



wwPDB X-ray Structure Validation Summary Report

Apr 1, 2014 – 08:39 PM BST

PDB ID : 4FY1
Title : The Crystallographic Structure of Panicum Mosaic Virus
Authors : Makino, D.L.; Larson, S.B.; McPherson, A.
Deposited on : 2012-07-04
Resolution : 2.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

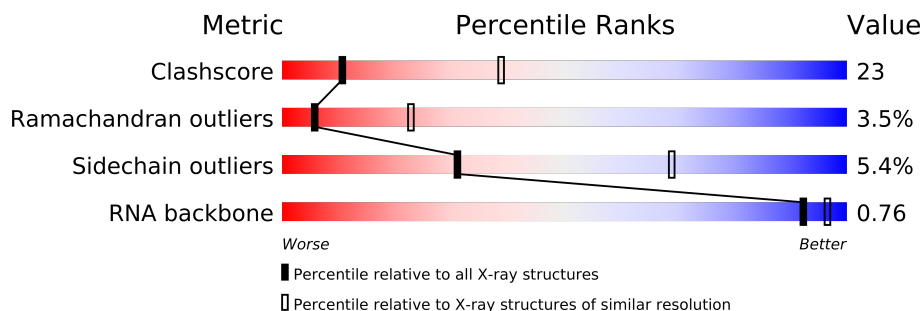
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	242	
1	4	242	
1	5	242	
1	6	242	
1	A	242	
1	B	242	
1	C	242	
1	F	242	
1	G	242	
1	H	242	
1	K	242	
1	L	242	
1	M	242	
1	P	242	
1	Q	242	

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Mol	Chain	Length	Quality of chain
1	R	242	
1	U	242	
1	V	242	
1	W	242	
1	Z	242	
1	a	242	
1	b	242	
1	e	242	
1	f	242	
1	g	242	
1	j	242	
1	k	242	
1	l	242	
1	o	242	
1	p	242	
1	q	242	
1	t	242	
1	u	242	
1	v	242	
1	y	242	
1	z	242	
2	2	17	
2	7	17	
2	D	17	
2	I	17	
2	N	17	
2	S	17	
2	X	17	
2	c	17	
2	h	17	
2	m	17	
2	r	17	
2	w	17	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 58812 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	B	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	C	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	F	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	G	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	H	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	K	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	L	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	M	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	P	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Q	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	R	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	U	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	V	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	W	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Z	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	b	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	e	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	f	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	g	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	j	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	k	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	l	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	o	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	p	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	q	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	t	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	u	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	v	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	y	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	z	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	1	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	4	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	5	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	6	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0

- Molecule 2 is a RNA chain called 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	I	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	N	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	S	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	X	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	c	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	h	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	m	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	r	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	w	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total 1	Ca 1	0	0
3	j	1	Total 1	Ca 1	0	0
3	4	1	Total 1	Ca 1	0	0
3	Z	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	t	1	Total 1	Ca 1	0	0
3	f	1	Total 1	Ca 1	0	0
3	U	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	o	1	Total 1	Ca 1	0	0
3	y	1	Total 1	Ca 1	0	0
3	L	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0

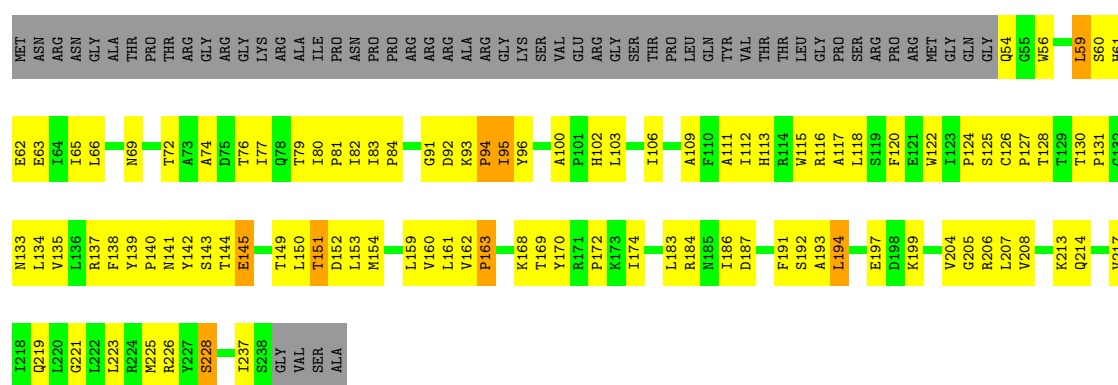
3 Residue-property plots

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 was not executed.

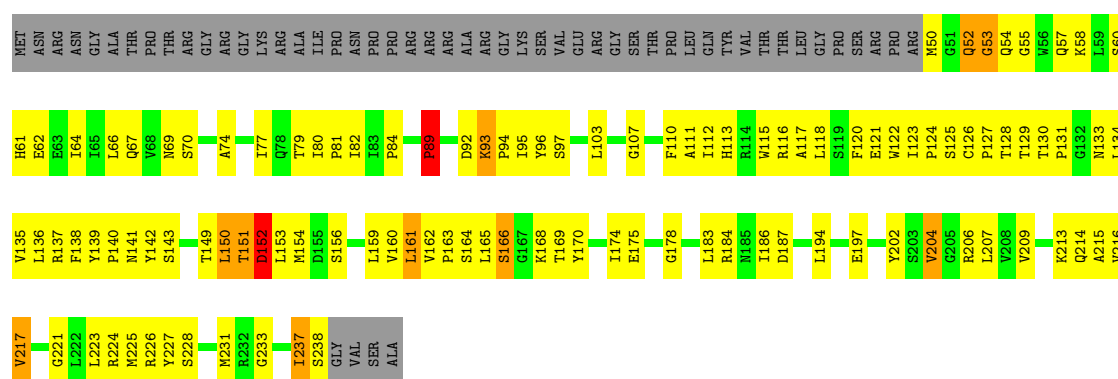
• Molecule 1: Capsid protein

Chain A:



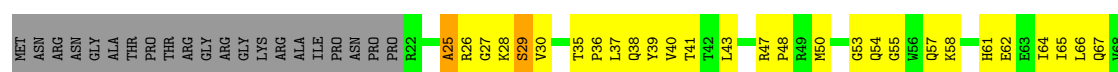
• Molecule 1: Capsid protein

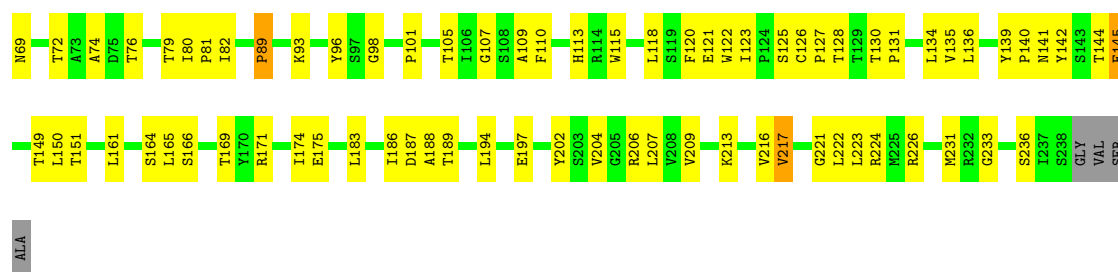
Chain B:



• Molecule 1: Capsid protein

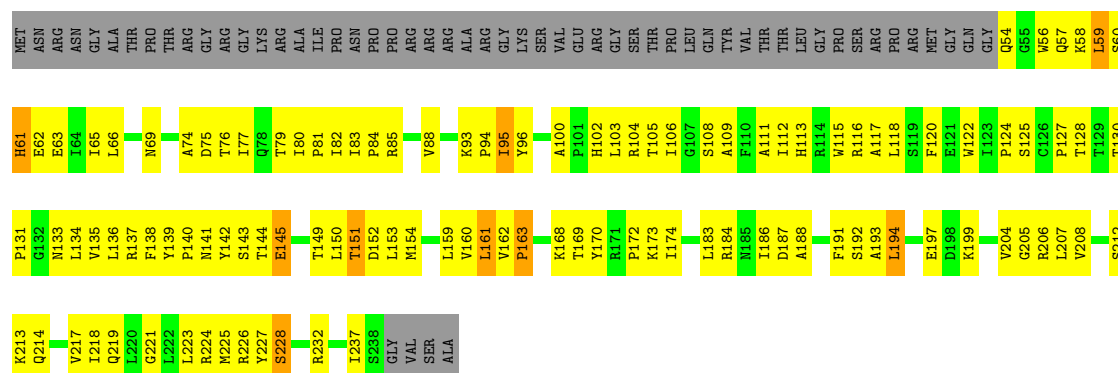
Chain C:





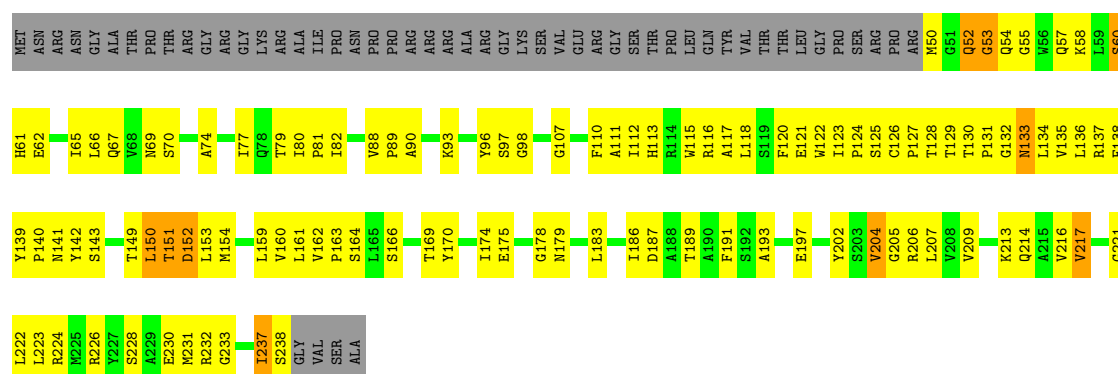
- Molecule 1: Capsid protein

Chain F:



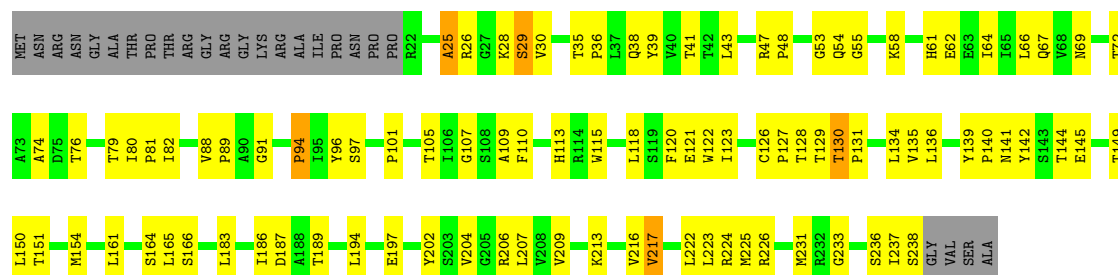
- Molecule 1: Capsid protein

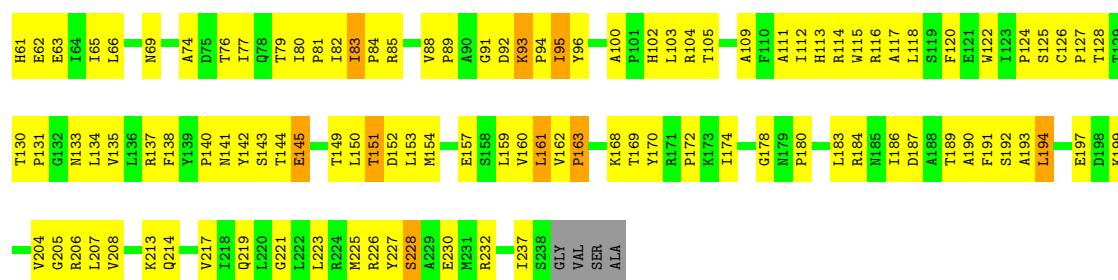
Chain G:



- Molecule 1: Capsid protein

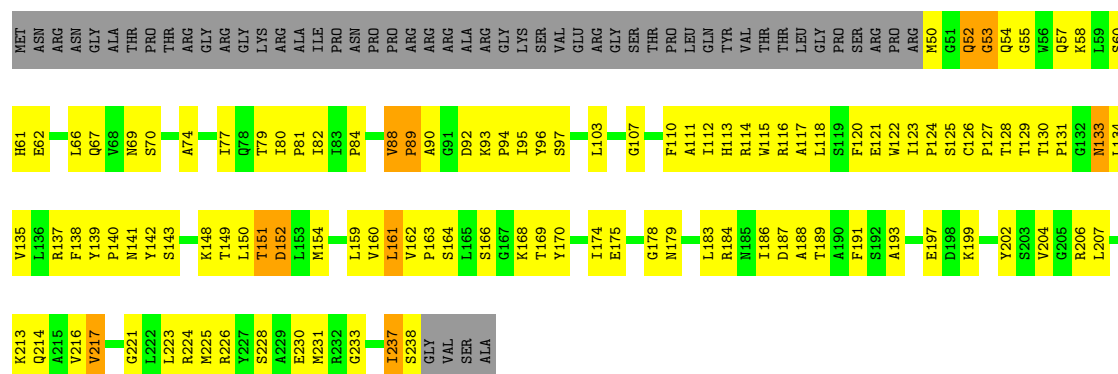
Chain H:





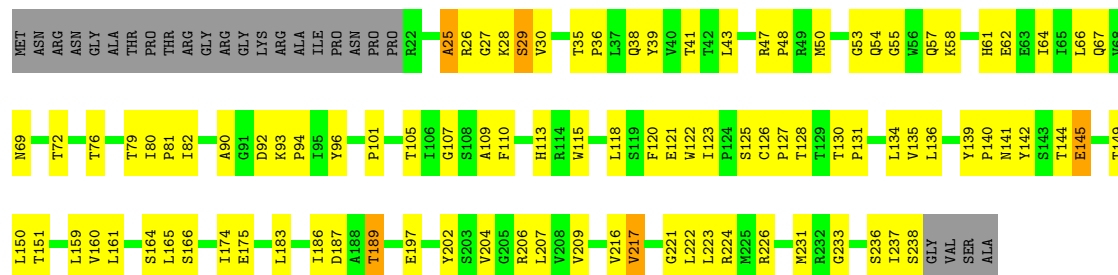
• Molecule 1: Capsid protein

Chain Q:



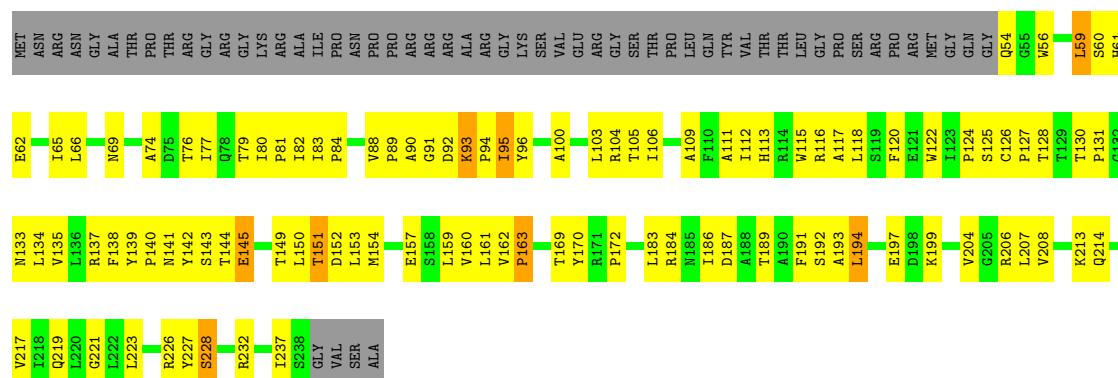
• Molecule 1: Capsid protein

Chain R:

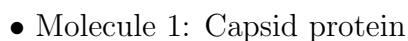


• Molecule 1: Capsid protein

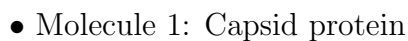
Chain U:



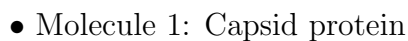
Chain V:



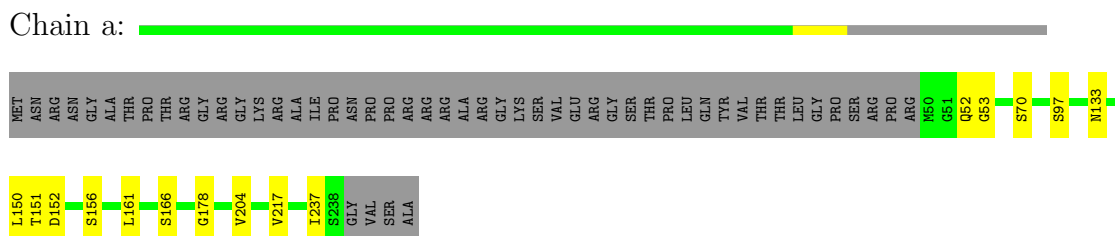
Chain W:



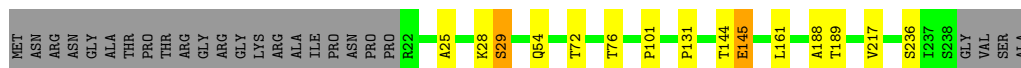
Chain Z:



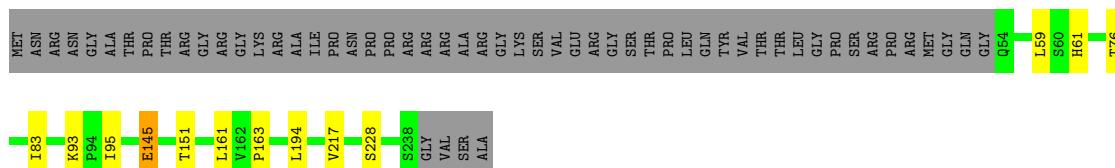
Chain a:



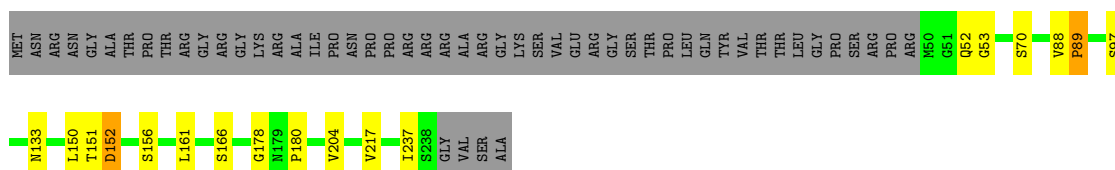
- Molecule 1: Capsid protein

Chain b: 

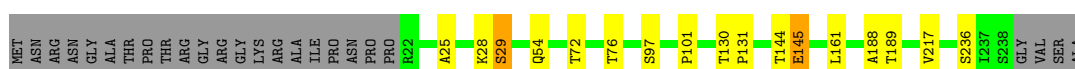
- Molecule 1: Capsid protein

Chain e: 

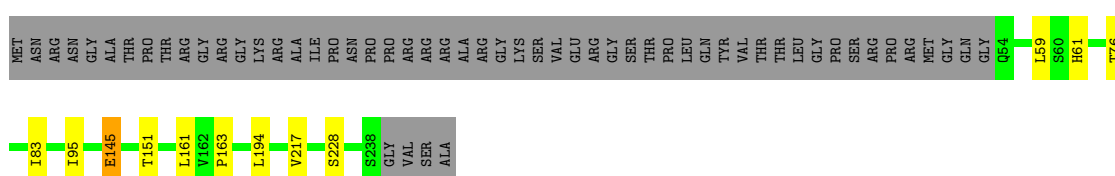
- Molecule 1: Capsid protein

Chain f: 

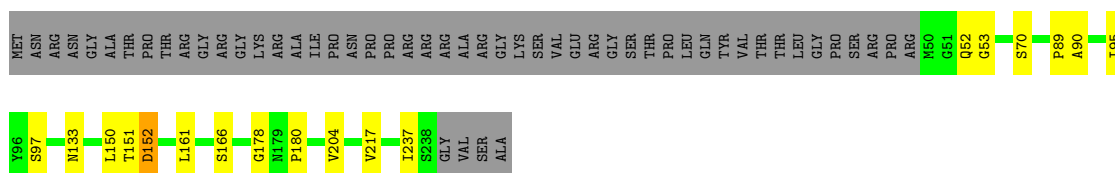
- Molecule 1: Capsid protein

Chain g: 

- Molecule 1: Capsid protein

Chain j: 

- Molecule 1: Capsid protein

Chain k: 

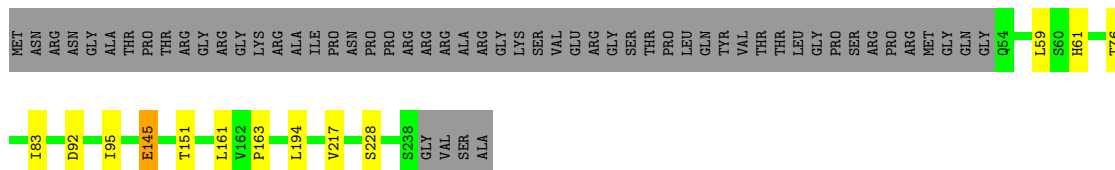
- Molecule 1: Capsid protein

Chain l: 



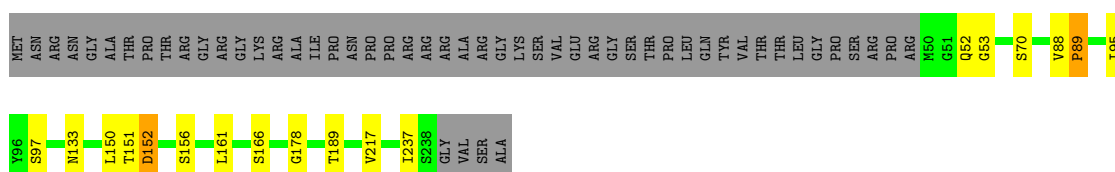
- Molecule 1: Capsid protein

Chain o: 



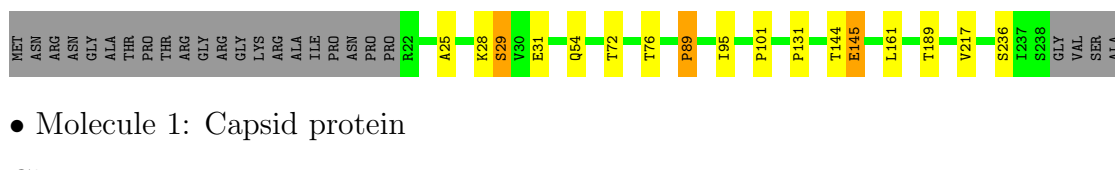
- Molecule 1: Capsid protein

Chain p: 



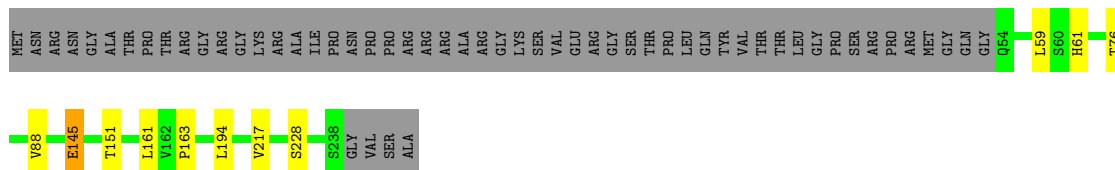
- Molecule 1: Capsid protein

Chain q: 



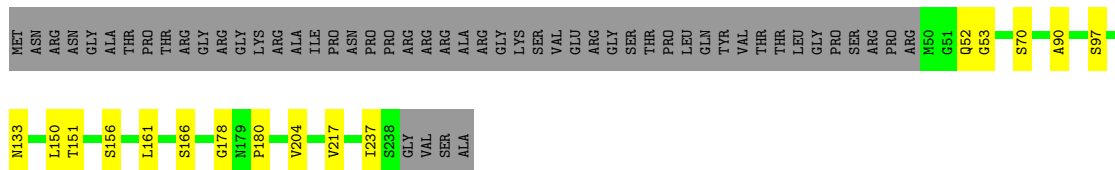
- Molecule 1: Capsid protein

Chain t: 



- Molecule 1: Capsid protein

Chain u: 



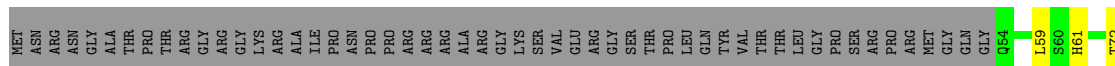
- Molecule 1: Capsid protein

Chain v: 



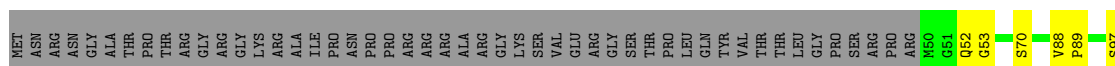
- Molecule 1: Capsid protein

Chain y:



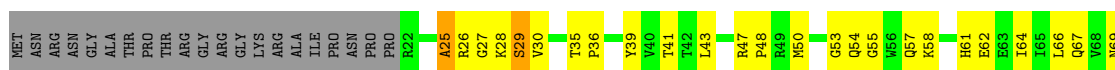
- Molecule 1: Capsid protein

Chain z:



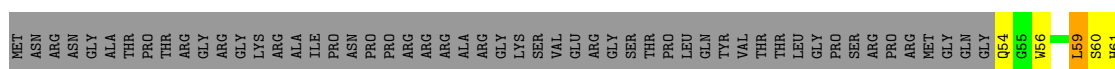
- Molecule 1: Capsid protein

Chain 1:



- Molecule 1: Capsid protein

Chain 4:

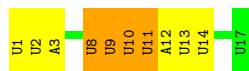


- Molecule 1: Capsid protein

Chain 5:

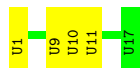
● Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3',

Chain X: 



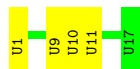
● Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3',

Chain c: 



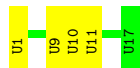
● Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3',

Chain h: 



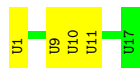
● Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3',

Chain m: 



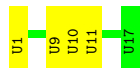
● Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3',

Chain r: 



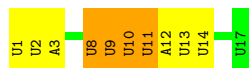
● Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3',

Chain w: 



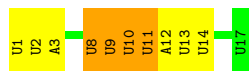
● Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3',

Chain 2: 



- Molecule 2: 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3',

Chain 7: 



4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	411.74Å 403.90Å 412.46Å 90.00° 89.65° 90.00°	Depositor
Resolution (Å)	50.01 – 2.90	Depositor
% Data completeness (in resolution range)	74.9 (50.01-2.90)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.91Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.251 , 0.285	Depositor
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.138	Xtriage
Estimated twinning fraction	0.025 for -l,k,h 0.034 for -h,-l,-k 0.024 for -h,l,k 0.044 for -k,-h,-l 0.024 for k,h,-l 0.017 for -l,-h,k 0.030 for -k,l,-h 0.038 for l,h,k 0.027 for k,-l,-h 0.035 for h,-k,-l 0.030 for -l,-k,-h	Xtriage
L-test for twinning	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 2217465 reflections	Xtriage
Total number of atoms	58812	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1	0.46	1/1710 (0.1%)	0.72	0/2323
1	4	0.45	0/1458	0.72	0/1986
1	5	0.41	0/1483	0.67	0/2018
1	6	0.46	2/1710 (0.1%)	0.71	0/2323
1	A	0.48	1/1458 (0.1%)	0.74	1/1986 (0.1%)
1	B	0.43	0/1483	0.71	0/2018
1	C	0.48	1/1710 (0.1%)	0.72	0/2323
1	F	0.51	1/1458 (0.1%)	0.75	0/1986
1	G	0.47	0/1483	0.71	0/2018
1	H	0.47	0/1710	0.72	0/2323
1	K	0.49	1/1458 (0.1%)	0.74	0/1986
1	L	0.46	0/1483	0.69	0/2018
1	M	0.48	1/1710 (0.1%)	0.73	0/2323
1	P	0.49	1/1458 (0.1%)	0.75	0/1986
1	Q	0.43	0/1483	0.69	0/2018
1	R	0.48	2/1710 (0.1%)	0.72	0/2323
1	U	0.45	1/1458 (0.1%)	0.71	0/1986
1	V	0.39	0/1483	0.67	0/2018
1	W	0.45	0/1710	0.70	0/2323
1	Z	0.52	2/1458 (0.1%)	0.76	0/1986
1	a	0.45	0/1483	0.70	0/2018
1	b	0.49	2/1710 (0.1%)	0.73	0/2323
1	e	0.50	1/1458 (0.1%)	0.76	0/1986
1	f	0.46	0/1483	0.70	0/2018
1	g	0.51	2/1710 (0.1%)	0.74	0/2323
1	j	0.47	1/1458 (0.1%)	0.73	0/1986
1	k	0.44	0/1483	0.70	0/2018
1	l	0.51	2/1710 (0.1%)	0.73	0/2323
1	o	0.51	1/1458 (0.1%)	0.76	0/1986
1	p	0.49	0/1483	0.70	0/2018
1	q	0.51	1/1710 (0.1%)	0.74	0/2323
1	t	0.51	2/1458 (0.1%)	0.76	0/1986

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	u	0.45	0/1483	0.69	0/2018
1	v	0.51	1/1710 (0.1%)	0.73	0/2323
1	y	0.46	1/1458 (0.1%)	0.72	0/1986
1	z	0.40	0/1483	0.67	0/2018
2	2	0.56	1/386 (0.3%)	0.70	0/594
2	7	0.56	1/386 (0.3%)	0.70	0/594
2	D	0.55	1/386 (0.3%)	0.69	0/594
2	I	0.56	1/386 (0.3%)	0.69	0/594
2	N	0.55	1/386 (0.3%)	0.68	0/594
2	S	0.56	1/386 (0.3%)	0.69	0/594
2	X	0.54	1/386 (0.3%)	0.70	0/594
2	c	0.56	1/386 (0.3%)	0.70	0/594
2	h	0.55	1/386 (0.3%)	0.69	0/594
2	m	0.55	1/386 (0.3%)	0.69	0/594
2	r	0.55	1/386 (0.3%)	0.70	0/594
2	w	0.55	1/386 (0.3%)	0.69	0/594
All	All	0.48	40/60444 (0.1%)	0.72	1/83052 (0.0%)

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1	U	OP3-P	-7.42	1.52	1.61
2	m	1	U	OP3-P	-7.36	1.52	1.61
2	I	1	U	OP3-P	-7.35	1.52	1.61
2	c	1	U	OP3-P	-7.32	1.52	1.61
2	S	1	U	OP3-P	-7.32	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	GLY	N-CA-C	-5.08	100.40	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1674	0	1700	63	0
1	4	1426	0	1439	87	0
1	5	1451	0	1462	79	0
1	6	1674	0	1700	60	0
1	A	1426	0	1439	122	0
1	B	1451	0	1462	119	0
1	C	1674	0	1700	77	0
1	F	1426	0	1439	147	0
1	G	1451	0	1462	115	0
1	H	1674	0	1700	86	0
1	K	1426	0	1439	120	0
1	L	1451	0	1462	101	0
1	M	1674	0	1700	102	0
1	P	1426	0	1439	135	0
1	Q	1451	0	1462	109	0
1	R	1674	0	1700	77	0
1	U	1426	0	1439	122	0
1	V	1451	0	1462	107	0
1	W	1674	0	1700	63	0
1	Z	1426	0	1439	109	0
1	a	1451	0	1462	0	0
1	b	1674	0	1700	0	0
1	e	1426	0	1439	0	0
1	f	1451	0	1462	0	0
1	g	1674	0	1700	0	0
1	j	1426	0	1439	0	0
1	k	1451	0	1462	0	0
1	l	1674	0	1700	0	0
1	o	1426	0	1439	0	0
1	p	1451	0	1462	0	0
1	q	1674	0	1700	0	0
1	t	1426	0	1439	0	0
1	u	1451	0	1462	0	0
1	v	1674	0	1700	0	0
1	y	1426	0	1439	0	0
1	z	1451	0	1462	0	0
2	2	349	0	175	22	0
2	7	349	0	175	22	0
2	D	349	0	175	24	0
2	I	349	0	175	32	0
2	N	349	0	175	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	349	0	175	28	0
2	X	349	0	175	23	0
2	c	349	0	175	0	0
2	h	349	0	175	0	0
2	m	349	0	175	0	0
2	r	349	0	175	0	0
2	w	349	0	175	0	0
3	4	1	0	0	0	0
3	A	1	0	0	0	0
3	F	1	0	0	0	0
3	L	1	0	0	0	0
3	P	1	0	0	0	0
3	U	1	0	0	0	0
3	Z	1	0	0	0	0
3	f	1	0	0	0	0
3	j	1	0	0	0	0
3	o	1	0	0	0	0
3	t	1	0	0	0	0
3	y	1	0	0	0	0
All	All	58812	0	57312	2040	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

The worst 5 of 2040 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:54:GLN:N	2:I:13:U:OP1	1.80	1.14
1:F:95:ILE:HD12	1:F:95:ILE:H	1.11	1.06
1:4:95:ILE:H	1:4:95:ILE:HD12	1.22	1.00
1:U:95:ILE:H	1:U:95:ILE:HD12	1.22	1.00
1:P:95:ILE:HD12	1:P:95:ILE:H	1.24	0.98

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 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	1	215/242 (89%)	187 (87%)	19 (9%)	9 (4%)	4	16
1	4	183/242 (76%)	165 (90%)	14 (8%)	4 (2%)	10	37
1	5	187/242 (77%)	160 (86%)	19 (10%)	8 (4%)	4	15
1	6	215/242 (89%)	187 (87%)	18 (8%)	10 (5%)	4	13
1	A	183/242 (76%)	165 (90%)	13 (7%)	5 (3%)	8	30
1	B	187/242 (77%)	158 (84%)	21 (11%)	8 (4%)	4	15
1	C	215/242 (89%)	187 (87%)	18 (8%)	10 (5%)	4	13
1	F	183/242 (76%)	167 (91%)	12 (7%)	4 (2%)	10	37
1	G	187/242 (77%)	161 (86%)	20 (11%)	6 (3%)	6	25
1	H	215/242 (89%)	189 (88%)	17 (8%)	9 (4%)	4	16
1	K	183/242 (76%)	163 (89%)	14 (8%)	6 (3%)	6	24
1	L	187/242 (77%)	160 (86%)	19 (10%)	8 (4%)	4	15
1	M	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	5	20
1	P	183/242 (76%)	164 (90%)	13 (7%)	6 (3%)	6	24
1	Q	187/242 (77%)	163 (87%)	18 (10%)	6 (3%)	6	25
1	R	215/242 (89%)	188 (87%)	19 (9%)	8 (4%)	5	20
1	U	183/242 (76%)	165 (90%)	11 (6%)	7 (4%)	5	19
1	V	187/242 (77%)	159 (85%)	22 (12%)	6 (3%)	6	25
1	W	215/242 (89%)	190 (88%)	16 (7%)	9 (4%)	4	16
1	Z	183/242 (76%)	167 (91%)	12 (7%)	4 (2%)	10	37
1	a	187/242 (77%)	161 (86%)	20 (11%)	6 (3%)	6	25
1	b	215/242 (89%)	189 (88%)	17 (8%)	9 (4%)	4	16
1	e	183/242 (76%)	164 (90%)	14 (8%)	5 (3%)	8	30
1	f	187/242 (77%)	160 (86%)	19 (10%)	8 (4%)	4	15
1	g	215/242 (89%)	188 (87%)	18 (8%)	9 (4%)	4	16
1	j	183/242 (76%)	165 (90%)	14 (8%)	4 (2%)	10	37
1	k	187/242 (77%)	159 (85%)	21 (11%)	7 (4%)	5	20
1	l	215/242 (89%)	185 (86%)	21 (10%)	9 (4%)	4	16
1	o	183/242 (76%)	166 (91%)	13 (7%)	4 (2%)	10	37
1	p	187/242 (77%)	160 (86%)	20 (11%)	7 (4%)	5	20
1	q	215/242 (89%)	185 (86%)	21 (10%)	9 (4%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	t	183/242 (76%)	163 (89%)	16 (9%)	4 (2%)	10	37
1	u	187/242 (77%)	159 (85%)	21 (11%)	7 (4%)	5	20
1	v	215/242 (89%)	186 (86%)	20 (9%)	9 (4%)	4	16
1	y	183/242 (76%)	163 (89%)	16 (9%)	4 (2%)	10	37
1	z	187/242 (77%)	161 (86%)	19 (10%)	7 (4%)	5	20
All	All	7020/8712 (81%)	6147 (88%)	624 (9%)	249 (4%)	6	23

5 of 249 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	28	LYS
1	C	29	SER
1	H	28	LYS
1	H	29	SER
1	M	28	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	186/204 (91%)	177 (95%)	9 (5%)	35	74
1	4	160/204 (78%)	151 (94%)	9 (6%)	30	66
1	5	162/204 (79%)	151 (93%)	11 (7%)	22	55
1	6	186/204 (91%)	177 (95%)	9 (5%)	35	74
1	A	160/204 (78%)	152 (95%)	8 (5%)	34	73
1	B	162/204 (79%)	152 (94%)	10 (6%)	26	61
1	C	186/204 (91%)	177 (95%)	9 (5%)	35	74
1	F	160/204 (78%)	153 (96%)	7 (4%)	39	77
1	G	162/204 (79%)	152 (94%)	10 (6%)	26	61
1	H	186/204 (91%)	177 (95%)	9 (5%)	35	74
1	K	160/204 (78%)	150 (94%)	10 (6%)	25	60
1	L	162/204 (79%)	152 (94%)	10 (6%)	26	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	186/204 (91%)	177 (95%)	9 (5%)	35	74
1	P	160/204 (78%)	150 (94%)	10 (6%)	25	60
1	Q	162/204 (79%)	152 (94%)	10 (6%)	26	61
1	R	186/204 (91%)	178 (96%)	8 (4%)	40	78
1	U	160/204 (78%)	153 (96%)	7 (4%)	39	77
1	V	162/204 (79%)	152 (94%)	10 (6%)	26	61
1	W	186/204 (91%)	179 (96%)	7 (4%)	44	83
1	Z	160/204 (78%)	152 (95%)	8 (5%)	34	73
1	a	162/204 (79%)	153 (94%)	9 (6%)	30	66
1	b	186/204 (91%)	179 (96%)	7 (4%)	44	83
1	e	160/204 (78%)	152 (95%)	8 (5%)	34	73
1	f	162/204 (79%)	150 (93%)	12 (7%)	20	50
1	g	186/204 (91%)	177 (95%)	9 (5%)	35	74
1	j	160/204 (78%)	152 (95%)	8 (5%)	34	73
1	k	162/204 (79%)	150 (93%)	12 (7%)	20	50
1	l	186/204 (91%)	178 (96%)	8 (4%)	40	78
1	o	160/204 (78%)	151 (94%)	9 (6%)	30	66
1	p	162/204 (79%)	149 (92%)	13 (8%)	17	45
1	q	186/204 (91%)	176 (95%)	10 (5%)	31	69
1	t	160/204 (78%)	153 (96%)	7 (4%)	39	77
1	u	162/204 (79%)	153 (94%)	9 (6%)	30	66
1	v	186/204 (91%)	176 (95%)	10 (5%)	31	69
1	y	160/204 (78%)	150 (94%)	10 (6%)	25	60
1	z	162/204 (79%)	152 (94%)	10 (6%)	26	61
All	All	6096/7344 (83%)	5765 (95%)	331 (5%)	31	69

5 of 331 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	204	VAL
1	g	161	LEU
1	4	83	ILE
1	b	131	PRO
1	f	88	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	113	HIS
1	g	57	GLN
1	4	133	ASN
1	a	52	GLN
1	b	69	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	16/17 (94%)	3 (18%)	3 (18%)
2	7	16/17 (94%)	3 (18%)	3 (18%)
2	D	16/17 (94%)	3 (18%)	3 (18%)
2	I	16/17 (94%)	3 (18%)	3 (18%)
2	N	16/17 (94%)	3 (18%)	3 (18%)
2	S	16/17 (94%)	3 (18%)	3 (18%)
2	X	16/17 (94%)	3 (18%)	3 (18%)
2	c	16/17 (94%)	3 (18%)	0
2	h	16/17 (94%)	3 (18%)	0
2	m	16/17 (94%)	3 (18%)	0
2	r	16/17 (94%)	3 (18%)	0
2	w	16/17 (94%)	3 (18%)	0
All	All	192/204 (94%)	36 (18%)	21 (10%)

5 of 36 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	9	U
2	D	10	U
2	D	11	U
2	I	9	U
2	I	10	U

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	S	8	U
2	S	10	U
2	2	10	U
2	N	10	U
2	7	8	U

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 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.

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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.