wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 11:06 PM GMT

PDB ID	:	1WCE
Title	:	Crystal structure of the T13 IBDV viral particle reveals a missing link in icosahedral viruses evolution
Authors	:	Coulibaly, F.; Chevalier, C.; Gutsche, I.; Pous, J.; Bressanelli, S.; Navaza, J.; Delmas, B.; Rey, F.A.
Deposited on	:	2004-11-12
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

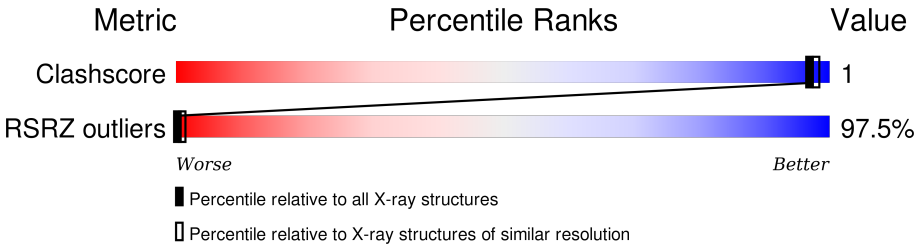
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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	102246	1063 (10.00-3.70)
RSRZ outliers	91569	1013 (9.50-3.66)

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. 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	441	95% 96% ·
1	B	441	95% 97% ·
1	C	441	95% 98% ·
1	D	441	94% 96% ·
1	E	441	94% 97% ·
1	F	441	97% 98% ·
1	G	441	93% 96% ·
1	H	441	93% 96% ·
1	I	441	91% 95% 5%

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Mol	Chain	Length	Quality of chain
1	J	441	95% 96%
1	K	441	93% 94% 6%
1	L	441	95% 97%
1	M	441	94% 96%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5533 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 STRUCTURAL PROTEIN VP2.

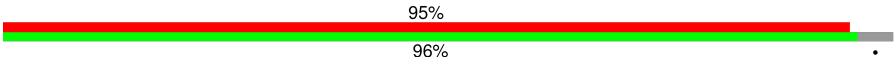
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	425	Total C 425 425	0	0	425
1	B	430	Total C 430 430	0	0	430
1	C	430	Total C 430 430	0	0	430
1	D	424	Total C 424 424	0	0	424
1	E	429	Total C 429 429	0	0	429
1	F	436	Total C 436 436	0	0	436
1	G	426	Total C 426 426	0	0	426
1	H	423	Total C 423 423	0	0	423
1	I	417	Total C 417 417	0	0	417
1	J	423	Total C 423 423	0	0	423
1	K	416	Total C 416 416	0	0	416
1	L	429	Total C 429 429	0	0	429
1	M	425	Total C 425 425	0	0	425

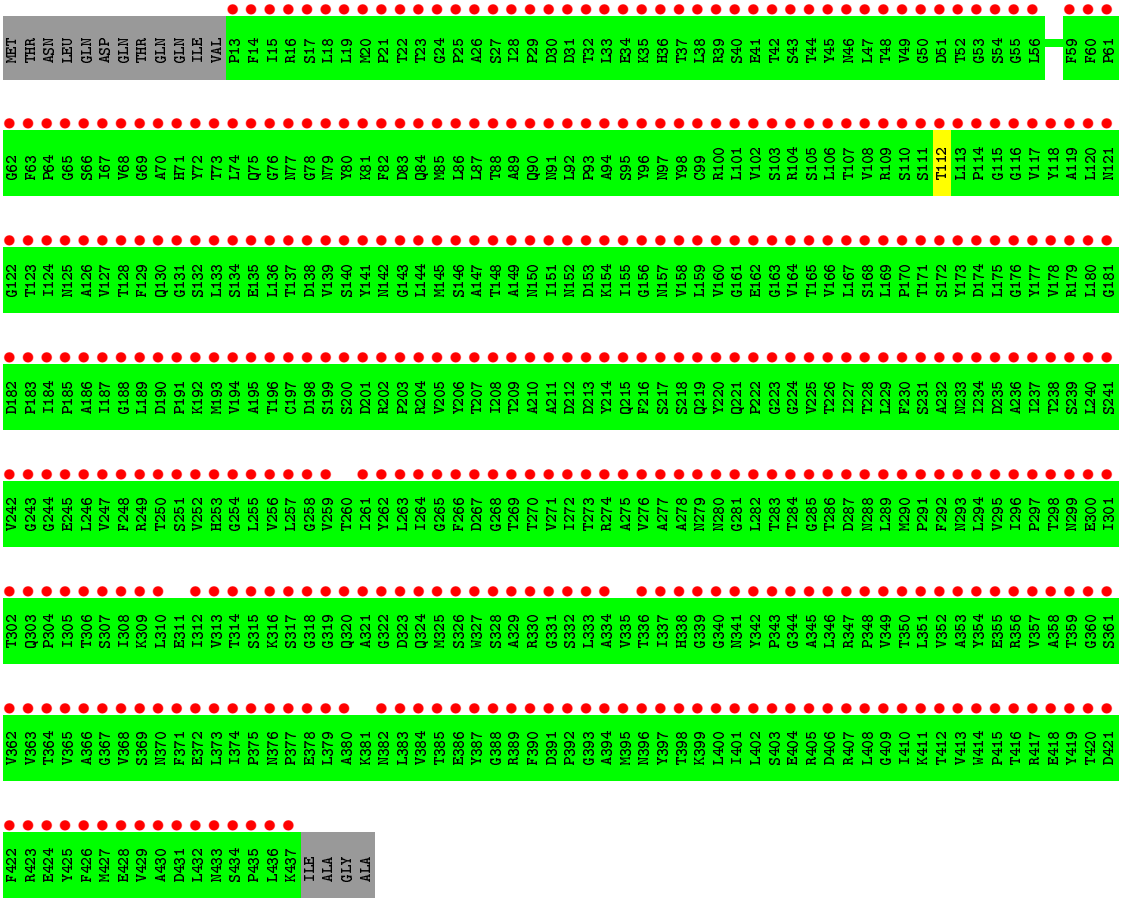
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 STRUCTURAL PROTEIN VP2

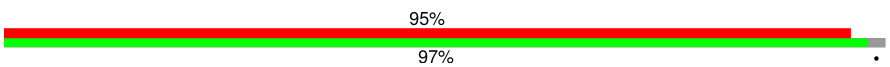
Chain A:

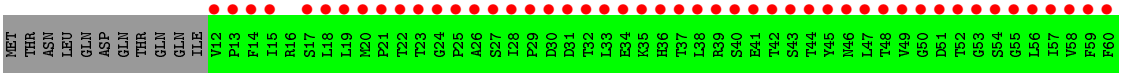


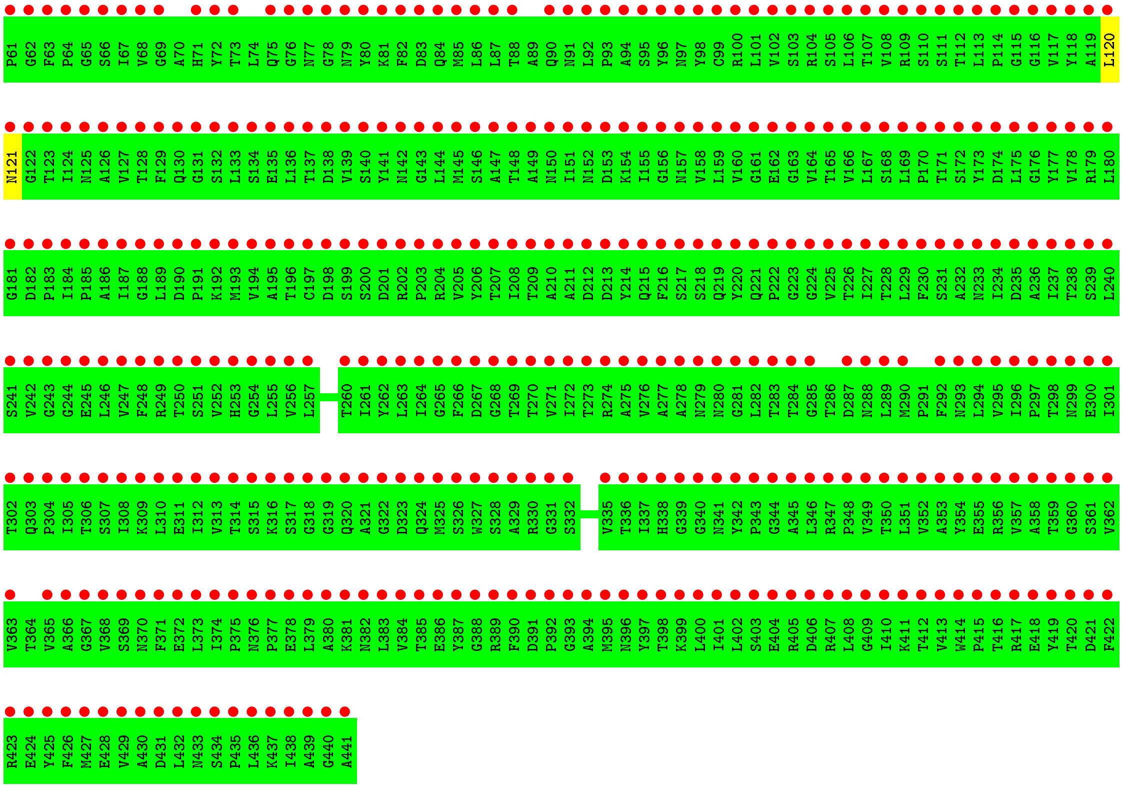


- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain B:

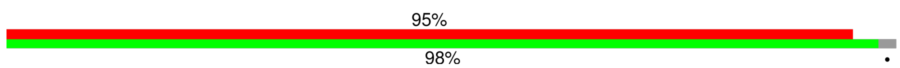


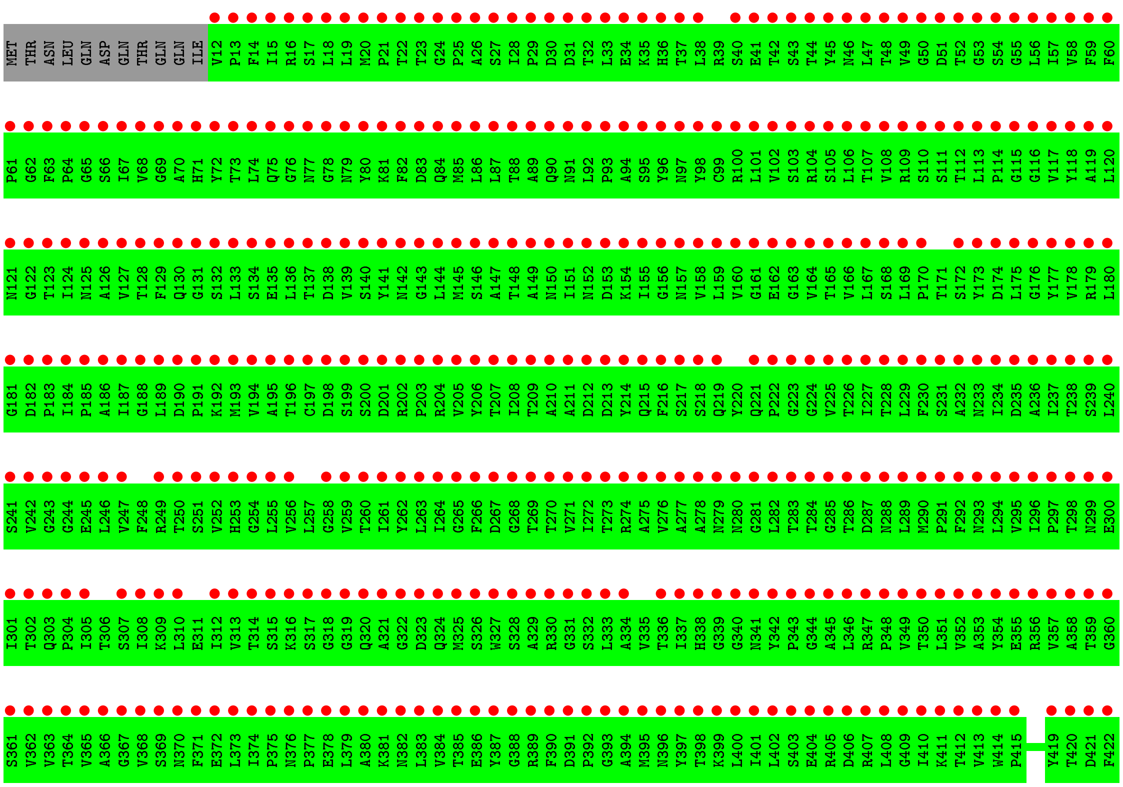


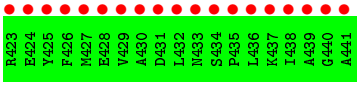


- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain C:

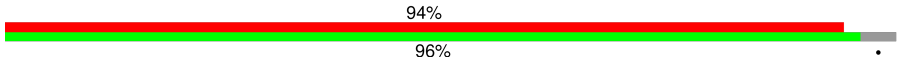


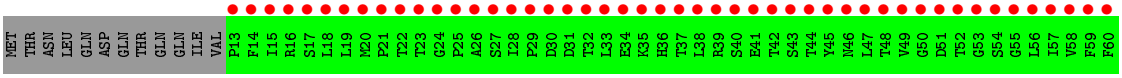


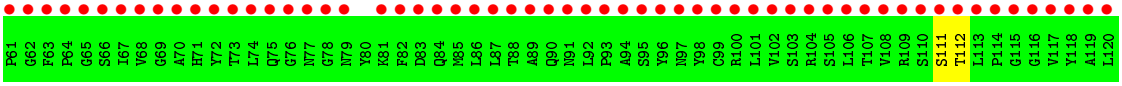


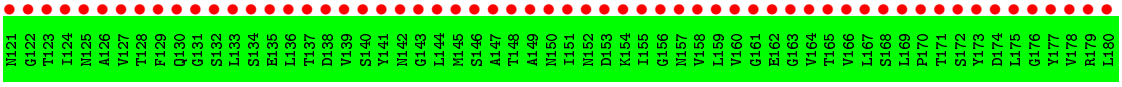
• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

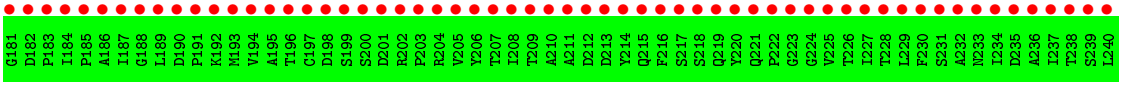
Chain D:

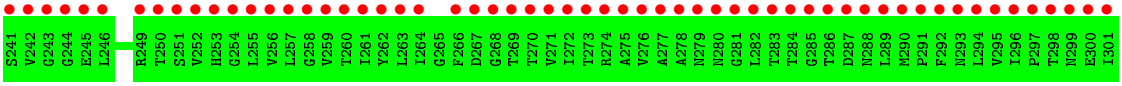


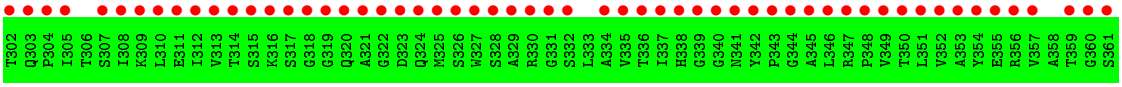


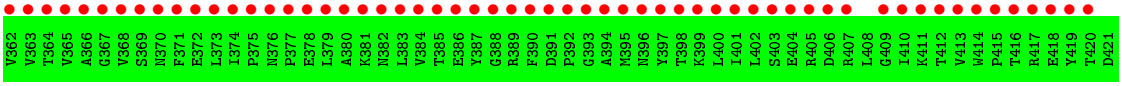


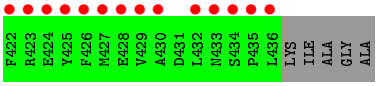






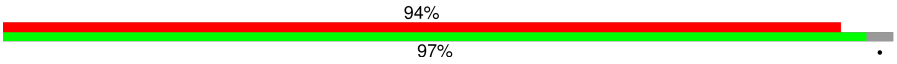


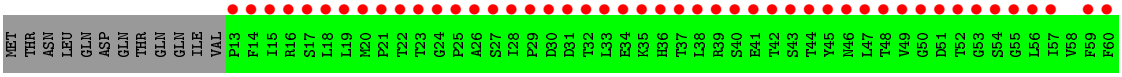


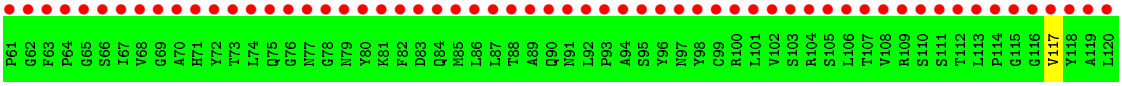


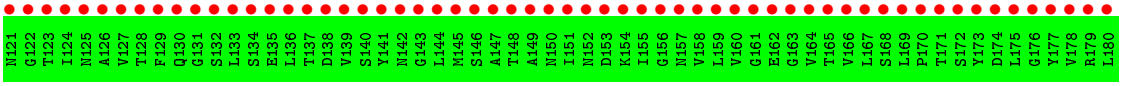
• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

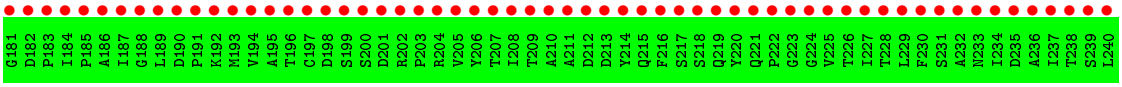
Chain E:





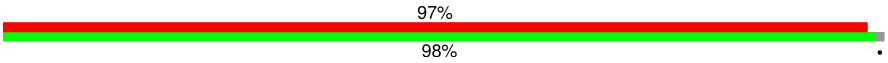


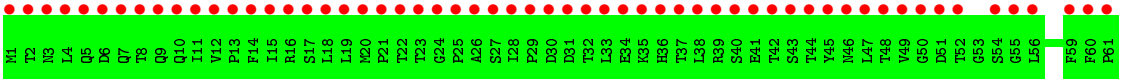


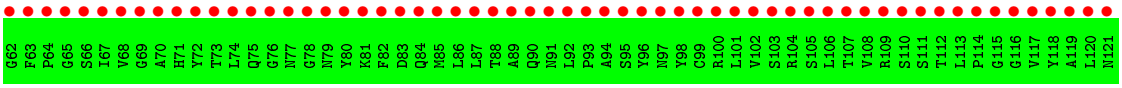


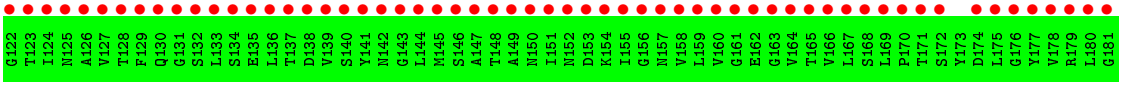
• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

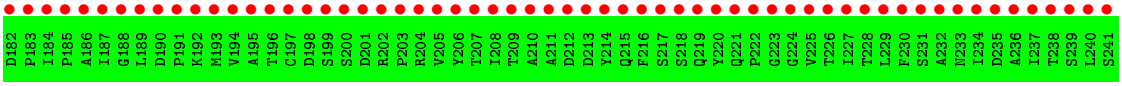
Chain F:

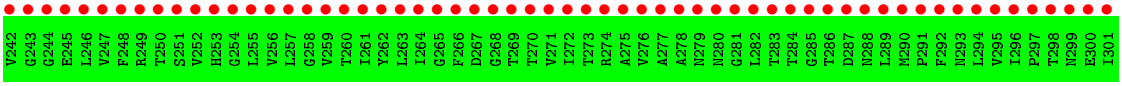


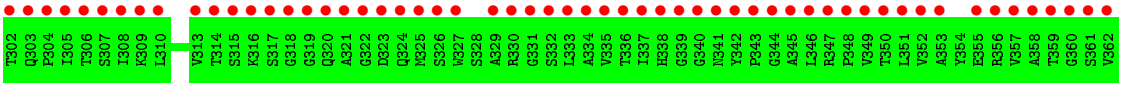






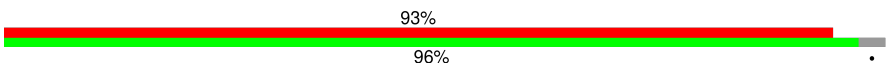


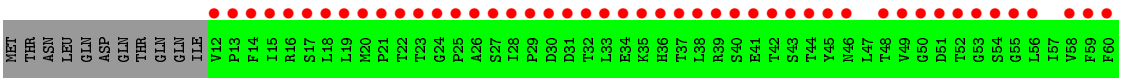


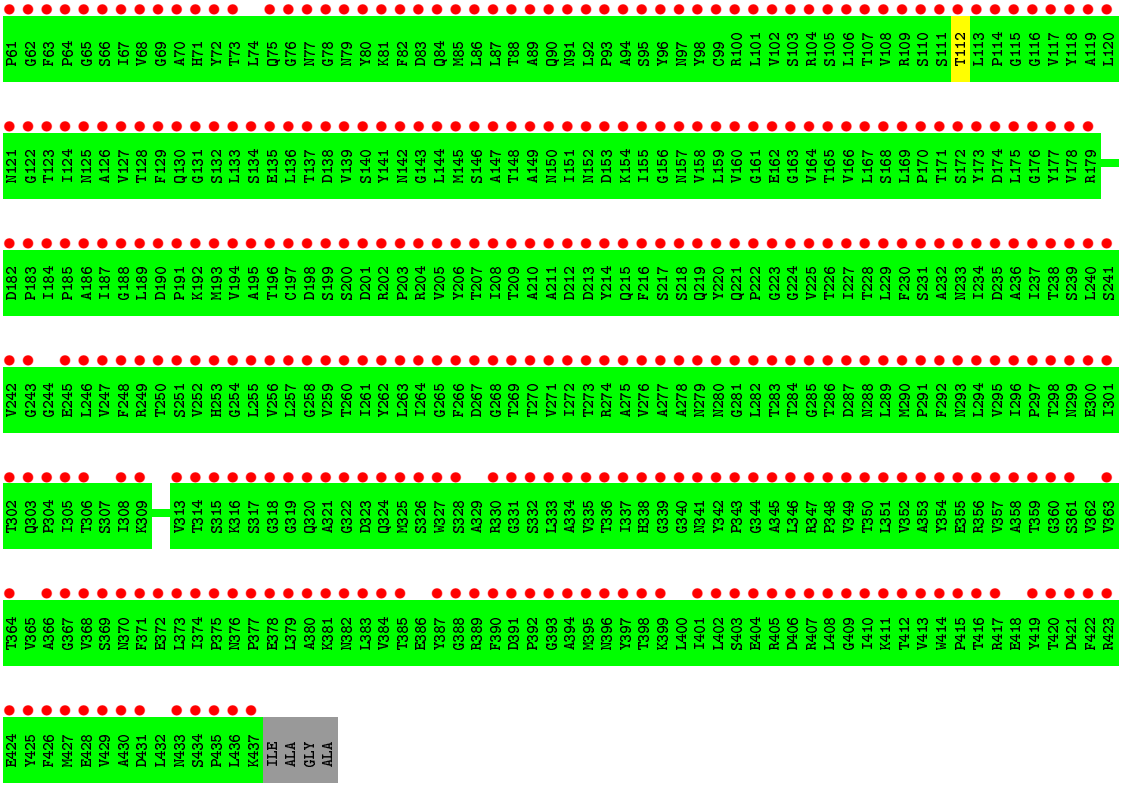


• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain G:

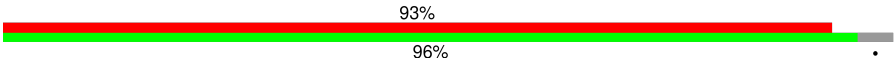


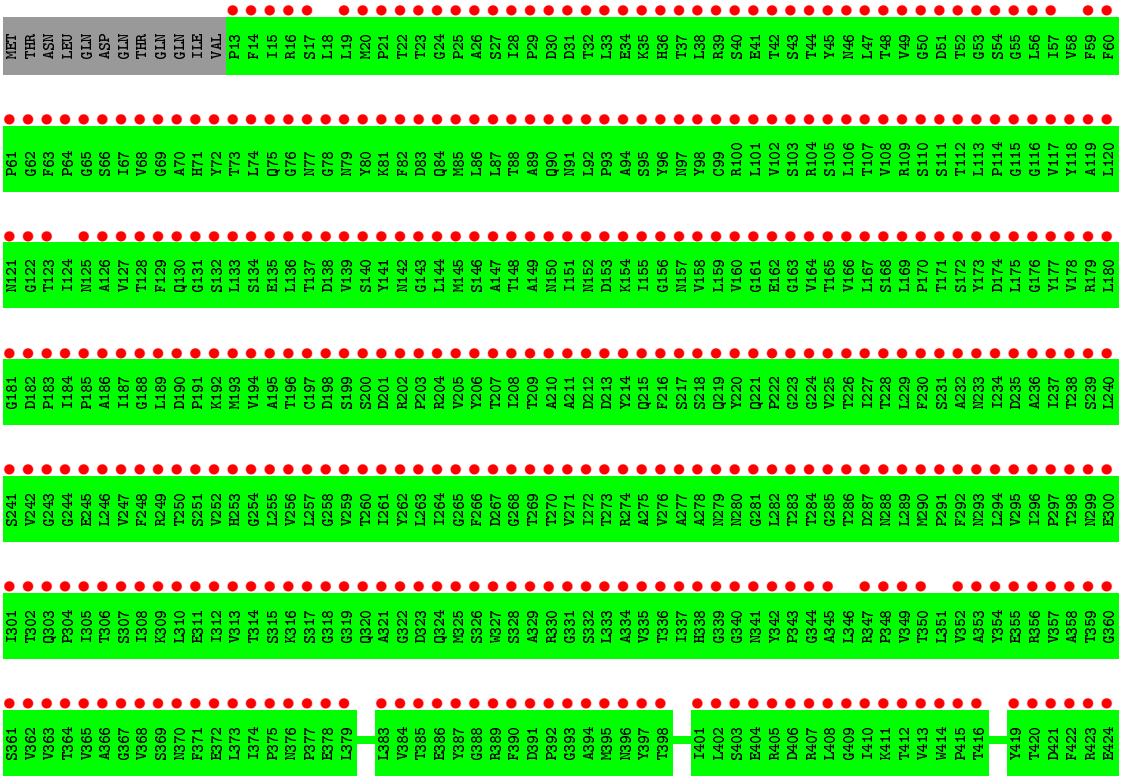


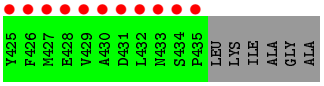


- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain H:

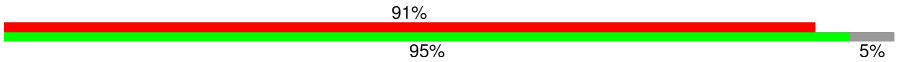


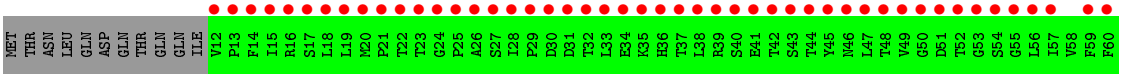


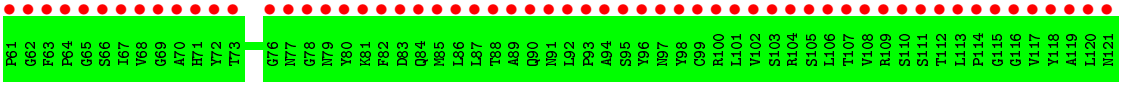


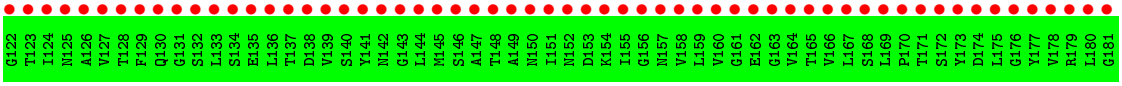
• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

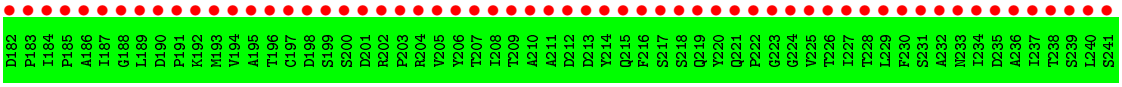
Chain I:

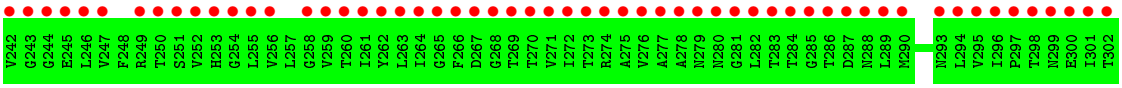


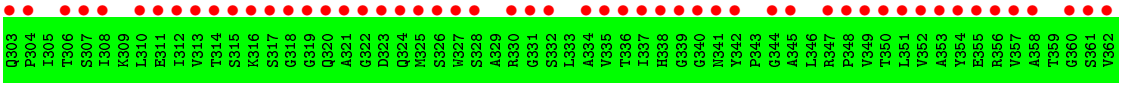


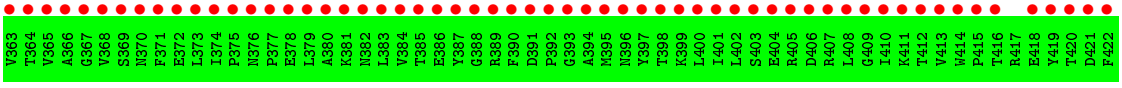


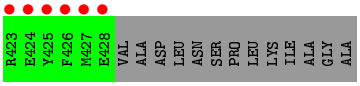






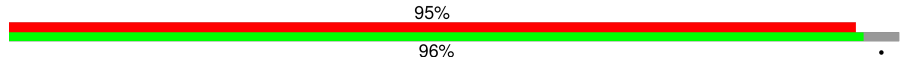


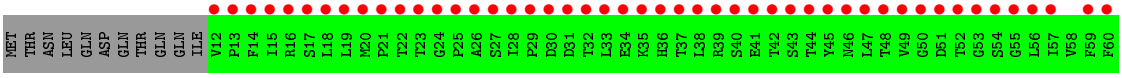


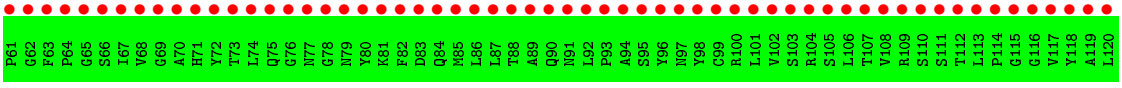


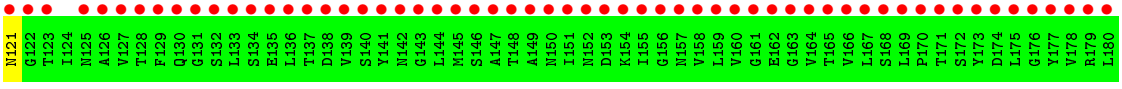
• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

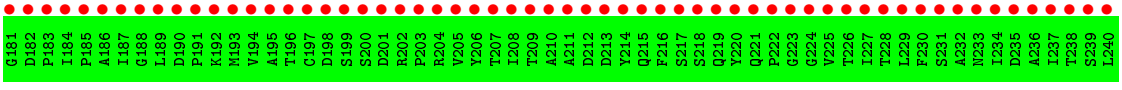
Chain J:

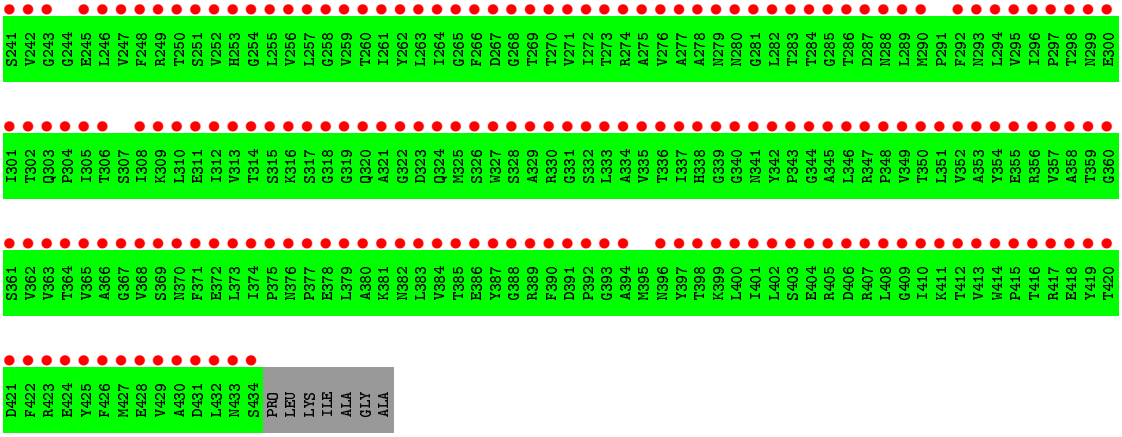






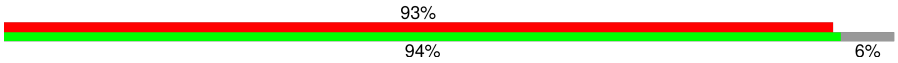


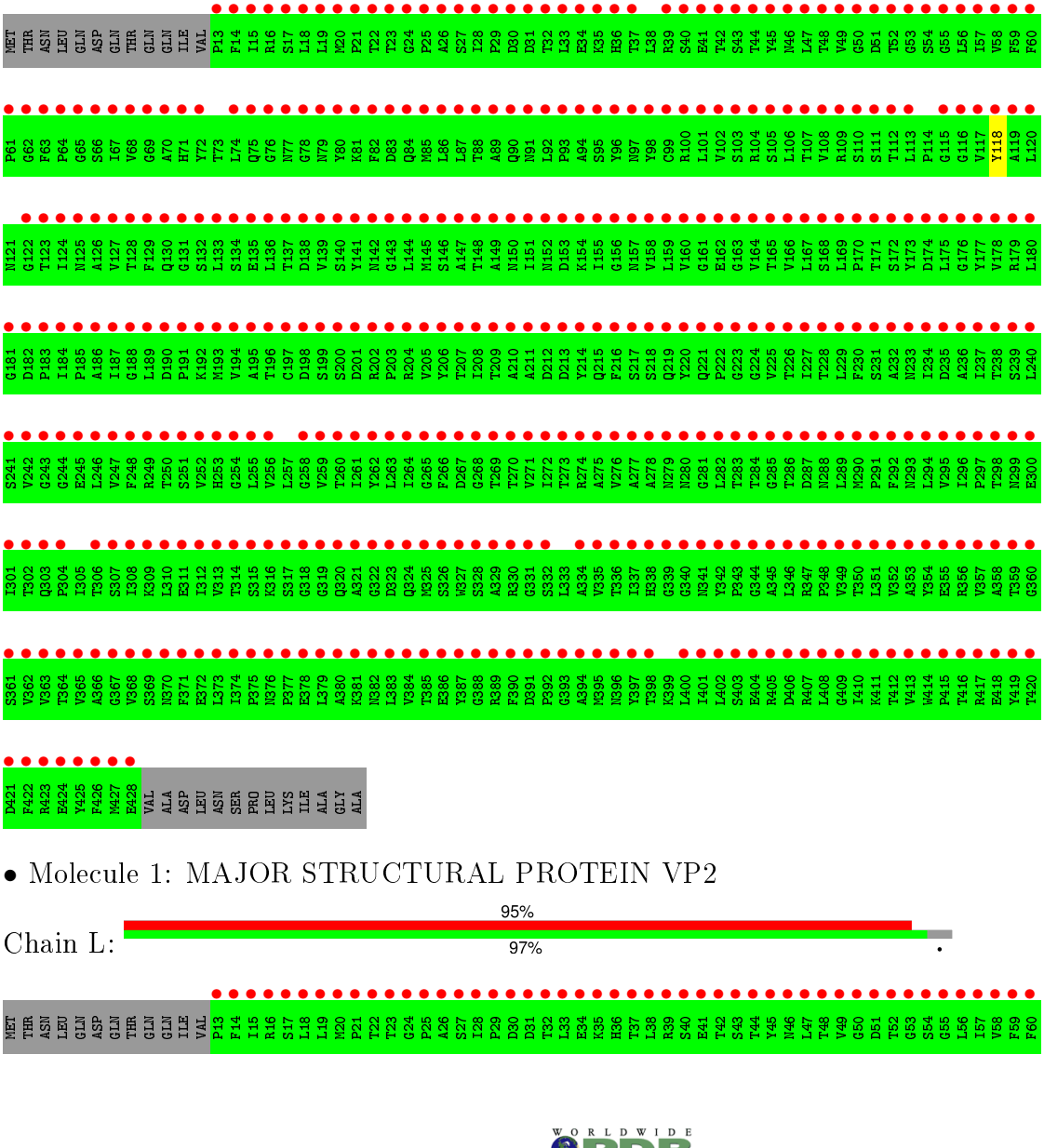




• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

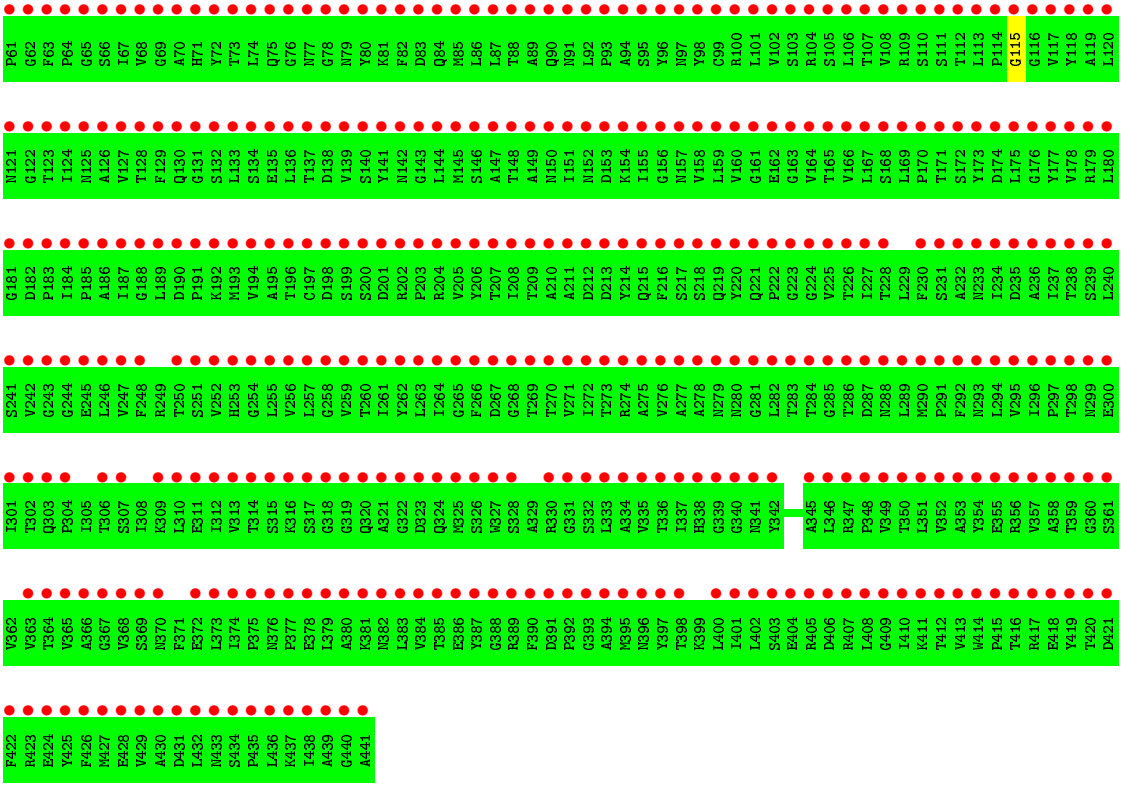
Chain K:





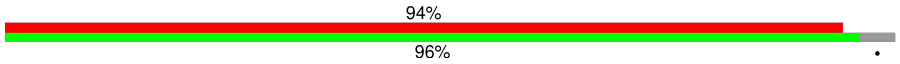
• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

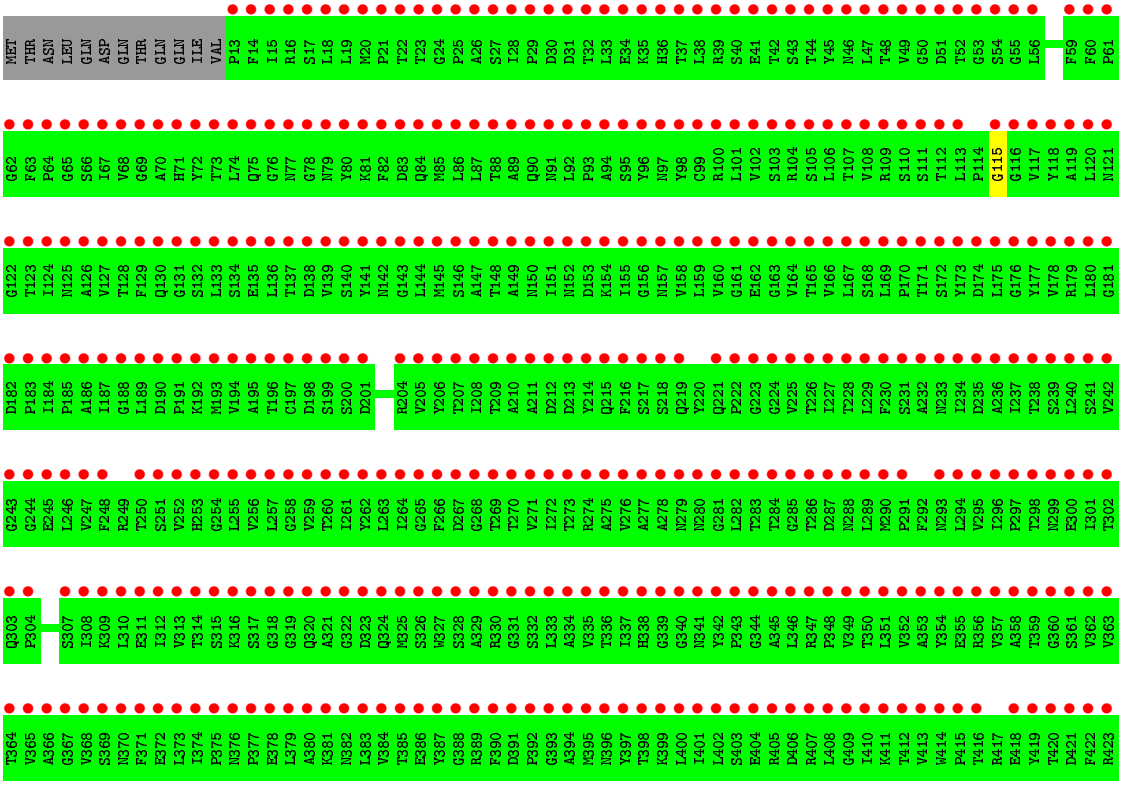
Chain L:

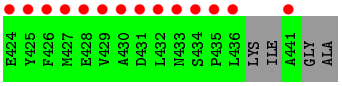


- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain M:






E424
Y425
F426
N427
E428
V429
A430
D431
L432
N433
S434
P435
L436
LYS
ILE
A441
GLY
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	854.01Å 692.23Å 792.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 7.00 49.86 – 6.97	Depositor EDS
% Data completeness (in resolution range)	75.1 (50.00-7.00) 74.8 (49.86-6.97)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 6.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	(Not available) , (Not available) 0.411 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	190.2	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 27.2	EDS
Estimated twinning fraction	0.327 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	2 of 1089556 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.65	EDS
Total number of atoms	5533	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	425	0	0	2	0
1	B	430	0	0	2	0
1	C	430	0	0	0	0
1	D	424	0	0	1	0
1	E	429	0	0	1	0
1	F	436	0	0	1	0
1	G	426	0	0	1	0
1	H	423	0	0	0	0
1	I	417	0	0	0	0
1	J	423	0	0	1	0
1	K	416	0	0	1	0
1	L	429	0	0	1	0
1	M	425	0	0	1	0
All	All	5533	0	0	7	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 1.

The worst 5 of 7 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:D:111:SER:CA	1:D:112:THR:CA	1.85	1.51
1:E:117:VAL:CA	1:M:115:GLY:CA	2.26	1.13
1:A:112:THR:CA	1:B:121:ASN:CA	2.64	0.76
1:K:118:TYR:CA	1:L:115:GLY:CA	2.82	0.58
1:A:112:THR:CA	1:B:120:LEU:CA	2.96	0.43

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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, 95^{th} 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	425/441 (96%)	7.27	419 (98%)	0	0	20, 47, 95, 99	0
1	B	430/441 (97%)	6.81	419 (97%)	0	1	20, 47, 95, 99	0
1	C	430/441 (97%)	6.88	419 (97%)	0	1	20, 47, 95, 99	0
1	D	424/441 (96%)	6.85	414 (97%)	0	1	20, 47, 95, 99	0
1	E	429/441 (97%)	6.77	416 (96%)	0	1	20, 47, 95, 99	0
1	F	436/441 (98%)	7.11	427 (97%)	0	1	20, 46, 95, 99	0
1	G	426/441 (96%)	6.86	409 (96%)	0	1	20, 47, 95, 99	0
1	H	423/441 (95%)	6.76	411 (97%)	0	1	20, 47, 95, 99	0
1	I	417/441 (94%)	7.04	402 (96%)	0	1	20, 47, 96, 99	0
1	J	423/441 (95%)	7.20	417 (98%)	0	0	20, 47, 95, 99	0
1	K	416/441 (94%)	6.70	408 (98%)	0	1	20, 47, 96, 99	0
1	L	429/441 (97%)	7.03	419 (97%)	0	1	20, 47, 95, 99	0
1	M	425/441 (96%)	6.97	414 (97%)	0	1	20, 47, 95, 99	0
All	All	5533/5733 (96%)	6.94	5394 (97%)	0	1	20, 47, 96, 99	0

The worst 5 of 5394 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	150	ASN	25.7
1	C	209	THR	25.7
1	A	64	PRO	23.9
1	F	83	ASP	23.4
1	D	391	ASP	23.1

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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.