



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:48 am GMT

PDB ID : 3ZX8
EMDB ID: : EMD-1863
Title : Cryo-EM reconstruction of native and expanded Turnip Crinkle virus
Authors : Bakker, S.E.; Robottom, J.; Hogle, J.M.; Maeda, A.; Pearson, A.R.; Stockley, P.G.; Ranson, N.A.; Harrison, S.C.
Deposited on : 2011-08-08
Resolution : 11.50 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

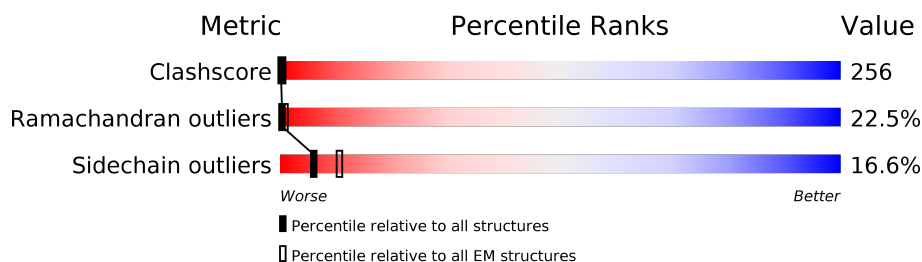
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.50 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	347	
1	B	347	
1	C	347	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6290 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 CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	267	Total	C	N	O	S	0	0
			2026	1280	344	397	5		
1	B	267	Total	C	N	O	S	0	0
			2026	1280	344	397	5		
1	C	295	Total	C	N	O	S	0	0
			2238	1410	386	437	5		

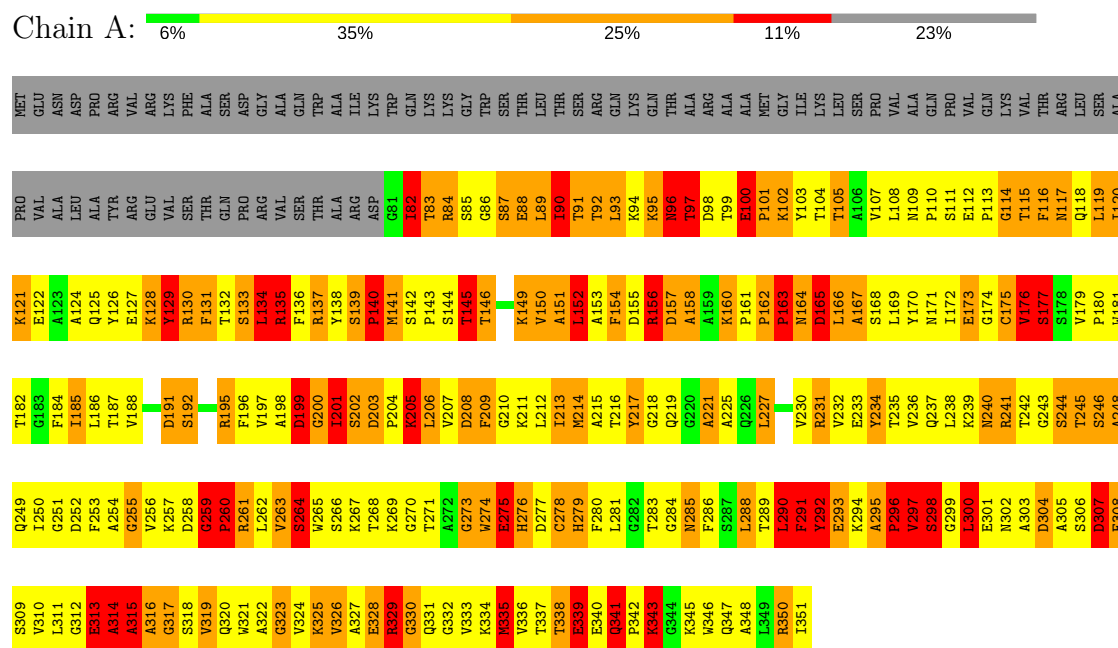
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	.	-	ASN	DELETION	UNP P06663
A	.	-	ASP	DELETION	UNP P06663
A	.	-	ALA	DELETION	UNP P06663
A	.	-	ASP	DELETION	UNP P06663
A	346	TRP	LEU	VARIANT	UNP P06663
B	.	-	ASN	DELETION	UNP P06663
B	.	-	ASP	DELETION	UNP P06663
B	.	-	ALA	DELETION	UNP P06663
B	.	-	ASP	DELETION	UNP P06663
B	346	TRP	LEU	VARIANT	UNP P06663
C	.	-	ASN	DELETION	UNP P06663
C	.	-	ASP	DELETION	UNP P06663
C	.	-	ALA	DELETION	UNP P06663
C	.	-	ASP	DELETION	UNP P06663
C	346	TRP	LEU	VARIANT	UNP P06663

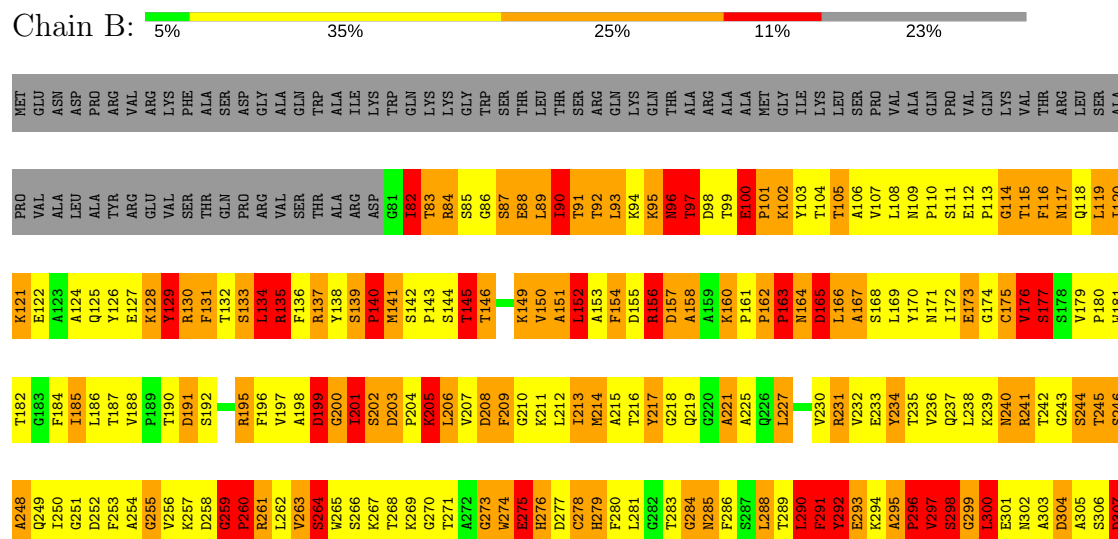
3 Residue-property plots

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: CAPSID PROTEIN



• Molecule 1: CAPSID PROTEIN



F308	S309	V310	L311	G312	E313	A314	A315	A316	G317	S318	V319	Q320	W321	A322	G323	V324	K325	V326	A327	E328	G329	G330	Q331	G332	V333	K334	K335	V336	T337	T338	E339	E340	Q341	P342	K343	G344	K345	W346	Q347	A348	L349	R350	I351
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● Molecule 1: CAPSID PROTEIN



MET	GLU	ASN	ASP	PRO	ARG	VAL	ARG	LYS	PHE	ALA	SER	ASP	GLY	ALA	GLN	TRP	ALA	ILE	LYS	TRP	THR	LEU	THR	SER	ARG	GLN	LYS	THR	ALA	ARG	ALA	ALA	MET	GLY	ILE	LYS	LEU	SER	PRO	VAL	ALA	GLN	PRO	VAL	Q53	K54	V55	T56	R57	L58	S59	A60
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P61	V62	A63	L64	A65	Y66	R67	E68	V69	S70	T71	Q72	P73	R74	V75	S76	T77	A78	R79	D80	G81	I82	T83	R84	S85	G86	S87	E88	L89	I90	T91	T92	L93	K94	K95	N96	T97	D98	T99	E100	P101	K102	Y103	T104	T105	A106	V107	L108	N109	P110	S111	E112	P113	G114	T115	F116	N117	Q118	L119	I120
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K121	E122	A123	A124	Q125	Y126	E127	K128	Y129	R130	F131	T132	S133	L134	R135	F136	R137	Y138	S139	P140	M141	S142	P143	S144	T145	T146	K149	V150	A151	L152	A153	D154	D155	R156	D157	A158	A159	K160	P161	P162	P163	N164	D165	L166	A167	S168	Y169	Y170	M171	I172	E173	G174	C175	Y176	S177	S178	V179	P180	W181
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T182	G183	F184	I185	L186	T187	V188	D191	S192	R195	F196	V197	A198	D199	G200	L201	S202	D203	P204	K205	L206	T207	D208	F209	G210	K211	L212	T213	M214	A215	L216	Y217	G218	Q219	G220	A221	A225	Q226	L227	V230	R231	V232	E233	Y234	T235	V236	Q237	L238	K239	N240	R241	T242	G243	S244	T245	S246	A248
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Q249	I250	G251	D252	F253	A254	G255	V256	K257	D258	G259	P260	R261	L262	V263	S264	W265	S266	K267	T268	K269	G270	T271	A272	G273	W274	E275	H276	D277	C278	H279	F280	L281	G282	G284	N285	F286	S287	L288	T289	L290	F291	Y292	E293	K294	A295	P296	Y297	S298	G299	L300	E301	N302	A303	D304	A305	S306	D307	F308
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S309	V310	L311	G312	E313	A314	A315	A316	G317	S318	V319	Q320	W321	A322	G323	K325	V326	A327	E328	G329	G330	Q331	G332	V333	K334	K335	V336	T337	T338	E339	E340	Q341	P342	K343	G344	K345	W346	Q347	A348	L349	R350	I351
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE-FLIPPING EACH PARTICLE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	52911	Depositor
Image detector	KODAK SO163 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	2.49	42/2070 (2.0%)	2.48	130/2806 (4.6%)
1	B	2.49	42/2070 (2.0%)	2.48	130/2806 (4.6%)
1	C	2.51	56/2285 (2.5%)	2.46	145/3099 (4.7%)
All	All	2.50	140/6425 (2.2%)	2.47	405/8711 (4.6%)

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	A	0	8
1	B	0	8
1	C	0	10
All	All	0	26

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	ILE	C-N	-42.35	0.36	1.34
1	B	201	ILE	C-N	-42.34	0.36	1.34
1	C	201	ILE	C-N	-42.34	0.36	1.34
1	B	93	LEU	N-CA	-41.12	0.64	1.46
1	C	93	LEU	N-CA	-41.10	0.64	1.46

The worst 5 of 405 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ILE	O-C-N	-59.09	28.16	122.70
1	A	201	ILE	O-C-N	-59.06	28.20	122.70
1	C	201	ILE	O-C-N	-59.04	28.24	122.70
1	A	82	ILE	O-C-N	-16.84	95.76	122.70
1	C	82	ILE	O-C-N	-16.83	95.77	122.70

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLU	Mainchain
1	A	177	SER	Mainchain
1	A	201	ILE	Mainchain
1	A	260	PRO	Mainchain
1	A	92	THR	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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2026	0	1961	1032	0
1	B	2026	0	1962	1050	0
1	C	2238	0	2183	1152	0
All	All	6290	0	6106	3179	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 256.

The worst 5 of 3179 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:C:138:TYR:CB	1:C:184:PHE:CE1	1.75	1.66
1:B:101:PRO:CD	1:B:166:LEU:CD1	1.75	1.65
1:A:138:TYR:CB	1:A:184:PHE:CE1	1.75	1.65
1:A:114:GLY:HA2	1:A:283:THR:CG2	1.25	1.64
1:A:138:TYR:HB2	1:A:184:PHE:CZ	1.15	1.63

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	A	263/347 (76%)	144 (55%)	60 (23%)	59 (22%)	0	2
1	B	263/347 (76%)	144 (55%)	60 (23%)	59 (22%)	0	2
1	C	291/347 (84%)	161 (55%)	64 (22%)	66 (23%)	0	2
All	All	817/1041 (78%)	449 (55%)	184 (22%)	184 (22%)	0	2

5 of 184 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	87	SER
1	A	90	ILE
1	A	95	LYS
1	A	96	ASN

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	215/282 (76%)	178 (83%)	37 (17%)	2	14
1	B	215/282 (76%)	179 (83%)	36 (17%)	2	16
1	C	238/282 (84%)	200 (84%)	38 (16%)	3	18
All	All	668/846 (79%)	557 (83%)	111 (17%)	6	16

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	152	LEU
1	B	217	TYR
1	C	264	SER
1	B	154	PHE
1	B	192	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	GLN
1	B	237	GLN
1	C	249	GLN
1	B	164	ASN
1	B	171	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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.