



wwPDB X-ray Structure Validation Summary Report i

Feb 1, 2016 – 10:11 AM GMT

PDB ID : 3KZ4
Title : Crystal Structure of the Rotavirus Double Layered Particle
Authors : Mcclain, B.; Settembre, E.C.; Bellamy, A.R.; Harrison, S.C.
Deposited on : 2009-12-07
Resolution : 3.80 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:

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

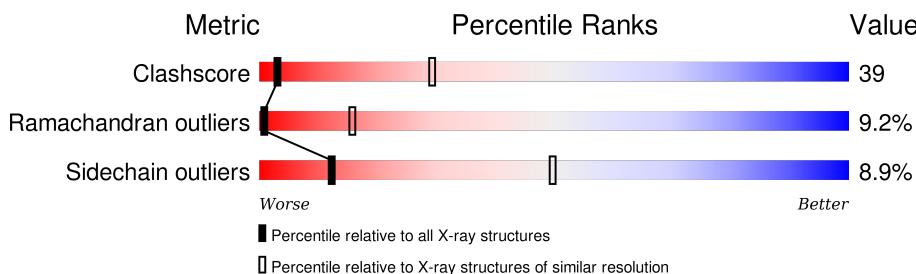
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

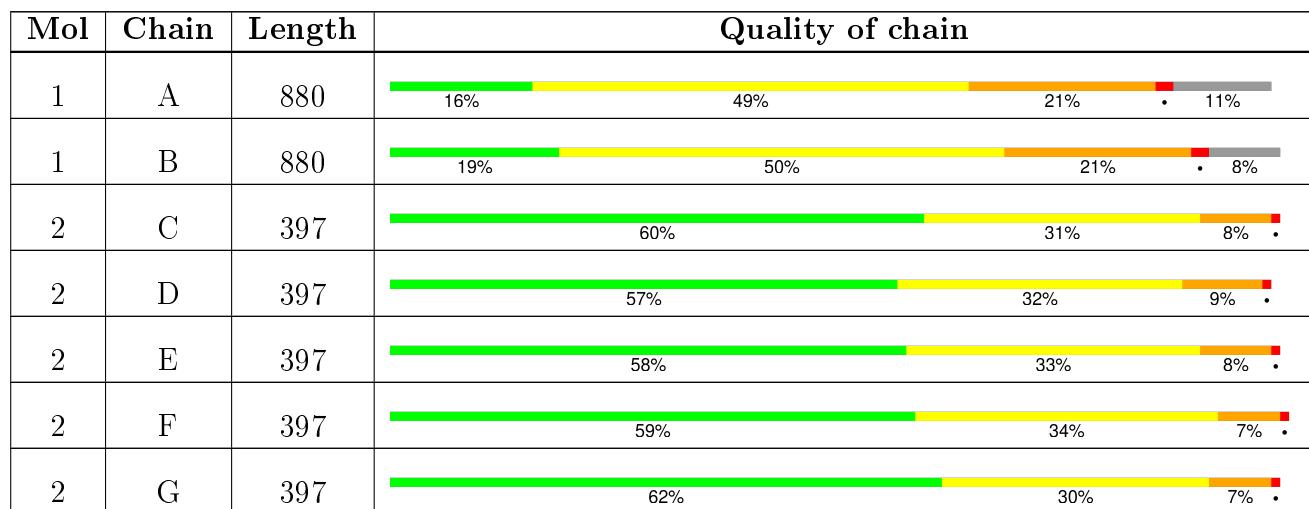
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)

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.

Note EDS failed to run properly.



Continued on next page...

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Mol	Chain	Length	Quality of chain		
2	H	397	60%	32%	7% •
2	I	397	58%	33%	9%
2	J	397	58%	34%	8% •
2	K	397	59%	33%	8% •
2	L	397	57%	35%	7% •
2	M	397	58%	35%	6% •
2	N	397	56%	34%	9% •
2	O	397	57%	33%	9% •

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 54109 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 Inner capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C 6374	N 4049	O 1099	S 1190	36	0	0
1	B	810	Total	C 6624	N 4211	O 1138	S 1239	36	0	0

- Molecule 2 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	397	Total	C 3162	N 2001	O 550	S 596	15	0	0
2	D	397	Total	C 3162	N 2001	O 550	S 596	15	0	0
2	E	397	Total	C 3162	N 2001	O 550	S 596	15	0	0
2	F	397	Total	C 3162	N 2001	O 550	S 596	15	0	0
2	G	397	Total	C 3162	N 2001	O 550	S 596	15	0	0
2	H	397	Total	C 3162	N 2001	O 550	S 596	15	0	0
2	I	397	Total	C 3162	N 2001	O 550	S 596	15	0	0
2	J	397	Total	C 3162	N 2001	O 550	S 596	15	0	0
2	K	397	Total	C 3162	N 2001	O 550	S 596	15	0	0
2	L	397	Total	C 3162	N 2001	O 550	S 596	15	0	0
2	M	397	Total	C 3162	N 2001	O 550	S 596	15	0	0
2	N	397	Total	C 3162	N 2001	O 550	S 596	15	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	O	397	3162	2001	550	596	15	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

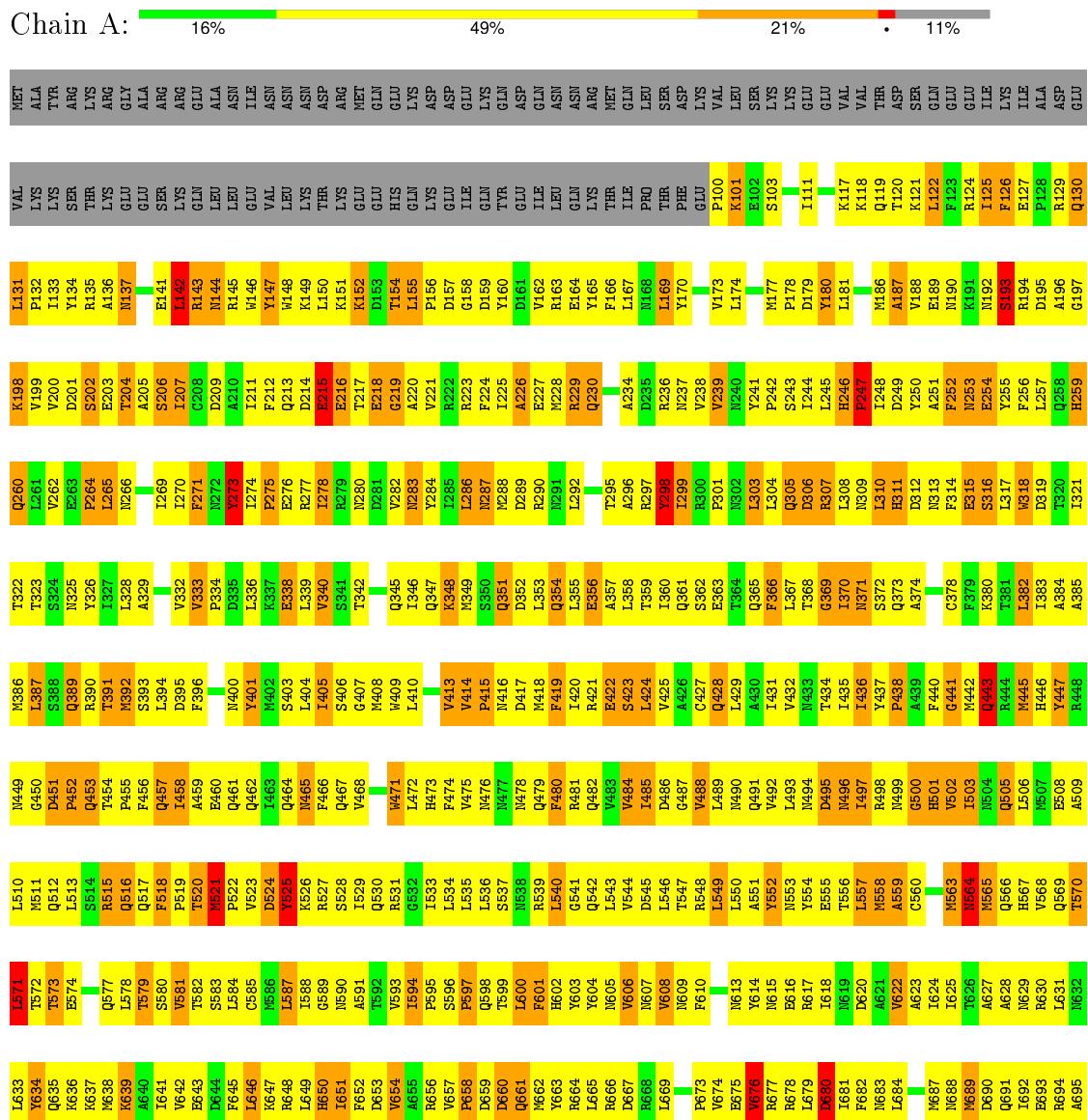
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

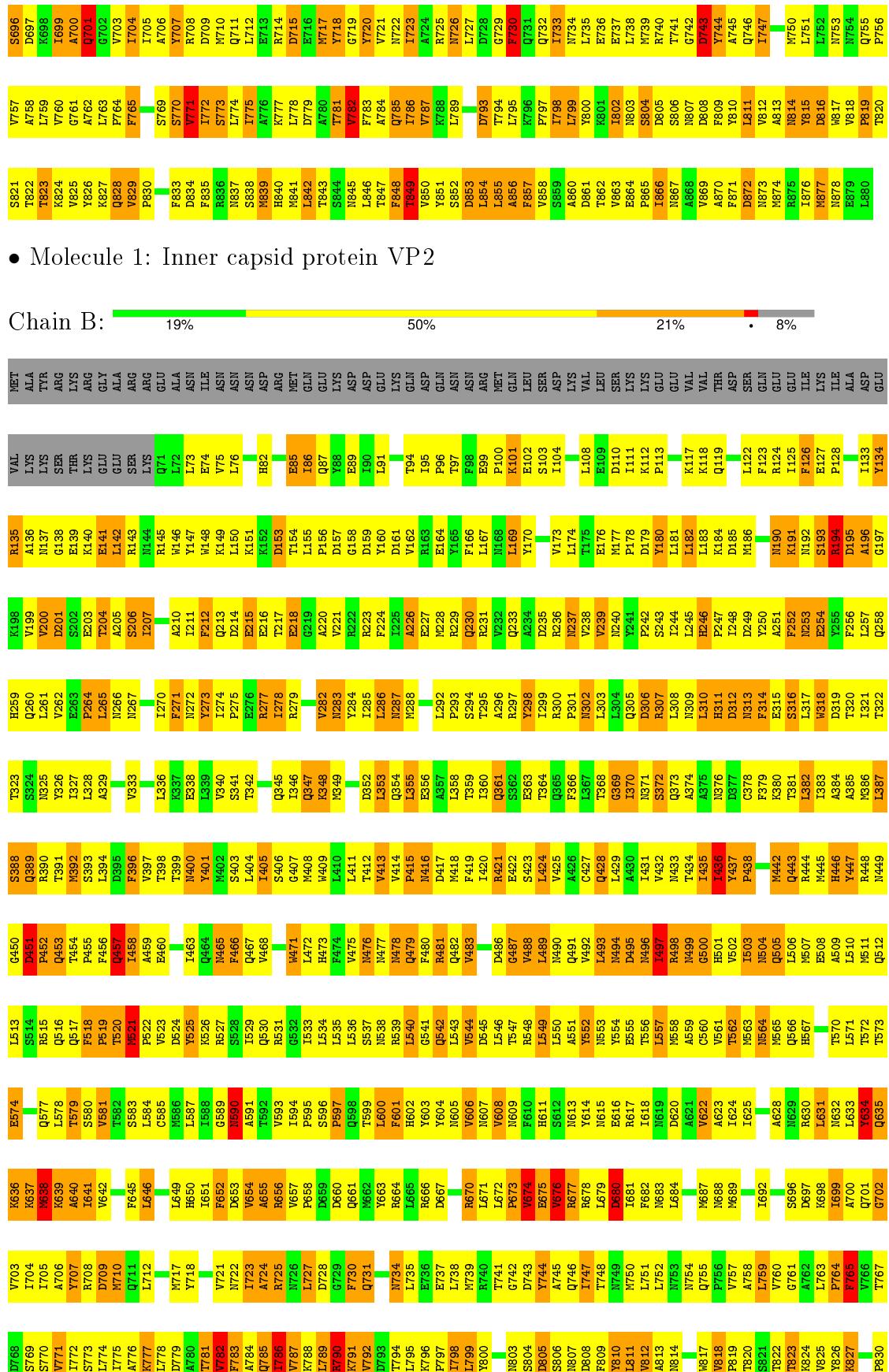
3 Residue-property plots

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

Note EDS failed to run properly.

- Molecule 1: Inner capsid protein VP2







- Molecule 2: Intermediate capsid protein VP6

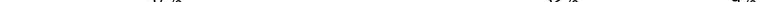
Chain C:



T148	C449	F150	T151	F152	K154	P155	N156	L157	F158	S163	M167	R168	S169	Q170	M175	L176	M177	G178	W181	V190	D204	E210	I214	P215	E216	V217	L225	P227	D228	D239	T246	F249	N250	P251	V252	I253	E254	R255	E260
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27273 27474 27777 28383 28484 28585 28686 28996 29000 29112 29113 29119 29128 29137 29140 29141 29142 29146 29154 29160 29170 29171 29174 29178 29181 29182 29183 29184 29185 29186 29187 29188 29197

- Molecule 2: Intermediate capsid protein VP6

Chain D:  57% 32% 9%

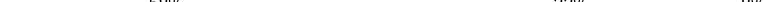


L71 N72 L73 D74 A75 N76 Y77 V78 AB1 R52 N53 T64 I85 F88 V89 D90 F91 V92 D93 M97 N98 E99 M100 E103 S104 K105 M107 G108 L109 A110 P111 S115 L116 R117 K118 L119 K120 F124 K125 R126 L127 N128 F129 D130 M131 S132 S133 E134 Y135 L136 E137 W138 W139

Q142 **M143** **R144** **R145** **Q146** **R147** **T148** **T149** **F150** **F151** **E151** **F152** **H153** **K154** **P155** **M156** **I157** **F158** **S163** **M167** **R168** **S169** **Q170** **M175** **L176** **G177** **C178** **A181** **S186** **V190** **D204** **E210** **L214** **R215** **R216** **V217** **L226** **R226** **F234** **P235** **R236** **R237** **D239** **T246** **F249**

100250 **10251** **10252** **10253** **10254** **10255** **10256** **10257** **10258** **10259** **10260** **10261** **10262** **10263** **10264** **10265** **10266** **10267** **10268** **10269** **10270** **10271** **10272** **10273** **10274** **10275** **10276** **10277** **10278** **10279** **10280** **10281** **10282** **10283** **10284** **10285** **10286** **10287** **10288** **10289** **10290** **10291** **10292** **10293** **10294** **10295** **10296** **10297** **10298** **10299** **102100** **102101** **102102** **102103** **102104** **102105** **102106** **102107** **102108** **102109** **102110** **102111** **102112** **102113** **102114** **102115** **102116** **102117** **102118** **102119** **102120** **102121** **102122** **102123** **102124** **102125** **102126** **102127** **102128** **102129** **102130** **102131** **102132** **102133** **102134** **102135** **102136** **102137** **102138** **102139** **102140** **102141** **102142** **102143** **102144** **102145** **102146** **102147** **102148** **102149** **102150** **102151** **102152** **102153** **102154** **102155** **102156** **102157** **102158** **102159** **102160** **102161** **102162** **102163** **102164** **102165** **102166** **102167** **102168** **102169** **102170** **102171** **102172** **102173** **102174** **102175** **102176** **102177** **102178** **102179** **102180** **102181** **102182** **102183** **102184** **102185** **102186** **102187** **102188** **102189** **102190** **102191** **102192** **102193** **102194** **102195** **102196** **102197** **102198** **102199** **102200** **102201** **102202** **102203** **102204** **102205** **102206** **102207** **102208** **102209** **102210** **102211** **102212** **102213** **102214** **102215** **102216** **102217** **102218** **102219** **102220** **102221** **102222** **102223** **102224** **102225** **102226** **102227** **102228** **102229** **102230** **102231** **102232** **102233** **102234** **102235** **102236** **102237** **102238** **102239** **102240** **102241** **102242** **102243** **102244** **102245** **102246** **102247** **102248** **102249** **102250** **102251** **102252** **102253** **102254** **102255** **102256** **102257** **102258** **102259** **102260** **102261** **102262** **102263** **102264** **102265** **102266** **102267** **102268** **102269** **102270** **102271** **102272** **102273** **102274** **102275** **102276** **102277** **102278** **102279** **102280** **102281** **102282** **102283** **102284** **102285** **102286** **102287** **102288** **102289** **102290** **102291** **102292** **102293** **102294** **102295** **102296** **102297** **102298** **102299** **102300** **102301** **102302** **102303** **102304** **102305** **102306** **102307** **102308** **102309** **102310** **102311** **102312** **102313** **102314** **102315** **102316** **102317** **102318** **102319** **102320** **102321** **102322** **102323** **102324** **102325** **102326** **102327** **102328** **102329** **102330** **102331** **102332** **102333** **102334** **102335** **102336** **102337** **102338** **102339** **102340** **102341** **102342** **102343** **102344** **102345** **102346** **102347** **102348** **102349** **102350** **102351** **102352** **102353** **102354** **102355** **102356** **102357** **102358** **102359** **102360** **102361** **102362** **102363** **102364** **102365** **102366** **102367** **102368** **102369** **102370** **102371** **102372** **102373** **102374** **102375** **102376** **102377** **102378** **102379** **102380** **102381** **102382** **102383** **102384** **102385** **102386** **102387** **102388** **102389** **102390**

- Molecule 2: Intermediate capsid protein VP6

Chain E:  58% 33% 8%



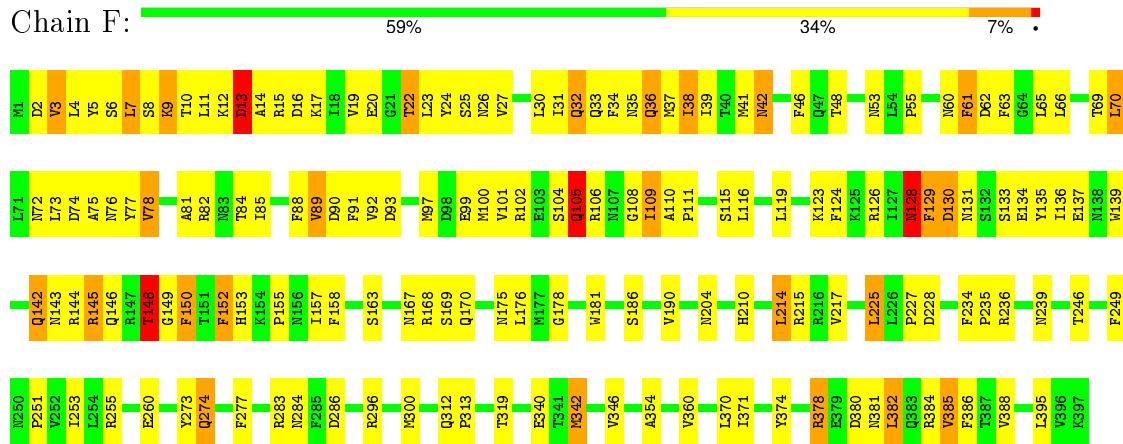
T69
L70
L71
L72
L73
D74
A75
N76
V77
S181
R82
I85
F88
V89
D90
F91
V92
D93
H94
V95
C96
M97
D98
B99
M100
V101
E102
P106
N107
G108
I109
A110
P111
S115
L116
L117
K125
R126
P128
F129
D130
M131
S132
S133
E134
I135
N136
E137

109 1139
110 Q142
111 Q143
112 R144
113 T148
114 C149
115 F150
116 L151
117 F152
118 K153
119 K154
120 I157
121 N157
122 F158
123 S163
124 M167
125 A168
126 S169
127 J170
128 H175
129 L176
130 M177
131 G178
132 W181
133 S186
134 Y190
135 P210
136 D214
137 C215
138 C216
139 V217
140 D226
141 D228
142 P227
143 C228
144 P234
145 C235
146 R236
147 D246
148 P249
149 C250
150 P251
151 C252
152 S253

[#252525](#) [#2A2B2C](#) [#2B2B2D](#) [#2C2C2D](#) [#2E2E2F](#) [#2F2F30](#) [#303031](#) [#313132](#) [#323233](#) [#333334](#) [#343435](#) [#353536](#) [#363637](#) [#373738](#) [#383839](#) [#39393A](#) [#3A3A3B](#) [#3B3B3C](#) [#3C3C3D](#) [#3D3D3E](#) [#3E3E3F](#) [#3F3F40](#) [#404041](#) [#414142](#) [#424243](#) [#434344](#) [#444445](#) [#454546](#) [#464647](#) [#474748](#) [#484849](#) [#49494A](#) [#4A4A4B](#) [#4B4B4C](#) [#4C4C4D](#) [#4D4D4E](#) [#4E4E4F](#) [#4F4F50](#) [#505051](#) [#515152](#) [#525253](#) [#535354](#) [#545455](#) [#555556](#) [#565657](#) [#575758](#) [#585859](#) [#59595A](#) [#5A5A5B](#) [#5B5B5C](#) [#5C5C5D](#) [#5D5D5E](#) [#5E5E5F](#) [#5F5F60](#) [#606061](#) [#616162](#) [#626263](#) [#636364](#) [#646465](#) [#656566](#) [#666667](#) [#676768](#) [#686869](#) [#69696A](#) [#6A6A6B](#) [#6B6B6C](#) [#6C6C6D](#) [#6D6D6E](#) [#6E6E6F](#) [#6F6F70](#) [#707071](#) [#717172](#) [#727273](#) [#737374](#) [#747475](#) [#757576](#) [#767677](#) [#777778](#) [#787879](#) [#79797A](#) [#7A7A7B](#) [#7B7B7C](#) [#7C7C7D](#) [#7D7D7E](#) [#7E7E7F](#) [#7F7F80](#) [#808081](#) [#818182](#) [#828283](#) [#838384](#) [#848485](#) [#858586](#) [#868687](#) [#878788](#) [#888889](#) [#89898A](#) [#8A8A8B](#) [#8B8B8C](#) [#8C8C8D](#) [#8D8D8E](#) [#8E8E8F](#) [#8F8F90](#) [#909091](#) [#919192](#) [#929293](#) [#939394](#) [#949495](#) [#959596](#) [#969697](#) [#979798](#) [#989899](#) [#99999A](#) [#9A9A9B](#) [#9B9B9C](#) [#9C9C9D](#) [#9D9D9E](#) [#9E9E9F](#) [#9F9F99](#) [#999999](#)

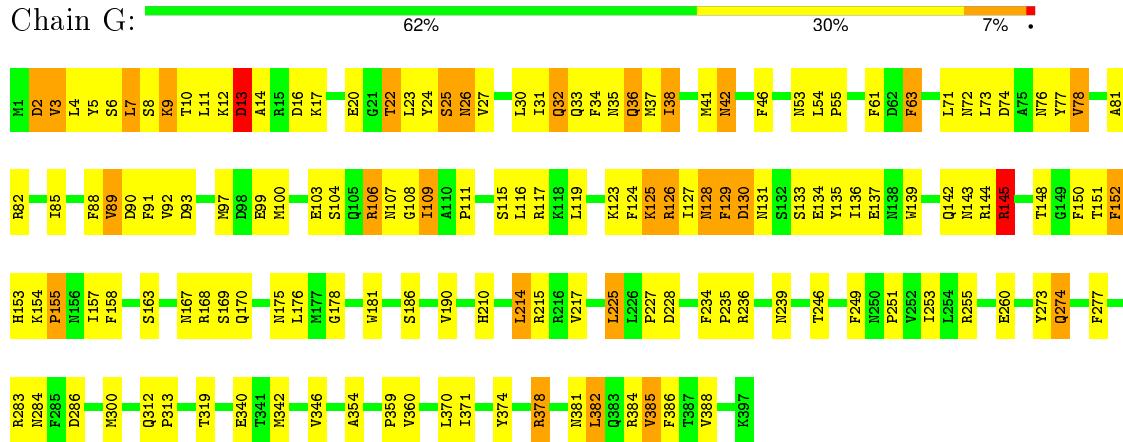
- Molecule 2: Intermediate capsid protein VP6

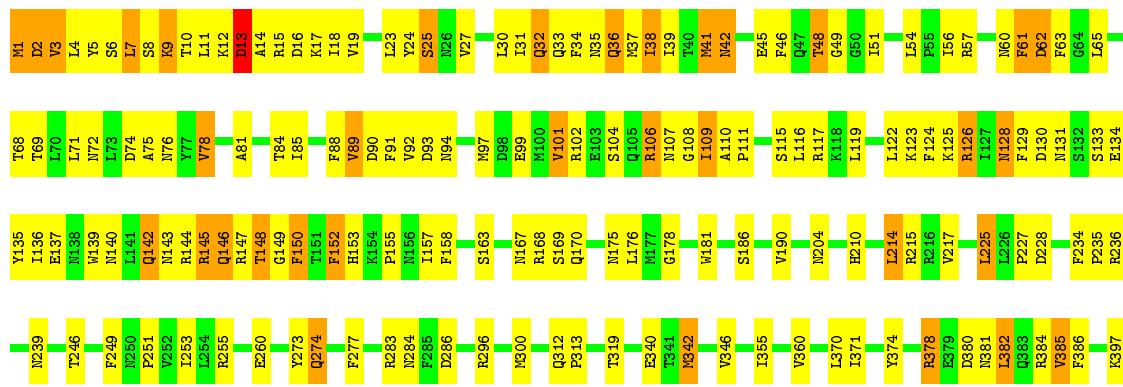
Chain F:



- Molecule 2: Intermediate capsid protein VP6

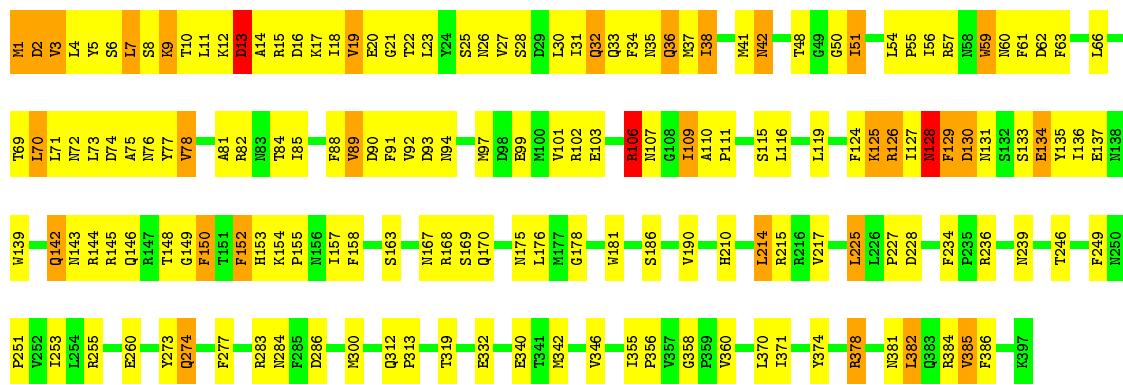
Chain G:





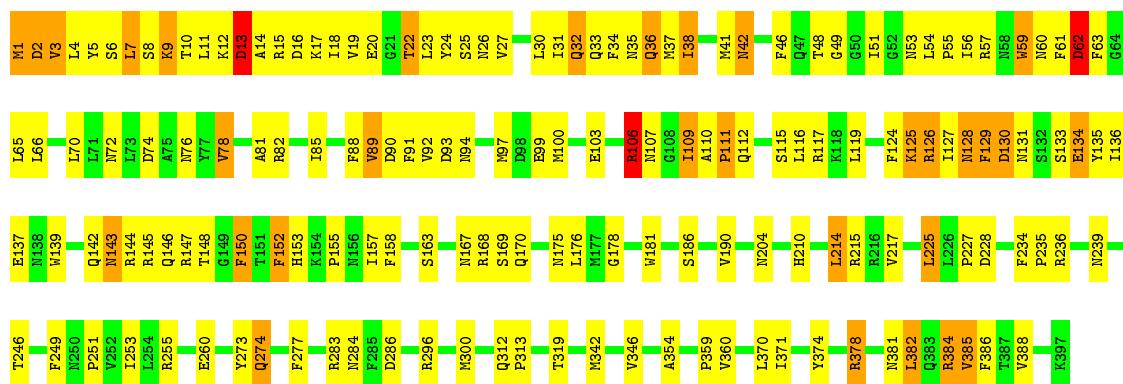
- Molecule 2: Intermediate capsid protein VP6

Chain J:



- Molecule 2: Intermediate capsid protein VP6

Chain K:



- Molecule 2: Intermediate capsid protein VP6

Chain L:





- Molecule 2: Intermediate capsid protein VP6

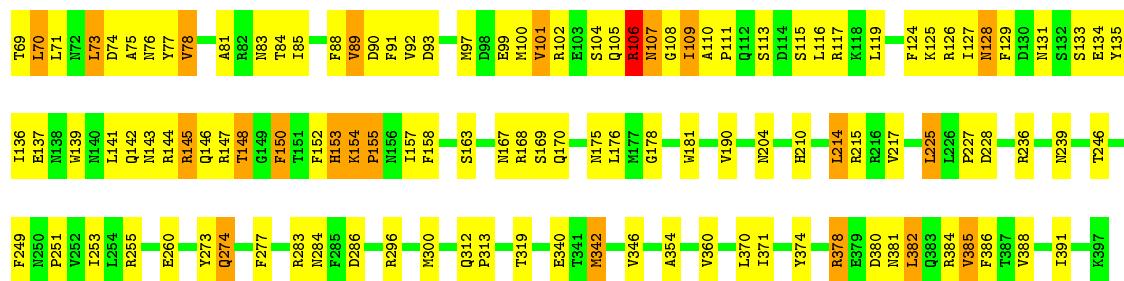


- Molecule 2: Intermediate capsid protein VP6



- Molecule 2: Intermediate capsid protein VP6





4 Data and refinement statistics i

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	740.75Å 1198.07Å 1345.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80	Depositor
% Data completeness (in resolution range)	15.9 (30.00-3.80)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	0.49 (at 3.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.328 , 0.339	Depositor
Wilson B-factor (Å ²)	167.1	Xtriage
Anisotropy	0.043	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45, \langle L^2 \rangle = 0.29$	Xtriage
Outliers	4 of 2393850 reflections (0.000%)	Xtriage
Total number of atoms	54109	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.48	0/6491	0.84	9/8806 (0.1%)
1	B	0.50	0/6745	0.82	10/9149 (0.1%)
2	C	0.51	0/3232	0.78	5/4397 (0.1%)
2	D	0.51	0/3232	0.78	5/4397 (0.1%)
2	E	0.51	0/3232	0.77	5/4397 (0.1%)
2	F	0.50	0/3232	0.76	5/4397 (0.1%)
2	G	0.50	0/3232	0.77	5/4397 (0.1%)
2	H	0.50	0/3232	0.76	5/4397 (0.1%)
2	I	0.50	0/3232	0.77	5/4397 (0.1%)
2	J	0.51	0/3232	0.78	5/4397 (0.1%)
2	K	0.51	0/3232	0.77	5/4397 (0.1%)
2	L	0.51	0/3232	0.77	5/4397 (0.1%)
2	M	0.51	0/3232	0.77	5/4397 (0.1%)
2	N	0.51	0/3232	0.77	5/4397 (0.1%)
2	O	0.52	0/3232	0.79	7/4397 (0.2%)
All	All	0.50	0/55252	0.79	86/75116 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TYR	CB-CG-CD2	10.70	127.42	121.00

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TYR	CB-CG-CD1	-9.86	115.08	121.00
1	A	273	TYR	CA-CB-CG	9.85	132.12	113.40
1	B	273	TYR	CB-CG-CD1	9.85	126.91	121.00
1	B	273	TYR	CB-CG-CD2	-9.21	115.48	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	TYR	Sidechain

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	6374	0	6394	992	0
1	B	6624	0	6652	1122	0
2	C	3162	0	3101	170	0
2	D	3162	0	3101	179	0
2	E	3162	0	3101	164	0
2	F	3162	0	3101	160	0
2	G	3162	0	3101	149	0
2	H	3162	0	3101	175	0
2	I	3162	0	3101	215	0
2	J	3162	0	3101	187	0
2	K	3162	0	3101	166	0
2	L	3162	0	3101	178	0
2	M	3162	0	3101	173	0
2	N	3162	0	3101	191	0
2	O	3162	0	3101	163	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
3	O	1	0	0	0	0
All	All	54109	0	53359	4148	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

The worst 5 of 4148 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:771:VAL:HB	1:B:809:PHE:HB3	1.23	1.18
1:A:333:VAL:HG11	1:A:380:LYS:HA	1.27	1.15
1:A:428:GLN:OE1	1:A:456:PHE:HB2	1.46	1.13
1:A:563:MET:HA	1:A:563:MET:HE3	1.22	1.12
2:G:145:ARG:HB3	2:G:145:ARG:HH11	1.10	1.12

There are no symmetry-related clashes.

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	779/880 (88%)	431 (55%)	199 (26%)	149 (19%)	0 3
1	B	808/880 (92%)	458 (57%)	204 (25%)	146 (18%)	0 3
2	C	395/397 (100%)	318 (80%)	54 (14%)	23 (6%)	2 28
2	D	395/397 (100%)	315 (80%)	50 (13%)	30 (8%)	1 20
2	E	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	2 28
2	F	395/397 (100%)	324 (82%)	47 (12%)	24 (6%)	2 27
2	G	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	2 28
2	H	395/397 (100%)	323 (82%)	50 (13%)	22 (6%)	2 29
2	I	395/397 (100%)	320 (81%)	51 (13%)	24 (6%)	2 27
2	J	395/397 (100%)	320 (81%)	53 (13%)	22 (6%)	2 29
2	K	395/397 (100%)	318 (80%)	52 (13%)	25 (6%)	2 26
2	L	395/397 (100%)	322 (82%)	47 (12%)	26 (7%)	1 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	M	395/397 (100%)	322 (82%)	52 (13%)	21 (5%)	2 30
2	N	395/397 (100%)	317 (80%)	50 (13%)	28 (7%)	1 23
2	O	395/397 (100%)	317 (80%)	47 (12%)	31 (8%)	1 20
All	All	6722/6921 (97%)	5051 (75%)	1054 (16%)	617 (9%)	1 16

5 of 617 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	130	GLN
1	A	193	SER
1	A	198	LYS
1	A	220	ALA

5.3.2 Protein sidechains [\(1\)](#)

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	715/809 (88%)	603 (84%)	112 (16%)	3 24
1	B	744/809 (92%)	635 (85%)	109 (15%)	4 27
2	C	350/350 (100%)	325 (93%)	25 (7%)	18 59
2	D	350/350 (100%)	322 (92%)	28 (8%)	15 54
2	E	350/350 (100%)	325 (93%)	25 (7%)	18 59
2	F	350/350 (100%)	327 (93%)	23 (7%)	21 62
2	G	350/350 (100%)	327 (93%)	23 (7%)	21 62
2	H	350/350 (100%)	329 (94%)	21 (6%)	24 65
2	I	350/350 (100%)	327 (93%)	23 (7%)	21 62
2	J	350/350 (100%)	327 (93%)	23 (7%)	21 62
2	K	350/350 (100%)	327 (93%)	23 (7%)	21 62
2	L	350/350 (100%)	321 (92%)	29 (8%)	14 52
2	M	350/350 (100%)	325 (93%)	25 (7%)	18 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	N	350/350 (100%)	324 (93%)	26 (7%)	17 57
2	O	350/350 (100%)	329 (94%)	21 (6%)	24 65
All	All	6009/6168 (97%)	5473 (91%)	536 (9%)	12 50

5 of 536 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	374	TYR
2	F	13	ASP
2	N	73	LEU
2	D	19	VAL
2	D	382	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 220 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	345	ASN
2	H	26	ASN
2	N	167	ASN
2	F	72	ASN
2	F	345	ASN

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 [\(i\)](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

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

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

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates [\(i\)](#)

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands [\(i\)](#)

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers [\(i\)](#)

EDS failed to run properly - this section will therefore be empty.