wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1F15
Title	:	CUCUMBER MOSAIC VIRUS (STRAIN FNY)
Authors	:	Smith, T.J.; Chase, E.; Schmidt, T.; Perry, K.
Deposited on	:	2000-05-18
Resolution	:	3.20 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

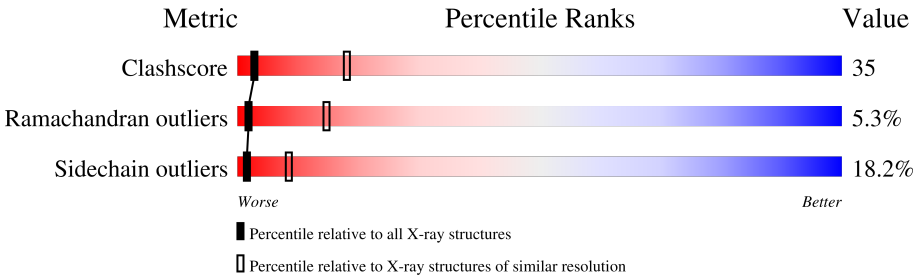
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	218	30% 30% 10% • 28%
1	B	218	32% 40% 14% • 13%
1	C	218	35% 43% 8% • 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4200 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	157	Total	C	N	O	S	0	0	0
			1229	784	209	232	4			
1	B	190	Total	C	N	O	S	0	0	0
			1483	942	259	278	4			
1	C	191	Total	C	N	O	S	0	0	0
			1488	945	260	279	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	LEU	ILE	conflict	UNP P69466
B	107	LEU	ILE	conflict	UNP P69466
C	107	LEU	ILE	conflict	UNP P69466

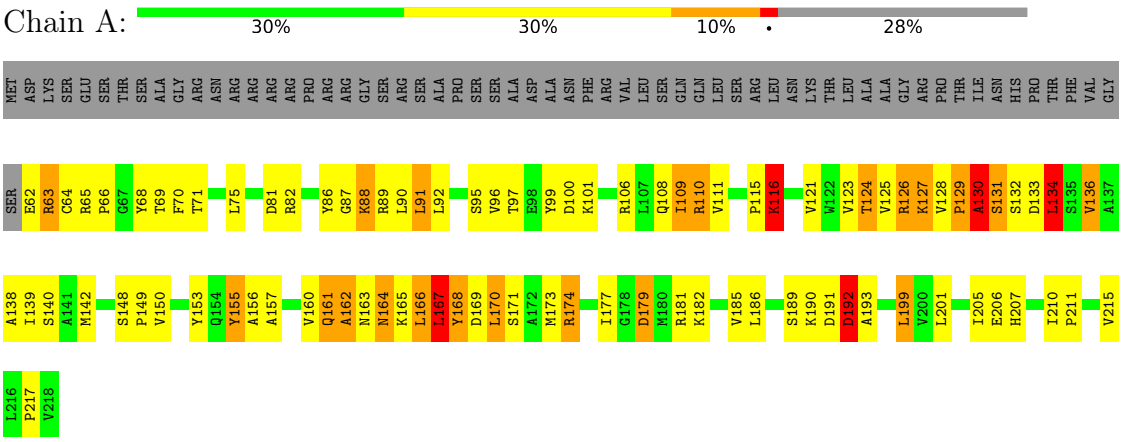
3 Residue-property plots (i)

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. 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.

Note EDS was not executed.

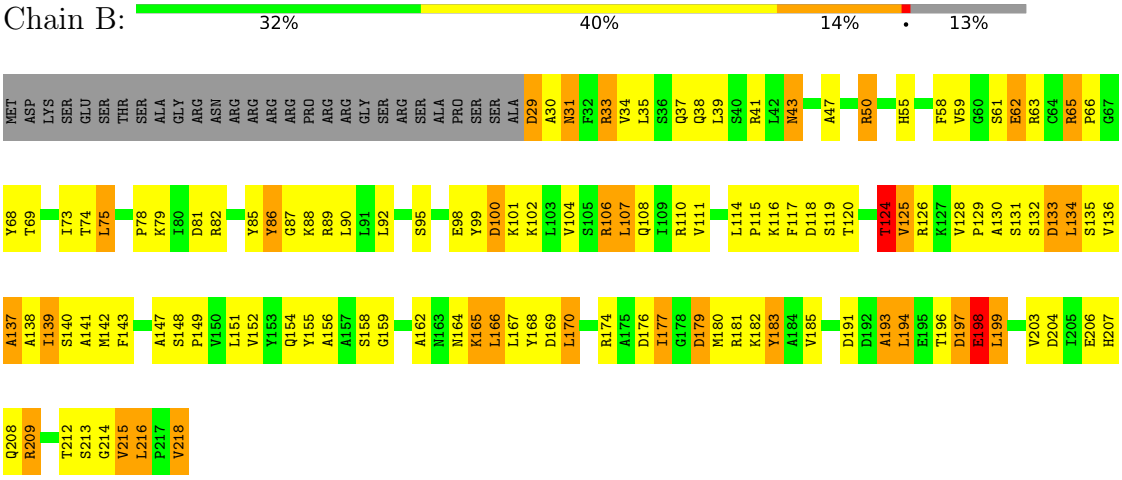
• Molecule 1: COAT PROTEIN

Chain A:



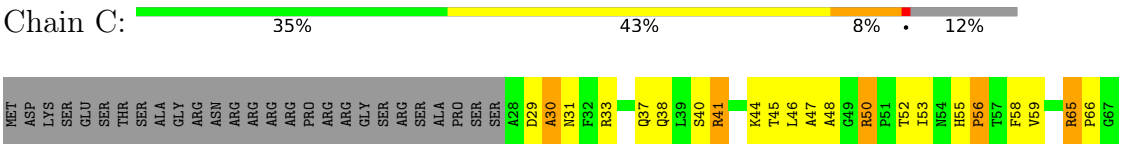
• Molecule 1: COAT PROTEIN

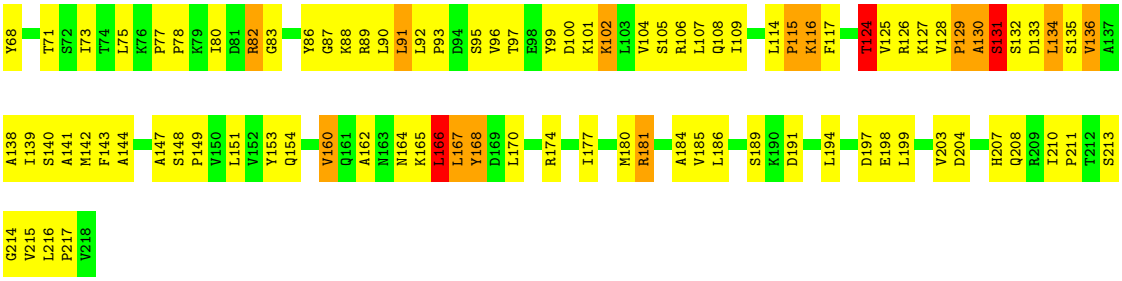
Chain B:



• Molecule 1: COAT PROTEIN

Chain C:




Y68
T71
S72
I73
T74
L75
K76
P77
P78
K79
I80
D81
R82
G83
Y86
G87
K88
R89
L90
L91
L92
P93
D94
S95
V96
T97
E98
Y99
D100
K101
K102
L103
V104
S105
R106
L107
Q108
I109
L114
P115
K116
F117
T124
V125
R126
K127
V128
P129
A130
S131
S132
D133
L134
S135
V136
A137
A138
I139
S140
A141
M142
F143
A144
A147
S148
P149
V150
L151
V152
Y153
Q154
V160
Q161
A162
N163
N164
K165
L166
L167
Y168
D169
L170
R174
I177
M180
R181
A184
V185
L186
S189
K190
D191
L194
D197
E198
L199
V203
D204
H207
Q208
R209
I210
P211
T212
S213
G214
V215
L216
P217
V218

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α, β, γ	336.00Å 336.00Å 336.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.246 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4200	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

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	0.92	1/1254 (0.1%)	1.15	9/1704 (0.5%)
1	B	0.81	1/1513 (0.1%)	1.12	3/2056 (0.1%)
1	C	0.75	0/1518	1.09	2/2063 (0.1%)
All	All	0.83	2/4285 (0.0%)	1.11	14/5823 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	ALA	CA-CB	7.97	1.69	1.52
1	B	198	GLU	CG-CD	5.01	1.59	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	198	GLU	N-CA-C	-9.71	84.78	111.00
1	C	166	LEU	CA-CB-CG	7.28	132.05	115.30
1	A	167	LEU	C-N-CA	7.04	139.29	121.70
1	B	193	ALA	N-CA-C	-6.47	93.52	111.00
1	A	130	ALA	N-CA-C	-6.30	94.00	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	1229	0	1254	90	0
1	B	1483	0	1513	124	0
1	C	1488	0	1518	109	0
All	All	4200	0	4285	301	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 35.

The worst 5 of 301 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:A:130:ALA:HB3	1:A:133:ASP:HB3	1.23	1.10
1:A:64:CYS:SG	1:B:214:GLY:HA2	1.98	1.03
1:B:134:LEU:HD23	1:B:135:SER:H	1.31	0.96
1:A:69:THR:HG21	1:B:212:THR:HB	1.47	0.96
1:C:134:LEU:CD2	1:C:136:VAL:HG22	2.02	0.90

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	A	155/218 (71%)	116 (75%)	27 (17%)	12 (8%)	1 6
1	B	188/218 (86%)	151 (80%)	29 (15%)	8 (4%)	2 20
1	C	189/218 (87%)	149 (79%)	32 (17%)	8 (4%)	3 20
All	All	532/654 (81%)	416 (78%)	88 (16%)	28 (5%)	2 15

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ALA

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Mol	Chain	Res	Type
1	A	162	ALA
1	B	133	ASP
1	B	193	ALA
1	C	30	ALA

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	A	137/188 (73%)	113 (82%)	24 (18%)	2 9
1	B	165/188 (88%)	127 (77%)	38 (23%)	1 3
1	C	165/188 (88%)	142 (86%)	23 (14%)	3 16
All	All	467/564 (83%)	382 (82%)	85 (18%)	1 8

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	204	ASP
1	C	115	PRO
1	B	215	VAL
1	C	65	ARG
1	C	131	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	GLN
1	B	55	HIS
1	C	55	HIS
1	C	31	ASN
1	C	54	ASN

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.