wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2023 – 01:03 pm GMT

PDB ID	:	7PA7
Title	:	BK polyomavirus VP1 in complex with scFv 29B1
Authors	:	Harprecht, C.; Stroeh, L.J.; Freytag, J.; Stehle, T.
Deposited on	:	2021-07-29
Resolution	:	2.60 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

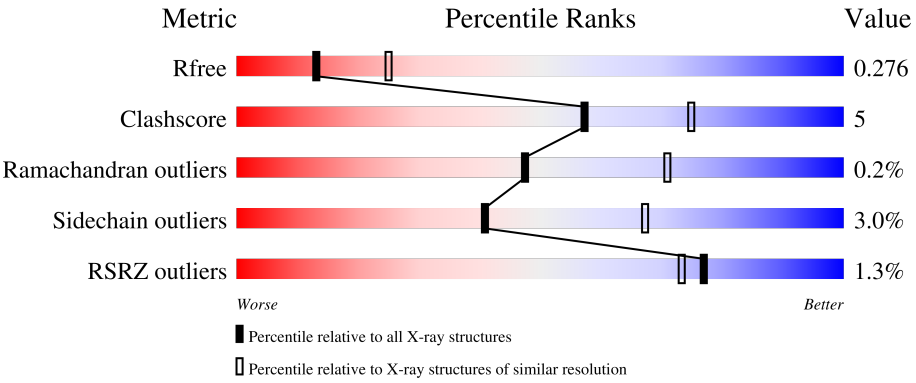
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	aaa	252	3% 89% · 8%
1	bbb	252	90% · 8%
1	ccc	252	9% 88% · 10%
1	ddd	252	91% · 7%
1	eee	252	91% · 7%

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Mol	Chain	Length	Quality of chain
1	mmm	252	2% 89% 8%
1	nnn	252	90% 8%
1	ooo	252	% 88% 8%
1	ppp	252	90% 8%
1	qqq	252	3% 90% 8%
2	AAA	275	77% 14% 9%
2	BBB	275	% 85% 7% 8%
2	CCC	275	81% 10% 8%
2	DDD	275	% 81% 8% 10%
2	EEE	275	84% 12%
2	MMM	275	78% 12% 8%
2	NNN	275	% 79% 12% 9%
2	OOO	275	85% 12%
2	PPP	275	81% 10% 9%
2	QQQ	275	% 84% 8% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 37703 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 scFv 29B1 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	eee	235	Total	C	N	O	S	0	0	0
			1777	1111	309	349	8			
1	aaa	231	Total	C	N	O	S	0	0	0
			1753	1096	309	340	8			
1	bbb	231	Total	C	N	O	S	0	0	0
			1733	1086	299	340	8			
1	ccc	228	Total	C	N	O	S	0	0	0
			1656	1035	283	331	7			
1	ddd	234	Total	C	N	O	S	0	0	0
			1768	1105	309	346	8			
1	mmm	231	Total	C	N	O	S	0	0	0
			1722	1074	298	342	8			
1	nnn	232	Total	C	N	O	S	0	0	0
			1739	1089	299	343	8			
1	ooo	233	Total	C	N	O	S	0	0	0
			1760	1100	308	344	8			
1	ppp	231	Total	C	N	O	S	0	0	0
			1744	1091	302	343	8			
1	qqq	232	Total	C	N	O	S	0	0	0
			1729	1082	297	342	8			

- Molecule 2 is a protein called Major capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AAA	251	Total	C	N	O	S	0	0	0
			1937	1217	336	372	12			
2	BBB	254	Total	C	N	O	S	0	0	0
			1959	1232	338	377	12			
2	CCC	253	Total	C	N	O	S	0	0	0
			1953	1231	337	373	12			
2	DDD	248	Total	C	N	O	S	0	0	0
			1903	1194	332	365	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	EEE	268	Total	C	N	O	S	0	0	0
			2052	1288	355	396	13			
2	MMM	252	Total	C	N	O	S	0	0	0
			1923	1209	333	369	12			
2	NNN	250	Total	C	N	O	S	0	0	0
			1921	1206	335	368	12			
2	OOO	269	Total	C	N	O	S	0	0	0
			2068	1298	355	402	13			
2	PPP	250	Total	C	N	O	S	0	0	0
			1930	1214	335	369	12			
2	QQQ	254	Total	C	N	O	S	0	0	0
			1950	1225	339	374	12			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	27	GLY	-	expression tag	UNP P03088
AAA	28	SER	-	expression tag	UNP P03088
AAA	29	HIS	-	expression tag	UNP P03088
AAA	30	MET	-	expression tag	UNP P03088
AAA	158	ASP	GLU	variant	UNP P03088
AAA	171	THR	SER	variant	UNP P03088
AAA	219	THR	ALA	variant	UNP P03088
BBB	27	GLY	-	expression tag	UNP P03088
BBB	28	SER	-	expression tag	UNP P03088
BBB	29	HIS	-	expression tag	UNP P03088
BBB	30	MET	-	expression tag	UNP P03088
BBB	158	ASP	GLU	variant	UNP P03088
BBB	171	THR	SER	variant	UNP P03088
BBB	219	THR	ALA	variant	UNP P03088
CCC	27	GLY	-	expression tag	UNP P03088
CCC	28	SER	-	expression tag	UNP P03088
CCC	29	HIS	-	expression tag	UNP P03088
CCC	30	MET	-	expression tag	UNP P03088
CCC	158	ASP	GLU	variant	UNP P03088
CCC	171	THR	SER	variant	UNP P03088
CCC	219	THR	ALA	variant	UNP P03088
DDD	27	GLY	-	expression tag	UNP P03088
DDD	28	SER	-	expression tag	UNP P03088
DDD	29	HIS	-	expression tag	UNP P03088
DDD	30	MET	-	expression tag	UNP P03088
DDD	158	ASP	GLU	variant	UNP P03088
DDD	171	THR	SER	variant	UNP P03088

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	219	THR	ALA	variant	UNP P03088
EEE	27	GLY	-	expression tag	UNP P03088
EEE	28	SER	-	expression tag	UNP P03088
EEE	29	HIS	-	expression tag	UNP P03088
EEE	30	MET	-	expression tag	UNP P03088
EEE	158	ASP	GLU	variant	UNP P03088
EEE	171	THR	SER	variant	UNP P03088
EEE	219	THR	ALA	variant	UNP P03088
MMM	27	GLY	-	expression tag	UNP P03088
MMM	28	SER	-	expression tag	UNP P03088
MMM	29	HIS	-	expression tag	UNP P03088
MMM	30	MET	-	expression tag	UNP P03088
MMM	158	ASP	GLU	variant	UNP P03088
MMM	171	THR	SER	variant	UNP P03088
MMM	219	THR	ALA	variant	UNP P03088
NNN	27	GLY	-	expression tag	UNP P03088
NNN	28	SER	-	expression tag	UNP P03088
NNN	29	HIS	-	expression tag	UNP P03088
NNN	30	MET	-	expression tag	UNP P03088
NNN	158	ASP	GLU	variant	UNP P03088
NNN	171	THR	SER	variant	UNP P03088
NNN	219	THR	ALA	variant	UNP P03088
OOO	27	GLY	-	expression tag	UNP P03088
OOO	28	SER	-	expression tag	UNP P03088
OOO	29	HIS	-	expression tag	UNP P03088
OOO	30	MET	-	expression tag	UNP P03088
OOO	158	ASP	GLU	variant	UNP P03088
OOO	171	THR	SER	variant	UNP P03088
OOO	219	THR	ALA	variant	UNP P03088
PPP	27	GLY	-	expression tag	UNP P03088
PPP	28	SER	-	expression tag	UNP P03088
PPP	29	HIS	-	expression tag	UNP P03088
PPP	30	MET	-	expression tag	UNP P03088
PPP	158	ASP	GLU	variant	UNP P03088
PPP	171	THR	SER	variant	UNP P03088
PPP	219	THR	ALA	variant	UNP P03088
QQQ	27	GLY	-	expression tag	UNP P03088
QQQ	28	SER	-	expression tag	UNP P03088
QQQ	29	HIS	-	expression tag	UNP P03088
QQQ	30	MET	-	expression tag	UNP P03088
QQQ	158	ASP	GLU	variant	UNP P03088
QQQ	171	THR	SER	variant	UNP P03088

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Chain	Residue	Modelled	Actual	Comment	Reference
QQQ	219	THR	ALA	variant	UNP P03088

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	eee	29	Total O 29 29	0	0
3	AAA	52	Total O 52 52	0	0
3	BBB	36	Total O 36 36	0	0
3	CCC	39	Total O 39 39	0	0
3	DDD	50	Total O 50 50	0	0
3	EEE	63	Total O 63 63	0	0
3	MMM	39	Total O 39 39	0	0
3	NNN	58	Total O 58 58	0	0
3	OOO	42	Total O 42 42	0	0
3	PPP	51	Total O 51 51	0	0
3	QQQ	38	Total O 38 38	0	0
3	aaa	25	Total O 25 25	0	0
3	bbb	18	Total O 18 18	0	0
3	ccc	35	Total O 35 35	0	0
3	ddd	31	Total O 31 31	0	0
3	mmm	30	Total O 30 30	0	0
3	nnn	20	Total O 20 20	0	0
3	ooo	32	Total O 32 32	0	0
3	ppp	22	Total O 22 22	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	qqq	16	Total	O	0	0
			16	16		

3 Residue-property plots (i)

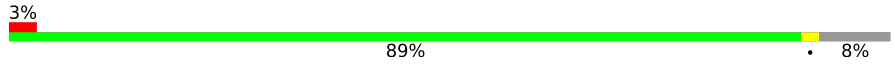
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

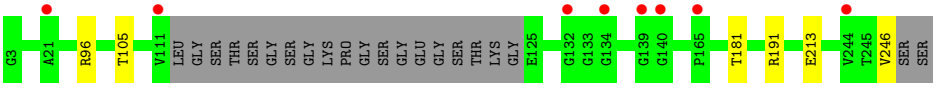
- Molecule 1: scFv 29B1 antibody heavy chain

Chain eee:

- Molecule 1: scFv 29B1 antibody heavy chain

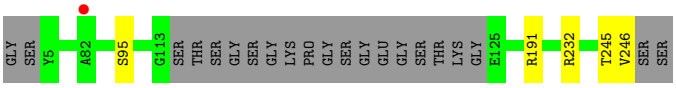
Chain aaa:





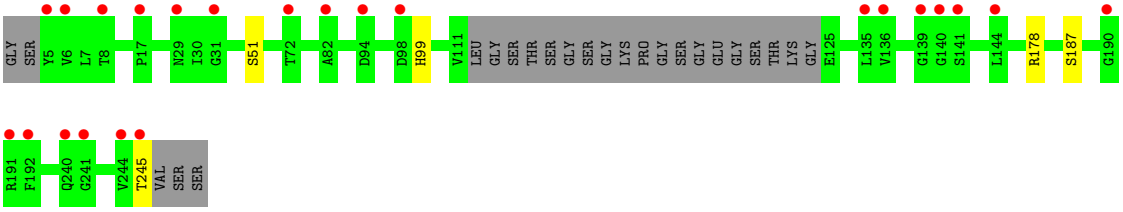
- Molecule 1: scFv 29B1 antibody heavy chain

Chain bbb:



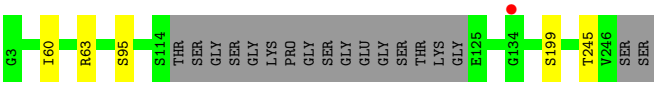
- Molecule 1: scFv 29B1 antibody heavy chain

Chain ccc:



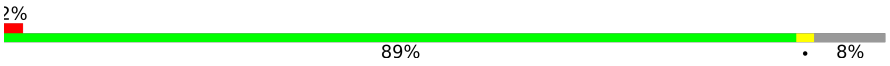
- Molecule 1: scFv 29B1 antibody heavy chain

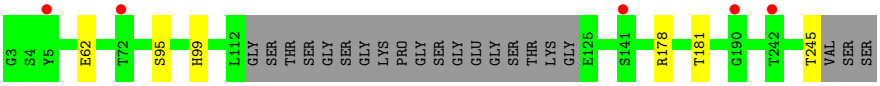
Chain ddd:



• Molecule 1: scFv 29B1 antibody heavy chain

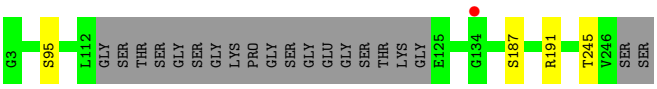
Chain mmm:





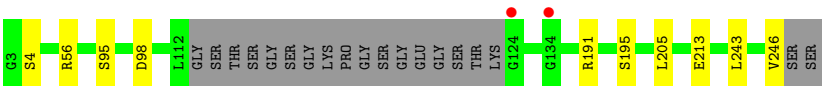
• Molecule 1: scFv 29B1 antibody heavy chain

Chain nnn:



• Molecule 1: scFv 29B1 antibody heavy chain

Chain ooo:

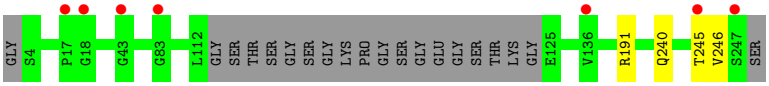


• Molecule 1: scFv 29B1 antibody heavy chain

Chain ppp:

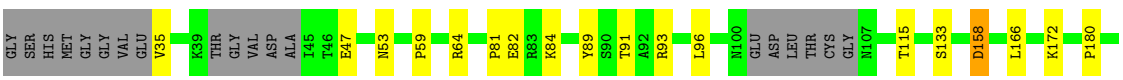
• Molecule 1: scFv 29B1 antibody heavy chain

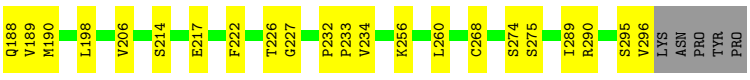
Chain qqq:



• Molecule 2: Major capsid protein VP1

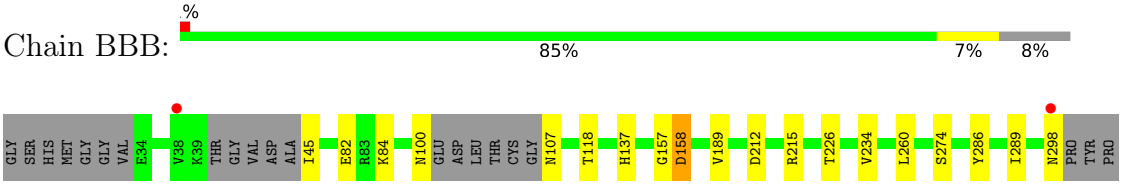
Chain AAA:





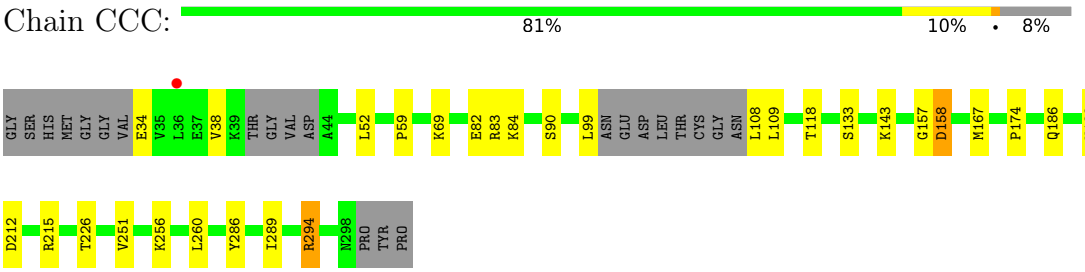
• Molecule 2: Major capsid protein VP1

Chain BBB:



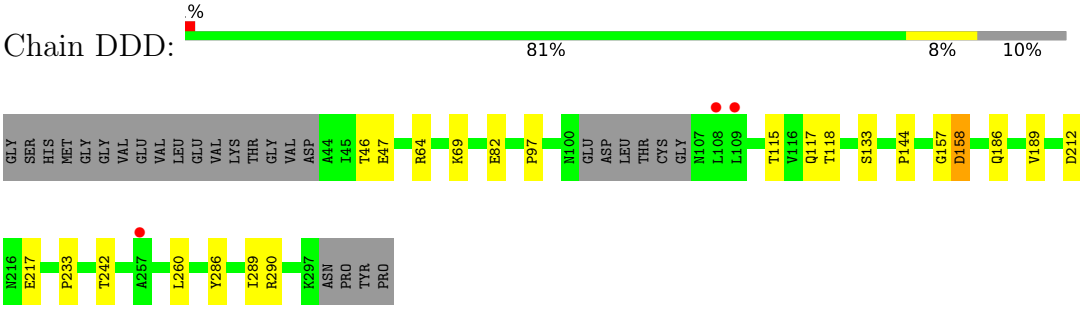
• Molecule 2: Major capsid protein VP1

Chain CCC:



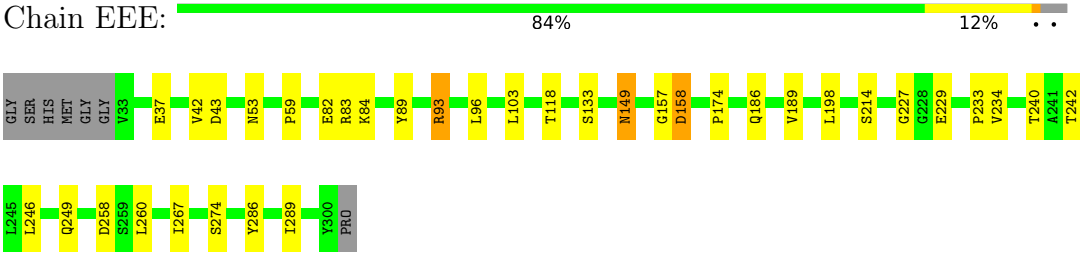
• Molecule 2: Major capsid protein VP1

Chain DDD:



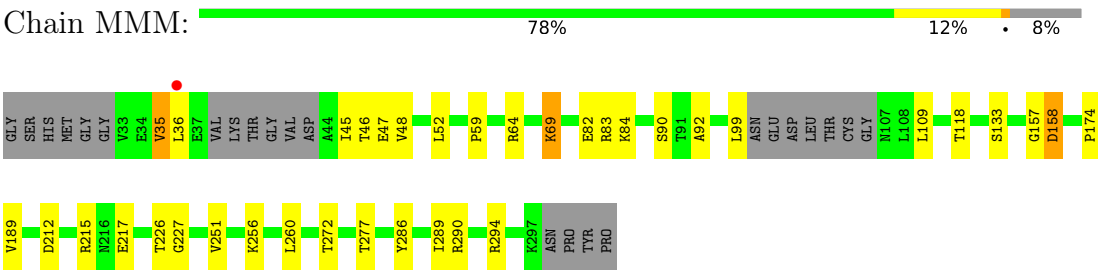
• Molecule 2: Major capsid protein VP1

Chain EEE:



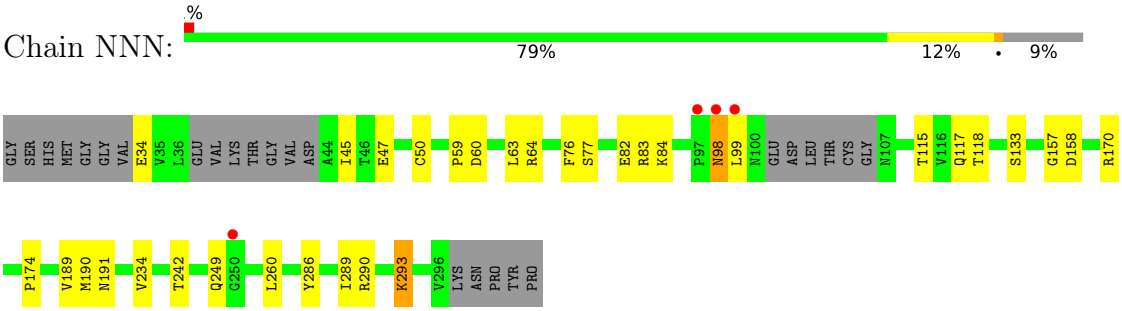
• Molecule 2: Major capsid protein VP1

Chain MMM:



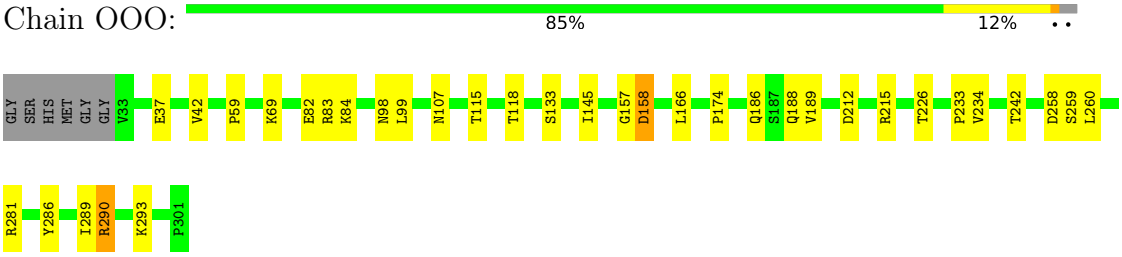
• Molecule 2: Major capsid protein VP1

Chain NNN:



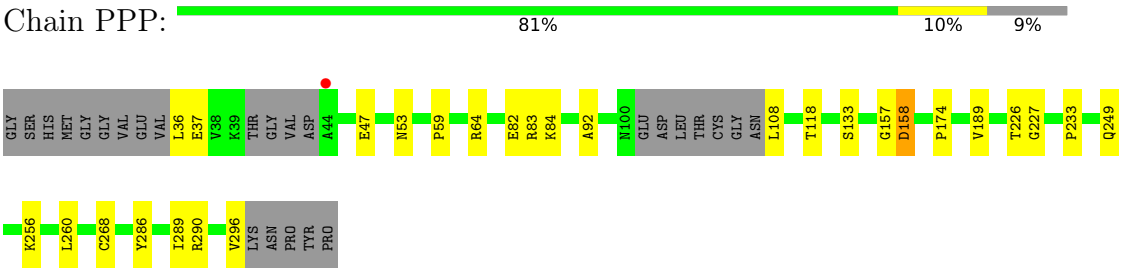
• Molecule 2: Major capsid protein VP1

Chain OOO:



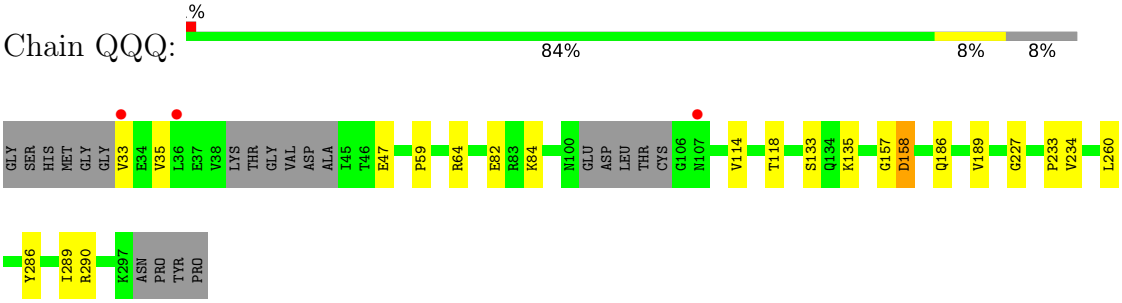
• Molecule 2: Major capsid protein VP1

Chain PPP:



• Molecule 2: Major capsid protein VP1

Chain QQQ:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	114.59Å 114.61Å 142.37Å 92.31° 106.00° 111.41°	Depositor
Resolution (Å)	48.44 – 2.60 48.44 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.9 (48.44-2.60) 91.9 (48.44-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.247 , 0.272 0.249 , 0.276	Depositor DCC
R_{free} test set	1810 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	37703	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.26% 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, 0.333 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	aaa	0.68	0/1796	0.79	0/2443
1	bbb	0.68	0/1775	0.76	0/2419
1	ccc	0.70	0/1698	0.80	0/2324
1	ddd	0.69	0/1811	0.79	0/2464
1	eee	0.67	0/1820	0.78	0/2476
1	mmm	0.69	0/1764	0.77	0/2406
1	nnn	0.70	0/1782	0.77	0/2430
1	ooo	0.67	0/1803	0.80	0/2453
1	ppp	0.68	0/1787	0.80	0/2435
1	qqq	0.68	0/1770	0.79	0/2413
2	AAA	0.61	0/1981	0.80	1/2692 (0.0%)
2	BBB	0.64	0/2003	0.79	1/2722 (0.0%)
2	CCC	0.65	0/1997	0.83	1/2713 (0.0%)
2	DDD	0.65	0/1948	0.79	1/2649 (0.0%)
2	EEE	0.63	0/2100	0.83	1/2861 (0.0%)
2	MMM	0.65	0/1967	0.82	1/2677 (0.0%)
2	NNN	0.66	0/1965	0.79	0/2672
2	OOO	0.65	0/2117	0.83	1/2884 (0.0%)
2	PPP	0.66	0/1974	0.80	1/2682 (0.0%)
2	QQQ	0.66	0/1994	0.78	1/2712 (0.0%)
All	All	0.66	0/37852	0.80	9/51527 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	158	ASP	CB-CG-OD2	5.42	123.18	118.30
2	QQQ	158	ASP	CB-CG-OD2	5.24	123.01	118.30
2	EEE	158	ASP	CB-CG-OD2	5.22	123.00	118.30
2	AAA	158	ASP	CB-CG-OD2	5.21	122.99	118.30
2	MMM	158	ASP	CB-CG-OD2	5.20	122.98	118.30

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	aaa	1753	0	1662	0	0
1	bbb	1733	0	1626	0	0
1	ccc	1656	0	1482	0	1
1	ddd	1768	0	1672	0	0
1	eee	1777	0	1681	0	0
1	mmm	1722	0	1595	0	0
1	nnn	1739	0	1622	0	0
1	ooo	1760	0	1660	0	0
1	ppp	1744	0	1631	0	0
1	qqq	1729	0	1617	0	0
2	AAA	1937	0	1870	19	0
2	BBB	1959	0	1890	11	0
2	CCC	1953	0	1897	17	0
2	DDD	1903	0	1827	11	0
2	EEE	2052	0	1976	22	0
2	MMM	1923	0	1839	23	0
2	NNN	1921	0	1849	23	0
2	OOO	2068	0	1991	20	1
2	PPP	1930	0	1871	22	0
2	QQQ	1950	0	1880	11	0
3	AAA	52	0	0	3	0
3	BBB	36	0	0	5	0
3	CCC	39	0	0	6	0
3	DDD	50	0	0	3	0
3	EEE	63	0	0	5	0
3	MMM	39	0	0	7	0
3	NNN	58	0	0	10	0
3	OOO	42	0	0	4	0
3	PPP	51	0	0	11	0
3	QQQ	38	0	0	1	0
3	aaa	25	0	0	0	0
3	bbb	18	0	0	0	0
3	ccc	35	0	0	0	0
3	ddd	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	eee	29	0	0	0	0
3	mmm	30	0	0	0	0
3	nnn	20	0	0	0	0
3	ooo	32	0	0	0	0
3	ppp	22	0	0	0	0
3	qqq	16	0	0	0	0
All	All	37703	0	35138	164	1

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 5.

The worst 5 of 164 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)
2:BBB:298:ASN:HA	3:BBB:414:HOH:O	1.48	1.13
2:NNN:117:GLN:HB3	3:NNN:444:HOH:O	1.58	1.01
2:MMM:109:LEU:CB	3:MMM:429:HOH:O	2.12	0.97
2:NNN:293:LYS:HE3	3:NNN:432:HOH:O	1.75	0.86
2:PPP:37:GLU:CA	3:PPP:414:HOH:O	2.23	0.85

All (1) 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)
2:OOO:107:ASN:OD1	1:ccc:178:ARG:NH2[1_445]	2.19	0.01

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	aaa	227/252 (90%)	221 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	bbb	227/252 (90%)	220 (97%)	7 (3%)	0	100	100
1	ccc	224/252 (89%)	219 (98%)	5 (2%)	0	100	100
1	ddd	230/252 (91%)	225 (98%)	5 (2%)	0	100	100
1	eee	231/252 (92%)	223 (96%)	8 (4%)	0	100	100
1	mmm	227/252 (90%)	224 (99%)	3 (1%)	0	100	100
1	nnn	228/252 (90%)	220 (96%)	8 (4%)	0	100	100
1	ooo	229/252 (91%)	223 (97%)	6 (3%)	0	100	100
1	ppp	227/252 (90%)	222 (98%)	5 (2%)	0	100	100
1	qqq	228/252 (90%)	224 (98%)	4 (2%)	0	100	100
2	AAA	245/275 (89%)	233 (95%)	11 (4%)	1 (0%)	34	57
2	BBB	248/275 (90%)	237 (96%)	10 (4%)	1 (0%)	34	57
2	CCC	247/275 (90%)	236 (96%)	10 (4%)	1 (0%)	34	57
2	DDD	244/275 (89%)	234 (96%)	9 (4%)	1 (0%)	34	57
2	EEE	266/275 (97%)	252 (95%)	13 (5%)	1 (0%)	34	57
2	MMM	246/275 (90%)	234 (95%)	11 (4%)	1 (0%)	34	57
2	NNN	244/275 (89%)	235 (96%)	8 (3%)	1 (0%)	34	57
2	OOO	267/275 (97%)	256 (96%)	10 (4%)	1 (0%)	34	57
2	PPP	244/275 (89%)	234 (96%)	9 (4%)	1 (0%)	34	57
2	QQQ	248/275 (90%)	235 (95%)	12 (5%)	1 (0%)	34	57
All	All	4777/5270 (91%)	4607 (96%)	160 (3%)	10 (0%)	47	71

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AAA	189	VAL
2	BBB	189	VAL
2	CCC	189	VAL
2	EEE	189	VAL
2	MMM	189	VAL

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	aaa	186/204 (91%)	180 (97%)	6 (3%)	39	65
1	bbb	182/204 (89%)	177 (97%)	5 (3%)	44	71
1	ccc	166/204 (81%)	162 (98%)	4 (2%)	49	74
1	ddd	188/204 (92%)	183 (97%)	5 (3%)	44	71
1	eee	189/204 (93%)	183 (97%)	6 (3%)	39	65
1	mmm	180/204 (88%)	174 (97%)	6 (3%)	38	64
1	nnn	183/204 (90%)	179 (98%)	4 (2%)	52	76
1	ooo	186/204 (91%)	176 (95%)	10 (5%)	22	44
1	ppp	184/204 (90%)	181 (98%)	3 (2%)	62	82
1	qqq	182/204 (89%)	178 (98%)	4 (2%)	52	76
2	AAA	213/236 (90%)	202 (95%)	11 (5%)	23	46
2	BBB	215/236 (91%)	210 (98%)	5 (2%)	50	75
2	CCC	214/236 (91%)	209 (98%)	5 (2%)	50	75
2	DDD	207/236 (88%)	201 (97%)	6 (3%)	42	68
2	EEE	225/236 (95%)	217 (96%)	8 (4%)	35	61
2	MMM	208/236 (88%)	198 (95%)	10 (5%)	25	49
2	NNN	210/236 (89%)	203 (97%)	7 (3%)	38	64
2	OOO	228/236 (97%)	222 (97%)	6 (3%)	46	72
2	PPP	212/236 (90%)	210 (99%)	2 (1%)	78	91
2	QQQ	214/236 (91%)	209 (98%)	5 (2%)	50	75
All	All	3972/4400 (90%)	3854 (97%)	118 (3%)	41	67

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	NNN	293	LYS
1	ooo	246	VAL
1	aaa	96	ARG
1	ooo	243	LEU
1	nnn	191	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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

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	aaa	231/252 (91%)	-0.02	8 (3%) 44 36	13, 35, 59, 69	0
1	bbb	231/252 (91%)	-0.28	1 (0%) 92 91	18, 35, 55, 76	0
1	ccc	228/252 (90%)	0.59	23 (10%) 7 4	26, 53, 81, 96	0
1	ddd	234/252 (92%)	-0.15	1 (0%) 92 91	15, 34, 58, 66	0
1	eee	235/252 (93%)	-0.36	0 100 100	12, 26, 48, 85	0
1	mmm	231/252 (91%)	0.22	5 (2%) 62 56	21, 43, 65, 80	0
1	nnn	232/252 (92%)	-0.22	1 (0%) 92 91	17, 33, 55, 69	0
1	ooo	233/252 (92%)	-0.28	2 (0%) 84 82	15, 30, 52, 70	0
1	ppp	231/252 (91%)	-0.27	0 100 100	14, 33, 56, 79	0
1	qqq	232/252 (92%)	-0.05	7 (3%) 50 43	18, 37, 61, 74	0
2	AAA	251/275 (91%)	-0.36	0 100 100	9, 19, 45, 68	0
2	BBB	254/275 (92%)	-0.41	2 (0%) 86 84	11, 20, 47, 92	0
2	CCC	253/275 (92%)	-0.34	1 (0%) 92 91	9, 21, 50, 69	0
2	DDD	248/275 (90%)	-0.28	3 (1%) 79 76	7, 19, 48, 70	0
2	EEE	268/275 (97%)	-0.43	0 100 100	9, 18, 40, 67	0
2	MMM	252/275 (91%)	-0.31	1 (0%) 92 91	8, 21, 51, 64	0
2	NNN	250/275 (90%)	-0.31	4 (1%) 72 68	9, 20, 49, 74	0
2	OOO	269/275 (97%)	-0.39	0 100 100	10, 19, 45, 84	0
2	PPP	250/275 (90%)	-0.41	1 (0%) 92 91	9, 18, 43, 71	0
2	QQQ	254/275 (92%)	-0.39	3 (1%) 79 76	11, 21, 50, 78	0
All	All	4867/5270 (92%)	-0.23	63 (1%) 77 73	7, 26, 58, 96	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	ccc	191	ARG	4.2
2	QQQ	107	ASN	3.9
1	ddd	134	GLY	3.7
2	NNN	98	ASN	3.5
1	ccc	190	GLY	3.4

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 monosaccharides 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.