



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:58 PM UTC

PDB ID : 2W0C / pdb_00002w0c
Title : X-ray structure of the entire lipid-containing bacteriophage PM2
Authors : Abrescia, N.G.A.; Grimes, J.M.; Kivela, H.M.; Assenberg, R.; Sutton, G.C.;
Butcher, S.J.; Bamford, J.K.H.; Bamford, D.H.; Stuart, D.I.
Deposited on : 2008-08-13
Resolution : 7.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

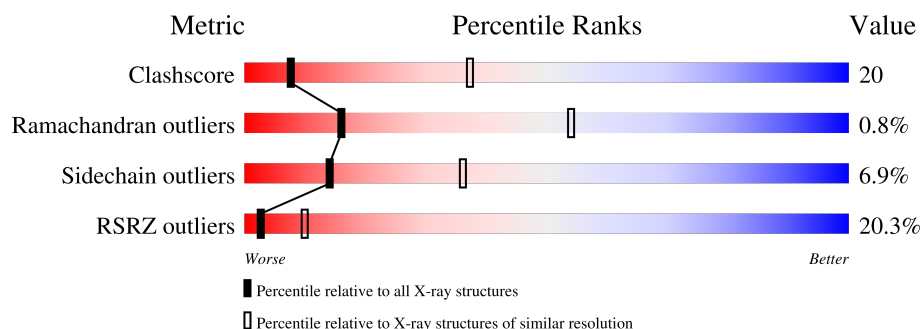
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 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	1007 (9.70-4.04)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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 $\leq 5\%$. 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	269	24% 66% 31% .
1	B	269	23% 65% 32% .
1	C	269	16% 67% 31% .
1	D	269	22% 67% 30% .
1	E	269	23% 64% 33% .
1	F	269	11% 66% 32% .
1	G	269	24% 66% 31% .

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Mol	Chain	Length	Quality of chain
1	H	269	
1	I	269	
1	J	269	
2	L	335	
3	P	104	
3	Q	104	
3	R	104	
3	S	104	
4	T	127	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26447 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 MAJOR CAPSID PROTEIN P2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	B	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	C	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	D	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	E	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	F	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	G	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	H	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	I	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			
1	J	269	Total	C	N	O	S	0	0	0
			2123	1347	366	400	10			

- Molecule 2 is a protein called PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	335	Total	C	N	O	S	0	0	0
			2634	1660	439	529	6			

- Molecule 3 is a protein called PROTEIN P3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	65	Total	C	N	O	S	0	0	0
			451	275	82	92	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	60	Total	C	N	O	S	0	0	0
			432	265	77	89	1			
3	R	63	Total	C	N	O	S	0	0	0
			453	280	80	92	1			
3	S	84	Total	C	N	O	S	0	0	0
			608	386	107	113	2			

- Molecule 4 is a protein called PROTEIN P6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	T	127	Total	C	N	O	0	0	0
			628	374	127	127			

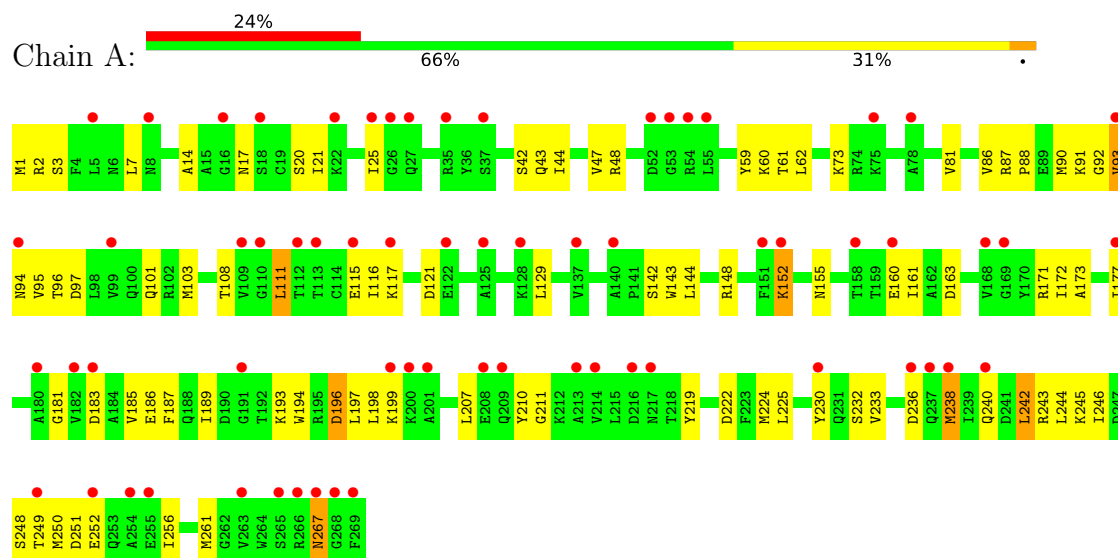
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	G	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		
5	I	1	Total	Ca	0	0
			1	1		
5	J	1	Total	Ca	0	0
			1	1		
5	L	1	Total	Ca	0	0
			1	1		

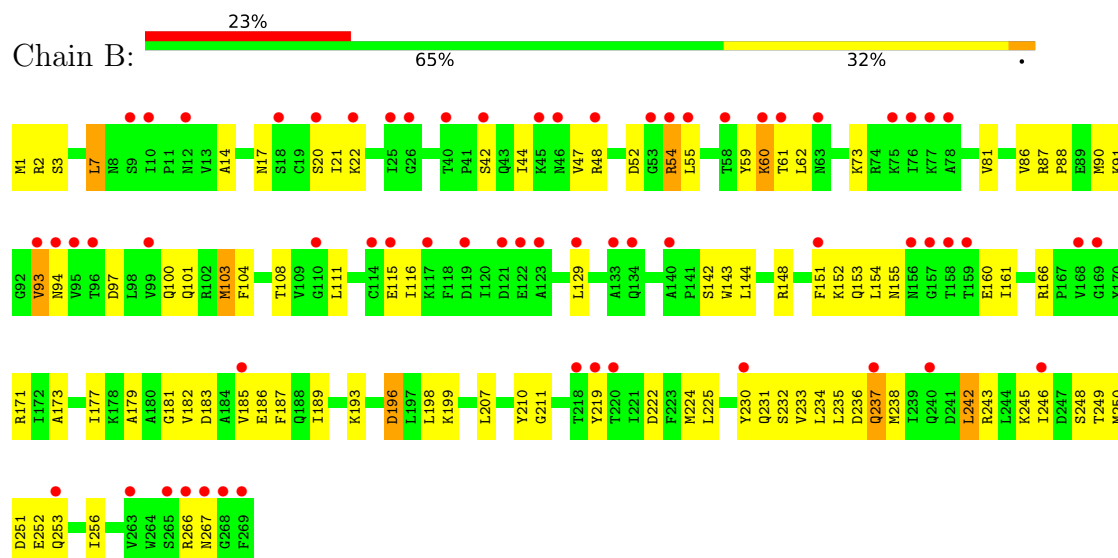
3 Residue-property plots [i](#)

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 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: MAJOR CAPSID PROTEIN P2

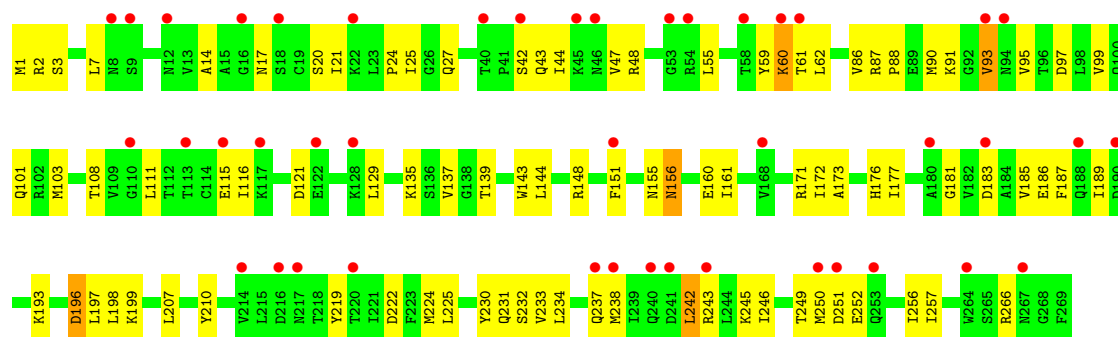


• Molecule 1: MAJOR CAPSID PROTEIN P2

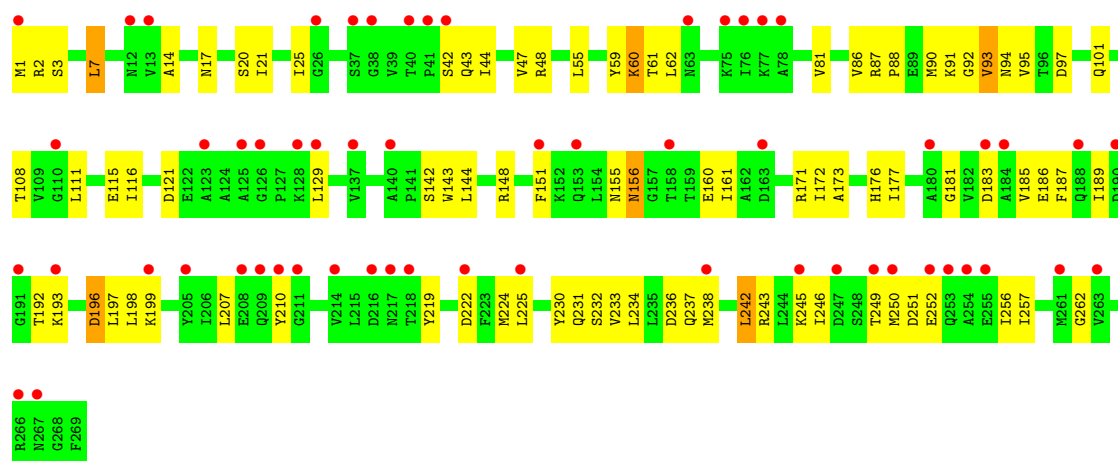


• Molecule 1: MAJOR CAPSID PROTEIN P2

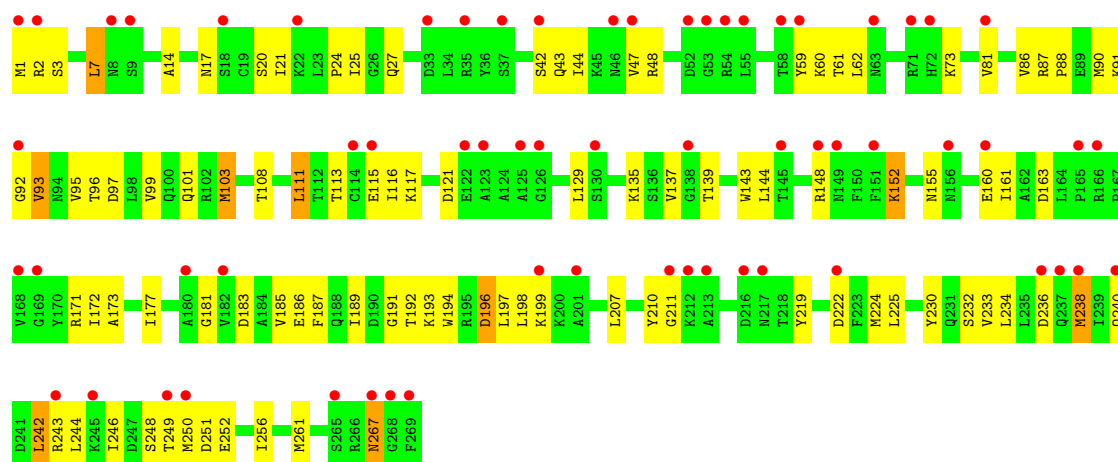




• Molecule 1: MAJOR CAPSID PROTEIN P2

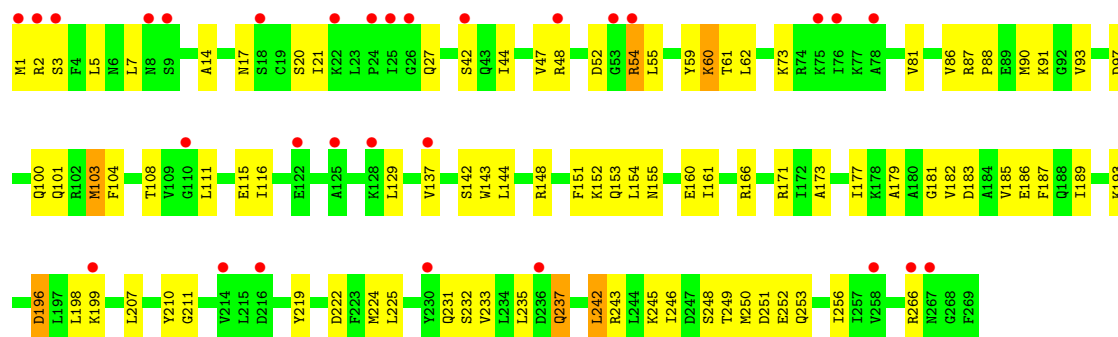


• Molecule 1: MAJOR CAPSID PROTEIN P2

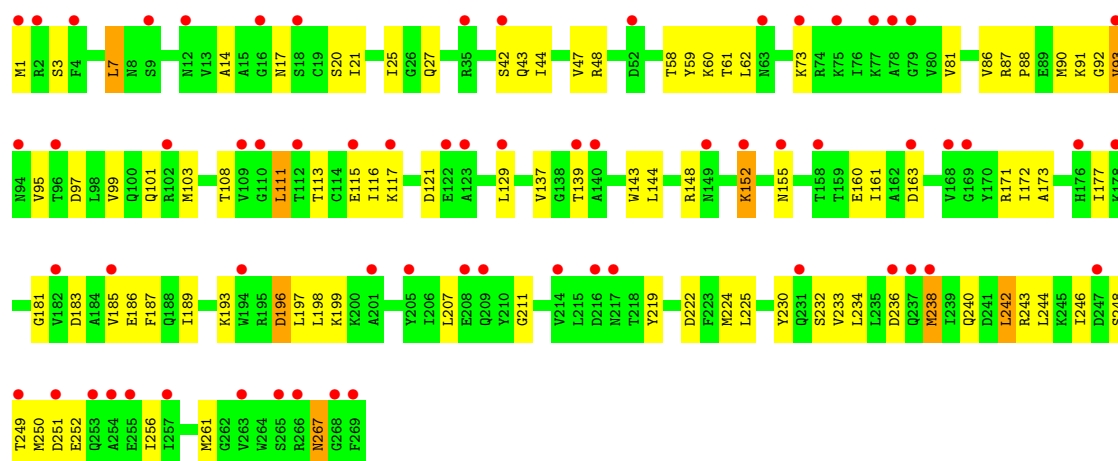


• Molecule 1: MAJOR CAPSID PROTEIN P2

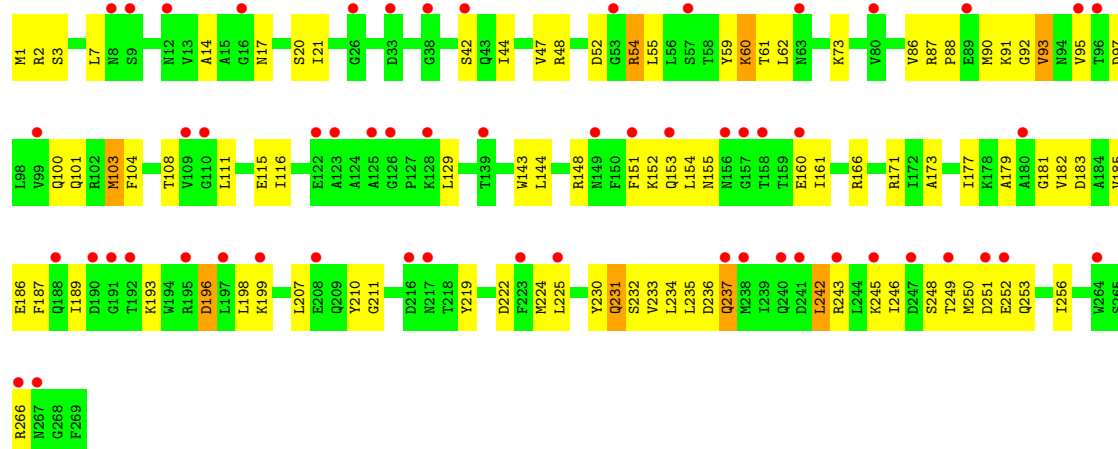




• Molecule 1: MAJOR CAPSID PROTEIN P2

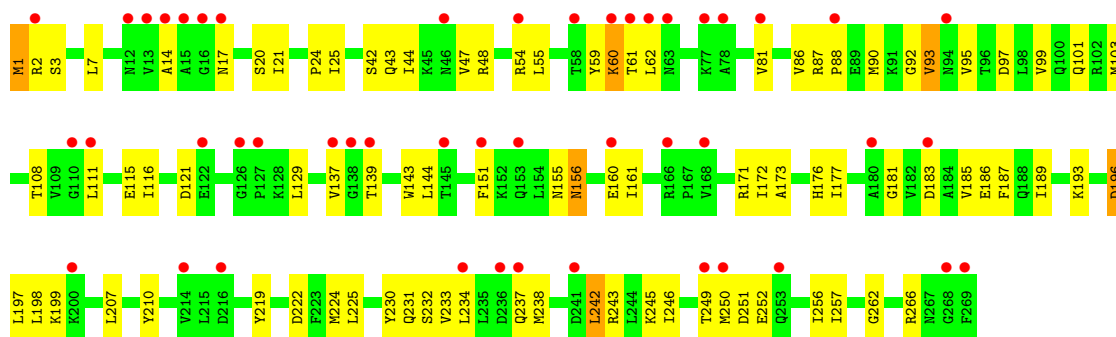


• Molecule 1: MAJOR CAPSID PROTEIN P2

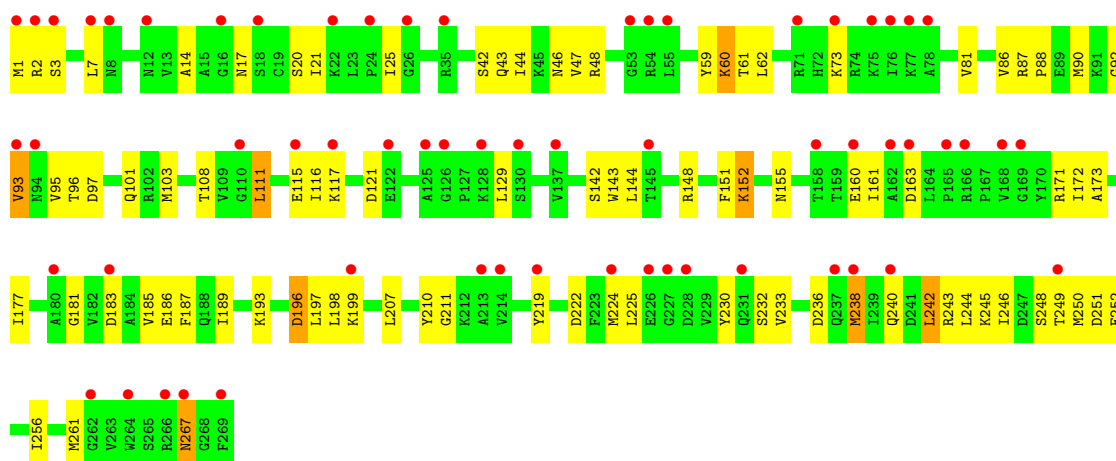


• Molecule 1: MAJOR CAPSID PROTEIN P2

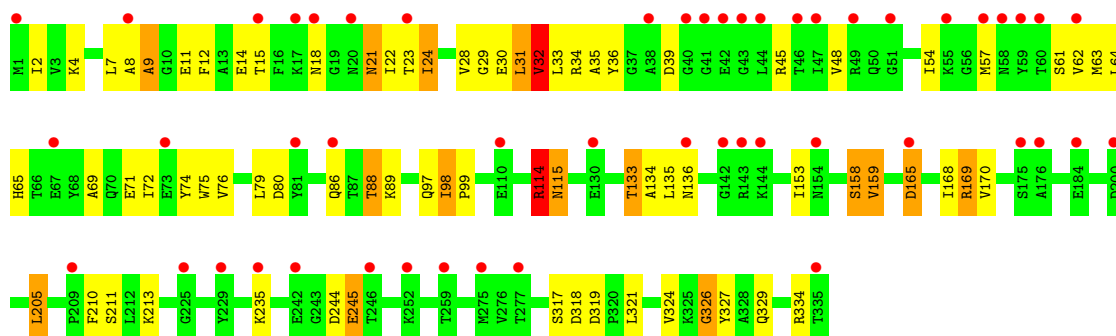
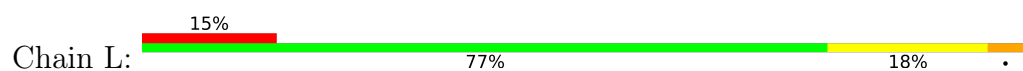




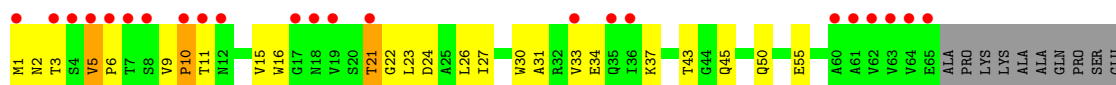
• Molecule 1: MAJOR CAPSID PROTEIN P2



• Molecule 2: PROTEIN 2

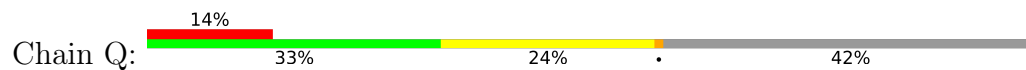


• Molecule 3: PROTEIN P3



THR
LEU
VAL
PHE
SER
GLY
VAL
PRO
GLN
LEU
THR
LEU
LEU
LEU
GLY
PHE
GLY
GLY
LEU
VAL
LEU
GLY
VAL
MET
ARG
GLY
ASN
LYS

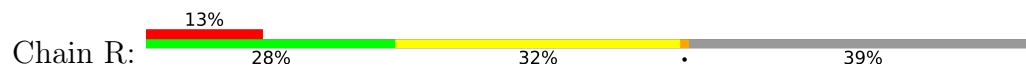
• Molecule 3: PROTEIN P3



MET ASN THR SER PRO T7 S8 V9 P10 T11 N12 W16 G17 N18 T21 G22 L23 D24 I27 S28 G29 W30 A31 V33 E34 Q35 T36 K37 A38 A39 K40 A41 S42 T43 G44 Q45 G46 R47 V48 E49 Q50 T53 P54 E55 L56 D57 N58 G59 A60 V63 V64 E65 A66

PRO LYS LYS ALA ALA GLN PRO SER GLU THR LEU THR VAL PHE GLY VAL PRO GLN LYS THR LEU LEU LEU LEU LEU LEU PHE GLY GLY LEU VAL LEU LEU LEU LEU VAL MET ARG GLY ASN LYS

• Molecule 3: PROTEIN P3



MET ASN THR SER V5 P6 V9 N12 Q13 S14 W16 G17 N18 V19 S20 T21 G22 L23 D24 A25 L26 I27 S28 G29 W30 A31 V33 E34 Q35 T36 K37 A41 S42 T43 G44 Q45 G46 R47 V48 E49 Q50 A51 M52 E55 L56 D57 A61 V62 V63 V64 E65 A66 P67

LYS LYS ALA ALA GLN PRO SER GLU THR LEU THR VAL PHE GLY VAL PRO GLN LYS THR LEU LEU LEU LEU LEU PHE GLY GLY LEU VAL LEU LEU LEU LEU VAL MET ARG GLY ASN LYS

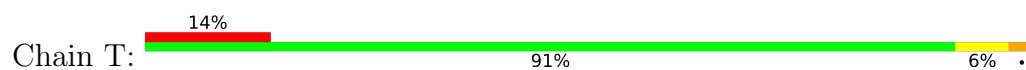
• Molecule 3: PROTEIN P3



MET ASN THR SER PRO VAL THR SER VAL PRO THR VAL THR ASN GLN SER SER TRP GLY ASN VAL SER T21 G22 L23 D24 A25 L26 I27 W30 A31 R32 V33 E34 Q35 I36 K37 A38 A41 S42 T43 G44 Q45 G46 R47 V48 E49 Q50 A51 M52 E55 L56 D57 V62 V63 V64 E65 A66

P67 K68 K69 A70 A71 Q72 P73 S74 E75 T76 L77 V78 V81 P82 Q83 K84 L87 L88 G89 F90 G91 G92 G93 L94 L95 L96 G97 L98 H103 K104

• Molecule 4: PROTEIN P6



W1 A2 N3 K34 P35 I36 A37 D38 F39 P56 N57 D69 D76 A80 H85 E94 I95 L96 D97 H98 E99 R100 R101 P104 A116 S117 T118 A122 S123 G124 V125 E126 L127

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	946.90Å 677.60Å 1067.60Å 90.00° 102.90° 90.00°	Depositor
Resolution (Å)	96.00 – 7.00 96.00 – 7.00	Depositor EDS
% Data completeness (in resolution range)	82.9 (96.00-7.00) 82.9 (96.00-7.00)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 6.73Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.419 , (Not available) 0.466 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	132.6	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.36	EDS
Total number of atoms	26447	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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

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	0.35	2/2158 (0.1%)	0.73	1/2917 (0.0%)
1	B	0.29	0/2158	0.73	0/2917
1	C	0.33	1/2158 (0.0%)	0.75	1/2917 (0.0%)
1	D	0.33	1/2158 (0.0%)	0.75	1/2917 (0.0%)
1	E	0.35	2/2158 (0.1%)	0.73	1/2917 (0.0%)
1	F	0.29	0/2158	0.73	0/2917
1	G	0.35	2/2158 (0.1%)	0.73	1/2917 (0.0%)
1	H	0.29	0/2158	0.72	0/2917
1	I	0.33	1/2158 (0.0%)	0.75	1/2917 (0.0%)
1	J	0.35	2/2158 (0.1%)	0.73	1/2917 (0.0%)
2	L	1.21	5/2688 (0.2%)	1.16	19/3646 (0.5%)
3	P	0.46	0/457	0.72	0/624
3	Q	0.42	0/437	0.67	0/596
3	R	0.45	0/460	0.68	0/630
3	S	0.45	0/615	0.73	0/831
4	T	0.49	0/627	0.97	3/872 (0.3%)
All	All	0.50	16/26864 (0.1%)	0.79	29/36369 (0.1%)

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	L	0	5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	169	ARG	C-N	49.53	1.94	1.33
2	L	324	VAL	C-N	19.70	1.63	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	111	LEU	CG-CD1	-6.13	1.32	1.52
1	J	111	LEU	CG-CD1	-6.13	1.32	1.52
1	G	111	LEU	CG-CD1	-6.12	1.32	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	169	ARG	O-C-N	-30.41	87.56	122.84
2	L	115	ASN	N-CA-C	15.31	136.62	111.37
2	L	98	ILE	CA-C-N	14.87	138.43	119.84
2	L	98	ILE	C-N-CA	14.87	138.43	119.84
2	L	169	ARG	CA-C-N	12.43	141.71	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	114	ARG	Peptide
2	L	158	SER	Peptide
2	L	165	ASP	Mainchain
2	L	326	GLY	Peptide
2	L	98	ILE	Peptide

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	2123	0	2155	99	0
1	B	2123	0	2156	85	0
1	C	2123	0	2155	127	0
1	D	2123	0	2156	71	0
1	E	2123	0	2153	149	0
1	F	2123	0	2156	66	0
1	G	2123	0	2153	105	0
1	H	2123	0	2156	84	0
1	I	2123	0	2154	126	0
1	J	2123	0	2154	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	2634	0	2479	80	0
3	P	451	0	425	94	0
3	Q	432	0	425	114	0
3	R	453	0	443	144	0
3	S	608	0	641	134	0
4	T	628	0	311	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
All	All	26447	0	26272	1061	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 20.

The worst 5 of 1061 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:230:TYR:CE1	3:P:1:MET:HG2	1.24	1.70
1:A:230:TYR:CZ	3:P:1:MET:HG2	1.32	1.59
1:E:113:THR:HG21	3:S:56:LEU:CD2	1.37	1.50
1:A:230:TYR:CE1	3:P:1:MET:CG	1.92	1.47
1:D:234:LEU:H	3:R:47:ARG:NH1	1.10	1.47

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	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	30	67
1	B	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
1	C	267/269 (99%)	252 (94%)	14 (5%)	1 (0%)	30	67
1	D	267/269 (99%)	251 (94%)	15 (6%)	1 (0%)	30	67
1	E	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	30	67
1	F	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
1	G	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	30	67
1	H	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
1	I	267/269 (99%)	252 (94%)	14 (5%)	1 (0%)	30	67
1	J	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	30	67
2	L	331/335 (99%)	306 (92%)	19 (6%)	6 (2%)	6	34
3	P	63/104 (61%)	56 (89%)	5 (8%)	2 (3%)	3	21
3	Q	58/104 (56%)	51 (88%)	6 (10%)	1 (2%)	7	36
3	R	61/104 (59%)	53 (87%)	6 (10%)	2 (3%)	3	21
3	S	82/104 (79%)	74 (90%)	6 (7%)	2 (2%)	4	27
4	T	125/127 (98%)	112 (90%)	7 (6%)	6 (5%)	2	16
All	All	3390/3568 (95%)	3160 (93%)	204 (6%)	26 (1%)	16	54

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	32	VAL
2	L	99	PRO
3	R	65	GLU
3	S	72	GLN
4	T	35	PRO

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	232/232 (100%)	213 (92%)	19 (8%)	10	30
1	B	232/232 (100%)	213 (92%)	19 (8%)	10	30
1	C	232/232 (100%)	216 (93%)	16 (7%)	14	36
1	D	232/232 (100%)	216 (93%)	16 (7%)	14	36
1	E	232/232 (100%)	213 (92%)	19 (8%)	10	30
1	F	232/232 (100%)	213 (92%)	19 (8%)	10	30
1	G	232/232 (100%)	212 (91%)	20 (9%)	10	29
1	H	232/232 (100%)	213 (92%)	19 (8%)	10	30
1	I	232/232 (100%)	216 (93%)	16 (7%)	14	36
1	J	232/232 (100%)	213 (92%)	19 (8%)	10	30
2	L	272/285 (95%)	265 (97%)	7 (3%)	40	62
3	P	44/81 (54%)	42 (96%)	2 (4%)	24	46
3	Q	45/81 (56%)	44 (98%)	1 (2%)	45	64
3	R	48/81 (59%)	48 (100%)	0	100	100
3	S	62/81 (76%)	61 (98%)	1 (2%)	55	70
All	All	2791/2929 (95%)	2598 (93%)	193 (7%)	14	36

5 of 193 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	93	VAL
1	H	237	GLN
1	G	152	LYS
1	H	7	LEU
1	I	42	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	100	GLN
1	G	155	ASN
2	L	152	GLN
1	G	27	GLN
1	H	27	GLN

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](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	88:THR	C	89:LYS	N	2.88
1	L	169:ARG	C	170:VAL	N	1.94

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	324:VAL	C	325:LYS	N	1.63

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(Å ²)	Q<0.9
1	A	269/269 (100%)	1.12	65 (24%) 2 9	40, 40, 40, 40	0
1	B	269/269 (100%)	1.33	63 (23%) 2 9	40, 40, 40, 40	0
1	C	269/269 (100%)	0.67	43 (15%) 5 12	40, 40, 40, 40	0
1	D	269/269 (100%)	0.97	58 (21%) 2 9	40, 40, 40, 40	0
1	E	269/269 (100%)	1.23	63 (23%) 2 9	40, 40, 40, 40	0
1	F	269/269 (100%)	0.44	30 (11%) 10 18	40, 40, 40, 40	0
1	G	269/269 (100%)	1.09	65 (24%) 2 9	40, 40, 40, 40	0
1	H	269/269 (100%)	0.99	57 (21%) 2 10	40, 40, 40, 40	0
1	I	269/269 (100%)	0.88	47 (17%) 4 12	40, 40, 40, 40	0
1	J	269/269 (100%)	1.16	61 (22%) 2 9	40, 40, 40, 40	0
2	L	335/335 (100%)	0.69	50 (14%) 5 14	40, 40, 40, 40	0
3	P	65/104 (62%)	1.94	23 (35%) 1 6	40, 40, 40, 40	0
3	Q	60/104 (57%)	1.55	15 (25%) 2 8	40, 40, 40, 40	0
3	R	63/104 (60%)	1.58	14 (22%) 2 9	40, 40, 40, 40	0
3	S	84/104 (80%)	1.64	23 (27%) 1 8	40, 40, 40, 40	0
4	T	127/127 (100%)	0.78	18 (14%) 6 15	40, 40, 40, 40	0
All	All	3424/3568 (95%)	1.01	695 (20%) 3 10	40, 40, 40, 40	0

The worst 5 of 695 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	S	21	THR	19.1
1	E	237	GLN	16.6
3	P	64	VAL	14.8
2	L	42	GLU	13.0
1	J	78	ALA	12.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	J	1270	1/1	0.93	0.32	40,40,40,40	0
5	CA	D	1270	1/1	0.99	0.04	40,40,40,40	0
5	CA	G	1270	1/1	0.99	0.05	40,40,40,40	0
5	CA	H	1270	1/1	0.99	0.09	40,40,40,40	0
5	CA	C	1270	1/1	0.99	0.11	40,40,40,40	0
5	CA	L	400	1/1	0.99	0.07	40,40,40,40	0
5	CA	A	1270	1/1	1.00	0.09	40,40,40,40	0
5	CA	B	1270	1/1	1.00	0.10	40,40,40,40	0
5	CA	I	1270	1/1	1.00	0.06	40,40,40,40	0
5	CA	E	1270	1/1	1.00	0.20	40,40,40,40	0
5	CA	F	1270	1/1	1.00	0.11	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.