



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5FMO / pdb\_00005fmo  
Title : Crystal structure and proteomics analysis of empty virus like particles of Cowpea mosaic virus  
Authors : Huynh, N.; Hesketh, E.L.; Saxena, P.; Meshcheriakova, Y.; Ku, Y.C.; Hoang, L.; Johnson, J.E.; Ranson, N.A.; Lomonossoff, G.P.; Reddy, V.S.  
Deposited on : 2015-11-07  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : **FAILED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

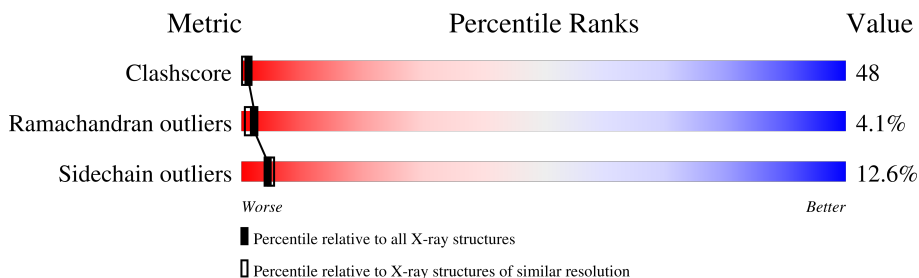
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	L	374	 35% 53% 10% ..
2	S	213	 32% 47% 11% • 9%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4440 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 EMPTY VIRUS LIKE PARTICLES OF COWPEA MOSAIC VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	370	2866	1822	481	541	22	0	0	1

- Molecule 2 is a protein called EMPTY VIRUS LIKE PARTICLES OF COWPEA MOSAIC VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S	194	1516	971	256	280	9	0	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	45	Total	O	0	0
			45	45		
3	S	13	Total	O	0	0
			13	13		



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	655.97Å 655.97Å 571.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	58.3 (10.00-2.30)	Depositor
$R_{merge}$	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.29Å)	Xtrriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.359 , 0.362	Depositor
Wilson B-factor (Å <sup>2</sup> )	7.7	Xtrriage
Anisotropy	0.283	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.32$ , $\langle L^2 \rangle = 0.15$	Xtrriage
Estimated twinning fraction	0.105 for -k,-h,-l	Xtrriage
Total number of atoms	4440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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  >5	RMSZ	# Z  >5
1	L	0.56	0/2933	1.04	18/3985 (0.5%)
2	S	0.65	1/1564 (0.1%)	1.19	16/2143 (0.7%)
All	All	0.59	1/4497 (0.0%)	1.10	34/6128 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	562	PRO	N-CA	-6.54	1.39	1.47

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	384	VAL	CB-CA-C	-15.39	91.82	110.91
2	S	561	PRO	CB-CA-C	-9.72	99.06	110.92
1	L	361	PRO	CB-CA-C	-8.82	99.24	112.11
2	S	383	ASP	CA-C-N	7.91	132.57	122.37
2	S	383	ASP	C-N-CA	7.91	132.57	122.37

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	L	2866	0	2813	287	0
2	S	1516	0	1456	147	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	45	0	0	22	0
3	S	13	0	0	7	0
All	All	4440	0	4269	417	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 48.

The worst 5 of 417 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:L:22:ASP:O	1:L:58:ALA:HB2	1.60	1.01
1:L:113:MET:HE3	1:L:125:PHE:HD1	1.27	0.96
1:L:113:MET:HE3	1:L:125:PHE:CD1	2.02	0.94
2:S:466:VAL:CG2	2:S:482:PHE:HB2	2.03	0.89
1:L:96:VAL:HG12	2:S:550:LEU:HB2	1.55	0.87

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 X-ray entries followed by that with respect to entries of similar resolution.

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	L	368/374 (98%)	301 (82%)	54 (15%)	13 (4%)	3	1
2	S	192/213 (90%)	164 (85%)	18 (9%)	10 (5%)	1	1
All	All	560/587 (95%)	465 (83%)	72 (13%)	23 (4%)	2	1

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	39	GLY
1	L	54	GLN

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Mol	Chain	Res	Type
2	S	458	ALA
2	S	567	ARG
1	L	217	ILE

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	L	318/320 (99%)	274 (86%)	44 (14%)	3	4
2	S	167/183 (91%)	150 (90%)	17 (10%)	7	8
All	All	485/503 (96%)	424 (87%)	61 (13%)	4	5

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	228	LEU
2	S	497	ASP
1	L	263	THR
2	S	492	LEU
2	S	558	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	343	ASN
2	S	473	ASN
2	S	470	GLN
2	S	486	GLN
1	L	128	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 oligosaccharides 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.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.