



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:28 am GMT

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

This is a wwPDB/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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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) : recalc29047

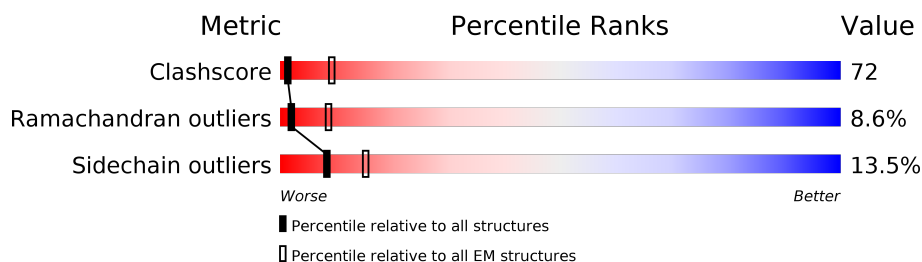
1 Overall quality at a glance

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.



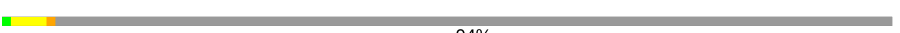

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	A	648	94%
1	B	648	27% 51% 14% 7%
1	C	648	94%
1	D	648	22% 55% 14% 7%
1	E	648	94%
1	F	648	22% 54% 15% 7%
1	G	648	94%
1	H	648	22% 55% 15% 7%
1	I	648	94%

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

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

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

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 80985 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Outer capsid VP4.

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

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

- Molecule 2 is a protein called Core protein VP6.

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

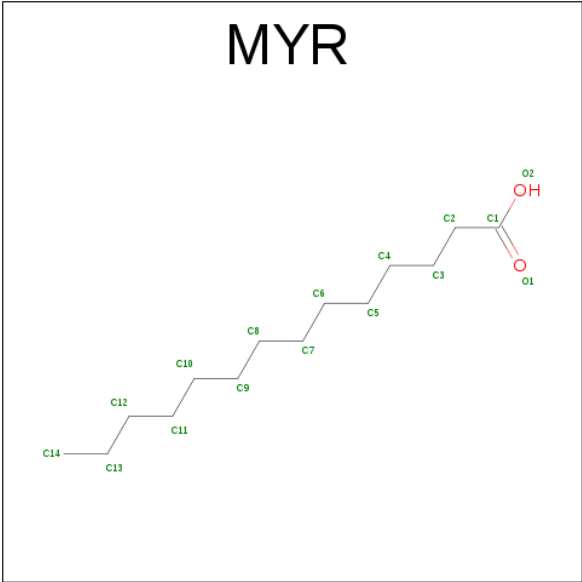
- Molecule 3 is a protein called VP1.

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

- Molecule 4 is a protein called VP3.

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

- Molecule 5 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



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

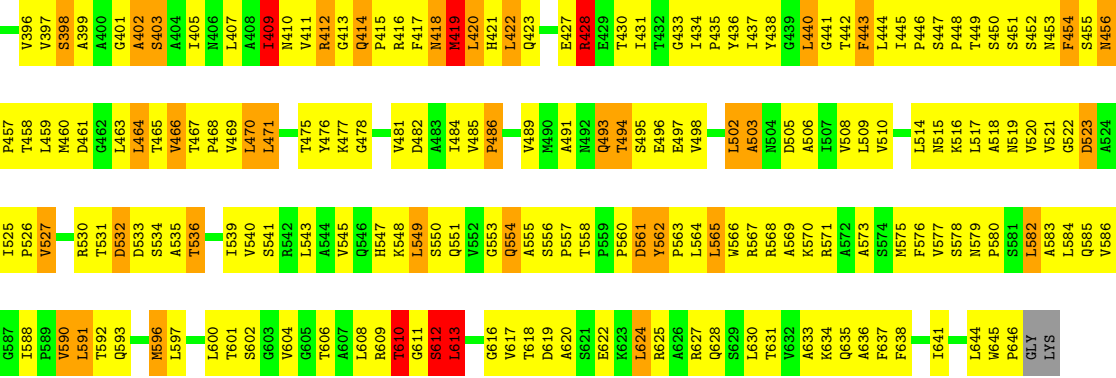
- Molecule 1: Outer capsid VP4

- Molecule 1: Outer capsid VP4

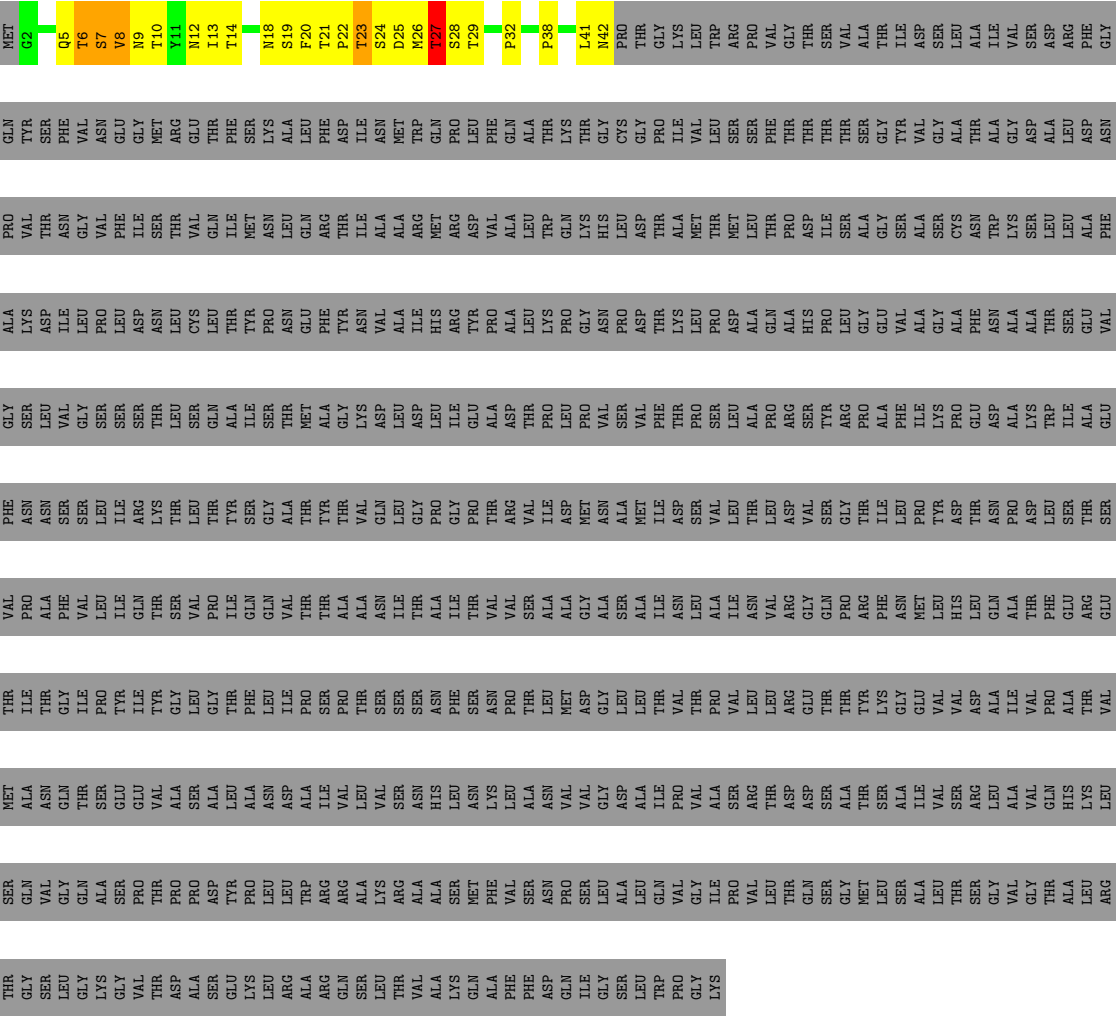




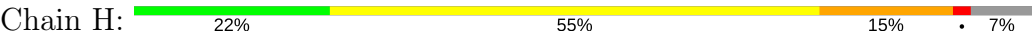


• Molecule 1: Outer capsid VP4



• Molecule 1: Outer capsid VP4



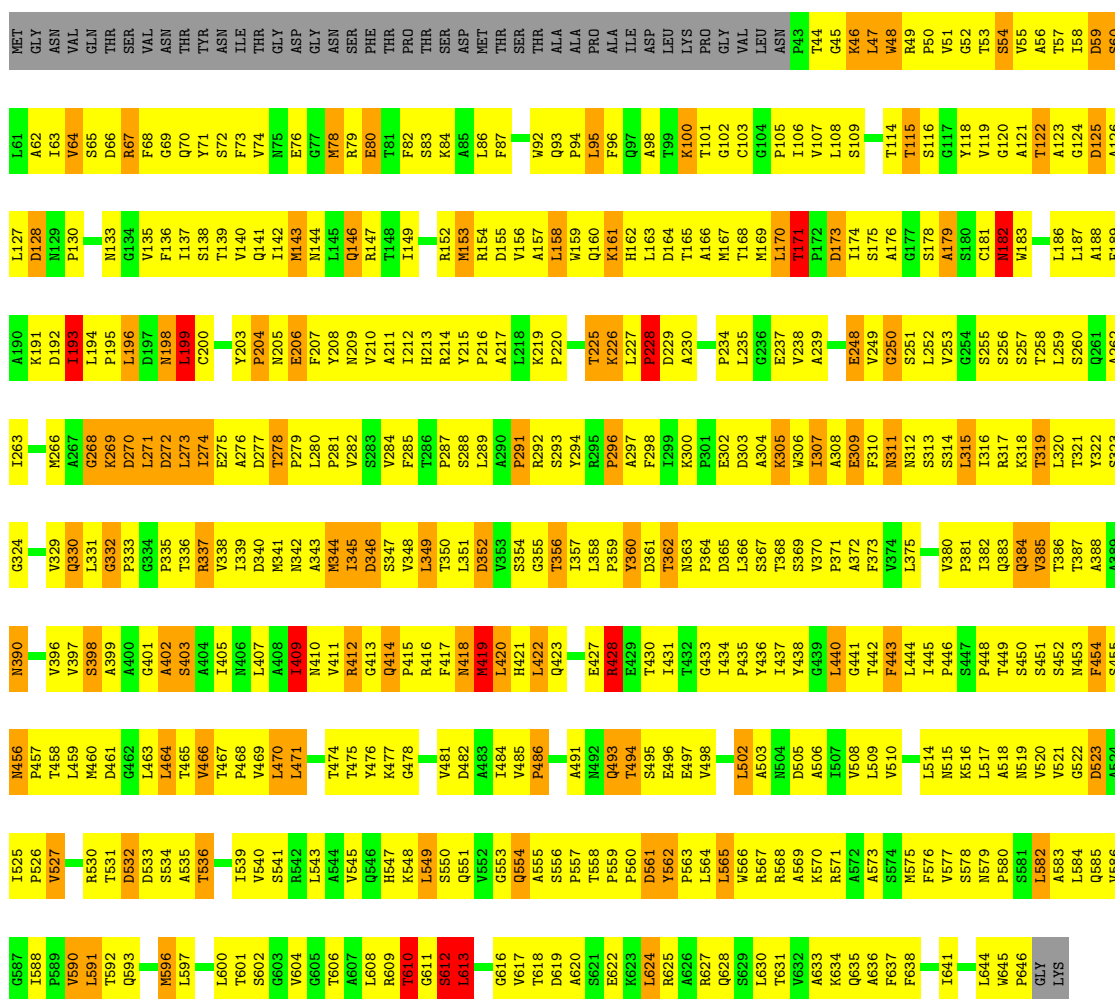
● Molecule 1: Outer capsid VP4

Chain I: 94%

[illegible]

- Molecule 1: Outer capsid VP4

Chain J:  22% 55% 15% 7%



- Molecule 1: Outer capsid VP4

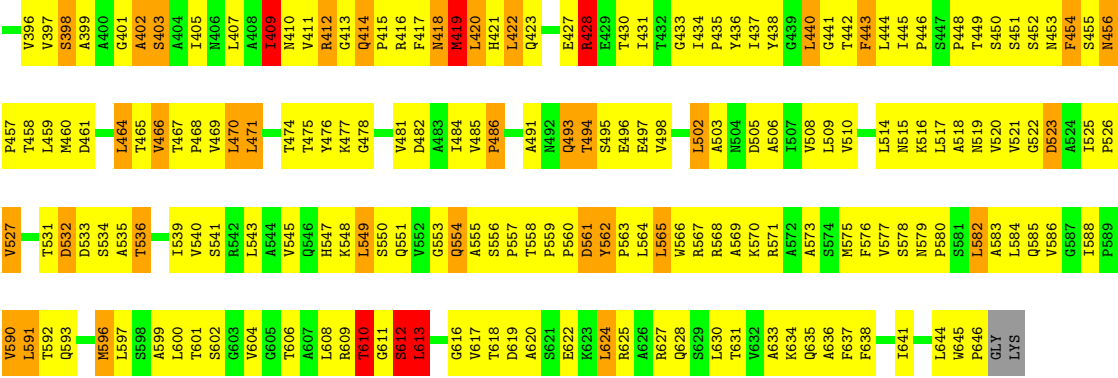
Chain K: ... 94%

[illegible]

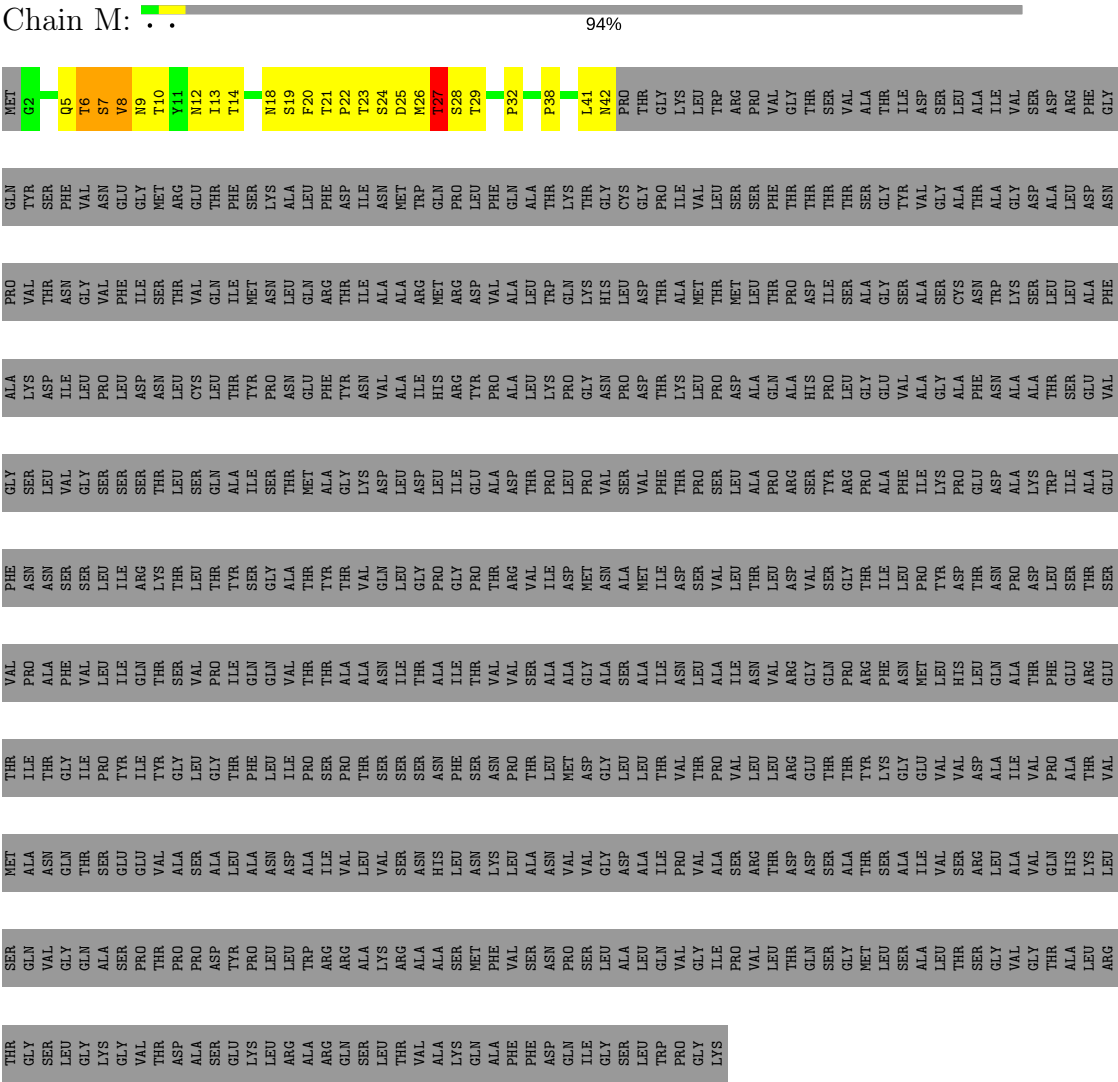
- Molecule 1: Outer capsid VP4

Chain L:  23% 54% 15% • 7%

V329	T265	K191	D128	I63	MET
G330	A266	D192	N129	I64	GLY
L331	G267	I193	P130	O64	ASN
G332	G268	L194		S65	VAL
P333	G269	P195	N133	D66	GLN
G334	D270	L196	G134	R67	THR
P335	L271	D197	V135	F68	SER
T336	D272	N198	F136	G69	VAL
R337	L273	I199	I137	Y70	ASN
V338	L274	C200	S138	Q71	THR
I339	E275		T139	S72	TYR
M341	A276	Y203	V140	F73	ASN
N342	D277	P204	Q141	V74	ILE
A343	T278	N205	I142	N75	THR
A344	P279	E206	M143	E76	GLY
M345	L280	F207	N144	G77	ASP
D346	P281	Y208	L145	N78	GLY
S347	V282	N209	Q146	R79	ASN
V348	S283	V210	R147	E80	SER
L349	V284	A211	T148	T81	PHE
T350	F285	I212	I149	F82	THR
L351	T286	H213		S83	PRO
D352	P287	R214	R152	K84	THR
S353	S288	Y215	M153	A85	SER
G354	L289	P216	R154	L86	ASP
G355	V290	A217	D155	F87	MET
T356	A291	L218	V156		THR
L357	R292	K219	A157	W92	SER
L358	S293	P220	L158	Q93	THR
V359	K295		W159	P94	ALA
P360	P296	T225	K161	L96	ALA
D361	A297	L227	H162	F96	PRO
T362	F298	P228	L163	Q97	ALA
M363	T299	D229	D164	T99	ILE
P364	K300	A230	T165	K100	ASP
L366	E302	P234	A166	T101	LEU
S367	D303	P235	T168	G102	LYS
T368	A304	L235	G169	C103	PRO
G369	K305	G336	M170	G104	GLY
V370	W306	E237	L171	P105	VAL
P371	T307	V238	P172	I106	LEU
A372	A308	E248	D173	V107	ASN
F373	F310	V249	I174	L108	P43
V374	N311	G250	A176	S109	T44
L375	N312	S251	G177	T114	K46
V380	S313	L252	T178	T115	L47
P381	S314	V253	A179	I116	W48
L382	L315	G254	S180	G117	R49
Q383	T316	S255	K181	Y118	P50
Q384	R317	S256	N182	V119	V51
T386	K318	S257	W183	G120	G52
T387	T319	L258		A121	S64
A388	L320	T259	L186	T122	T53
L389	V321		L187	G124	S64
	T322	A262	A188	D125	T58
	S323	L263	F189	A126	D59



● Molecule 1: Outer capsid VP4



● Molecule 1: Outer capsid VP4



L584	G522	S455	A389	G324	S264	K191	D128	MET
Q585	A523	M456	N390		T265	D192	N129	GLY
G587	L525	T458	V396	V329	M266	L193	P130	ASN
P526	G525	L459	V397	G330	A267	L194		VAL
P589	P527	M460	S398	G332	K269	L196	N133	GLN
V590		D461	A399	P333	L270	D197	G134	THR
	R530		A400	G334	D271	N198	V136	SER
L591	T531	L464	G401	P335	L272	L199	I137	VAL
Q593	D532	T465	A402	T336	L273	C200	S138	ASN
	D533	V466	S403	R337	L274		T139	TVR
S534	T467	A404	A404	V338	E275	Y203	V140	ASN
A535	P468	I405	I405	I339	A276	P204	Q141	ILE
	V469	A406	A406	D340	D277	N205	I142	THR
L600	L470	L407	L407	M341	T278	E206	M143	GLY
S601	R471	L471	A408	A342	T279	F207	N144	ASP
G603	R472	R472	A409	A343	L280	Y208	L145	GLY
S604	R542	T474	N410	M344	P281	N209	Q146	ASN
G605	L543	T475	R412	I345	S282	V210	L147	SER
T606	A544	V476	G413	D346	S283	A211	T148	PHE
A607	V545	K477	Q414	V348	F285	L212	I149	THR
L608	Q546	G478	P415	L349	T286	H213		PRO
R609	H547		R416	T350	P287	R214	R152	THR
	K548	V481	R417	L351	S288	Y215	M153	SER
T610	K549	D482	F417	D352	L289	P216	R154	ASP
G611	S550	A483	N418	V353	A290	L218	D155	MET
S612	Q551	L494	A420	S354	P291	K219	A157	THR
L613	V552	V485	H421	G355	R292	L219	L158	SER
	G553	P486	L422	T356	S293	P220	V159	ALA
G616			Q423	I357	T294	T225	Q160	PRO
V617	V489			L358	R295	K226	K161	ALA
S655	M490	A491	A428	P359	P296	L162	H162	PRO
A620	P557	A491	R428	V360	A297	P228	L163	ALA
S621	T558	M492	A429	D361	F298	D229	D164	ILE
P559	P559	Q493	T430	T362	T298	A230	T165	ASP
E622	S560	T494	I431	M363	K300		A166	LEU
G623	L624	S495	T432	P364	P301	P234	M167	LYS
R625	V562	A496	G433	D365	E302	L235	T168	PRO
A626	P563	V497	I434	L366	D303	G236	M169	GLY
R627	L564	A498	P435	S367	A304	E237	K170	VAL
			Y436	T368	K305	V238	T171	LEU
Q628	L665	L502	I437	S369	W306	A239	P172	ASN
S629	S629	A503	V438	V370	T307		D173	P43
L630	R567	M504	G439	A371	E308	E248	I174	T44
T631	S568	D505	L440	P372	A309	V249	S175	G45
G632	A569	V506	G439	A373	E309	K251	G177	R46
K630	K570	A507	G441	R373	F310	G260	A176	L47
A634	R571	L506	T442	G374	N311	S251	G177	L48
K635	V508	V508	F443	L375	N312	L262	S178	R49
A636	L509	L509	L444		S313	V253	A179	R49
F637	S574	V510	T445		S314	G264	R180	P50
F638	M575		P446	V380	L315	S255	C181	G52
	F576		S447	P381	T316	S256	N182	G52
	V577		P448	I382	R317	S257	W183	T53
	S578		T449	Q383	T318	T258		S54
	L514	M515	A445	V385	L319	L269	L186	V55
L644	L517	A516	S450	Q384	R319	L269	A123	A56
W645	P580	A518	S451	R385	L320	S260	L187	T57
P646	S581	M519	S452	T386	T321	Q261	A188	L58
GLY	L582	V520	N453	T387	V322	A262	F189	D59
	A582	W521	F454	A388	S223	T262	L195	D59

- Molecule 1: Outer capsid VP4

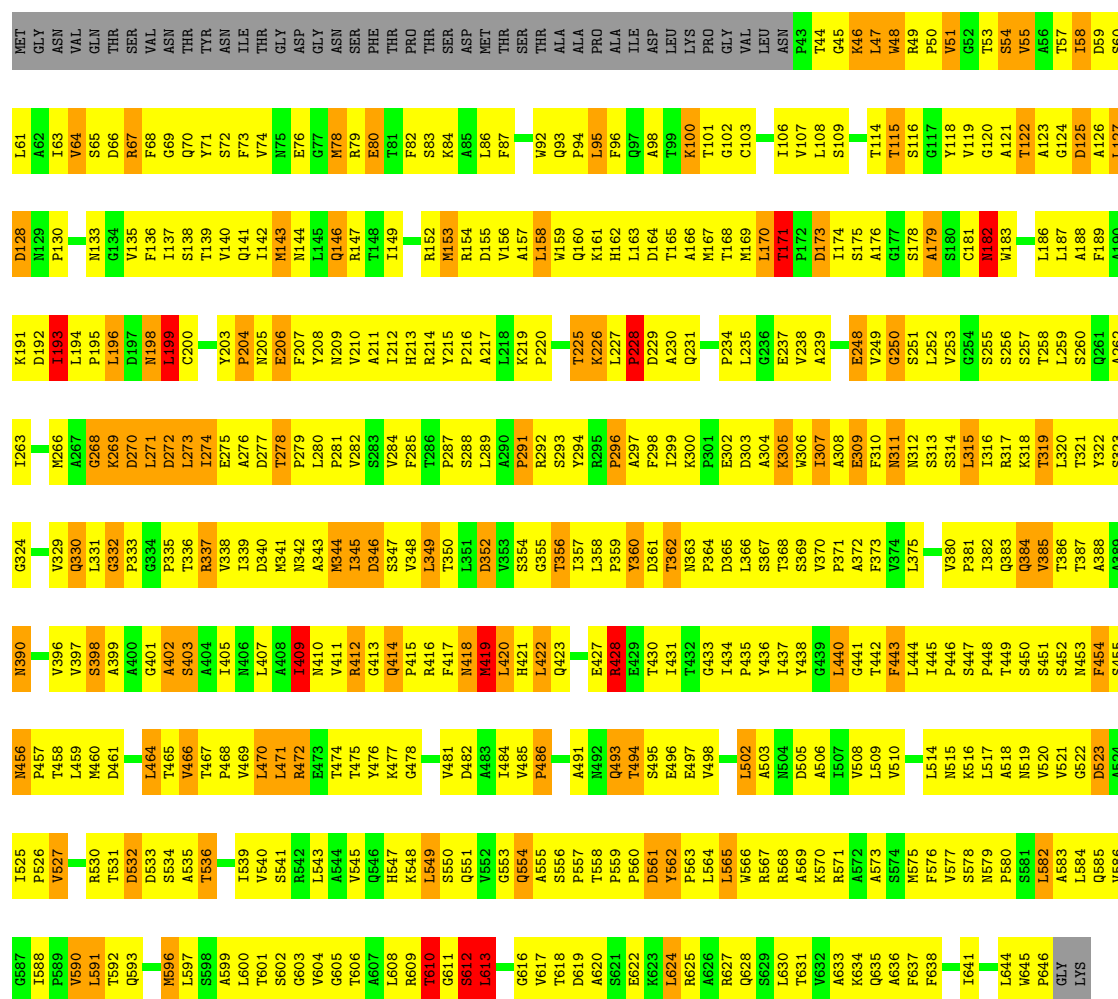
Chain 0: 94%

Lys	Ala	Ser	Asp	Met
Thr	Leu	Leu	Ala	Asp
Ser	Leu	Leu	Leu	Arg
Ile	Ser	Leu	Ala	Phe
Ala	Val	Phe	Asn	Gly
Glu	Gly	Ala	Pro	Gln
Phe	Ser	Lys	Val	Tyr
Asn	Ser	Leu	Val	Thr
Asn	Leu	Asp	Thr	Ser
Ser	Val	Ile	Thr	Phe
Ser	Gly	Leu	Gly	Val
Ser	Ser	Pro	Val	Asn
Leu	Ser	Leu	Phe	Asn
Ile	Ser	Leu	Ile	Gly
Arg	Ser	Asp	Ile	Gly
Lys	Thr	Asn	Ser	Met
Thr	Leu	Leu	Thr	Arg
Leu	Ser	Cys	Val	Glu
Thr	Gln	Leu	Gln	Thr
Tyr	Ala	Thr	Ile	Phe
Ser	Ile	Tyr	Met	Ser
Gly	Ser	Pro	Asn	Lys
Ala	Thr	Asn	Leu	Ala
Thr	Met	Glu	Gln	Leu
Ala	Ala	Phe	Arg	Phe
Tyr	Gly	Tyr	Thr	Asp
Thr	Gly	Leu	Thr	Asp
Val	Lys	Asn	Ile	Ile
Gln	Asp	Val	Ala	Asn
Leu	Leu	Val	Ala	Met
Leu	Leu	Ile	Arg	Met
Gly	Leu	His	Met	Gln
Gly	Ile	Arg	Arg	Pro
Pro	Glu	Tyr	Asp	Leu
Thr	Ala	Pro	Val	Phe
Arg	Asp	Ala	Ala	Gln
Val	Thr	Leu	Leu	Ala
Val	Thr	Leu	Leu	Ala
Ile	Pro	Lys	Trp	Thr
Asp	Leu	Pro	Gln	Lys
Met	Pro	Gly	Lys	Lys
Met	Pro	Leu	Lys	Lys
Asn	Val	Asn	His	Thr
Ala	Ser	Pro	Leu	Gly
Ala	Met	Asp	Asp	Pro
Met	Val	Thr	Thr	Thr
Ile	Phe	Thr	Ala	Gly
Asp	Thr	Lys	Ala	Lys
Ser	Pro	Leu	Met	Val
Val	Ser	Pro	Thr	Trp
Leu	Leu	Asp	Met	Arg
Thr	Ala	Ala	Leu	Pro
Leu	Pro	Gln	Thr	Val
Asp	Arg	Ala	Pro	Gly
Val	Ser	His	Asp	Thr
Val	Ser	Pro	Asp	Thr
Thr	Tyr	Pro	Ile	Ser
Gly	Arg	Leu	Ser	Val
Thr	Pro	Gly	Ala	Ala
Ile	Ala	Val	Gly	Thr
Leu	Phe	Val	Ser	Ile
Pro	Ile	Gly	Ala	Thr
Pro	Lys	Ala	Ala	Asp
Asn	Ala	Asn	Cys	Leu
Pro	Thr	Thr	Thr	Ala
Thr	Thr	Phe	Thr	Ala
Pro	Asp	Ala	Trp	Ile
Asn	Ala	Ala	Lys	Val

[illegible]

- Molecule 1: Outer capsid VP4

Chain P: 22% 55% 15% 7%



- Molecule 1: Outer capsid VP4

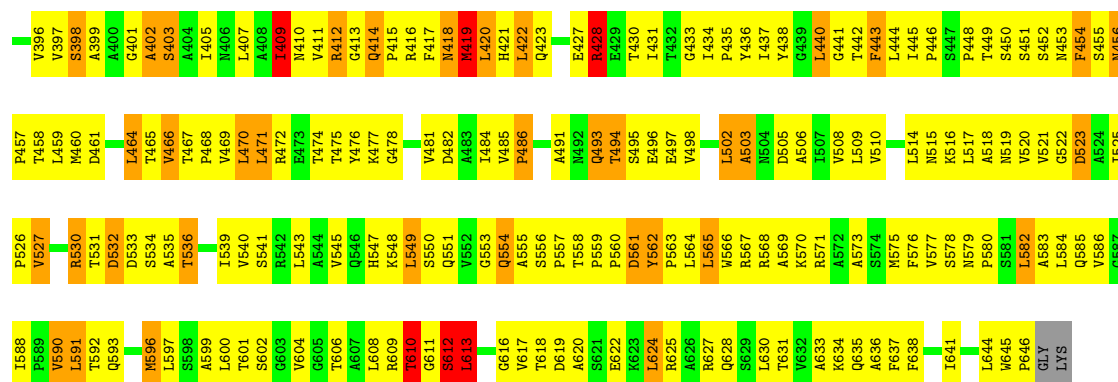
Chain Q: 94%

[illegible]

- Molecule 1: Outer capsid VP4

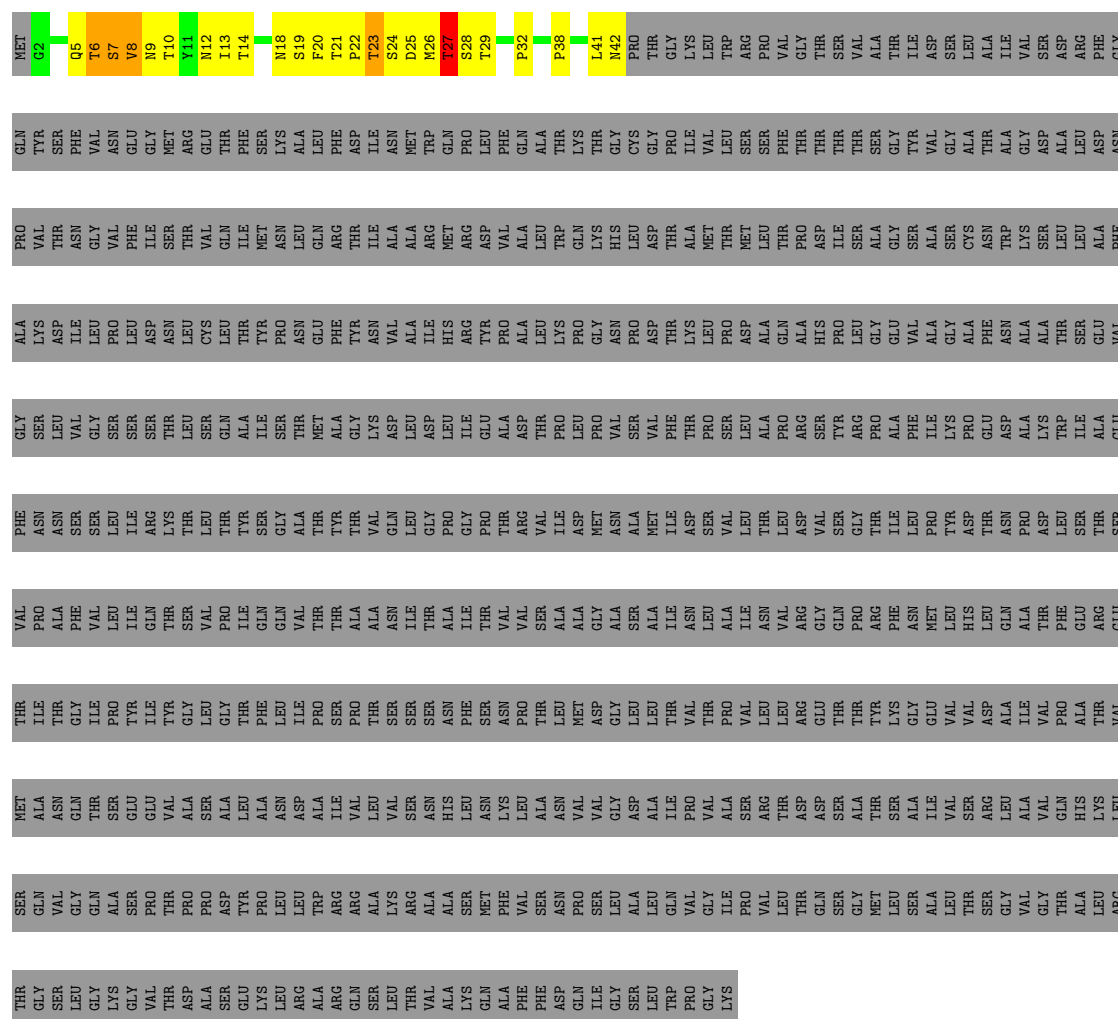
Chain R:  23% 54% 15% • 7%

[illegible]



- Molecule 1: Outer capsid VP4

Chain S: 94%



- Molecule 1: Outer capsid VP4

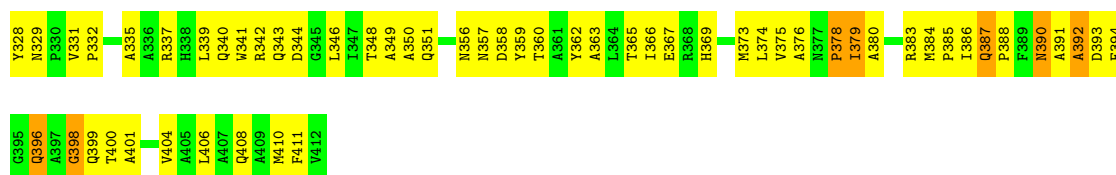
Chain T: 22% 55% 15% 7%

LYS

- Molecule 2: Core protein VP6

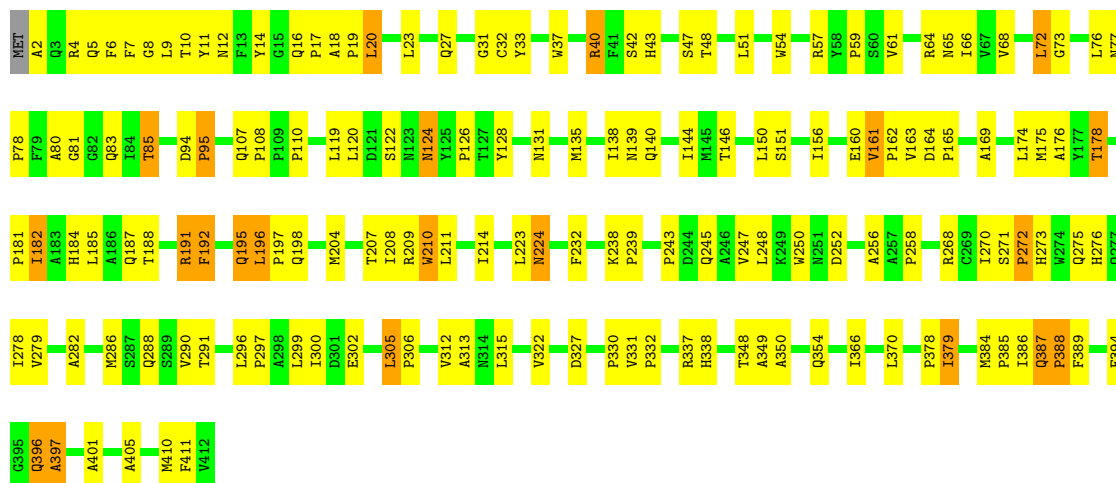
Chain U: 27% 61% 12%

[illegible]



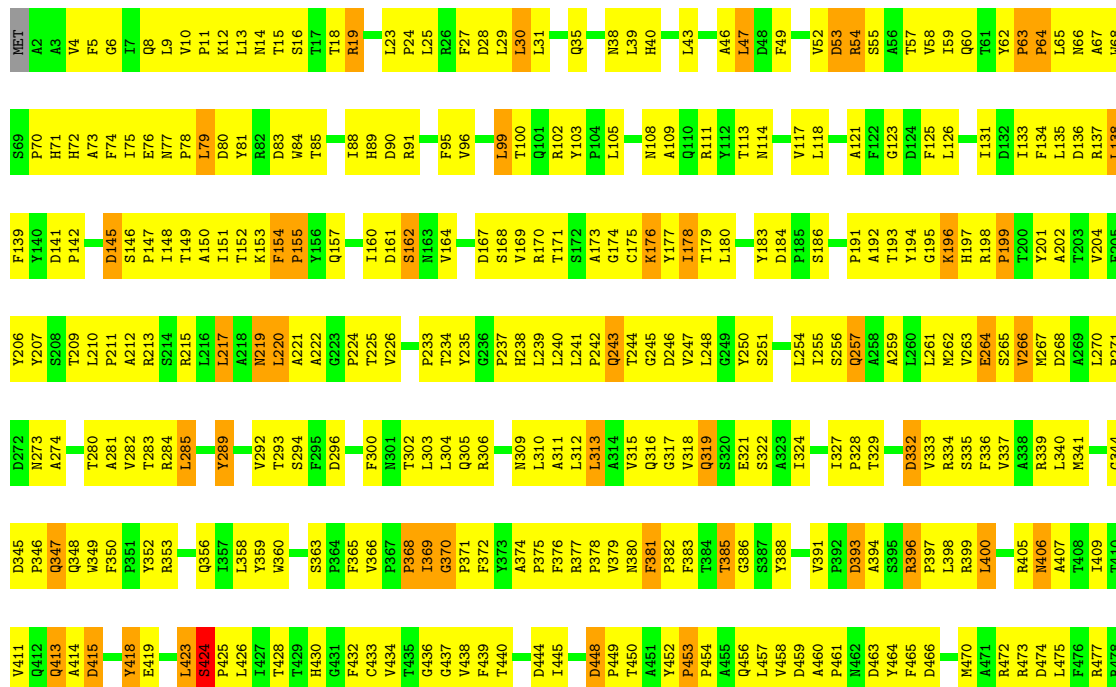
• Molecule 2: Core protein VP6

Chain V: 61% 34% 5%



• Molecule 3: VP1

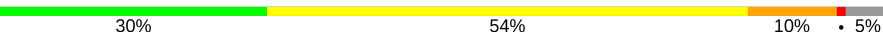
Chain W: 33% 58% 9%





THR	A1151	L1085	P1024	I957	T894	C824	V761	S685	N632	T570	S503	R438	L376	K310	T247
	A1152	H1086	N1025	H958	S895	T827	T762	A696	P633	L571	E502	T439	L376	I311	N248
	S1153	Y1087	G1026	R959	A897	T828	T763	M697	Q634	A572	D506	I440	I377	N312	N249
	D1155	D1089	L1027	A960	A898	T829	T764	S698	Q635	G573		L441		K313	A250
	P1090	P1089	Q1030	Q961	A899	R830	Q768	N699	A636	P574	S509	C442	E380	S314	S251
	Q1091	Q1091	L1031	Q963	E900	L831	Q769	W700	P637	M575	P510	W444	P316	L252	G253
	L1094	L1094	I1032	V964	M902	L832	Q770	I701	L638	T576	I511	F445	D254	T316	G254
	D1095	D1095	I1033	E965	H903	P833	F771	T704	R639	S577	P512	A446	E255	F317	
	E1096	E1096	D1034	Q966	H904	S834	T772	T705	L640	D578	S513	K384	E256		
	A1097	A1097	D1035	T967	A904	H835	R773	A706	A641	H580	E514	S447	G257	D320	
	P1098	P1098	G1035	F968	N905	H836	L774	F707	E643	S581	L515	E449	R257	T323	
	I1099	I1099	N1036	E971	N906	Y837	Q775	F708	E644	P582	R516	W450	L258	I324	
	E1100	E1100	V1037	M972	D907	C838	Q776	I709	H645	V583	L517	D450	E260	T325	
	L1101	L1101	P1038	N973	K910	R839	T777	R710	I646	F586	L518	L453	V261	S326	
	R1168	R1168	R1039	L974	T911	A840	D778	V711	R647	M587	D519	Q454	R262	S327	
	S1105	S1105	D1040	F975		H841	V779	W712	A648	A588	P520	Q455	R263	K328	
	K1106	K1106		N976	D914	P843	T781	T718	N649	M589	GLY	V456	P264	M329	
	G1171	G1171	D1044	Q977	L915	L844	T782	T719	P651	A590	ASN	M457	P265	I330	
	N1108	N1108	W1045	N978	D916	P845	R783	T720	Q652	M591	D524	H458	P266	R331	
	P1109	P1109	A978	R979	L917	T844	R784	T721	P653	L592	Y525	L459	T267	F333	
	D1173	D1173	Y1046	Q980	A918	F851	L785	W722	S654	L593	A526	N461	D268	GLU	
	A1110	A1110	Y1047	G981	G917	T852	R786	T723	E655	A594	A527	I462	S269	GLY	
	P1175	P1175	P1048	N981	L919	R853	R787	D723	P656	Q595	F528	S463	S270	ARG	
	G1112	G1112	S1049	L982	L920	N854	R788	L724	G657	P586	N529	S464	V271	P337	
	P1113	P1113	D1050	Y983	D921	H854	V788	T725	G658	E597	K530	N465		T401	
	P1114	P1114	V1051	L984	G922	R855	D789	R726	Y658	P598	C531	T402	Y274	E338	
	V1115	V1115	I1052	N985	L923	R856	P790	R727	G659	L597	A532	T403	K275	L339	
	P1116	P1116	Q1053	Q986	A924	A857	A791	T728	S660	A600	L532	N404	T276	L340	
	F1117	F1117	V1054	T987	L925	V858	R792	M729	S661	I601	A533	A468	V277	A341	
	K1118	K1118	S1055	N988	Y926	T859	R793	T730	L662	G602	S534	A469	L278	L342	
	I1119	I1119	V1056	T989	G927	T860	Q794	T731	Q663	V603	N535	L470	S279	L343	
	P1120	P1120	A1057	N992	D928	R861	D795	V732	G664	P604	A536	P471	R280	Y344	
	I1121	I1121	V1058	W992	P929	T862		T733	L668	G605	N538	N473	G281	R347	
	P1122	P1122	R1060	S994	R930	A863	D799	T734	P669	M606	L540	E474	Y282	A348	
	V1124	V1124	D1061	P995	A932	V865	I800	M736	I670	H607	G539	A475	D284	V349	
	Y1125	Y1125	Y1062	M996	D933		R801	R737	P671	Q608	V541	L476	N285	L350	
	P1126	P1126	W1064	A997	L934		A902	Q738	S672	T609	T542		A286	P351	
	C1127	C1127	P1065	P998	S935		T803	V739	N672	T610	T543	L479	Q287	T352	
	I1128	I1128	M1066	P1002	A936		H804	T741	N675	P611	V544	R480	F288	Q353	
	T1129	T1129	A937	P1003	Y938		A805	T742	V676	A612	L545	R481	N289	T354	
	A1130	A1130	Y1067	P1004	L939		T806	T743	Y677	S613		S482	P290	K355	
	R1131	R1131	K1068	F1004	L939		F807	T744	P678	Q614	D552	V483	L291	N356	
	R1132	R1132	A1069	V1005	Q940		A908	F745	P678	F615		T484	A292	A357	
	Y1135	Y1135	G1070	R1006	G943		A809	F746	W679	S616	Q555	P485	L293	L299	
	F1136	F1136	T1071	G1007	N944		A810	Y746	P680	H617	S556	L488	L294	Q358	
	A1137	A1137	R1073	N1010	E945		L811	T747	N681	G619	T558	E422	R294	L360	
	E1140	E1140	V1074	V946	N946		P812	Q748	Q682	G618	T559	C423	S295	S361	
	N1143	N1143	V1075	R1012	E948		V813	H749	P683	V620	H559	A424	V297	T362	
	D1144	D1144	L1076	V1013	N947		D814	M750	L684	W621	L560	N425	L298	A363	
	S1145	S1145	E1077	V1014	H949		A816	T751	P685	P622	S562	N426	L299	L364	
	L1146	L1146	G1078	G1015	D886		P752	F752	R686	P623		L427	L299	L364	
	Y1209	Y1209	F1017	R1016	A887		T753	L754	L687			N429	L300		
	F1147	F1147	H1080	F1017	P951		R818	E754	T688	L626	N563	N494	L301	R367	
	V1210	V1210	Y1081	G1018	G953		V819	L755	P691	W627	K564	A496	L302	I368	
	S1148	S1148	Y1082	T1019	P954		V820	S756	T692	P628	K565	I497	Q303	G369	
	T1149	T1149	Y1083	M922	S954		A821	V757	T692	Q629	L567	T498	S307	I370	
	ALA	ALA	N1150	V1021	H956		L823	L758	D694	I631	F569	L436	N308	D372	

• Molecule 4: VP3

Chain Y:  30% 54% 10% • 5%

T1084	G942	V871	H804	K740	T543	T478	D412	A341	V277	L215	THR	G76	MET
L1085	G943	A872	F807	T741	T544	L479	P413	L342	L278	T216	PRO	D77	PRO
Y1087	A944	Q873	A808	T742	V544	L480	Q415	A343		K217	MET	I78	ARG
Y1088	Y945	C874	A809	T743	S546	R481	I416	R347	Y282	E218	ILE	I79	ARG
D1089	R947	Q875	A810	T744	S547	R482	V417	R348	O284	L220	ASN	R81	ALA
P1090	R947	D876	L811	T745	D548	T484	Q418	Y349	D284	C221	N155	R82	ARG
Q1091	P952	Q876	P812	Y746	A549	P485	I419	L350	N285	F223	A156	P83	LYS
L1092	G953	F879	V813	T747	F550	L486	V420	P351	Q287	T222	I157	T82	LYS
S1093	P954	Q879	D814	Q748	P551	V487	I420	R352	F288	R223	R158	S94	ALA
L1094	S955	P882	P815	H749	D552	L488	N421	Q353	F289	W224	F159	D85	GLN
D1095	H956	H883	A816	Q882	S553	D489		T354	N289	F225	F160	S86	SER
E1096	I957	P884	A817	C751	S554	P490	A424	T355	P290	M226	L161	I87	ALA
A1097	Q1030	L885	I818	P752	Q555	T491	N425	K355	P291	Q227			ILE
P1098	L1031	D886		P753	S556	V492	N426	N356	A292		V164	A97	ALA
L1099	I1032		A821	T754	S557	L493	L427	A357	L293	Y229	D165	V100	
E1100	Y964	R889	C824	V757	T558	A496	L428	Q358	R294	Q230	D166		
E1102	E965	Q890	Q825	L758	H559	T497	L430	F359	S295	Q238	I167	P103	
V1103	F968	P891	Q826	A759	P561	T498	I432	L360	N296	L235	R168	Q104	
L1104	P969	D892		V761	S562	T499	A433	L361	V297	P236	I169	S105	
S1105	N973	A897	T830	V763	L567	S501	T431	T364	L298	E237	P172	M106	
K1106	L974	A898	L831	T764	F568	GLU	L436	A365	M300	Q239	ASP	K107	
T1107	F975	A899	I832	P765	L569	THR	L437	D366	L302	A238	VAL	V108	
L1108	N976	E900	P833	P766	Q634	SER	R437	R367	Q303	N241	SER	T109	
P1109	Y977	I901	S834	P767	Q635	THR	P438	R370	F304	R242	LYS	I111	
G1110	A978	N902	G835	F767	A636	THR	T439	L371	T305	J243	SER	V112	
P1111	Y979	H903	H836	V768	L630	THR	I441	D372	L306	V244	LEU	N113	
L1112	Q980	A904	Y837	Q769	L631	ILE	C442	A374	S307	C245	SER	Y117	
P1113	N981	V905	Q838	P770	Q640	SER	P443	A375	N308	M246	ALA	V118	
L1114	L982	N906	K839	F771	L641	PRO	W444	L376	L309	T247	TVR	V119	
P1115			A840	T772	F642	ILE		I377	K310	N248	LEU	C119	
F1116	Y985	K910	F841	T773	H645	SER	S448	A383	I311	W249	D194	N120	
G1117	Q986	F913	A842	L774	H646	GLU	Q449	A389	K312	A250	S185	V121	
L1119	T987	D914	P843	V775	L646	ILE	D450	L390	S314	S251		C122	
P1120	A988	N915	L844	Q776	P647	LEU	L451	V384	S315	L252	A188	N123	
L1121	T989	L915		N777	L648	ARG	R452	E386	T316	D254		A124	
Q1122	N990	D916	S847	D778	F586	LEU	L453	C387	F317	E255	P191	H125	
	G991	G917	N848	V779	M587	LEU	Q454	M388		Q256	L192	F126	
C1127	N992	A918	A849	L780	A588	GLN	Q455	E389	D320	R257	L193	T128	
L1128	Y993	L919	M850	T781	L589	PRO	V456	L390	V321	C258	I195	N129	
T1129	S994	L920	F851	N782	A590	MET	H457	C391	T322	L259	E196	S130	
A1130	P995	D921	T852	V783	N591	GLY	H459	D392	T323	E260	D197	A131	
R1131	N996	G922	R853	L784	L592	ASN	L459	A393	I324	V261	T198	L132	
R1132	A997	L923		V785	L593	D524	I462	L394	T325	R262	G199	S133	
L1133	P998	A924	R856	A786	F656	Y525	S463	I398		L263	L200	E134	
H1134	P1002	Y926	A857	V788	Q594	A526	S464	R399	M329	P264	C201	H135	
A1135	P1003		V858	D789	P596	K530	N465	E400	I330	P265	T202	L136	
L1136	F1004	P929	I859	P790	E597		T466	T401	R331	T267	S203		
F1137	L1005		T860	V791	P598	C531	A467	Y402	A332	D268	L206	H140	
S1139	R1006	A930	R861	T792	A600		A468	L403	F333	D269	L207	ASP	
E1140	E1077	A932	E862	Q793	Q599		A469	M404	S334	S270	D208	P68	
L1141	P1009		F864	V798	G602		L470	G335	V271	V271	N209	ALA	
N1142	V1010	A937	V865	V799	V603		P471	R407	R336	H272	I210	SER	
N1143	V1011	Y938	C866	D799	L657		E474	S408	P337	A273	P211	THR	
L1144	R1012	Y939	A867	R800	M606			M409	E338	Y274	S212	LEU	
L1145	G1015	Q940	R868	R801	H607			H410	L339	T276	A213	LEU	
		Y941			Q808			Q411	L340	T276	H214	ALA	

L1146	F1147	S1148	T1149	N1150	A1151	A1152	S1153	I1154	D1155	T1156	A1157	F1158	G1159	E1160	N1161	A1162		L1167	R1168	W1169	P1170	G1171	L1172	V1173		R1178	V1179		N1182	D1183	L1184	P1185		T1189	L1190	Y1191	N1192	S1193	L1194	Y1195	R1196	Y1197	N1198		Y1201	P1202	T1203	L1204	D1205	G1206	I1207	M1208	Y1209	V1210	R1211	S1212	A1213	T1214
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	18464	Depositor
Resolution determination method	FSC at 0.143 cut-off	Depositor
CTF correction method	Each particle	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	57700	Depositor
Image detector	Kodak SO163 film	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.60	0/295	1.00	0/405
1	B	0.52	0/4601	0.80	0/6295
1	C	0.60	0/295	1.00	0/405
1	D	0.51	0/4601	0.80	1/6295 (0.0%)
1	E	0.60	0/295	0.99	0/405
1	F	0.52	0/4601	0.80	0/6295
1	G	0.60	0/286	0.95	0/391
1	H	0.52	0/4601	0.80	0/6295
1	I	0.60	0/295	1.00	0/405
1	J	0.51	0/4601	0.80	0/6295
1	K	0.60	0/295	0.99	0/405
1	L	0.52	0/4601	0.80	0/6295
1	M	0.60	0/286	0.95	0/391
1	N	0.52	0/4601	0.80	0/6295
1	O	0.60	0/295	0.99	0/405
1	P	0.51	0/4601	0.80	0/6295
1	Q	0.60	0/295	0.99	0/405
1	R	0.52	0/4601	0.80	0/6295
1	S	0.60	0/286	0.95	0/391
1	T	0.52	0/4601	0.80	0/6295
2	U	0.33	0/3233	0.55	0/4443
2	V	0.31	0/3233	0.49	0/4443
3	W	0.32	0/10148	0.60	0/13935
4	X	0.53	0/8078	0.75	2/11071 (0.0%)
4	Y	0.38	0/9056	0.66	2/12412 (0.0%)
All	All	0.47	0/82681	0.75	5/113262 (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	1
1	D	0	1
1	F	0	1
1	H	0	1
1	J	0	1
1	L	0	1
1	N	0	1
1	P	0	1
1	R	0	1
1	T	0	1
4	X	0	3
4	Y	0	2
All	All	0	15

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	934	LEU	CA-CB-CG	-5.76	102.06	115.30
1	D	51	VAL	N-CA-C	5.75	126.53	111.00
4	Y	1002	PRO	N-CA-CB	5.60	110.02	103.30
4	Y	1003	PRO	N-CA-CB	5.52	109.93	103.30
4	X	428	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

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

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	291	0	277	54	0
1	B	4508	0	4555	643	0
1	C	291	0	277	78	0
1	D	4508	0	4555	904	0
1	E	291	0	277	77	0
1	F	4508	0	4555	874	0
1	G	284	0	267	56	0
1	H	4508	0	4555	864	0
1	I	291	0	277	81	0
1	J	4508	0	4555	891	0
1	K	291	0	277	78	0
1	L	4508	0	4555	872	0
1	M	284	0	267	57	0
1	N	4508	0	4555	882	0
1	O	291	0	277	76	0
1	P	4508	0	4555	898	0
1	Q	291	0	277	85	0
1	R	4508	0	4555	883	0
1	S	284	0	267	58	0
1	T	4508	0	4555	879	0
2	U	3138	0	3061	444	0
2	V	3138	0	3061	174	0
3	W	9882	0	9821	1051	0
4	X	7873	0	7851	1242	0
4	Y	8835	0	8748	1054	0
5	A	15	0	27	27	0
5	C	15	0	27	33	0
5	E	15	0	27	27	0
5	G	15	0	27	29	0
5	I	15	0	27	29	0
5	K	15	0	27	27	0
5	M	15	0	27	26	0
5	O	15	0	27	28	0
5	Q	15	0	27	27	0
5	S	15	0	27	30	0
All	All	80985	0	81102	11617	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 72.

The worst 5 of 11617 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

5.3 Torsion angles [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	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	2
1	B	602/648 (93%)	407 (68%)	134 (22%)	61 (10%)	1	4
1	C	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	2
1	D	602/648 (93%)	416 (69%)	129 (21%)	57 (10%)	1	5
1	E	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	2
1	F	602/648 (93%)	408 (68%)	133 (22%)	61 (10%)	1	4
1	G	37/648 (6%)	24 (65%)	8 (22%)	5 (14%)	0	2
1	H	602/648 (93%)	409 (68%)	132 (22%)	61 (10%)	1	4
1	I	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	2
1	J	602/648 (93%)	411 (68%)	132 (22%)	59 (10%)	1	4
1	K	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	2
1	L	602/648 (93%)	409 (68%)	132 (22%)	61 (10%)	1	4
1	M	37/648 (6%)	24 (65%)	8 (22%)	5 (14%)	0	2
1	N	602/648 (93%)	408 (68%)	133 (22%)	61 (10%)	1	4
1	O	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	2
1	P	602/648 (93%)	410 (68%)	132 (22%)	60 (10%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	39/648 (6%)	25 (64%)	9 (23%)	5 (13%)	0	2
1	R	602/648 (93%)	406 (67%)	135 (22%)	61 (10%)	1	4
1	S	37/648 (6%)	24 (65%)	8 (22%)	5 (14%)	0	2
1	T	602/648 (93%)	406 (67%)	135 (22%)	61 (10%)	1	4
2	U	409/412 (99%)	283 (69%)	81 (20%)	45 (11%)	0	3
2	V	409/412 (99%)	330 (81%)	60 (15%)	19 (5%)	3	19
3	W	1276/1299 (98%)	1063 (83%)	173 (14%)	40 (3%)	5	30
4	X	1012/1214 (83%)	714 (71%)	219 (22%)	79 (8%)	1	8
4	Y	1146/1214 (94%)	860 (75%)	204 (18%)	82 (7%)	1	10
All	All	10656/17511 (61%)	7587 (71%)	2151 (20%)	918 (9%)	2	6

5 of 918 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	34/536 (6%)	27 (79%)	7 (21%)	1	6
1	B	499/536 (93%)	426 (85%)	73 (15%)	3	18
1	C	34/536 (6%)	27 (79%)	7 (21%)	1	6
1	D	499/536 (93%)	425 (85%)	74 (15%)	3	17
1	E	34/536 (6%)	27 (79%)	7 (21%)	1	6
1	F	499/536 (93%)	426 (85%)	73 (15%)	3	18
1	G	32/536 (6%)	25 (78%)	7 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	499/536 (93%)	426 (85%)	73 (15%)	3	18
1	I	34/536 (6%)	27 (79%)	7 (21%)	1	6
1	J	499/536 (93%)	425 (85%)	74 (15%)	3	17
1	K	34/536 (6%)	27 (79%)	7 (21%)	1	6
1	L	499/536 (93%)	425 (85%)	74 (15%)	3	17
1	M	32/536 (6%)	25 (78%)	7 (22%)	1	5
1	N	499/536 (93%)	424 (85%)	75 (15%)	3	16
1	O	34/536 (6%)	27 (79%)	7 (21%)	1	6
1	P	499/536 (93%)	423 (85%)	76 (15%)	3	16
1	Q	34/536 (6%)	27 (79%)	7 (21%)	1	6
1	R	499/536 (93%)	425 (85%)	74 (15%)	3	17
1	S	32/536 (6%)	25 (78%)	7 (22%)	1	5
1	T	499/536 (93%)	424 (85%)	75 (15%)	3	16
2	U	325/326 (100%)	305 (94%)	20 (6%)	21	56
2	V	325/326 (100%)	305 (94%)	20 (6%)	21	56
3	W	1082/1092 (99%)	977 (90%)	105 (10%)	9	35
4	X	869/1030 (84%)	736 (85%)	133 (15%)	3	16
4	Y	976/1030 (95%)	864 (88%)	112 (12%)	6	28
All	All	8901/14524 (61%)	7700 (86%)	1201 (14%)	8	20

5 of 1201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	422	LEU
1	R	158	LEU
4	Y	231	MET
1	N	561	ASP
1	P	309	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 351 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	410	ASN
1	T	383	GLN
4	Y	429	ASN

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Mol	Chain	Res	Type
1	P	515	ASN
1	R	406	ASN

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 ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	MYR	A	649	1	14,14,15	0.54	0	13,13,15	0.58	0
5	MYR	C	649	1	14,14,15	0.54	0	13,13,15	0.57	0
5	MYR	E	649	1	14,14,15	0.54	0	13,13,15	0.58	0
5	MYR	G	649	1	14,14,15	0.54	0	13,13,15	0.57	0
5	MYR	I	649	1	14,14,15	0.54	0	13,13,15	0.57	0
5	MYR	K	649	1	14,14,15	0.54	0	13,13,15	0.58	0
5	MYR	M	649	1	14,14,15	0.54	0	13,13,15	0.58	0
5	MYR	O	649	1	14,14,15	0.55	0	13,13,15	0.58	0
5	MYR	Q	649	1	14,14,15	0.55	0	13,13,15	0.58	0
5	MYR	S	649	1	14,14,15	0.54	0	13,13,15	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MYR	A	649	1	-	0/11/12/13	0/0/0/0
5	MYR	C	649	1	-	0/11/12/13	0/0/0/0
5	MYR	E	649	1	-	0/11/12/13	0/0/0/0
5	MYR	G	649	1	-	0/11/12/13	0/0/0/0
5	MYR	I	649	1	-	0/11/12/13	0/0/0/0
5	MYR	K	649	1	-	0/11/12/13	0/0/0/0
5	MYR	M	649	1	-	0/11/12/13	0/0/0/0
5	MYR	O	649	1	-	0/11/12/13	0/0/0/0
5	MYR	Q	649	1	-	0/11/12/13	0/0/0/0
5	MYR	S	649	1	-	0/11/12/13	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 283 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	649	MYR	27	0
5	C	649	MYR	33	0
5	E	649	MYR	27	0
5	G	649	MYR	29	0
5	I	649	MYR	29	0
5	K	649	MYR	27	0
5	M	649	MYR	26	0
5	O	649	MYR	28	0
5	Q	649	MYR	27	0
5	S	649	MYR	30	0

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.