wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:38 PM GMT

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
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:

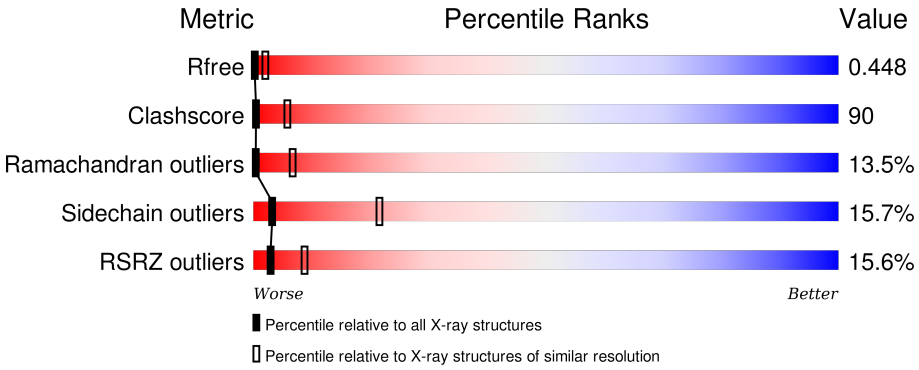
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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	545	12% 19% 53% 18% • 8%
1	B	545	19% 19% 54% 18% • 8%
1	C	545	18% 18% 54% 18% • 8%
1	D	545	14% 18% 54% 18% • 8%
1	E	545	19% 19% 53% 18% • 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	545	11% 18% 54% 18% • 8%
1	G	545	18% 19% 53% 18% • 8%
1	H	545	9% 18% 54% 18% • 8%
1	I	545	11% 19% 53% 18% • 8%
1	J	545	11% 18% 54% 18% • 8%
1	K	545	12% 18% 54% 18% • 8%
1	L	545	14% 17% 55% 18% • 8%
1	M	545	14% 17% 54% 19% • 8%
1	N	545	15% 18% 54% 18% • 8%
1	O	545	10% 19% 53% 18% • 8%
1	P	545	17% 19% 53% 19% • 8%
1	Q	545	12% 19% 54% 18% • 8%
1	R	545	22% 18% 54% 18% • 8%
1	S	545	18% 19% 53% 18% • 8%
1	T	545	12% 18% 54% 19% • 8%

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
1	A	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	B	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	C	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	D	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	E	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	F	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	G	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	H	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	I	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	J	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	K	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	L	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	M	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	N	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	O	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	P	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			

Continued on next page...

Continued from previous page...

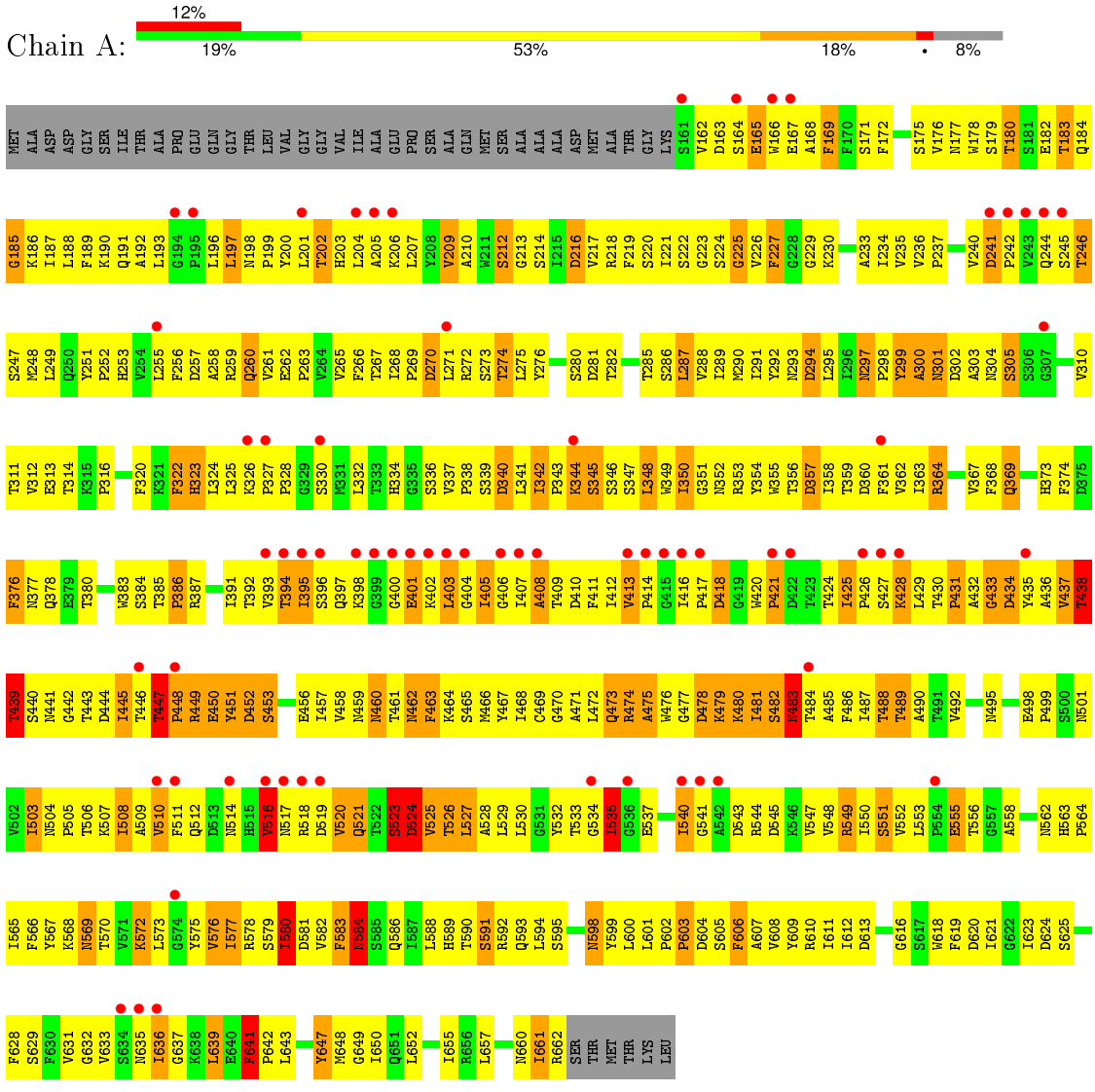
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	R	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	S	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	T	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			

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.

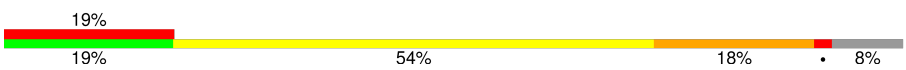
- Molecule 1: VP1

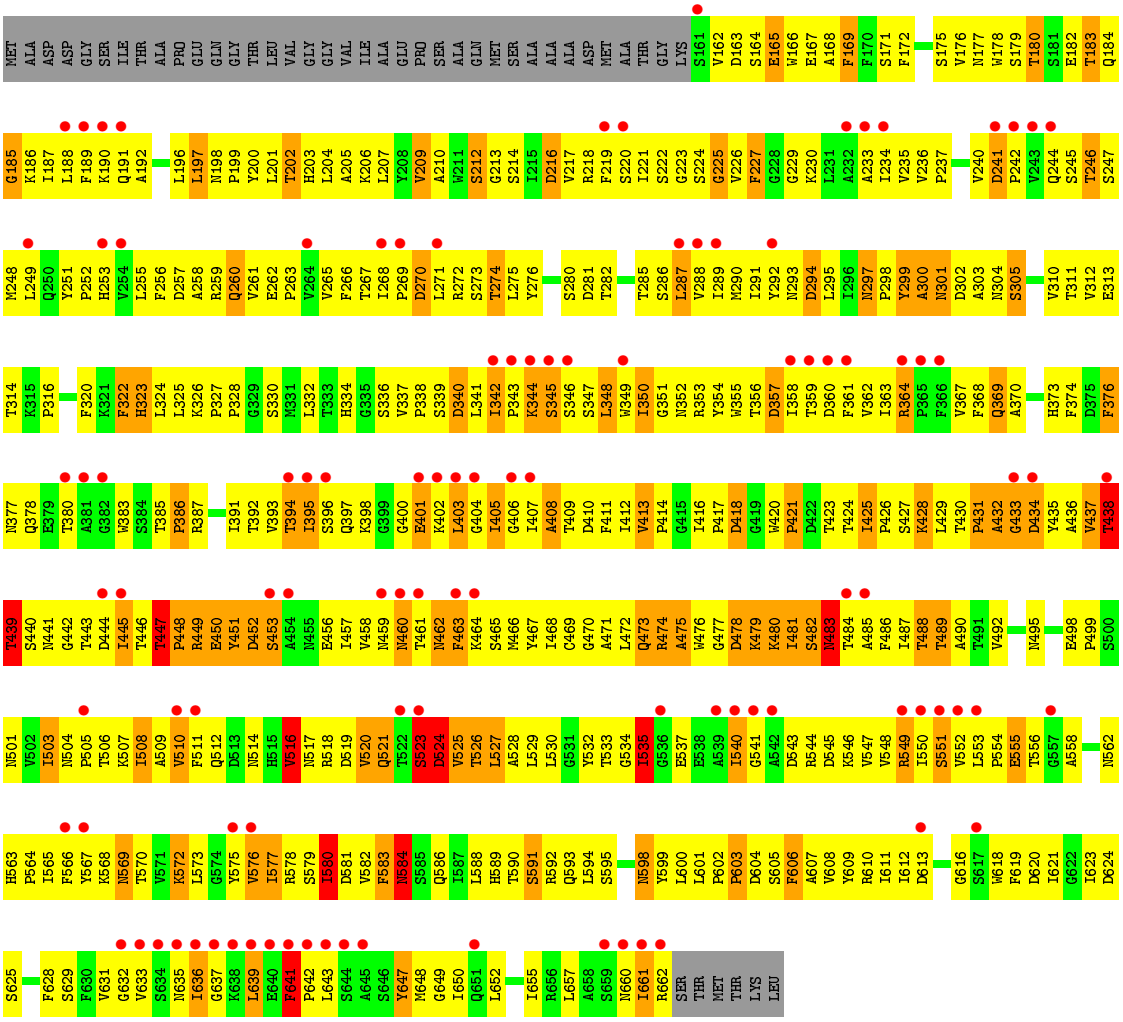
Chain A:



- Molecule 1: VP1

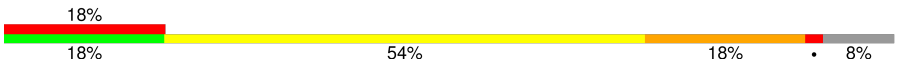
Chain B:

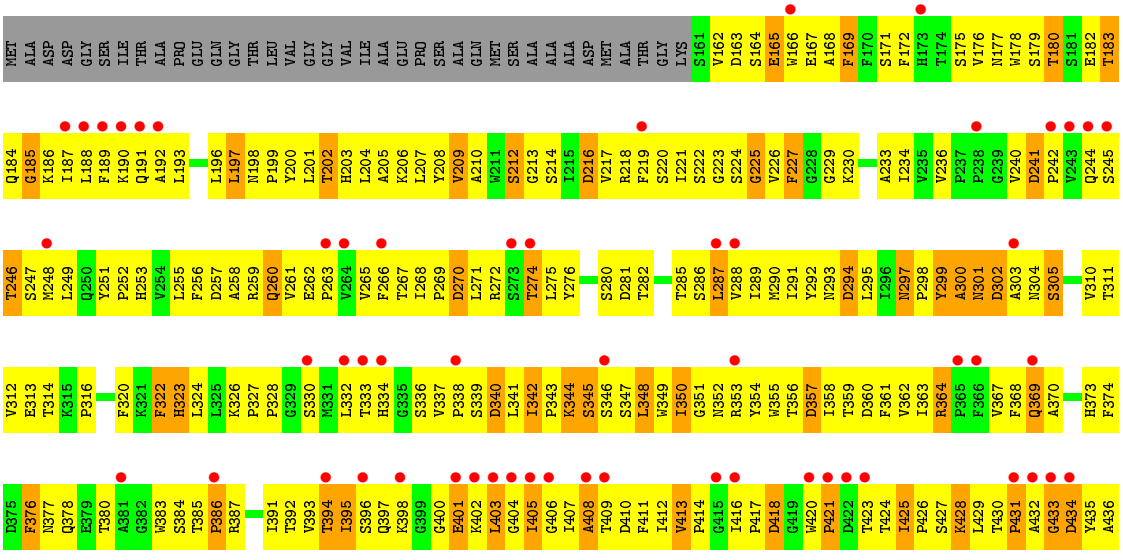


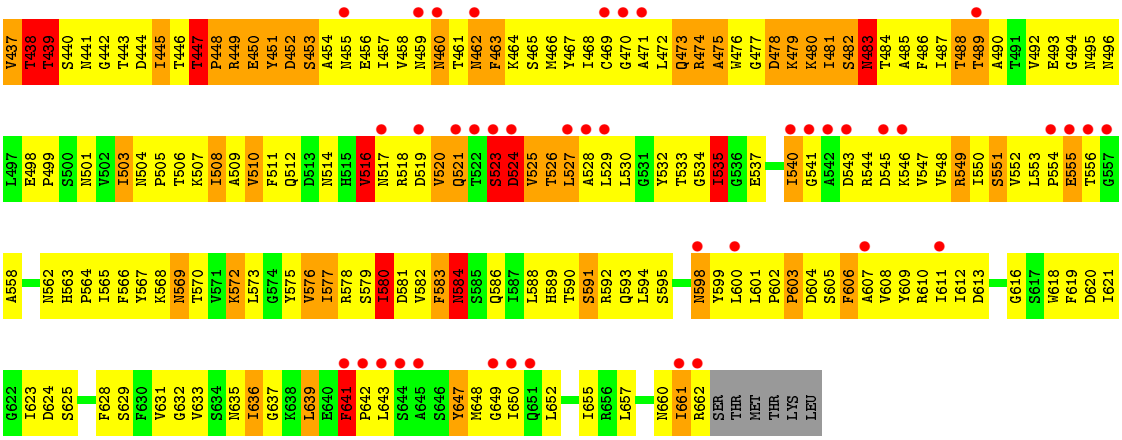


• Molecule 1: VP1

Chain C:

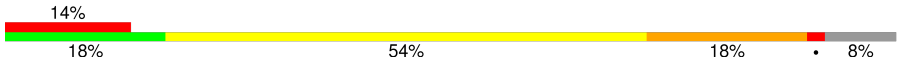


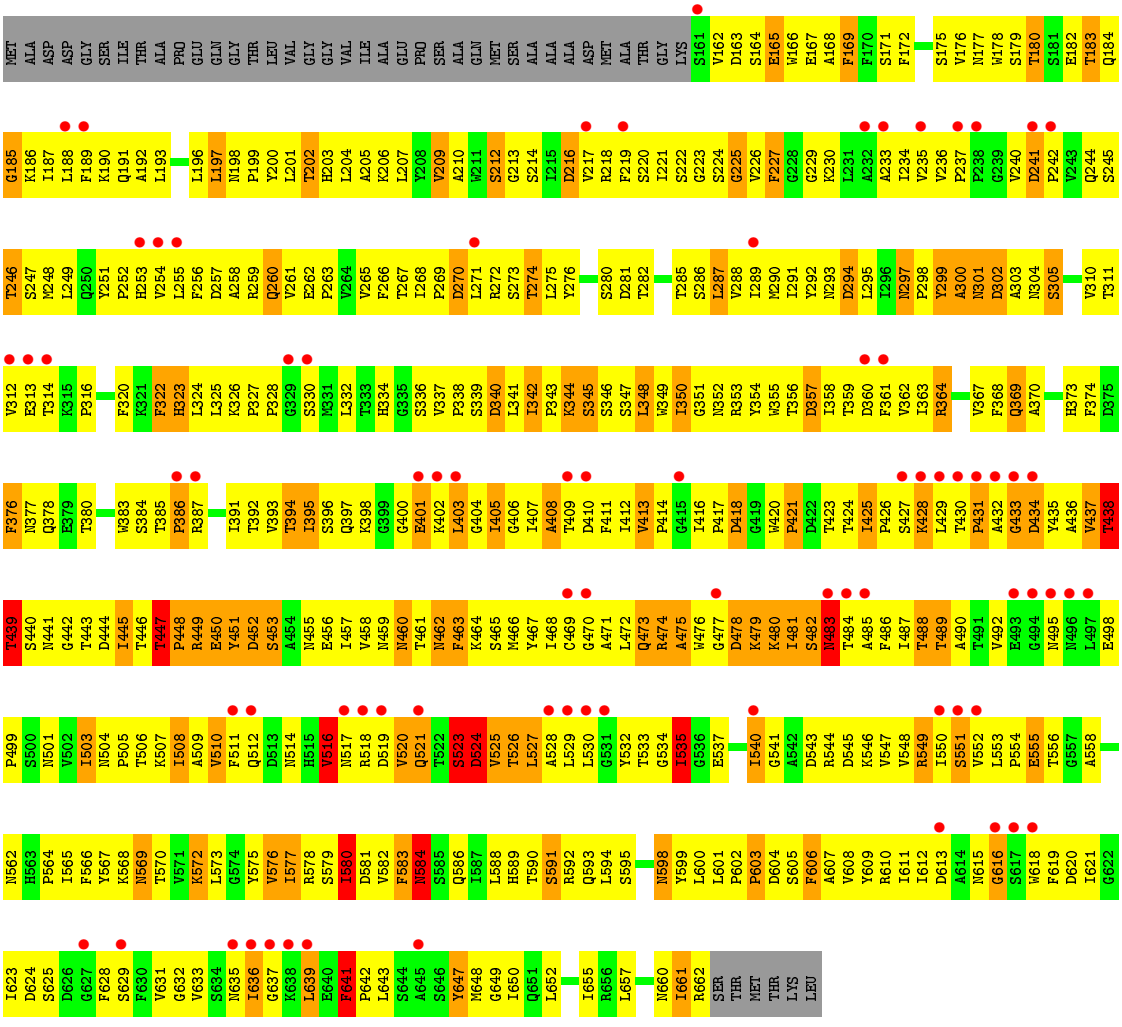




• Molecule 1: VP1

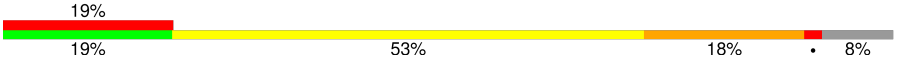
Chain D:

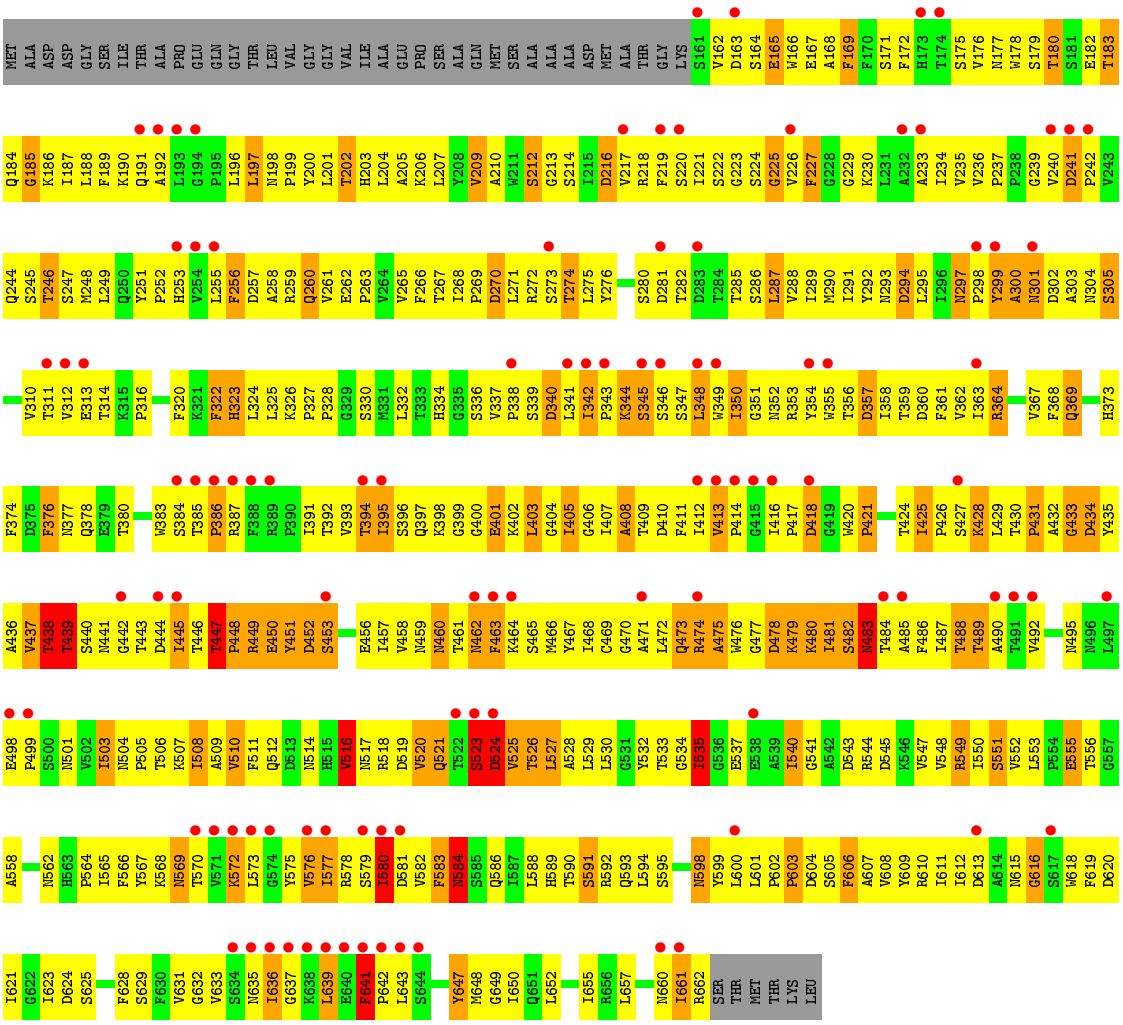




• Molecule 1: VP1

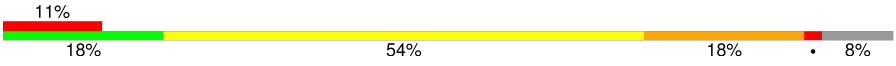
Chain E:

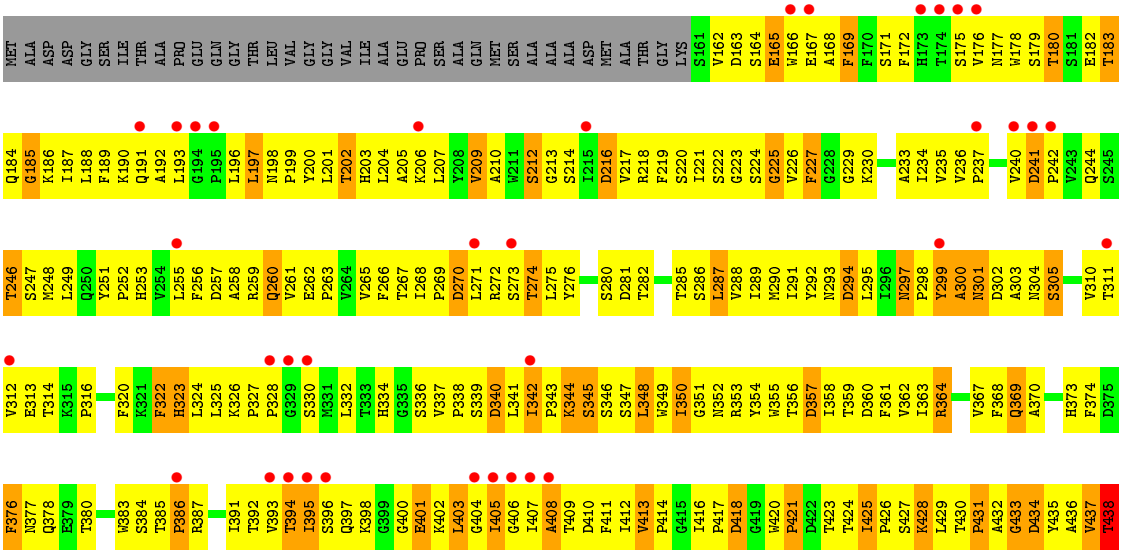


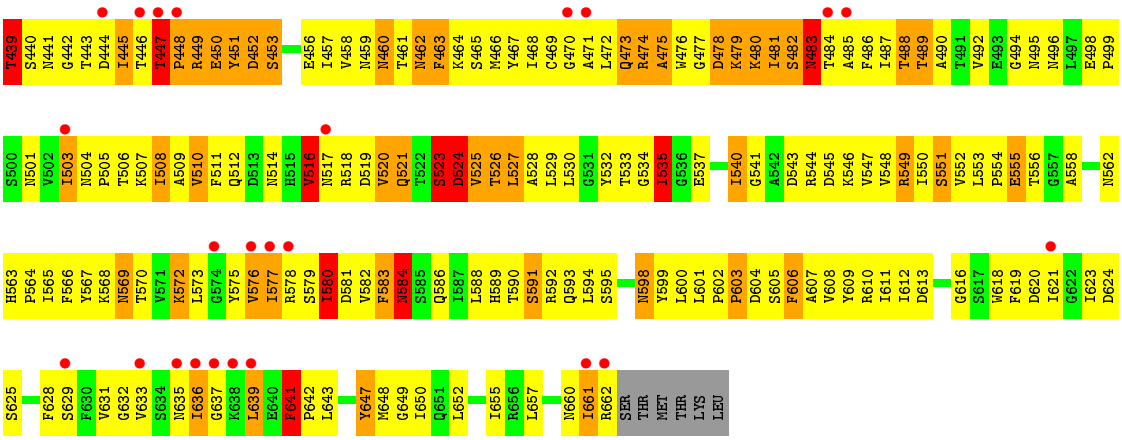


• Molecule 1: VP1

Chain F:

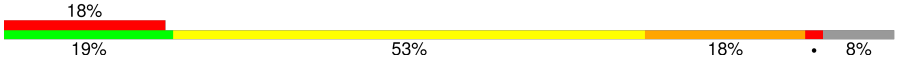


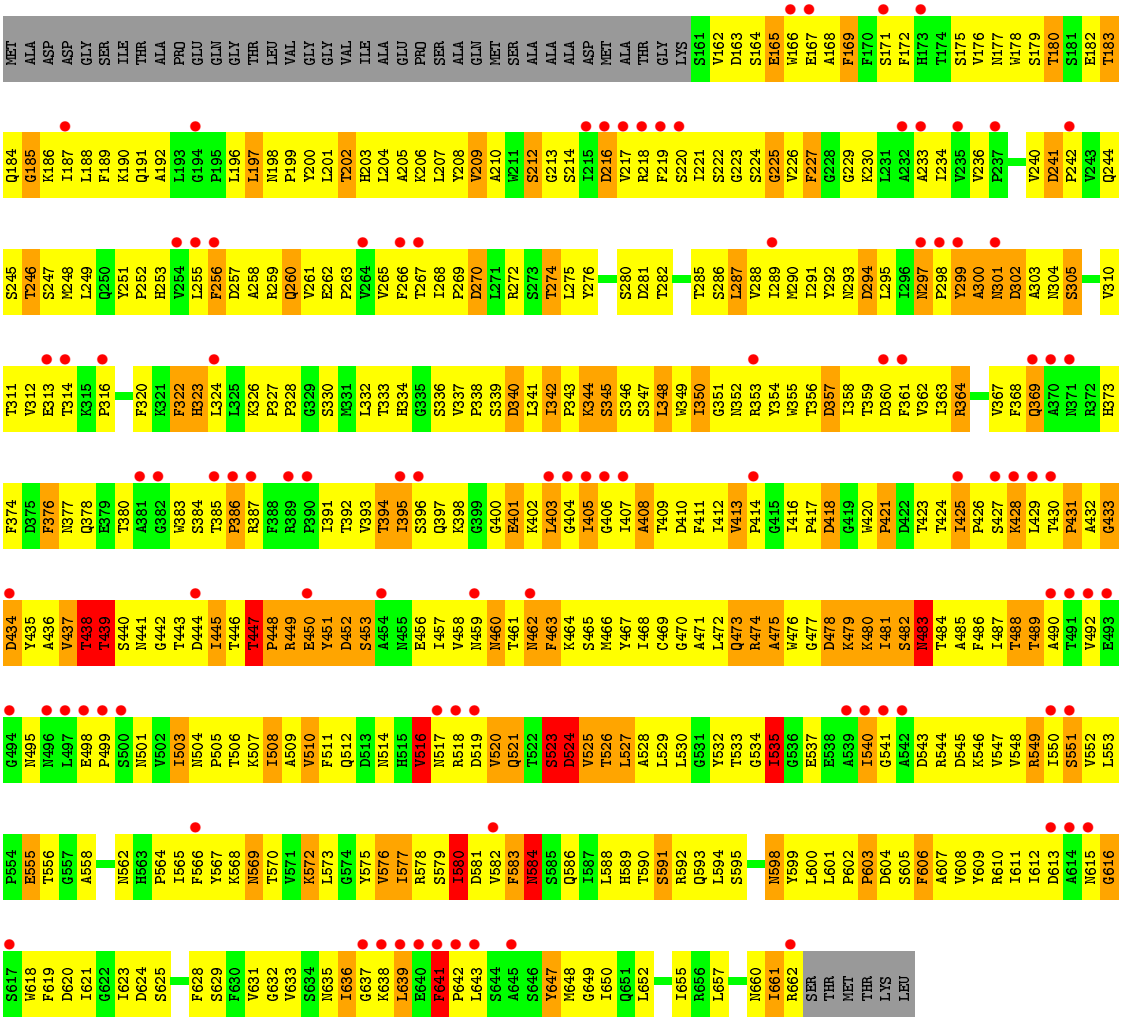




• Molecule 1: VP1

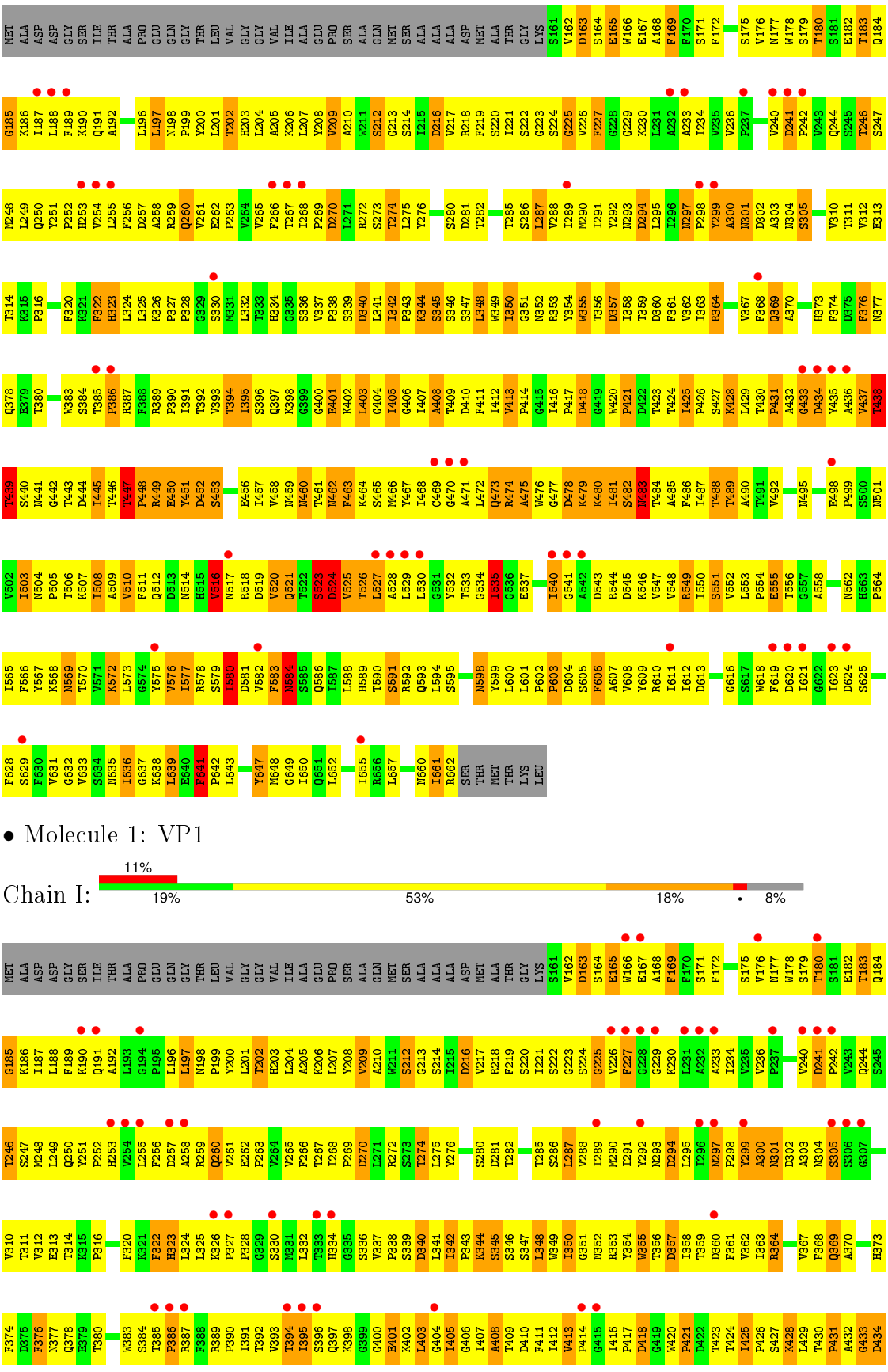
Chain G:





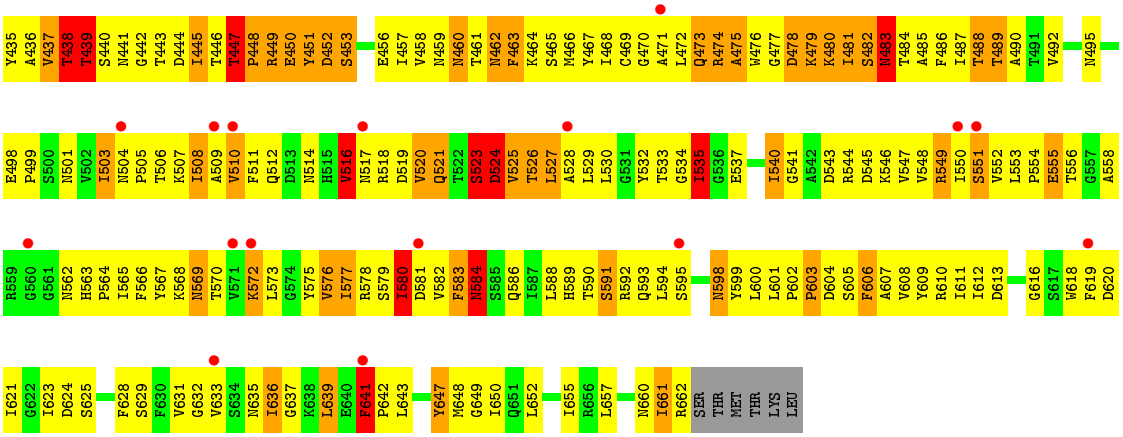
• Molecule 1: VP1

Chain H:



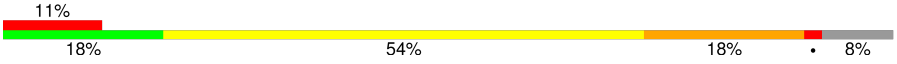
• Molecule 1: VP1

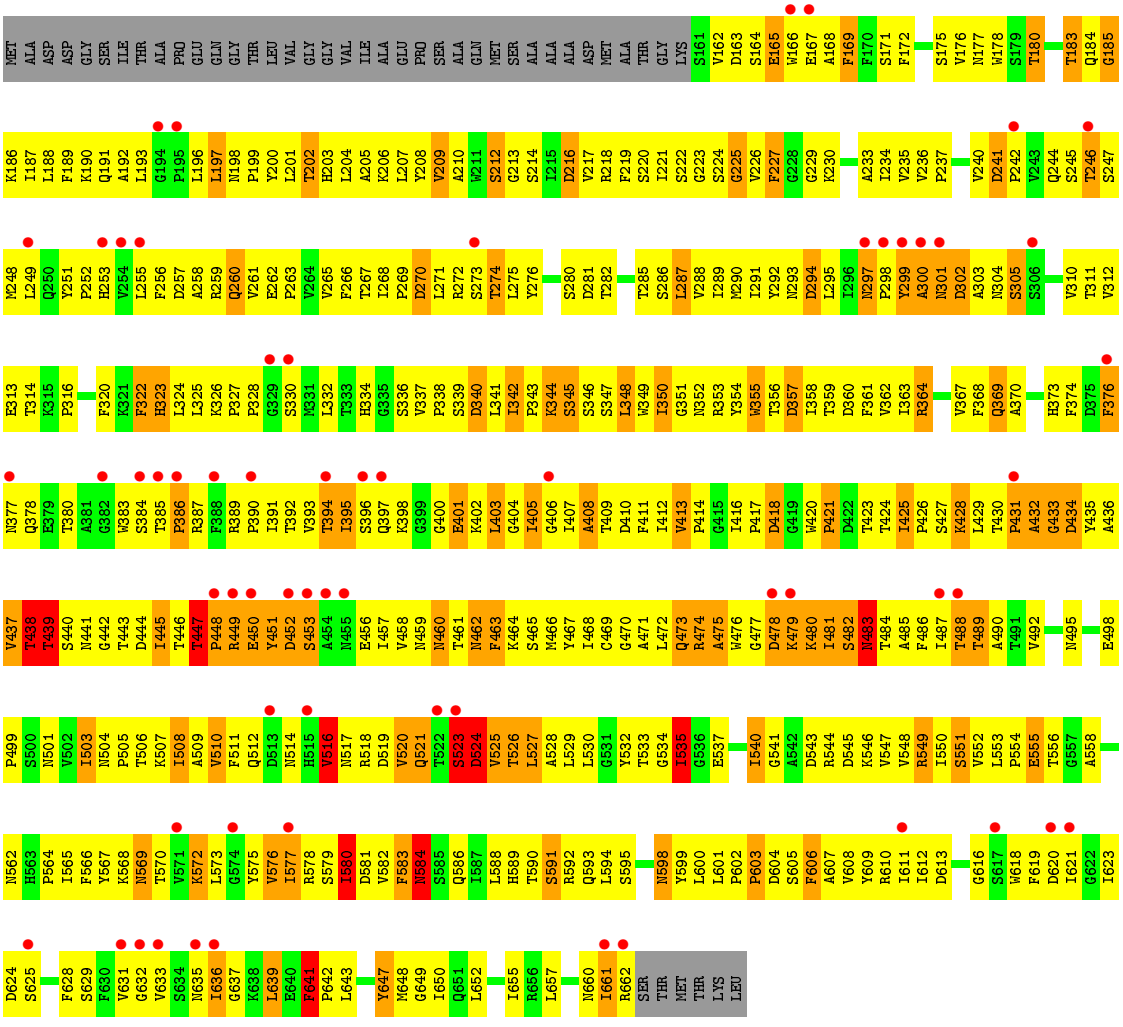
Chain I:



• Molecule 1: VP1

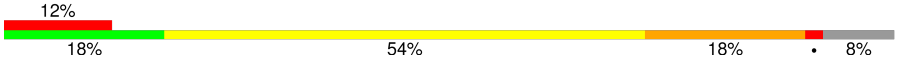
Chain J:

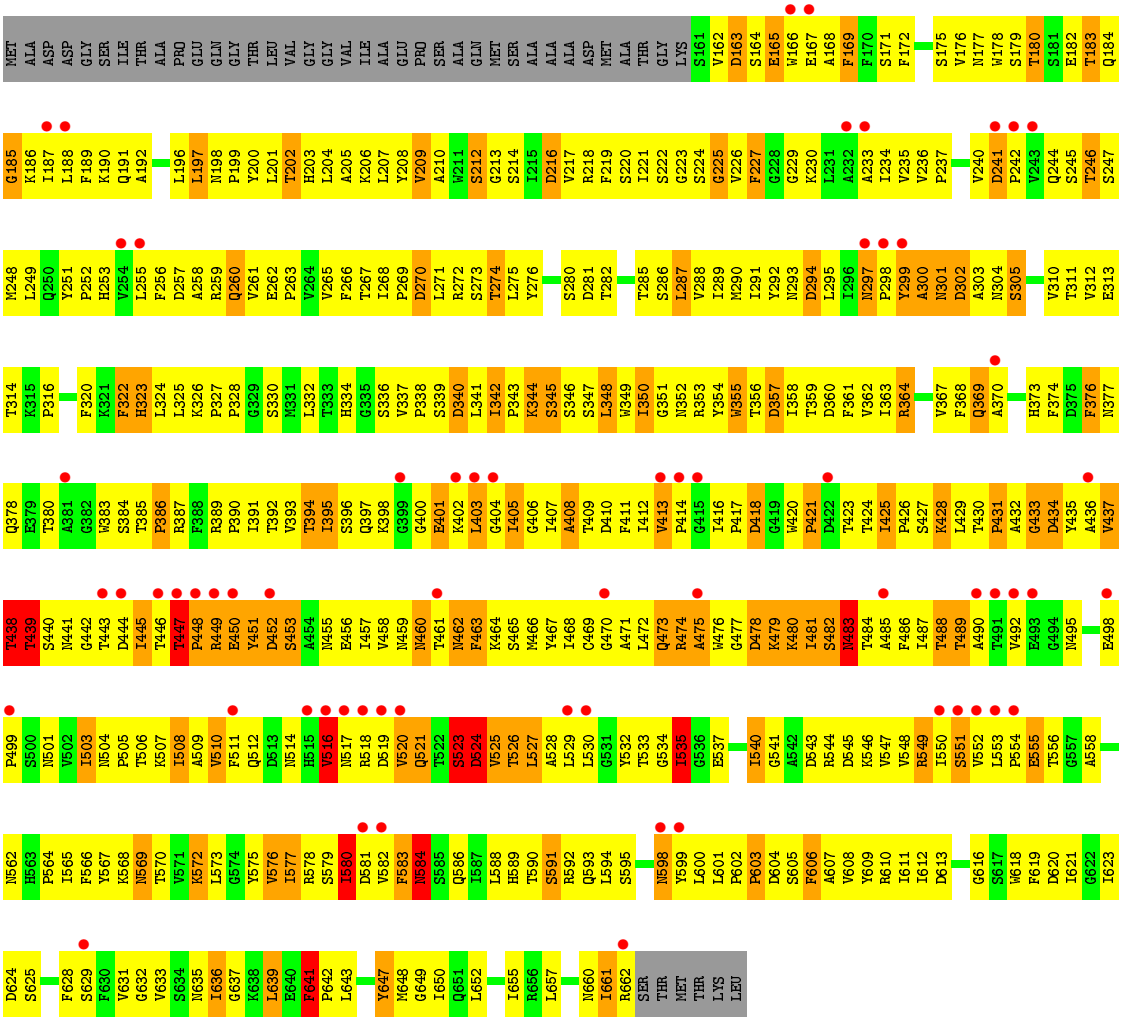




• Molecule 1: VP1

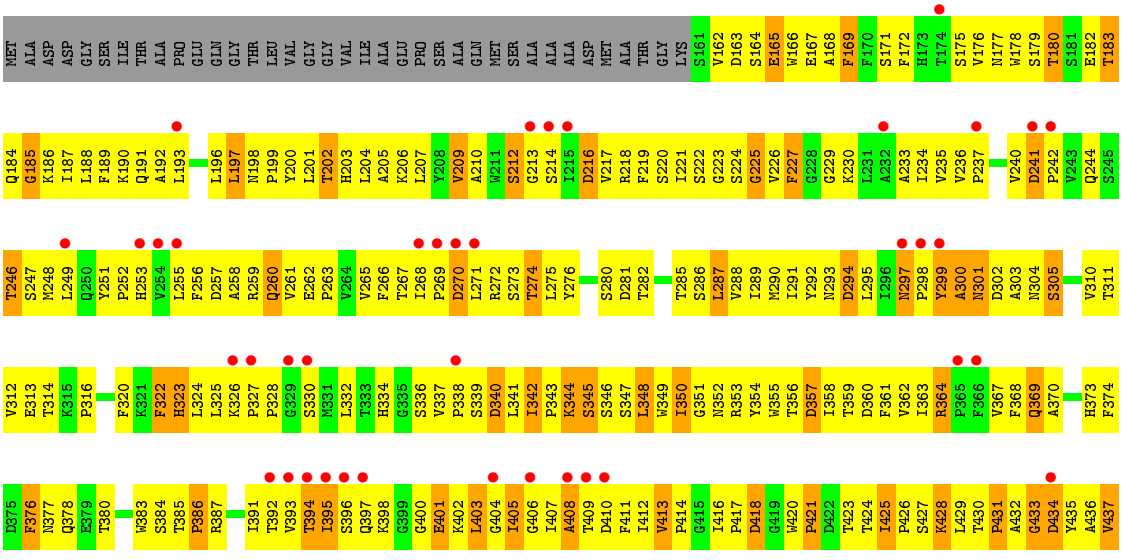
Chain K:

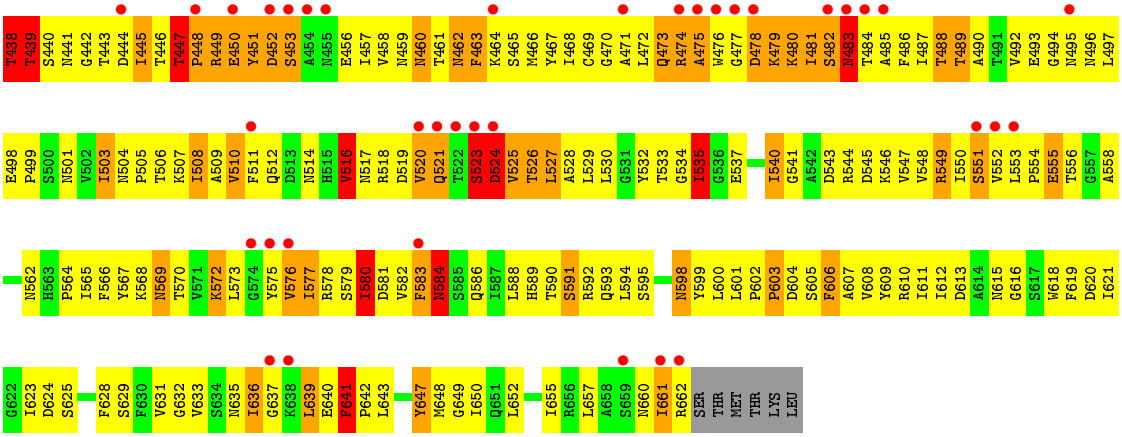




• Molecule 1: VP1

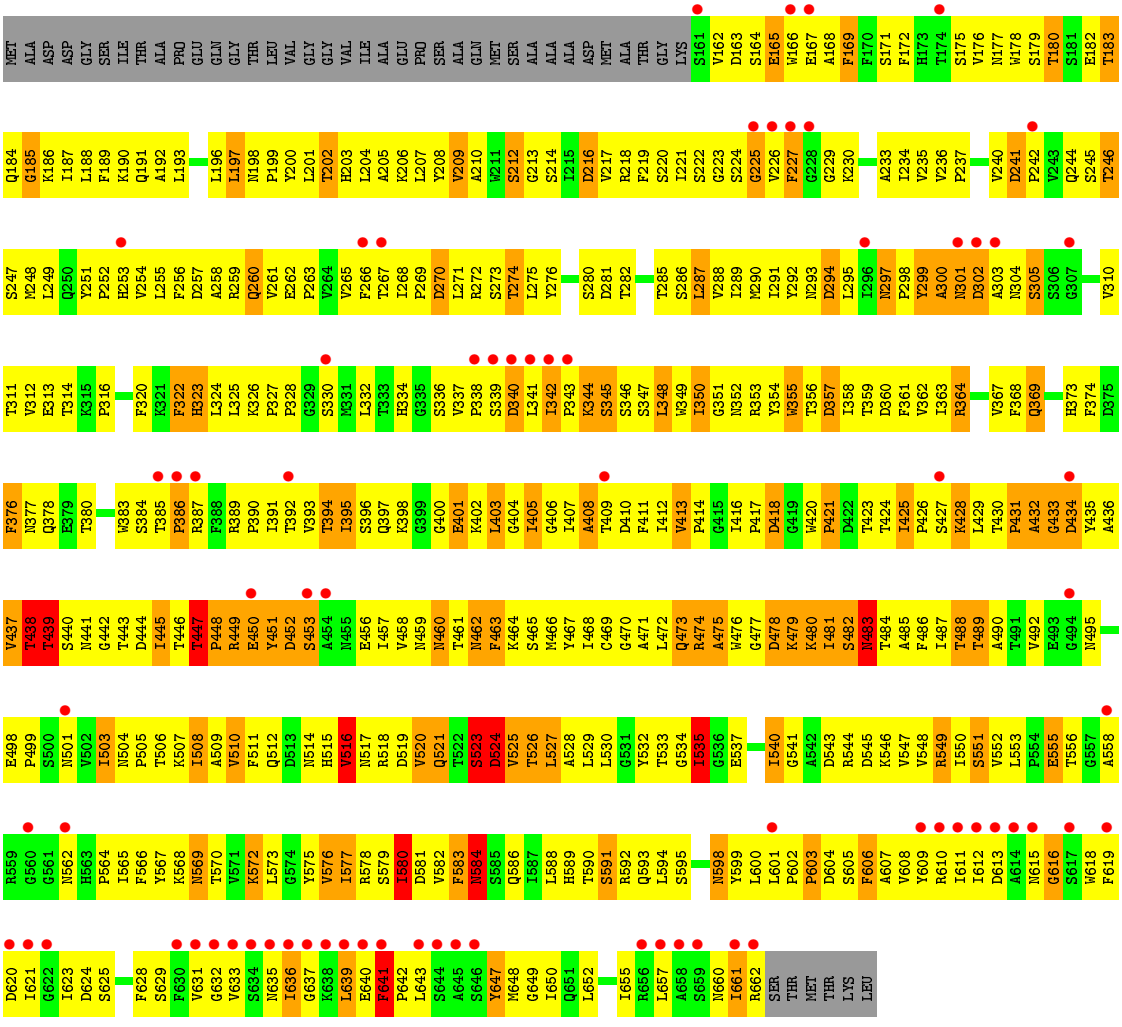
Chain L:





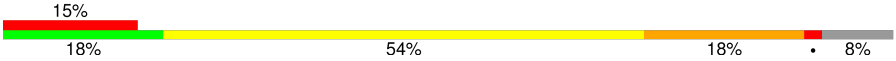
• Molecule 1: VP1

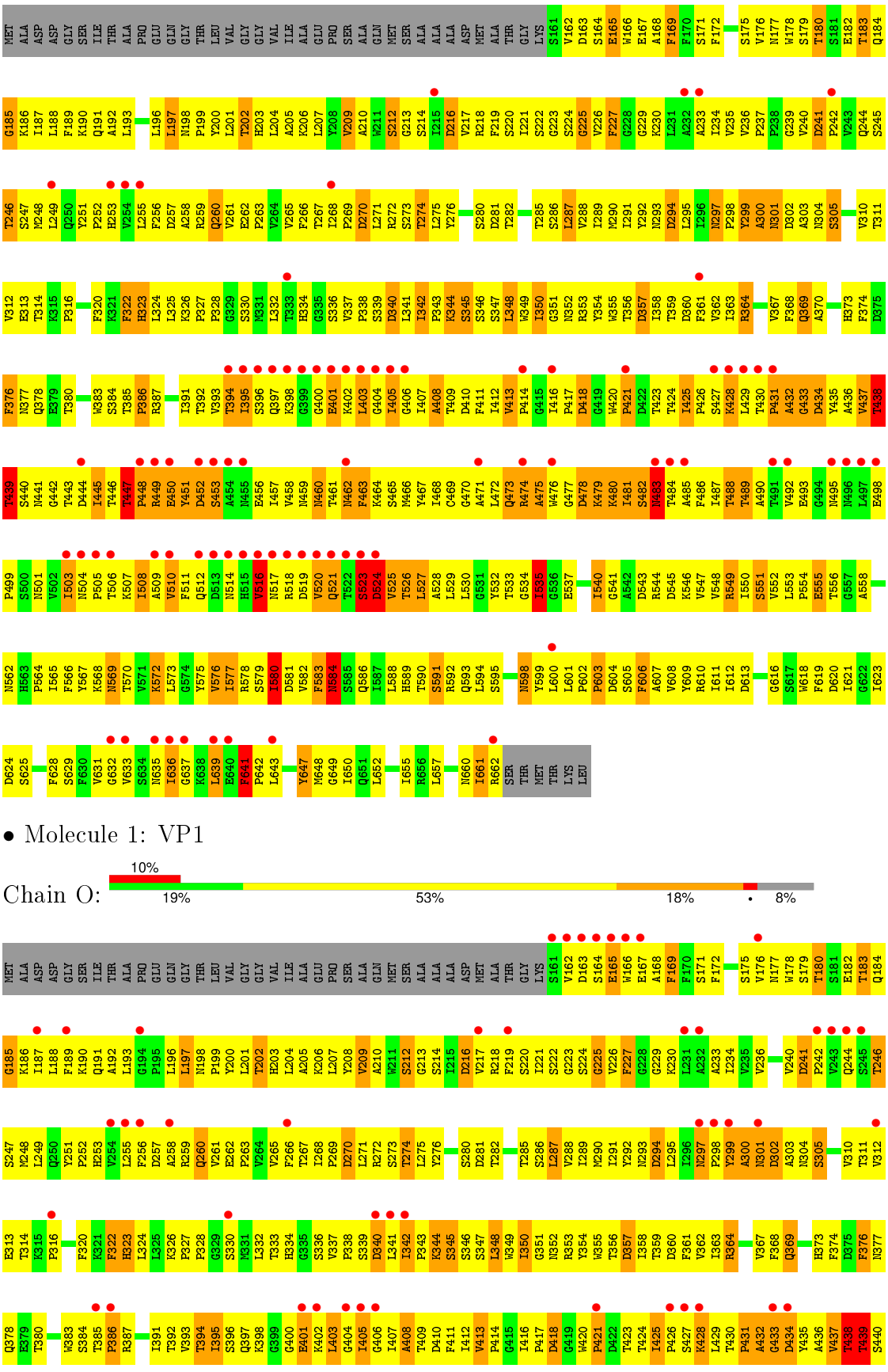
Chain M:



• Molecule 1: VP1

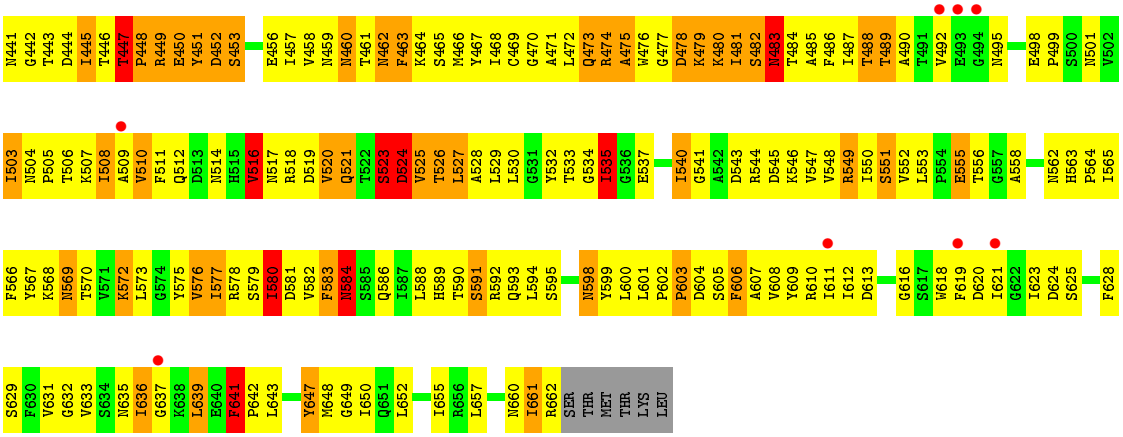
Chain N:





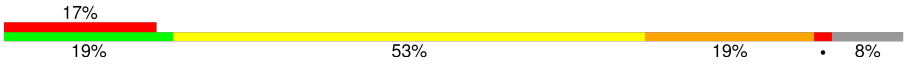
• Molecule 1: VP1

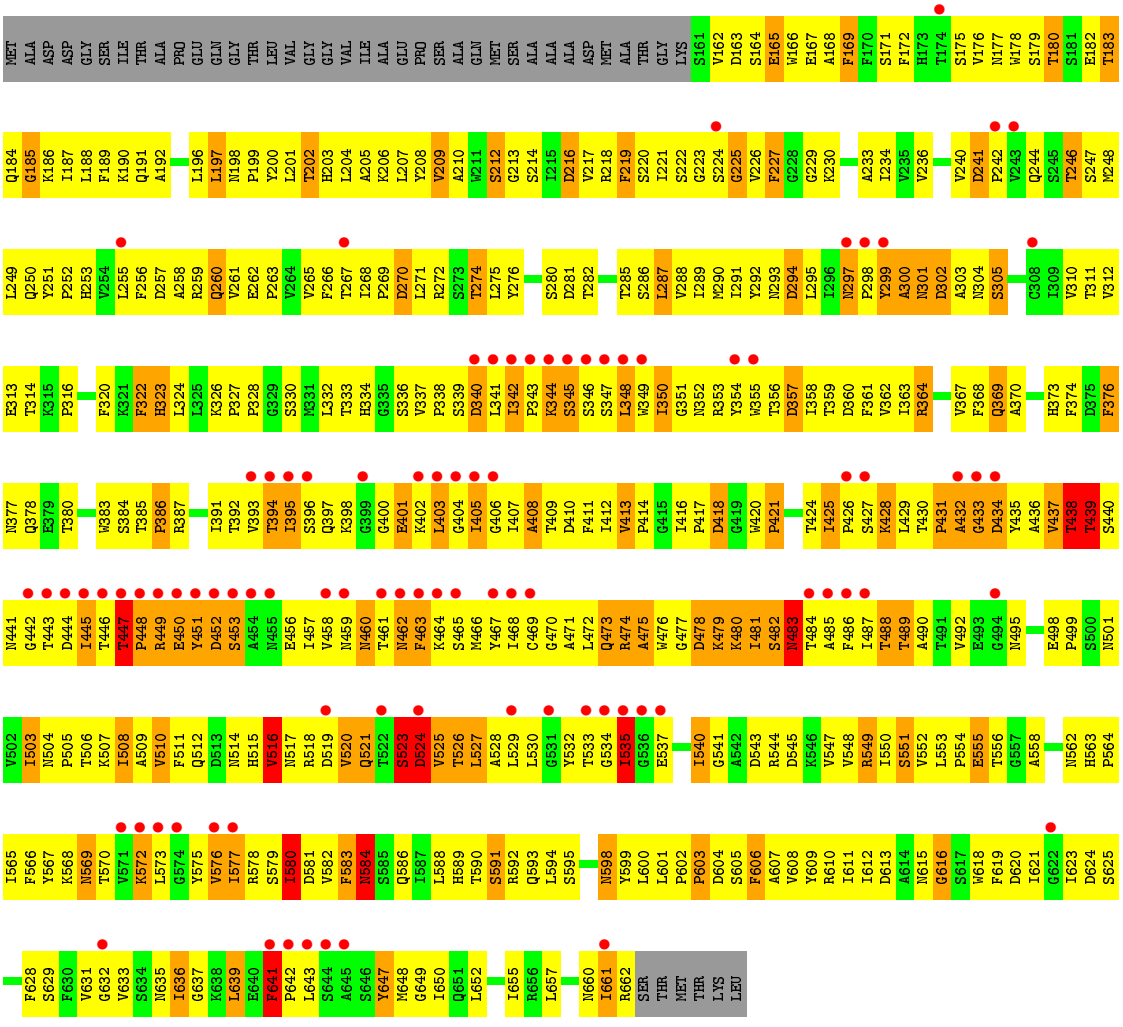
Chain O:



• Molecule 1: VP1

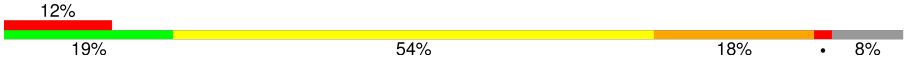
Chain P:

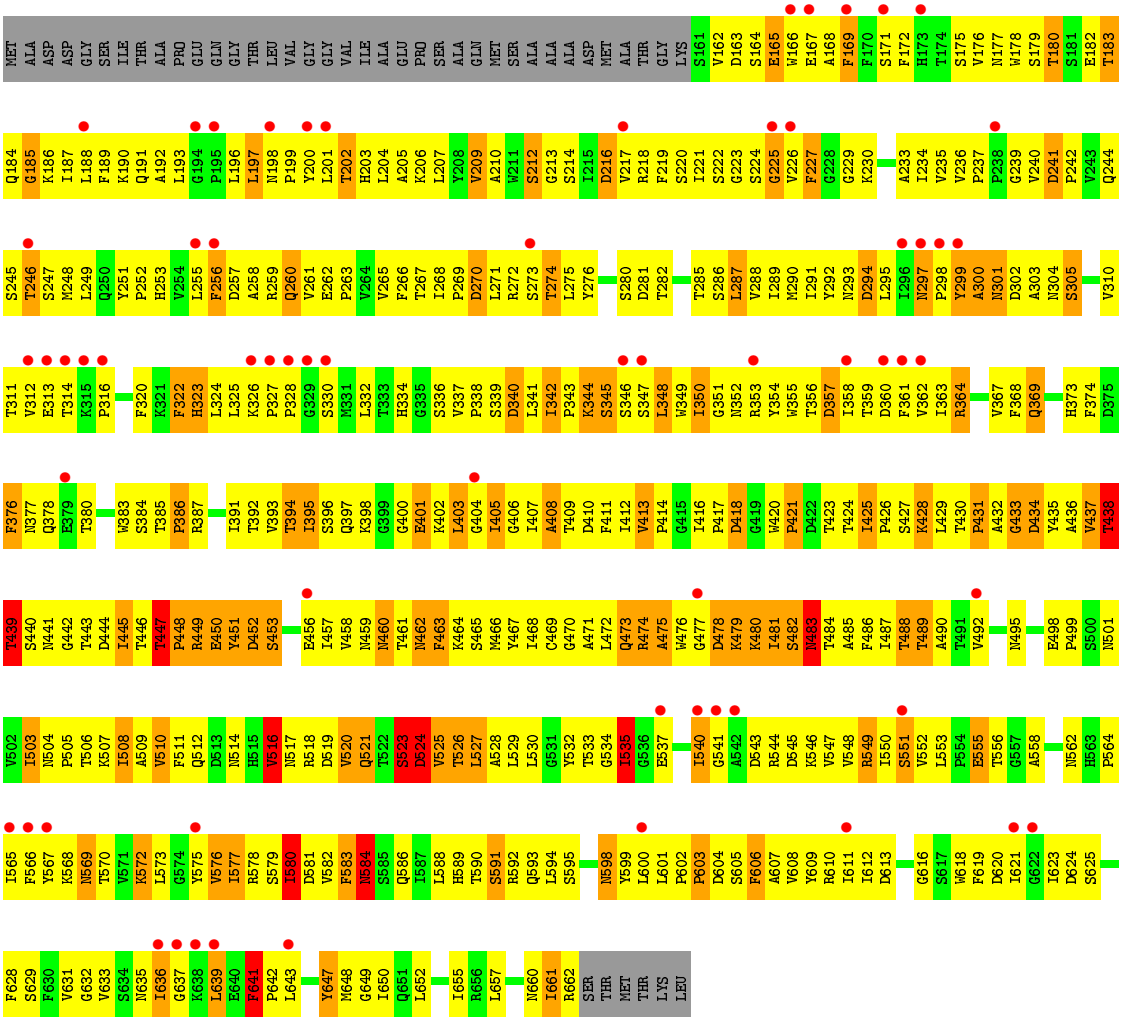




• Molecule 1: VP1

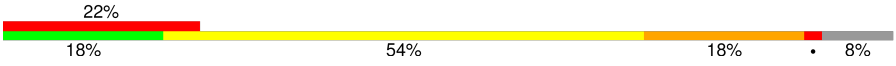
Chain Q:

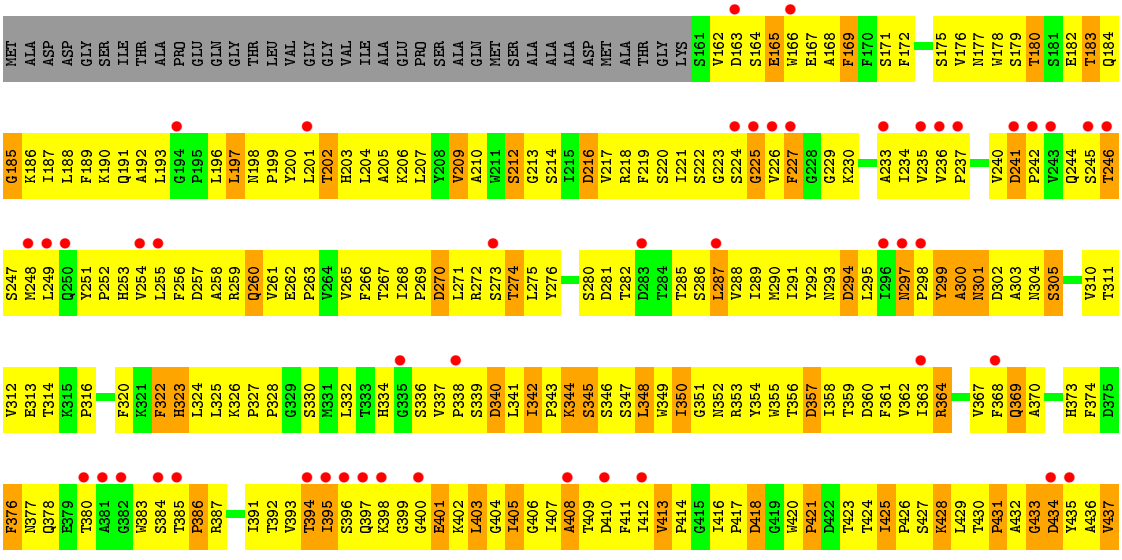


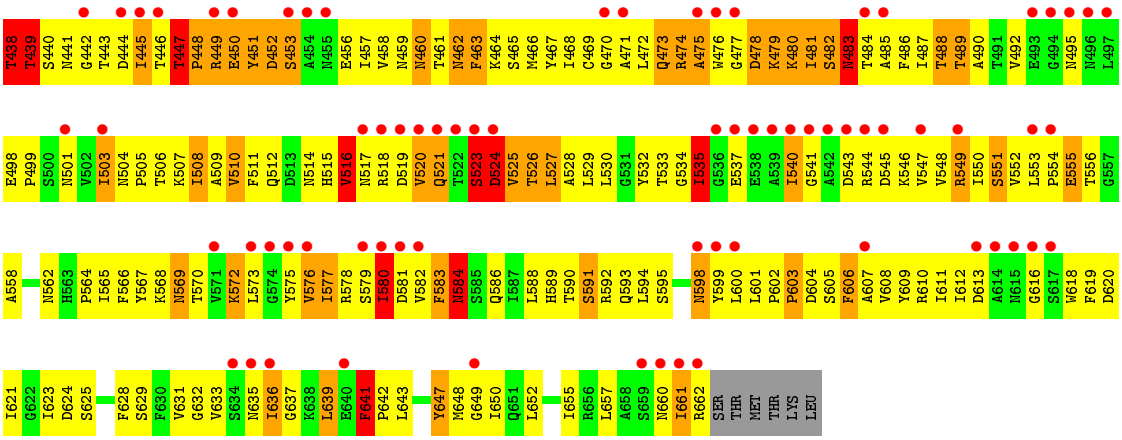


• Molecule 1: VP1

Chain R:

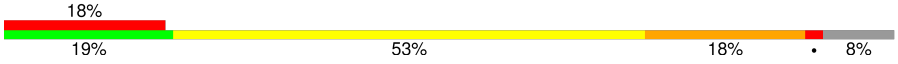


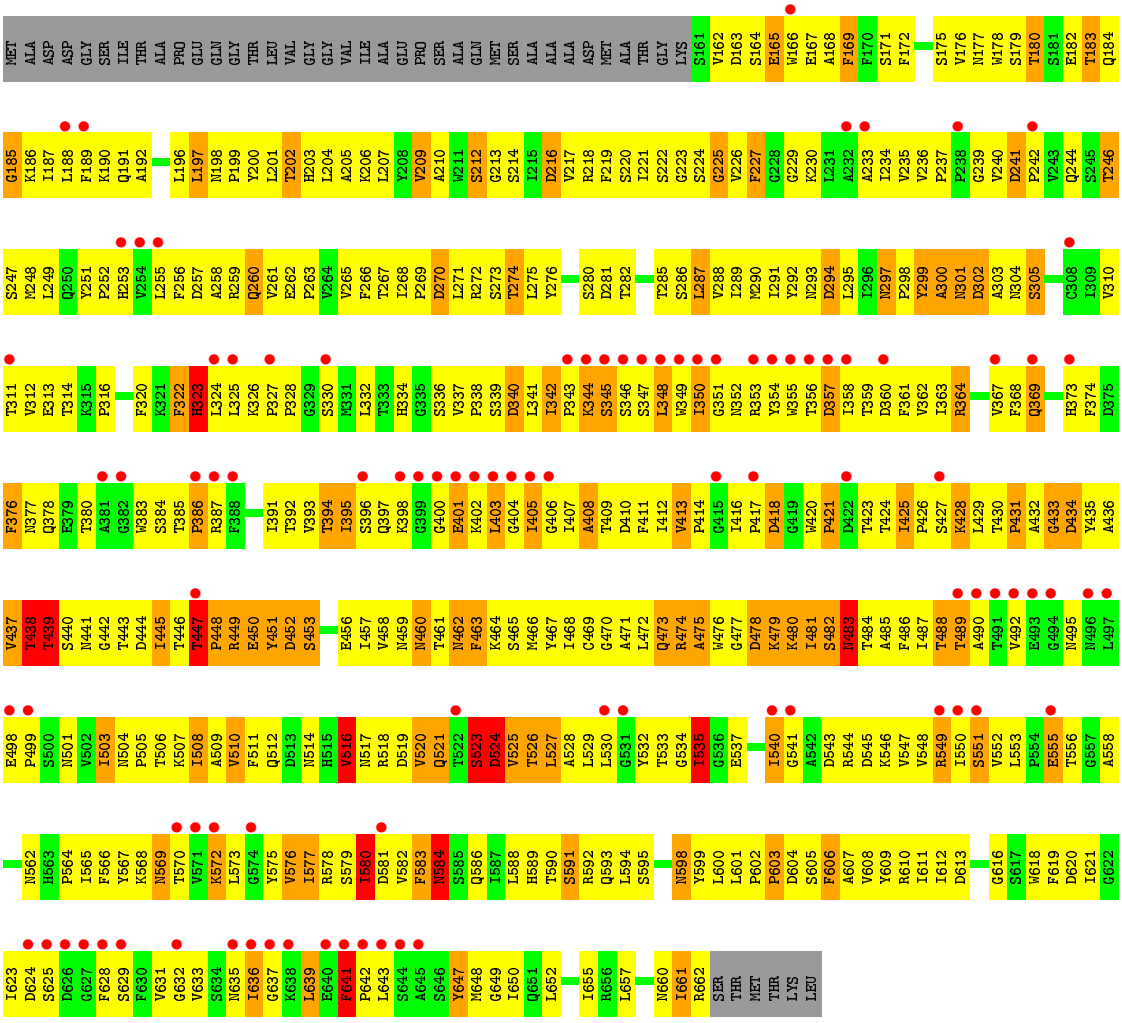




• Molecule 1: VP1

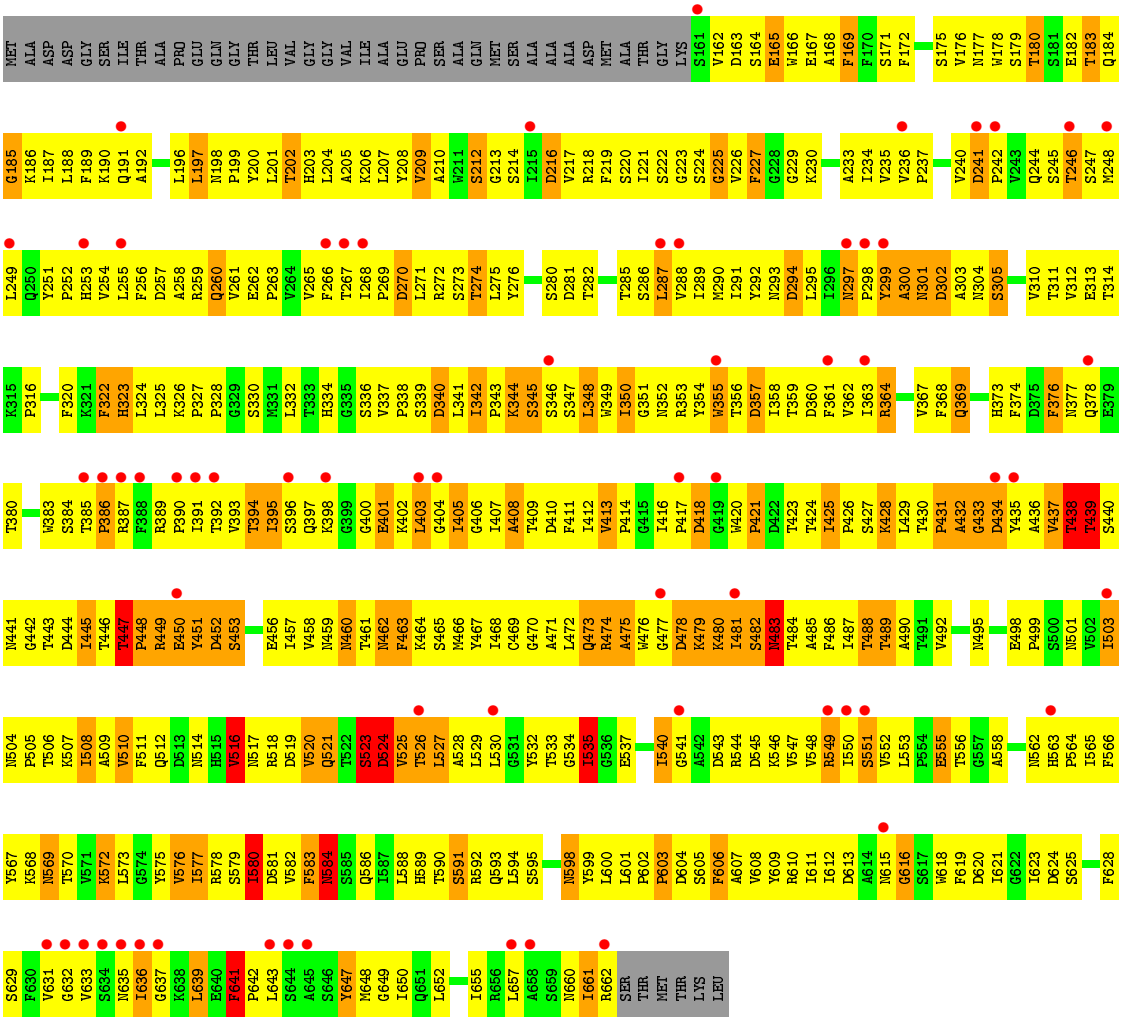
Chain S:





• Molecule 1: VP1

Chain T:


MET ALA ASP ASP GLY SER ILE THR ALA PRO GLU GLN GLY THR LEU VAL GLY GLY VAL ILE ALA GLU PRO SER ALA GLN MET SER ALA ALA ALA ASP MET ALA THR GLY LYS S161 V162 D163 S164 E165 W166 E167 A168 F169 F170 S171 F172 S175 V176 N177 W178 S179 T180 S181 E182 T183 Q184
G185 K186 I187 L188 F189 K190 Q191 A192 L196 L197 N198 P199 Y200 L201 T202 H203 L204 A205 K206 L207 Y208 V209 A210 W211 S212 G213 S214 I215 D216 V217 R218 F219 S220 I221 S222 G223 S224 G225 V226 F227 G228 G229 K230 A233 I234 V235 V236 P237 V240 D241 P242 V243 Q244 S245 T246 S247 M248
L249 Q250 Y251 P252 H253 V254 L255 F256 D257 A258 R259 Q260 V261 E262 P263 V264 V265 F266 T267 I268 P269 D270 L271 R272 S273 T274 L275 Y276 S280 D281 T282 T285 S286 L287 V288 I289 M290 I291 Y292 N293 D294 L295 I296 N297 P298 Y299 A300 N301 D302 A303 N304 S305 V310 T311 V312 E313 T314
K315 P316 F320 K321 F322 H323 L324 L325 K326 P327 P328 G329 S330 M331 L332 T333 H334 G335 S336 V337 P338 S339 D340 L341 I342 P343 K344 S345 S346 S347 L348 W349 I350 G351 N352 R353 Y354 W355 T356 D357 I358 T359 D360 F361 V362 I363 R364 V367 F368 Q369 H373 F374 D375 F376 N377 Q378 E379
T380 W383 S384 T385 P386 R387 F388 R389 P390 I391 T392 V393 T394 I395 S396 Q397 K398 G399 G400 E401 K402 L403 G404 I405 G406 I407 A408 T409 D410 F411 I412 V413 P414 G415 I416 P417 D418 G419 W420 P421 D422 T423 T424 I425 P426 S427 K428 L429 T430 P431 A432 G433 D434 Y435 A436 V437 T438 T439 S440
N441 G442 T443 D444 I445 T446 T447 P448 R449 E450 Y451 D452 S453 E456 I457 V458 N459 N460 T461 N462 F463 K464 S465 M466 Y467 I468 C469 G470 A471 L472 Q473 R474 A475 W476 G477 D478 K479 K480 I481 S482 N483 T484 A485 F486 I487 T488 T489 A490 T491 V492 N495 E498 P499 S500 N501 V502 I503
N504 P505 T506 K507 I508 A509 V510 F511 Q512 D513 N514 H515 V516 N517 R518 D519 V520 Q521 T522 S523 D524 V525 T526 L527 A528 L529 I530 G531 Y532 T533 G534 I535 G536 E537 I540 G541 A542 D543 R544 D545 K546 V547 V548 R549 I550 S551 V552 L553 P554 E555 T556 G557 A558 N562 H563 P564 I565 P566
Y567 K568 N569 T570 V571 K572 L573 G574 Y575 V576 I577 R578 S579 I580 D581 V582 F583 N584 S585 Q586 I587 L588 H589 T590 S591 R592 Q593 L594 S595 N598 Y599 L600 L601 P602 P603 D604 S605 F606 A607 V608 Y609 R610 I611 I612 D613 A614 N615 G616 S617 W618 F619 D620 I621 G622 I623 D624 S625 F628
S629 F630 V631 G632 V633 S634 N635 I636 G637 K638 L639 E640 F641 P642 L643 S644 A645 S646 Y647 M648 G649 I650 Q651 L652 I655 R656 L657 A658 S659 N660 I661 R662 SER THR MET THR LYS LEU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.41 (at 8.38Å)	Xtriage
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 (5.16%)	DCC
Wilson B-factor (Å^2)	426.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.108 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.16$	Xtriage
Outliers	0 of 14491 reflections	Xtriage
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

Xtriage'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.*

[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).

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(^{o})	Ideal(^{o})
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

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	159
1	D	3892	0	3823	913	3
1	E	3892	0	3824	824	65
1	F	3892	0	3823	917	7
1	G	3892	0	3825	684	110
1	H	3892	0	3825	678	97
1	I	3892	0	3825	675	69
1	J	3892	0	3824	761	70
1	K	3892	0	3824	760	81
1	L	3892	0	3823	910	29
1	M	3892	0	3824	772	90
1	N	3892	0	3824	826	83
1	O	3892	0	3825	676	118
1	P	3892	0	3825	684	109
1	Q	3892	0	3824	845	66
1	R	3892	0	3823	912	12
1	S	3892	0	3824	823	62
1	T	3892	0	3824	761	65
All	All	77840	0	76480	13874	709

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 709 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 7
1	B	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0 7
1	C	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0 7
1	D	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0 7
1	E	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0 7
1	F	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0 7
1	G	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0 7
1	H	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0 7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	7
1	J	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	7
1	K	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	7
1	L	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	7
1	M	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	7
1	N	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	7
1	O	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	7
1	P	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	7
1	Q	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	7
1	R	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	7
1	S	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	7
1	T	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	7
All	All	9960/10900 (91%)	6341 (64%)	2279 (23%)	1340 (14%)	0	7

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%)	3	21
1	B	434/464 (94%)	367 (85%)	67 (15%)	3	22
1	C	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	D	434/464 (94%)	366 (84%)	68 (16%)	3	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	F	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	G	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	H	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	I	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	J	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	K	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	L	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	M	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	N	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	O	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	P	434/464 (94%)	365 (84%)	69 (16%)	3	21
1	Q	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	R	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	S	434/464 (94%)	366 (84%)	68 (16%)	3	21
1	T	434/464 (94%)	366 (84%)	68 (16%)	3	21
All	All	8680/9280 (94%)	7320 (84%)	1360 (16%)	3	21

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

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

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

Continued on next page...

Continued from previous page...

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

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	502/545 (92%)	0.87	68 (13%) 4 10	95, 95, 95, 95	0
1	B	502/545 (92%)	1.10	105 (20%) 1 7	95, 95, 95, 95	0
1	C	502/545 (92%)	0.99	97 (19%) 2 7	95, 95, 95, 95	0
1	D	502/545 (92%)	0.80	77 (15%) 3 9	95, 95, 95, 95	0
1	E	502/545 (92%)	0.99	102 (20%) 1 7	95, 95, 95, 95	0
1	F	502/545 (92%)	0.70	60 (11%) 6 11	95, 95, 95, 95	0
1	G	502/545 (92%)	1.05	98 (19%) 1 7	95, 95, 95, 95	0
1	H	502/545 (92%)	0.64	48 (9%) 10 14	95, 95, 95, 95	0
1	I	502/545 (92%)	0.76	62 (12%) 5 11	95, 95, 95, 95	0
1	J	502/545 (92%)	0.78	62 (12%) 5 11	95, 95, 95, 95	0
1	K	502/545 (92%)	0.71	63 (12%) 5 11	95, 95, 95, 95	0
1	L	502/545 (92%)	0.88	76 (15%) 3 9	95, 95, 95, 95	0
1	M	502/545 (92%)	0.81	74 (14%) 3 9	95, 95, 95, 95	0
1	N	502/545 (92%)	0.88	82 (16%) 2 8	95, 95, 95, 95	0
1	O	502/545 (92%)	0.61	55 (10%) 7 12	95, 95, 95, 95	0
1	P	502/545 (92%)	1.01	90 (17%) 2 7	95, 95, 95, 95	0
1	Q	502/545 (92%)	0.81	63 (12%) 5 11	95, 95, 95, 95	0
1	R	502/545 (92%)	1.20	120 (23%) 1 6	95, 95, 95, 95	0
1	S	502/545 (92%)	1.12	96 (19%) 2 7	95, 95, 95, 95	0
1	T	502/545 (92%)	0.80	64 (12%) 5 11	95, 95, 95, 95	0
All	All	10040/10900 (92%)	0.88	1562 (15%) 3 9	95, 95, 95, 95	0

The worst 5 of 1562 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	491	THR	9.9
1	G	498	GLU	9.4
1	F	406	GLY	8.6
1	G	404	GLY	8.4
1	L	522	THR	8.2

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.