



Full wwPDB EM Validation Report ⓘ

Jul 1, 2023 – 02:03 PM EDT

PDB ID : 8FJK
EMDB ID : EMD-29243
Title : Golden Shiner Reovirus Core Polar Vertex
Authors : Stevens, A.S.; Zhou, Z.H.
Deposited on : 2022-12-19
Resolution : 3.30 Å (reported)

This is a Full wwPDB EM Validation 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.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

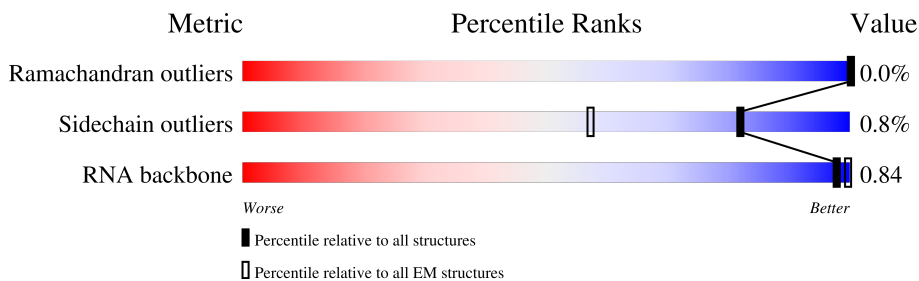
1 Overall quality at a glance

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.



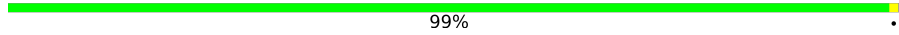
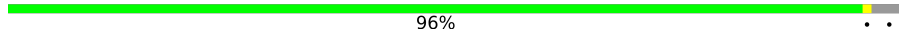
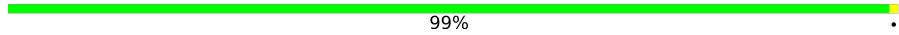
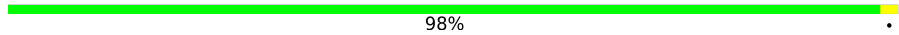




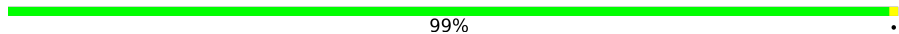
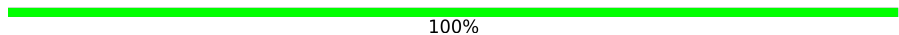
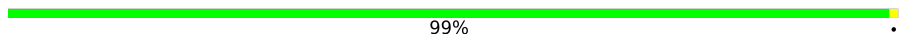
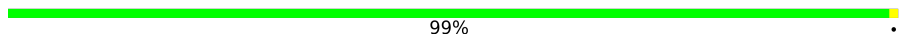
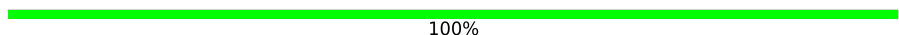
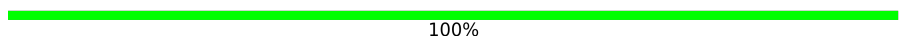
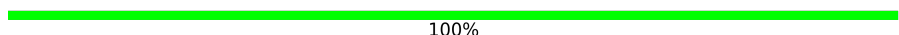
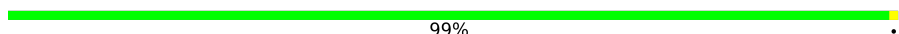
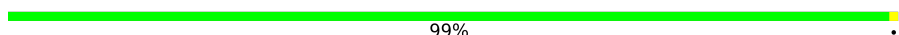
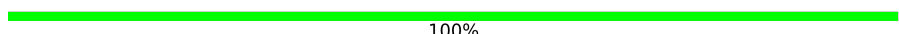
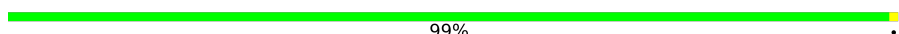
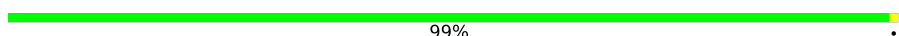
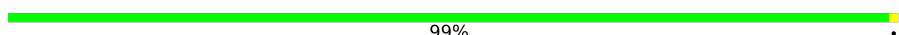
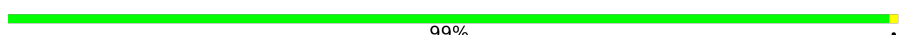
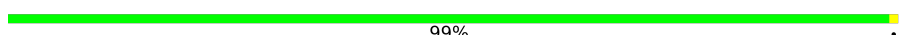
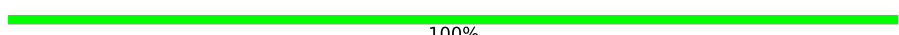
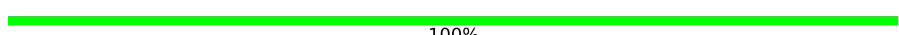
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1273	99% .
2	B	718	99% .
3	C	1138	94% 6%
3	D	1138	100%
3	E	1138	96% ..
3	F	1138	99% .
3	G	1138	96% .
3	H	1138	98% ..
3	I	1138	93% 6%

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Mol	Chain	Length	Quality of chain
3	J	1138	 99%
3	K	1138	 96%
3	L	1138	 99%
4	M	94	 98%
4	N	94	 32% 68%
4	k	94	 32% 68%
4	l	94	 32% 68%
4	m	94	 32% 68%
5	V	411	 99%
5	W	411	 100%
5	X	411	 99%
5	a	411	 99%
5	b	411	 100%
5	d	411	 100%
5	e	411	 100%
5	g	411	 99%
5	h	411	 99%
5	n	411	 100%
6	Y	1297	 99%
6	Z	1297	 99%
6	c	1297	 99%
6	f	1297	 99%
6	i	1297	 99%
7	a1	52	 100%
7	b1	52	 100%

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Mol	Chain	Length	Quality of chain
8	a2	60	 100%
8	b2	60	 100%
9	a3	40	 100%
9	b3	40	 100%
10	a4	18	 100%
10	b4	18	 100%
11	a5	38	 100%
11	b5	38	 100%
12	a6	30	 100%
12	b6	30	 100%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 193908 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 RNA-directed RNA polymerase VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1273	9978	6375	1736	1822	45	0	0

- Molecule 2 is a protein called Microtubule-associated protein VP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	718	5593	3588	971	1016	18	0	0

- Molecule 3 is a protein called Major inner capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	1075	8300	5296	1421	1534	49	0	0
3	D	1138	8761	5578	1502	1628	53	0	0
3	E	1106	8534	5440	1463	1579	52	0	0
3	F	1138	8761	5578	1502	1628	53	0	0
3	G	1098	8477	5403	1454	1568	52	0	0
3	H	1130	8699	5540	1491	1615	53	0	0
3	I	1065	8226	5244	1412	1519	51	0	0
3	J	1130	8699	5540	1491	1615	53	0	0
3	K	1098	8477	5403	1454	1568	52	0	0
3	L	1138	8761	5578	1502	1628	53	0	0

- Molecule 4 is a protein called Major inner capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	94	Total	C	N	O	S	0	0
			640	377	113	149	1		
4	N	30	Total	C	N	O	S	0	0
			210	128	36	45	1		
4	k	30	Total	C	N	O	S	0	0
			211	128	36	46	1		
4	l	30	Total	C	N	O	S	0	0
			211	128	36	46	1		
4	m	30	Total	C	N	O	S	0	0
			211	128	36	46	1		

- Molecule 5 is a protein called Clamp protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	W	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	X	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	a	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	b	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	d	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	e	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	g	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	h	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	n	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		

- Molecule 6 is a protein called Outer capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		
6	Z	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		
6	c	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		
6	i	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		

- Molecule 7 is a RNA chain called RNA (52-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a1	52	Total	C	N	O	P	0	0
			1089	494	182	362	51		
7	b1	52	Total	C	N	O	P	0	0
			1089	494	182	362	51		

- Molecule 8 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a2	60	Total	C	N	O	P	0	0
			1257	570	210	418	59		
8	b2	60	Total	C	N	O	P	0	0
			1257	570	210	418	59		

- Molecule 9 is a RNA chain called RNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a3	40	Total	C	N	O	P	0	0
			837	380	140	278	39		
9	b3	40	Total	C	N	O	P	0	0
			837	380	140	278	39		

- Molecule 10 is a RNA chain called RNA (18-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a4	18	Total	C	N	O	P	0	0
			375	171	63	124	17		
10	b4	18	Total	C	N	O	P	0	0
			375	171	63	124	17		

- Molecule 11 is a RNA chain called RNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a5	38	Total	C	N	O	P	0	0
			795	361	133	264	37		
11	b5	38	Total	C	N	O	P	0	0
			795	361	133	264	37		

- Molecule 12 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a6	30	Total	C	N	O	P	0	0
			627	285	105	208	29		
12	b6	30	Total	C	N	O	P	0	0
			627	285	105	208	29		

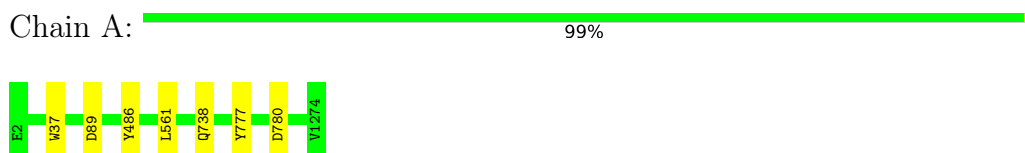
- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	E	1	Total	Zn	0
			1	1	
13	G	1	Total	Zn	0
			1	1	
13	I	1	Total	Zn	0
			1	1	
13	K	1	Total	Zn	0
			1	1	

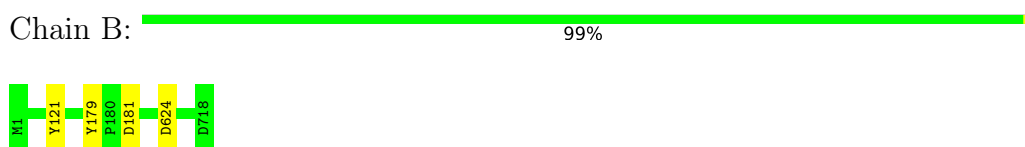
3 Residue-property plots [i](#)

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. 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.

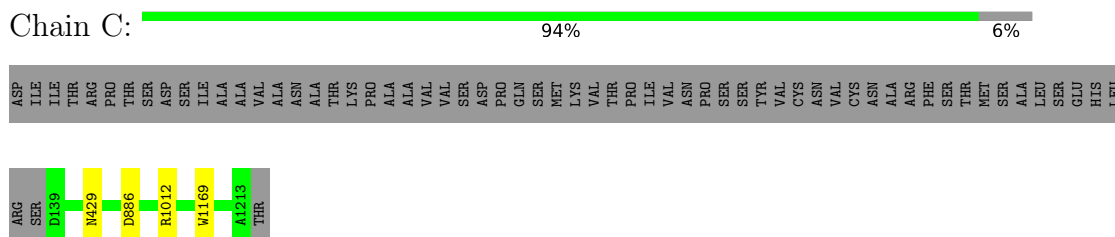
- Molecule 1: RNA-directed RNA polymerase VP2



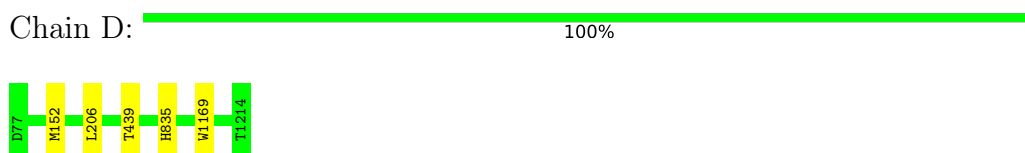
- Molecule 2: Microtubule-associated protein VP5



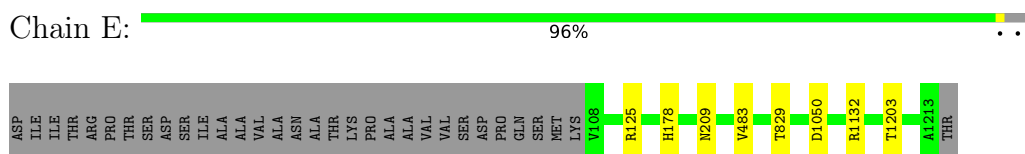
- Molecule 3: Major inner capsid protein VP3



- Molecule 3: Major inner capsid protein VP3



- Molecule 3: Major inner capsid protein VP3



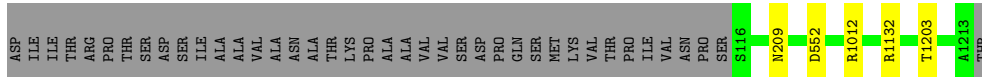
- Molecule 3: Major inner capsid protein VP3

Chain F:  99%



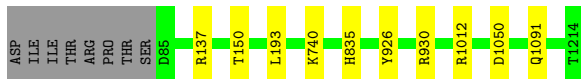
- Molecule 3: Major inner capsid protein VP3

Chain G:  96%



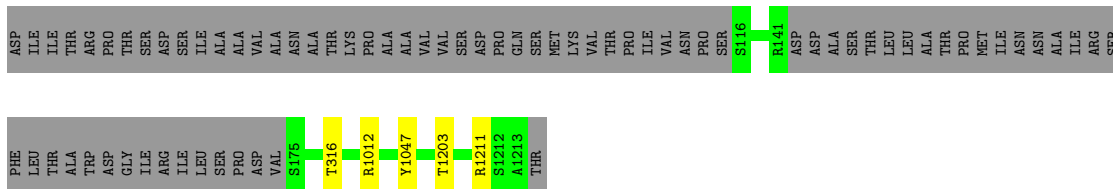
- Molecule 3: Major inner capsid protein VP3

Chain H:  98%



- Molecule 3: Major inner capsid protein VP3

Chain I:  93% 6%



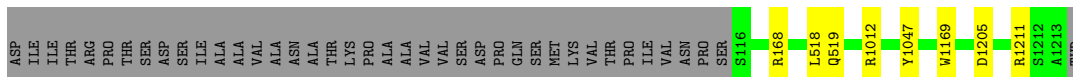
- Molecule 3: Major inner capsid protein VP3

Chain J:  99%



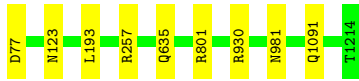
- Molecule 3: Major inner capsid protein VP3

Chain K:  96%



- Molecule 3: Major inner capsid protein VP3

Chain L:  99%



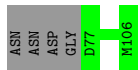
• Molecule 4: Major inner capsid protein VP3



• Molecule 4: Major inner capsid protein VP3



THR	ALA	SER	PRO	ALA	ASP	THR	ASN	VAL	VAL	PRO	PRO	LYS	ASP	ALA	THR	THR	ASN	SER	PRO	SER	THR	SER	PRO	ASN	GLN	ALA	ALA	ALA	ASP	ALA	ALA	ASN	GLN	GLN	ALA	GLY	ILE	VAL	SER	SER	GLN	GLY	PRO	ASN	ALA	VAL	GLY	ASP	SER	ALA	PRO	SER	THR	SER	VAL
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• Molecule 4: Major inner capsid protein VP3



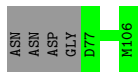
THR	ALA	SER	PRO	ALA	ASP	THR	ASN	VAL	VAL	PRO	PRO	LYS	ASP	ALA	THR	THR	ASN	SER	PRO	SER	THR	SER	PRO	ASN	GLN	ALA	ALA	ALA	ASP	ALA	ALA	ASN	GLN	GLN	ALA	GLY	ILE	VAL	SER	SER	GLN	GLY	PRO	ASN	ALA	VAL	GLY	ASP	SER	ALA	PRO	SER	THR	SER	VAL
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• Molecule 4: Major inner capsid protein VP3



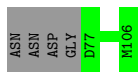
THR	ALA	SER	PRO	ALA	ASP	THR	ASN	VAL	VAL	PRO	PRO	LYS	ASP	ALA	THR	THR	ASN	SER	PRO	SER	THR	SER	PRO	ASN	GLN	ALA	ALA	ALA	ASP	ALA	ALA	ASN	GLN	GLN	ALA	GLY	ILE	VAL	SER	SER	GLN	GLY	PRO	ASN	ALA	VAL	GLY	ASP	SER	ALA	PRO	SER	THR	SER	VAL
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• Molecule 4: Major inner capsid protein VP3



THR	ALA	SER	PRO	ALA	ASP	THR	ASN	VAL	VAL	PRO	PRO	LYS	ASP	ALA	THR	THR	ASN	SER	PRO	SER	THR	SER	PRO	ASN	GLN	ALA	ALA	ALA	ASP	ALA	ALA	ASN	GLN	GLN	ALA	GLY	ILE	VAL	SER	SER	GLN	GLY	PRO	ASN	ALA	VAL	GLY	ASP	SER	ALA	PRO	SER	THR	SER	VAL
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• Molecule 5: Clamp protein VP6

Chain V:  99%



● Molecule 5: Clamp protein VP6

Chain W:  100%



● Molecule 5: Clamp protein VP6

Chain X:  99%



● Molecule 5: Clamp protein VP6

Chain a:  99%



● Molecule 5: Clamp protein VP6

Chain b:  100%



● Molecule 5: Clamp protein VP6

Chain d:  100%



● Molecule 5: Clamp protein VP6

Chain e:  100%



● Molecule 5: Clamp protein VP6

Chain g:  99%



- Molecule 5: Clamp protein VP6

Chain h:  99%



- Molecule 5: Clamp protein VP6

Chain n:  100%



- Molecule 6: Outer capsid protein VP1

Chain Y:  99%



- Molecule 6: Outer capsid protein VP1

Chain Z:  99%



- Molecule 6: Outer capsid protein VP1

Chain c:  99%



- Molecule 6: Outer capsid protein VP1

Chain f:  99%



- Molecule 6: Outer capsid protein VP1

Chain i:  99%



- Molecule 7: RNA (52-MER)

Chain a1:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: RNA (52-MER)

Chain b1:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: RNA (60-MER)

Chain a2:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: RNA (60-MER)

Chain b2:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: RNA (40-MER)

Chain a3:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: RNA (40-MER)

Chain b3:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: RNA (18-MER)

Chain a4:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: RNA (18-MER)

Chain b4:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: RNA (38-MER)

Chain a5:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: RNA (38-MER)

Chain b5:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: RNA (30-MER)

Chain a6:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: RNA (30-MER)

Chain b6:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119182	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.32	0/10261	0.50	0/14016
2	B	0.31	0/5734	0.52	0/7849
3	C	0.33	0/8516	0.49	0/11674
3	D	0.33	0/8985	0.49	0/12316
3	E	0.33	0/8755	0.49	0/12001
3	F	0.33	0/8985	0.49	0/12316
3	G	0.33	0/8696	0.49	0/11917
3	H	0.33	0/8922	0.49	0/12229
3	I	0.33	0/8439	0.49	0/11562
3	J	0.33	0/8922	0.49	0/12229
3	K	0.33	0/8696	0.49	0/11917
3	L	0.33	0/8985	0.49	0/12316
4	M	0.28	0/650	0.46	0/898
4	N	0.30	0/212	0.46	0/291
4	k	0.28	0/213	0.47	0/291
4	l	0.27	0/213	0.46	0/291
4	m	0.26	0/213	0.47	0/291
5	V	0.32	0/3234	0.47	0/4444
5	W	0.33	0/3234	0.48	0/4444
5	X	0.32	0/3234	0.47	0/4444
5	a	0.33	0/3234	0.48	0/4444
5	b	0.32	0/3234	0.47	0/4444
5	d	0.33	0/3234	0.48	0/4444
5	e	0.32	0/3234	0.47	0/4444
5	g	0.32	0/3234	0.48	0/4444
5	h	0.32	0/3234	0.47	0/4444
5	n	0.33	0/3234	0.48	0/4444
6	Y	0.31	0/10233	0.51	0/14057
6	Z	0.31	0/10233	0.51	0/14057
6	c	0.31	0/10233	0.51	0/14057
6	f	0.31	0/10233	0.51	0/14057
6	i	0.31	0/10233	0.51	0/14057

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	a1	0.16	0/1218	0.73	0/1890
7	b1	0.17	0/1218	0.77	0/1890
8	a2	0.17	0/1406	0.77	0/2182
8	b2	0.16	0/1406	0.73	0/2182
9	a3	0.16	0/936	0.73	0/1452
9	b3	0.17	0/936	0.77	0/1452
10	a4	0.18	0/419	0.76	0/649
10	b4	0.16	0/419	0.72	0/649
11	a5	0.16	0/889	0.73	0/1379
11	b5	0.17	0/889	0.76	0/1379
12	a6	0.16	0/701	0.72	0/1087
12	b6	0.17	0/701	0.76	0/1087
All	All	0.31	0/200040	0.51	0/276407

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 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	1271/1273 (100%)	1212 (95%)	59 (5%)	0	100	100
2	B	716/718 (100%)	688 (96%)	28 (4%)	0	100	100
3	C	1073/1138 (94%)	1026 (96%)	47 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1136/1138 (100%)	1097 (97%)	39 (3%)	0	100	100
3	E	1104/1138 (97%)	1064 (96%)	40 (4%)	0	100	100
3	F	1136/1138 (100%)	1094 (96%)	42 (4%)	0	100	100
3	G	1096/1138 (96%)	1056 (96%)	40 (4%)	0	100	100
3	H	1128/1138 (99%)	1070 (95%)	58 (5%)	0	100	100
3	I	1061/1138 (93%)	1022 (96%)	39 (4%)	0	100	100
3	J	1128/1138 (99%)	1075 (95%)	53 (5%)	0	100	100
3	K	1096/1138 (96%)	1047 (96%)	49 (4%)	0	100	100
3	L	1136/1138 (100%)	1083 (95%)	53 (5%)	0	100	100
4	M	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
4	N	28/94 (30%)	28 (100%)	0	0	100	100
4	k	28/94 (30%)	26 (93%)	2 (7%)	0	100	100
4	l	28/94 (30%)	27 (96%)	1 (4%)	0	100	100
4	m	28/94 (30%)	27 (96%)	1 (4%)	0	100	100
5	V	409/411 (100%)	401 (98%)	8 (2%)	0	100	100
5	W	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
5	X	409/411 (100%)	403 (98%)	6 (2%)	0	100	100
5	a	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
5	b	409/411 (100%)	402 (98%)	7 (2%)	0	100	100
5	d	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
5	e	409/411 (100%)	403 (98%)	6 (2%)	0	100	100
5	g	409/411 (100%)	397 (97%)	12 (3%)	0	100	100
5	h	409/411 (100%)	401 (98%)	8 (2%)	0	100	100
5	n	409/411 (100%)	397 (97%)	12 (3%)	0	100	100
6	Y	1295/1297 (100%)	1254 (97%)	41 (3%)	0	100	100
6	Z	1295/1297 (100%)	1255 (97%)	40 (3%)	0	100	100
6	c	1295/1297 (100%)	1255 (97%)	40 (3%)	0	100	100
6	f	1295/1297 (100%)	1253 (97%)	42 (3%)	0	100	100
6	i	1295/1297 (100%)	1255 (97%)	39 (3%)	1 (0%)	51	81
All	All	23850/24436 (98%)	23009 (96%)	840 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	i	1291	ALA

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 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	1092/1092 (100%)	1085 (99%)	7 (1%)	86	91
2	B	619/619 (100%)	615 (99%)	4 (1%)	86	91
3	C	917/972 (94%)	913 (100%)	4 (0%)	91	95
3	D	972/972 (100%)	967 (100%)	5 (0%)	88	93
3	E	946/972 (97%)	938 (99%)	8 (1%)	81	89
3	F	972/972 (100%)	961 (99%)	11 (1%)	73	85
3	G	938/972 (96%)	933 (100%)	5 (0%)	88	93
3	H	964/972 (99%)	954 (99%)	10 (1%)	76	86
3	I	910/972 (94%)	905 (100%)	5 (0%)	88	93
3	J	964/972 (99%)	958 (99%)	6 (1%)	86	91
3	K	938/972 (96%)	930 (99%)	8 (1%)	78	87
3	L	972/972 (100%)	963 (99%)	9 (1%)	78	87
4	M	73/73 (100%)	71 (97%)	2 (3%)	44	71
4	N	24/73 (33%)	24 (100%)	0	100	100
4	k	24/73 (33%)	24 (100%)	0	100	100
4	l	24/73 (33%)	24 (100%)	0	100	100
4	m	24/73 (33%)	24 (100%)	0	100	100
5	V	325/325 (100%)	322 (99%)	3 (1%)	78	87
5	W	325/325 (100%)	323 (99%)	2 (1%)	86	91
5	X	325/325 (100%)	322 (99%)	3 (1%)	78	87
5	a	325/325 (100%)	322 (99%)	3 (1%)	78	87
5	b	325/325 (100%)	324 (100%)	1 (0%)	92	96
5	d	325/325 (100%)	323 (99%)	2 (1%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	325/325 (100%)	323 (99%)	2 (1%)	86	91
5	g	325/325 (100%)	322 (99%)	3 (1%)	78	87
5	h	325/325 (100%)	322 (99%)	3 (1%)	78	87
5	n	325/325 (100%)	323 (99%)	2 (1%)	86	91
6	Y	1089/1089 (100%)	1077 (99%)	12 (1%)	73	85
6	Z	1089/1089 (100%)	1081 (99%)	8 (1%)	84	90
6	c	1089/1089 (100%)	1082 (99%)	7 (1%)	86	91
6	f	1089/1089 (100%)	1081 (99%)	8 (1%)	84	90
6	i	1089/1089 (100%)	1079 (99%)	10 (1%)	78	87
All	All	20068/20491 (98%)	19915 (99%)	153 (1%)	82	89

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	TRP
1	A	89	ASP
1	A	486	TYR
1	A	561	LEU
1	A	738	GLN
1	A	777	TYR
1	A	780	ASP
2	B	121	TYR
2	B	179	TYR
2	B	181	ASP
2	B	624	ASP
3	C	429	ASN
3	C	886	ASP
3	C	1012	ARG
3	C	1169	TRP
3	D	152	MET
3	D	206	LEU
3	D	439	THR
3	D	835	HIS
3	D	1169	TRP
3	E	125	ARG
3	E	178	HIS
3	E	209	ASN
3	E	483	VAL
3	E	829	THR

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Mol	Chain	Res	Type
3	E	1050	ASP
3	E	1132	ARG
3	E	1203	THR
3	F	105	SER
3	F	106	MET
3	F	143	ASP
3	F	232	THR
3	F	523	ASN
3	F	740	LYS
3	F	801	ARG
3	F	835	HIS
3	F	926	TYR
3	F	930	ARG
3	F	1012	ARG
3	G	209	ASN
3	G	552	ASP
3	G	1012	ARG
3	G	1132	ARG
3	G	1203	THR
3	H	137	ARG
3	H	150	THR
3	H	193	LEU
3	H	740	LYS
3	H	835	HIS
3	H	926	TYR
3	H	930	ARG
3	H	1012	ARG
3	H	1050	ASP
3	H	1091	GLN
3	I	316	THR
3	I	1012	ARG
3	I	1047	TYR
3	I	1203	THR
3	I	1211	ARG
3	J	232	THR
3	J	322	THR
3	J	483	VAL
3	J	617	HIS
3	J	835	HIS
3	J	958	HIS
3	K	168	ARG
3	K	518	LEU

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Mol	Chain	Res	Type
3	K	519	GLN
3	K	1012	ARG
3	K	1047	TYR
3	K	1169	TRP
3	K	1205	ASP
3	K	1211	ARG
3	L	77	ASP
3	L	123	ASN
3	L	193	LEU
3	L	257	ARG
3	L	635	GLN
3	L	801	ARG
3	L	930	ARG
3	L	981	ASN
3	L	1091	GLN
4	M	85	ASP
4	M	94	THR
5	V	35	ARG
5	V	158	HIS
5	V	255	ARG
5	W	11	TYR
5	W	255	ARG
5	X	35	ARG
5	X	44	LEU
5	X	255	ARG
6	Y	71	HIS
6	Y	243	GLN
6	Y	711	ASP
6	Y	929	MET
6	Y	932	GLN
6	Y	955	VAL
6	Y	963	ARG
6	Y	1204	LEU
6	Y	1209	ASP
6	Y	1225	ASP
6	Y	1283	GLN
6	Y	1296	TYR
6	Z	164	VAL
6	Z	243	GLN
6	Z	410	THR
6	Z	439	SER
6	Z	676	ARG

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Mol	Chain	Res	Type
6	Z	711	ASP
6	Z	929	MET
6	Z	1296	TYR
5	a	11	TYR
5	a	252	ASP
5	a	255	ARG
5	b	255	ARG
6	c	243	GLN
6	c	658	VAL
6	c	711	ASP
6	c	929	MET
6	c	1205	LEU
6	c	1283	GLN
6	c	1296	TYR
5	d	11	TYR
5	d	255	ARG
5	e	245	GLN
5	e	255	ARG
6	f	71	HIS
6	f	243	GLN
6	f	610	THR
6	f	711	ASP
6	f	929	MET
6	f	1225	ASP
6	f	1283	GLN
6	f	1296	TYR
5	g	11	TYR
5	g	38	THR
5	g	255	ARG
5	h	158	HIS
5	h	195	GLN
5	h	255	ARG
6	i	71	HIS
6	i	197	HIS
6	i	243	GLN
6	i	309	ASN
6	i	711	ASP
6	i	929	MET
6	i	1225	ASP
6	i	1261	THR
6	i	1283	GLN
6	i	1296	TYR

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Mol	Chain	Res	Type
5	n	11	TYR
5	n	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1206	HIS
3	D	209	ASN
3	F	104	GLN
3	F	906	ASN
3	G	748	GLN
3	I	287	GLN
3	J	353	GLN
3	J	580	HIS
3	J	962	GLN
3	K	748	GLN
3	L	135	HIS
3	L	140	HIS
3	L	1091	GLN
5	X	273	HIS
6	Y	630	GLN
6	Z	685	ASN
5	a	338	HIS
5	b	158	HIS
6	f	630	GLN
5	g	158	HIS
6	i	309	ASN
6	i	1151	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	a4	17/18 (94%)	0	0
10	b4	17/18 (94%)	0	0
11	a5	37/38 (97%)	0	0
11	b5	37/38 (97%)	0	0
12	a6	29/30 (96%)	0	0
12	b6	29/30 (96%)	0	0
7	a1	51/52 (98%)	0	0
7	b1	51/52 (98%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	a2	59/60 (98%)	0	0
8	b2	59/60 (98%)	0	0
9	a3	39/40 (97%)	0	0
9	b3	39/40 (97%)	0	0
All	All	464/476 (97%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 [i](#)

Of 4 ligands modelled in this entry, 4 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 Map visualisation

This section contains visualisations of the EMDB entry EMD-29243. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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.