



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:51 am 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28972

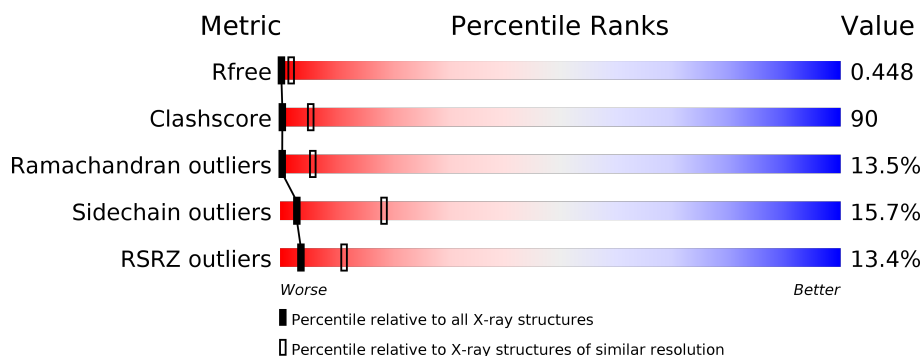
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1100 (10.00-3.70)
Clashscore	112137	1036 (11.50-3.80)
Ramachandran outliers	110173	1004 (11.50-3.76)
Sidechain outliers	110143	1099 (11.50-3.70)
RSRZ outliers	101464	1004 (11.50-3.72)

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 $\leq 5\%$. 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> <div>12%</div> <div> <div>19%</div> <div>53%</div> <div>18%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	545	<div> <div>16%</div> <div> <div>19%</div> <div>54%</div> <div>18%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	545	<div> <div>15%</div> <div> <div>18%</div> <div>54%</div> <div>18%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	545	<div> <div>12%</div> <div> <div>18%</div> <div>54%</div> <div>18%</div> <div>•</div> <div>8%</div> </div> </div>
1	E	545	<div> <div>17%</div> <div> <div>19%</div> <div>53%</div> <div>18%</div> <div>•</div> <div>8%</div> </div> </div>
1	F	545	<div> <div>9%</div> <div> <div>18%</div> <div>54%</div> <div>18%</div> <div>•</div> <div>8%</div> </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
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			

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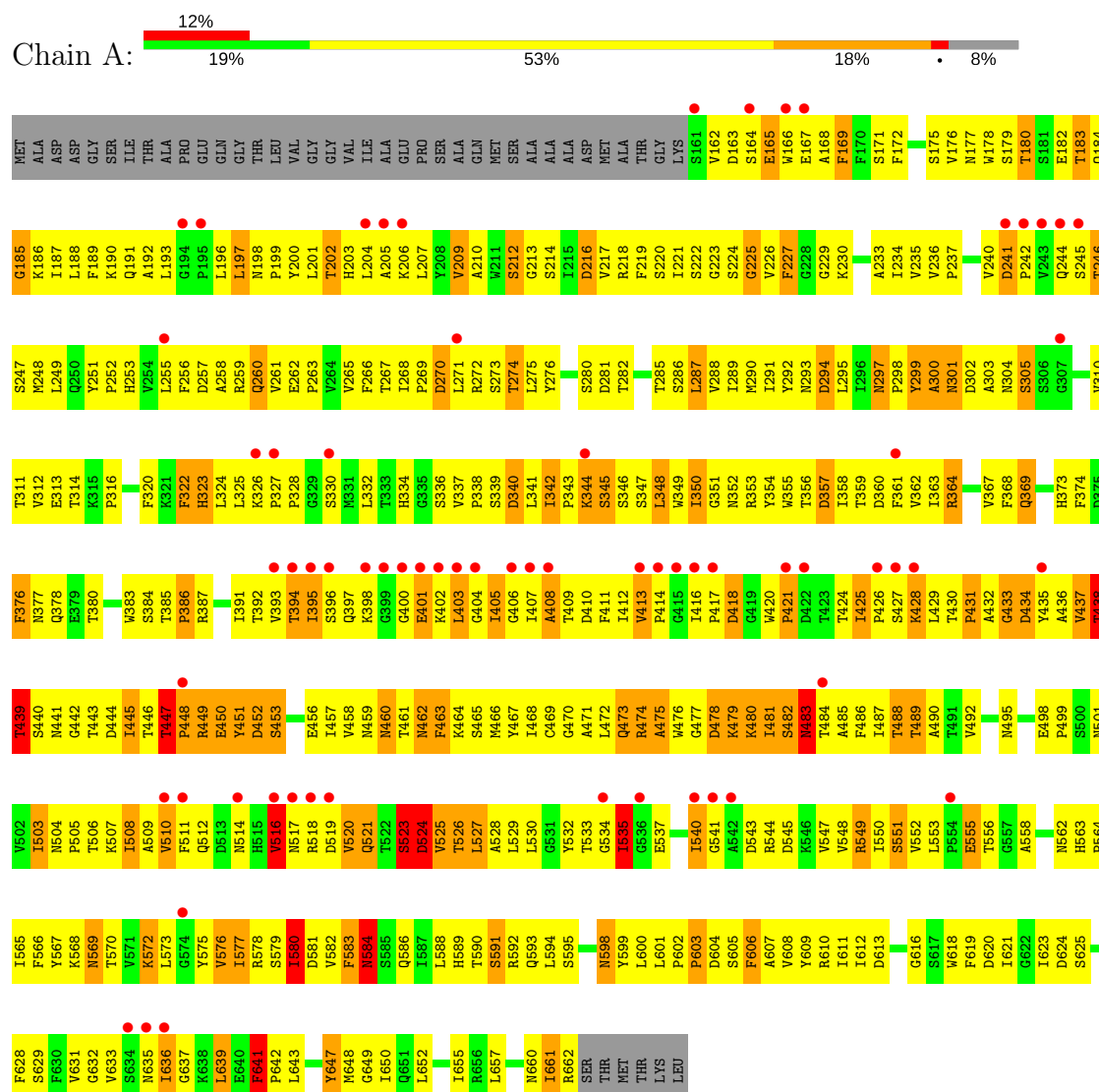
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	R	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	S	502	Total	C	N	O	S	0	0	0
			3892	2491	651	742	8			
1	T	502	Total	C	N	O	S	0	0	0
			3892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

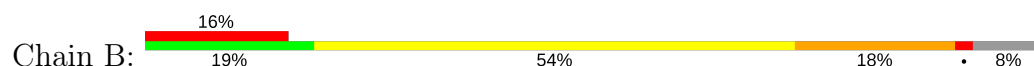
3 Residue-property plots

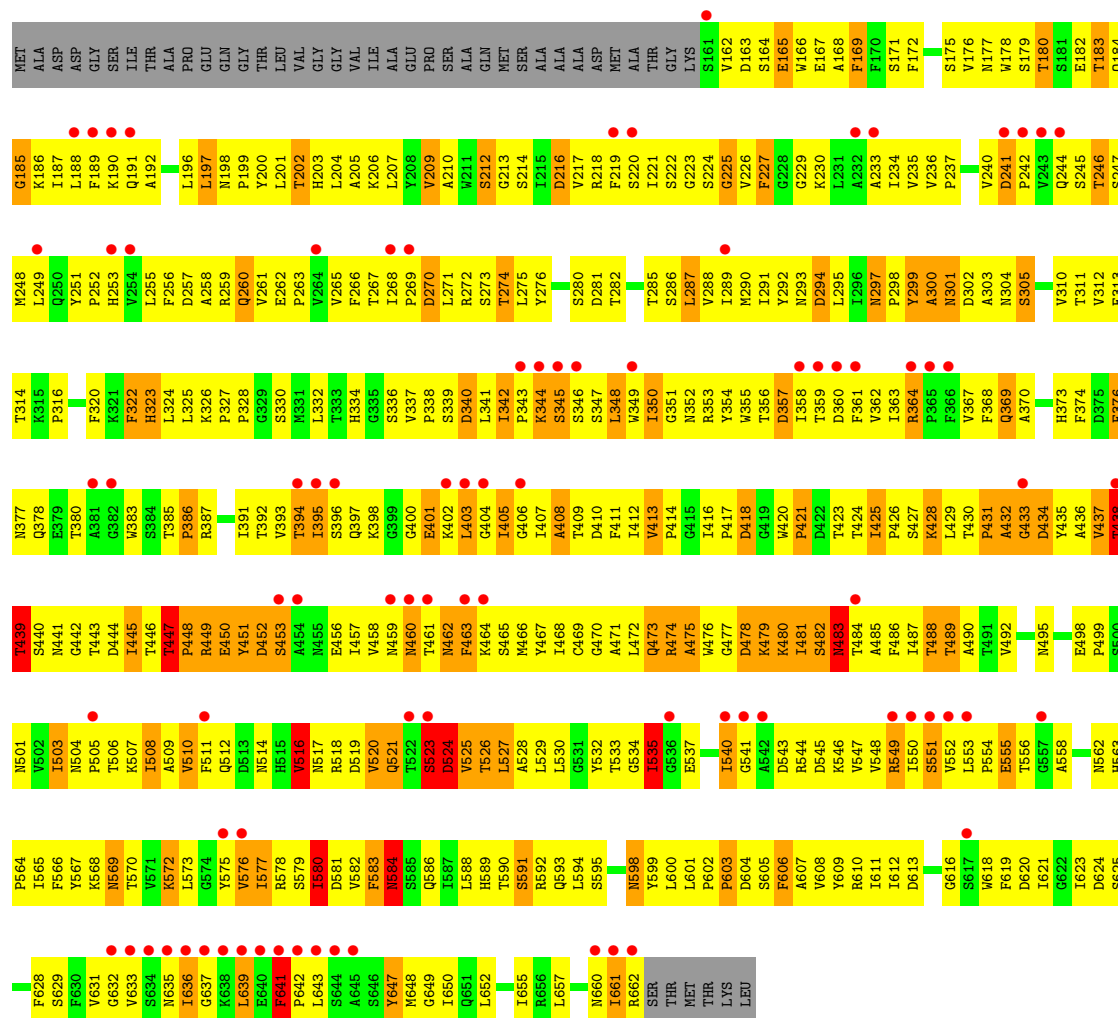
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

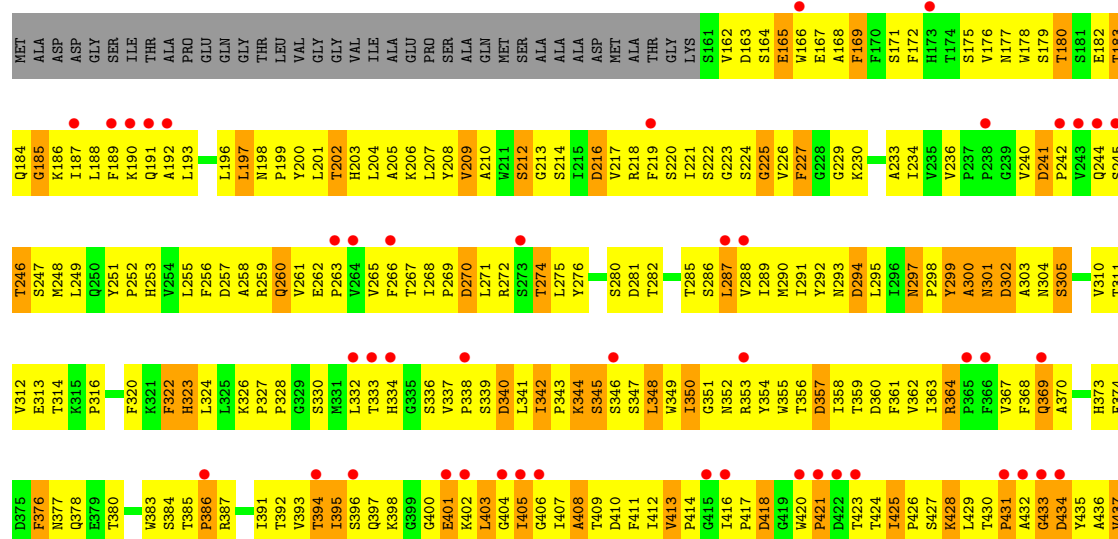
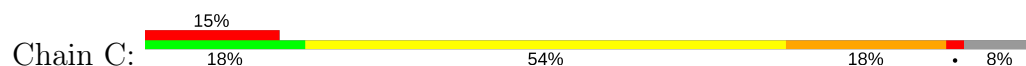


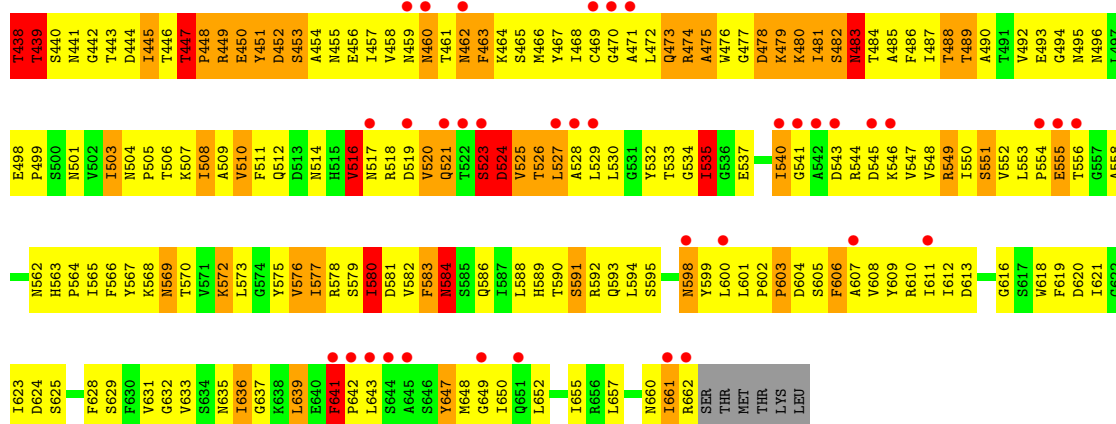
• Molecule 1: VP1



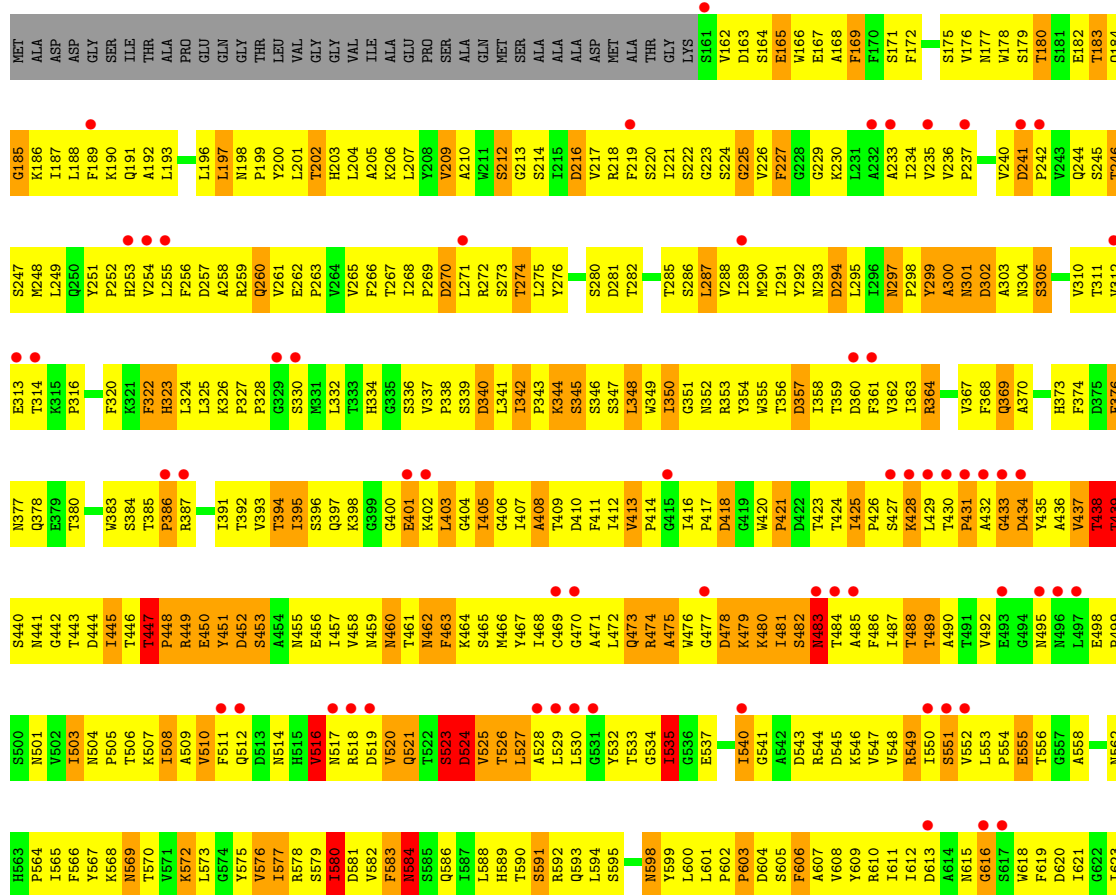
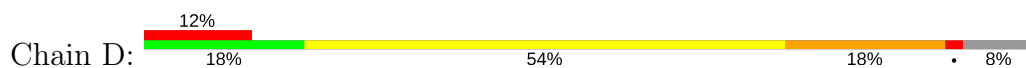


• Molecule 1: VP1

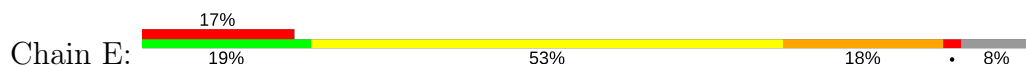


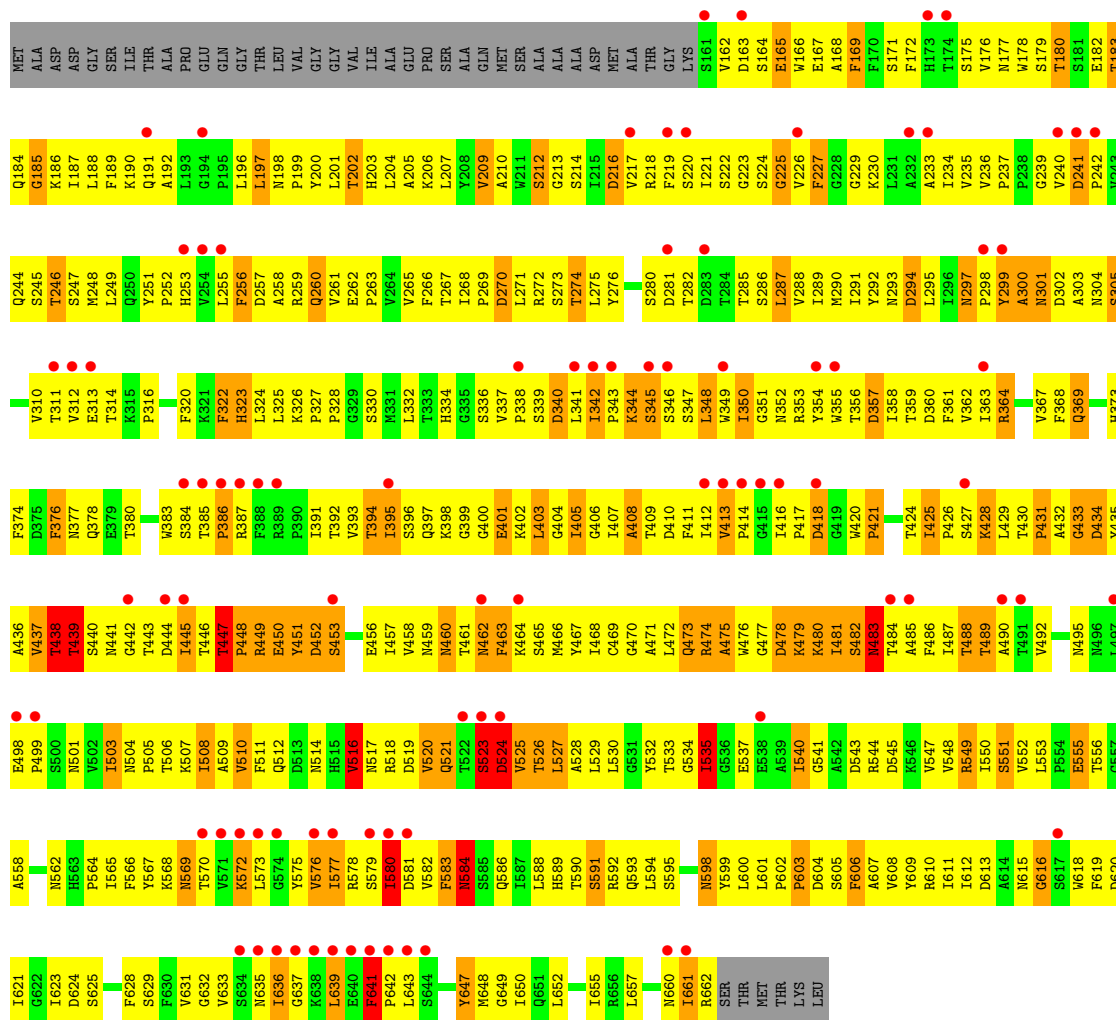


• Molecule 1: VP1

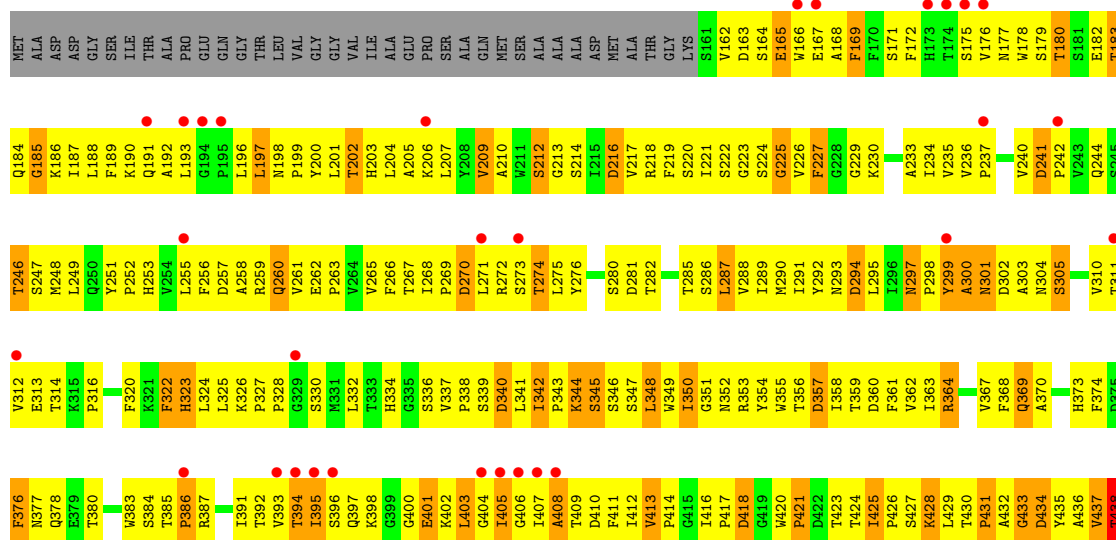
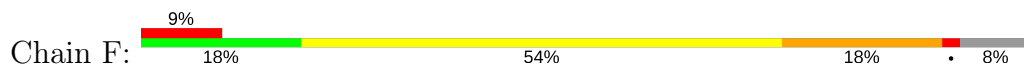


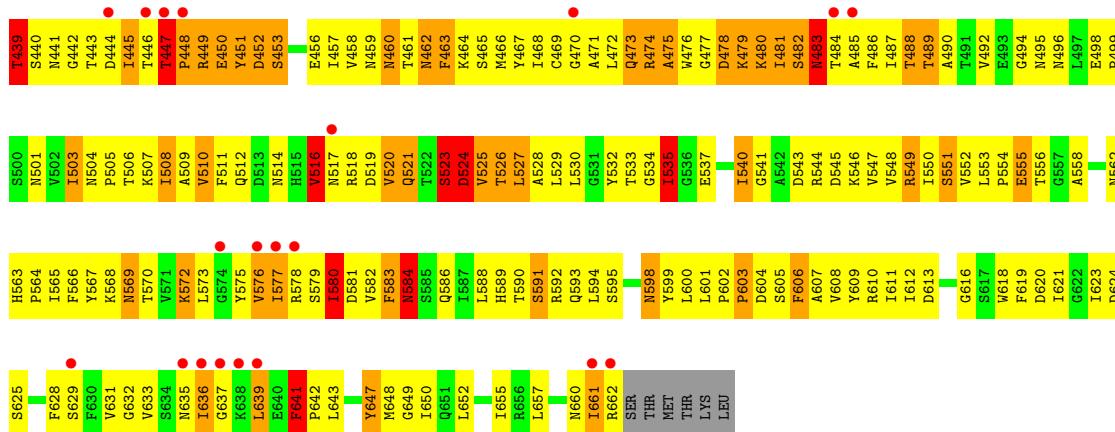
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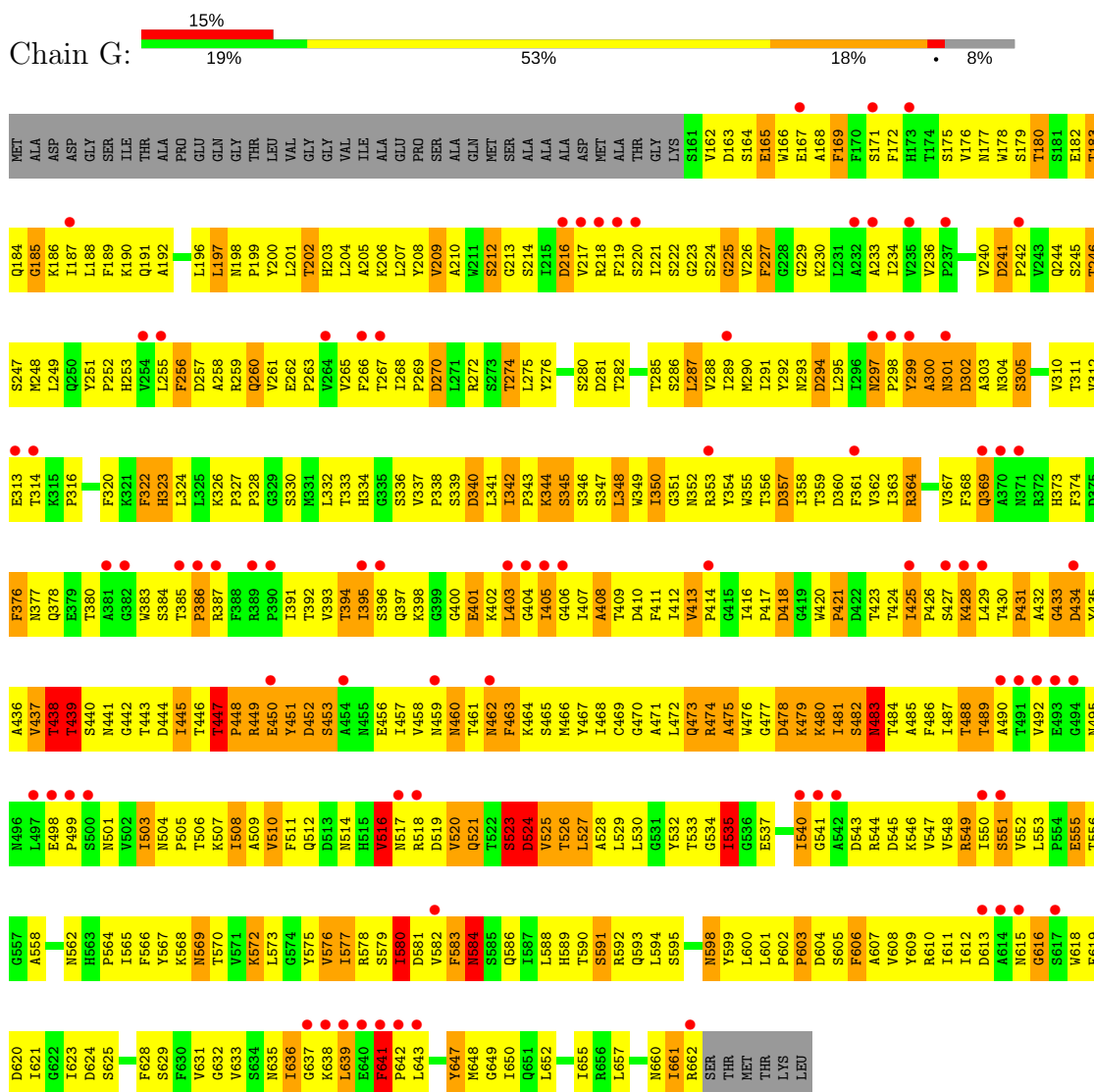


• Molecule 1: VP1

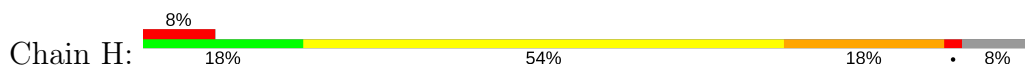


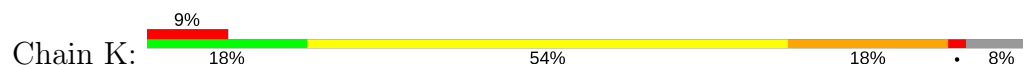


• Molecule 1: VP1

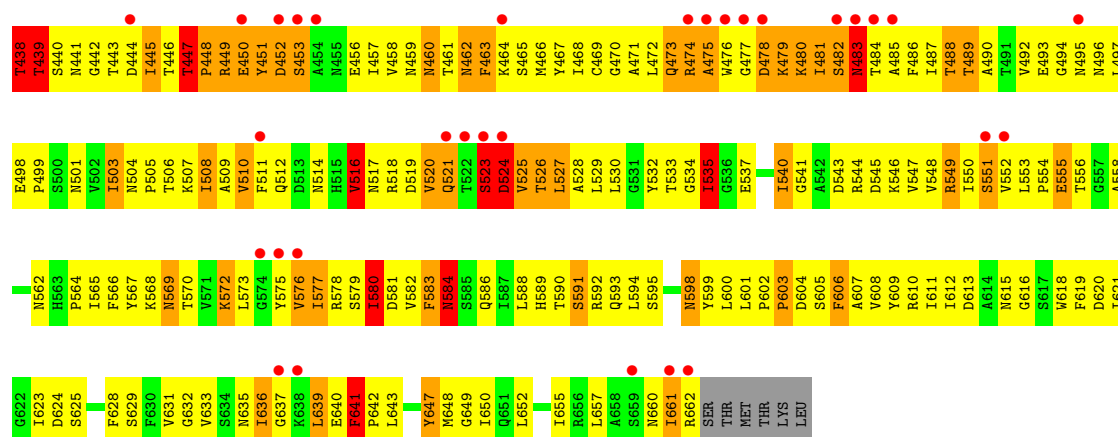


• Molecule 1: VP1

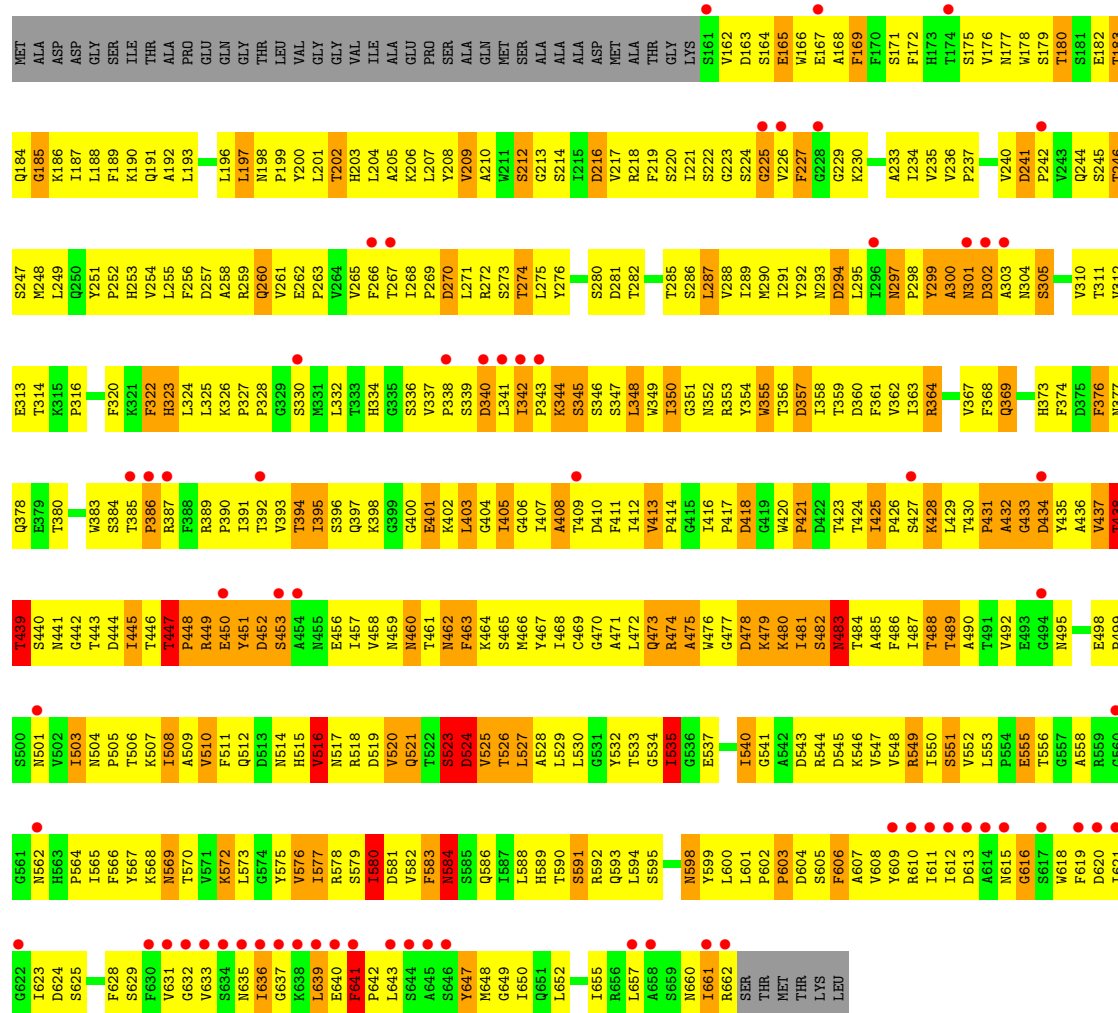
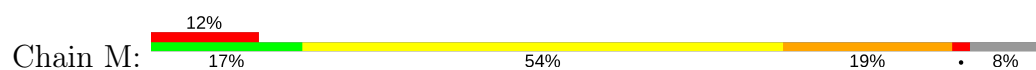




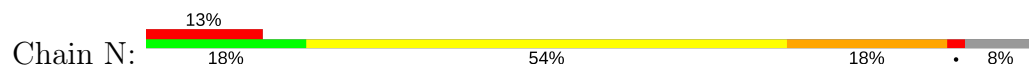




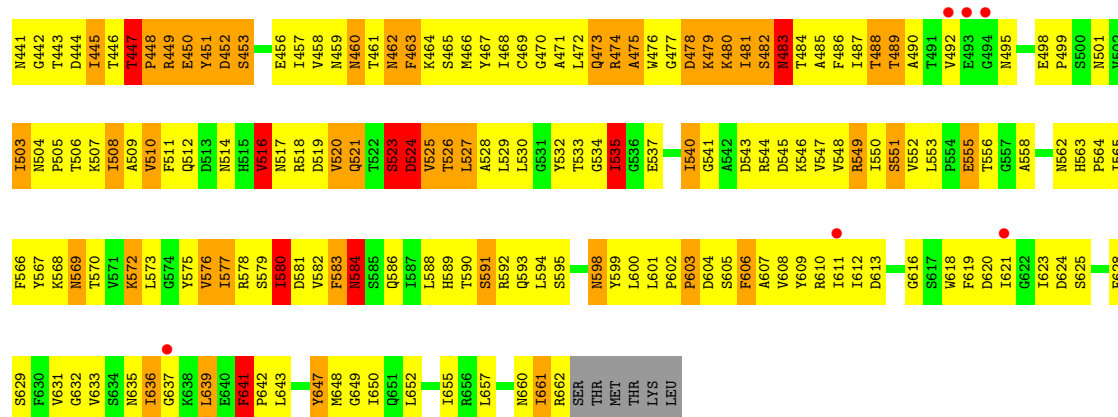
• Molecule 1: VP1



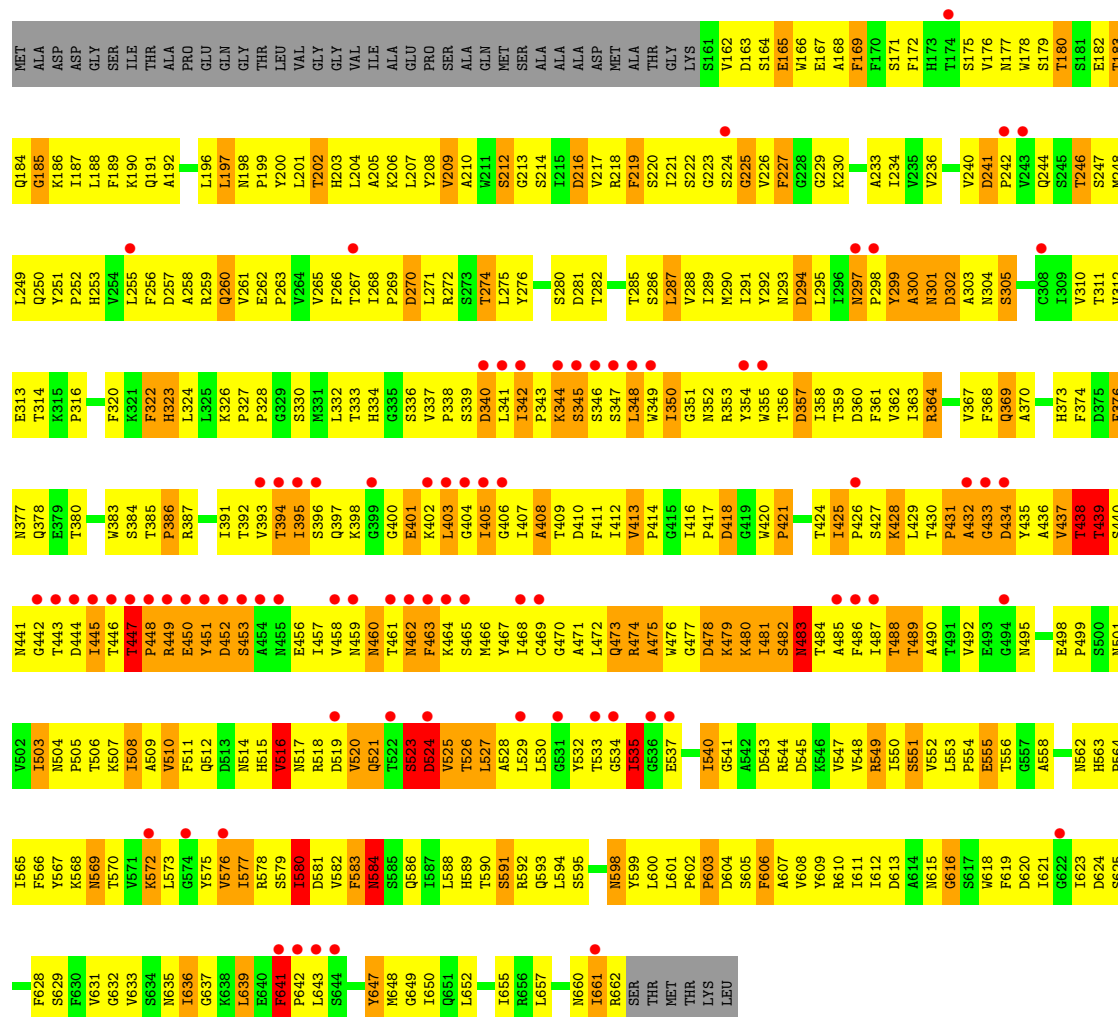
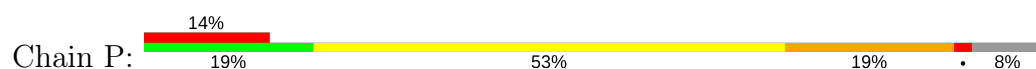
• Molecule 1: VP1



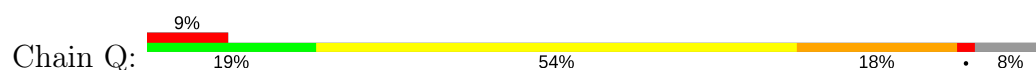


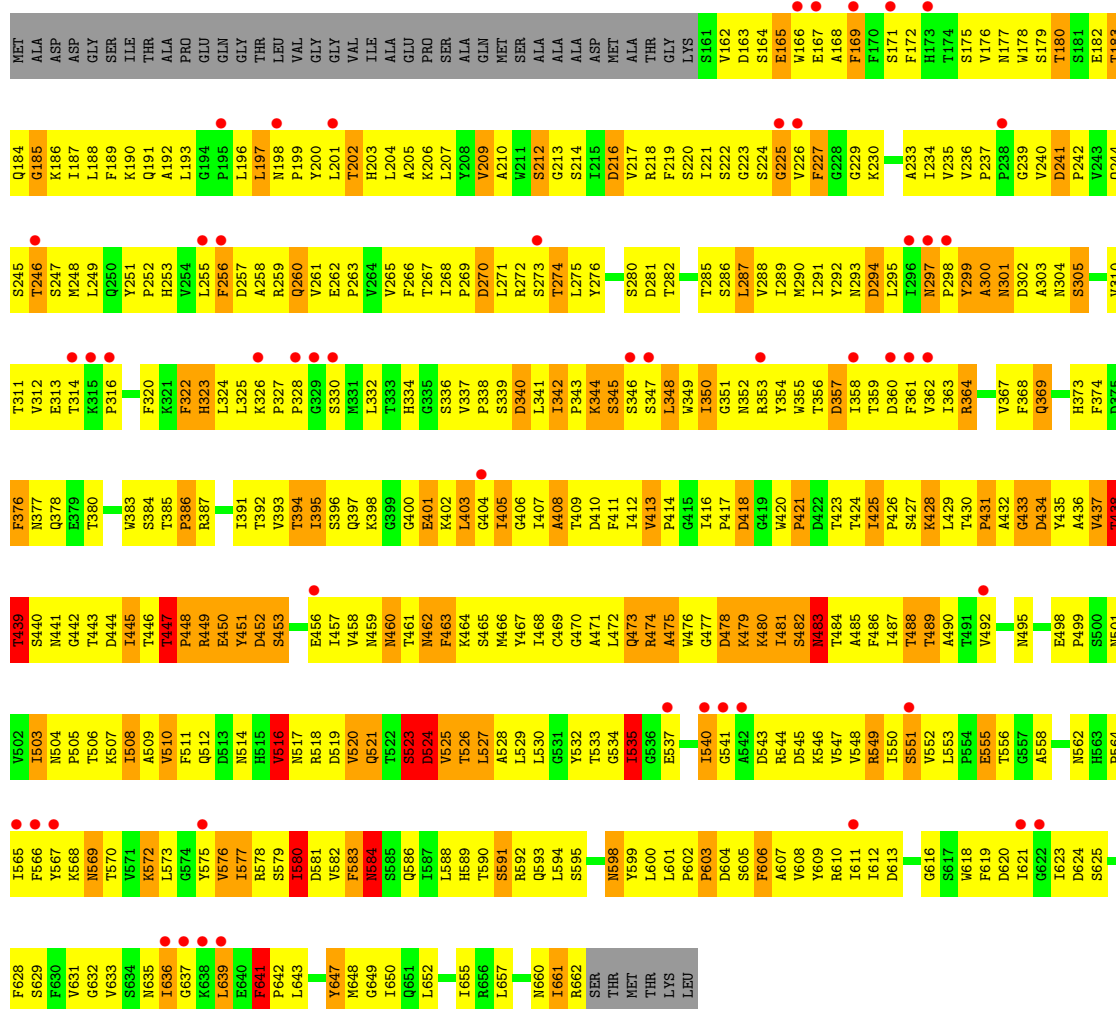


• Molecule 1: VP1



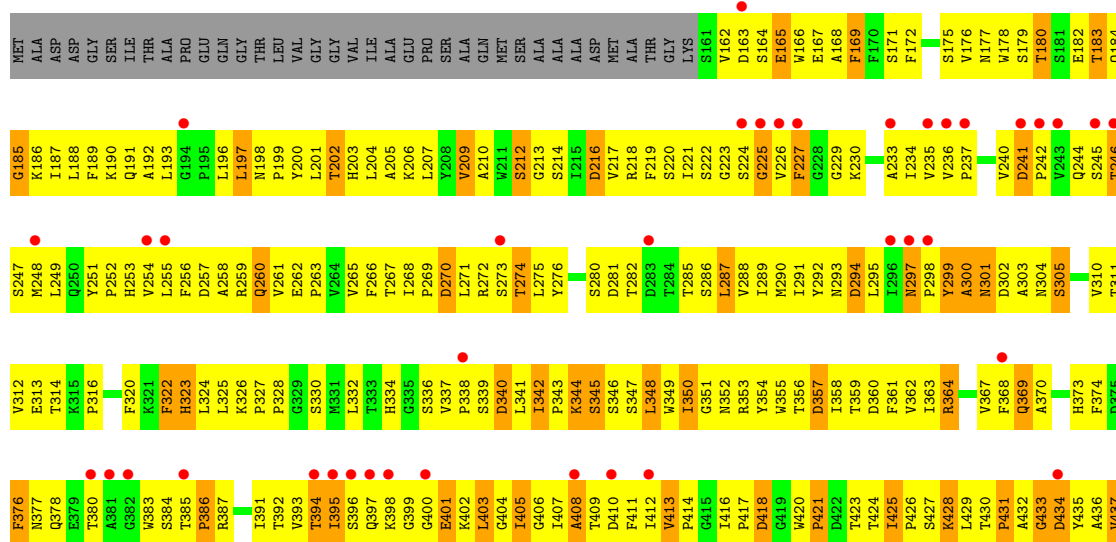
• Molecule 1: VP1

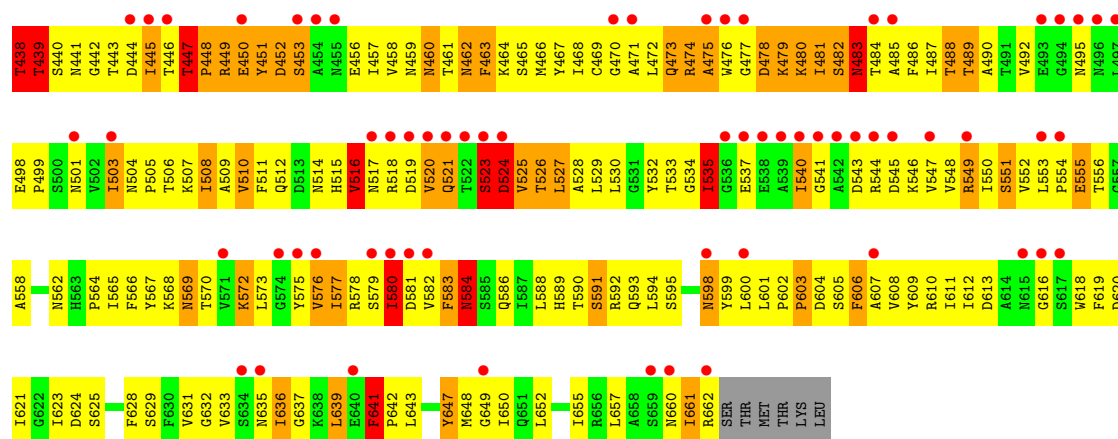




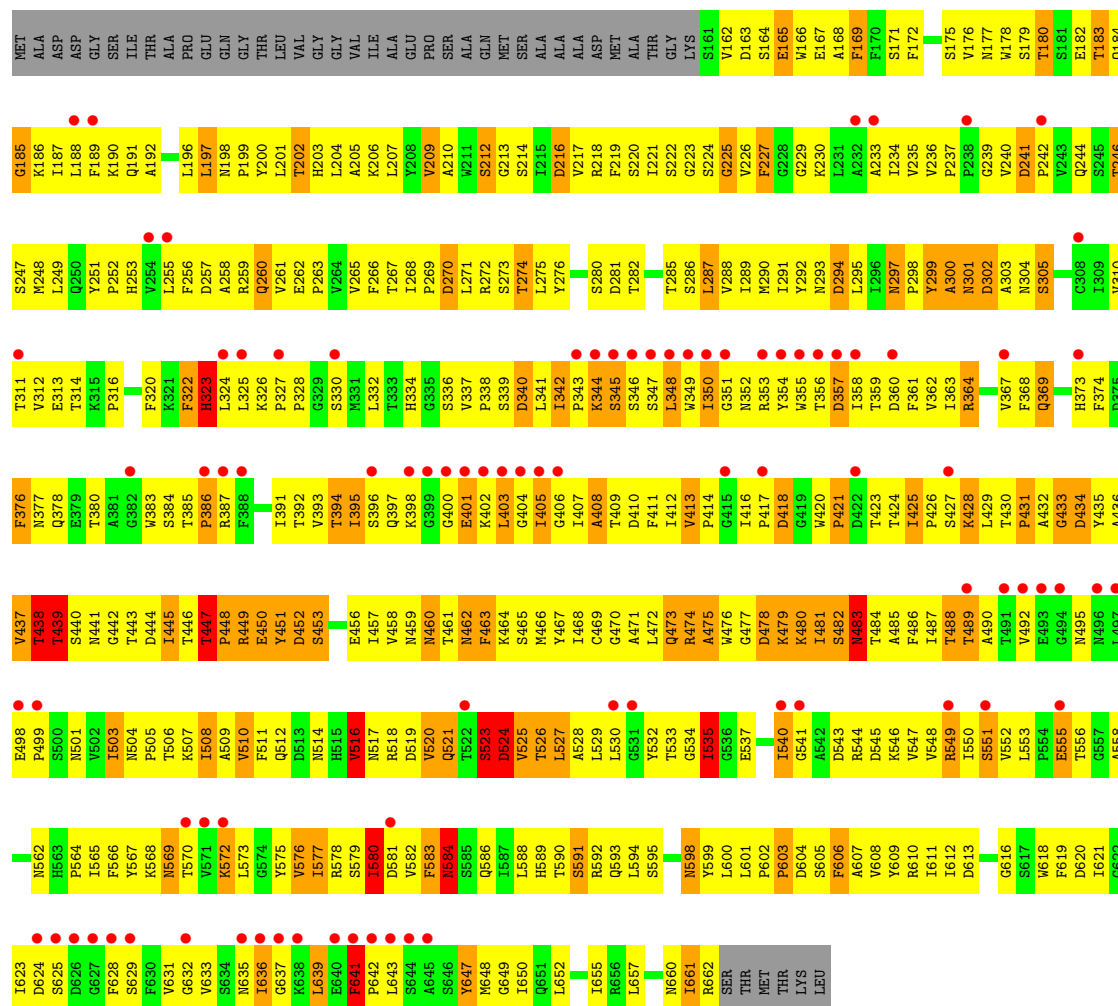
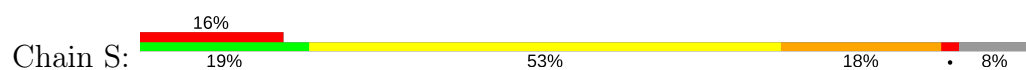
• Molecule 1: VP1

Chain R:

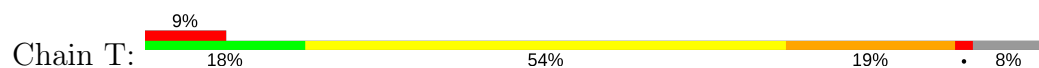


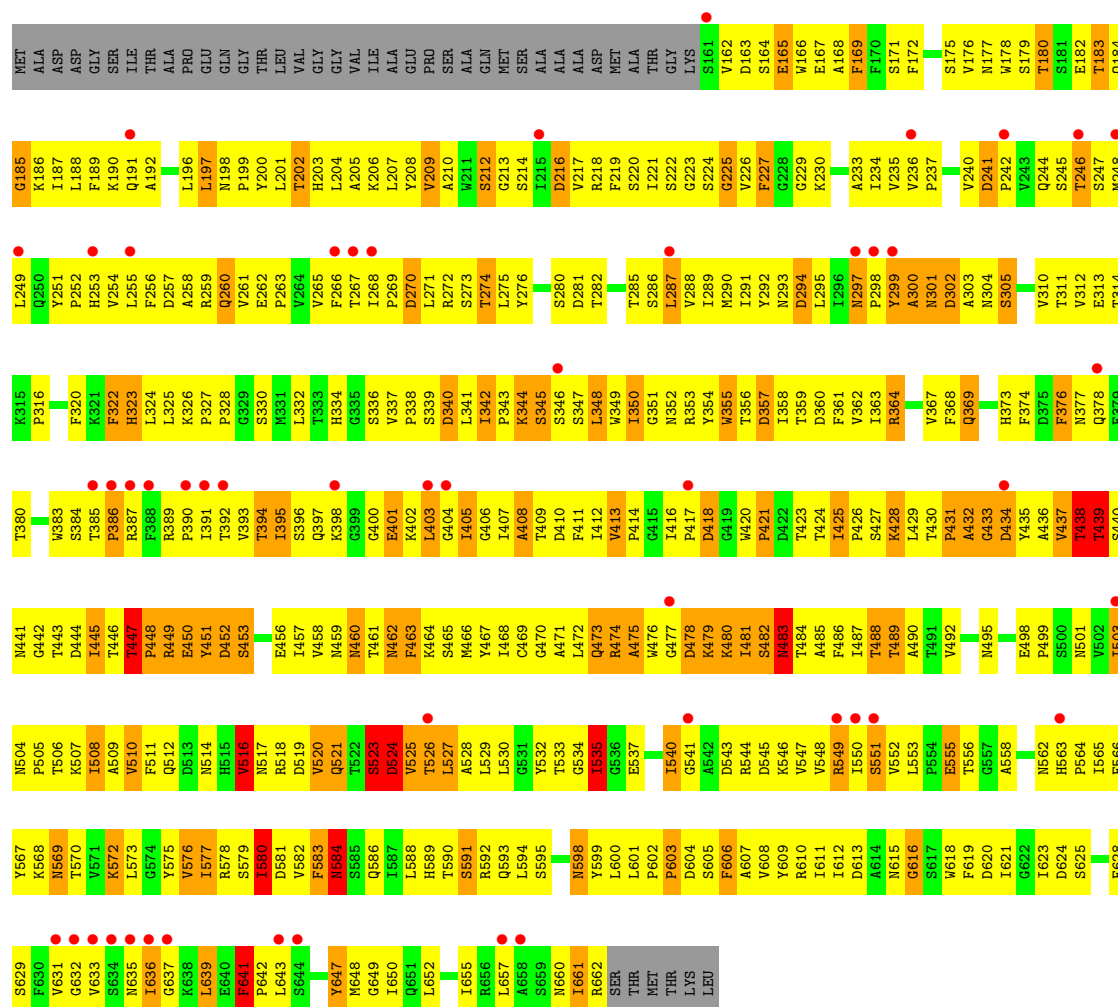


• Molecule 1: VP1



• 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)	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)	0.83 , 94.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	0.108 for l,-k,h	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.*

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 ⓘ

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(°)	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

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 ⓘ

5.3.1 Protein backbone ⓘ

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	6
1	B	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	6
1	C	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	6
1	D	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	6
1	E	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	6
1	F	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	6
1	G	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	6
1	H	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	6
1	J	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	6
1	K	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	6
1	L	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	6
1	M	498/545 (91%)	316 (64%)	115 (23%)	67 (14%)	0	6
1	N	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	6
1	O	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	6
1	P	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	6
1	Q	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	6
1	R	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	6
1	S	498/545 (91%)	318 (64%)	113 (23%)	67 (14%)	0	6
1	T	498/545 (91%)	317 (64%)	114 (23%)	67 (14%)	0	6
All	All	9960/10900 (91%)	6341 (64%)	2279 (23%)	1340 (14%)	0	6

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 ⓘ

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	18
1	B	434/464 (94%)	367 (85%)	67 (15%)	3	19
1	C	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	D	434/464 (94%)	366 (84%)	68 (16%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	F	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	G	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	H	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	I	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	J	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	K	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	L	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	M	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	N	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	O	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	P	434/464 (94%)	365 (84%)	69 (16%)	3	18
1	Q	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	R	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	S	434/464 (94%)	366 (84%)	68 (16%)	3	18
1	T	434/464 (94%)	366 (84%)	68 (16%)	3	18
All	All	8680/9280 (94%)	7320 (84%)	1360 (16%)	3	18

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 ⓘ

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