



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:24 am GMT

PDB ID : 3IZX
EMDB ID: : EMD-5256
Title : 3.1 Angstrom cryoEM structure of cytoplasmic polyhedrosis virus
Authors : Yu, X.; Ge, P.; Jiang, J.; Atanasov, I.; Zhou, Z.H.
Deposited on : 2011-01-15
Resolution : 3.10 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) : recalc29047

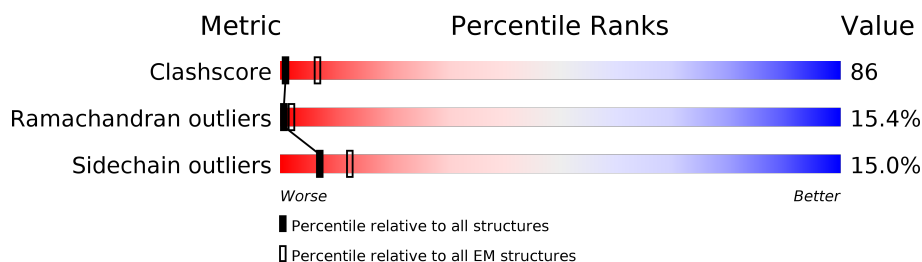
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	1058	
2	B	1333	
2	C	1333	
3	D	448	
3	E	448	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32209 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1057	Total	C	N	O	S	0	0
			8434	5345	1457	1587	45		

- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1191	Total	C	N	O	S	0	0
			9397	5937	1634	1789	37		
2	C	1249	Total	C	N	O	S	0	0
			9844	6213	1712	1882	37		

- Molecule 3 is a protein called Viral structural protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	290	Total	C	N	O	S	0	0
			2267	1440	398	422	7		
3	E	290	Total	C	N	O	S	0	0
			2267	1440	398	422	7		

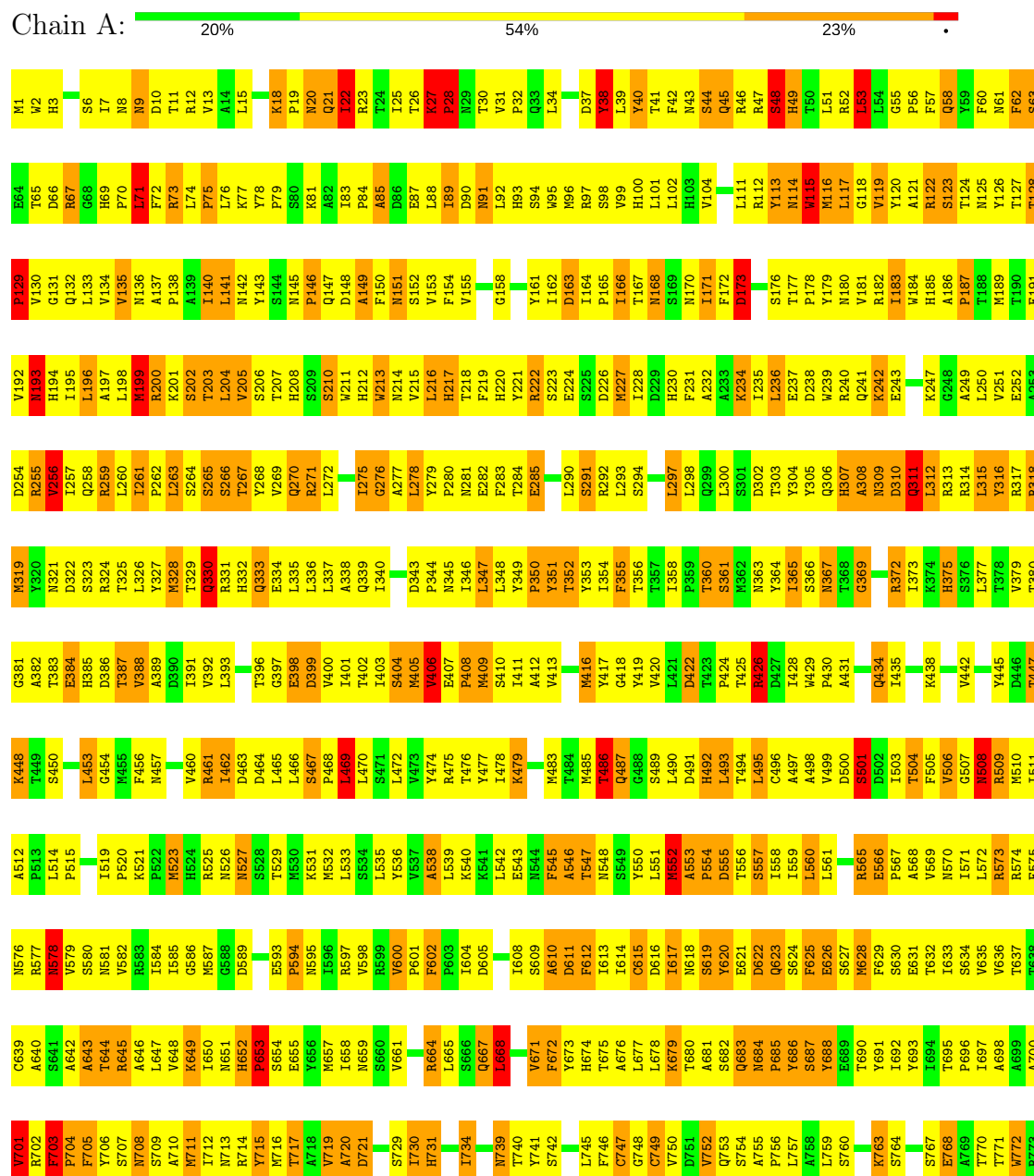
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	37	TRP	TYR	ENGINEERED MUTATION	UNP C6K2M8
E	37	TRP	TYR	ENGINEERED MUTATION	UNP C6K2M8

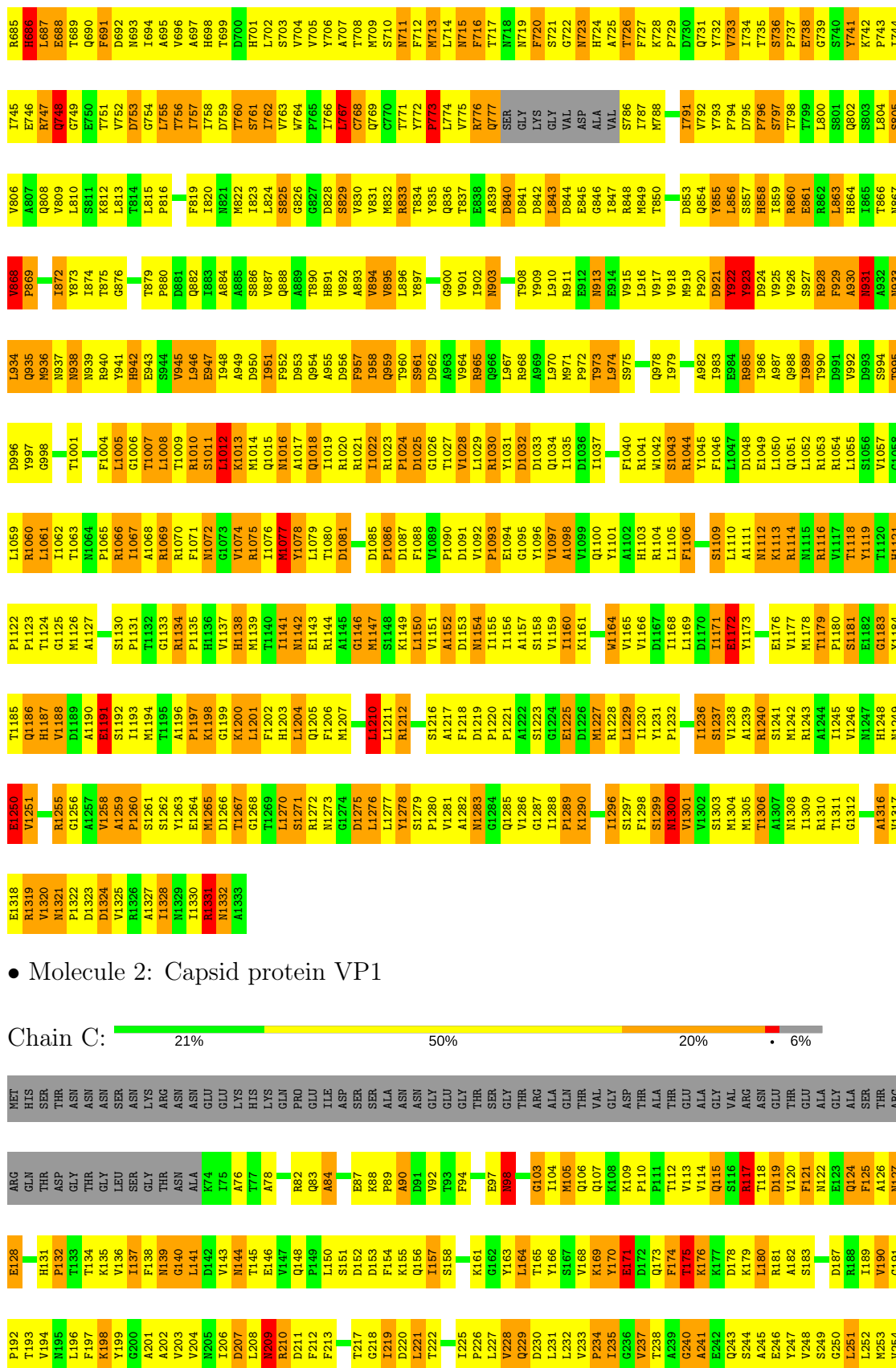
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: Structural protein VP3

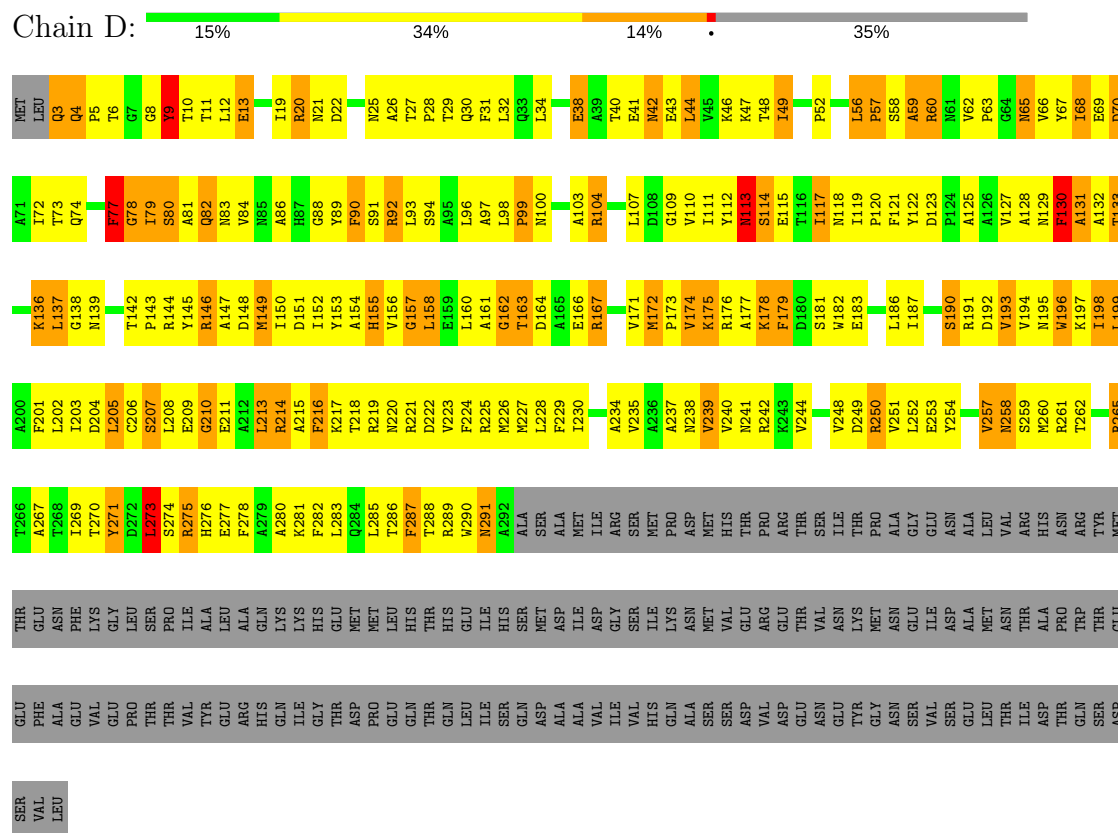




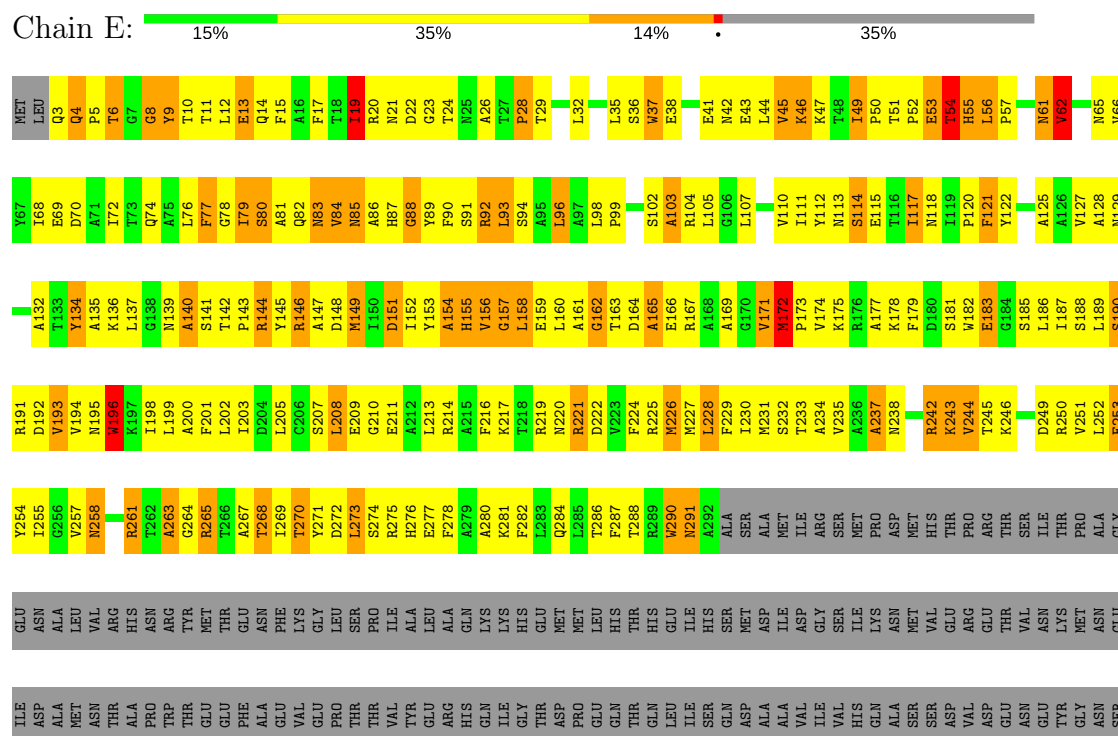


M1283	R1212	A1145	Y1078	N1016	D953	A893	S829	C768	V704	T638	D576	L512	S444	A381	N316	L255
G1284	S1216	G1146	L1079	A1017	Q954	V894	V830	Q769	V705	M639	Q577	E513	E445	H382	M317	F256
V1285		S1147	T1080	Q1018	A955	L895	V831	C770	A706	Q640	A578	F514	K446	S383	L318	K257
Q1286		S1148		I1019	D956	L896	M832	T771	T708	R641	L579	L515	R447	M384	Q319	V258
I1287	D1226	K1149	D1083	R1020	F957	Q998	R834	Y772	T709	G643	L581	L516	Y448	L385	Q320	M259
L1288	L1150	L1150	P1084	R1021	F958	Q989	T834	P773	M710	T644	S582	F517	F449	S386		T260
P1289	L1151	L1151	D1085	I1022	Q959	S899	Y835	L774	M711	T645	E583	F521	E451	Q388	Y325	R263
K1290	L1229	D1153	P1086	R1023	T960	G900	Q836	W775	F712	T646	H584	F522	M452	F389	L327	L264
L1291	L1230	A1154		P1024	S961	V901	T837	Q777	M713	T647	F584	F523	L453	H390	G328	L266
E1292	V1231	I1155	P1089	D1025	D962	I902	E838	T776	L714	F648	F586	E524	E454	H391	L329	L266
V1293	P1232	N1156	P1090	G1026	A963	N903	A839	Q777	M715	T649	A587	F525	Q455	P392	T330	V267
L1294	L1233	I1156	D1091	T1027	V964	G904	D840	GLY	M716	S650	L588	N526	Q455	N393	E331	G268
H1295	Q1234		V1092	L1028	R965	P905	D841	L1Y5	F717	G651	F589	R527	A459	Q394	T332	E269
L1296	P1235	V1159	P1093	L1029	Q966	A906	D842	GLY	T717	R651			A460	G395	R333	T270
S1297	T1236	I1160		R1030	L967	S907	L843	VAL	M718	F652	V592	F528	A460	G396	R334	T271
P1298	S1237	K1161	Y1096	Y1031	R968	T908		ASP	M719	R653	P593	K529	R461	A396	L334	T272
M1300	V1238	S1162	V1097	Q1034	A969	Y909	G846	ALA	F720	T654	L594	D530	L462	L397	D335	P273
	R1240	N1163	Q1100	I1035	L970	R911	I847	VAL	S721	M655	L594	D531	V463	R398	Y336	P273
M1304	S1241	V1165	Y1101	D1036	M971	R911	R848	SER	G722	V656	A595	I532	S464	P399	V337	M274
M1305	T1242	V1166	A1102	I1037	P972	E912	M849	ILE	M723	A657	G596	Q533	A465	E400	R338	S275
T1306	R1243	D1167	H1103	E1038	T973	E914	T850	MET	H724	T658	G597	N534	V466	L401	L339	S275
A1307	L1244	I1168	R1104	A1039	L974	E915	T851	E789	F727	A660	T599	L536	A468	A402	V340	L277
N1308	L1245	L1169	F1105	R1040	Q978	L916	D853	E790	K728	N661	I600	L537	A468	D404	T342	L278
I1309	V1246	D1170	F1106	R1041	Q979	V917	Q854	V792	T729	V662	I601	L538	A470	H405	I343	S279
R1310	N1247	I1171		W1042	R980	V918	V855	Y793	D730	V663	A692	F539	A473	D406	V344	V281
T1311	H1248	E1172	S1109	I1043	H981	M919	L856	P794	Q731	N664	I603	F540	A473	H407	G345	V282
G1312	N1249	Y1173	L1110	R1044	A982	P920	S857	D795	Y732	M604	M604	S541		L408	H346	N283
	E1251	A1175	A1111	F1046	L983	D921	H858	P796	F733	R605	R605	N542	S476	L409	A347	N284
M1315	V1251	T1176	N1112	F1046	E984	Y922	I859	S797	T734	N606	L606	N543	S477	R410	L348	N284
A1316	R1252	E1176	K1113	L1047	R985	Y923	R860	T798	T735	F607	F607	V544	I478	C411	N349	L286
V1317	R1253	V1177	R1114		R866	D924	E861	T799	T736	K674	P608	F545		L412	I350	L287
E1318	P1254	M1178	N1115	L1050	A987	V925	R862	L900	F737	A675	P609	V546	R484	M413	D351	T288
R1319		T1179	R1116	Q1051	Q988	V926	L863	S801	E738	T676		E547	E485	L414	H352	T289
	A1257	P1180	V1117	L1052	T989	S927	H864	Q802	G739	R677	F612	Y548	V486	A415	F353	T290
V1320	V1258	S1181	T1118	R1053	T990	R928	I865	S803	S740	C679	R614	Q549	S487	A416	A354	N291
N1321	A1259	E1182	Y1119	R1054	D991	F929	T866	L804	Y741	C679	R614	Q549	M488	A417	N292	N292
P1322	P1260	G1183	T1120	L1055	V992	A930	M867	S805	K742	T680	T615	F551	M489	N418		V293
	S1261	Y1184	H1121	S1056	D993	N931	V868	V806	F743	R681	D616	V552	F490	Y419	V357	V293
R1326	T1262	T1185	P1122	V1057	S994	A932	P869	A907	T744	Q882	D617		M491	P420		V294
A1327	Y1263	Q1186	P1123	G1058	T995	N933	D870	Q808	I745	L684	L618	A556	V492	R421	N361	G295
I1328	E1264	H1187	T1124	L1059	D996	L934	P871	V909	E746	L684	A619	A556	H493	L422	L362	V296
M1329	M1265	V1188	G1125	R1060	Y997	Q935	I872	L810	Q747	R685	I620	T557	E494	L422	R363	P298
N1330	D1266		M1126	L1061	G998	M936	V873	S811	Q748	H686	A621	V558	L495	L426	A364	A299
R1331	T1267	S1192		I1062	K999	M937	I874	K812	G749	L687	A622	T559	K486	V427	L365	L300
N1332	G1268	I1193	P1129	T1063	L1000	N938	T875	L813	E750	E888	M623	I560	K497	Q428	M366	L301
A1333	T1269	M1194	S1130	N1064	T1001	N939	G876	T814	T751	Q690	F624	N561	I498	L422	E367	R302
	L1270		P1131	P1065	L1002	R940	A877	P815	V752	F691	P625	A562	A499	T431	A368	D303
	S1271	G1199	T1132	R1066	R1003	Y941	Q882	P816	T756	T694	R626	A563	E500	G432	N369	F304
R1272	L1201	K1200	G1133	I1067	F1004	H942	I883	D817	I757	A695	A627	Q564	S601	Y433	V370	T305
N1273	F1202	L201	P1134	A1068	L1005	E943	I883	A818			S628	E565	F502	V433	T371	Q306
G1274			H1136	R1069		S944	A884	F819	T758	A695	R629	E566	F503	A435	A372	Q307
	D1275		T1009	F1070	L1008	V945	A885	R819	D759	V696	M630	E567	D504	S436	D373	N308
L1276	Q1205	Q1205	T1009	F1071	T1009	L946	A885	I820	T759	A697	P631	F568	P505	A437	D374	W309
Y1277	L1276	L1276	R1010	E947	R1010	S886	V887	M822	T762	H698	Q632	S569	S506	N438	R375	L310
Y1278	M1207	M1207	G1073	Q888	S1011	I948	V887	I823	V763	T699	T633		S507	V439	I376	X311
S1279	D1208	D1208	L1012	Y1074	L1012	A949	A889	I823	W764	D700	Y634	N572	I508	I440	K377	R312
P1280	P1280	P1280	K1013	R1075	L1013	H909	T890	G826	P765	H701	P635	E573	V509	R441	A378	R312
Y1281	L1210	G1210	M1014	T1076	M1014	I951	H891	G827	T766	L702	P636	K574	V511	P442	L379	L313
A1282	L1211	L1211	R1144	M1077	Q1015	F952	V892	D828	L767	S703	Y637	N575		Y443	Q380	T315

● Molecule 3: Viral structural protein 5



● Molecule 3: Viral structural protein 5



VAL
SER
GLU
LEU
THR
ILE
ASP
THR
GLN
SER
ASP
SER
VAL
LEU

4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images used	28993	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	Kodak SO 163 film	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 2	RMSZ	# Z > 2
1	A	0.68	9/8619 (0.1%)	1.04	42/11737 (0.4%)
2	B	0.77	16/9590 (0.2%)	1.08	49/13056 (0.4%)
2	C	0.69	7/10045 (0.1%)	1.07	42/13678 (0.3%)
3	D	0.63	0/2314	1.03	17/3147 (0.5%)
3	E	0.65	0/2314	0.98	12/3147 (0.4%)
All	All	0.71	32/32882 (0.1%)	1.06	162/44765 (0.4%)

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	ALA	CA-CB	11.75	1.77	1.52
2	B	1098	ALA	CA-CB	8.29	1.69	1.52
2	C	114	VAL	CA-CB	8.29	1.72	1.54
2	C	1320	VAL	CA-CB	7.62	1.70	1.54
1	A	232	ALA	CA-CB	-7.29	1.37	1.52

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	550	ILE	CB-CA-C	-9.49	92.62	111.60
2	C	1059	LEU	CA-CB-CG	9.28	136.65	115.30
2	C	1316	ALA	CB-CA-C	8.39	122.68	110.10
1	A	971	LEU	CA-CB-CG	-8.22	96.39	115.30
2	B	863	LEU	CA-CB-CG	-8.15	96.55	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8434	0	8395	1501	0
2	B	9397	0	9313	1584	0
2	C	9844	0	9749	1701	0
3	D	2267	0	2260	343	0
3	E	2267	0	2260	348	0
All	All	32209	0	31977	5388	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 86.

The worst 5 of 5388 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:C:1242:MET:HE1	2:C:1260:PRO:CD	1.25	1.60
2:C:615:THR:CG2	2:C:632:GLN:HB3	1.26	1.60
3:D:26:ALA:CB	3:D:30:GLN:HE21	1.13	1.60
2:C:832:MET:CE	2:C:946:LEU:HD12	1.34	1.56
2:B:202:ALA:CA	2:B:202:ALA:CB	1.77	1.56

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	1055/1058 (100%)	659 (62%)	233 (22%)	163 (16%)	0	0
2	B	1187/1333 (89%)	800 (67%)	183 (15%)	204 (17%)	0	0
2	C	1245/1333 (93%)	861 (69%)	207 (17%)	177 (14%)	0	1
3	D	288/448 (64%)	203 (70%)	46 (16%)	39 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	288/448 (64%)	191 (66%)	55 (19%)	42 (15%)	0	1
All	All	4063/4620 (88%)	2714 (67%)	724 (18%)	625 (15%)	1	0

5 of 625 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	63	SER
1	A	123	SER
1	A	135	VAL
1	A	202	SER

5.3.2 Protein sidechains [i](#)

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	942/943 (100%)	786 (83%)	156 (17%)	2	11
2	B	1038/1153 (90%)	891 (86%)	147 (14%)	4	17
2	C	1088/1153 (94%)	928 (85%)	160 (15%)	3	16
3	D	238/379 (63%)	204 (86%)	34 (14%)	4	17
3	E	238/379 (63%)	203 (85%)	35 (15%)	3	16
All	All	3544/4007 (88%)	3012 (85%)	532 (15%)	7	15

5 of 532 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	773	PRO
2	B	1290	LYS
3	D	271	TYR
2	B	922	TYR
2	B	1112	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	711	ASN
2	B	978	GLN
3	D	25	ASN
2	B	719	ASN
2	B	854	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.