Full wwPDB Geometry-Only Validation Report (i)

Jun 12, 2024 – 05:41 PM EDT

PDB ID	:	1CGM
Title	:	STRUCTURE DETERMINATION OF CUCUMBER GREEN MOTTLE MOSAIC VIRUS BY X-RAY FIBER DIFFRACTION. SIGNIFICANCE FOR THE EVOLUTION OF TOBAMOVIRUSES
Authors	:	Wang, H.; Stubbs, G.
Deposited on	:	1993-11-17
Resolution	:	3.40 Å(reported)

This is a Full wwPDB Geometry-Only Validation 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 (1)) were used in the production of this report:

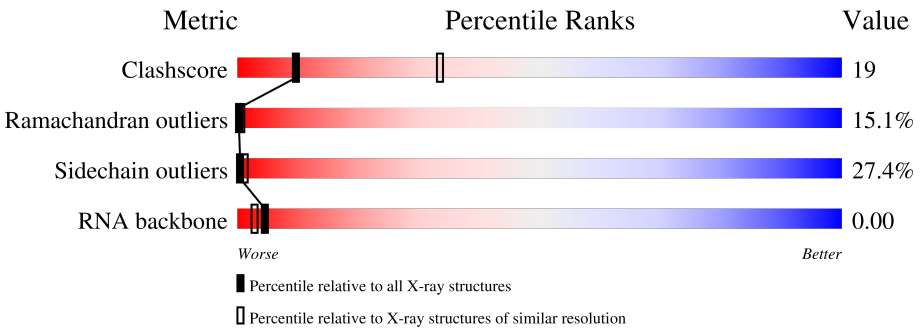
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
FIBER DIFFRACTION

The reported resolution of this entry is 3.40 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	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RNA backbone	3102	1006 (3.84-2.96)

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	I	3	33% 67%
2	E	161	38% 39% 18% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1296 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 RNA chain called RNA (5'-R(P*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	I	3	67	30	15	19	3	0	0	0

- Molecule 2 is a protein called CUCUMBER GREEN MOTTLE MOSAIC VIRUS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	161	1224	773	206	245	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	E	5	5	5	0	0

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.

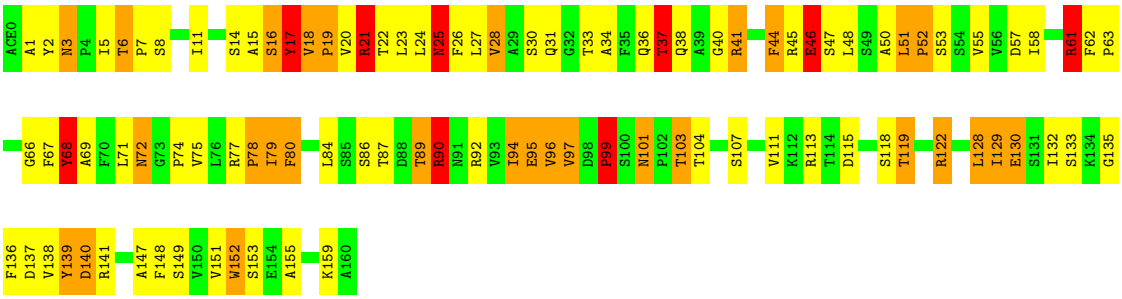
Note EDS was not executed.

• Molecule 1: RNA (5'-R(P*GP*AP*A)-3')

Chain I: 33% 67%

• Molecule 2: CUCUMBER GREEN MOTTLE MOSAIC VIRUS

Chain E: 38% 39% 18% 6%



4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE

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	I	2.01	3/75 (4.0%)	3.00	9/115 (7.8%)
2	E	0.80	0/1247	1.89	33/1701 (1.9%)
All	All	0.91	3/1322 (0.2%)	1.98	42/1816 (2.3%)

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
2	E	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1	G	O3'-P	7.30	1.70	1.61
1	I	3	A	C3'-O3'	5.85	1.50	1.42
1	I	1	G	C4'-C3'	-5.63	1.47	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	2	A	N9-C1'-C2'	-13.01	97.08	114.00
1	I	2	A	O4'-C1'-N9	11.97	117.78	108.20
1	I	1	G	C3'-C2'-C1'	10.91	110.23	101.50
1	I	1	G	O4'-C1'-N9	9.71	115.97	108.20
2	E	17	TYR	CB-CG-CD2	-9.17	115.50	121.00
2	E	113	ARG	NE-CZ-NH2	-8.98	115.81	120.30
2	E	95	GLU	CA-C-N	-8.24	99.07	117.20
1	I	3	A	O4'-C1'-N9	7.94	114.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	90	ARG	N-CA-C	7.79	132.02	111.00
2	E	17	TYR	CB-CG-CD1	7.76	125.66	121.00
2	E	17	TYR	CA-CB-CG	7.76	128.14	113.40
2	E	95	GLU	N-CA-C	7.58	131.47	111.00
1	I	1	G	O4'-C4'-C3'	7.11	111.79	106.10
2	E	152	TRP	CD1-CG-CD2	6.93	111.84	106.30
2	E	57	ASP	N-CA-C	-6.80	92.63	111.00
1	I	2	A	C1'-O4'-C4'	-6.76	104.49	109.90
2	E	152	TRP	CE2-CD2-CG	-6.72	101.93	107.30
2	E	36	GLN	CA-C-N	-6.61	102.67	117.20
2	E	6	THR	CA-C-N	6.47	135.23	117.10
2	E	77	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	E	37	THR	CA-C-N	-6.33	103.26	117.20
2	E	18	VAL	N-CA-C	6.26	127.90	111.00
2	E	95	GLU	O-C-N	6.19	132.61	122.70
2	E	68	TYR	CA-CB-CG	6.19	125.16	113.40
2	E	141	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	I	1	G	C2'-C3'-O3'	5.73	122.86	113.70
2	E	136	PHE	N-CA-C	5.61	126.16	111.00
2	E	20	VAL	CA-CB-CG2	-5.55	102.57	110.90
2	E	92	ARG	CA-C-N	-5.54	105.00	117.20
2	E	21	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	E	36	GLN	O-C-N	5.51	131.51	122.70
2	E	94	ILE	CB-CA-C	-5.42	100.75	111.60
2	E	155	ALA	N-CA-C	5.32	125.36	111.00
2	E	18	VAL	N-CA-CB	-5.29	99.87	111.50
2	E	119	THR	CA-CB-CG2	5.25	119.75	112.40
2	E	25	ASN	CA-CB-CG	5.23	124.90	113.40
2	E	5	ILE	N-CA-C	5.21	125.06	111.00
2	E	99	PRO	N-CA-C	5.21	125.64	112.10
1	I	1	G	C5'-C4'-C3'	-5.18	107.71	116.00
2	E	61	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	E	8	SER	CA-C-N	-5.12	105.94	117.20
2	E	77	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	101	ASN	Peptide
2	E	3	ASN	Peptide
2	E	51	LEU	Peptide

4.2 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	I	67	0	34	3	0
2	E	1224	0	1202	48	0
3	E	5	0	0	0	0
All	All	1296	0	1236	49	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 19.

All (49) 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:E:19:PRO:HG3	2:E:68:TYR:HA	1.43	1.00
2:E:119:THR:HG23	2:E:122:ARG:HE	1.48	0.78
2:E:19:PRO:HB3	2:E:69:ALA:HB3	1.76	0.68
2:E:66:GLY:HA3	2:E:140:ASP:HA	1.77	0.66
2:E:38:GLN:HA	2:E:41:ARG:CZ	2.28	0.64
2:E:15:ALA:HB1	2:E:18:VAL:HG11	1.80	0.62
2:E:139:TYR:OH	2:E:147:ALA:HB2	2.00	0.61
2:E:24:LEU:HD12	2:E:129:ILE:HG12	1.84	0.60
2:E:14:SER:HB3	2:E:72:ASN:HD21	1.67	0.60
2:E:44:PHE:HE1	2:E:48:LEU:HD12	1.66	0.60
2:E:30:SER:HB3	2:E:44:PHE:CZ	2.39	0.57
2:E:19:PRO:O	2:E:23:LEU:HB2	2.04	0.57
2:E:89:THR:HB	2:E:90:ARG:HH21	1.69	0.57
2:E:75:VAL:O	2:E:78:PRO:HD2	2.05	0.56
2:E:21:ARG:HH22	2:E:67:PHE:HE1	1.53	0.55
2:E:41:ARG:CZ	2:E:90:ARG:HA	2.37	0.54
1:I:1:G:N2	2:E:118:SER:HB3	2.22	0.53
2:E:69:ALA:HA	2:E:139:TYR:H	1.73	0.53
2:E:44:PHE:CE1	2:E:48:LEU:HD12	2.44	0.53
2:E:18:VAL:HG22	2:E:23:LEU:HG	1.91	0.52
2:E:25:ASN:O	2:E:28:VAL:HG23	2.09	0.52
2:E:15:ALA:HB3	2:E:71:LEU:O	2.10	0.52
2:E:128:LEU:O	2:E:132:ILE:HG13	2.10	0.52
2:E:103:THR:HB	2:E:107:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:80:PHE:O	2:E:84:LEU:HB2	2.10	0.51
2:E:23:LEU:O	2:E:27:LEU:HD13	2.11	0.50
2:E:22:THR:HG22	2:E:26:PHE:CE1	2.47	0.49
2:E:22:THR:HA	2:E:26:PHE:CD1	2.47	0.49
2:E:128:LEU:CD2	2:E:132:ILE:HG12	2.43	0.49
2:E:16:SER:HA	2:E:69:ALA:O	2.13	0.48
2:E:23:LEU:HD13	2:E:132:ILE:HD13	1.94	0.48
2:E:18:VAL:HB	2:E:52:PRO:HB3	1.94	0.48
1:I:1:G:H2'	2:E:119:THR:HB	1.95	0.47
2:E:79:ILE:HG21	2:E:128:LEU:HG	1.96	0.46
2:E:94:ILE:HG21	2:E:104:THR:HG23	1.98	0.46
2:E:34:ALA:O	2:E:40:GLY:HA3	2.15	0.46
2:E:128:LEU:HD23	2:E:132:ILE:HG12	1.99	0.45
2:E:2:TYR:HA	2:E:149:SER:O	2.17	0.44
2:E:19:PRO:HB3	2:E:69:ALA:CB	2.44	0.44
2:E:130:GLU:H	2:E:130:GLU:HG3	1.59	0.44
2:E:96:VAL:HG12	2:E:97:VAL:HG12	2.01	0.43
1:I:3:A:N3	1:I:3:A:H5"	2.34	0.43
2:E:17:TYR:CE1	2:E:55:VAL:HG23	2.54	0.43
2:E:27:LEU:O	2:E:31:GLN:HB2	2.19	0.43
2:E:45:ARG:NH2	2:E:89:THR:HA	2.33	0.42
2:E:46:GLU:O	2:E:50:ALA:HB3	2.19	0.42
2:E:68:TYR:CE1	2:E:139:TYR:HB3	2.55	0.42
2:E:21:ARG:HG3	2:E:22:THR:H	1.85	0.41
2:E:61:ARG:NH2	2:E:139:TYR:O	2.55	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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
2	E	159/161 (99%)	96 (60%)	39 (24%)	24 (15%)	0 0

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	1	ALA
2	E	6	THR
2	E	90	ARG
2	E	16	SER
2	E	19	PRO
2	E	21	ARG
2	E	37	THR
2	E	52	PRO
2	E	53	SER
2	E	78	PRO
2	E	79	ILE
2	E	96	VAL
2	E	122	ARG
2	E	137	ASP
2	E	46	GLU
2	E	47	SER
2	E	63	PRO
2	E	74	PRO
2	E	97	VAL
2	E	135	GLY
2	E	111	VAL
2	E	7	PRO
2	E	99	PRO
2	E	151	VAL

4.3.2 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
2	E	135/135 (100%)	98 (73%)	37 (27%)	0 1

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	3	ASN

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Mol	Chain	Res	Type
2	E	11	ILE
2	E	17	TYR
2	E	25	ASN
2	E	28	VAL
2	E	33	THR
2	E	37	THR
2	E	41	ARG
2	E	44	PHE
2	E	46	GLU
2	E	51	LEU
2	E	58	ILE
2	E	61	ARG
2	E	62	PHE
2	E	68	TYR
2	E	72	ASN
2	E	80	PHE
2	E	86	SER
2	E	87	THR
2	E	89	THR
2	E	90	ARG
2	E	95	GLU
2	E	99	PRO
2	E	101	ASN
2	E	103	THR
2	E	115	ASP
2	E	128	LEU
2	E	129	ILE
2	E	130	GLU
2	E	133	SER
2	E	138	VAL
2	E	139	TYR
2	E	140	ASP
2	E	148	PHE
2	E	152	TRP
2	E	153	SER
2	E	159	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	3	ASN
2	E	72	ASN

4.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	3/3 (100%)	2 (66%)	2 (66%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	2	A
1	I	3	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	1	G
1	I	2	A

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.