



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 24, 2023 – 04:57 AM EDT

PDB ID : 5KOV
Title : Crystal structure of the human astrovirus 2 capsid protein spike in complex with a single chain variable fragment of an astrovirus neutralizing antibody at 3.24-Å resolution
Authors : Bogdanoff, W.A.; DuBois, R.M.
Deposited on : 2016-07-01
Resolution : 3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

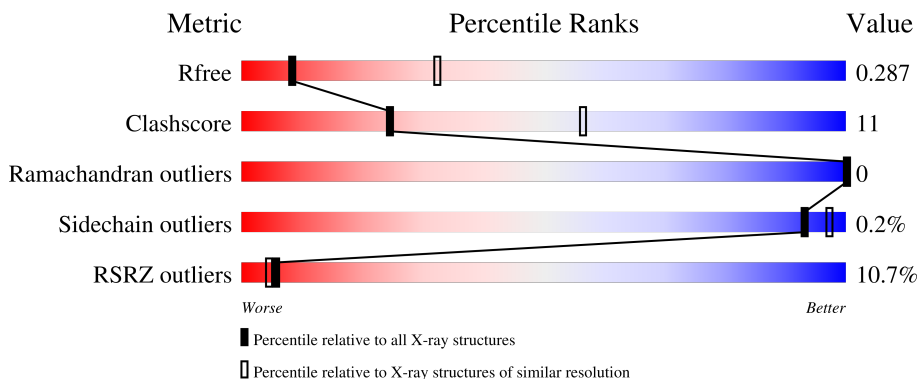
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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.



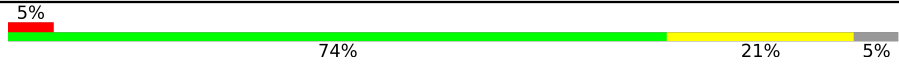

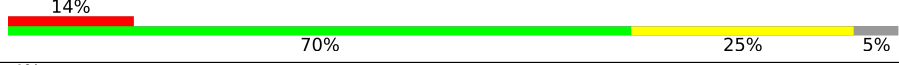


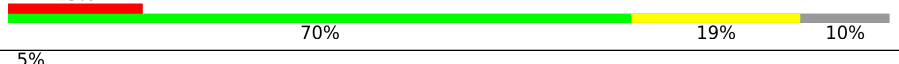
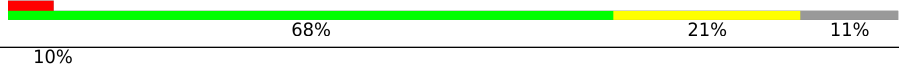



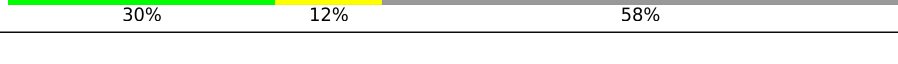
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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 $\leq 5\%$. 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	228	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
1	B	228	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
1	G	228	<div style="display: flex; align-items: center;"> <div style="width: 13%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
1	H	228	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
1	M	228	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	N	228	
1	S	228	
1	T	228	
2	C	251	
2	E	251	
2	I	251	
2	K	251	
2	O	251	
2	Q	251	
2	U	251	
2	W	251	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1201	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 25943 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 Capsid polyprotein VP90.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	Total 1745	C 1118	N 290	O 328	S 9	0	0	0
1	B	218	Total 1756	C 1125	N 292	O 330	S 9	0	0	0
1	H	216	Total 1745	C 1118	N 290	O 328	S 9	0	0	0
1	G	219	Total 1760	C 1127	N 293	O 331	S 9	0	0	0
1	N	217	Total 1750	C 1121	N 291	O 329	S 9	0	0	0
1	M	216	Total 1745	C 1118	N 290	O 328	S 9	0	0	0
1	S	218	Total 1755	C 1124	N 292	O 330	S 9	0	0	0
1	T	216	Total 1745	C 1118	N 290	O 328	S 9	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	427	MET	-	initiating methionine	UNP Q82446
A	428	GLY	-	expression tag	UNP Q82446
A	645	ALA	-	expression tag	UNP Q82446
A	646	ALA	-	expression tag	UNP Q82446
A	647	ALA	-	expression tag	UNP Q82446
A	648	GLU	-	expression tag	UNP Q82446
A	649	LEU	-	expression tag	UNP Q82446
A	650	ALA	-	expression tag	UNP Q82446
A	651	LEU	-	expression tag	UNP Q82446
A	652	VAL	-	expression tag	UNP Q82446
A	653	PRO	-	expression tag	UNP Q82446
A	654	ARG	-	expression tag	UNP Q82446
B	427	MET	-	initiating methionine	UNP Q82446

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Chain	Residue	Modelled	Actual	Comment	Reference
B	428	GLY	-	expression tag	UNP Q82446
B	645	ALA	-	expression tag	UNP Q82446
B	646	ALA	-	expression tag	UNP Q82446
B	647	ALA	-	expression tag	UNP Q82446
B	648	GLU	-	expression tag	UNP Q82446
B	649	LEU	-	expression tag	UNP Q82446
B	650	ALA	-	expression tag	UNP Q82446
B	651	LEU	-	expression tag	UNP Q82446
B	652	VAL	-	expression tag	UNP Q82446
B	653	PRO	-	expression tag	UNP Q82446
B	654	ARG	-	expression tag	UNP Q82446
H	427	MET	-	initiating methionine	UNP Q82446
H	428	GLY	-	expression tag	UNP Q82446
H	645	ALA	-	expression tag	UNP Q82446
H	646	ALA	-	expression tag	UNP Q82446
H	647	ALA	-	expression tag	UNP Q82446
H	648	GLU	-	expression tag	UNP Q82446
H	649	LEU	-	expression tag	UNP Q82446
H	650	ALA	-	expression tag	UNP Q82446
H	651	LEU	-	expression tag	UNP Q82446
H	652	VAL	-	expression tag	UNP Q82446
H	653	PRO	-	expression tag	UNP Q82446
H	654	ARG	-	expression tag	UNP Q82446
G	427	MET	-	initiating methionine	UNP Q82446
G	428	GLY	-	expression tag	UNP Q82446
G	645	ALA	-	expression tag	UNP Q82446
G	646	ALA	-	expression tag	UNP Q82446
G	647	ALA	-	expression tag	UNP Q82446
G	648	GLU	-	expression tag	UNP Q82446
G	649	LEU	-	expression tag	UNP Q82446
G	650	ALA	-	expression tag	UNP Q82446
G	651	LEU	-	expression tag	UNP Q82446
G	652	VAL	-	expression tag	UNP Q82446
G	653	PRO	-	expression tag	UNP Q82446
G	654	ARG	-	expression tag	UNP Q82446
N	427	MET	-	initiating methionine	UNP Q82446
N	428	GLY	-	expression tag	UNP Q82446
N	645	ALA	-	expression tag	UNP Q82446
N	646	ALA	-	expression tag	UNP Q82446
N	647	ALA	-	expression tag	UNP Q82446
N	648	GLU	-	expression tag	UNP Q82446
N	649	LEU	-	expression tag	UNP Q82446

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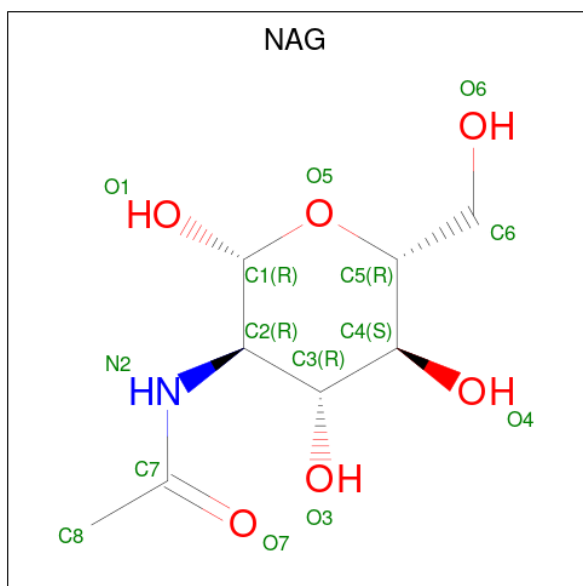
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Chain	Residue	Modelled	Actual	Comment	Reference
N	650	ALA	-	expression tag	UNP Q82446
N	651	LEU	-	expression tag	UNP Q82446
N	652	VAL	-	expression tag	UNP Q82446
N	653	PRO	-	expression tag	UNP Q82446
N	654	ARG	-	expression tag	UNP Q82446
M	427	MET	-	initiating methionine	UNP Q82446
M	428	GLY	-	expression tag	UNP Q82446
M	645	ALA	-	expression tag	UNP Q82446
M	646	ALA	-	expression tag	UNP Q82446
M	647	ALA	-	expression tag	UNP Q82446
M	648	GLU	-	expression tag	UNP Q82446
M	649	LEU	-	expression tag	UNP Q82446
M	650	ALA	-	expression tag	UNP Q82446
M	651	LEU	-	expression tag	UNP Q82446
M	652	VAL	-	expression tag	UNP Q82446
M	653	PRO	-	expression tag	UNP Q82446
M	654	ARG	-	expression tag	UNP Q82446
S	427	MET	-	initiating methionine	UNP Q82446
S	428	GLY	-	expression tag	UNP Q82446
S	645	ALA	-	expression tag	UNP Q82446
S	646	ALA	-	expression tag	UNP Q82446
S	647	ALA	-	expression tag	UNP Q82446
S	648	GLU	-	expression tag	UNP Q82446
S	649	LEU	-	expression tag	UNP Q82446
S	650	ALA	-	expression tag	UNP Q82446
S	651	LEU	-	expression tag	UNP Q82446
S	652	VAL	-	expression tag	UNP Q82446
S	653	PRO	-	expression tag	UNP Q82446
S	654	ARG	-	expression tag	UNP Q82446
T	427	MET	-	initiating methionine	UNP Q82446
T	428	GLY	-	expression tag	UNP Q82446
T	645	ALA	-	expression tag	UNP Q82446
T	646	ALA	-	expression tag	UNP Q82446
T	647	ALA	-	expression tag	UNP Q82446
T	648	GLU	-	expression tag	UNP Q82446
T	649	LEU	-	expression tag	UNP Q82446
T	650	ALA	-	expression tag	UNP Q82446
T	651	LEU	-	expression tag	UNP Q82446
T	652	VAL	-	expression tag	UNP Q82446
T	653	PRO	-	expression tag	UNP Q82446
T	654	ARG	-	expression tag	UNP Q82446

- Molecule 2 is a protein called PL-2 scFv chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	223	Total	C	N	O	S	0	0	0
			1726	1087	290	342	7			
2	E	224	Total	C	N	O	S	0	0	0
			1727	1087	288	345	7			
2	K	223	Total	C	N	O	S	0	0	0
			1726	1087	290	342	7			
2	I	225	Total	C	N	O	S	0	0	0
			1738	1093	292	346	7			
2	Q	93	Total	C	N	O	S	0	0	0
			746	482	122	138	4			
2	O	212	Total	C	N	O	S	0	0	0
			1651	1043	276	325	7			
2	W	105	Total	C	N	O	S	0	0	0
			853	548	141	159	5			
2	U	222	Total	C	N	O	S	0	0	0
			1719	1082	289	341	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		

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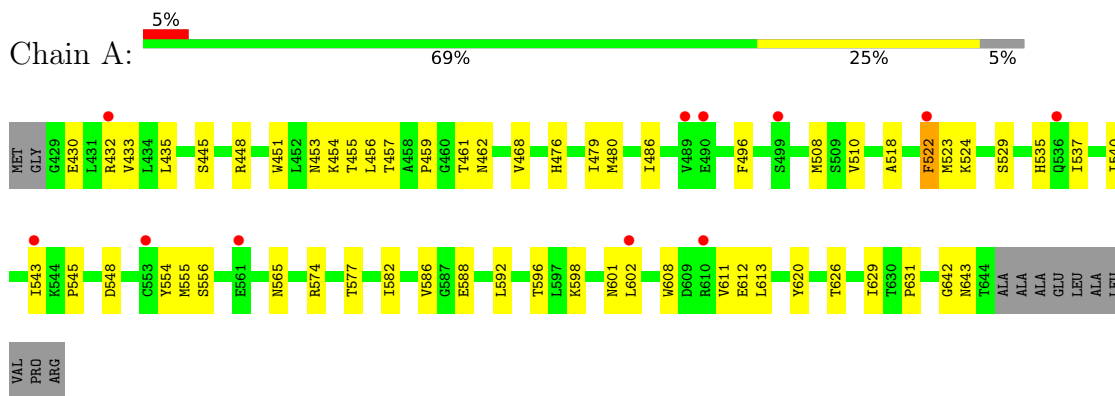
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	I	1	14	8	1	5	0	0

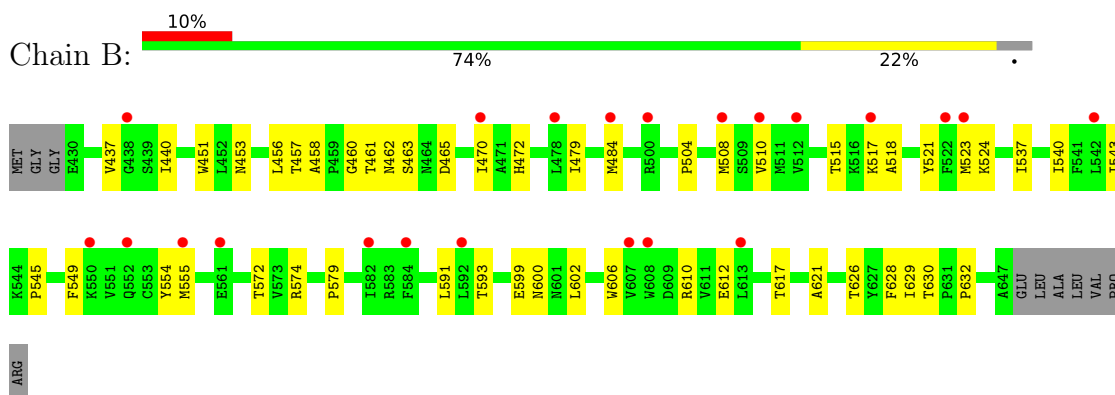
3 Residue-property plots [i](#)

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.

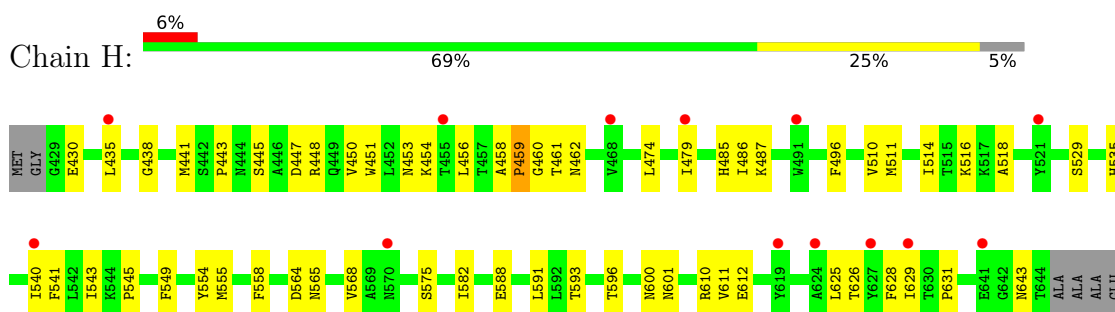
- Molecule 1: Capsid polyprotein VP90



- Molecule 1: Capsid polyprotein VP90

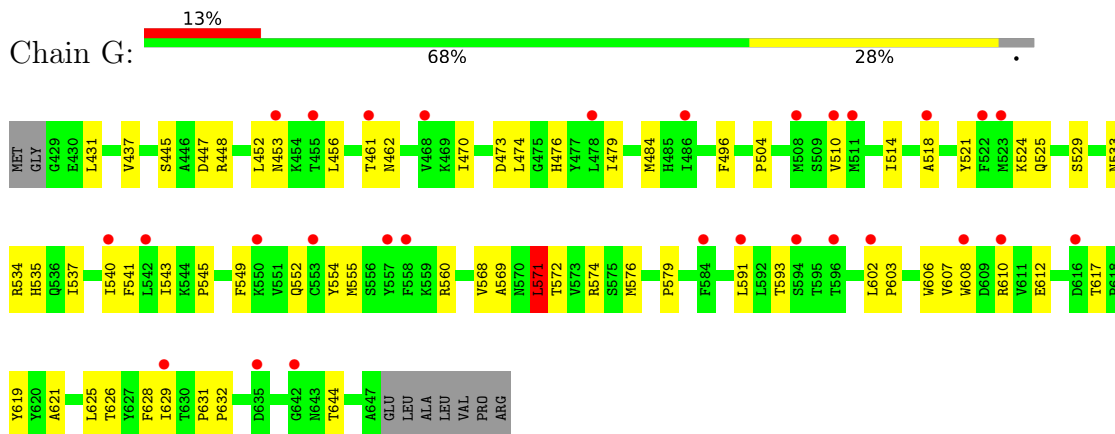


- Molecule 1: Capsid polyprotein VP90

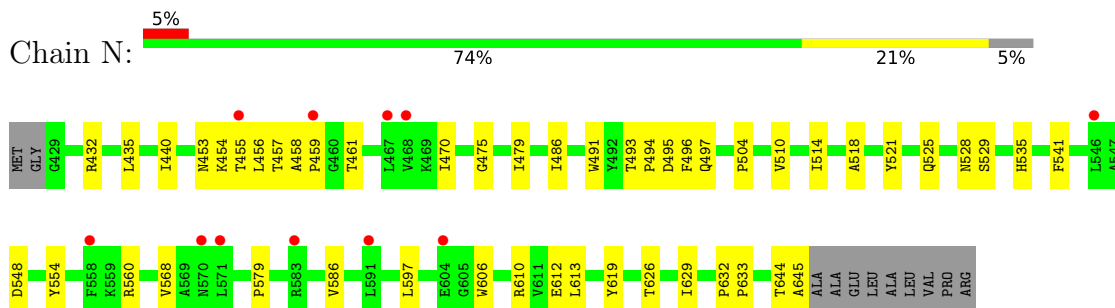


LEU
ALA
LEU
VAL
PRO
ARG

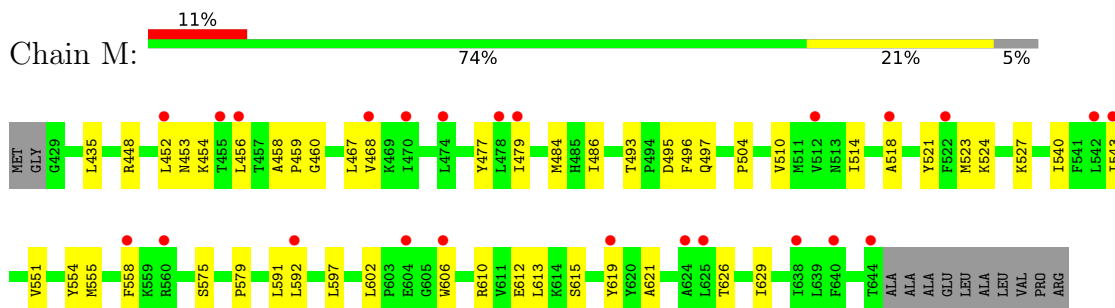
• Molecule 1: Capsid polyprotein VP90



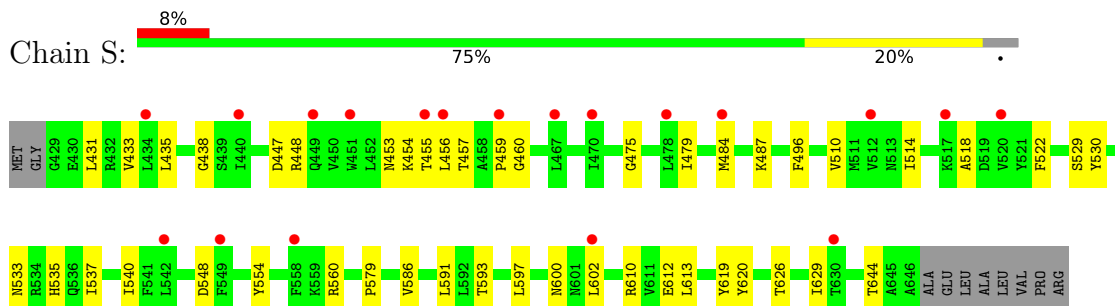
• Molecule 1: Capsid polyprotein VP90

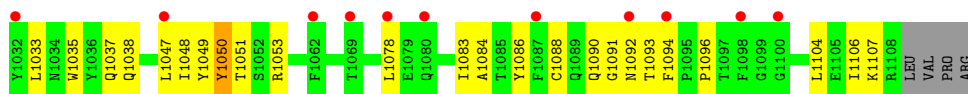


• Molecule 1: Capsid polyprotein VP90

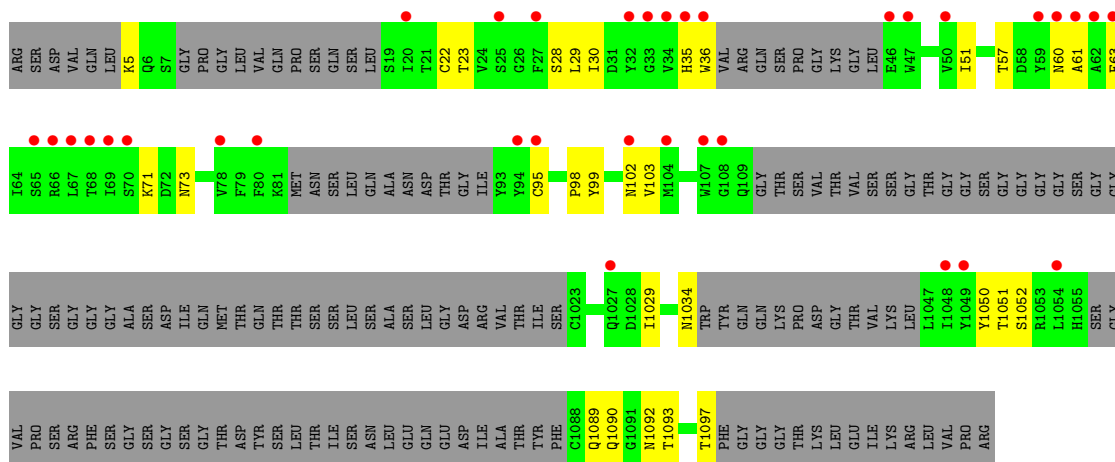
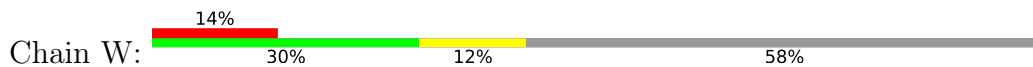


• Molecule 1: Capsid polyprotein VP90

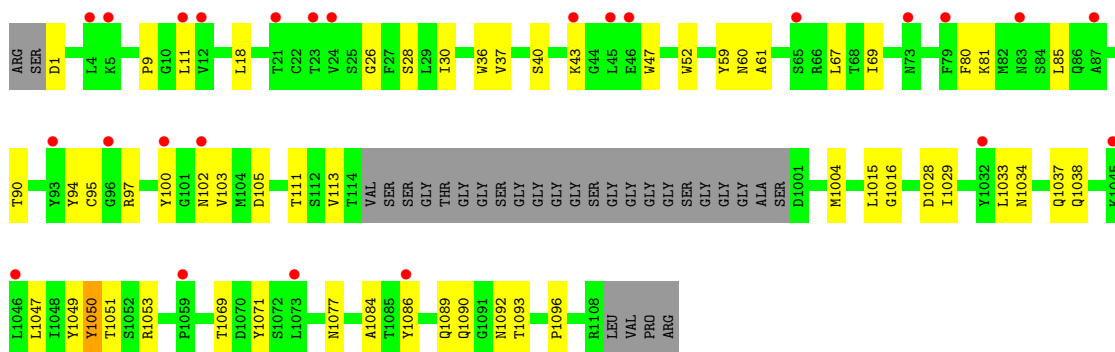




● Molecule 2: PL-2 scFv chain



● Molecule 2: PL-2 scFv chain



4 Data and refinement statistics i

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	200.00Å 200.00Å 157.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 50.00 – 3.24	Depositor EDS
% Data completeness (in resolution range)	88.1 (50.00-3.25) 81.5 (50.00-3.24)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.25Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.241 , 0.288 0.241 , 0.287	Depositor DCC
R_{free} test set	4185 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtrriage
Anisotropy	0.523	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.417 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25943	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/1792	0.54	1/2441 (0.0%)
1	B	0.30	0/1803	0.53	0/2457
1	G	0.30	0/1807	0.55	1/2462 (0.0%)
1	H	0.29	0/1792	0.52	0/2441
1	M	0.27	0/1792	0.53	0/2441
1	N	0.28	0/1797	0.51	0/2448
1	S	0.28	0/1802	0.55	0/2455
1	T	0.29	0/1792	0.53	0/2441
2	C	0.36	1/1765 (0.1%)	0.54	0/2395
2	E	0.27	0/1766	0.52	0/2397
2	I	0.29	0/1777	0.54	1/2411 (0.0%)
2	K	0.30	0/1765	0.53	0/2395
2	O	0.27	0/1686	0.53	0/2283
2	Q	0.24	0/764	0.48	0/1031
2	U	0.27	0/1758	0.52	0/2385
2	W	0.25	0/874	0.47	0/1179
All	All	0.29	1/26532 (0.0%)	0.53	3/36062 (0.0%)

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	H	0	1
2	O	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1087	PHE	CG-CD2	-5.03	1.31	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	571	LEU	CA-CB-CG	6.79	130.91	115.30
1	A	601	ASN	C-N-CA	5.64	135.81	121.70
2	I	97	ARG	NE-CZ-NH1	-5.45	117.57	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	459	PRO	Peptide
2	O	111	THR	Peptide

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	1745	0	1709	43	0
1	B	1756	0	1721	34	0
1	G	1760	0	1724	46	0
1	H	1745	0	1709	44	0
1	M	1745	0	1709	36	0
1	N	1750	0	1714	35	0
1	S	1755	0	1719	32	0
1	T	1745	0	1709	52	0
2	C	1726	0	1661	38	0
2	E	1727	0	1658	48	0
2	I	1738	0	1671	34	0
2	K	1726	0	1661	37	0
2	O	1651	0	1587	49	0
2	Q	746	0	701	14	0
2	U	1719	0	1653	45	0
2	W	853	0	788	22	0
3	C	14	0	13	1	0
3	E	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	14	0	13	0	0
3	K	14	0	13	1	0
All	All	25943	0	25146	555	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 11.

The worst 5 of 555 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:H:514:ILE:HD11	2:K:30:ILE:HB	1.54	0.90
1:T:554:TYR:HA	1:T:579:PRO:HA	1.55	0.89
1:S:484:MET:HB3	1:S:591:LEU:HB3	1.56	0.88
1:B:461:THR:HG22	1:B:463:SER:H	1.42	0.84
1:G:461:THR:HG22	1:G:462:ASN:H	1.42	0.83

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	214/228 (94%)	206 (96%)	8 (4%)	0	100	100
1	B	216/228 (95%)	205 (95%)	11 (5%)	0	100	100
1	G	217/228 (95%)	207 (95%)	10 (5%)	0	100	100
1	H	214/228 (94%)	206 (96%)	8 (4%)	0	100	100
1	M	214/228 (94%)	204 (95%)	10 (5%)	0	100	100
1	N	215/228 (94%)	201 (94%)	14 (6%)	0	100	100
1	S	216/228 (95%)	204 (94%)	12 (6%)	0	100	100
1	T	214/228 (94%)	202 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	219/251 (87%)	213 (97%)	6 (3%)	0	100	100
2	E	220/251 (88%)	211 (96%)	9 (4%)	0	100	100
2	I	221/251 (88%)	212 (96%)	9 (4%)	0	100	100
2	K	219/251 (87%)	209 (95%)	10 (5%)	0	100	100
2	O	202/251 (80%)	194 (96%)	8 (4%)	0	100	100
2	Q	81/251 (32%)	69 (85%)	12 (15%)	0	100	100
2	U	218/251 (87%)	209 (96%)	9 (4%)	0	100	100
2	W	91/251 (36%)	84 (92%)	7 (8%)	0	100	100
All	All	3191/3832 (83%)	3036 (95%)	155 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	197/204 (97%)	196 (100%)	1 (0%)	88	94
1	B	197/204 (97%)	197 (100%)	0	100	100
1	G	197/204 (97%)	196 (100%)	1 (0%)	88	94
1	H	197/204 (97%)	197 (100%)	0	100	100
1	M	197/204 (97%)	197 (100%)	0	100	100
1	N	197/204 (97%)	197 (100%)	0	100	100
1	S	197/204 (97%)	197 (100%)	0	100	100
1	T	197/204 (97%)	196 (100%)	1 (0%)	88	94
2	C	193/206 (94%)	193 (100%)	0	100	100
2	E	194/206 (94%)	193 (100%)	1 (0%)	88	94
2	I	195/206 (95%)	194 (100%)	1 (0%)	88	94
2	K	193/206 (94%)	193 (100%)	0	100	100
2	O	185/206 (90%)	184 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	82/206 (40%)	82 (100%)	0	100	100
2	U	192/206 (93%)	191 (100%)	1 (0%)	88	94
2	W	93/206 (45%)	93 (100%)	0	100	100
All	All	2903/3280 (88%)	2896 (100%)	7 (0%)	93	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	571	LEU
2	O	1050	TYR
1	T	444	ASN
2	U	1050	TYR
2	I	1092	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	K	6	GLN
2	I	1034	ASN
1	G	513	ASN
2	O	6	GLN
1	T	552	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 monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1201	2	14,14,15	0.39	0	17,19,21	0.45	0
3	NAG	K	1201	2	14,14,15	0.32	0	17,19,21	0.44	0
3	NAG	I	1201	2	14,14,15	0.26	0	17,19,21	0.51	0
3	NAG	E	1201	2	14,14,15	0.33	0	17,19,21	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1201	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1201	2	-	2/6/23/26	0/1/1/1
3	NAG	I	1201	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1201	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1201	NAG	O5-C5-C6-O6
3	K	1201	NAG	O5-C5-C6-O6
3	C	1201	NAG	O5-C5-C6-O6
3	I	1201	NAG	C4-C5-C6-O6
3	C	1201	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1201	NAG	1	0
3	K	1201	NAG	1	0

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](#)

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	216/228 (94%)	0.62	11 (5%) 28 18	50, 81, 124, 168	0
1	B	218/228 (95%)	0.73	22 (10%) 7 5	59, 106, 136, 152	0
1	G	219/228 (96%)	0.83	29 (13%) 3 2	64, 108, 146, 163	0
1	H	216/228 (94%)	0.59	13 (6%) 21 14	52, 82, 127, 165	0
1	M	216/228 (94%)	0.91	24 (11%) 5 4	66, 103, 135, 151	0
1	N	217/228 (95%)	0.55	11 (5%) 28 18	59, 91, 129, 147	0
1	S	218/228 (95%)	0.60	19 (8%) 10 7	58, 92, 131, 149	0
1	T	216/228 (94%)	0.90	32 (14%) 2 2	70, 103, 138, 164	0
2	C	223/251 (88%)	0.54	11 (4%) 29 19	48, 70, 122, 147	3 (1%)
2	E	224/251 (89%)	0.81	23 (10%) 6 5	86, 121, 149, 166	3 (1%)
2	I	225/251 (89%)	0.90	37 (16%) 1 1	93, 126, 157, 175	3 (1%)
2	K	223/251 (88%)	0.67	12 (5%) 25 16	46, 72, 125, 146	3 (1%)
2	O	212/251 (84%)	0.70	24 (11%) 5 4	97, 131, 155, 167	3 (1%)
2	Q	93/251 (37%)	1.02	21 (22%) 0 1	120, 145, 163, 172	0
2	U	222/251 (88%)	0.83	25 (11%) 5 4	96, 129, 166, 193	3 (1%)
2	W	105/251 (41%)	1.36	34 (32%) 0 0	114, 145, 162, 173	0
All	All	3263/3832 (85%)	0.76	348 (10%) 6 4	46, 107, 151, 193	18 (0%)

The worst 5 of 348 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	37	VAL	6.0
2	W	69	ILE	6.0
1	M	468	VAL	5.9
2	W	1027	GLN	5.6
1	B	608	TRP	5.6

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	C	1201	14/15	0.65	0.42	146,163,170,174	0
3	NAG	K	1201	14/15	0.65	0.29	140,179,188,188	0
3	NAG	I	1201	14/15	0.79	0.19	133,147,156,157	0
3	NAG	E	1201	14/15	0.84	0.29	138,153,158,158	0

6.5 Other polymers [i](#)

There are no such residues in this entry.