	
	D492			A114	N190	W262	Q339			
	V493			A115	F191	E263	Q340			
				C116	Y192	S264	H341			
	G498			W117	I193	S264	N343			
				G118	D194		T344			
				W119		Y267	G345			
	N442			W120	G197	T268	G346			
	N443					F269	P347			
							I349			
	F47			A124	P200	P273	Q353			
	N48			Q127	R202		P354			
	Y49			Q128	A203	L276	P355			
	N54			L129	S204	Q281	Q356			
	T55			I130	L206	S282	A357			
	I56				K205	Q283	Q358			
	I57				P207	R284	A358			
	C58			C133	T208	E285	P359			
	H59			R134	Y209	R286	G361			
				E135	C210	G287	W360			
				I136	T211	C287	G362			
	R62			K137	H212	S288	A361			
	L63			P138	Y213	C289	S362			
	L64			S139	D214	E290	T363			
	H65			E140	T215	P291	W364			
	I66			F141	W216	S292	A433			
						T293	N434			
	N68						T370			
	S69			I145	I219	E298	Q371			
	D70			E146	D220	C299	A372			
	M71			N147	R221	G300	G373			
				I148	I222	G301	T374			
				V149	R223	Q302	C375			
	R75			I150	Q223	G302	A376			
					A224	T303	A377			
	L84			V153	D225	R226	I378			
	P85				R227	C309	P379			
	P86			T156	R228	C310	D380			
				A157	Q229	W311	N381			
	Q89			G159	E232	Q312	H383			
	D90			E160			G384			
	L91			Q32			D385			
	Q93			Q161	G236	R317	Q386			
	D94			E162	I237	N318	H387			
	N95			T163	Q238	P319	A471			
	T96			T164			I472			
	I97			Q185			L474			
	N98				I242		G477			
					Q243	A322	P478			
	D99			L173	F244	S323	F479			
	S100			L174	T245	R324	N390			
	Y101			Q175	R246	R325	R391			
	H102			V176	L247	W326	E392			
	A103			A177	S248	S327				
	K104			Q178	T249	N328	G389			
	E105			D179	N250	G332	F473			
	E106			T178	I251	G332	L474			
	T107			L183	D252	G332				
	P108			W184	H253	G333	N398			
				H185	S254	S334	E399			



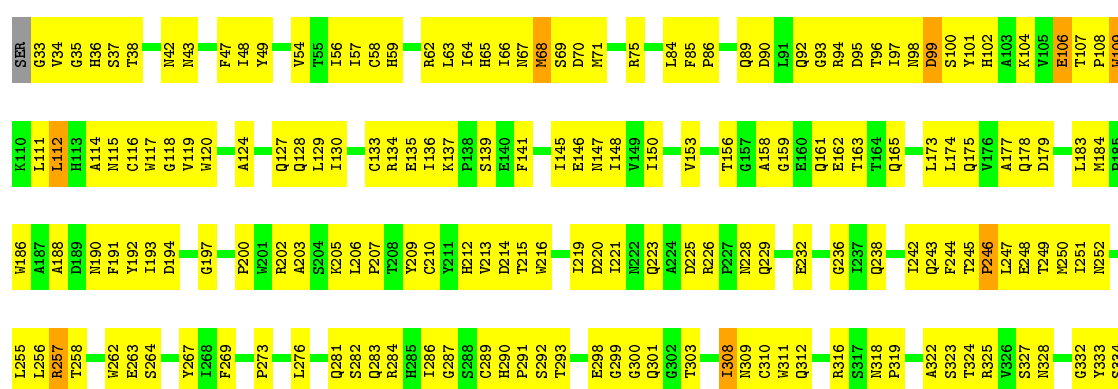
• Molecule 1: VP2

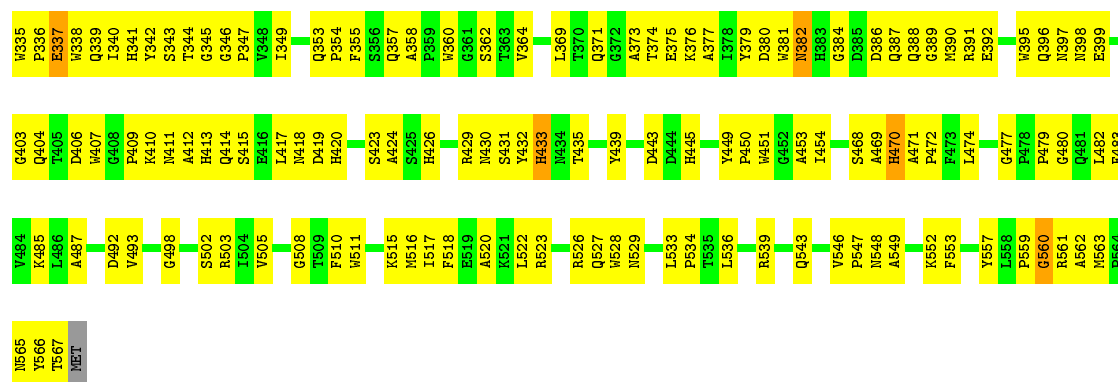
Chain P: 42% 55%



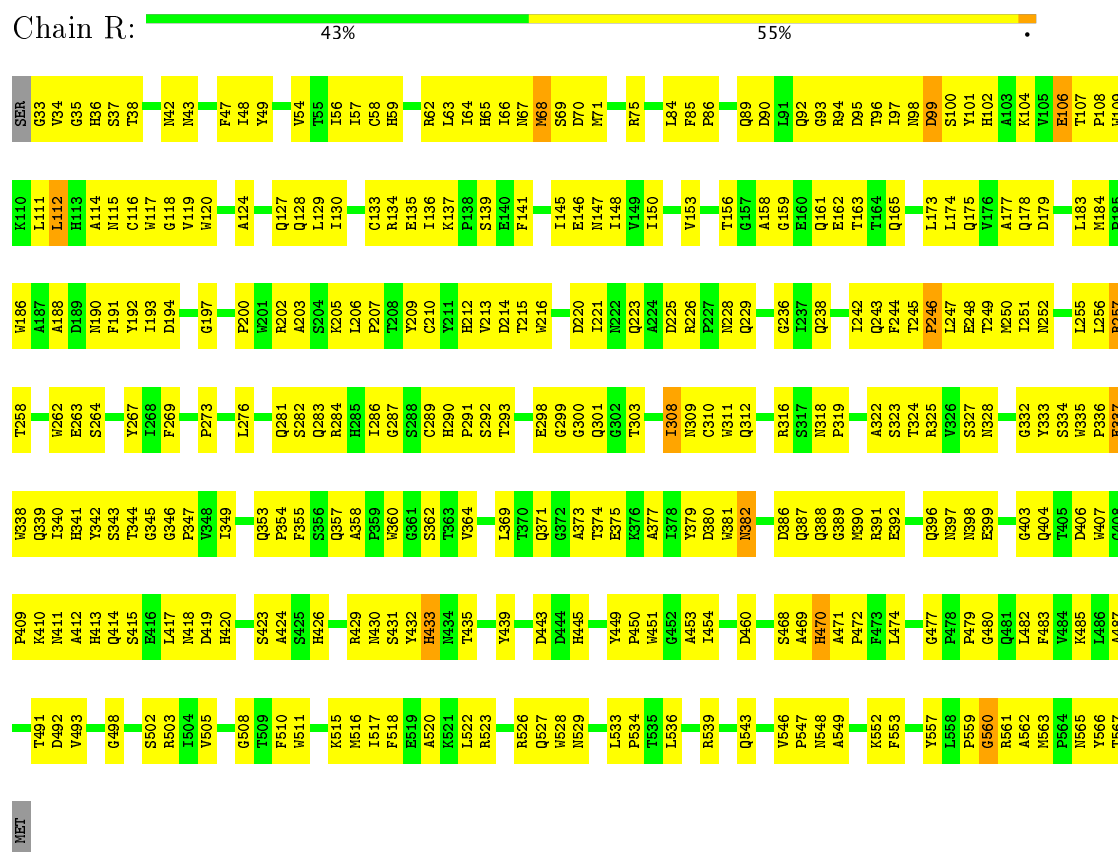
• Molecule 1: VP2

Chain Q: 42% 55%

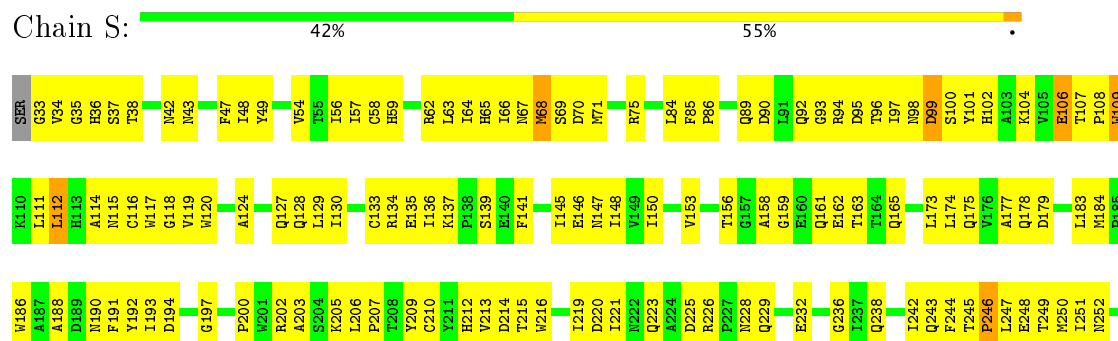


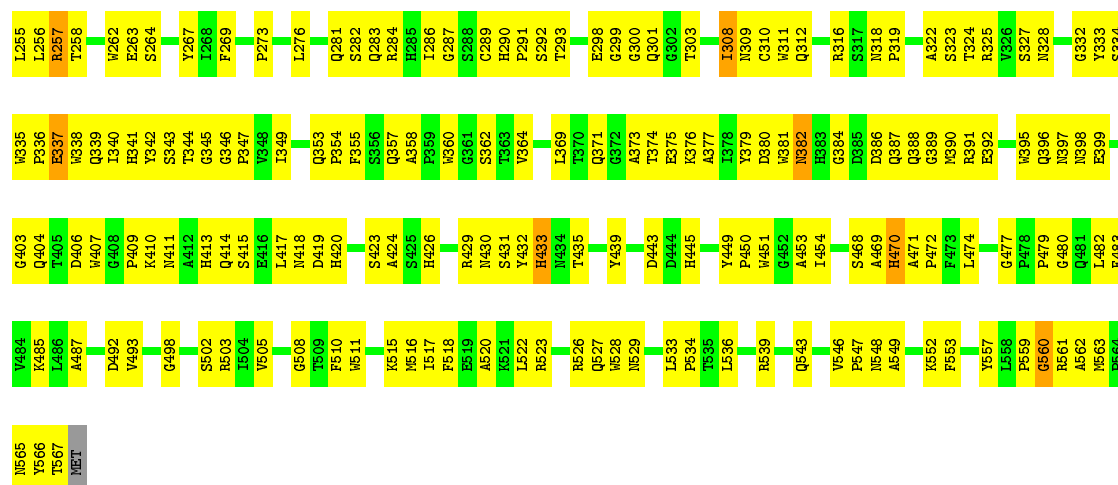


• Molecule 1: VP2



• Molecule 1: VP2





K110	L111	L112	H113	A114	N115	C116	W117	G118	V119	W120	A124	Q127	Q128	L129	I130	C133	R134	E135	I136	K137	F141	I145	E146	N147	I148	V149	I150	V153	T156	G157	A158	G159	E160	Q161	E162	T163	T164	Q165	L173	L174	Q175	V176	A177	Q178	D179	L183	M184	P185	W186	A187								
A188	D189	N190	F191	G262	E263	S264	D194	G197	P200	W201	R202	A203	S204	Q283	L206	P207	T208	Y209	C210	Y211	H212	V213	D214	T215	W216	I219	D220	I221	I222	Q223	A224	R226	P227	N228	Q229	E232	G236	I237	Q238	I242	Q243	F244	T245	T246	L247	E248	T249	K250	N251	N252	L255	L256	L257					
R257	T258	W262	E263	S264	D194	G197	P200	W201	R202	A203	S204	Q283	L206	P207	T208	Y209	C210	Y211	H212	V213	D214	T215	W216	I219	D220	I221	I222	Q223	A224	R226	P227	N228	Q229	E232	G236	I237	Q238	I242	Q243	F244	T245	T246	L247	E248	T249	K250	N251	N252	L255	L256	L257							
H341	Y342	S343	T344	G345	E346	S264	P347	V348	I349	Q353	P354	F355	Q356	Q357	A358	P359	W360	G361	S362	T363	V364	A365	G366	T367	R368	L369	T370	Q371	G372	A373	T374	E375	K376	A377	L378	Y379	D380	N381	N382	R383	G384	D385	D386	Q387	Q388	R389	K390	R391	E392	Q396	N397	N398	E399	Q403	Q404	K405	Y406	T407
H407	G408	P409	K410	N411	A412	H413	Q414	S415	E416	L417	N418	D419	H420	S423	A424	W425	H426	R429	M430	S431	H432	H433	H434	T435	Y439	D443	D444	Y449	P450	W451	G452	A453	I454	S468	A469	H470	A471	F472	F473	L474	G477	P478	N479	O480	A103	K104	V105	E106	T107	P108	W109							
D492	V493	G498	S502	R503	L504	V505	G508	T509	F510	W511	K515	M516	I517	F518	E519	S528	C529	R530	T531	H532	L533	M534	L535	L536	R539	Q543	V546	P547	N548	A549	K552	F553	Y557	L558	P559	G560	R561	A562	K563	P564	N565	Y566	T567	MET														

• Molecule 1: VP2

Chain X:  42% 55%

Y666	T567	MET	L486	A487	T405	Q339	R257	A188	K110	SER

• Molecule 1: VP2

Chain Y:  42% 55%

SER	G33	V34	G35	R36	S37	T38	N42	N43	F47	L48	Y49	V54	T55	I56	I57	C58	H59	R62	L63	I64	R65	I66	N67	P68	G69	S69	D70	W71	R75	L84	F85	P86	Q89	D90	L91	Q92	Q93	R94	T96	I97	N98	D99	S100	Y101	H102	A103	K104	V105	E106	T107	P108	W109
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• Molecule 1: VP2

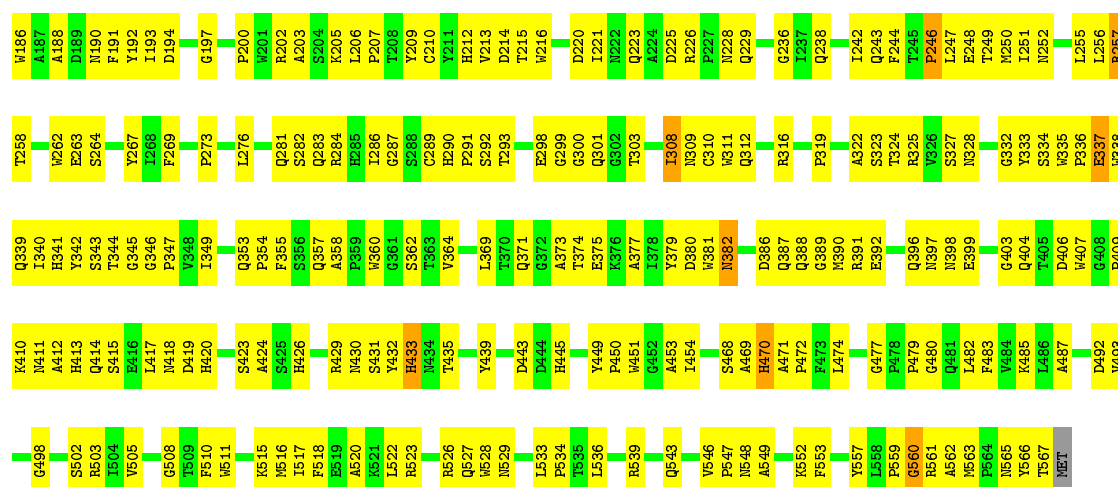
Chain 3: 44% 54%

	G498	K410	Q339	R257	A188	K110	SER
		M411		T258		L111	G33
		A412	H341		D189	L112	V34
	S502	H413	Y342	Y262	M190	H113	G35
	R503	Q414	S343	E263	F191	N115	R36
	I504	S415	T344	S264	Y192	A114	S37
	V505	E416	G345		I193	C116	T38
		L417	G346	Y267	D194	W117	
	G508	M418	P347			G118	
	T509	D419	V348	P273	G197	V119	N42
	F510	H420	I349			W120	N43
	W511			L276	P200		
		S423	Q353		R201	A124	F47
	K515	A424	P354	Q281	A203		L48
	M516	S425	F355	S282	S204	Q127	Y49
	I517	H426	S356	Q283	K205	Q128	V54
	F518		Q357	Q284	L206	L129	T55
	E519		A358	H285	P207	I130	I56
	A520	R429	P359	T286	T208		
	K521	M430	W360	G287	Y209	C133	I57
	L522	S431	G361	S288	C210	R134	C58
	R523	H433	S362	C289	Y211	E135	H59
		N434	T363	H290	E212	I136	
	R526	T435	V364	P291	V213	K137	R62
	Q527			S292	D214	L64	L63
	W528	Y439	L369	T293	T215	F141	I64
	N529		T370		W216		H65
		D443	Q371	E298		I145	I66
	L533	H444	G372	G299	T219	E146	N67
	P534	H445	A373	G300	D220	N147	P68
	T535		T374	Q301	I221	I148	S69
	L536	Y449	E375	G302	N222	V149	D70
		P450	K376	T303	Q223	I150	W71
	R539	N451	A377		A224		
		G452	I378	I308	D225	V153	R75
	Q543	A453	Y379	N309	R226		
	V546	I454	D380	C310	P227	T156	L84
	N548		W381	W311	N228	G157	F95
	A549	S468	N382	Q312	Q229	A158	P86
		A469				G159	
		H470	D386	R316	E232	F160	Q89
		A471	Q387	S317		Q161	D90
	K552	P472	Q388	N318	G236	E162	L91
	F553	F473	G389	P319	T237	T163	Q92
		L474	N390	Q238	Q238	R94	G93
	Y557		R391	A322		Q165	R94
							D95
				S323	T242		T96
				T324	Q243	L173	I97
				R325	F244	L174	N98
				S326	T245	Q175	D99
				S327	P246	V176	S100
				N328	L247	A177	Y101
					E248	Q178	H102
					T249	D179	A103
				G332	K250		K104
				S333	I251	L183	Y105
				S334	N252	M184	E106
				W335		P185	T107
				P336		W186	P108
				E337		L492	
				W328			
			</				

• Molecule 1: VP2

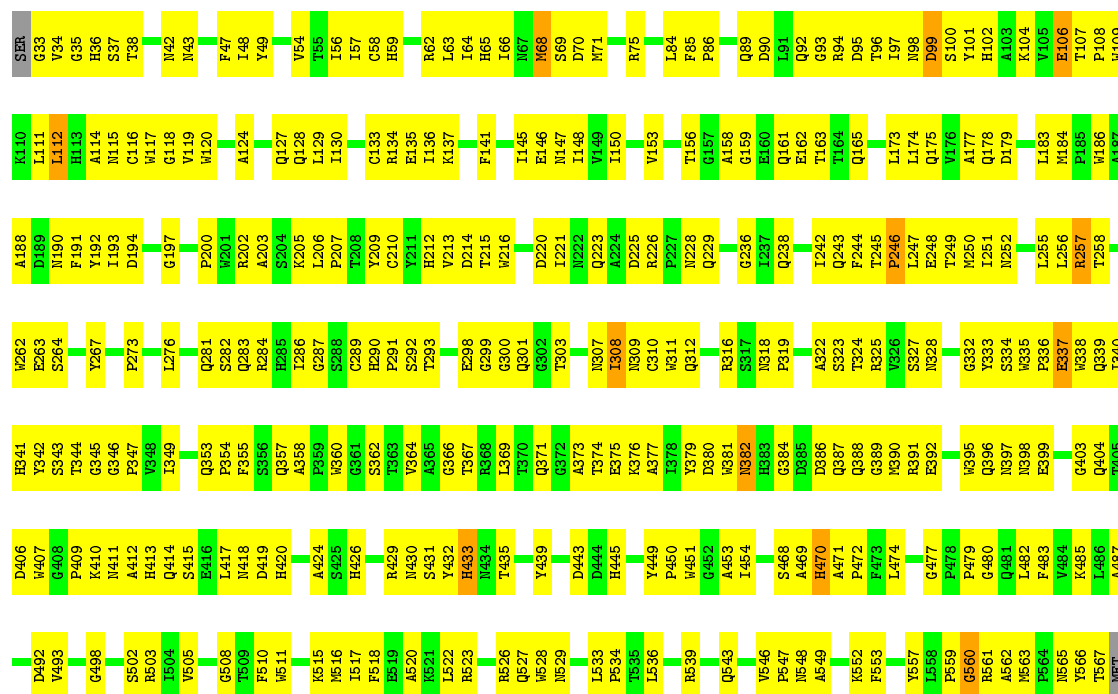
Chain 4: 44% 54%

SER	G33	V34	H35	R36	S37	T38	N42	N43	F47	L48	Y49	V54	T55	I56	I57	C58	H59	R62	L63	I64	H65	E66	N67	P68	S69	D70	W71	R75	L84	F85	P86	Q89	D90	L91	Q92	Q93	R94	D95	T96	I97	N98	D99	S100	Y101	H102	A103	L104	Y105	E106	T107	W108	W109
	K110	L111	L112	H113	A114	N115	C116	L117	G118	V119	W120	A124	Q127	Q128	L129	I130	C133	R134	E135	I136	K137	P138	S139	F141	I145	E146	N147	I148	V149	I150	V153	T156	G157	A158	G159	E160	Q161	E162	T163	T164	Q165	L173	L174	Q175	V176	A177	Q178	D179	L183	M184	P185	



• Molecule 1: VP2

Chain 5: 43% 55% .



• Molecule 1: VP2

Chain a: 96% .



• Molecule 1: VP2

Chain b: 97% .



- Molecule 1: VP2

Chain c: 96%



- Molecule 1: VP2

Chain d: 96%



- Molecule 1: VP2

Chain e: 96%



- Molecule 1: VP2

Chain f: 96%



- Molecule 1: VP2

Chain g: 96%



- Molecule 1: VP2

Chain h: 97%



- Molecule 1: VP2

Chain i: 97%



• Molecule 1: VP2

Chain j:  97%

• Molecule 1: VP2

Chain k:  96%

• Molecule 1: VP2

Chain l:  96%

• Molecule 1: VP2

Chain m:  96%

• Molecule 1: VP2

Chain n:  97%

• Molecule 1: VP2

Chain o:  96%

• Molecule 1: VP2

Chain p:  97%

• Molecule 1: VP2

Chain q:  96%



- Molecule 1: VP2

Chain r: 97%



- Molecule 1: VP2

Chain s: 96%



- Molecule 1: VP2

Chain t: 96%



- Molecule 1: VP2

Chain u: 96%



- Molecule 1: VP2

Chain v: 97%



- Molecule 1: VP2

Chain w: 96%



- Molecule 1: VP2

Chain x: 96%



- Molecule 1: VP2

Chain y:  97%



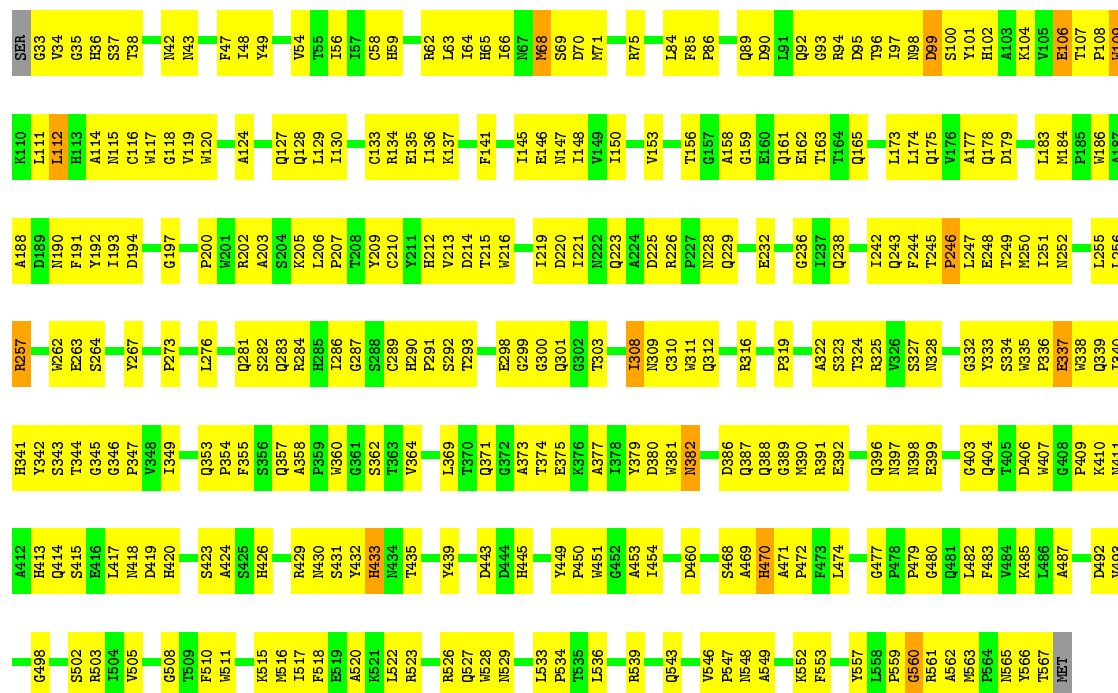
• Molecule 1: VP2

Chain z:  96%



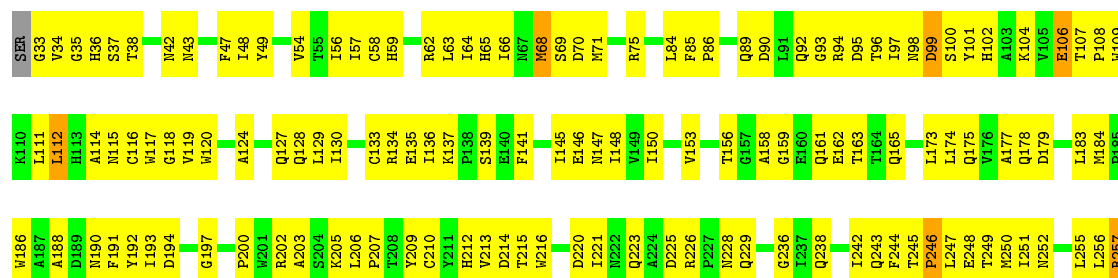
• Molecule 1: VP2

Chain 6:  44% 53%



• Molecule 1: VP2

Chain 7:  43% 54%



MIET	A487	D406	W338	T258
	D492	W407	Q339	
	V493	G408	I340	W262
		P409	H341	E263
	G498	K410	Y342	S264
		N411	S343	
	S502	A412	T344	Y267
	R503	H413	G345	L268
	I504	Q414	G346	F269
	V505	S415	P347	
		E416	V348	P273
	G508	L417	I349	
	T509	N418		L276
	W510	D419	Q353	
	W511	H420	P354	Q281
			F355	S282
	K515	S423	S356	Q283
	M516	A424	Q357	R284
	I517	S425	A358	H285
	F518	H426	F359	I286
	E519		W360	G287
	A520	R429	G361	S288
	R521	N430	S362	C289
	L522	S431	T363	H290
	R523	Y432	V364	P291
		H433	A365	S292
	R526	N434	G366	T293
	Q527	T435	T367	
	W528		R368	E298
	N529	Y439	L369	G299
			T370	G300
	L533	D443	Q371	Q301
	P534	D444	G372	G302
	T535	H445	A373	T303
	L536		T374	
	R539	Y449	E375	I308
		P450	K376	N309
		W451	A377	C310
	Q543	G452	I378	W311
		A453	Y379	Q312
	V546	I454	D380	
	P547		W381	R316
	N548	S468	N382	S317
	A549	A469		N318
		H470	D386	F319
	K552	A471	Q387	
	F553	P472	Q388	A322
		F473	G389	S323
	Y557	L474	M390	T324
	L558		R391	R325
	P559	G477	E392	V326
	G560	P478		S327
	R561	P479	Q396	N328
	A562	G480	N397	
	M563	Q481	N398	G332
	F564	L482	E399	Y333
	N565	F483		S334
	Y566	W484	G403	W335
	T567	K485	Q404	P336
		L486	T405	E337

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	7564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	0	0.52	0/4472	0.65	3/6114 (0.0%)
1	1	0.52	0/4472	0.65	3/6114 (0.0%)
1	2	0.52	0/4472	0.65	3/6114 (0.0%)
1	3	0.52	0/4472	0.65	3/6114 (0.0%)
1	4	0.52	0/4472	0.65	3/6114 (0.0%)
1	5	0.52	0/4472	0.65	3/6114 (0.0%)
1	6	0.52	0/4472	0.65	3/6114 (0.0%)
1	7	0.52	0/4472	0.65	3/6114 (0.0%)
1	A	0.52	0/4472	0.65	3/6114 (0.0%)
1	B	0.52	0/4472	0.65	3/6114 (0.0%)
1	C	0.52	0/4472	0.65	3/6114 (0.0%)
1	D	0.52	0/4472	0.65	3/6114 (0.0%)
1	E	0.52	0/4472	0.65	3/6114 (0.0%)
1	F	0.52	0/4472	0.65	3/6114 (0.0%)
1	G	0.52	0/4472	0.65	3/6114 (0.0%)
1	H	0.52	0/4472	0.65	3/6114 (0.0%)
1	I	0.52	0/4472	0.65	3/6114 (0.0%)
1	J	0.52	0/4472	0.65	3/6114 (0.0%)
1	K	0.52	0/4472	0.65	3/6114 (0.0%)
1	L	0.52	0/4472	0.65	3/6114 (0.0%)
1	M	0.52	0/4472	0.65	3/6114 (0.0%)
1	N	0.52	0/4472	0.65	3/6114 (0.0%)
1	O	0.52	0/4472	0.65	3/6114 (0.0%)
1	P	0.52	0/4472	0.65	3/6114 (0.0%)
1	Q	0.52	0/4472	0.65	3/6114 (0.0%)
1	R	0.52	0/4472	0.65	3/6114 (0.0%)
1	S	0.52	0/4472	0.65	3/6114 (0.0%)
1	T	0.52	0/4472	0.65	3/6114 (0.0%)
1	U	0.52	0/4472	0.65	3/6114 (0.0%)
1	V	0.52	0/4472	0.65	3/6114 (0.0%)
1	W	0.52	0/4472	0.65	3/6114 (0.0%)
1	X	0.52	0/4472	0.65	3/6114 (0.0%)
1	Y	0.52	0/4472	0.65	3/6114 (0.0%)
1	Z	0.52	0/4472	0.65	3/6114 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	a	0.52	0/4472	0.65	3/6114 (0.0%)
1	b	0.52	0/4472	0.65	3/6114 (0.0%)
1	c	0.52	0/4472	0.65	3/6114 (0.0%)
1	d	0.52	0/4472	0.65	3/6114 (0.0%)
1	e	0.52	0/4472	0.65	3/6114 (0.0%)
1	f	0.52	0/4472	0.65	3/6114 (0.0%)
1	g	0.52	0/4472	0.65	3/6114 (0.0%)
1	h	0.52	0/4472	0.65	3/6114 (0.0%)
1	i	0.52	0/4472	0.65	3/6114 (0.0%)
1	j	0.52	0/4472	0.65	3/6114 (0.0%)
1	k	0.52	0/4472	0.65	3/6114 (0.0%)
1	l	0.52	0/4472	0.65	3/6114 (0.0%)
1	m	0.52	0/4472	0.65	3/6114 (0.0%)
1	n	0.52	0/4472	0.65	3/6114 (0.0%)
1	o	0.52	0/4472	0.65	3/6114 (0.0%)
1	p	0.52	0/4472	0.65	3/6114 (0.0%)
1	q	0.52	0/4472	0.65	3/6114 (0.0%)
1	r	0.52	0/4472	0.65	3/6114 (0.0%)
1	s	0.52	0/4472	0.65	3/6114 (0.0%)
1	t	0.52	0/4472	0.65	3/6114 (0.0%)
1	u	0.52	0/4472	0.65	3/6114 (0.0%)
1	v	0.52	0/4472	0.65	3/6114 (0.0%)
1	w	0.52	0/4472	0.65	3/6114 (0.0%)
1	x	0.52	0/4472	0.65	3/6114 (0.0%)
1	y	0.52	0/4472	0.65	3/6114 (0.0%)
1	z	0.52	0/4472	0.65	3/6114 (0.0%)
All	All	0.52	0/268320	0.65	180/366840 (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	0	0	2
1	1	0	2
1	2	0	2
1	3	0	2
1	4	0	2
1	5	0	2
1	6	0	2
1	7	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
1	O	0	2
1	P	0	2
1	Q	0	2
1	R	0	2
1	S	0	2
1	T	0	2
1	U	0	2
1	V	0	2
1	W	0	2
1	X	0	2
1	Y	0	2
1	Z	0	2
1	a	0	2
1	b	0	2
1	c	0	2
1	d	0	2
1	e	0	2
1	f	0	2
1	g	0	2
1	h	0	2
1	i	0	2
1	j	0	2
1	k	0	2
1	l	0	2
1	m	0	2
1	n	0	2
1	o	0	2
1	p	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	0	2
1	r	0	2
1	s	0	2
1	t	0	2
1	u	0	2
1	v	0	2
1	w	0	2
1	x	0	2
1	y	0	2
1	z	0	2
All	All	0	120

There are no bond length outliers.

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	560	GLY	N-CA-C	5.99	128.06	113.10
1	g	560	GLY	N-CA-C	5.99	128.06	113.10
1	h	560	GLY	N-CA-C	5.99	128.06	113.10
1	l	560	GLY	N-CA-C	5.99	128.06	113.10
1	x	560	GLY	N-CA-C	5.99	128.06	113.10

There are no chirality outliers.

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	ASN	Peptide
1	A	68	MET	Peptide
1	B	382	ASN	Peptide
1	B	68	MET	Peptide
1	C	68	MET	Peptide

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
-----	-------	-------	----------	----------	---------	--------------

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4326	0	4014	457	0
1	1	4326	0	4013	452	0
1	2	4326	0	4014	453	0
1	3	4326	0	4014	461	0
1	4	4326	0	4013	459	0
1	5	4326	0	4013	455	0
1	6	4326	0	4014	451	0
1	7	4326	0	4013	456	0
1	A	4326	0	4014	672	0
1	B	4326	0	4013	680	0
1	C	4326	0	4014	670	0
1	D	4326	0	4013	669	0
1	E	4326	0	4014	676	0
1	F	4326	0	4013	661	0
1	G	4326	0	4014	670	0
1	H	4326	0	4013	675	0
1	I	4326	0	4014	676	0
1	J	4326	0	4013	671	0
1	K	4326	0	4013	679	0
1	L	4326	0	4014	674	0
1	M	4326	0	4014	676	0
1	N	4326	0	4014	670	0
1	O	4326	0	4014	670	0
1	P	4326	0	4013	628	0
1	Q	4326	0	4014	632	0
1	R	4326	0	4014	617	0
1	S	4326	0	4013	618	0
1	T	4326	0	4014	678	0
1	U	4326	0	4014	673	0
1	V	4326	0	4014	675	0
1	W	4326	0	4014	670	0
1	X	4326	0	4013	675	0
1	Y	4326	0	4014	675	0
1	Z	4326	0	4014	665	0
1	a	4326	0	4013	0	0
1	b	4326	0	4014	0	0
1	c	4326	0	4013	0	0
1	d	4326	0	4013	0	0
1	e	4326	0	4014	0	0
1	f	4326	0	4014	0	0
1	g	4326	0	4014	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	h	4326	0	4014	0	0
1	i	4326	0	4014	0	0
1	j	4326	0	4014	0	0
1	k	4326	0	4014	0	0
1	l	4326	0	4014	0	0
1	m	4326	0	4014	0	0
1	n	4326	0	4014	0	0
1	o	4326	0	4013	0	0
1	p	4326	0	4014	0	0
1	q	4326	0	4014	0	0
1	r	4326	0	4014	0	0
1	s	4326	0	4013	0	0
1	t	4326	0	4014	0	0
1	u	4326	0	4014	0	0
1	v	4326	0	4014	0	0
1	w	4326	0	4014	0	0
1	x	4326	0	4013	0	0
1	y	4326	0	4014	0	0
1	z	4326	0	4013	0	0
All	All	259560	0	240820	14764	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 30.

The worst 5 of 14764 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:X:34:VAL:N	1:5:36:HIS:CE1	1.71	1.58
1:A:34:VAL:N	1:E:36:HIS:CE1	11.02	1.58
1:J:36:HIS:CE1	1:O:34:VAL:N	1.72	1.58
1:G:36:HIS:CE1	1:M:34:VAL:H	152.11	1.57
1:A:34:VAL:H	1:B:36:HIS:CE1	1.22	1.57

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	0	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	1	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	2	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	3	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	4	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	5	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	6	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	7	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	A	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	B	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	C	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	D	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	E	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	F	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	G	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	H	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	I	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	J	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	K	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	L	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	M	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	N	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	O	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	P	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	Q	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	S	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	T	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	U	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	V	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	W	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	X	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	Y	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	Z	533/537 (99%)	507 (95%)	25 (5%)	1 (0%)	51	85
1	a	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	b	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	c	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	d	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	e	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	f	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	g	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	h	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	i	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	j	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	k	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	l	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	m	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	n	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	o	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	p	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	q	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	r	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	s	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	t	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	u	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	v	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	x	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	y	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
1	z	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	51	85
All	All	31980/32220 (99%)	30479 (95%)	1441 (4%)	60 (0%)	54	85

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	193	ILE
1	H	193	ILE
1	S	193	ILE
1	V	193	ILE
1	1	193	ILE

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	0	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	1	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	2	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	3	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	4	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	5	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	6	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	7	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	A	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	B	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	C	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	D	464/466 (100%)	453 (98%)	11 (2%)	54	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	F	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	G	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	H	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	I	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	J	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	K	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	L	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	M	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	N	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	O	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	P	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	Q	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	R	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	S	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	T	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	U	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	V	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	W	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	X	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	Y	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	Z	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	a	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	b	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	c	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	d	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	e	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	f	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	g	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	h	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	i	464/466 (100%)	454 (98%)	10 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	j	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	k	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	l	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	m	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	n	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	o	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	p	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	q	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	r	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	s	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	t	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	u	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	v	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	w	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	x	464/466 (100%)	453 (98%)	11 (2%)	54	80
1	y	464/466 (100%)	454 (98%)	10 (2%)	57	81
1	z	464/466 (100%)	453 (98%)	11 (2%)	54	80
All	All	27840/27960 (100%)	27201 (98%)	639 (2%)	59	80

5 of 639 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	109	TRP
1	b	337	GLU
1	x	112	LEU
1	1	536	LEU
1	4	112	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 892 such sidechains are listed below:

Mol	Chain	Res	Type
1	1	59	HIS
1	b	281	GLN
1	x	165	GLN
1	1	463	HIS

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Mol	Chain	Res	Type
1	4	281	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.