Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:35 am BST

PDB ID	:	1EI7
Title	:	TMV COAT PROTEIN REFINED FROM THE 4-LAYER AGGREGATE
Authors	:	Bhyravbhatla, B.; Watowich, S.J.; Caspar, D.L.
Deposited on	:	2000-02-24
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure 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 ⓘ symbol.

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

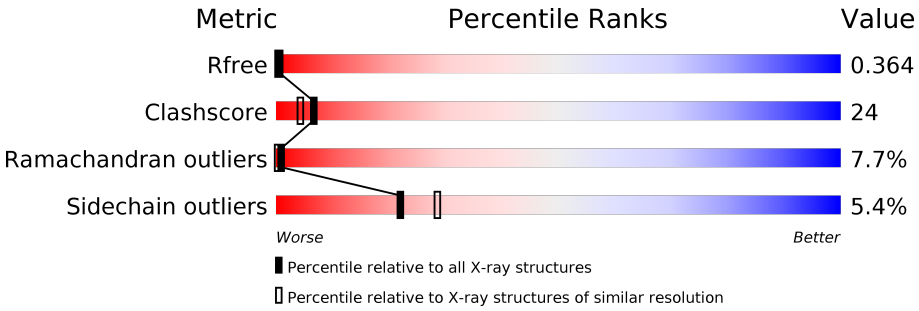
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.45 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))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)

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 on 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%

Mol	Chain	Length	Quality of chain
1	A	158	75% 18% 7%
1	B	158	66% 23% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2804 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	158	Total	C	N	O	S	0	0	0
			1235	776	215	243	1			
1	B	158	Total	C	N	O	S	0	0	0
			1235	776	215	243	1			

- Molecule 2 is water.

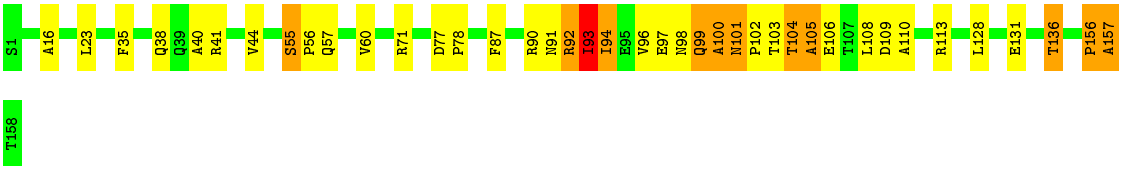
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	158	Total	O	0	0
			158	158		
2	B	176	Total	O	0	0
			176	176		

3 Residue-property plots (i)

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.

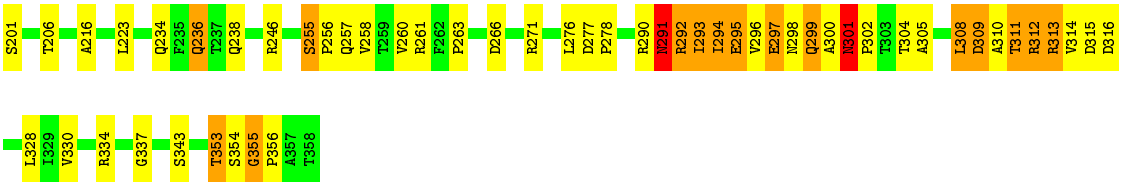
- Molecule 1: COAT PROTEIN

Chain A:



- Molecule 1: COAT PROTEIN

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	220.84Å 171.70Å 226.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.45 29.97 – 2.44	Depositor EDS
% Data completeness (in resolution range)	69.0 (29.90-2.45) 65.1 (29.97-2.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.45Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.195 , 0.225 0.364 , 0.364	Depositor DCC
R_{free} test set	10952 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	6.7	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	0.188 for l,-k,h	Xtriage
F_o,F_c correlation	0.56	EDS
Total number of atoms	2804	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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	0.38	0/1260	0.59	0/1723
1	B	0.38	0/1260	0.62	0/1723
All	All	0.38	0/2520	0.61	0/3446

There are no bond length outliers.

There are no bond angle outliers.

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	1235	0	1213	42	0
1	B	1235	0	1210	73	0
2	A	158	0	0	0	0
2	B	176	0	0	6	0
All	All	2804	0	2423	115	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 24.

All (115) 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:B:312:ARG:HA	1:B:315:ASP:HB2	1.53	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ALA:HA	1:B:308:LEU:HD22	1.52	0.88
1:B:313:ARG:HH11	1:B:313:ARG:HG2	1.44	0.82
1:A:38:GLN:HE22	1:A:90:ARG:HA	1.50	0.77
1:A:90:ARG:HB2	1:A:93:ILE:CG2	2.15	0.76
1:A:105:ALA:N	1:A:108:LEU:HD13	2.02	0.74
1:B:309:ASP:HA	1:B:312:ARG:NH1	2.03	0.73
1:B:291:ASN:ND2	1:B:291:ASN:H	1.88	0.72
1:B:355:GLY:H	1:B:356:PRO:HD3	1.57	0.70
1:A:77:ASP:HB3	1:A:78:PRO:HD3	1.73	0.70
1:B:313:ARG:NH1	1:B:313:ARG:HG2	2.05	0.67
1:B:301:ASN:ND2	1:B:302:PRO:HD3	2.09	0.67
1:A:40:ALA:O	1:A:44:VAL:HG22	1.93	0.67
1:B:305:ALA:O	1:B:308:LEU:HB3	1.96	0.66
1:A:90:ARG:HB2	1:A:93:ILE:HG22	1.77	0.65
1:B:309:ASP:HA	1:B:312:ARG:HH12	1.62	0.65
1:A:38:GLN:NE2	1:A:41:ARG:HH21	1.94	0.64
1:A:35:PHE:HE1	1:A:44:VAL:HG21	1.63	0.63
1:B:292:ARG:CB	1:B:296:VAL:HG22	2.29	0.63
1:A:93:ILE:O	1:A:93:ILE:HG12	1.99	0.62
1:B:255:SER:HB3	1:B:256:PRO:CD	2.30	0.62
1:A:38:GLN:NE2	1:A:90:ARG:HA	2.14	0.62
1:B:293:ILE:O	1:B:294:ILE:HB	2.00	0.60
1:B:234:GLN:HB3	1:B:236:GLN:HE22	1.67	0.60
1:A:55:SER:HB3	1:A:56:PRO:CD	2.31	0.60
1:A:103:THR:O	1:A:105:ALA:N	2.35	0.60
1:B:292:ARG:HG3	1:B:293:ILE:HG12	1.84	0.59
1:A:101:ASN:N	1:A:102:PRO:HD2	2.16	0.59
1:B:292:ARG:O	1:B:293:ILE:HG23	2.03	0.59
1:B:355:GLY:N	1:B:356:PRO:HD3	2.18	0.58
1:B:310:ALA:O	1:B:312:ARG:N	2.35	0.58
1:B:305:ALA:CA	1:B:308:LEU:HD22	2.31	0.58
1:B:300:ALA:O	1:B:301:ASN:HB3	2.03	0.57
1:B:276:LEU:HD22	1:B:337:GLY:HA3	1.86	0.56
1:B:292:ARG:HB2	1:B:296:VAL:HG22	1.87	0.56
1:B:309:ASP:O	1:B:312:ARG:HG2	2.06	0.56
1:A:108:LEU:HD12	1:A:108:LEU:H	1.71	0.56
1:B:308:LEU:HD23	1:B:308:LEU:N	2.20	0.55
1:B:308:LEU:O	1:B:310:ALA:N	2.40	0.55
1:B:291:ASN:O	1:B:292:ARG:HB2	2.07	0.54
1:A:92:ARG:HE	1:A:106:GLU:CG	2.20	0.54
1:B:304:THR:C	1:B:308:LEU:HD13	2.28	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:HB3	1:B:296:VAL:HG22	1.89	0.54
1:A:35:PHE:CE1	1:A:44:VAL:HG21	2.44	0.53
1:A:92:ARG:HH21	1:A:106:GLU:HA	1.74	0.53
1:A:92:ARG:O	1:A:94:ILE:HG22	2.07	0.53
1:B:238:GLN:OE1	1:B:290:ARG:HD2	2.08	0.53
1:B:292:ARG:HG2	1:B:296:VAL:HA	1.92	0.52
1:B:304:THR:O	1:B:308:LEU:HD13	2.09	0.52
1:B:309:ASP:O	1:B:311:THR:HG22	2.10	0.51
1:A:109:ASP:O	1:A:113:ARG:HG3	2.10	0.51
1:A:16:ALA:HB1	1:A:71:ARG:HB3	1.91	0.51
1:B:311:THR:O	1:B:313:ARG:N	2.43	0.51
1:B:291:ASN:ND2	1:B:291:ASN:N	2.58	0.51
1:B:312:ARG:HB3	1:B:316:ASP:CG	2.32	0.49
1:A:44:VAL:HG23	1:A:87:PHE:CE1	2.48	0.49
1:B:236:GLN:HA	2:B:586:HOH:O	2.13	0.49
1:B:308:LEU:O	1:B:309:ASP:C	2.51	0.48
1:B:261:ARG:NH1	1:B:356:PRO:O	2.45	0.48
1:A:100:ALA:C	1:A:102:PRO:HD2	2.34	0.48
1:A:93:ILE:HD13	1:A:93:ILE:H	1.77	0.48
1:A:108:LEU:N	1:A:108:LEU:HD12	2.28	0.47
1:A:94:ILE:O	1:A:94:ILE:HG13	2.14	0.47
1:B:298:ASN:O	1:B:299:GLN:HB2	2.14	0.47
1:A:131:GLU:O	1:A:136:THR:HG23	2.14	0.47
1:B:355:GLY:H	1:B:356:PRO:CD	2.24	0.47
1:B:292:ARG:NE	1:B:296:VAL:HG13	2.31	0.46
1:A:92:ARG:HE	1:A:106:GLU:HG3	1.80	0.46
1:B:236:GLN:N	1:B:236:GLN:HE21	2.14	0.46
1:B:263:PRO:HB2	1:B:266:ASP:HB2	1.99	0.45
1:B:310:ALA:C	1:B:312:ARG:N	2.70	0.45
1:B:313:ARG:CG	1:B:313:ARG:HH11	2.20	0.45
1:B:309:ASP:CA	1:B:312:ARG:NH1	2.77	0.45
1:B:330:VAL:O	1:B:334:ARG:HG3	2.16	0.45
1:B:292:ARG:HE	1:B:297:GLU:CD	2.21	0.44
1:A:99:GLN:HE21	1:A:100:ALA:HB3	1.83	0.44
1:A:101:ASN:O	1:A:102:PRO:C	2.55	0.43
1:A:104:THR:O	1:A:105:ALA:HB2	2.18	0.43
1:A:38:GLN:NE2	1:A:41:ARG:NH2	2.65	0.43
1:A:92:ARG:HE	1:A:106:GLU:HG2	1.83	0.43
1:A:93:ILE:N	1:A:93:ILE:HD13	2.33	0.43
1:A:92:ARG:HD3	1:A:110:ALA:HB2	2.00	0.43
1:B:246:ARG:HG2	2:B:518:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HB2	1:A:93:ILE:HG23	1.97	0.43
1:B:312:ARG:HA	1:B:315:ASP:CB	2.38	0.43
1:B:353:THR:HG22	1:B:354:SER:H	1.82	0.43
1:B:258:VAL:HG23	2:B:467:HOH:O	2.19	0.43
1:A:57:GLN:HB2	1:A:60:VAL:HB	2.01	0.43
1:B:246:ARG:HD2	2:B:517:HOH:O	2.17	0.43
1:B:309:ASP:O	1:B:312:ARG:NH1	2.52	0.43
1:B:299:GLN:HE22	1:B:301:ASN:N	2.17	0.42
1:B:255:SER:CB	1:B:256:PRO:CD	2.97	0.42
1:B:290:ARG:C	1:B:292:ARG:H	2.22	0.42
1:B:292:ARG:CZ	1:B:296:VAL:HG13	2.50	0.42
1:A:105:ALA:O	1:A:108:LEU:N	2.53	0.42
1:A:156:PRO:O	1:A:157:ALA:HB3	2.20	0.42
1:B:255:SER:HB3	1:B:256:PRO:HD2	2.02	0.42
1:B:277:ASP:HB3	1:B:278:PRO:CD	2.50	0.42
1:B:308:LEU:N	1:B:308:LEU:CD2	2.82	0.42
1:B:311:THR:C	1:B:313:ARG:N	2.73	0.41
1:B:312:ARG:HD2	1:B:315:ASP:HB2	2.02	0.41
1:B:236:GLN:H	1:B:236:GLN:HE21	1.68	0.41
1:A:55:SER:HB3	1:A:56:PRO:HD3	2.02	0.41
1:B:312:ARG:C	1:B:314:VAL:N	2.72	0.41
1:B:355:GLY:N	1:B:356:PRO:CD	2.82	0.41
1:A:92:ARG:NH2	1:A:109:ASP:HB3	2.36	0.41
1:B:257:GLN:HB2	1:B:260:VAL:HB	2.02	0.41
1:A:100:ALA:O	1:A:101:ASN:C	2.59	0.41
1:B:343:SER:HA	2:B:735:HOH:O	2.21	0.41
1:B:292:ARG:HB3	1:B:295:GLU:O	2.20	0.41
1:B:299:GLN:NE2	1:B:300:ALA:H	2.19	0.41
1:A:96:VAL:O	1:A:97:GLU:C	2.60	0.40
1:B:311:THR:HG22	1:B:312:ARG:HH11	1.86	0.40
1:B:201:SER:N	2:B:453:HOH:O	2.54	0.40
1:B:216:ALA:HB1	1:B:271:ARG:HB3	2.04	0.40

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	156/158 (99%)	139 (89%)	6 (4%)	11 (7%)	1 0
1	B	156/158 (99%)	132 (85%)	11 (7%)	13 (8%)	1 0
All	All	312/316 (99%)	271 (87%)	17 (5%)	24 (8%)	1 0

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	104	THR
1	A	105	ALA
1	B	255	SER
1	B	292	ARG
1	B	293	ILE
1	B	301	ASN
1	B	308	LEU
1	B	311	THR
1	B	312	ARG
1	A	55	SER
1	A	91	ASN
1	A	93	ILE
1	A	98	ASN
1	A	99	GLN
1	A	100	ALA
1	B	355	GLY
1	A	156	PRO
1	B	291	ASN
1	B	294	ILE
1	B	297	GLU
1	B	309	ASP
1	A	157	ALA
1	B	299	GLN

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	138/138 (100%)	132 (96%)	6 (4%)	29 38
1	B	138/138 (100%)	129 (94%)	9 (6%)	17 21
All	All	276/276 (100%)	261 (95%)	15 (5%)	22 28

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	92	ARG
1	A	93	ILE
1	A	101	ASN
1	A	128	LEU
1	A	136	THR
1	B	206	THR
1	B	223	LEU
1	B	236	GLN
1	B	291	ASN
1	B	295	GLU
1	B	301	ASN
1	B	313	ARG
1	B	328	LEU
1	B	353	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	99	GLN
1	B	229	ASN
1	B	234	GLN
1	B	236	GLN
1	B	245	GLN
1	B	301	ASN
1	B	326	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 carbohydrates 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.