Full wwPDB EM Validation Report ⓘ

Jul 1, 2023 – 02:03 PM EDT

PDB ID	:	8FJL
EMDB ID	:	EMD-29244
Title	:	Golden Shiner Reovirus Core Tropical Vertex
Authors	:	Stevens, A.S.; Zhou, Z.H.
Deposited on	:	2022-12-19
Resolution	:	3.27 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:

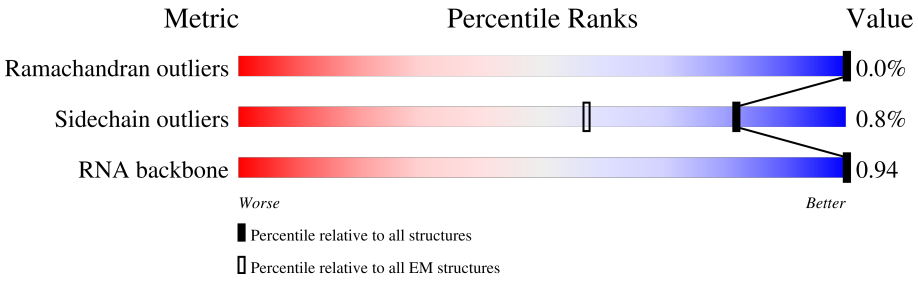
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.27 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 <=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	a5	28	100%
5	b5	28	100%
6	a6	38	100%
6	b6	38	100%
7	a1	52	100%
7	b1	52	100%
8	a3	40	100%
8	b3	40	100%
9	V	411	99%
9	W	411	100%
9	X	411	99%
9	a	411	99%
9	b	411	100%
9	d	411	100%
9	e	411	100%
9	g	411	99%
9	h	411	99%

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Mol	Chain	Length	Quality of chain
9	n	411	100%
10	Y	1297	99%
10	Z	1297	99%
10	c	1297	99%
10	f	1297	99%
10	i	1297	99%
11	a2	60	100%
11	b2	60	100%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 197669 atoms, of which 4598 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
1	A	1273	Total	C	N	O	S	0	0
			9978	6375	1736	1822	45		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1075	Total	C	N	O	S	0	0
			8300	5296	1421	1534	49		
3	D	1138	Total	C	N	O	S	0	0
			8761	5578	1502	1628	53		
3	E	1106	Total	C	N	O	S	0	0
			8534	5440	1463	1579	52		
3	F	1138	Total	C	N	O	S	0	0
			8761	5578	1502	1628	53		
3	G	1098	Total	C	N	O	S	0	0
			8477	5403	1454	1568	52		
3	H	1130	Total	C	N	O	S	0	0
			8699	5540	1491	1615	53		
3	I	1065	Total	C	N	O	S	0	0
			8226	5244	1412	1519	51		
3	J	1130	Total	C	N	O	S	0	0
			8696	5537	1491	1615	53		
3	K	1098	Total	C	N	O	S	0	0
			8477	5403	1454	1568	52		
3	L	1138	Total	C	N	O	S	0	0
			8761	5578	1502	1628	53		

- 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 RNA chain called RNA (38-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	a5	28	Total	C	H	N	O	P	0	0
			881	266	296	98	194	27		
5	b5	28	Total	C	H	N	O	P	0	0
			881	266	296	98	194	27		

- Molecule 6 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	b6	38	Total	C	H	N	O	P	0	0
			1196	361	401	133	264	37		
6	a6	38	Total	C	H	N	O	P	0	0
			1196	361	401	133	264	37		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	a1	52	Total	C	H	N	O	P	0	0
			1637	494	548	182	362	51		
7	b1	52	Total	C	H	N	O	P	0	0
			1637	494	548	182	362	51		

- Molecule 8 is a RNA chain called RNA (39-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	a3	40	Total	C	H	N	O	P	0	0
			1259	380	422	140	278	39		
8	b3	40	Total	C	H	N	O	P	0	0
			1259	380	422	140	278	39		

- Molecule 9 is a protein called Clamp protein VP6.

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

- Molecule 10 is a protein called Outer capsid protein VP1.

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

- Molecule 11 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
11	a2	60	Total	C	H	N	O	P	0	0
			1889	570	632	210	418	59		
11	b2	60	Total	C	H	N	O	P	0	0
			1889	570	632	210	418	59		

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

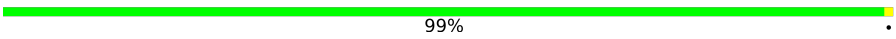
Mol	Chain	Residues	Atoms	AltConf
12	E	1	Total Zn 1 1	0
12	G	1	Total Zn 1 1	0
12	I	1	Total Zn 1 1	0
12	K	1	Total Zn 1 1	0

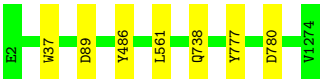
3 Residue-property plots (i)

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. 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

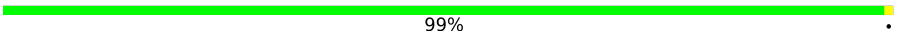
Chain A:





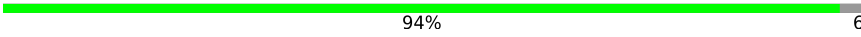
- Molecule 2: Microtubule-associated protein VP5

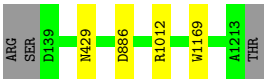
Chain B:



- Molecule 3: Major inner capsid protein VP3

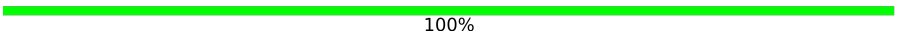
Chain C:

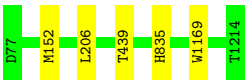




- Molecule 3: Major inner capsid protein VP3

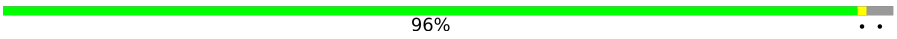
Chain D:





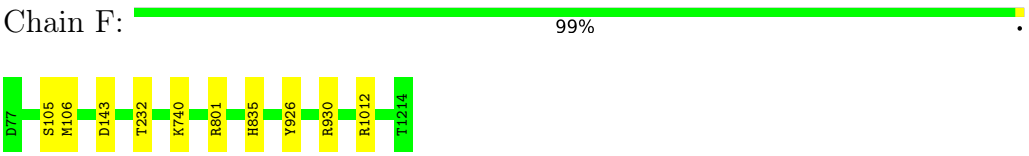
- Molecule 3: Major inner capsid protein VP3

Chain E:



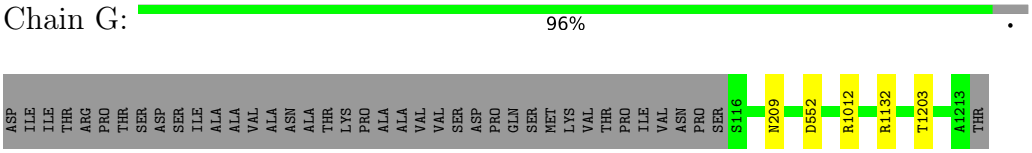
- Molecule 3: Major inner capsid protein VP3

Chain F:



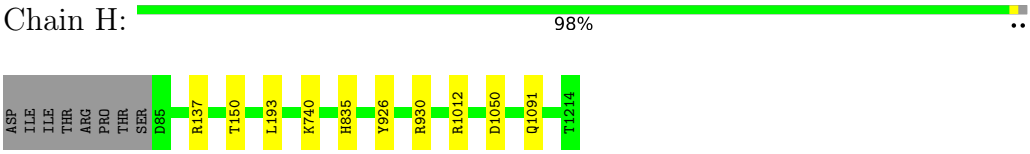
• Molecule 3: Major inner capsid protein VP3

Chain G:



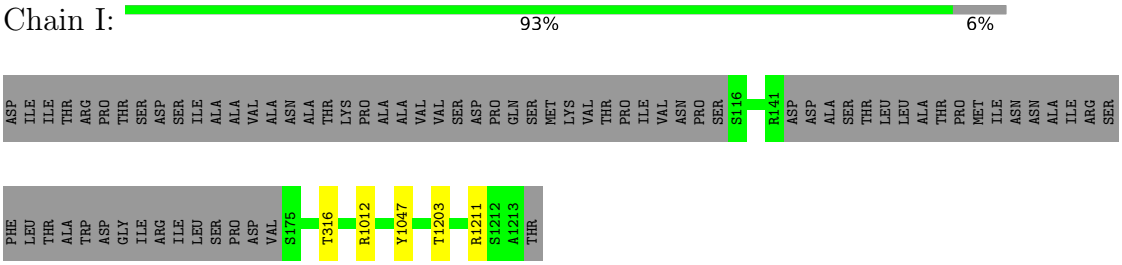
• Molecule 3: Major inner capsid protein VP3

Chain H:



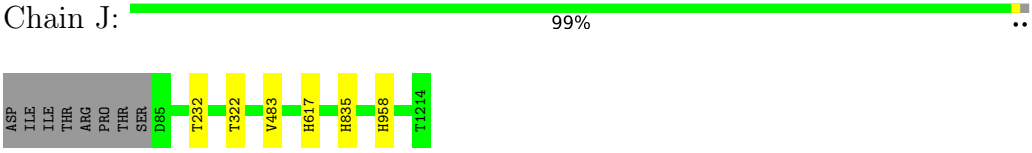
• Molecule 3: Major inner capsid protein VP3

Chain I:



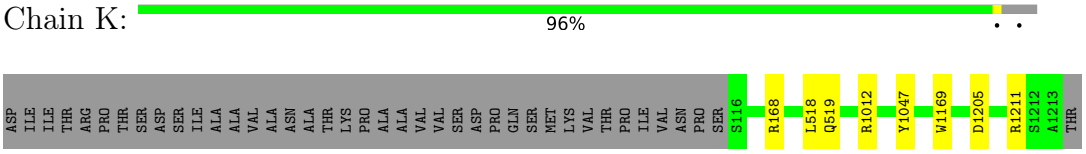
• Molecule 3: Major inner capsid protein VP3

Chain J:



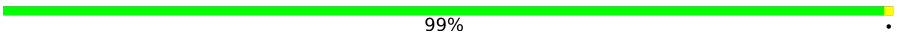
• Molecule 3: Major inner capsid protein VP3

Chain K:



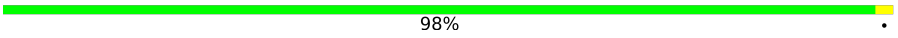
• Molecule 3: Major inner capsid protein VP3

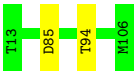
Chain L:



• Molecule 4: Major inner capsid protein VP3

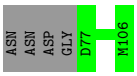
Chain M:





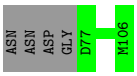
• Molecule 4: Major inner capsid protein VP3

Chain N:



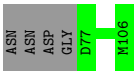
• Molecule 4: Major inner capsid protein VP3

Chain k:



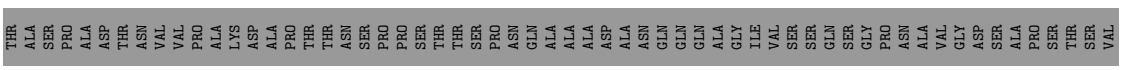
• Molecule 4: Major inner capsid protein VP3

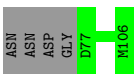
Chain l:



• Molecule 4: Major inner capsid protein VP3

Chain m:





• Molecule 5: RNA (38-MER)

Chain a5: 100%

There are no outlier residues recorded for this chain.

• Molecule 5: RNA (38-MER)

Chain b5: 100%

There are no outlier residues recorded for this chain.

• Molecule 6: RNA (30-MER)

Chain b6: 100%

There are no outlier residues recorded for this chain.

• Molecule 6: RNA (30-MER)

Chain a6: 100%

There are no outlier residues recorded for this chain.

• 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 (39-MER)

Chain a3: 100%

There are no outlier residues recorded for this chain.

• Molecule 8: RNA (39-MER)

Chain b3: 100%

There are no outlier residues recorded for this chain.

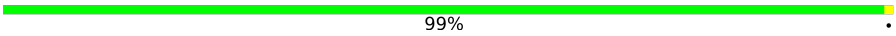
• Molecule 9: Clamp protein VP6

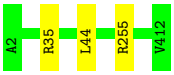
Chain V: 99%

• Molecule 9: Clamp protein VP6

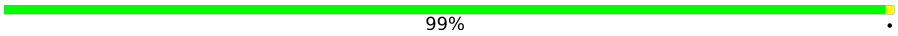
Chain W: 

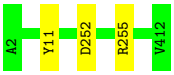
• Molecule 9: Clamp protein VP6

Chain X: 

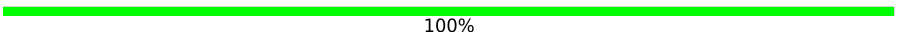


• Molecule 9: Clamp protein VP6

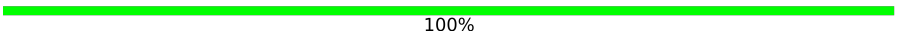
Chain a: 



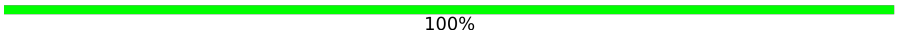
• Molecule 9: Clamp protein VP6

Chain b: 

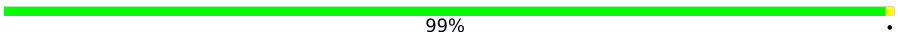
• Molecule 9: Clamp protein VP6

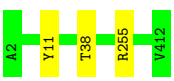
Chain d: 

• Molecule 9: Clamp protein VP6

Chain e: 

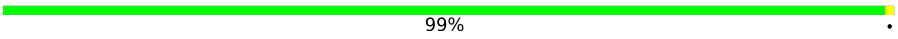
• Molecule 9: Clamp protein VP6

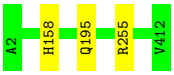
Chain g: 



• Molecule 9: Clamp protein VP6

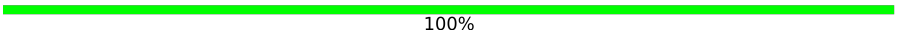
Chain h:





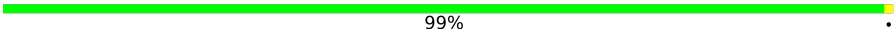
• Molecule 9: Clamp protein VP6

Chain n:



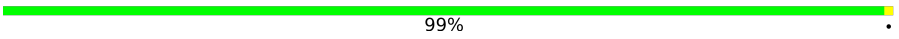
• Molecule 10: Outer capsid protein VP1

Chain Y:



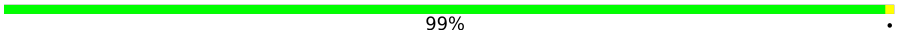
• Molecule 10: Outer capsid protein VP1

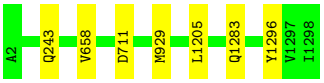
Chain Z:



• Molecule 10: Outer capsid protein VP1

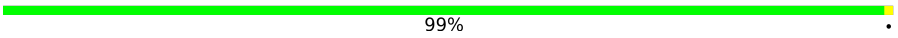
Chain c:





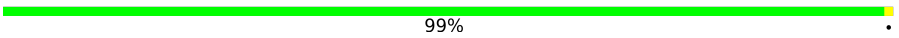
• Molecule 10: Outer capsid protein VP1

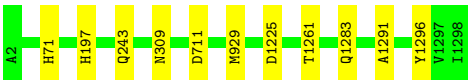
Chain f:



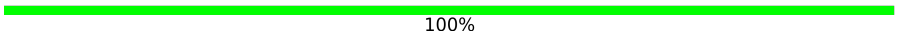
• Molecule 10: Outer capsid protein VP1

Chain i:



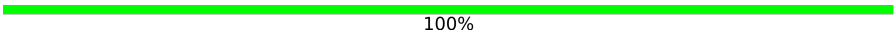


• Molecule 11: RNA (60-MER)

Chain a2: 

There are no outlier residues recorded for this chain.

• Molecule 11: RNA (60-MER)

Chain b2: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99323	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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.32	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	0/8919	0.49	0/12225
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	a5	0.15	0/654	0.73	0/1014
5	b5	0.10	0/654	0.67	0/1014
6	a6	0.10	0/889	0.68	0/1379
6	b6	0.17	0/889	0.74	0/1379
7	a1	0.16	0/1218	0.73	0/1890
7	b1	0.10	0/1218	0.68	0/1890
8	a3	0.16	0/936	0.73	0/1452
8	b3	0.10	0/936	0.68	0/1452
9	V	0.32	0/3234	0.47	0/4444
9	W	0.33	0/3234	0.48	0/4444
9	X	0.32	0/3234	0.47	0/4444
9	a	0.33	0/3234	0.48	0/4444
9	b	0.32	0/3234	0.47	0/4444
9	d	0.33	0/3234	0.48	0/4444
9	e	0.32	0/3234	0.47	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
9	g	0.32	0/3234	0.48	0/4444
9	h	0.32	0/3234	0.47	0/4444
9	n	0.33	0/3234	0.48	0/4444
10	Y	0.31	0/10233	0.51	0/14057
10	Z	0.31	0/10233	0.51	0/14057
10	c	0.31	0/10233	0.51	0/14057
10	f	0.31	0/10233	0.51	0/14057
10	i	0.31	0/10233	0.51	0/14057
11	a2	0.16	0/1406	0.74	0/2182
11	b2	0.10	0/1406	0.68	0/2182
All	All	0.31	0/199105	0.51	0/274959

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

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

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	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
3	D	1136/1138 (100%)	1097 (97%)	39 (3%)	0	100	100
3	E	1104/1138 (97%)	1064 (96%)	40 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
9	V	409/411 (100%)	401 (98%)	8 (2%)	0	100	100
9	W	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
9	X	409/411 (100%)	403 (98%)	6 (2%)	0	100	100
9	a	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
9	b	409/411 (100%)	402 (98%)	7 (2%)	0	100	100
9	d	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
9	e	409/411 (100%)	403 (98%)	6 (2%)	0	100	100
9	g	409/411 (100%)	397 (97%)	12 (3%)	0	100	100
9	h	409/411 (100%)	401 (98%)	8 (2%)	0	100	100
9	n	409/411 (100%)	397 (97%)	12 (3%)	0	100	100
10	Y	1295/1297 (100%)	1254 (97%)	41 (3%)	0	100	100
10	Z	1295/1297 (100%)	1255 (97%)	40 (3%)	0	100	100
10	c	1295/1297 (100%)	1255 (97%)	40 (3%)	0	100	100
10	f	1295/1297 (100%)	1253 (97%)	42 (3%)	0	100	100
10	i	1295/1297 (100%)	1255 (97%)	39 (3%)	1 (0%)	51	82
All	All	23850/24436 (98%)	23009 (96%)	840 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	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%)	962 (99%)	10 (1%)	76	85
3	G	938/972 (96%)	933 (100%)	5 (0%)	88	93
3	H	964/972 (99%)	954 (99%)	10 (1%)	76	85
3	I	910/972 (94%)	905 (100%)	5 (0%)	88	93
3	J	963/972 (99%)	957 (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
9	V	325/325 (100%)	322 (99%)	3 (1%)	78	87
9	W	325/325 (100%)	323 (99%)	2 (1%)	86	91
9	X	325/325 (100%)	322 (99%)	3 (1%)	78	87
9	a	325/325 (100%)	322 (99%)	3 (1%)	78	87
9	b	325/325 (100%)	324 (100%)	1 (0%)	92	96
9	d	325/325 (100%)	323 (99%)	2 (1%)	86	91
9	e	325/325 (100%)	323 (99%)	2 (1%)	86	91
9	g	325/325 (100%)	322 (99%)	3 (1%)	78	87
9	h	325/325 (100%)	322 (99%)	3 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	n	325/325 (100%)	323 (99%)	2 (1%)	86 91
10	Y	1089/1089 (100%)	1077 (99%)	12 (1%)	73 85
10	Z	1089/1089 (100%)	1081 (99%)	8 (1%)	84 90
10	c	1089/1089 (100%)	1082 (99%)	7 (1%)	86 91
10	f	1089/1089 (100%)	1081 (99%)	8 (1%)	84 90
10	i	1089/1089 (100%)	1079 (99%)	10 (1%)	78 87
All	All	20067/20491 (98%)	19915 (99%)	152 (1%)	82 89

All (152) 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
3	E	1050	ASP
3	E	1132	ARG
3	E	1203	THR
3	F	105	SER

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Mol	Chain	Res	Type
3	F	106	MET
3	F	143	ASP
3	F	232	THR
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
3	K	519	GLN
3	K	1012	ARG
3	K	1047	TYR
3	K	1169	TRP
3	K	1205	ASP

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Mol	Chain	Res	Type
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
9	V	35	ARG
9	V	158	HIS
9	V	255	ARG
9	W	11	TYR
9	W	255	ARG
9	X	35	ARG
9	X	44	LEU
9	X	255	ARG
10	Y	71	HIS
10	Y	243	GLN
10	Y	711	ASP
10	Y	929	MET
10	Y	932	GLN
10	Y	955	VAL
10	Y	963	ARG
10	Y	1204	LEU
10	Y	1209	ASP
10	Y	1225	ASP
10	Y	1283	GLN
10	Y	1296	TYR
10	Z	164	VAL
10	Z	243	GLN
10	Z	410	THR
10	Z	439	SER
10	Z	676	ARG
10	Z	711	ASP
10	Z	929	MET
10	Z	1296	TYR
9	a	11	TYR
9	a	252	ASP

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1206	HIS
3	D	209	ASN
3	F	104	GLN
3	F	523	ASN
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
9	X	273	HIS
10	Y	630	GLN
10	Z	685	ASN
9	a	338	HIS
9	b	158	HIS
10	f	630	GLN
9	g	158	HIS
10	i	309	ASN
10	i	1151	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	a2	59/60 (98%)	0	0
11	b2	59/60 (98%)	0	0
5	a5	27/28 (96%)	0	0
5	b5	27/28 (96%)	0	0
6	a6	37/38 (97%)	0	0
6	b6	37/38 (97%)	0	0
7	a1	51/52 (98%)	0	0
7	b1	51/52 (98%)	0	0
8	a3	39/40 (97%)	0	0
8	b3	39/40 (97%)	0	0
All	All	426/436 (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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29244. 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.