



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2026 – 12:29 AM UTC

PDB ID : 5VF3 / pdb_00005vf3
EMDB ID : EMD-8661
Title : Bacteriophage T4 isometric capsid
Authors : Chen, Z.; Sun, L.; Zhang, Z.; Fokine, A.; Padilla-Sanchez, V.; Hanein, D.;
Jiang, W.; Rossmann, M.G.; Rao, V.B.
Deposited on : 2017-04-06
Resolution : 3.30 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

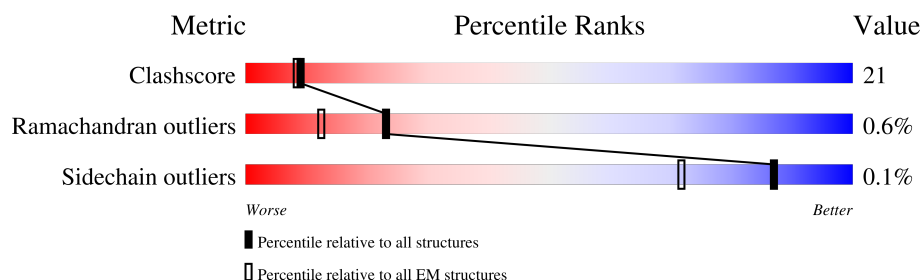
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



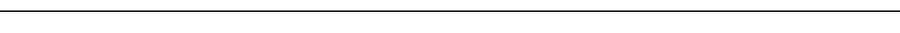
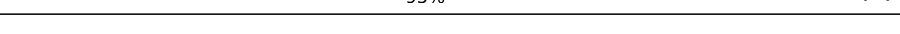
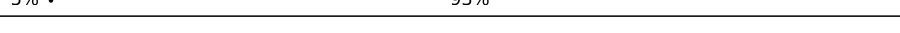
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	a	417	57% 41% .
2	A	456	58% 42%
2	B	456	52% 48%
2	C	456	56% 44%
2	D	456	55% 43% .
2	E	456	52% 48% .
2	F	456	53% 46% .
2	G	456	59% 40% .
2	H	456	57% 42%

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Mol	Chain	Length	Quality of chain
2	I	456	 55% 45%
2	J	456	 58% 41% .
2	K	456	 58% 41% .
2	L	456	 56% 43%
3	O	80	 69% 30% .
3	P	80	 60% 39% .
3	Q	80	 91% 8% .
3	R	80	 95% . .
3	S	80	 95% . .
3	T	80	 89% 10% .
3	U	80	 95% . .
3	V	80	 92% 6% .
3	W	80	 55% 44% .
3	X	80	 92% 6% .
3	Y	80	 95% . .
4	Z	376	 5% . 93%
5	z	15	 93% 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 51584 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 vertex protein gp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	415	Total	C	N	O	S	0	0
			3208	2039	521	640	8		

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	B	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	C	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	D	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	E	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	F	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	G	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	H	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	I	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	J	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	K	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	L	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	THR	ALA	conflict	UNP P04535
B	275	THR	ALA	conflict	UNP P04535
C	275	THR	ALA	conflict	UNP P04535
D	275	THR	ALA	conflict	UNP P04535
E	275	THR	ALA	conflict	UNP P04535
F	275	THR	ALA	conflict	UNP P04535
G	275	THR	ALA	conflict	UNP P04535
H	275	THR	ALA	conflict	UNP P04535
I	275	THR	ALA	conflict	UNP P04535
J	275	THR	ALA	conflict	UNP P04535
K	275	THR	ALA	conflict	UNP P04535
L	275	THR	ALA	conflict	UNP P04535

- Molecule 3 is a protein called Small outer capsid protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	79	Total 633	C 403	N 106	O 124	0	0
3	P	79	Total 633	C 403	N 106	O 124	0	0
3	Q	79	Total 633	C 403	N 106	O 124	0	0
3	R	79	Total 633	C 403	N 106	O 124	0	0
3	S	79	Total 633	C 403	N 106	O 124	0	0
3	T	79	Total 633	C 403	N 106	O 124	0	0
3	U	79	Total 633	C 403	N 106	O 124	0	0
3	V	79	Total 633	C 403	N 106	O 124	0	0
3	W	79	Total 633	C 403	N 106	O 124	0	0
3	X	79	Total 633	C 403	N 106	O 124	0	0
3	Y	79	Total 633	C 403	N 106	O 124	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	4	ALA	THR	conflict	UNP P03715

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Chain	Residue	Modelled	Actual	Comment	Reference
O	28	VAL	ILE	conflict	UNP P03715
P	4	ALA	THR	conflict	UNP P03715
P	28	VAL	ILE	conflict	UNP P03715
Q	4	ALA	THR	conflict	UNP P03715
Q	28	VAL	ILE	conflict	UNP P03715
R	4	ALA	THR	conflict	UNP P03715
R	28	VAL	ILE	conflict	UNP P03715
S	4	ALA	THR	conflict	UNP P03715
S	28	VAL	ILE	conflict	UNP P03715
T	4	ALA	THR	conflict	UNP P03715
T	28	VAL	ILE	conflict	UNP P03715
U	4	ALA	THR	conflict	UNP P03715
U	28	VAL	ILE	conflict	UNP P03715
V	4	ALA	THR	conflict	UNP P03715
V	28	VAL	ILE	conflict	UNP P03715
W	4	ALA	THR	conflict	UNP P03715
W	28	VAL	ILE	conflict	UNP P03715
X	4	ALA	THR	conflict	UNP P03715
X	28	VAL	ILE	conflict	UNP P03715
Y	4	ALA	THR	conflict	UNP P03715
Y	28	VAL	ILE	conflict	UNP P03715

- Molecule 4 is a protein called Highly immunogenic outer capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	25	Total	C	N	O	S	0	0
			214	140	32	39	3		

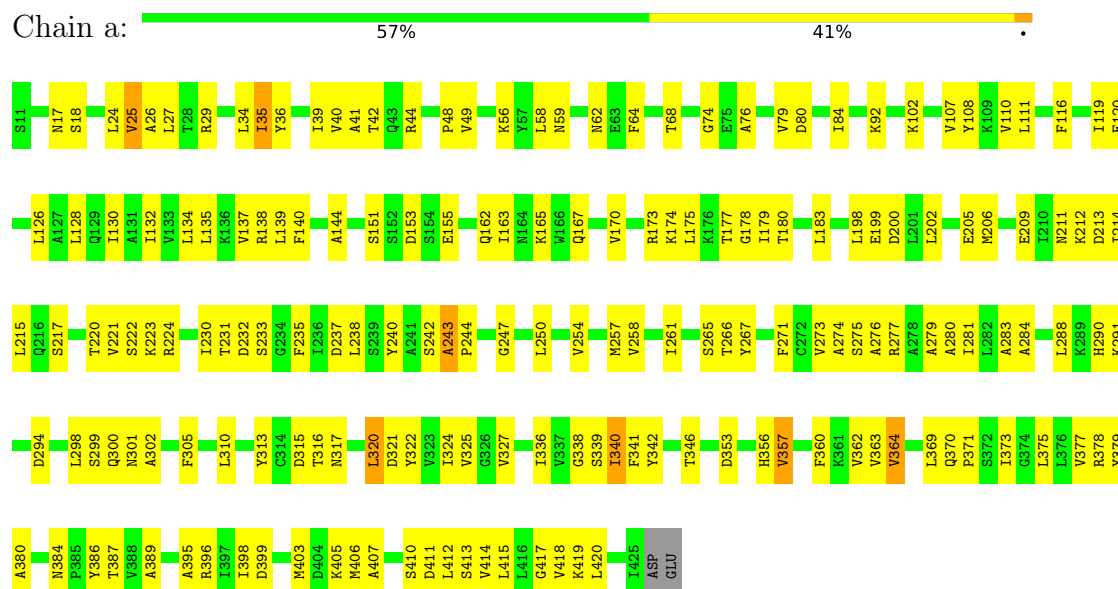
- Molecule 5 is a protein called Highly immunogenic outer capsid protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	z	15	Total	C	N	O	0	0
			75	45	15	15		

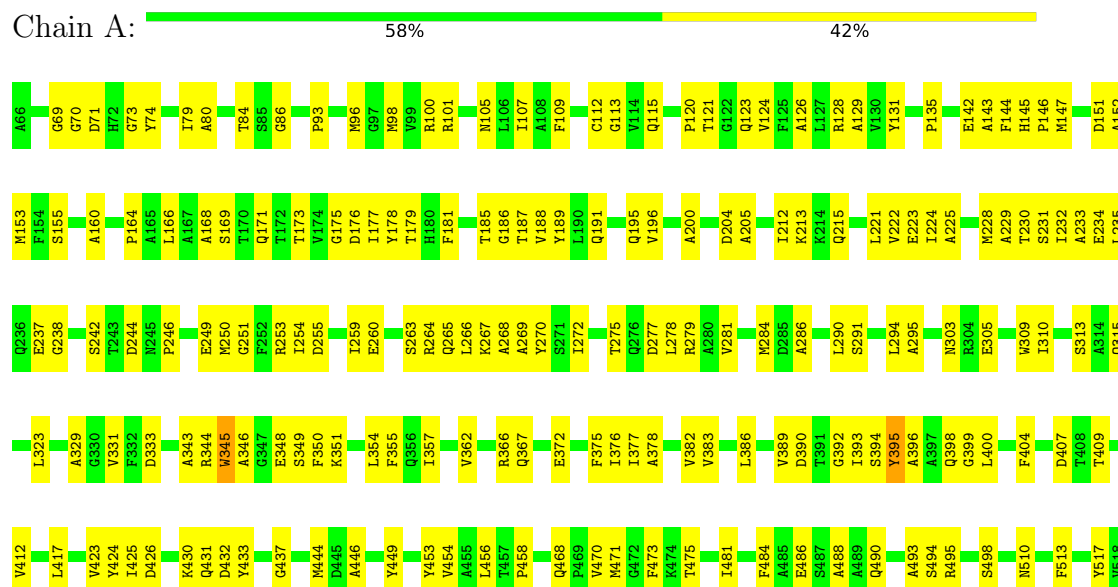
3 Residue-property plots

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. 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. 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 vertex protein gp24



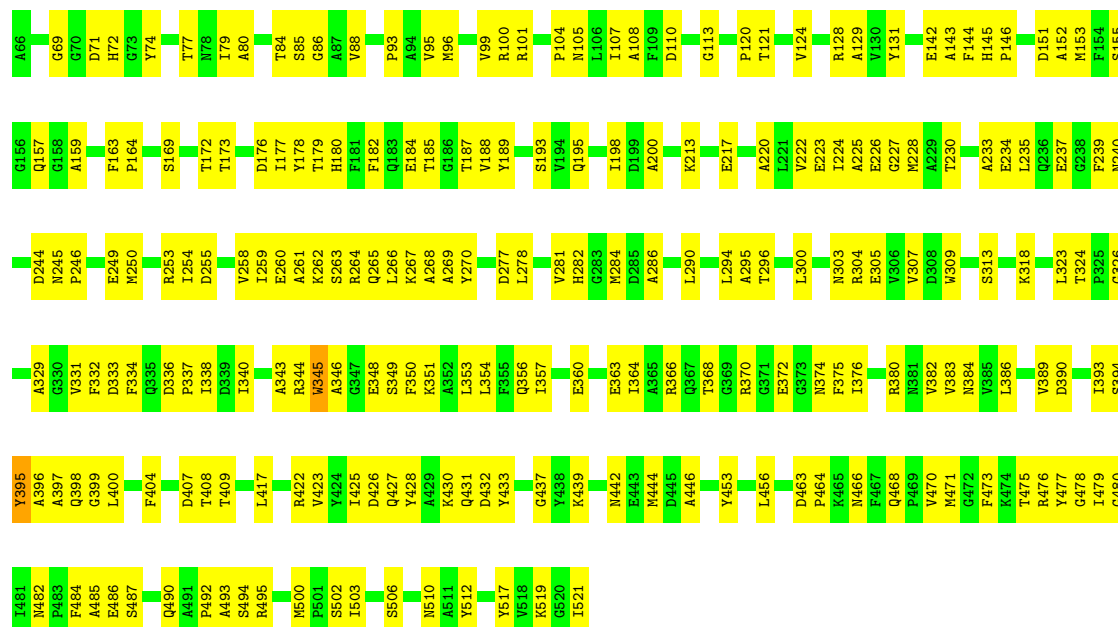
- Molecule 2: Major capsid protein



K519
G520
I521

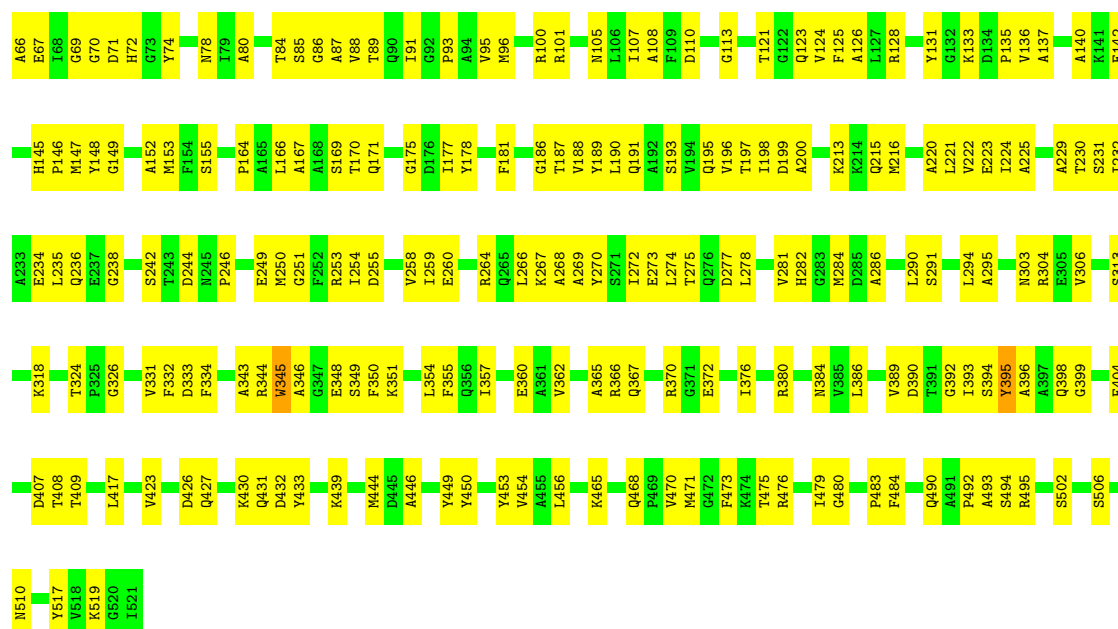
• Molecule 2: Major capsid protein

Chain B:  52% 48%



• Molecule 2: Major capsid protein

Chain C:  56% 44%



• Molecule 2: Major capsid protein

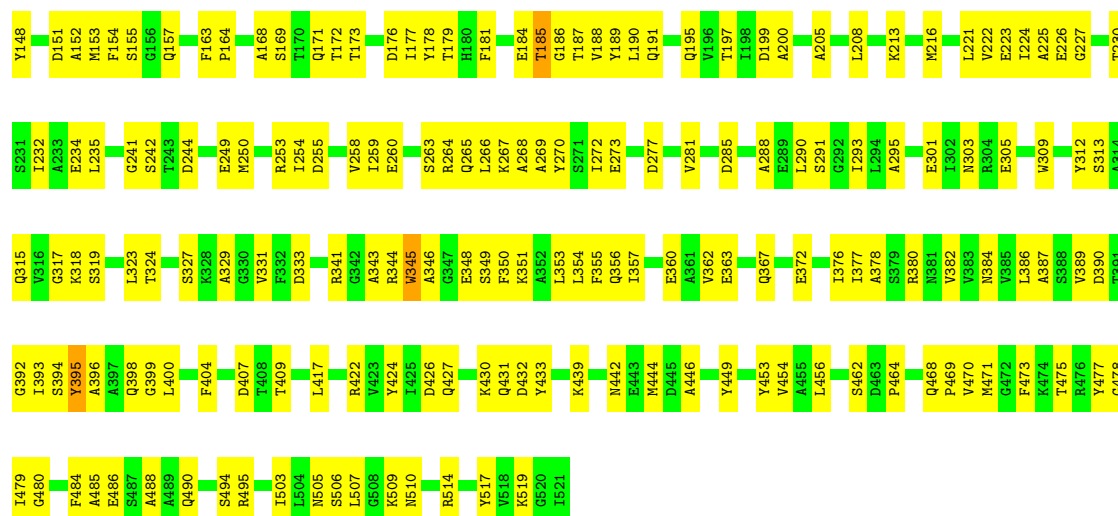
F513	F404	V331	M288	P164	A86
Y517	S405	F332	E249	P164	A86
V518	T406	D333	M250	L166	G69
K519	D407	D336	R253	A167	H72
G520	T408	P337	I254	A168	G73
I521	T409		D255	S169	Y74
		I340	K256		
	V423	R341		T172	T77
	G424	G342	I259	T173	N78
T425		A343	E260		I79
D426	R344			D176	A80
Q427	W345		S283	I177	
	A346		R284	Y178	
K430	G347		Q265	T179	S85
Q431	E348		K266	H180	
D432	S349		K267	F181	P93
Y433	F350		A288		
	K351		A289	G186	N96
	A352			T187	R100
Q437	L353		I272	V188	R101
M444	L354			Y189	
	F355		D277		N105
Y449	G356		L278	Q195	L106
	I357		R279	V196	I107
L456			A280	I197	
	V362		V281	D199	P120
D463	E363			A200	T121
P464	I364		M284		G122
	A365		D285		Q123
Q468	R366		A286	I212	
P469	Q367		D287	K213	F125
V470	T368				A126
M471			L290	E217	L127
	E372				R128
K474			I283	V222	A129
T475	F375		L294	E223	V130
D476	I376		W309	I224	
Y477	I377		L300	A225	G132
G478	A378			E226	K133
	S379		N303	G227	D134
	R380		R394		
M482	K381		E305	T230	A137
F483	V382			S231	
A484	F383		I310	I232	E142
E486	N384			A233	A143
S487	V385			E234	F144
A488	L386		S313	L235	H145
A489			A314	Q236	P146
Q490	V389		Q315	E237	M147
	D390			G238	Y148
			K318	F239	G149
A493	I393			N240	P150
S494	S394		L323	G241	D151
R495	Y395		T324	S242	A152
				T243	M153
L507	A396			D244	F154
G508	A397		S327	N245	S155
K509	Q398		K328	G246	G156
N510	G399		A329	P246	
	I400		G330	I247	G157

Chain E: 52% 48%

F467	N384	R304	T230	H145	A66
Q468	V385	E305	S231	P146	G69
P469	L386		T232	M147	D70
M470		W309	A233	Y148	G71
M471	V389		E234		H72
Q472	D390	S313	L235	D151	
P473		A314	E236	A152	G73
K474	I393	Q315	Q237	M153	Y74
T475	S394		G238	P154	N75
R476	Y395	K318		S155	A76
A396			G241	G156	T77
Q397	L323		S242	Q157	H78
I398	S327		T243	I158	I79
G399	S328	K328	D244	A159	A80
L400		A329	N245		
F404	G330	V246	P247	F163	T84
S405	V331	N248		P164	S85
T406	F332	E249		A165	S86
D407	D333	M250		L166	
T408	F334	G251	A167	A168	P83
		Q335	F252	S169	A94
Q490		D336	R253	T170	V95
	V412		T254	Q171	M96
		I340			R100
L417			V258	I177	R101
A511	R344		L259	Y178	
Y512	V423	W345	E260	T179	M105
	Y424	A346	A261	H190	L106
Y517	I425	G347	V262	F181	I107
D426		E348	S263		A108
K430	S349	R264	S264	T185	F109
Q431	F350	Q265	Q265	G186	D110
D432	K351	L266	L266	T187	
Y433	A352	K267	V188	V188	G113
	L353	A268		Y189	
V436	L354	A269		L190	M117
Q437				Q191	N118
Y438	I357	T272			S119
K439	E360	D277	V194	Q195	P120
		L278		V196	T121
M442	E363	R279			V124
E443		G283		A200	F125
M444	R366	Q284	A126		A126
A445	Q367	D285	K213		L127
A446		A286	G214		R128
	R370	D287	Q215		A129
A451	G371	D287	M216		V130
P452	E372		E217		Y131
Y453		L290		A220	G132
V454	F375	S291		L221	D133
A455	I376			V222	P135
L456	I377	L294		E223	V136
P457	A378	A295		T224	A137
T458	S379				
	R380	L300		A225	
	N381	E301		E226	E142
D463	V382	T302		G227	A143
		V382			F144
		V382			

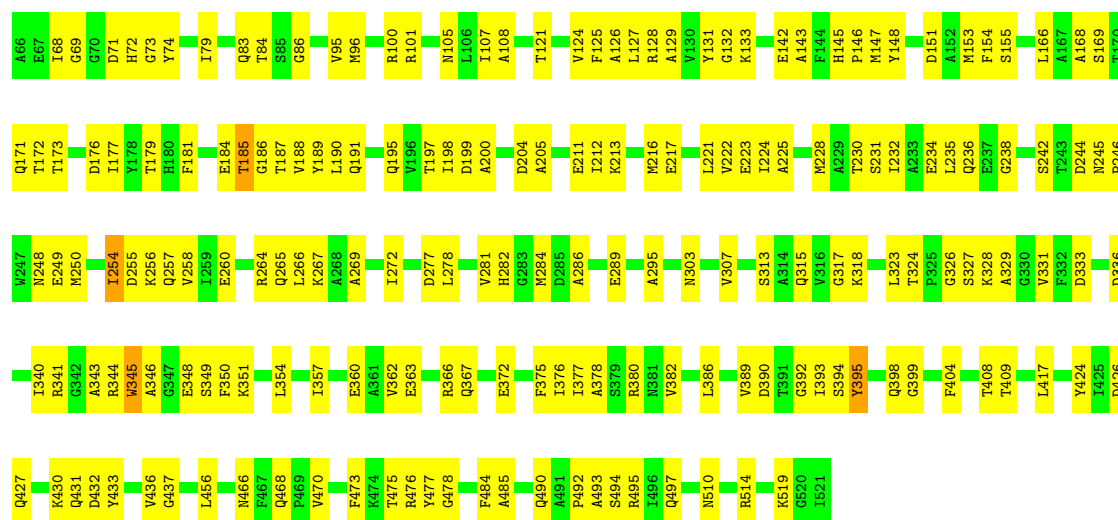
Chain F: 53% 46%

A66	E57	I68	G69	W72	G73	Y74	W75	A76		I79		Q83	T84	S85	G86	A87	V88	T89	Q90	Q91	G92	G93	A94	V95	M96		R100	R101		M105	L106	I107	D110	G113	P120	G122	Q123	W124		R128		Y131	G132	K133	D134		A137		E142	A143	F144	H145	P146	F147
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• Molecule 2: Major capsid protein

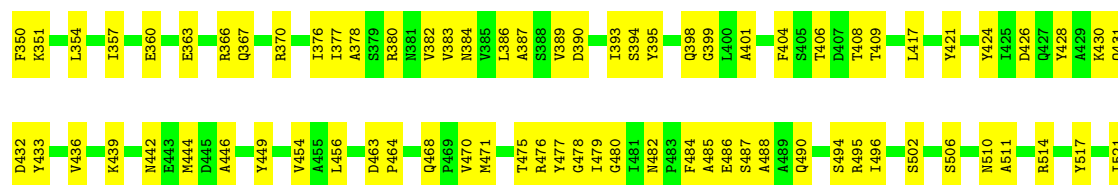
Chain G: 59% 40%



• Molecule 2: Major capsid protein

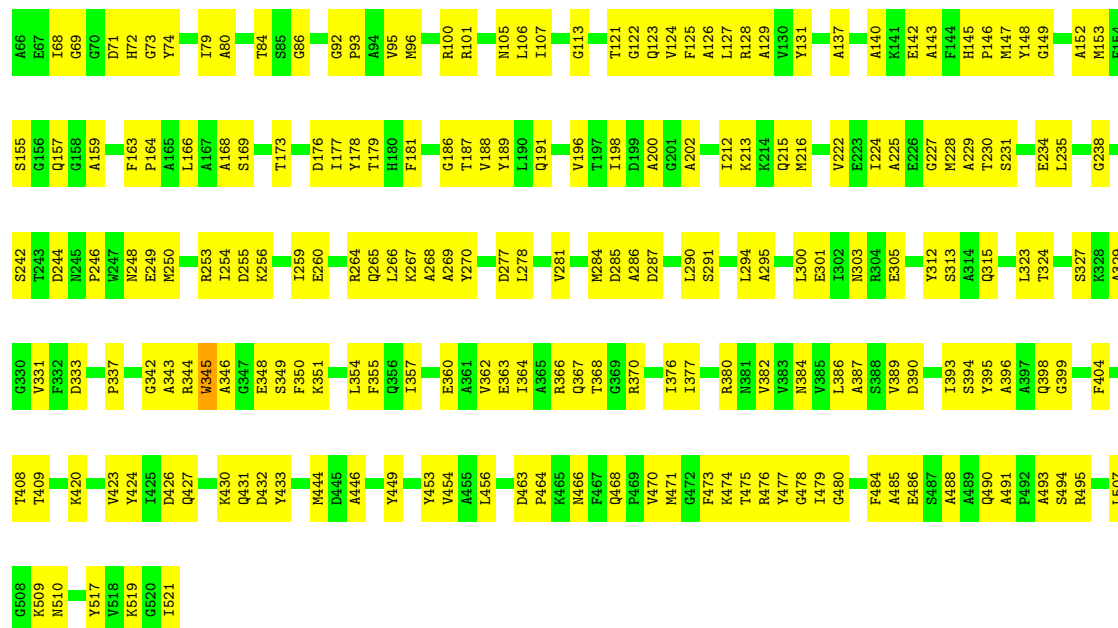
Chain H: 57% 42%





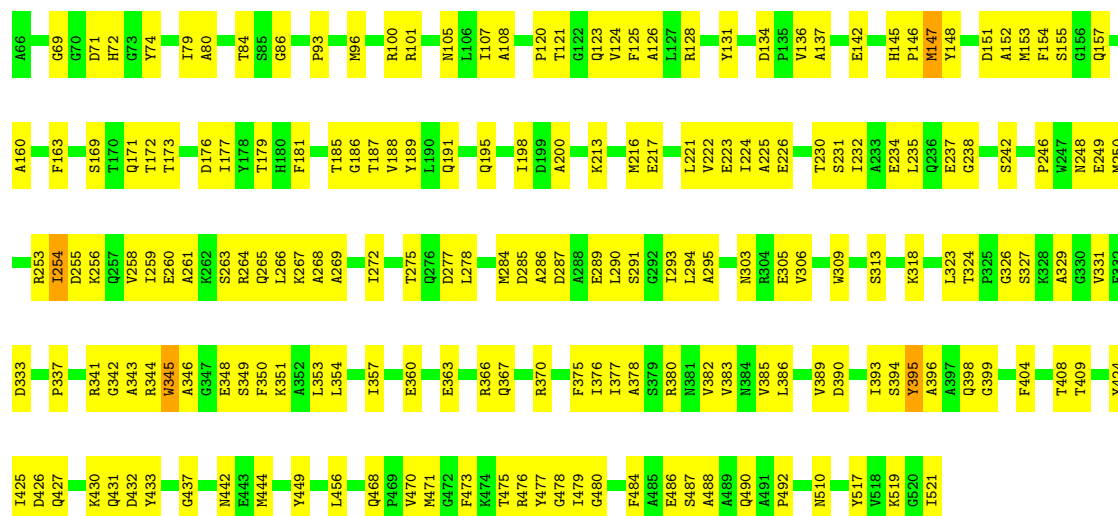
• Molecule 2: Major capsid protein

Chain I:  55% 45%



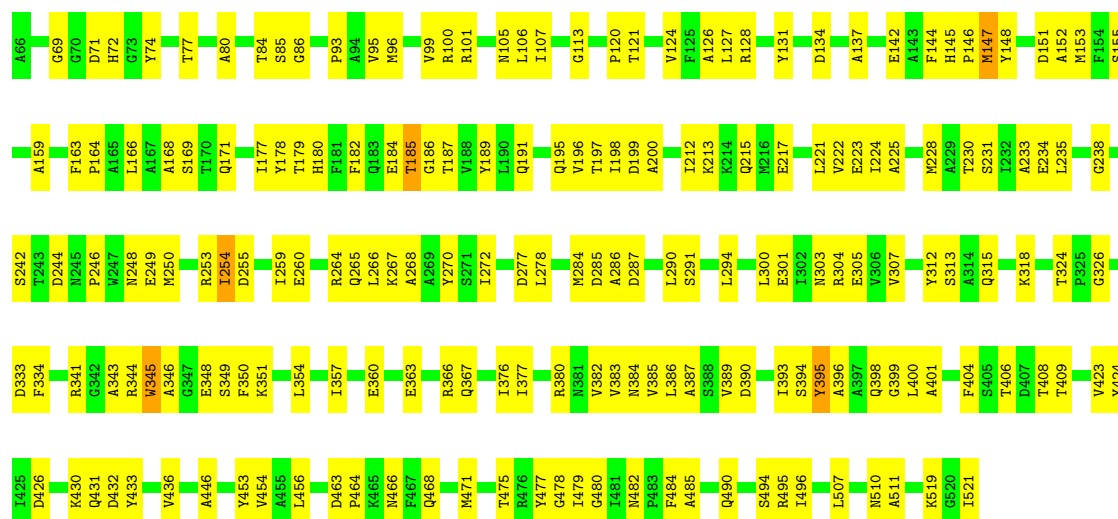
• Molecule 2: Major capsid protein

Chain J:  58% 41%



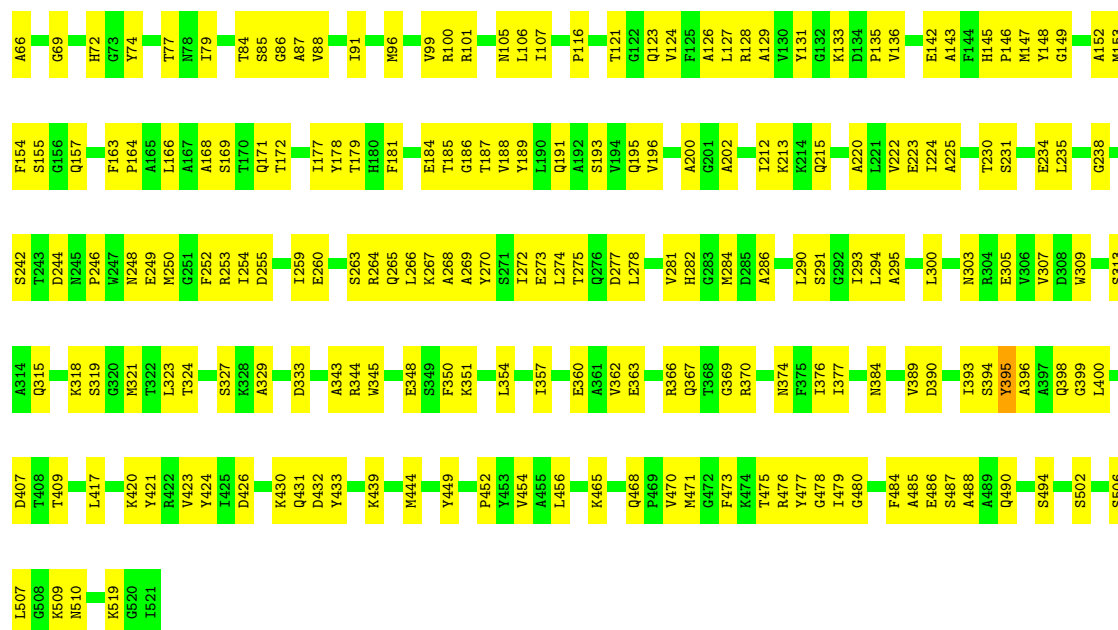
• Molecule 2: Major capsid protein

Chain K:  58% 41% .



• Molecule 2: Major capsid protein

Chain L:  56% 43% .



• Molecule 3: Small outer capsid protein

Chain O:  69% 30% .

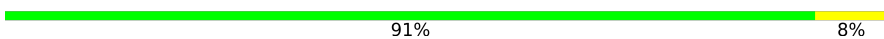


• Molecule 3: Small outer capsid protein

Chain P:  60% 39%

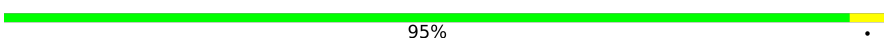


- Molecule 3: Small outer capsid protein

Chain Q:  91% 8%

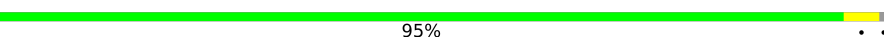


- Molecule 3: Small outer capsid protein

Chain R:  95%



- Molecule 3: Small outer capsid protein

Chain S:  95%

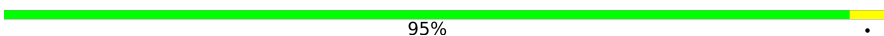


- Molecule 3: Small outer capsid protein

Chain T:  89% 10%

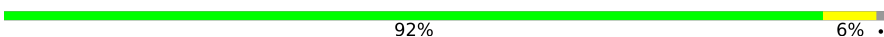


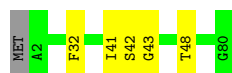
- Molecule 3: Small outer capsid protein

Chain U:  95%



- Molecule 3: Small outer capsid protein

Chain V:  92% 6%



- Molecule 3: Small outer capsid protein

MET
A2
R5
G6
V7
V8
N9
I10
K11
T12
F13
E14
D18
K21
K22
K26
E27
F32
P33
L34
X35
S36
D37
V38
H39
K40
I41
S42
Y46
S51
A54
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E67
W68
I69
A70
A71
N72
T73
D74
L75

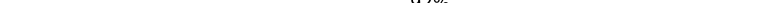
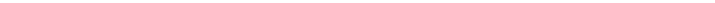
- Chain X:  92% 6%

Diagram illustrating the structure of the A2 domain of the A2 protein. The structure is shown as a yellow ribbon. The A2 domain is highlighted in yellow. The MET domain is shown in grey. The A2 domain is connected to the MET domain by a linker. The A2 domain is composed of several alpha-helices and beta-sheets. The A2 domain is labeled with residues A2, F13, F32, Y46, F49, P50, and G80.

- Chain Y:  95%

- Chain Z: 5% 93%

THR	TYR	PRO	SER	ASN	GLU	LEU	ALA	MET
			S302	VAL	VAL	ALA	GLY	
				TYR	SER	SER	GLN	PHE
			I305	THR	THR	GLN	LYS	THR
			W306	VAL	THR	PRO	THR	VAL
				ASP	VAL	ASP	ILE	ASP
			W309	THR	ASN	GLY	LYS	THR
				SER	LYS	SER	ALA	THR
			D313	VAL	THR	ALA	VAL	PRO
				GLY	MET	THR	THR	LYS
			E321	SER	ASN	TYR	THR	THR
					PRO	GLN	ASN	PRO
			R326	THR	GLN	TRP	LEU	GLY
				ASP	ILE	TYR	SER	ILE
				GLU	THR	VAL	GLY	ASP
				VAL	THR	ASP	GLY	GLU
				THR	THR	THR	GLY	ASP
				ALA	PRO	SER	PRO	GLU
				THR	ALA	GLN	GLU	LYS
				THR	THR	VAL	THR	THR
				THR	THR	VAL	ALA	PHE
				VAL	ALA	GLY	ALA	ALA
				ALA	ASN	GLY	GLU	THR
				ALA	VAL	GLU	ALA	ALA
				ASP	GLN	GLU	THR	THR
				TYR	GLN	ASN	THR	PRO
				ASN	ASP	SER	THR	SER
				PRO	ALA	THR	ILE	GLY
				VAL	SER	PHE	THR	GLN
				THR	ALA	SER	VAL	THR
				THR	PHE	THR	LYS	GLY
				THR	THR	THR	ASN	GLY
				LYS	THR	PRO	LYS	GLY
				THR	ALA	THR	THR	THR
				GLY	ASN	THR	GLN	ILE
				ASN	VAL	SER	THR	THR
				VAL	GLY	VAL	THR	TYR
				THR	VAL	LYS	THR	ALA
				ASP	ALA	ARG	LEU	TRP
				VAL	THR	ILE	VAL	SER
				ALA	GLU	ILE	VAL	VAL
				LYS	GLU	THR	THR	ASP
				VAL	ALA	CYS	PRO	ASN
				SER	VAL	VAL	ALA	VAL
				ARG	ALA	VAL	ALA	ASN
				ASN	PRO	ILE	SER	PRO
				GLY	GLU	GLN	PRO	GLN
				TYR	PRO	VAL	ALA	ASP
				ILE	THR	THR	ALA	GLY
				GLY	GLY	THR	GLY	ALA
				HIS	LYS	ASP	ILE	ALA
				THR	THR	TYR	GLY	THR
				ALA	SER	ASP	THR	PHE
				LEU	SER	ALA	PRO	SER
				THR	PRO	LEU	VAL	TYR
				THR	VAL	SER	GLN	VAL
				GLY	THR	VAL	PHE	THR
				ILE	GLY	THR	THR	LYS
				THR	SER	SER	ALA	GLY

- Chain z: 93% 7%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	18000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed during 3D reconstruction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	a	0.49	0/3263	0.66	0/4430
2	A	0.54	0/3495	0.65	2/4734 (0.0%)
2	B	0.53	0/3495	0.64	1/4734 (0.0%)
2	C	0.54	0/3495	0.64	1/4734 (0.0%)
2	D	0.53	0/3495	0.63	2/4734 (0.0%)
2	E	0.55	0/3495	0.65	1/4734 (0.0%)
2	F	0.54	0/3495	0.64	2/4734 (0.0%)
2	G	0.53	0/3495	0.65	1/4734 (0.0%)
2	H	0.53	0/3495	0.64	1/4734 (0.0%)
2	I	0.52	0/3495	0.64	1/4734 (0.0%)
2	J	0.53	0/3495	0.64	1/4734 (0.0%)
2	K	0.53	0/3495	0.65	1/4734 (0.0%)
2	L	0.53	0/3495	0.64	0/4734
3	O	0.28	0/648	0.43	0/876
3	P	0.30	0/648	0.48	0/876
3	Q	0.25	0/648	0.45	0/876
3	R	0.25	0/648	0.45	0/876
3	S	0.24	0/648	0.43	0/876
3	T	0.21	0/648	0.40	0/876
3	U	0.23	0/648	0.46	0/876
3	V	0.18	0/648	0.41	0/876
3	W	0.26	0/648	0.46	0/876
3	X	0.20	0/648	0.44	0/876
3	Y	0.22	0/648	0.44	0/876
4	Z	0.18	0/222	0.43	0/301
All	All	0.50	0/52553	0.62	14/71175 (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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
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Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	3
2	E	0	1
2	F	0	1
2	G	0	1
2	K	0	1
3	Q	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	186	GLY	N-CA-C	6.11	118.27	112.04
2	K	345	TRP	CA-CB-CG	5.90	124.81	113.60
2	H	345	TRP	CA-CB-CG	5.85	124.71	113.60
2	C	345	TRP	CA-CB-CG	5.72	124.48	113.60
2	D	345	TRP	CA-CB-CG	5.64	124.32	113.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	185	THR	Peptide
2	F	185	THR	Peptide
1	a	242	SER	Peptide
1	a	320	LEU	Peptide
1	a	35	ILE	Peptide

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	3208	0	3205	147	0
2	A	3427	0	3373	182	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3427	0	3373	204	0
2	C	3427	0	3373	207	0
2	D	3427	0	3373	192	0
2	E	3427	0	3373	213	0
2	F	3427	0	3373	207	0
2	G	3427	0	3373	184	0
2	H	3427	0	3373	172	0
2	I	3427	0	3373	192	0
2	J	3427	0	3373	178	0
2	K	3427	0	3373	184	0
2	L	3427	0	3373	194	0
3	O	633	0	608	21	0
3	P	633	0	608	25	0
3	Q	633	0	608	9	0
3	R	633	0	608	3	0
3	S	633	0	608	4	0
3	T	633	0	608	13	0
3	U	633	0	608	3	0
3	V	633	0	608	5	0
3	W	633	0	608	25	0
3	X	633	0	608	6	0
3	Y	633	0	608	3	0
4	Z	214	0	187	3	0
5	z	75	0	19	1	0
All	All	51584	0	50575	2109	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 21.

The worst 5 of 2109 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:A:152:ALA:HB1	2:A:225:ALA:HB2	1.51	0.92
2:J:431:GLN:HE22	2:K:217:GLU:HB2	1.35	0.92
2:J:152:ALA:HB1	2:J:225:ALA:HB2	1.51	0.91
1:a:378:ARG:HH21	2:F:273:GLU:HB3	1.35	0.90
2:H:152:ALA:HB1	2:H:225:ALA:HB2	1.54	0.89

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	413/417 (99%)	374 (91%)	34 (8%)	5 (1%)	10	37
2	A	454/456 (100%)	411 (90%)	41 (9%)	2 (0%)	30	60
2	B	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	18	49
2	C	454/456 (100%)	408 (90%)	43 (10%)	3 (1%)	18	49
2	D	454/456 (100%)	410 (90%)	41 (9%)	3 (1%)	18	49
2	E	454/456 (100%)	406 (89%)	44 (10%)	4 (1%)	14	43
2	F	454/456 (100%)	413 (91%)	39 (9%)	2 (0%)	30	60
2	G	454/456 (100%)	413 (91%)	38 (8%)	3 (1%)	18	49
2	H	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	18	49
2	I	454/456 (100%)	408 (90%)	44 (10%)	2 (0%)	30	60
2	J	454/456 (100%)	413 (91%)	37 (8%)	4 (1%)	14	43
2	K	454/456 (100%)	410 (90%)	41 (9%)	3 (1%)	18	49
2	L	454/456 (100%)	409 (90%)	43 (10%)	2 (0%)	30	60
3	O	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	P	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	Q	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	R	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	S	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	T	77/80 (96%)	71 (92%)	6 (8%)	0	100	100
3	U	77/80 (96%)	72 (94%)	5 (6%)	0	100	100
3	V	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	W	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	X	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	Y	77/80 (96%)	71 (92%)	6 (8%)	0	100	100
4	Z	23/376 (6%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6731/7145 (94%)	6083 (90%)	609 (9%)	39 (1%)	23	52

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	395	TYR
2	H	395	TYR
2	I	395	TYR
2	J	395	TYR
2	L	395	TYR

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 PDB entries followed by that with respect to all EM entries.

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	350/352 (99%)	350 (100%)	0	100	100
2	A	346/346 (100%)	346 (100%)	0	100	100
2	B	346/346 (100%)	346 (100%)	0	100	100
2	C	346/346 (100%)	346 (100%)	0	100	100
2	D	346/346 (100%)	346 (100%)	0	100	100
2	E	346/346 (100%)	346 (100%)	0	100	100
2	F	346/346 (100%)	346 (100%)	0	100	100
2	G	346/346 (100%)	346 (100%)	0	100	100
2	H	346/346 (100%)	346 (100%)	0	100	100
2	I	346/346 (100%)	346 (100%)	0	100	100
2	J	346/346 (100%)	346 (100%)	0	100	100
2	K	346/346 (100%)	346 (100%)	0	100	100
2	L	346/346 (100%)	346 (100%)	0	100	100
3	O	66/67 (98%)	66 (100%)	0	100	100
3	P	66/67 (98%)	66 (100%)	0	100	100
3	Q	66/67 (98%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	R	66/67 (98%)	66 (100%)	0	100	100
3	S	66/67 (98%)	66 (100%)	0	100	100
3	T	66/67 (98%)	65 (98%)	1 (2%)	57	72
3	U	66/67 (98%)	66 (100%)	0	100	100
3	V	66/67 (98%)	65 (98%)	1 (2%)	57	72
3	W	66/67 (98%)	66 (100%)	0	100	100
3	X	66/67 (98%)	66 (100%)	0	100	100
3	Y	66/67 (98%)	66 (100%)	0	100	100
4	Z	21/319 (7%)	19 (90%)	2 (10%)	8	29
All	All	5249/5560 (94%)	5245 (100%)	4 (0%)	87	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	T	41	ILE
3	V	41	ILE
4	Z	305	ILE
4	Z	321	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	282	HIS
3	P	45	HIS
2	H	427	GLN
3	P	15	GLN
3	X	45	HIS

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 [i](#)

There are no oligosaccharides 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](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8661. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.