wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:46 PM BST

PDB ID	:	3J9X
EMDB ID:	:	EMD-6310
Title	:	A Virus that Infects a Hyperthermophile Encapsidates A-Form DNA
Authors	:	DiMaio, F.; Yu, X.; Rensen, E.; Krupovic, M.; Prangishvili, D.; Egelman, E.
Deposited on	:	2015-03-21
Resolution	:	3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

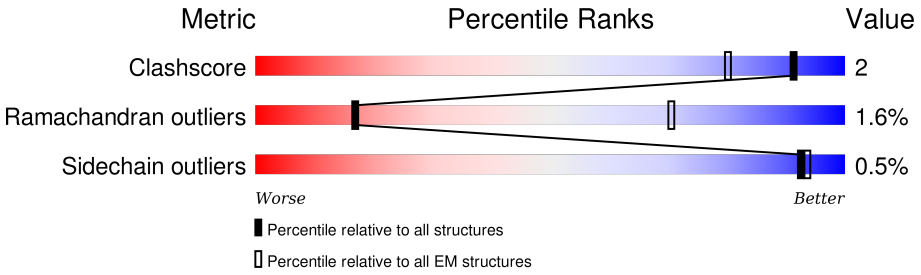
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	1	128	92% 7% •
1	2	128	91% 7% •
1	3	128	91% 9% •
1	4	128	91% 7% •
1	5	128	91% 9% •
1	6	128	91% 7% •
1	A	128	91% 9% •
1	B	128	90% 9% •
1	C	128	92% 7% •

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Mol	Chain	Length	Quality of chain
1	D	128	91% 7% •
1	E	128	90% 9% •
1	F	128	91% 8% •
1	G	128	90% 9% •
1	H	128	91% 8% •
1	I	128	91% 8% •
1	J	128	91% 7% •
1	K	128	89% 10% •
1	L	128	91% 7% •
1	M	128	90% 9% •
1	N	128	91% 8% •
1	O	128	91% 8% •
1	P	128	89% 9% •
1	Q	128	90% 9% •
1	R	128	90% 9% •
1	S	128	90% 9% •
1	T	128	91% 7% •
1	U	128	90% 9% •
1	V	128	91% 7% •
1	W	128	90% 9% •
1	X	128	91% 7% •
1	Y	128	90% 9% •
1	Z	128	91% 7% •
1	a	128	98% •
1	b	128	98% •

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Mol	Chain	Length	Quality of chain
1	c	128	98%
1	d	128	98%
1	e	128	98%
1	f	128	98%
1	g	128	98%
1	h	128	98%
1	i	128	98%
1	j	128	98%
1	k	128	98%
1	l	128	98%
1	m	128	98%
1	n	128	98%
1	o	128	98%
1	p	128	98%
1	q	128	98%
1	r	128	98%
1	s	128	98%
1	t	128	98%
1	u	128	98%
1	v	128	98%
1	w	128	98%
1	x	128	98%
1	y	128	98%
1	z	128	98%
2	7	348	100%

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Mol	Chain	Length	Quality of chain
2	8	348	92% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 70702 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 coat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	B	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	C	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	D	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	E	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	F	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	G	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	H	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	I	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	J	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	K	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	L	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	M	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	N	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	O	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	P	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	Q	128	Total	C	N	O	S	0	0
			973	618	171	183	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	S	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	T	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	U	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	V	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	W	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	X	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	Y	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	Z	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	a	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	b	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	c	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	d	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	e	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	f	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	g	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	h	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	i	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	j	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	k	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	l	128	Total	C	N	O	S	0	0
			973	618	171	183	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	n	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	o	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	p	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	q	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	r	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	s	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	t	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	u	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	v	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	w	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	x	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	y	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	z	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	1	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	2	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	3	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	4	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	5	128	Total	C	N	O	S	0	0
			973	618	171	183	1		
1	6	128	Total	C	N	O	S	0	0
			973	618	171	183	1		

- Molecule 2 is a DNA chain called DNA.

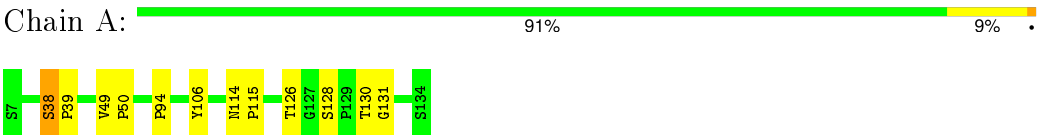
Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	348	Total 7134	C 3480	N 1218	O 2088	P 348	0	0
2	8	348	Total 7134	C 3480	N 1218	O 2088	P 348	0	0

3 Residue-property plots (i)

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. 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.

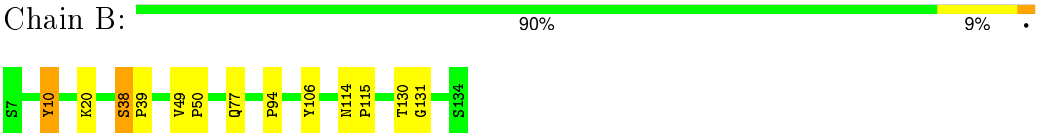
- Molecule 1: coat protein

Chain A:



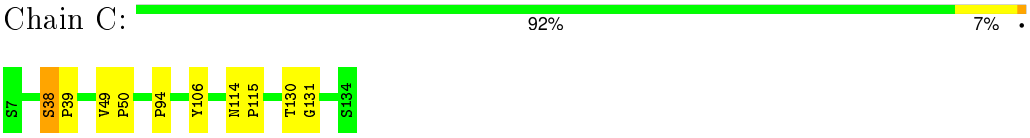
- Molecule 1: coat protein

Chain B:



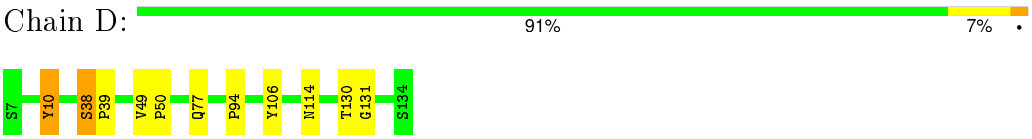
- Molecule 1: coat protein

Chain C:



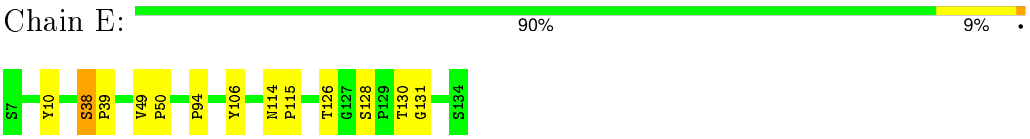
- Molecule 1: coat protein

Chain D:



- Molecule 1: coat protein

Chain E:



- Molecule 1: coat protein

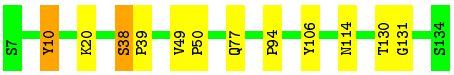
Chain F:

• Molecule 1: coat protein

Chain G:

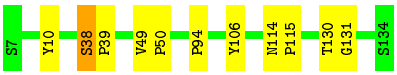
• Molecule 1: coat protein

Chain H:



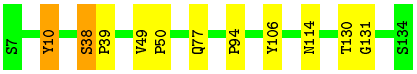
• Molecule 1: coat protein

Chain I:



• Molecule 1: coat protein

Chain J:

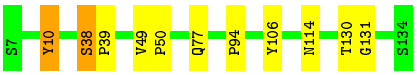


• Molecule 1: coat protein

Chain K:

• Molecule 1: coat protein

Chain L:

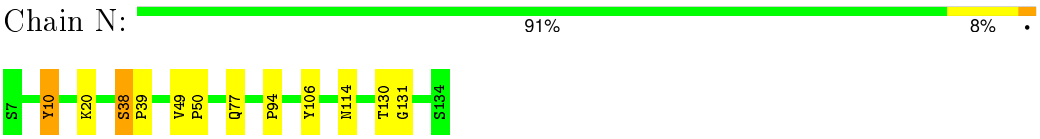


• Molecule 1: coat protein

Chain M:

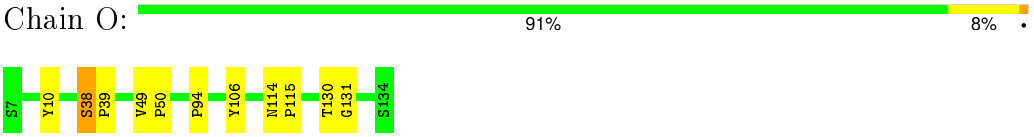
• Molecule 1: coat protein

Chain N:



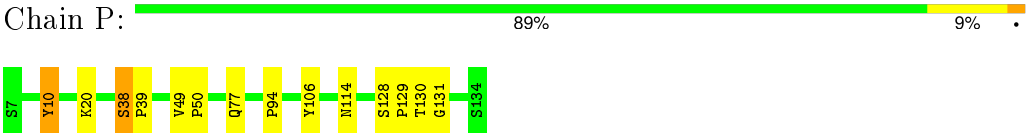
• Molecule 1: coat protein

Chain O:



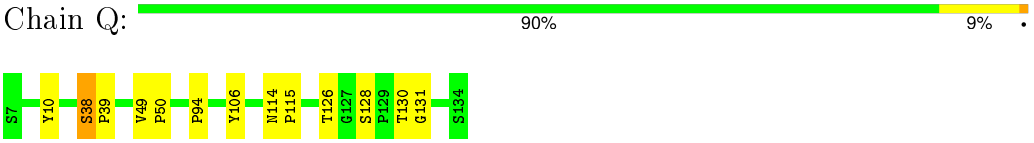
• Molecule 1: coat protein

Chain P:



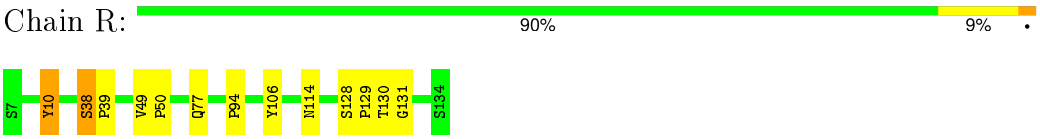
• Molecule 1: coat protein

Chain Q:



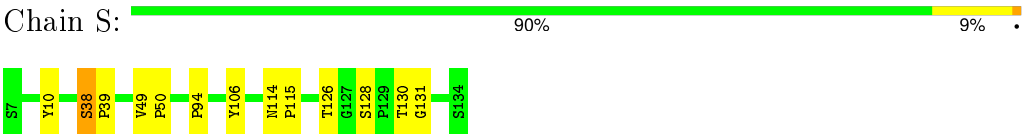
• Molecule 1: coat protein

Chain R:



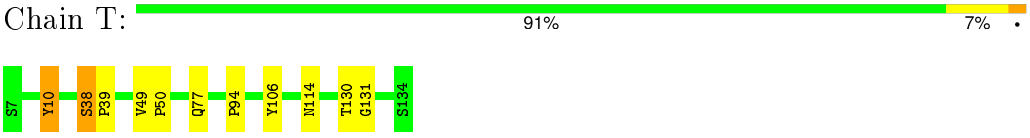
• Molecule 1: coat protein

Chain S:



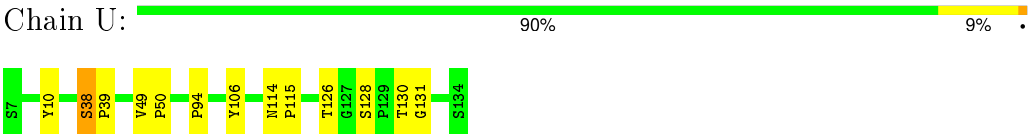
• Molecule 1: coat protein

Chain T:



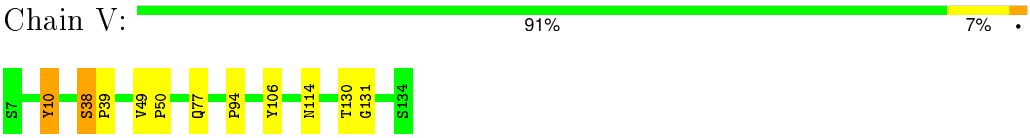
• Molecule 1: coat protein

Chain U:



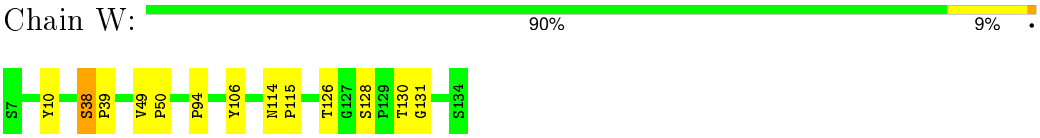
- Molecule 1: coat protein

Chain V:



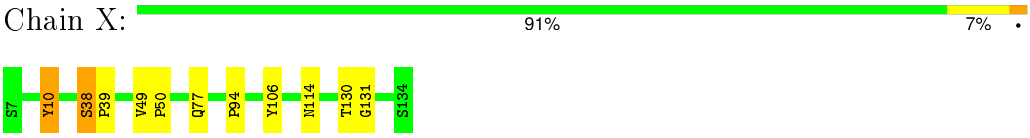
- Molecule 1: coat protein

Chain W:



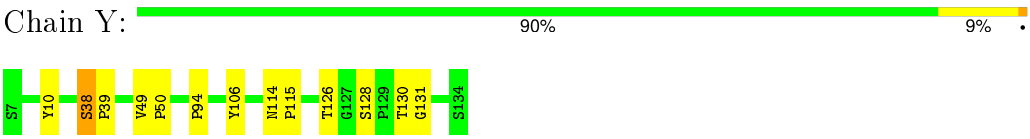
- Molecule 1: coat protein

Chain X:



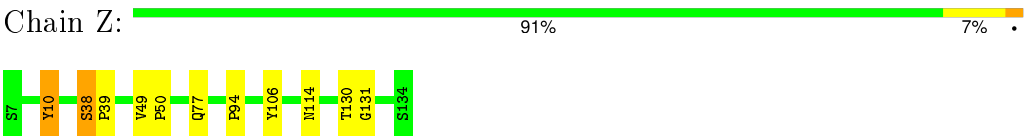
- Molecule 1: coat protein

Chain Y:



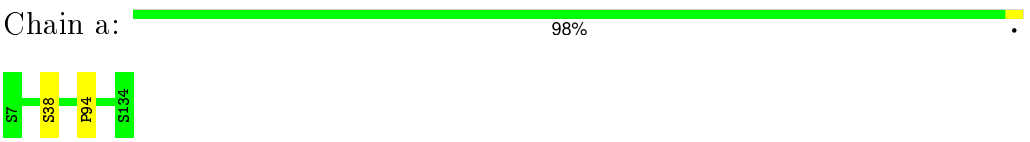
- Molecule 1: coat protein

Chain Z:



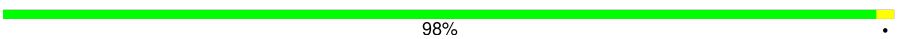
- Molecule 1: coat protein

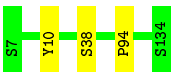
Chain a:



- Molecule 1: coat protein

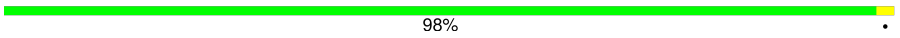
Chain b:

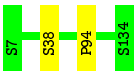




• Molecule 1: coat protein

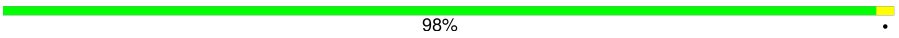
Chain c:

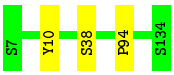




• Molecule 1: coat protein

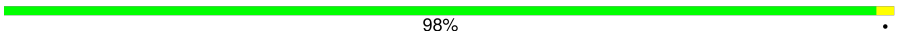
Chain d:

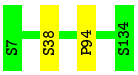




• Molecule 1: coat protein

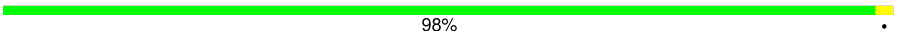
Chain e:

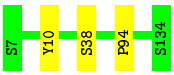




• Molecule 1: coat protein

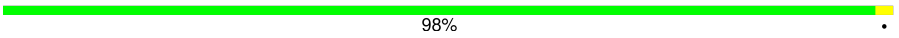
Chain f:

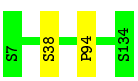




• Molecule 1: coat protein

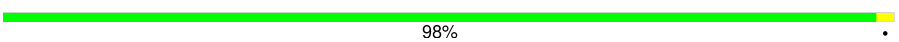
Chain g:

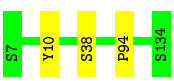




• Molecule 1: coat protein

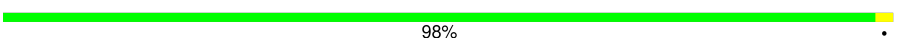
Chain h:

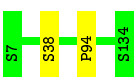




• Molecule 1: coat protein

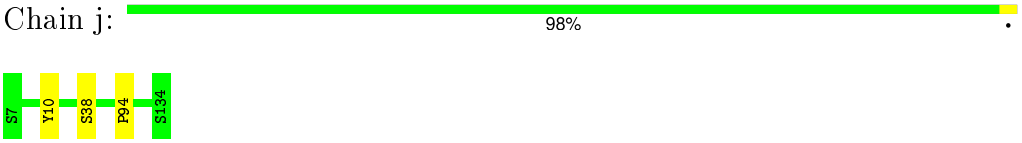
Chain i:





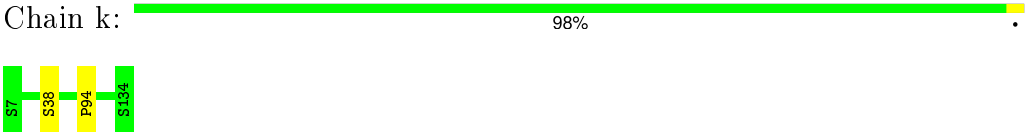
- Molecule 1: coat protein

Chain j:



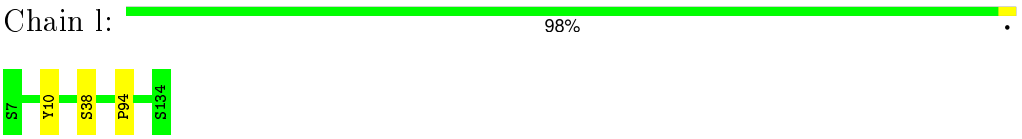
- Molecule 1: coat protein

Chain k:



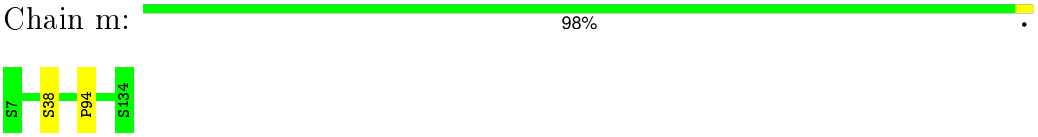
- Molecule 1: coat protein

Chain l:



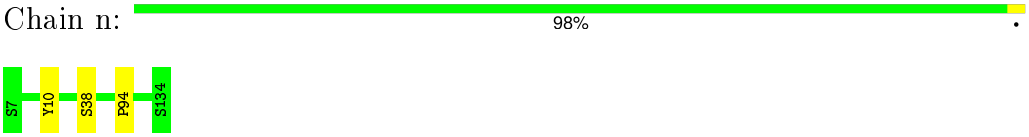
- Molecule 1: coat protein

Chain m:



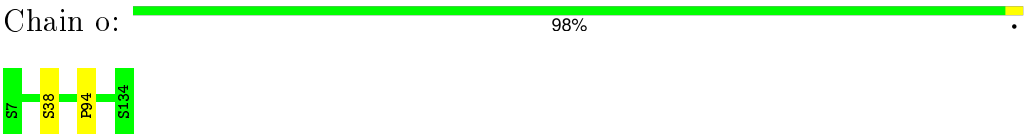
- Molecule 1: coat protein

Chain n:



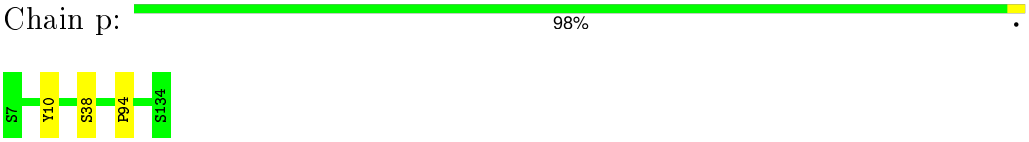
- Molecule 1: coat protein

Chain o:



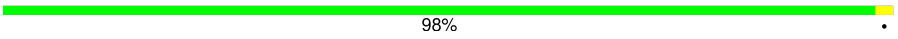
- Molecule 1: coat protein

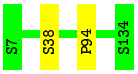
Chain p:



- Molecule 1: coat protein

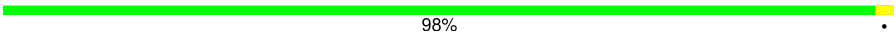
Chain q:

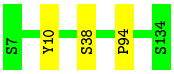




- Molecule 1: coat protein

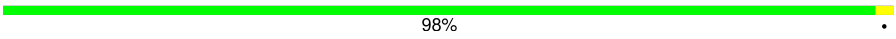
Chain r:





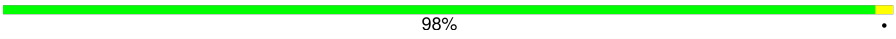
- Molecule 1: coat protein

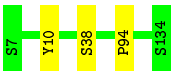
Chain s:



- Molecule 1: coat protein

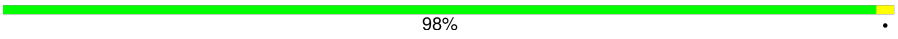
Chain t:

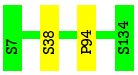




- Molecule 1: coat protein

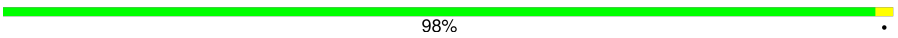
Chain u:

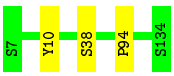




- Molecule 1: coat protein

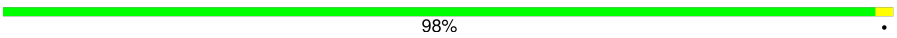
Chain v:

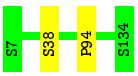




- Molecule 1: coat protein

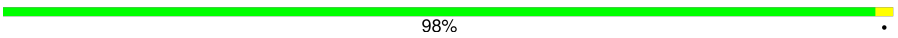
Chain w:

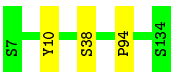




- Molecule 1: coat protein

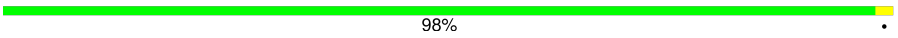
Chain x:





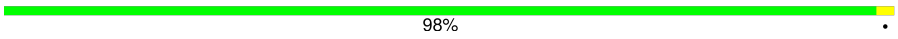
- Molecule 1: coat protein

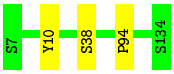
Chain y:



- Molecule 1: coat protein

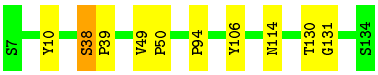
Chain z:





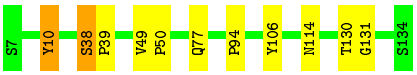
- Molecule 1: coat protein

Chain 1:



- Molecule 1: coat protein

Chain 2:

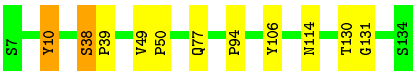


- Molecule 1: coat protein

Chain 3:

- Molecule 1: coat protein

Chain 4:

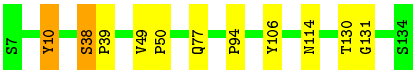


- Molecule 1: coat protein

Chain 5:

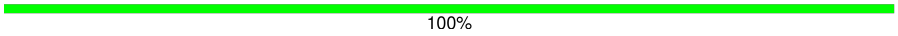
- Molecule 1: coat protein

Chain 6:



- Molecule 2: DNA

Chain 7:



There are no outlier residues recorded for this chain.

- Molecule 2: DNA

Chain 8:

4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	multiply images by CTF, divide reconstruction by sum of CTF**2	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	1	0.75	0/994	0.59	0/1354
1	2	0.74	0/994	0.61	0/1354
1	3	0.75	0/994	0.60	0/1354
1	4	0.74	0/994	0.61	0/1354
1	5	0.75	0/994	0.59	0/1354
1	6	0.74	0/994	0.61	0/1354
1	A	0.75	0/994	0.60	0/1354
1	B	0.74	0/994	0.61	0/1354
1	C	0.75	0/994	0.59	0/1354
1	D	0.74	0/994	0.61	0/1354
1	E	0.75	0/994	0.60	0/1354
1	F	0.74	0/994	0.61	0/1354
1	G	0.75	0/994	0.59	0/1354
1	H	0.74	0/994	0.61	0/1354
1	I	0.75	0/994	0.59	0/1354
1	J	0.74	0/994	0.61	0/1354
1	K	0.75	0/994	0.60	0/1354
1	L	0.74	0/994	0.61	0/1354
1	M	0.75	0/994	0.59	0/1354
1	N	0.74	0/994	0.61	0/1354
1	O	0.75	0/994	0.59	0/1354
1	P	0.74	0/994	0.61	0/1354
1	Q	0.75	0/994	0.60	0/1354
1	R	0.74	0/994	0.61	0/1354
1	S	0.75	0/994	0.59	0/1354
1	T	0.74	0/994	0.61	0/1354
1	U	0.75	0/994	0.59	0/1354
1	V	0.74	0/994	0.61	0/1354
1	W	0.75	0/994	0.60	0/1354
1	X	0.74	0/994	0.61	0/1354
1	Y	0.75	0/994	0.60	0/1354
1	Z	0.74	0/994	0.61	0/1354
1	a	0.75	0/994	0.59	0/1354
1	b	0.74	0/994	0.61	0/1354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
1	c	0.74	0/994	0.59	0/1354
1	d	0.74	0/994	0.61	0/1354
1	e	0.75	0/994	0.60	0/1354
1	f	0.74	0/994	0.61	0/1354
1	g	0.75	0/994	0.59	0/1354
1	h	0.74	0/994	0.61	0/1354
1	i	0.75	0/994	0.59	0/1354
1	j	0.74	0/994	0.61	0/1354
1	k	0.75	0/994	0.59	0/1354
1	l	0.74	0/994	0.61	0/1354
1	m	0.75	0/994	0.60	0/1354
1	n	0.74	0/994	0.61	0/1354
1	o	0.75	0/994	0.60	0/1354
1	p	0.74	0/994	0.61	0/1354
1	q	0.75	0/994	0.60	0/1354
1	r	0.74	0/994	0.61	0/1354
1	s	0.75	0/994	0.59	0/1354
1	t	0.74	0/994	0.61	0/1354
1	u	0.75	0/994	0.59	0/1354
1	v	0.74	0/994	0.61	0/1354
1	w	0.75	0/994	0.60	0/1354
1	x	0.74	0/994	0.61	0/1354
1	y	0.75	0/994	0.60	0/1354
1	z	0.74	0/994	0.61	0/1354
2	7	0.73	0/8003	0.89	0/12350
2	8	0.70	0/8003	1.01	35/12350 (0.3%)
All	All	0.74	0/73658	0.70	35/103232 (0.0%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	8	131	DA	O4'-C4'-C3'	-7.03	101.69	104.50
2	8	71	DA	O4'-C4'-C3'	-7.02	101.69	104.50
2	8	275	DA	O4'-C4'-C3'	-7.02	101.69	104.50
2	8	143	DA	O4'-C4'-C3'	-6.99	101.70	104.50
2	8	119	DA	O4'-C4'-C3'	-6.98	101.71	104.50
2	8	59	DA	O4'-C4'-C3'	-6.97	101.71	104.50
2	8	83	DA	O4'-C4'-C3'	-6.91	101.74	104.50
2	8	107	DA	O4'-C4'-C3'	-6.90	101.74	104.50
2	8	11	DA	O4'-C4'-C3'	-6.90	101.74	104.50
2	8	287	DA	O4'-C4'-C3'	-6.90	101.74	104.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	8	347	DA	O4'-C4'-C3'	-6.90	101.74	104.50
2	8	227	DA	O4'-C4'-C3'	-6.89	101.74	104.50
2	8	179	DA	O4'-C4'-C3'	-6.89	101.74	104.50
2	8	335	DA	O4'-C4'-C3'	-6.88	101.75	104.50
2	8	191	DA	O4'-C4'-C3'	-6.85	101.76	104.50
2	8	215	DA	O4'-C4'-C3'	-6.85	101.76	104.50
2	8	155	DA	O4'-C4'-C3'	-6.84	101.76	104.50
2	8	47	DA	O4'-C4'-C3'	-6.84	101.76	104.50
2	8	35	DA	O4'-C4'-C3'	-6.83	101.77	104.50
2	8	263	DA	O4'-C4'-C3'	-6.83	101.77	104.50
2	8	239	DA	O4'-C4'-C3'	-6.81	101.78	104.50
2	8	251	DA	O4'-C4'-C3'	-6.80	101.78	104.50
2	8	323	DA	O4'-C4'-C3'	-6.80	101.78	104.50
2	8	311	DA	O4'-C4'-C3'	-6.80	101.78	104.50
2	8	299	DA	O4'-C4'-C3'	-6.79	101.78	104.50
2	8	23	DA	O4'-C4'-C3'	-6.77	101.79	104.50
2	8	203	DA	O4'-C4'-C3'	-6.76	101.79	104.50
2	8	167	DA	O4'-C4'-C3'	-6.75	101.80	104.50
2	8	95	DA	O4'-C4'-C3'	-6.70	101.82	104.50
2	8	47	DA	C4'-C3'-C2'	-5.02	98.58	103.10
2	8	71	DA	C4'-C3'-C2'	-5.02	98.58	103.10
2	8	191	DA	C4'-C3'-C2'	-5.01	98.59	103.10
2	8	239	DA	C4'-C3'-C2'	-5.01	98.59	103.10
2	8	323	DA	C4'-C3'-C2'	-5.00	98.60	103.10
2	8	299	DA	C4'-C3'-C2'	-5.00	98.60	103.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	973	0	970	7	0
1	2	973	0	970	9	0
1	3	973	0	970	8	0
1	4	973	0	970	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	973	0	970	8	0
1	6	973	0	970	9	0
1	A	973	0	970	7	0
1	B	973	0	970	15	0
1	C	973	0	970	6	0
1	D	973	0	970	11	0
1	E	973	0	970	9	0
1	F	973	0	970	12	0
1	G	973	0	970	9	0
1	H	973	0	970	12	0
1	I	973	0	970	8	0
1	J	973	0	970	11	0
1	K	973	0	970	10	0
1	L	973	0	970	11	0
1	M	973	0	970	9	0
1	N	973	0	970	12	0
1	O	973	0	970	8	0
1	P	973	0	970	13	0
1	Q	973	0	970	9	0
1	R	973	0	970	12	0
1	S	973	0	970	9	0
1	T	973	0	970	11	0
1	U	973	0	970	9	0
1	V	973	0	970	11	0
1	W	973	0	970	9	0
1	X	973	0	970	11	0
1	Y	973	0	970	9	0
1	Z	973	0	970	11	0
1	a	973	0	970	0	0
1	b	973	0	970	0	0
1	c	973	0	970	0	0
1	d	973	0	970	0	0
1	e	973	0	970	0	0
1	f	973	0	970	0	0
1	g	973	0	970	0	0
1	h	973	0	970	0	0
1	i	973	0	970	0	0
1	j	973	0	970	0	0
1	k	973	0	970	0	0
1	l	973	0	970	0	0
1	m	973	0	970	0	0
1	n	973	0	970	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	o	973	0	970	0	0
1	p	973	0	970	0	0
1	q	973	0	970	0	0
1	r	973	0	970	0	0
1	s	973	0	970	0	0
1	t	973	0	970	0	0
1	u	973	0	970	0	0
1	v	973	0	970	0	0
1	w	973	0	970	0	0
1	x	973	0	970	0	0
1	y	973	0	970	0	0
1	z	973	0	970	0	0
2	7	7134	0	4003	0	0
2	8	7134	0	4003	0	0
All	All	70702	0	64266	270	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:10:TYR:HH	1:U:10:TYR:HE2	53.60	0.73
1:L:10:TYR:HH	1:O:10:TYR:HE2	53.61	0.73
1:J:10:TYR:HH	1:M:10:TYR:HE2	53.61	0.72
1:B:10:TYR:HH	1:E:10:TYR:HE2	53.60	0.71
1:F:10:TYR:HH	1:I:10:TYR:HE2	53.61	0.68
1:X:10:TYR:HH	1:1:10:TYR:HE2	1.40	0.67
1:N:10:TYR:HH	1:Q:10:TYR:HE2	53.61	0.65
1:V:10:TYR:HH	1:Y:10:TYR:HE2	53.61	0.65
1:P:10:TYR:HH	1:S:10:TYR:HE2	53.60	0.65
1:T:10:TYR:HH	1:W:10:TYR:HE2	53.60	0.64
1:B:10:TYR:HH	1:5:10:TYR:HE2	54.91	0.64
1:H:10:TYR:HH	1:K:10:TYR:HE2	53.61	0.63
1:D:10:TYR:HH	1:G:10:TYR:HE2	53.61	0.63
1:Z:10:TYR:HH	1:3:10:TYR:HE2	1.44	0.62
1:B:10:TYR:C	1:B:10:TYR:CD1	2.77	0.57
1:6:10:TYR:CD1	1:6:10:TYR:C	2.77	0.57
1:H:10:TYR:C	1:H:10:TYR:CD1	2.78	0.57
1:D:10:TYR:CD1	1:D:10:TYR:C	2.77	0.56
1:N:10:TYR:C	1:N:10:TYR:CD1	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:10:TYR:C	1:J:10:TYR:CD1	2.77	0.56
1:X:10:TYR:C	1:X:10:TYR:CD1	2.77	0.56
1:V:10:TYR:C	1:V:10:TYR:CD1	2.77	0.56
1:T:10:TYR:C	1:T:10:TYR:CD1	2.78	0.56
1:Z:10:TYR:C	1:Z:10:TYR:CD1	2.77	0.56
1:R:10:TYR:CD1	1:R:10:TYR:C	2.77	0.56
1:P:10:TYR:CD1	1:P:10:TYR:C	2.77	0.56
1:L:10:TYR:CD1	1:L:10:TYR:C	2.77	0.55
1:F:10:TYR:CD1	1:F:10:TYR:C	2.77	0.55
1:2:10:TYR:C	1:2:10:TYR:CD1	2.77	0.55
1:V:10:TYR:O	1:V:10:TYR:CD1	2.61	0.54
1:B:10:TYR:O	1:B:10:TYR:CD1	2.61	0.54
1:X:10:TYR:O	1:X:10:TYR:CD1	2.61	0.54
1:T:10:TYR:CD1	1:T:10:TYR:O	2.61	0.54
1:Z:10:TYR:O	1:Z:10:TYR:CD1	2.61	0.54
1:6:10:TYR:O	1:6:10:TYR:CD1	2.61	0.54
1:L:10:TYR:O	1:L:10:TYR:CD1	2.61	0.54
1:F:10:TYR:CD1	1:F:10:TYR:O	2.61	0.54
1:P:10:TYR:O	1:P:10:TYR:CD1	2.61	0.54
1:D:10:TYR:O	1:D:10:TYR:CD1	2.61	0.54
1:R:10:TYR:CD1	1:R:10:TYR:O	2.61	0.54
1:J:10:TYR:O	1:J:10:TYR:CD1	2.61	0.54
1:N:10:TYR:O	1:N:10:TYR:CD1	2.61	0.54
1:4:10:TYR:O	1:4:10:TYR:CD1	2.61	0.54
1:H:10:TYR:CD1	1:H:10:TYR:O	2.61	0.54
1:4:10:TYR:C	1:4:10:TYR:CD1	2.77	0.53
1:2:10:TYR:CD1	1:2:10:TYR:O	2.61	0.53
1:V:10:TYR:OH	1:Y:10:TYR:HE2	52.78	0.51
1:R:10:TYR:OH	1:U:10:TYR:HE2	52.78	0.51
1:Z:10:TYR:OH	1:3:10:TYR:HE2	1.94	0.51
1:N:10:TYR:OH	1:Q:10:TYR:HE2	52.78	0.51
1:H:10:TYR:OH	1:K:10:TYR:HE2	52.78	0.50
1:P:10:TYR:OH	1:S:10:TYR:HE2	52.78	0.50
1:B:10:TYR:OH	1:5:10:TYR:HE2	55.57	0.50
1:D:10:TYR:OH	1:G:10:TYR:HE2	52.78	0.49
1:J:10:TYR:OH	1:M:10:TYR:HE2	52.78	0.49
1:X:10:TYR:OH	1:1:10:TYR:HE2	1.94	0.49
1:T:10:TYR:OH	1:W:10:TYR:HE2	52.78	0.49
1:B:10:TYR:OH	1:E:10:TYR:HE2	52.78	0.47
1:F:10:TYR:OH	1:I:10:TYR:HE2	52.78	0.47
1:K:130:THR:OG1	1:K:131:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:THR:OG1	1:E:131:GLY:N	2.48	0.47
1:P:49:VAL:N	1:P:50:PRO:HD2	2.31	0.46
1:D:49:VAL:N	1:D:50:PRO:HD2	2.31	0.46
1:2:49:VAL:N	1:2:50:PRO:HD2	2.31	0.46
1:L:49:VAL:N	1:L:50:PRO:HD2	2.31	0.46
1:X:49:VAL:N	1:X:50:PRO:HD2	2.31	0.46
1:N:49:VAL:N	1:N:50:PRO:HD2	2.31	0.46
1:3:130:THR:OG1	1:3:131:GLY:N	2.48	0.46
1:6:49:VAL:N	1:6:50:PRO:HD2	2.31	0.46
1:H:49:VAL:N	1:H:50:PRO:HD2	2.31	0.46
1:V:49:VAL:N	1:V:50:PRO:HD2	2.31	0.46
1:R:49:VAL:N	1:R:50:PRO:HD2	2.31	0.46
1:L:10:TYR:OH	1:O:10:TYR:HE2	52.78	0.46
1:E:114:ASN:C	1:E:114:ASN:OD1	2.54	0.46
1:F:49:VAL:N	1:F:50:PRO:HD2	2.31	0.46
1:L:49:VAL:N	1:L:50:PRO:CD	2.79	0.46
1:X:49:VAL:N	1:X:50:PRO:CD	2.79	0.46
1:N:49:VAL:N	1:N:50:PRO:CD	2.79	0.46
1:T:49:VAL:N	1:T:50:PRO:HD2	2.31	0.46
1:J:49:VAL:N	1:J:50:PRO:HD2	2.31	0.46
1:V:49:VAL:N	1:V:50:PRO:CD	2.79	0.46
1:Z:49:VAL:N	1:Z:50:PRO:HD2	2.31	0.46
1:A:114:ASN:C	1:A:114:ASN:OD1	2.54	0.46
1:C:114:ASN:C	1:C:114:ASN:OD1	2.54	0.46
1:P:49:VAL:N	1:P:50:PRO:CD	2.79	0.46
1:6:49:VAL:N	1:6:50:PRO:CD	2.79	0.46
1:J:49:VAL:N	1:J:50:PRO:CD	2.79	0.46
1:B:49:VAL:N	1:B:50:PRO:HD2	2.31	0.46
1:C:130:THR:OG1	1:C:131:GLY:N	2.48	0.46
1:1:114:ASN:C	1:1:114:ASN:OD1	2.54	0.46
1:3:114:ASN:C	1:3:114:ASN:OD1	2.54	0.46
1:W:130:THR:OG1	1:W:131:GLY:N	2.48	0.46
1:Y:114:ASN:OD1	1:Y:114:ASN:C	2.54	0.46
1:O:114:ASN:C	1:O:114:ASN:OD1	2.54	0.46
1:I:114:ASN:OD1	1:I:114:ASN:C	2.54	0.46
1:H:49:VAL:N	1:H:50:PRO:CD	2.79	0.45
1:T:49:VAL:N	1:T:50:PRO:CD	2.79	0.45
1:B:49:VAL:N	1:B:50:PRO:CD	2.79	0.45
1:I:130:THR:OG1	1:I:131:GLY:N	2.48	0.45
1:W:114:ASN:OD1	1:W:114:ASN:C	2.54	0.45
1:4:49:VAL:N	1:4:50:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:49:VAL:N	1:4:50:PRO:HD2	2.31	0.45
1:R:49:VAL:N	1:R:50:PRO:CD	2.79	0.45
1:F:49:VAL:N	1:F:50:PRO:CD	2.79	0.45
1:M:114:ASN:OD1	1:M:114:ASN:C	2.54	0.45
1:G:114:ASN:C	1:G:114:ASN:OD1	2.54	0.45
1:6:77:GLN:OE1	1:6:77:GLN:HA	2.17	0.45
1:U:114:ASN:C	1:U:114:ASN:OD1	2.54	0.45
1:Z:49:VAL:N	1:Z:50:PRO:CD	2.79	0.45
1:S:114:ASN:OD1	1:S:114:ASN:C	2.54	0.45
1:5:114:ASN:C	1:5:114:ASN:OD1	2.54	0.45
1:H:77:GLN:HA	1:H:77:GLN:OE1	2.17	0.45
1:P:77:GLN:HA	1:P:77:GLN:OE1	2.17	0.45
1:D:77:GLN:HA	1:D:77:GLN:OE1	2.17	0.45
1:F:77:GLN:HA	1:F:77:GLN:OE1	2.17	0.45
1:Q:114:ASN:OD1	1:Q:114:ASN:C	2.54	0.45
1:Z:77:GLN:HA	1:Z:77:GLN:OE1	2.17	0.45
1:B:77:GLN:HA	1:B:77:GLN:OE1	2.17	0.45
1:L:77:GLN:HA	1:L:77:GLN:OE1	2.17	0.45
1:2:49:VAL:N	1:2:50:PRO:CD	2.79	0.45
1:2:77:GLN:OE1	1:2:77:GLN:HA	2.17	0.45
1:O:130:THR:OG1	1:O:131:GLY:N	2.48	0.45
1:Q:130:THR:OG1	1:Q:131:GLY:N	2.49	0.45
1:N:77:GLN:HA	1:N:77:GLN:OE1	2.17	0.45
1:1:130:THR:OG1	1:1:131:GLY:N	2.48	0.45
1:D:49:VAL:N	1:D:50:PRO:CD	2.79	0.45
1:R:77:GLN:OE1	1:R:77:GLN:HA	2.17	0.45
1:K:114:ASN:C	1:K:114:ASN:OD1	2.54	0.45
1:J:77:GLN:HA	1:J:77:GLN:OE1	2.17	0.45
1:X:77:GLN:HA	1:X:77:GLN:OE1	2.17	0.45
1:U:130:THR:OG1	1:U:131:GLY:N	2.48	0.45
1:S:130:THR:OG1	1:S:131:GLY:N	2.48	0.45
1:V:77:GLN:HA	1:V:77:GLN:OE1	2.17	0.44
1:T:77:GLN:OE1	1:T:77:GLN:HA	2.17	0.44
1:Y:130:THR:OG1	1:Y:131:GLY:N	2.48	0.44
1:A:130:THR:OG1	1:A:131:GLY:N	2.48	0.44
1:4:77:GLN:HA	1:4:77:GLN:OE1	2.17	0.44
1:G:130:THR:OG1	1:G:131:GLY:N	2.48	0.43
1:M:49:VAL:N	1:M:50:PRO:CD	2.82	0.43
1:G:49:VAL:N	1:G:50:PRO:CD	2.82	0.43
1:M:130:THR:OG1	1:M:131:GLY:N	2.49	0.43
1:K:49:VAL:N	1:K:50:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:VAL:N	1:E:50:PRO:CD	2.82	0.43
1:S:106:TYR:HB2	1:T:106:TYR:HB2	2.01	0.43
1:S:114:ASN:HA	1:S:115:PRO:HD3	1.92	0.43
1:S:49:VAL:N	1:S:50:PRO:CD	2.82	0.43
1:F:130:THR:OG1	1:F:131:GLY:N	2.51	0.43
1:O:106:TYR:HB2	1:P:106:TYR:HB2	2.01	0.43
1:M:106:TYR:HB2	1:N:106:TYR:HB2	2.01	0.43
1:U:49:VAL:N	1:U:50:PRO:CD	2.82	0.43
1:I:106:TYR:HB2	1:J:106:TYR:HB2	2.01	0.43
1:C:106:TYR:HB2	1:D:106:TYR:HB2	2.01	0.43
1:E:106:TYR:HB2	1:F:106:TYR:HB2	2.01	0.43
1:J:130:THR:OG1	1:J:131:GLY:N	2.51	0.43
1:D:130:THR:OG1	1:D:131:GLY:N	2.51	0.43
1:R:130:THR:OG1	1:R:131:GLY:N	2.51	0.43
1:Y:49:VAL:N	1:Y:50:PRO:CD	2.82	0.43
1:G:106:TYR:HB2	1:H:106:TYR:HB2	2.01	0.43
1:O:49:VAL:N	1:O:50:PRO:CD	2.82	0.43
1:I:49:VAL:N	1:I:50:PRO:CD	2.82	0.43
1:C:49:VAL:N	1:C:50:PRO:CD	2.82	0.42
1:5:49:VAL:N	1:5:50:PRO:CD	2.82	0.42
1:1:49:VAL:N	1:1:50:PRO:CD	2.82	0.42
1:H:130:THR:OG1	1:H:131:GLY:N	2.51	0.42
1:Q:49:VAL:N	1:Q:50:PRO:CD	2.82	0.42
1:Q:106:TYR:HB2	1:R:106:TYR:HB2	2.01	0.42
1:Y:114:ASN:HA	1:Y:115:PRO:HD3	1.92	0.42
1:K:126:THR:OG1	1:K:128:SER:O	2.37	0.42
1:3:126:THR:OG1	1:3:128:SER:O	2.37	0.42
1:K:106:TYR:HB2	1:L:106:TYR:HB2	2.01	0.42
1:A:114:ASN:HA	1:A:115:PRO:HD3	1.92	0.42
1:E:126:THR:OG1	1:E:128:SER:O	2.37	0.42
1:A:49:VAL:N	1:A:50:PRO:CD	2.82	0.42
1:W:106:TYR:HB2	1:X:106:TYR:HB2	2.01	0.42
1:L:130:THR:OG1	1:L:131:GLY:N	2.51	0.42
1:W:49:VAL:N	1:W:50:PRO:CD	2.82	0.42
1:W:114:ASN:HA	1:W:115:PRO:HD3	1.92	0.42
1:A:106:TYR:HB2	1:B:106:TYR:HB2	2.01	0.42
1:B:130:THR:OG1	1:B:131:GLY:N	2.51	0.42
1:6:130:THR:OG1	1:6:131:GLY:N	2.51	0.42
1:C:114:ASN:HA	1:C:115:PRO:HD3	1.92	0.42
1:U:106:TYR:HB2	1:V:106:TYR:HB2	2.01	0.42
1:5:130:THR:OG1	1:5:131:GLY:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:49:VAL:N	1:3:50:PRO:CD	2.82	0.42
1:Q:114:ASN:HA	1:Q:115:PRO:HD3	1.92	0.42
1:X:130:THR:OG1	1:X:131:GLY:N	2.51	0.42
1:5:106:TYR:HB2	1:6:106:TYR:HB2	2.01	0.42
1:W:126:THR:OG1	1:W:128:SER:O	2.37	0.42
1:1:106:TYR:HB2	1:2:106:TYR:HB2	2.01	0.42
1:U:114:ASN:HA	1:U:115:PRO:HD3	1.92	0.42
1:Y:106:TYR:HB2	1:Z:106:TYR:HB2	2.01	0.42
1:E:114:ASN:HA	1:E:115:PRO:HD3	1.92	0.41
1:Q:126:THR:OG1	1:Q:128:SER:O	2.37	0.41
1:3:106:TYR:HB2	1:4:106:TYR:HB2	2.01	0.41
1:Y:126:THR:OG1	1:Y:128:SER:O	2.37	0.41
1:5:38:SER:HB2	1:5:39:PRO:HD3	2.02	0.41
1:6:38:SER:HB2	1:6:39:PRO:HD3	2.02	0.41
1:U:38:SER:HB2	1:U:39:PRO:HD3	2.02	0.41
1:O:38:SER:HB2	1:O:39:PRO:HD3	2.02	0.41
1:K:38:SER:HB2	1:K:39:PRO:HD3	2.02	0.41
1:X:38:SER:HB2	1:X:39:PRO:HD3	2.02	0.41
1:4:38:SER:HB2	1:4:39:PRO:HD3	2.02	0.41
1:Y:38:SER:HB2	1:Y:39:PRO:HD3	2.02	0.41
1:1:38:SER:HB2	1:1:39:PRO:HD3	2.02	0.41
1:G:38:SER:HB2	1:G:39:PRO:HD3	2.02	0.41
1:2:130:THR:OG1	1:2:131:GLY:N	2.51	0.41
1:I:38:SER:HB2	1:I:39:PRO:HD3	2.02	0.41
1:P:38:SER:HB2	1:P:39:PRO:HD3	2.02	0.41
1:Z:114:ASN:C	1:Z:114:ASN:OD1	2.59	0.41
1:D:114:ASN:C	1:D:114:ASN:OD1	2.59	0.41
1:N:20:LYS:HA	1:N:20:LYS:HD2	1.90	0.41
1:P:20:LYS:HD2	1:P:20:LYS:HA	1.90	0.41
1:M:38:SER:HB2	1:M:39:PRO:HD3	2.02	0.41
1:N:38:SER:HB2	1:N:39:PRO:HD3	2.02	0.41
1:B:38:SER:HB2	1:B:39:PRO:HD3	2.02	0.41
1:V:114:ASN:C	1:V:114:ASN:OD1	2.59	0.41
1:P:114:ASN:OD1	1:P:114:ASN:C	2.59	0.41
1:X:114:ASN:OD1	1:X:114:ASN:C	2.59	0.41
1:R:114:ASN:OD1	1:R:114:ASN:C	2.59	0.41
1:Z:130:THR:OG1	1:Z:131:GLY:N	2.51	0.41
1:Q:38:SER:HB2	1:Q:39:PRO:HD3	2.02	0.41
1:P:130:THR:OG1	1:P:131:GLY:N	2.51	0.41
1:Z:38:SER:HB2	1:Z:39:PRO:HD3	2.02	0.41
1:T:114:ASN:C	1:T:114:ASN:OD1	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:114:ASN:OD1	1:6:114:ASN:C	2.59	0.41
1:D:38:SER:HB2	1:D:39:PRO:HD3	2.02	0.41
1:O:114:ASN:HA	1:O:115:PRO:HD3	1.92	0.41
1:G:114:ASN:HA	1:G:115:PRO:HD3	1.92	0.41
1:S:126:THR:OG1	1:S:128:SER:O	2.37	0.41
1:4:114:ASN:OD1	1:4:114:ASN:C	2.59	0.41
1:B:114:ASN:C	1:B:114:ASN:OD1	2.59	0.41
1:W:38:SER:HB2	1:W:39:PRO:HD3	2.02	0.41
1:E:38:SER:HB2	1:E:39:PRO:HD3	2.02	0.41
1:R:38:SER:HB2	1:R:39:PRO:HD3	2.02	0.41
1:L:38:SER:HB2	1:L:39:PRO:HD3	2.02	0.41
1:P:128:SER:HA	1:P:129:PRO:HD3	1.93	0.41
1:B:114:ASN:HA	1:B:115:PRO:HD3	1.93	0.41
1:H:38:SER:HB2	1:H:39:PRO:HD3	2.02	0.41
1:C:38:SER:HB2	1:C:39:PRO:HD3	2.02	0.41
1:K:20:LYS:HA	1:K:20:LYS:HD2	1.96	0.41
1:L:114:ASN:C	1:L:114:ASN:OD1	2.59	0.41
1:T:130:THR:OG1	1:T:131:GLY:N	2.51	0.41
1:N:130:THR:OG1	1:N:131:GLY:N	2.51	0.41
1:4:130:THR:OG1	1:4:131:GLY:N	2.51	0.41
1:A:38:SER:HB2	1:A:39:PRO:HD3	2.02	0.41
1:T:38:SER:HB2	1:T:39:PRO:HD3	2.02	0.41
1:J:114:ASN:OD1	1:J:114:ASN:C	2.59	0.41
1:F:114:ASN:OD1	1:F:114:ASN:C	2.59	0.41
1:M:126:THR:OG1	1:M:128:SER:O	2.37	0.41
1:G:126:THR:OG1	1:G:128:SER:O	2.37	0.41
1:2:114:ASN:OD1	1:2:114:ASN:C	2.59	0.41
1:H:20:LYS:HD2	1:H:20:LYS:HA	1.90	0.41
1:B:20:LYS:HA	1:B:20:LYS:HD2	1.90	0.41
1:2:38:SER:HB2	1:2:39:PRO:HD3	2.02	0.41
1:R:128:SER:HA	1:R:129:PRO:HD3	1.93	0.40
1:H:114:ASN:OD1	1:H:114:ASN:C	2.59	0.40
1:J:38:SER:HB2	1:J:39:PRO:HD3	2.02	0.40
1:5:126:THR:OG1	1:5:128:SER:O	2.37	0.40
1:F:38:SER:HB2	1:F:39:PRO:HD3	2.02	0.40
1:I:114:ASN:HA	1:I:115:PRO:HD3	1.92	0.40
1:A:126:THR:OG1	1:A:128:SER:O	2.37	0.40
1:N:114:ASN:OD1	1:N:114:ASN:C	2.59	0.40
1:V:130:THR:OG1	1:V:131:GLY:N	2.51	0.40
1:S:38:SER:HB2	1:S:39:PRO:HD3	2.02	0.40
1:M:114:ASN:HA	1:M:115:PRO:HD3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:LYS:HA	1:F:20:LYS:HD2	1.90	0.40
1:V:38:SER:HB2	1:V:39:PRO:HD3	2.02	0.40
1:K:114:ASN:HA	1:K:115:PRO:HD3	1.92	0.40
1:U:126:THR:OG1	1:U:128:SER:O	2.37	0.40
1:3:38:SER:HB2	1:3:39:PRO:HD3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	2	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	3	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	4	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	5	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	6	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	A	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	B	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	C	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	D	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	E	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	F	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	G	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	H	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	I	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	J	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	L	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	M	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	N	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	O	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	P	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	Q	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	R	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	S	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	T	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	U	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	V	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	W	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	X	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	Y	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	Z	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	a	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	b	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	c	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	d	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	e	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	f	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	g	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	h	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	i	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	j	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	k	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	l	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	m	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	n	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	o	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	p	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	q	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	r	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	s	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	t	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	u	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	v	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	w	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	x	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
1	y	126/128 (98%)	120 (95%)	4 (3%)	2 (2%)	12	58
1	z	126/128 (98%)	121 (96%)	3 (2%)	2 (2%)	12	58
All	All	7308/7424 (98%)	6989 (96%)	203 (3%)	116 (2%)	17	58

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	B	38	SER
1	C	38	SER
1	D	38	SER
1	E	38	SER
1	F	38	SER
1	G	38	SER
1	H	38	SER
1	I	38	SER
1	J	38	SER
1	K	38	SER
1	L	38	SER
1	M	38	SER
1	N	38	SER
1	O	38	SER
1	P	38	SER
1	Q	38	SER
1	R	38	SER
1	S	38	SER
1	T	38	SER
1	U	38	SER
1	V	38	SER

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Mol	Chain	Res	Type
1	W	38	SER
1	X	38	SER
1	Y	38	SER
1	Z	38	SER
1	a	38	SER
1	b	38	SER
1	c	38	SER
1	d	38	SER
1	e	38	SER
1	f	38	SER
1	g	38	SER
1	h	38	SER
1	i	38	SER
1	k	38	SER
1	m	38	SER
1	n	38	SER
1	o	38	SER
1	p	38	SER
1	q	38	SER
1	r	38	SER
1	s	38	SER
1	t	38	SER
1	u	38	SER
1	v	38	SER
1	w	38	SER
1	x	38	SER
1	y	38	SER
1	z	38	SER
1	1	38	SER
1	2	38	SER
1	3	38	SER
1	4	38	SER
1	5	38	SER
1	6	38	SER
1	j	38	SER
1	l	38	SER
1	L	94	PRO
1	P	94	PRO
1	R	94	PRO
1	X	94	PRO
1	z	94	PRO
1	A	94	PRO

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Mol	Chain	Res	Type
1	B	94	PRO
1	C	94	PRO
1	D	94	PRO
1	E	94	PRO
1	F	94	PRO
1	G	94	PRO
1	H	94	PRO
1	I	94	PRO
1	J	94	PRO
1	K	94	PRO
1	M	94	PRO
1	N	94	PRO
1	O	94	PRO
1	Q	94	PRO
1	S	94	PRO
1	T	94	PRO
1	U	94	PRO
1	V	94	PRO
1	W	94	PRO
1	Y	94	PRO
1	Z	94	PRO
1	a	94	PRO
1	b	94	PRO
1	c	94	PRO
1	d	94	PRO
1	e	94	PRO
1	f	94	PRO
1	g	94	PRO
1	h	94	PRO
1	i	94	PRO
1	j	94	PRO
1	k	94	PRO
1	l	94	PRO
1	m	94	PRO
1	n	94	PRO
1	o	94	PRO
1	p	94	PRO
1	q	94	PRO
1	r	94	PRO
1	s	94	PRO
1	t	94	PRO
1	u	94	PRO

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Mol	Chain	Res	Type
1	v	94	PRO
1	w	94	PRO
1	x	94	PRO
1	y	94	PRO
1	1	94	PRO
1	2	94	PRO
1	3	94	PRO
1	4	94	PRO
1	5	94	PRO
1	6	94	PRO

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	1	105/105 (100%)	105 (100%)	0	100 100
1	2	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	3	105/105 (100%)	105 (100%)	0	100 100
1	4	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	5	105/105 (100%)	105 (100%)	0	100 100
1	6	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	A	105/105 (100%)	105 (100%)	0	100 100
1	B	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	C	105/105 (100%)	105 (100%)	0	100 100
1	D	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	E	105/105 (100%)	105 (100%)	0	100 100
1	F	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	G	105/105 (100%)	105 (100%)	0	100 100
1	H	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	I	105/105 (100%)	105 (100%)	0	100 100
1	J	105/105 (100%)	104 (99%)	1 (1%)	82 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	105/105 (100%)	105 (100%)	0	100	100
1	L	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	M	105/105 (100%)	105 (100%)	0	100	100
1	N	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	O	105/105 (100%)	105 (100%)	0	100	100
1	P	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	Q	105/105 (100%)	105 (100%)	0	100	100
1	R	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	S	105/105 (100%)	105 (100%)	0	100	100
1	T	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	U	105/105 (100%)	105 (100%)	0	100	100
1	V	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	W	105/105 (100%)	105 (100%)	0	100	100
1	X	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	Y	105/105 (100%)	105 (100%)	0	100	100
1	Z	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	a	105/105 (100%)	105 (100%)	0	100	100
1	b	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	c	105/105 (100%)	105 (100%)	0	100	100
1	d	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	e	105/105 (100%)	105 (100%)	0	100	100
1	f	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	g	105/105 (100%)	105 (100%)	0	100	100
1	h	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	i	105/105 (100%)	105 (100%)	0	100	100
1	j	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	k	105/105 (100%)	105 (100%)	0	100	100
1	l	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	m	105/105 (100%)	105 (100%)	0	100	100
1	n	105/105 (100%)	104 (99%)	1 (1%)	82	92
1	o	105/105 (100%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	p	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	q	105/105 (100%)	105 (100%)	0	100 100
1	r	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	s	105/105 (100%)	105 (100%)	0	100 100
1	t	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	u	105/105 (100%)	105 (100%)	0	100 100
1	v	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	w	105/105 (100%)	105 (100%)	0	100 100
1	x	105/105 (100%)	104 (99%)	1 (1%)	82 92
1	y	105/105 (100%)	105 (100%)	0	100 100
1	z	105/105 (100%)	104 (99%)	1 (1%)	82 92
All	All	6090/6090 (100%)	6061 (100%)	29 (0%)	92 97

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	TYR
1	D	10	TYR
1	F	10	TYR
1	H	10	TYR
1	J	10	TYR
1	L	10	TYR
1	N	10	TYR
1	P	10	TYR
1	R	10	TYR
1	T	10	TYR
1	V	10	TYR
1	X	10	TYR
1	Z	10	TYR
1	b	10	TYR
1	d	10	TYR
1	f	10	TYR
1	h	10	TYR
1	j	10	TYR
1	l	10	TYR
1	n	10	TYR
1	p	10	TYR
1	r	10	TYR

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Mol	Chain	Res	Type
1	t	10	TYR
1	v	10	TYR
1	x	10	TYR
1	z	10	TYR
1	2	10	TYR
1	4	10	TYR
1	6	10	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.