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wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID	:	1QJZ
Title	:	Three Dimensional Structure of Physalis Mottle Virus : Implications for the Viral Assembly
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Deposited on	:	1999-07-07
Resolution	:	3.80 Å(reported)

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 3.80 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	Percentile Ranks	Value
Clashscore		39
Ramachandran outliers		7.8%
Sidechain outliers		14.6%
RSRZ outliers		1.6%

Worse ··· *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
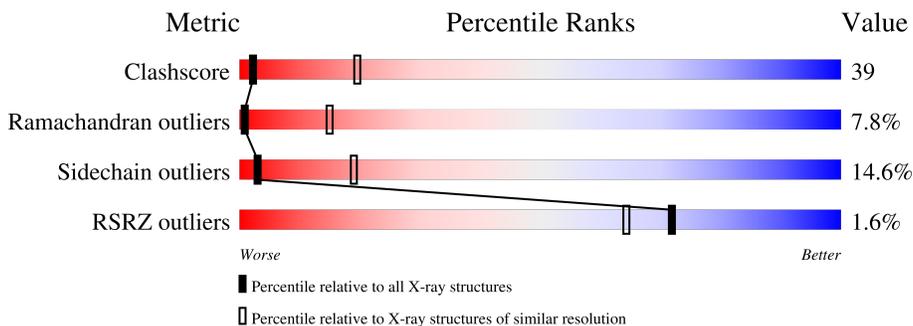
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	188	3% 30% 49% 16% • 5%
1	B	188	2% 40% 50% 9% •
1	C	188	% 34% 57% 7% •

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 4038 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 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1283	819	211	250	3			
1	B	188	Total	C	N	O	S	0	0	0
			1375	872	232	267	4			
1	C	188	Total	C	N	O	S	0	0	0
			1380	876	230	270	4			

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: COAT PROTEIN

Chain A:

- Molecule 1: COAT PROTEIN

Chain B:

- Molecule 1: COAT PROTEIN

Chain C:

N139 R140 M141 L142 K143 V146 T147 Y148 T149 D150 T151 P152 K153 L154 L155 A156 Y157 S158 R159 A160 P161 T162 N163 P164 S165 K166 I167 P168 T169 A170 S171 I172 Q173 I174 S175 G176 R177 S181 L185 N188

4　Data and refinement statistics　ⓘ

Property	Value	Source
Space group	R 3	Depositor
Cell constants a, b, c, α, β, γ	294.65Å　　294.65Å　　294.65Å 59.91°　　59.91°　　59.91°	Depositor
Resolution (Å)	10.00　–　3.80 49.07　–　3.79	Depositor EDS
% Data completeness (in resolution range)	40.0 (10.00-3.80) 58.9 (49.07-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.326　,　(Not available) 0.348　,　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , -65.5	EDS
L-test for twinning[1]	$< |L| > =$ (Not available), $< L^2 > =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.36	EDS
Total number of atoms	4038	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

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[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.24	0/1311	0.41	0/1807
1	B	0.56	0/1403	0.83	0/1926
1	C	0.55	0/1409	0.84	1/1936 (0.1%)
All	All	0.48	0/4123	0.73	1/5669 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	14	ILE	N-CA-C	-5.14	97.11	111.00

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	1283	0	1281	99	0
1	B	1375	0	1390	111	0
1	C	1380	0	1395	128	0
All	All	4038	0	4066	318	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 39.

The worst 5 of 318 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLN:HB2	1:B:151:THR:HG21	1.25	1.13
1:B:71:GLN:HB3	1:B:141:MET:SD	2.07	0.95
1:C:139:ASN:OD1	1:C:150:ASP:HB2	1.74	0.88
1:B:184:MET:HB3	1:B:186:ILE:HD11	1.59	0.82
1:C:32:ILE:HG22	1:C:34:LEU:HG	1.62	0.81

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 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	A	177/188 (94%)	118 (67%)	39 (22%)	20 (11%)	0	7
1	B	186/188 (99%)	144 (77%)	30 (16%)	12 (6%)	1	19
1	C	186/188 (99%)	140 (75%)	35 (19%)	11 (6%)	1	21
All	All	549/564 (97%)	402 (73%)	104 (19%)	43 (8%)	1	15

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ILE
1	A	186	ILE
1	B	24	PRO
1	B	108	ILE
1	B	112	TYR

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 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	A	137/159 (86%)	110 (80%)	27 (20%)	1	9
1	B	150/159 (94%)	133 (89%)	17 (11%)	6	28
1	C	152/159 (96%)	132 (87%)	20 (13%)	4	22
All	All	439/477 (92%)	375 (85%)	64 (15%)	3	19

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	136	ASP
1	C	147	THR
1	A	175	SER
1	A	165	SER
1	C	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	88	ASN
1	C	23	GLN
1	C	115	GLN
1	C	25	ASN
1	B	28	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	179/188 (95%)	0.71	5 (2%)	53	43	20, 20, 20, 20	0
1	B	188/188 (100%)	0.66	3 (1%)	72	64	20, 20, 20, 20	0
1	C	188/188 (100%)	0.59	1 (0%)	91	87	20, 20, 20, 20	0
All	All	555/564 (98%)	0.66	9 (1%)	72	64	20, 20, 20, 20	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	THR	2.7
1	A	150	ASP	2.5
1	A	149	THR	2.4
1	A	136	ASP	2.3
1	A	90	LEU	2.2

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.