



wwPDB EM Map/Model Validation Report

Apr 10, 2016 – 01:46 PM BST

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 EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

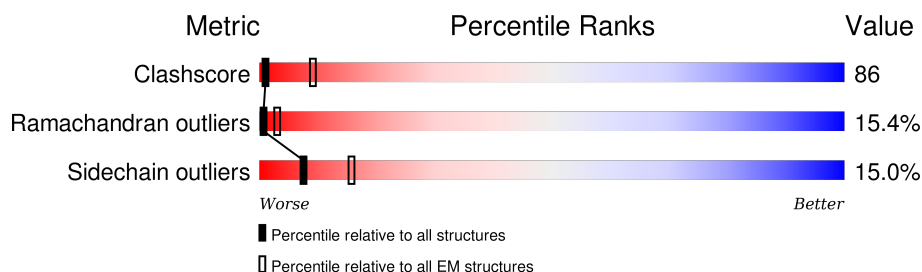
1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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		

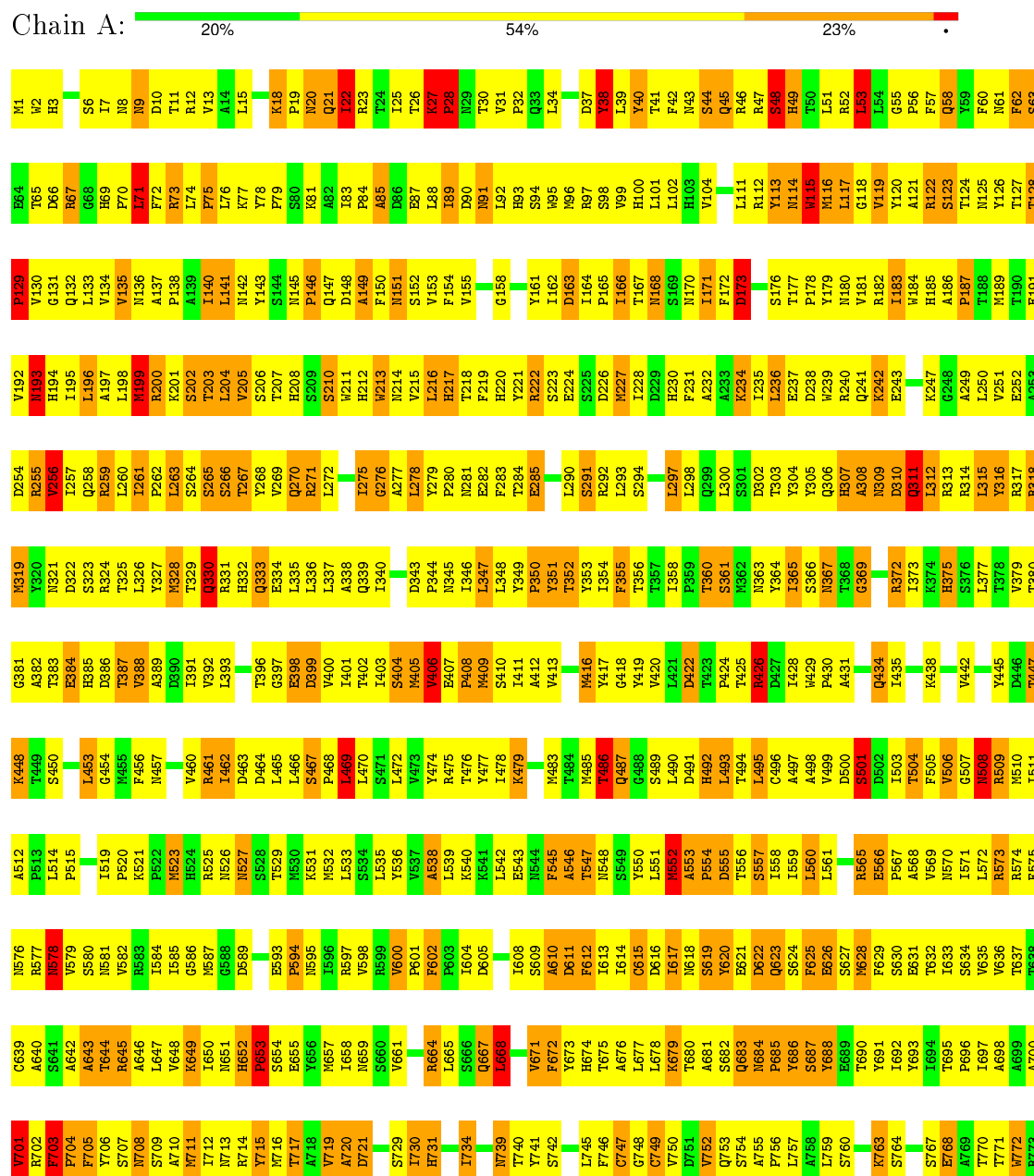
There are 2 discrepancies between the modelled and reference sequences:

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 errors 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



V774	K338	V899	V963	E1023	ARG	ARG	PHE	D186	V248	W309	V370	T431	L495	N561	N623
D775	K339	Q900	E964	L1024	HIS	GLN	ASN	D187	S249	L310	T371	G432	K496	A562	F624
N779	M340	S901	A965	I1025	THR	THR	GLU	R188	G250	N311	A372	G433	K497	A563	P625
L780	M341	F903	G966	C1028	ASN	GLY	PHE	I189	L251	D312	D373	G434	L498	E565	P626
V781	Y342	F904	Y967	S1029	THR	THR	ALA	G190	L252	D313	D374	A435	A499	F566	G628
V782	A843	Q905	T969	H1030	ASN	LEU	ASN	V194	V254	T314	L376	A436	E500	F567	S628
V783	L844	F906	A970	G1031	SER	GLY	GLU	V195	L255	T315	K377	A437	S503	F568	R629
V784	L845	D907	L971	Y1032	ASN	SER	ALA	N196	F256	M317	A378	M438	E503	R571	N630
A785	R346	A908	D972	R1033	THR	GLY	LEU	L196	D257	L318	L379	I440	D504	N572	Q632
V786	R347	A909	Q973	R1034	ARG	THR	HIS	F197	V258	Q319	Q380	R441	V504	E573	T633
V787	R348	N910	S974	L1035	ASN	ASN	PRO	K198	V259	Q320	A381	V442	V510	K574	Y634
V788	L849	N911	T975	G1036	ALA	ALA	THR	Y199	V260	A321	H382	V443	V511	M575	J635
V789	E853	D912	A976	S1037	GLU	LYS	THR	G200	N262	G322	S383	S444	L512	E576	P636
A790	N854	L913	H977	T1038	GLU	ILE	K136	A201	R263	Y325	S384	E445	E513	Q577	T637
V791	N855	E914	K978	G1039	ALA	LYS	V136	A202	L264	Y326	L385	K446	F514	A578	T638
A793	M855	N915	T979	V203	THR	THR	I137	V204	V265	G326	S386	R447	L515	L579	N639
V794	T856	N916	N980	V1042	ALA	LYS	L141	N205	V267	G328	T387	Y448	L516	Q640	Q641
V795	Q857	S917	R981	L1043	SER	GLN	L142	N206	G268	L329	Q388	F449	F517	L581	R641
V796	V858	N918	V982	D1044	PRO	ALA	V143	L207	G269	T330	F390	F450	A518	S582	Q642
V797	V859	N919	E983	F1046	ARG	ASP	N144	N208	E269	E331	G391	E451	F521	E583	T643
V798	S860	F921	Q985	N1047	ASP	ASP	T145	N209	T270	E332	P392	N452	P522	F584	V644
V799	G862	N922	R986	H1048	SER	ALA	E146	R210	T271	R333	N393	E454	T523	P586	N645
S800	G863	A923	L987	Y1049	SER	ASP	V147	R211	T272	L334	Q394	E455	E524	A587	E647
N801	R864	V924	K988	S1050	ALA	VAL	Q148	F212	N274	D335	G395	N456	F525	L588	F648
S802	N865	N925	V989	V1051	ASN	GLU	P149	F213	S275	Y336	A396	Q457	N526	F589	A649
S803	L866	N926	A990	V1052	LYS	LYS	L150	D214	T276	V337	L397	S458	N527	S590	S650
A804	A867	N927	L992	L1053	GLY	PRO	T155	T215	L277	R338	R398	A459	L528	D591	R651
V805	D868	E928	Y992	K1054	ALA	ALA	F154	T216	L278	R339	P399	A460	K529	V592	F652
S806	I869	P929	V993	L1055	GLY	ASP	P156	G217	S279	V340	E400	L462	G530	P603	R653
S807	S870	N930	P994	V1056	THR	VAL	Q156	G218	T280	K341	L401	V463	D531	L594	T654
V808	V871	G931	V995	R1057	SER	THR	Q157	L219	V281	T342	A402	V464	L532	A595	T655
N809	P873	A932	T997	THR	GLY	PHE	I157	D220	N282	I343	F403	S464	Q533	G596	V656
V810	L874	P935	V998	L998	THR	THR	P160	L221	N283	V344	D404	A465	V536	A597	V657
V811	N875	N938	V999	L999	ILE	ARG	K161	T222	N284	G345	H407	V466	L537	N598	T658
V812	N876	N938	E1000	E1000	ALA	ALA	G162	K223	V285	H346	L403	K467	L538	T599	L659
P813	R877	Q939	A1001	D1002	THR	GLN	G163	G224	L286	A347	L403	A468	L539	I600	A660
S815	Y878	N940	D1002	ASP	VAL	VAL	V163	L225	R287	L348	L409	R469	F539	I601	N661
L816	V879	D941	V1003	ASP	GLY	GLY	L164	P226	T288	N349	R410	V470	F540	A602	V662
G817	V880	K942	T1004	ASP	VAL	VAL	T165	L227	T289	I350	C411	E472	S541	M603	V663
V818	I881	L943	L1005	GLY	THR	THR	V168	V228	H291	D351	L412	A473	R542	M604	N664
V819	D882	N944	M1006	ILE	ALA	ALA	K169	Q229	N292	R352	N413	S476	N543	R605	E665
V820	P883	A947	L1007	THR	THR	THR	Y170	D230	N293	F354	L414	S477	P544	L606	R666
R821	A884	T948	D1008	GLU	GLU	GLN	E171	L232	N294	A354	A415	S478	P545	P607	Q669
R822	T885	T948	D1009	GLN	ALA	ALA	D172	V233	V296	A355	A416	L478	V546	T608	D670
T823	R886	A949	A949	GLY	GLY	GLY	T173	P234	G296	S356	A417	R479	E547	P609	D671
R824	I887	N950	G1011	LYS	VAL	VAL	Q174	I235	N297	V357	N418	L480	Y548	Q610	Q677
R825	E888	L951	I1012	ARG	ARG	ARG	T175	T238	P298	L358	Y419	P420	G549	G611	T674
F826	T889	T952	T1013	ASN	ASN	ASN	K176	A239	A299	N359	P420	R484	F551	F612	L613
R827	L890	R953	H1014	GLU	GLU	GLU	K177	G238	L300	I360	R421	E485	F552	R614	L614
T828	T891	T954	E1015	VAL	THR	THR	D178	A240	L301	N361	L422	V486	V552	R615	T676
N829	Q892	N955	I1016	VAL	THR	THR	K179	G241	R302	L362	E423	S487	Q553	T616	R677
H830	E934	C956	I1017	GLN	ALA	ALA	K180	E242	R303	R363	G424	P488	R554	D616	S678
R831	K394	N957	R1018	SER	GLY	GLY	L181	Q243	F304	A364	T425	M489	G555	D617	C679
E832	K395	A958	P1019	ARG	ALA	ALA	H182	S244	T305	N366	T426	P490	A556	L618	T680
R833	N896	T959	S1020	THR	SER	THR	S183	E245	V307	E367	Q428	V492	T557	A619	K681
T834	I897	N959	ASP	THR	THR	THR	E184	E246	Q308	A368	L429	V493	T558	L620	Q682
F835	E398	F962	P1022	ARG	ARG	ARG	A185	Y247	N308	N369	N430	E494	T560	A622	L684

• Molecule 2: Capsid protein VP1

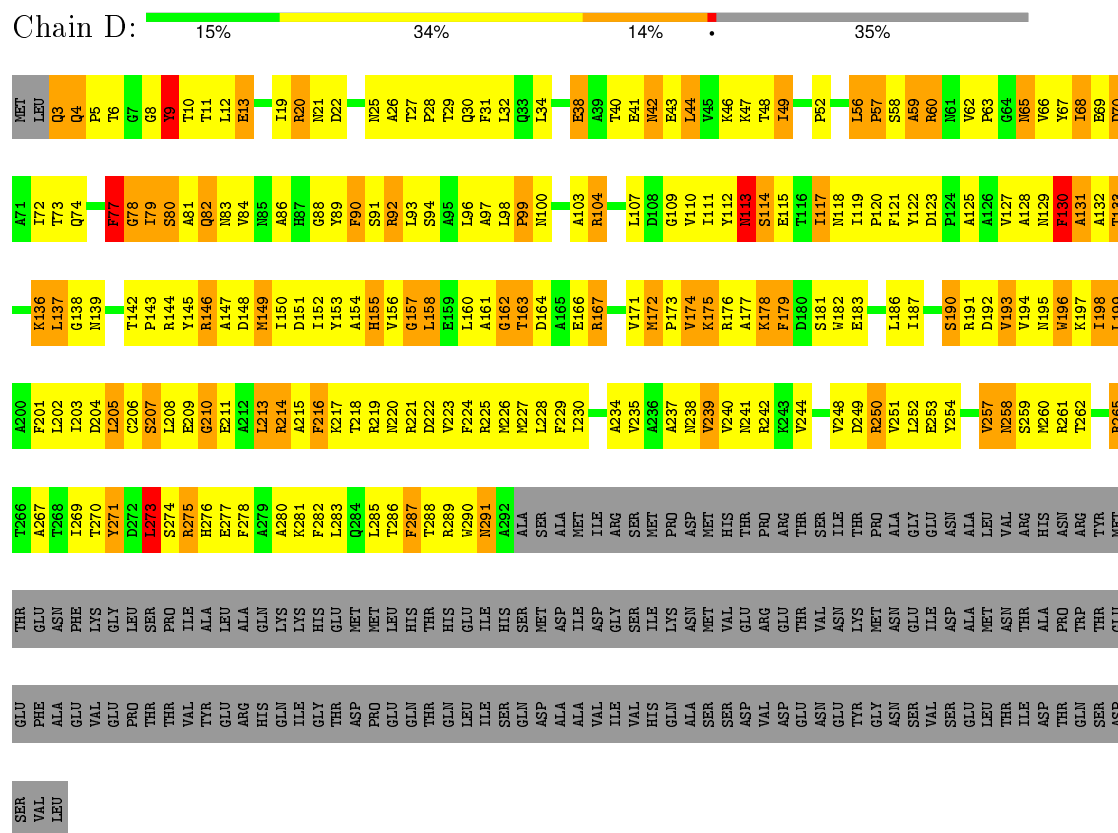
Chain B: 17% 49% 21% 11%

MET	ARG	PHE	D186	V248	W309	V370	T431	L495	N561	N623
HIS	GLN	ASN	D187	S249	L310	T371	G432	K496	A562	F624
SER	THR	GLU	R188	G250	N311	A372	G433	K497	A563	P625
THR	ASP	GLN	I189	L251	D312	D373	V434	L498	E565	R626
ASN	GLY	PHE	V190	L252	D313	D374	A435	A499	F566	A627
ASN	THR	ALA	G191	M253	L314	S375	S436	E500	E567	S628
ASN	GLY	ASN	V194	V254	T315	K376	A437	S501	F568	R629
SER	LEU	GLU	N195	L255	N316	K377	M438	F502	N630	P631
ASN	GLY	ALA	M195	F256	L317	A378	V439	E503	N572	Q632
LYS	SER	ALA	L196	K257	L318	L379	I440	D504	E573	T633
ARG	THR	HIS	F197	V258	Q319	Q380	R441	V504	K574	Y634
ASN	ASN	PRO	K198	M259	Q320	A381	V442	V510	E575	P636
ASN	THR	THR	Y199	V259	A321	H382	V443	V511	M575	J635
GLU	LYS	THR	G200	N262	G322	S383	S444	L512	E576	T637
LYS	ILE	K135	A201	R263	Y325	M384	E445	E513	Q577	T638
HIS	ALA	V136	M202	L264	Y326	L385	K446	F514	A578	N639
LYS	THR	I137	V203	V265	G326	S386	R447	L515	L579	Q640
LYS	ALA	L137	V204	L266	L327	T387	Y448	L516	V580	R641
GLN	SER	L141	N205	V267	G328	Q388	F449	F517	L581	E642
PRO	SER	D142	N206	G268	L329	F389	P450	A518	S582	Q643
GLU	ALA	V143	D207	E269	T330	E390	E451	F521	E583	T644
ILE	ARG	N144	L208	T270	E331	G391	N452	P522	F584	V644
ASP	GLN	T145	M209	T271	T332	P392	L463	E622	F585	T645
SER	ALA	E146	R210	T272	R333	N393	E454	T523	P586	N646
SER	ASP	V147	R211	T273	L334	Q394	E455	E524	A587	E647
ALA	VAL	Q148	F212	N274	D335	G395	N456	F525	L588	F648
ASN	GLU	P149	F213	S275	Y336	A396	Q457	N526	F589	A649
ASN	LYS	L150	D214	T276	V337	L397	S458	N527	S590	S650
GLY	PRO	T155	T215	T277	R338	R398	A459	L528	D591	R651
GLU	ALA	D153	A216	L278	L339	P399	A460	K529	V592	F652
GLY	ASP	F154	T217	S279	V340	E400	R461	G530	P603	R653
THR	VAL	K155	G218	T280	K341	L401	L462	D531	L594	T654
SER	THR	Q156	L219	V281	T342	A402	V463	L532	A595	P655
GLY	PHE	I157	D220	N282	V343	F403	S464	Q533	G596	V656
THR	THR	L157	L221	N283	V344	H404	A465	Q533	A597	A657
ARG	ILE	P160	T222	N284	G345	D404	V466	L536	N598	T658
ALA	GLU	K161	K223	V285	H346	H407	R467	L537	T599	L659
GLN	ASN	G162	G224	L286	A347	I408	A468	L538	I600	A660
THR	VAL	V163	L225	R287	L348	I409	R469	F539	N661	T601
VAL	ASP	L164	P226	T288	N349	R410	V470	F540	A602	V662
GLY	ASP	T165	L227	T289	I350	C411	E472	S541	M603	V663
ASP	THR	V168	V228	H291	D351	L412	A473	R542	R604	N664
THR	GLY	L168	Q229	N291	R352	N413	S476	N543	L605	E665
ALA	ALA	K169	D230	N292	F353	L414	S477	Y544	L606	R666
THR	THR	Y170	L231	N293	A354	A415	S477	P545	F607	T607
GLU	GLN	E171	L232	N294	A355	A416	L478	V546	T608	Q669
ALA	GLY	D172	V233	G295	S356	A417	R479	E547	P609	D670
GLY	GLY	Q173	P234	V296	V357	N418	L480	Y548	Q610	D671
VAL	LYS	F174	I235	N297	L358	Y419	P420	G549	G611	T674
ARG	PRO	T175	T238	P298	N359	R420	R484	F551	F612	K674
GLU	THR	K176	A239	A299	N360	R421	E485	F552	R613	A675
THR	THR	D177	G240	L300	I361	L422	V486	V552	R614	T676
GLU	VAL	K178	A241	R302	L362	E423	S487	Q553	T615	R677
LYS	VAL	K179	G241	R302	A363	T424	P488	R554	D616	S678
GLU	GLU	K180	E242	R303	A364	T425	M489	G555	D617	C679
ALA	GLN	L181	Q243	F304	L365	T426	P490	A556	L618	T680
GLY	SER	H182	S244	T305	N366	T427	P491	A557	A619	K681
ALA	ARG	A183	E245	V306	E367	Q428	V492	Y558	T620	Q682
SER	THR	R183	A246	V307	A368	Q429	R493	T559	E621	R683
THR	ASP	E184	E246	V307	A368	I429	E404	L560	A622	R684
ARG	VAL	L195	V247	V308	T260	N260	T260	T260	T260	T260

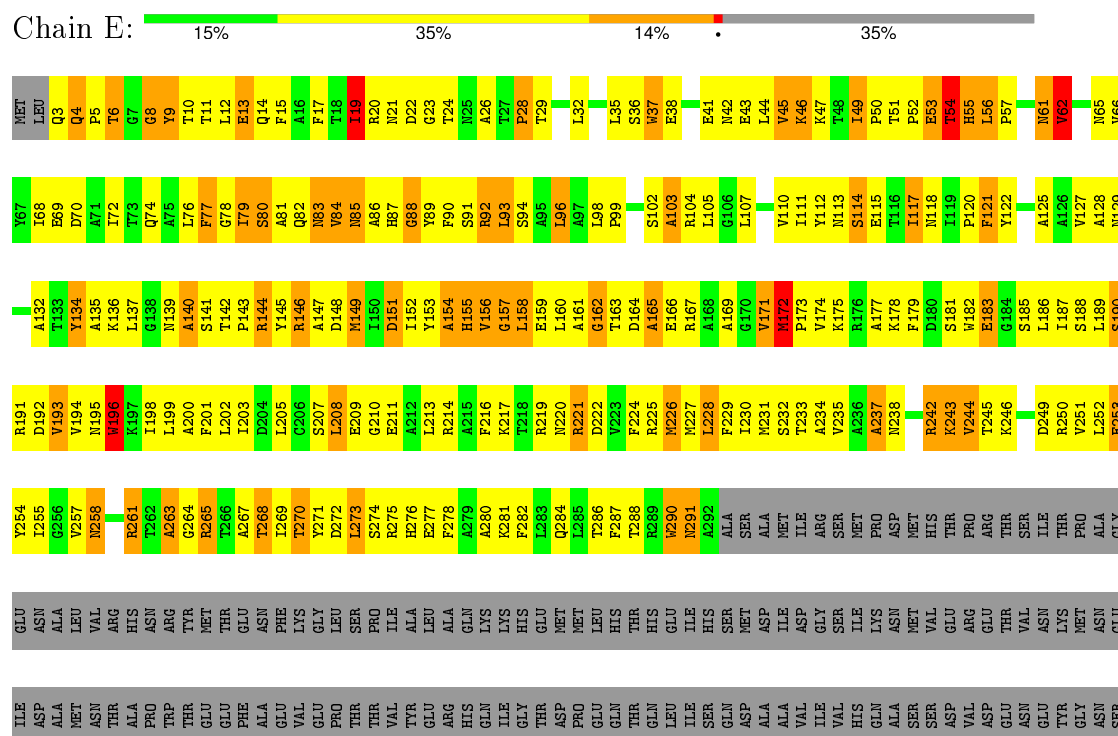





- Molecule 3: Viral structural protein 5



- 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	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 ⓘ

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	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 ⓘ

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:CB	2:B:202:ALA:CA	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%)	3	12
2	B	1038/1153 (90%)	891 (86%)	147 (14%)	4	18
2	C	1088/1153 (94%)	928 (85%)	160 (15%)	4	16
3	D	238/379 (63%)	204 (86%)	34 (14%)	4	17
3	E	238/379 (63%)	203 (85%)	35 (15%)	4	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.