



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 02:50 am BST

PDB ID : 4PB6
Title : Feline calicivirus VP1 T=1 virus-like particle
Authors : Burmeister, W.P.; Buisson, M.
Deposited on : 2014-04-11
Resolution : 8.00 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 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

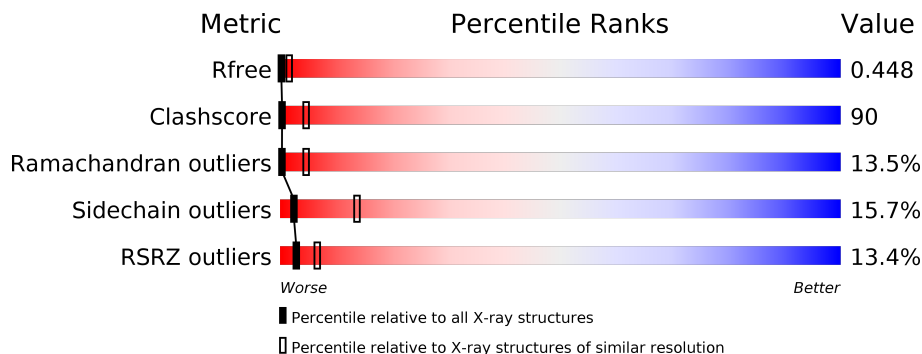
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.00 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))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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 $\leq 5\%$. 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	545	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 53%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	B	545	<div style="display: flex; align-items: center;"> <div style="width: 16%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	C	545	<div style="display: flex; align-items: center;"> <div style="width: 15%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	D	545	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	E	545	<div style="display: flex; align-items: center;"> <div style="width: 17%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 53%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	F	545	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	545	
1	H	545	
1	I	545	
1	J	545	
1	K	545	
1	L	545	
1	M	545	
1	N	545	
1	O	545	
1	P	545	
1	Q	545	
1	R	545	
1	S	545	
1	T	545	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 77840 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	502	3892	2491	651	742	8	0	0	0
1	B	502	3892	2491	651	742	8	0	0	0
1	C	502	3892	2491	651	742	8	0	0	0
1	D	502	3892	2491	651	742	8	0	0	0
1	E	502	3892	2491	651	742	8	0	0	0
1	F	502	3892	2491	651	742	8	0	0	0
1	G	502	3892	2491	651	742	8	0	0	0
1	H	502	3892	2491	651	742	8	0	0	0
1	I	502	3892	2491	651	742	8	0	0	0
1	J	502	3892	2491	651	742	8	0	0	0
1	K	502	3892	2491	651	742	8	0	0	0
1	L	502	3892	2491	651	742	8	0	0	0
1	M	502	3892	2491	651	742	8	0	0	0
1	N	502	3892	2491	651	742	8	0	0	0
1	O	502	3892	2491	651	742	8	0	0	0
1	P	502	3892	2491	651	742	8	0	0	0

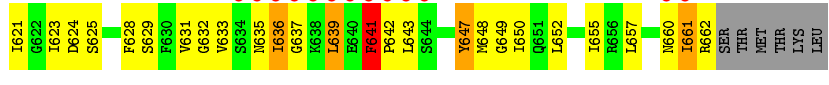
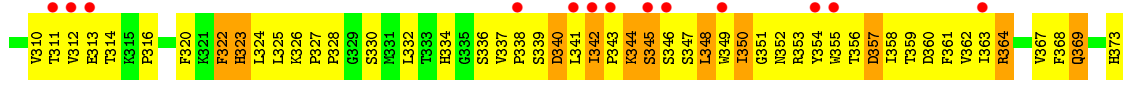
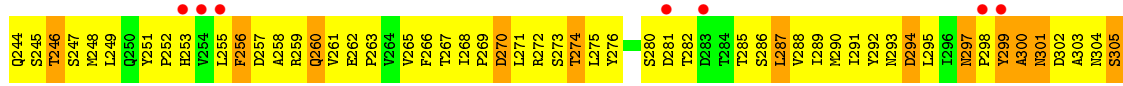
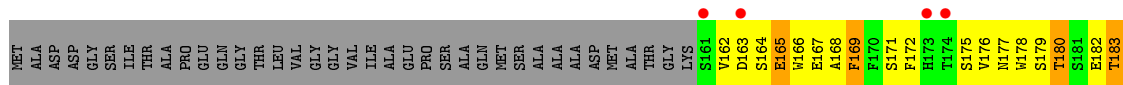
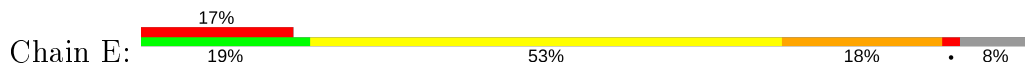
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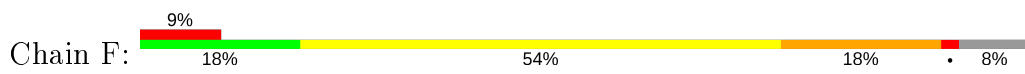
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	502	Total 3892	C 2491	N 651	O 742	S 8	0	0	0
1	R	502	Total 3892	C 2491	N 651	O 742	S 8	0	0	0
1	S	502	Total 3892	C 2491	N 651	O 742	S 8	0	0	0
1	T	502	Total 3892	C 2491	N 651	O 742	S 8	0	0	0

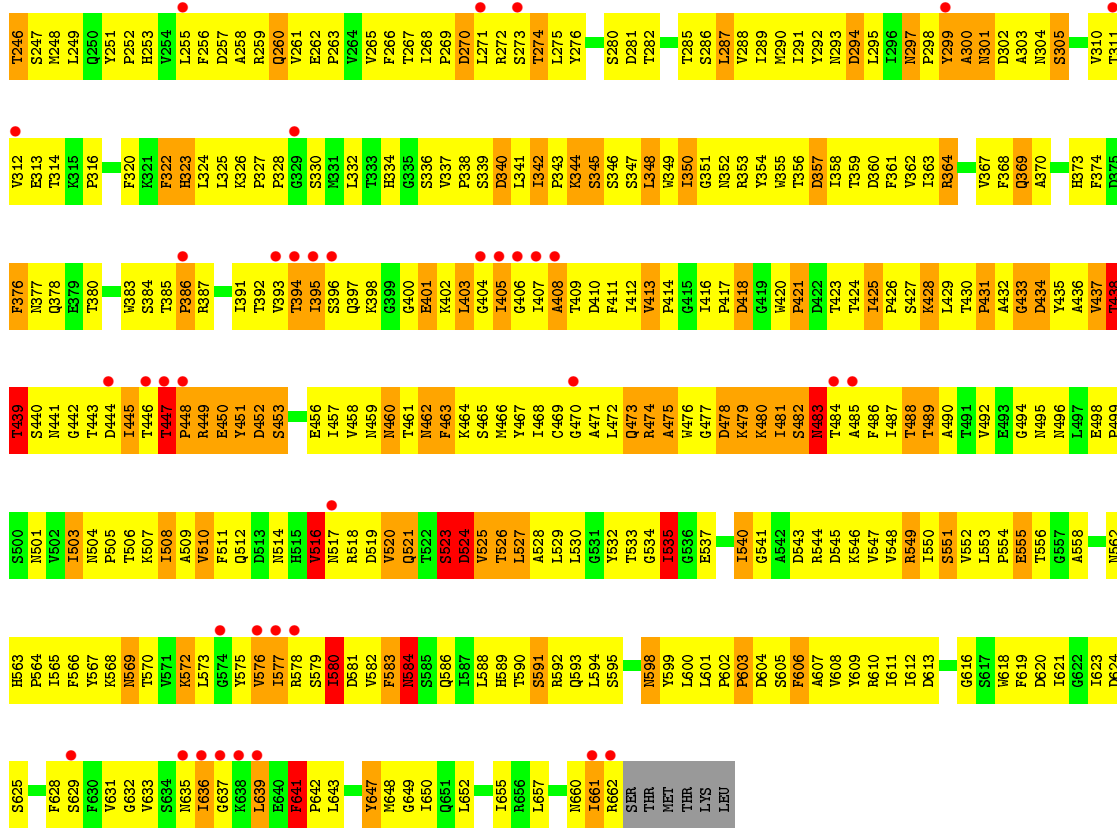


• Molecule 1: VP1

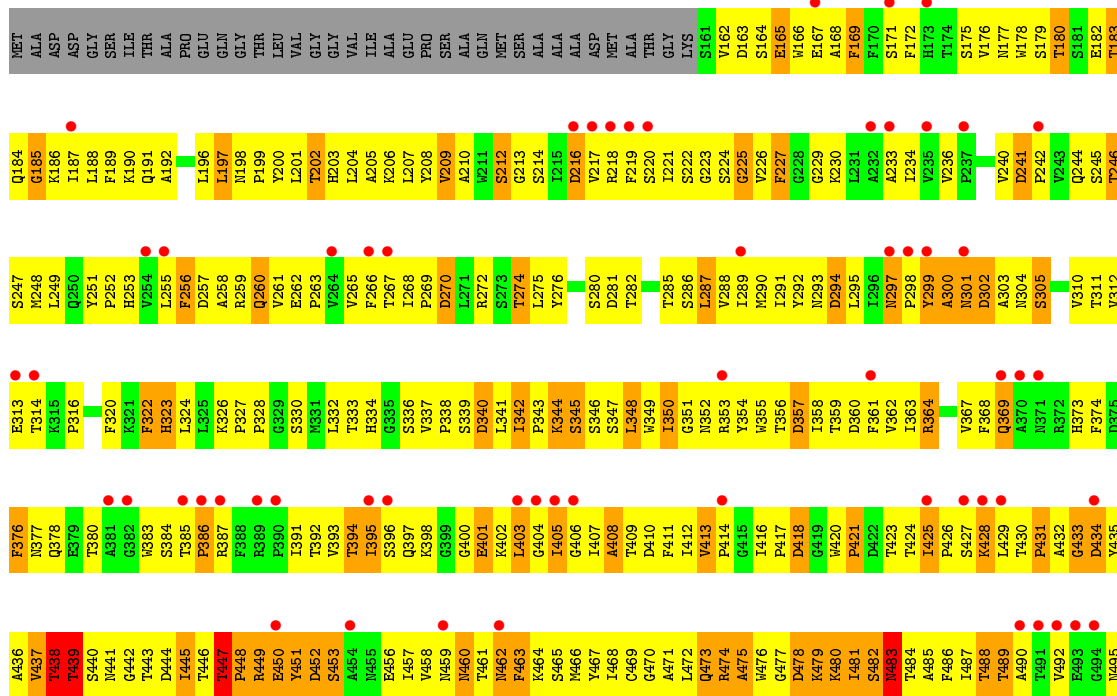
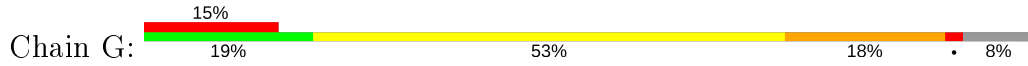


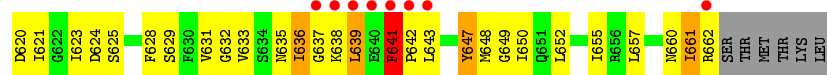
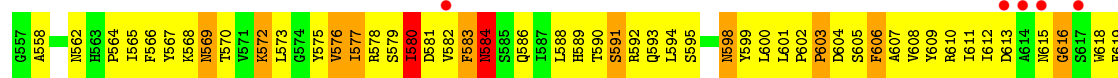
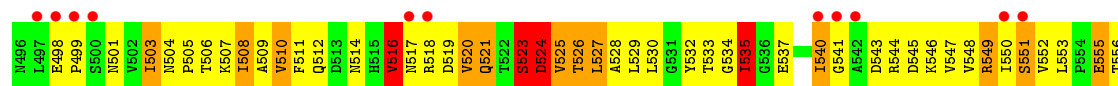
• Molecule 1: VP1



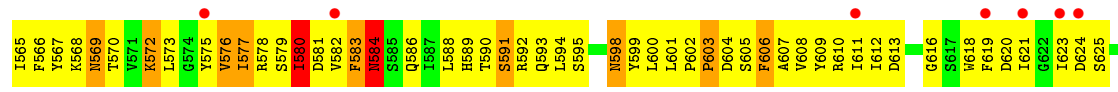
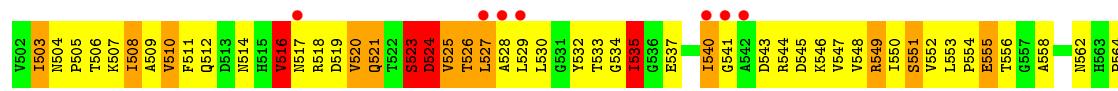
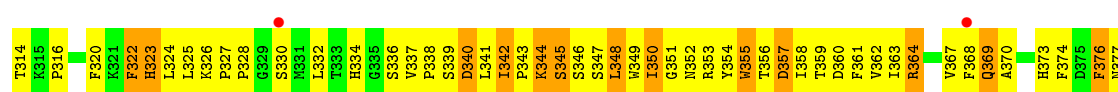
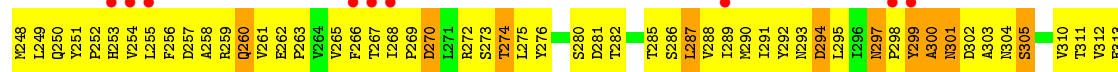
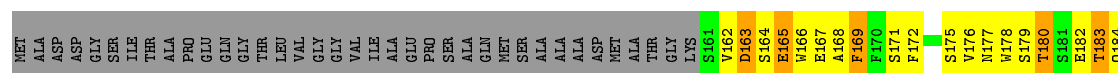
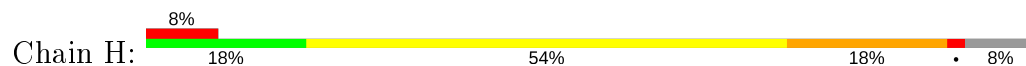


• Molecule 1: VP1

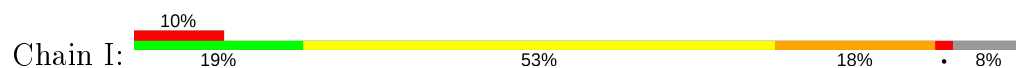


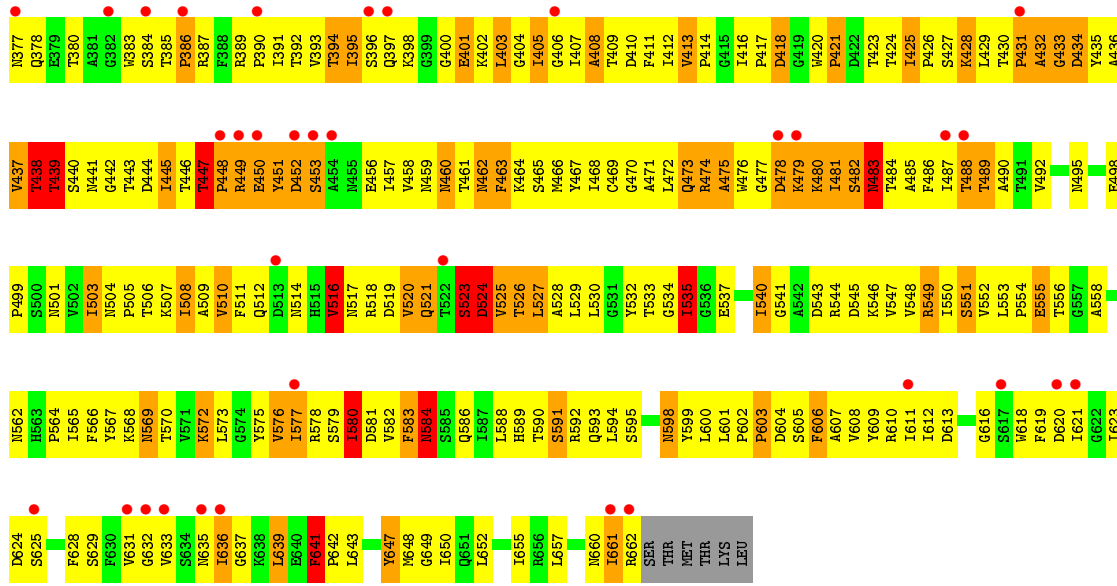


• Molecule 1: VP1

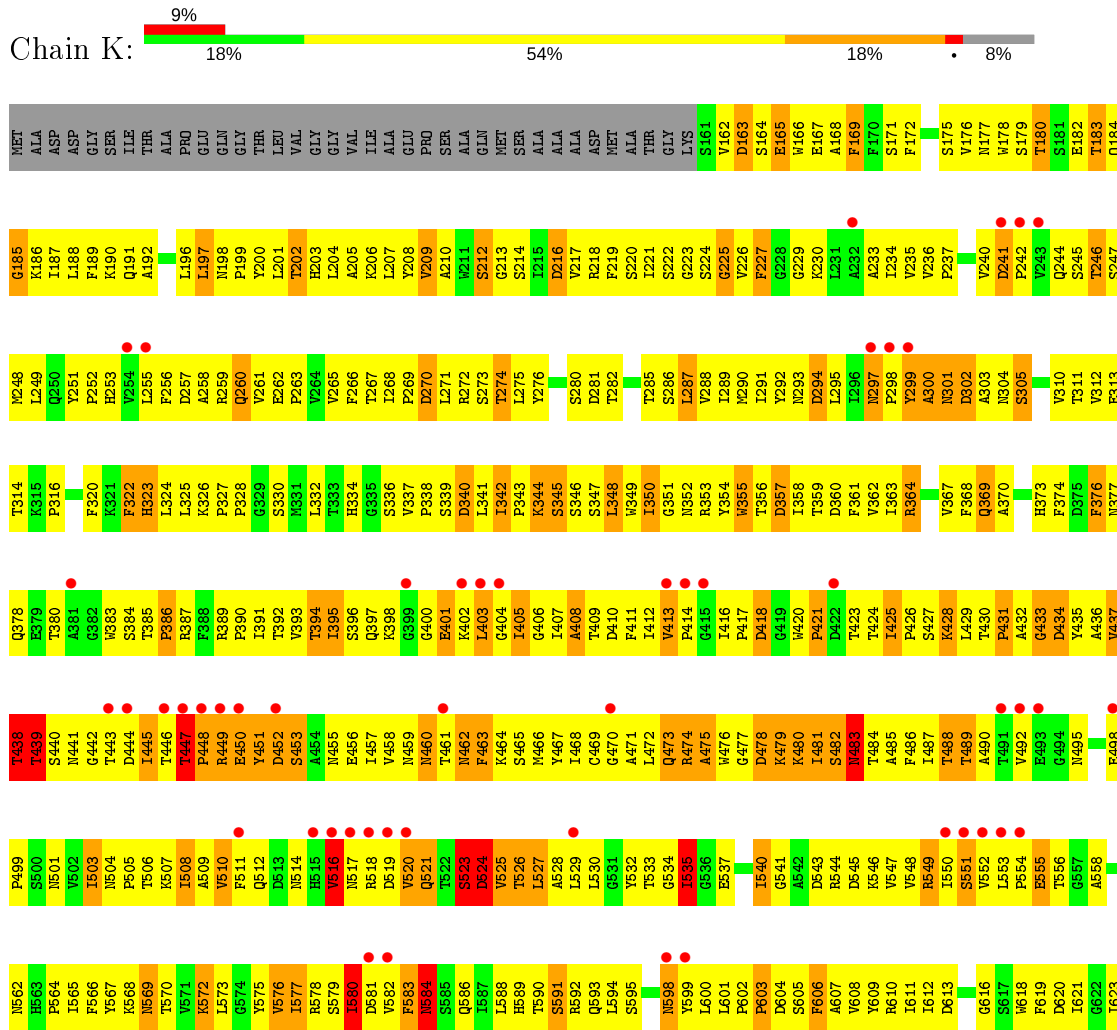


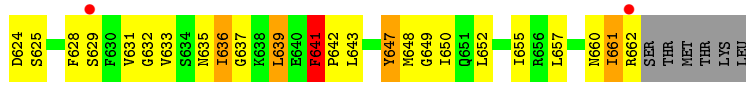
• Molecule 1: VP1



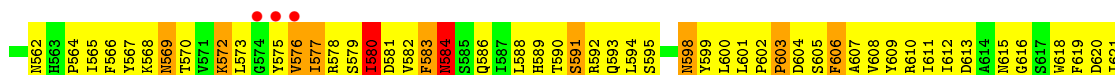
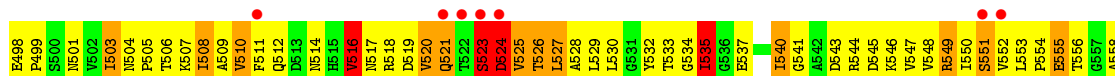
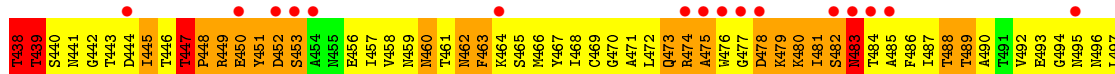
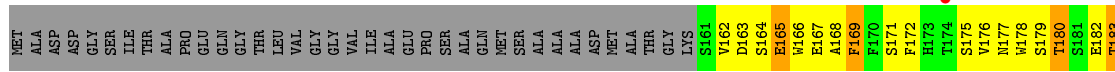
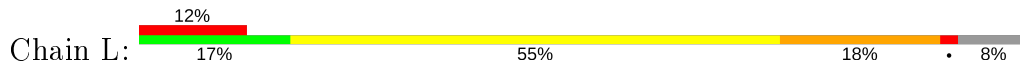


• Molecule 1: VP1

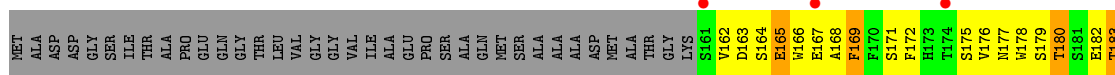
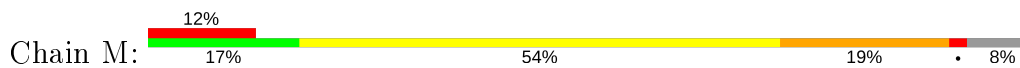


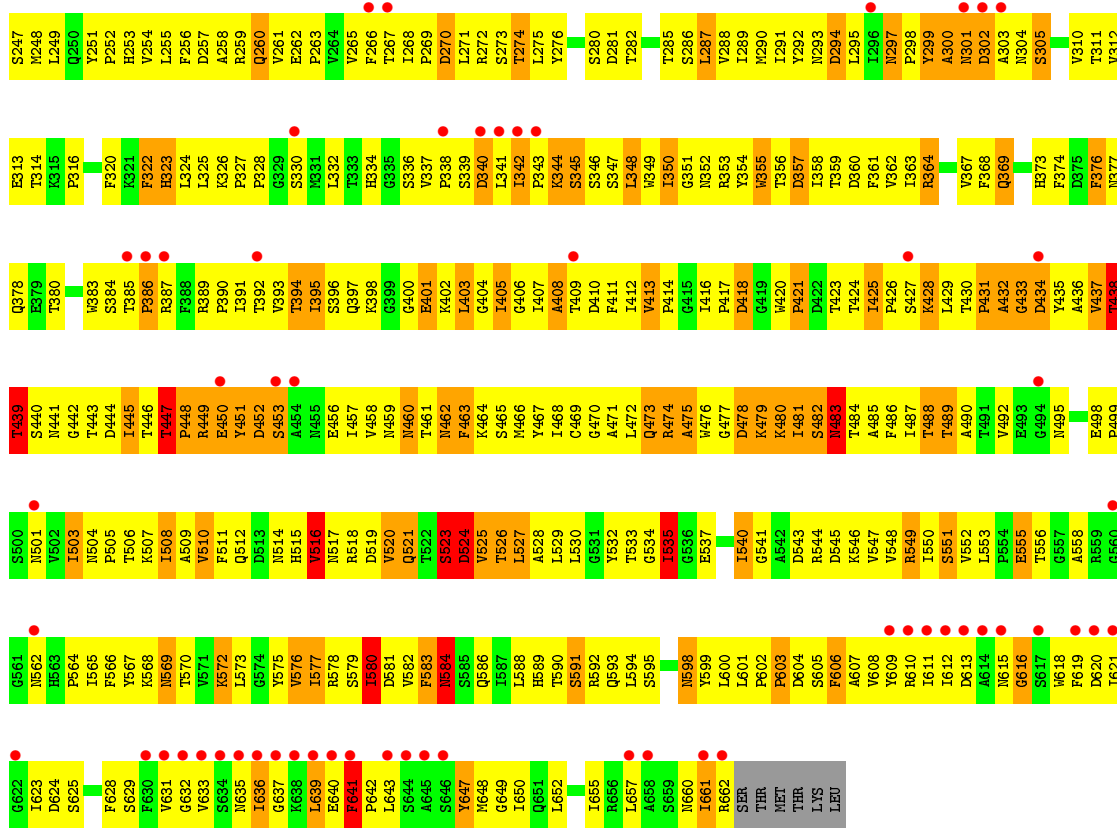


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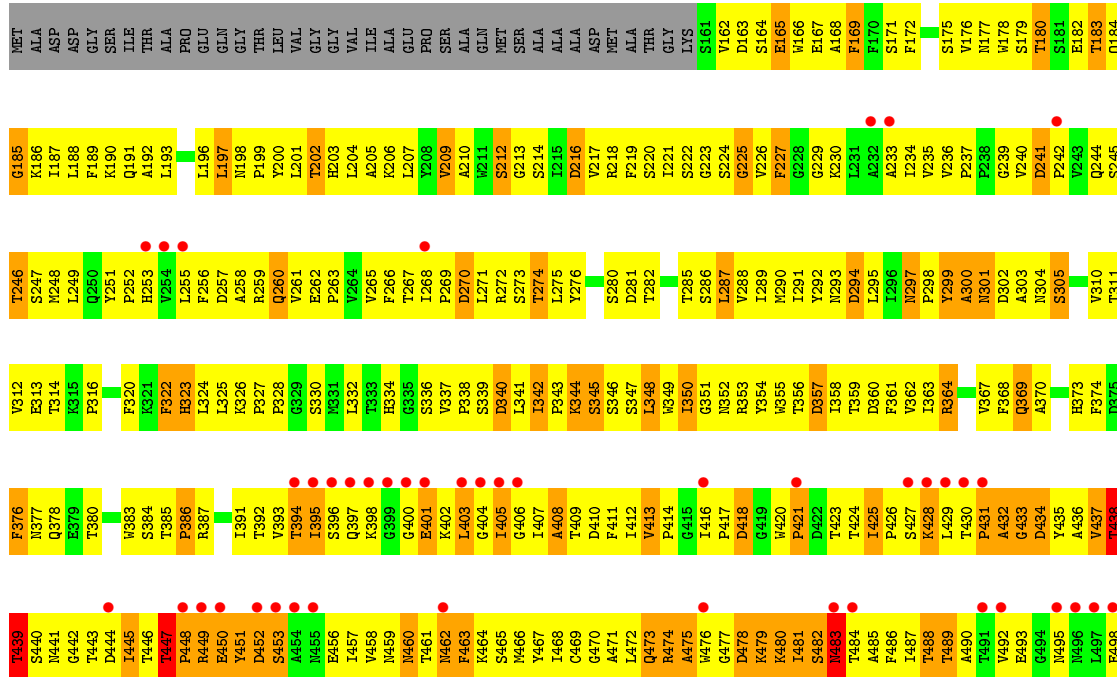
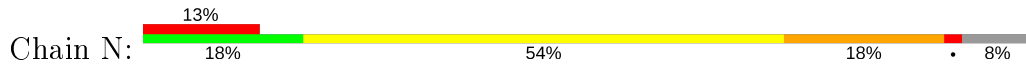


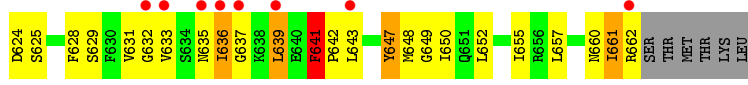
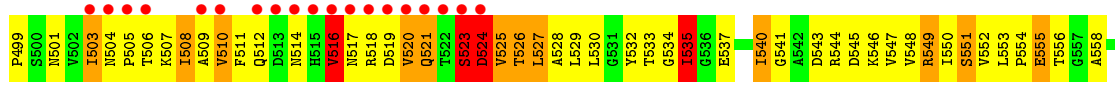
• Molecule 1: VP1



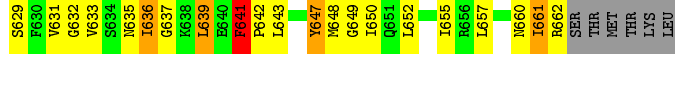
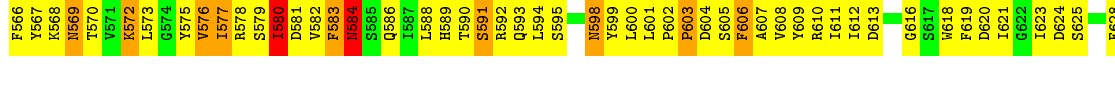
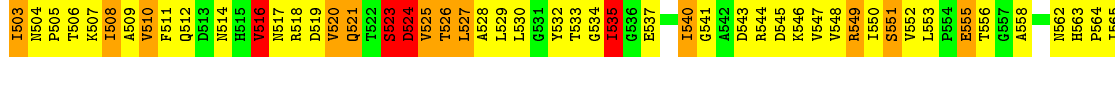
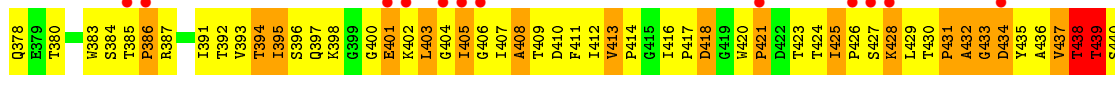
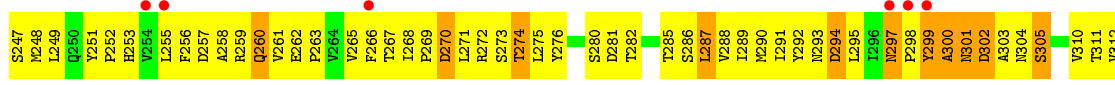
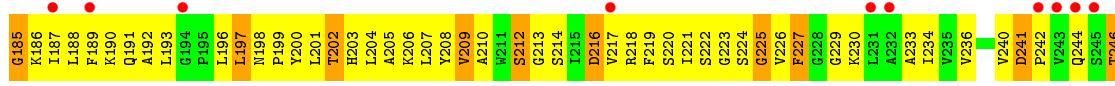
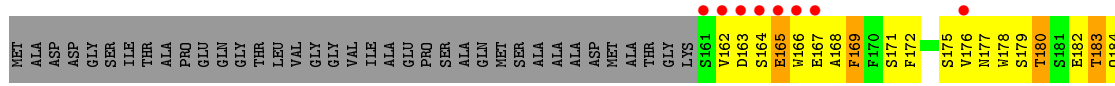
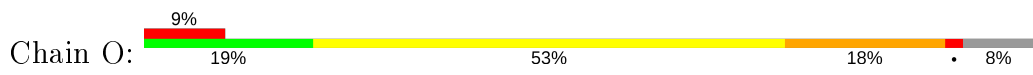


• Molecule 1: VP1

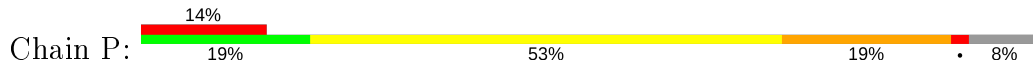


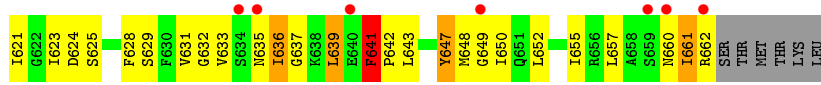


• Molecule 1: VP1

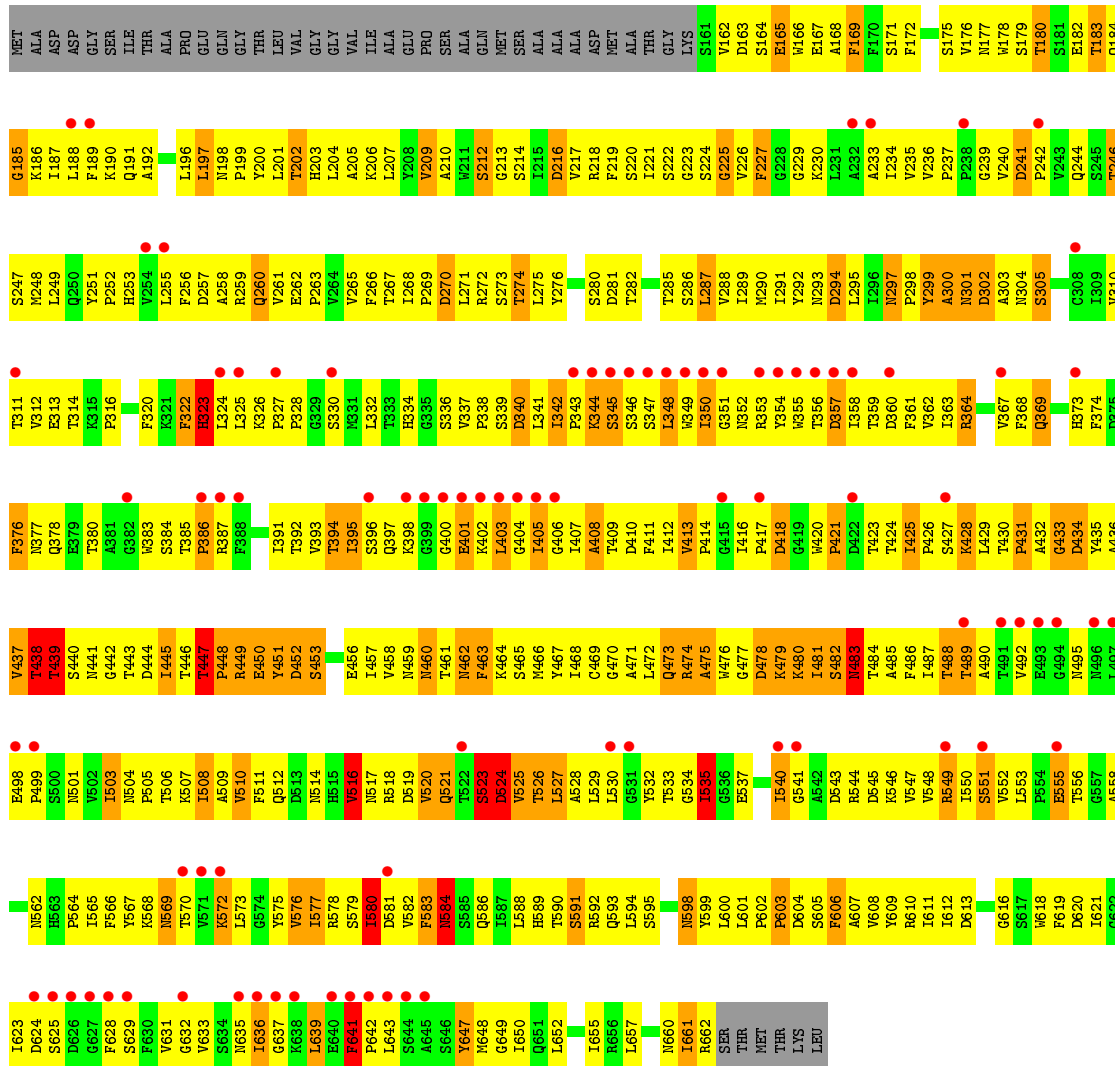
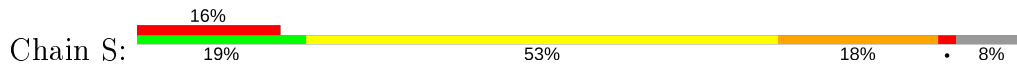


• Molecule 1: VP1

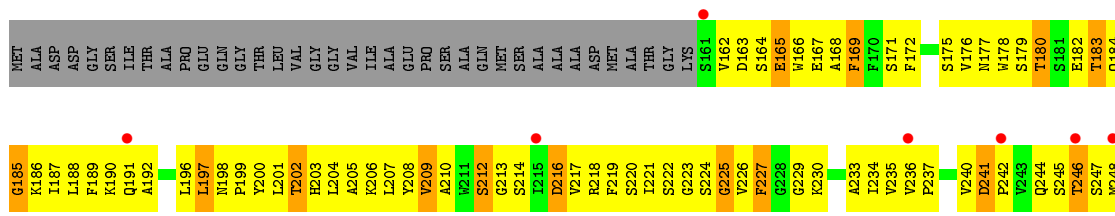
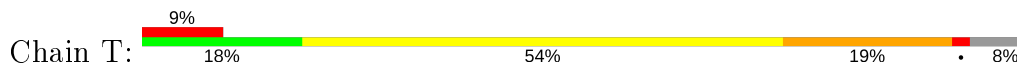


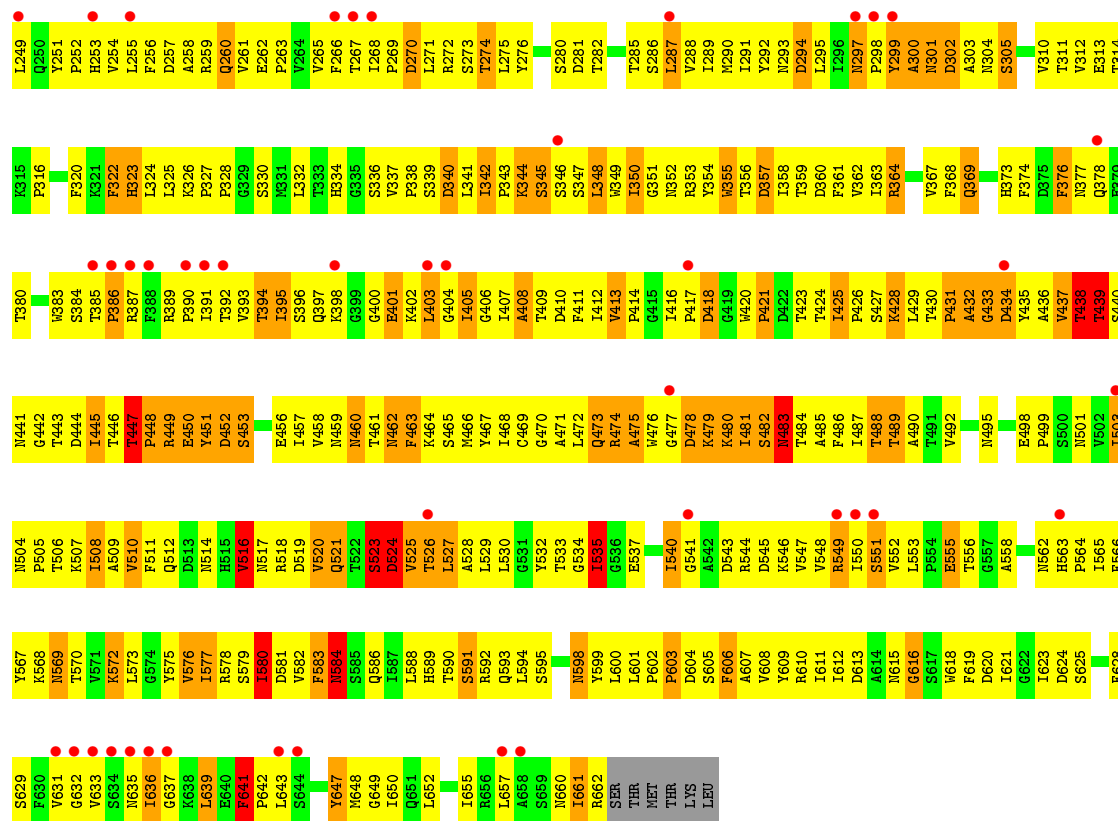


• Molecule 1: VP1



• Molecule 1: VP1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	358.34Å 358.34Å 358.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.51 – 8.00 65.42 – 8.00	Depositor EDS
% Data completeness (in resolution range)	87.8 (65.51-8.00) 88.1 (65.42-8.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 8.38Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.441 , 0.463 0.426 , 0.448	Depositor DCC
R_{free} test set	710 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	426.8	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.83 , 94.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.16$	Xtrriage
Estimated twinning fraction	0.108 for l,-k,h	Xtrriage
F_o, F_c correlation	0.54	EDS
Total number of atoms	77840	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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](#)

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	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	B	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	C	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	D	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	E	0.67	2/3991 (0.1%)	0.89	11/5446 (0.2%)
1	F	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	G	0.67	2/3991 (0.1%)	0.89	11/5446 (0.2%)
1	H	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	I	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	J	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	K	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	L	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	M	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	N	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	O	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	P	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	Q	0.67	2/3991 (0.1%)	0.89	11/5446 (0.2%)
1	R	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	S	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
1	T	0.67	1/3991 (0.0%)	0.89	11/5446 (0.2%)
All	All	0.67	23/79820 (0.0%)	0.89	220/108920 (0.2%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	476	TRP	CB-CG	5.99	1.61	1.50
1	H	476	TRP	CB-CG	5.97	1.60	1.50
1	Q	476	TRP	CB-CG	5.97	1.60	1.50
1	E	476	TRP	CB-CG	5.96	1.60	1.50
1	K	476	TRP	CB-CG	5.96	1.60	1.50

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	451	TYR	CB-CA-C	-8.92	92.56	110.40
1	C	451	TYR	CB-CA-C	-8.90	92.60	110.40
1	N	451	TYR	CB-CA-C	-8.90	92.60	110.40
1	F	451	TYR	CB-CA-C	-8.89	92.62	110.40
1	I	451	TYR	CB-CA-C	-8.88	92.64	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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	A	3892	0	3823	914	5
1	B	3892	0	3823	911	0
1	C	3892	0	3825	678	207
1	D	3892	0	3823	913	3
1	E	3892	0	3824	824	88
1	F	3892	0	3823	917	8
1	G	3892	0	3825	684	143
1	H	3892	0	3825	678	124
1	I	3892	0	3825	675	88
1	J	3892	0	3824	761	91
1	K	3892	0	3824	760	104
1	L	3892	0	3823	910	38
1	M	3892	0	3824	772	123
1	N	3892	0	3824	826	115
1	O	3892	0	3825	676	152
1	P	3892	0	3825	684	149
1	Q	3892	0	3824	845	85
1	R	3892	0	3823	912	14
1	S	3892	0	3824	823	82
1	T	3892	0	3824	761	85
All	All	77840	0	76480	13874	928

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 90.

The worst 5 of 13874 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:325:LEU:HD22	1:D:165:GLU:CG	1.29	1.62
1:Q:325:LEU:HD22	1:R:165:GLU:CG	1.29	1.61
1:A:325:LEU:HD22	1:E:165:GLU:CG	1.29	1.60
1:L:325:LEU:HD22	1:S:165:GLU:CG	1.29	1.59
1:Q:165:GLU:CD	1:R:325:LEU:HD22	1.20	1.58

The worst 5 of 928 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:GLU:O	1:C:518:ARG:CD[7_564]	0.17	2.03
1:G:251:TYR:CE1	1:M:327:PRO:O[9_555]	0.34	1.86
1:R:435:TYR:CD1	1:R:519:ASP:OD1[11_455]	0.35	1.85
1:O:251:TYR:CE1	1:T:327:PRO:O[5_555]	0.38	1.82
1:H:272:ARG:O	1:H:276:TYR:CE1[9_555]	0.40	1.80

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	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	4
1	B	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	4
1	C	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	4
1	D	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	4
1	E	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	4
1	F	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	4
1	G	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	4
1	H	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	4
1	J	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	4
1	K	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	4
1	L	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	4
1	M	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	4
1	N	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	4
1	O	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	4
1	P	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	4
1	Q	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	4
1	R	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	4
1	S	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	4
1	T	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	4
All	All	9960/10900 (91%)	6341 (64%)	2279 (23%)	1340 (14%)	0	4

5 of 1340 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	A	300	ALA
1	A	301	ASN
1	A	303	ALA
1	A	305	SER

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	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	B	434/464 (94%)	367 (85%)	67 (15%)	2	14
1	C	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	D	434/464 (94%)	366 (84%)	68 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	F	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	G	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	H	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	I	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	J	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	K	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	L	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	M	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	N	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	O	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	P	434/464 (94%)	365 (84%)	69 (16%)	2	13
1	Q	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	R	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	S	434/464 (94%)	366 (84%)	68 (16%)	2	14
1	T	434/464 (94%)	366 (84%)	68 (16%)	2	14
All	All	8680/9280 (94%)	7320 (84%)	1360 (16%)	2	14

5 of 1360 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	183	THR
1	L	287	LEU
1	S	410	ASP
1	J	348	LEU
1	K	266	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 311 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	244	GLN
1	L	297	ASN
1	S	378	GLN
1	J	371	ASN
1	K	244	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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
1	P	1
1	G	1
1	J	1
1	Q	1
1	D	1
1	K	1
1	E	1
1	H	1
1	B	1
1	I	1
1	C	1
1	A	1
1	T	1
1	N	1
1	O	1
1	R	1

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Mol	Chain	Number of breaks
1	L	1
1	S	1
1	F	1
1	M	1

The worst 5 of 20 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	330:SER	C	331:MET	N	3.54
1	B	330:SER	C	331:MET	N	3.54
1	C	330:SER	C	331:MET	N	3.54
1	D	330:SER	C	331:MET	N	3.54
1	E	330:SER	C	331:MET	N	3.54

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	502/545 (92%)	0.79	66 (13%) 3 7	95, 95, 95, 95	0
1	B	502/545 (92%)	1.01	85 (16%) 1 4	95, 95, 95, 95	0
1	C	502/545 (92%)	0.90	82 (16%) 1 4	95, 95, 95, 95	0
1	D	502/545 (92%)	0.73	67 (13%) 3 7	95, 95, 95, 95	0
1	E	502/545 (92%)	0.90	90 (17%) 1 4	95, 95, 95, 95	0
1	F	502/545 (92%)	0.62	50 (9%) 7 10	95, 95, 95, 95	0
1	G	502/545 (92%)	0.96	83 (16%) 1 4	95, 95, 95, 95	0
1	H	502/545 (92%)	0.57	46 (9%) 9 11	95, 95, 95, 95	0
1	I	502/545 (92%)	0.68	53 (10%) 6 9	95, 95, 95, 95	0
1	J	502/545 (92%)	0.70	53 (10%) 6 9	95, 95, 95, 95	0
1	K	502/545 (92%)	0.64	51 (10%) 6 10	95, 95, 95, 95	0
1	L	502/545 (92%)	0.79	67 (13%) 3 7	95, 95, 95, 95	0
1	M	502/545 (92%)	0.73	65 (12%) 3 7	95, 95, 95, 95	0
1	N	502/545 (92%)	0.80	72 (14%) 2 6	95, 95, 95, 95	0
1	O	502/545 (92%)	0.54	47 (9%) 8 11	95, 95, 95, 95	0
1	P	502/545 (92%)	0.92	79 (15%) 2 5	95, 95, 95, 95	0
1	Q	502/545 (92%)	0.73	51 (10%) 6 10	95, 95, 95, 95	0
1	R	502/545 (92%)	1.10	103 (20%) 1 3	95, 95, 95, 95	0
1	S	502/545 (92%)	1.02	88 (17%) 1 4	95, 95, 95, 95	0
1	T	502/545 (92%)	0.72	50 (9%) 7 10	95, 95, 95, 95	0
All	All	10040/10900 (92%)	0.79	1348 (13%) 3 6	95, 95, 95, 95	0

The worst 5 of 1348 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	491	THR	9.3
1	G	498	GLU	9.0
1	F	406	GLY	8.2
1	T	298	PRO	8.0
1	G	404	GLY	8.0

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 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.