



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:24 PM BST

PDB ID : 3J9G
EMDB ID: : EMD-2699
Title : Atomic model of the VipA/VipB, the type six secretion system contractile sheath of *Vibrio cholerae* from cryo-EM
Authors : Kudryashev, M.; Wang, R.Y.-R.; Brackmann, M.; Scherer, S.; Maier, T.; Baker, D.; DiMaio, F.; Stahlberg, H.; Egelman, E.H.; Basler, M.
Deposited on : 2015-01-16
Resolution : 3.50 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

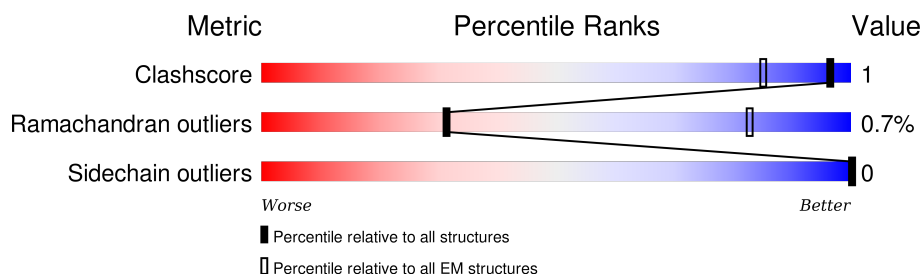
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



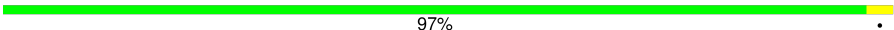
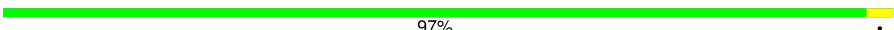
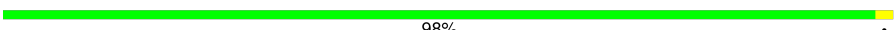
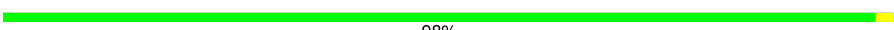






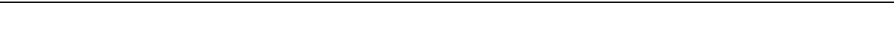

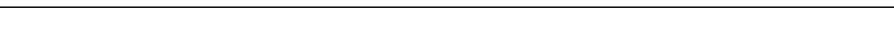
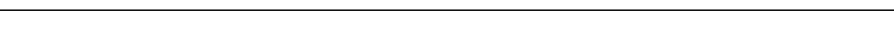
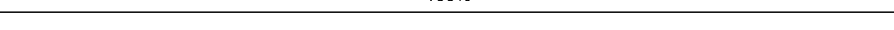
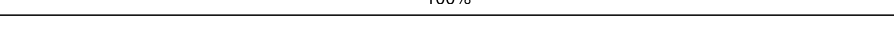
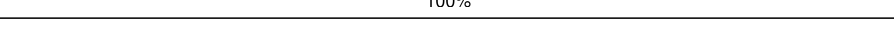
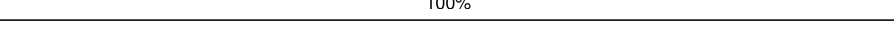
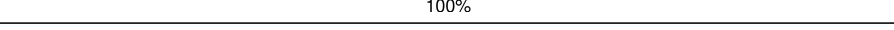
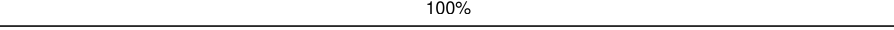
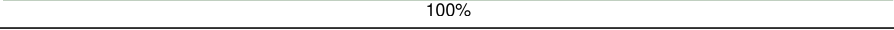
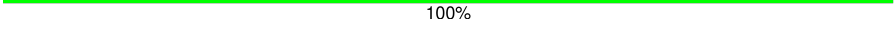
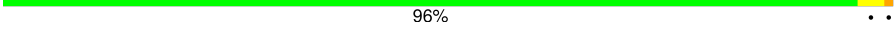
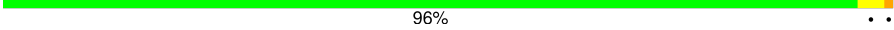
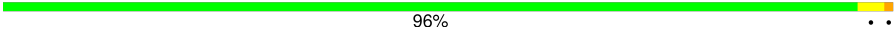
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	125	98% .
1	3	125	96% .
1	5	125	98% .
1	7	125	98% .
1	A	125	94% 6% .
1	C	125	98% .
1	E	125	98% .
1	G	125	98% .
1	I	125	98% .

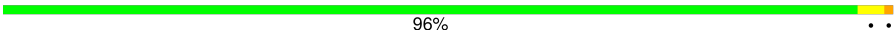
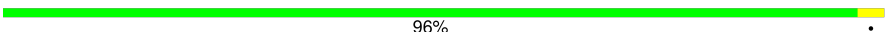
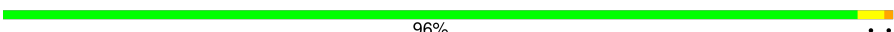

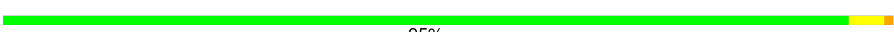







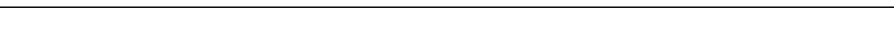

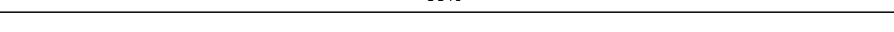
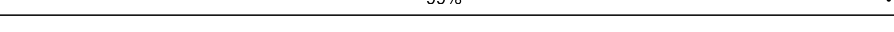
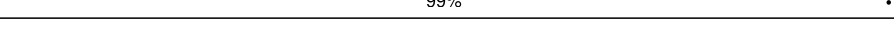
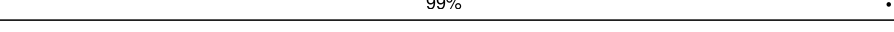
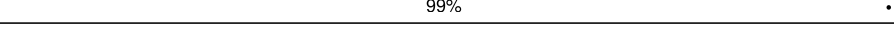
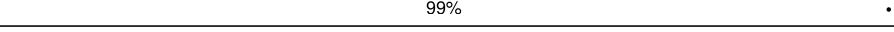
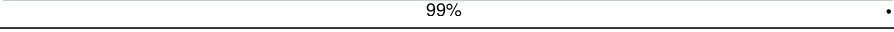
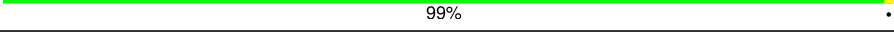
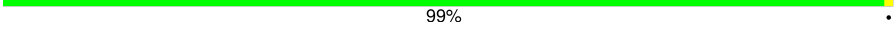
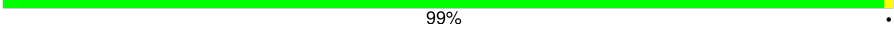
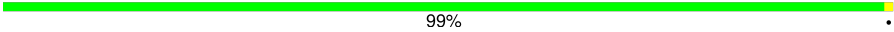
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Mol	Chain	Length	Quality of chain
1	K	125	 97% .
1	M	125	 97% .
1	O	125	 98% .
1	Q	125	 98% .
1	S	125	 97% .
1	U	125	 97% .
1	W	125	 98% .
1	Y	125	 98% .
1	a	125	 100%
1	c	125	 100%
1	e	125	 100%
1	g	125	 100%
1	i	125	 100%
1	k	125	 100%
1	m	125	 100%
1	o	125	 100%
1	q	125	 100%
1	s	125	 100%
1	u	125	 100%
1	w	125	 100%
1	y	125	 100%
2	2	432	 96% . .
2	4	432	 96% . .
2	6	432	 96% . .
2	8	432	 97% .


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Mol	Chain	Length	Quality of chain
2	B	432	 96% ..
2	D	432	 96% .
2	F	432	 96% ..
2	H	432	 96% ..
2	J	432	 95% ..
2	L	432	 96% ..
2	N	432	 96% ..
2	P	432	 96% ..
2	R	432	 96% ..
2	T	432	 96% ..
2	V	432	 96% ..
2	X	432	 96% ..
2	Z	432	 96% ..
2	b	432	 99% .
2	d	432	 99% .
2	f	432	 99% .
2	h	432	 99% .
2	j	432	 99% .
2	l	432	 99% .
2	n	432	 99% .
2	p	432	 99% .
2	r	432	 99% .
2	t	432	 99% .
2	v	432	 99% .
2	x	432	 99% .

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Mol	Chain	Length	Quality of chain
2	z	432	 99%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 132930 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 VipA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	C	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	E	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	G	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	I	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	K	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	M	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	O	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	Q	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	S	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	U	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	W	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	Y	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	a	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	c	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	e	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	g	125	Total 963	C 608	N 160	O 194	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	k	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	m	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	o	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	q	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	s	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	u	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	w	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	y	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	1	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	3	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	5	125	Total 963	C 608	N 160	O 194	S 1	0	0
1	7	125	Total 963	C 608	N 160	O 194	S 1	0	0

- Molecule 2 is a protein called VipB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	D	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	F	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	H	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	J	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	L	432	Total 3468	C 2215	N 590	O 650	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	P	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	R	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	T	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	V	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	X	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	Z	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	b	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	d	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	f	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	h	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	j	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	l	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	n	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	p	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	r	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	t	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	v	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	x	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	z	432	Total 3468	C 2215	N 590	O 650	S 13	0	0
2	2	432	Total 3468	C 2215	N 590	O 650	S 13	0	0

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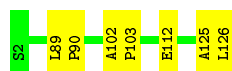
Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	432	Total	C	N	O	S	0	0
			3468	2215	590	650	13		
2	6	432	Total	C	N	O	S	0	0
			3468	2215	590	650	13		
2	8	432	Total	C	N	O	S	0	0
			3468	2215	590	650	13		

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: VipA

Chain A:  94% 6%



- Molecule 1: VipA

Chain C:  98% .



- Molecule 1: VipA

Chain E:  98% .



- Molecule 1: VipA

Chain G:  98% .



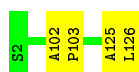
- Molecule 1: VipA

Chain I:  98% .



- Molecule 1: VipA

Chain K:  97% .



- Molecule 1: VipA

Chain M:  97%



- Molecule 1: VipA

Chain O:  98%



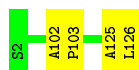
- Molecule 1: VipA

Chain Q:  98%



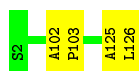
- Molecule 1: VipA

Chain S:  97%



- Molecule 1: VipA

Chain U:  97%



- Molecule 1: VipA

Chain W:  98%



- Molecule 1: VipA

Chain Y:  98%



- Molecule 1: VipA

Chain a:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: VipA

Chain 1:  98%



- Molecule 1: VipA

Chain 3:  96%



- Molecule 1: VipA

Chain 5:  98%



- Molecule 1: VipA

Chain 7:  98%



- Molecule 2: VipB

Chain B:  96% ..



• Molecule 2: VipB

Chain D:  96% .



• Molecule 2: VipB

Chain F:  96% ..



• Molecule 2: VipB

Chain H:  96% ..



• Molecule 2: VipB

Chain J:  95% ..



• Molecule 2: VipB

Chain L:  96% ..



• Molecule 2: VipB

Chain N:  96% ..



• Molecule 2: VipB

Chain P:  96% ..



- Molecule 2: VipB

Chain R: 96%



- Molecule 2: VipB

Chain T: 96%



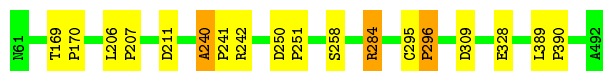
- Molecule 2: VipB

Chain V: 96%



- Molecule 2: VipB

Chain X: 96%



- Molecule 2: VipB

Chain Z: 96%



- Molecule 2: VipB

Chain b: 99%



- Molecule 2: VipB

Chain d: 99%



● Molecule 2: VipB

Chain f:  99%

● Molecule 2: VipB

Chain h:  99%

● Molecule 2: VipB

Chain j:  99%

● Molecule 2: VipB

Chain l:  99%

● Molecule 2: VipB

Chain n:  99%

● Molecule 2: VipB

Chain p:  99%

● Molecule 2: VipB

Chain r:  99%

● Molecule 2: VipB

Chain t:  99%



- Molecule 2: VipB

Chain v:  99%



- Molecule 2: VipB

Chain x:  99%



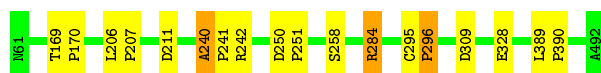
- Molecule 2: VipB

Chain z:  99%



- Molecule 2: VipB

Chain 2:  96%



- Molecule 2: VipB

Chain 4:  96%



- Molecule 2: VipB

Chain 6:  96%



- Molecule 2: VipB

Chain 8:  97%

861	T169 P170	L206 P207	A240 P241 R242	S258	R284	P296	D309	E328	L389 P390	1492
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4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	96000	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Phase Flip, CTF detection by CTFFIND	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 (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	0.84	0/975	0.60	0/1321
1	3	0.84	0/975	0.60	0/1321
1	5	0.84	0/975	0.60	0/1321
1	7	0.84	0/975	0.60	0/1321
1	A	0.84	0/975	0.60	0/1321
1	C	0.84	0/975	0.60	0/1321
1	E	0.84	0/975	0.60	0/1321
1	G	0.84	0/975	0.60	0/1321
1	I	0.84	0/975	0.60	0/1321
1	K	0.84	0/975	0.60	0/1321
1	M	0.84	0/975	0.60	0/1321
1	O	0.84	0/975	0.60	0/1321
1	Q	0.84	0/975	0.60	0/1321
1	S	0.84	0/975	0.60	0/1321
1	U	0.84	0/975	0.60	0/1321
1	W	0.84	0/975	0.60	0/1321
1	Y	0.84	0/975	0.60	0/1321
1	a	0.84	0/975	0.60	0/1321
1	c	0.84	0/975	0.60	0/1321
1	e	0.84	0/975	0.60	0/1321
1	g	0.84	0/975	0.60	0/1321
1	i	0.84	0/975	0.60	0/1321
1	k	0.84	0/975	0.60	0/1321
1	m	0.84	0/975	0.60	0/1321
1	o	0.84	0/975	0.60	0/1321
1	q	0.84	0/975	0.60	0/1321
1	s	0.84	0/975	0.60	0/1321
1	u	0.84	0/975	0.60	0/1321
1	w	0.84	0/975	0.60	0/1321
1	y	0.84	0/975	0.60	0/1321
2	2	0.74	0/3556	0.67	2/4811 (0.0%)
2	4	0.74	0/3556	0.67	2/4811 (0.0%)
2	6	0.74	0/3556	0.67	2/4811 (0.0%)
2	8	0.74	0/3556	0.67	2/4811 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	B	0.74	0/3556	0.67	2/4811 (0.0%)
2	D	0.74	0/3556	0.67	2/4811 (0.0%)
2	F	0.74	0/3556	0.67	2/4811 (0.0%)
2	H	0.74	0/3556	0.67	2/4811 (0.0%)
2	J	0.74	0/3556	0.67	2/4811 (0.0%)
2	L	0.74	0/3556	0.67	2/4811 (0.0%)
2	N	0.74	0/3556	0.67	2/4811 (0.0%)
2	P	0.74	0/3556	0.67	2/4811 (0.0%)
2	R	0.74	0/3556	0.67	2/4811 (0.0%)
2	T	0.74	0/3556	0.67	2/4811 (0.0%)
2	V	0.74	0/3556	0.67	2/4811 (0.0%)
2	X	0.74	0/3556	0.67	2/4811 (0.0%)
2	Z	0.74	0/3556	0.67	2/4811 (0.0%)
2	b	0.74	0/3556	0.67	2/4811 (0.0%)
2	d	0.74	0/3556	0.67	2/4811 (0.0%)
2	f	0.74	0/3556	0.67	2/4811 (0.0%)
2	h	0.74	0/3556	0.67	2/4811 (0.0%)
2	j	0.74	0/3556	0.67	2/4811 (0.0%)
2	l	0.74	0/3556	0.67	2/4811 (0.0%)
2	n	0.74	0/3556	0.67	2/4811 (0.0%)
2	p	0.74	0/3556	0.67	2/4811 (0.0%)
2	r	0.74	0/3556	0.67	2/4811 (0.0%)
2	t	0.74	0/3556	0.67	2/4811 (0.0%)
2	v	0.74	0/3556	0.67	2/4811 (0.0%)
2	x	0.74	0/3556	0.67	2/4811 (0.0%)
2	z	0.74	0/3556	0.67	2/4811 (0.0%)
All	All	0.77	0/135930	0.66	60/183960 (0.0%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	242	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	v	242	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	2	242	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	P	242	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	n	242	ARG	NE-CZ-NH2	-5.93	117.34	120.30
2	6	242	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	d	242	ARG	NE-CZ-NH2	-5.91	117.34	120.30
2	B	242	ARG	NE-CZ-NH2	-5.91	117.35	120.30
2	J	242	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	R	242	ARG	NE-CZ-NH2	-5.90	117.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	r	242	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	Z	242	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	z	242	ARG	NE-CZ-NH2	-5.87	117.36	120.30
2	L	242	ARG	NE-CZ-NH2	-5.87	117.37	120.30
2	T	242	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	V	242	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	F	242	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	f	242	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	H	242	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	b	242	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	x	242	ARG	NE-CZ-NH2	-5.85	117.37	120.30
2	4	242	ARG	NE-CZ-NH2	-5.85	117.38	120.30
2	t	242	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	h	242	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	N	242	ARG	NE-CZ-NH2	-5.83	117.39	120.30
2	X	242	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	8	242	ARG	NE-CZ-NH2	-5.81	117.39	120.30
2	D	242	ARG	NE-CZ-NH2	-5.81	117.39	120.30
2	l	242	ARG	NE-CZ-NH2	-5.79	117.40	120.30
2	p	242	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	L	284	ARG	NE-CZ-NH2	-5.37	117.61	120.30
2	j	284	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	v	284	ARG	NE-CZ-NH2	-5.35	117.63	120.30
2	p	284	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	4	284	ARG	NE-CZ-NH2	-5.33	117.63	120.30
2	H	284	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	8	284	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	Z	284	ARG	NE-CZ-NH2	-5.31	117.64	120.30
2	n	284	ARG	NE-CZ-NH2	-5.31	117.64	120.30
2	d	284	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	h	284	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	V	284	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	T	284	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	D	284	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	2	284	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	F	284	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	P	284	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	x	284	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	l	284	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	R	284	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	b	284	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	B	284	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	284	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	6	284	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	t	284	ARG	NE-CZ-NH2	-5.25	117.68	120.30
2	N	284	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	J	284	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	z	284	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	f	284	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	r	284	ARG	NE-CZ-NH2	-5.21	117.70	120.30

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	963	0	986	3	0
1	3	963	0	986	4	0
1	5	963	0	986	2	0
1	7	963	0	986	3	0
1	A	963	0	986	6	0
1	C	963	0	986	4	0
1	E	963	0	986	2	0
1	G	963	0	986	3	0
1	I	963	0	986	2	0
1	K	963	0	986	4	0
1	M	963	0	986	4	0
1	O	963	0	986	4	0
1	Q	963	0	986	4	0
1	S	963	0	986	4	0
1	U	963	0	986	3	0
1	W	963	0	986	3	0
1	Y	963	0	986	2	0
1	a	963	0	986	0	0
1	c	963	0	986	0	0
1	e	963	0	986	0	0
1	g	963	0	986	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	i	963	0	986	0	0
1	k	963	0	986	0	0
1	m	963	0	986	0	0
1	o	963	0	986	0	0
1	q	963	0	986	0	0
1	s	963	0	986	0	0
1	u	963	0	986	0	0
1	w	963	0	986	0	0
1	y	963	0	986	0	0
2	2	3468	0	3386	14	0
2	4	3468	0	3386	13	0
2	6	3468	0	3386	13	0
2	8	3468	0	3386	11	0
2	B	3468	0	3386	14	0
2	D	3468	0	3386	14	0
2	F	3468	0	3386	13	0
2	H	3468	0	3386	16	0
2	J	3468	0	3386	18	0
2	L	3468	0	3386	14	0
2	N	3468	0	3386	14	0
2	P	3468	0	3386	14	0
2	R	3468	0	3386	15	0
2	T	3468	0	3386	15	0
2	V	3468	0	3386	16	0
2	X	3468	0	3386	16	0
2	Z	3468	0	3386	15	0
2	b	3468	0	3386	0	0
2	d	3468	0	3386	0	0
2	f	3468	0	3386	0	0
2	h	3468	0	3386	0	0
2	j	3468	0	3386	0	0
2	l	3468	0	3386	0	0
2	n	3468	0	3386	0	0
2	p	3468	0	3386	0	0
2	r	3468	0	3386	0	0
2	t	3468	0	3386	0	0
2	v	3468	0	3386	0	0
2	x	3468	0	3386	0	0
2	z	3468	0	3386	0	0
All	All	132930	0	131160	302	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 1.

All (302) 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:A:126:LEU:O	1:A:126:LEU:HG	1.92	0.70
1:1:126:LEU:HG	1:1:126:LEU:O	1.92	0.70
1:G:126:LEU:HG	1:G:126:LEU:O	1.92	0.69
1:O:126:LEU:HG	1:O:126:LEU:O	1.92	0.69
1:C:126:LEU:O	1:C:126:LEU:HG	1.92	0.69
1:Y:126:LEU:HG	1:Y:126:LEU:O	1.92	0.69
1:M:126:LEU:HG	1:M:126:LEU:O	1.92	0.69
1:U:126:LEU:HG	1:U:126:LEU:O	1.92	0.69
1:7:126:LEU:HG	1:7:126:LEU:O	1.92	0.69
1:W:126:LEU:HG	1:W:126:LEU:O	1.92	0.69
1:S:126:LEU:O	1:S:126:LEU:HG	1.92	0.69
1:K:126:LEU:O	1:K:126:LEU:HG	1.92	0.69
1:3:126:LEU:O	1:3:126:LEU:HG	1.92	0.68
1:5:126:LEU:O	1:5:126:LEU:HG	1.92	0.68
1:E:126:LEU:HG	1:E:126:LEU:O	1.92	0.68
1:Q:126:LEU:HG	1:Q:126:LEU:O	1.92	0.68
1:I:126:LEU:O	1:I:126:LEU:HG	1.92	0.68
2:B:240:ALA:HB3	2:B:241:PRO:HD3	1.92	0.53
2:D:240:ALA:HB3	2:D:241:PRO:HD3	1.91	0.53
2:R:240:ALA:HB3	2:R:241:PRO:HD3	1.92	0.52
2:4:240:ALA:HB3	2:4:241:PRO:HD3	1.91	0.52
2:P:240:ALA:HB3	2:P:241:PRO:HD3	1.92	0.52
2:2:240:ALA:HB3	2:2:241:PRO:HD3	1.91	0.52
2:F:240:ALA:HB3	2:F:241:PRO:HD3	1.92	0.52
2:N:240:ALA:HB3	2:N:241:PRO:HD3	1.92	0.52
2:6:240:ALA:HB3	2:6:241:PRO:HD3	1.92	0.52
2:T:240:ALA:HB3	2:T:241:PRO:HD3	1.92	0.52
2:Z:240:ALA:HB3	2:Z:241:PRO:HD3	1.91	0.52
2:L:240:ALA:HB3	2:L:241:PRO:HD3	1.91	0.52
2:F:169:THR:HB	2:F:170:PRO:HD3	1.92	0.51
2:X:240:ALA:HB3	2:X:241:PRO:HD3	1.91	0.51
2:R:169:THR:HB	2:R:170:PRO:HD3	1.92	0.51
2:6:169:THR:HB	2:6:170:PRO:HD3	1.92	0.51
2:H:240:ALA:HB3	2:H:241:PRO:HD3	1.92	0.51
2:T:169:THR:HB	2:T:170:PRO:HD3	1.92	0.51
2:8:240:ALA:HB3	2:8:241:PRO:HD3	1.91	0.51
2:J:240:ALA:HB3	2:J:241:PRO:HD3	1.91	0.51
2:2:240:ALA:HB3	2:2:241:PRO:CD	2.41	0.51
2:V:240:ALA:HB3	2:V:241:PRO:CD	2.41	0.51
2:B:240:ALA:HB3	2:B:241:PRO:CD	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:240:ALA:HB3	2:Z:241:PRO:CD	2.41	0.51
2:L:240:ALA:HB3	2:L:241:PRO:CD	2.41	0.51
2:D:169:THR:HB	2:D:170:PRO:HD3	1.92	0.51
2:8:169:THR:HB	2:8:170:PRO:HD3	1.92	0.51
2:V:240:ALA:HB3	2:V:241:PRO:HD3	1.91	0.51
2:L:169:THR:HB	2:L:170:PRO:HD3	1.92	0.51
2:B:240:ALA:CB	2:B:241:PRO:CD	2.89	0.51
2:4:240:ALA:HB3	2:4:241:PRO:CD	2.41	0.51
2:2:240:ALA:CB	2:2:241:PRO:CD	2.89	0.51
2:6:240:ALA:HB3	2:6:241:PRO:CD	2.41	0.51
2:T:240:ALA:HB3	2:T:241:PRO:CD	2.41	0.51
2:8:240:ALA:HB3	2:8:241:PRO:CD	2.41	0.51
2:Z:169:THR:HB	2:Z:170:PRO:HD3	1.92	0.51
2:N:169:THR:HB	2:N:170:PRO:HD3	1.92	0.51
2:D:240:ALA:HB3	2:D:241:PRO:CD	2.41	0.51
2:P:240:ALA:CB	2:P:241:PRO:CD	2.89	0.51
2:F:240:ALA:HB3	2:F:241:PRO:CD	2.41	0.51
2:N:240:ALA:CB	2:N:241:PRO:CD	2.89	0.51
2:4:328:GLU:N	2:4:328:GLU:OE1	2.38	0.51
2:J:328:GLU:N	2:J:328:GLU:OE1	2.38	0.51
2:X:169:THR:HB	2:X:170:PRO:HD3	1.92	0.51
2:4:169:THR:HB	2:4:170:PRO:HD3	1.92	0.51
2:P:240:ALA:HB3	2:P:241:PRO:CD	2.41	0.50
2:X:240:ALA:HB3	2:X:241:PRO:CD	2.41	0.50
2:H:240:ALA:HB3	2:H:241:PRO:CD	2.41	0.50
2:H:169:THR:HB	2:H:170:PRO:HD3	1.92	0.50
2:L:240:ALA:CB	2:L:241:PRO:CD	2.89	0.50
2:Z:328:GLU:N	2:Z:328:GLU:OE1	2.38	0.50
2:B:169:THR:HB	2:B:170:PRO:HD3	1.92	0.50
2:D:240:ALA:CB	2:D:241:PRO:CD	2.89	0.50
2:R:240:ALA:HB3	2:R:241:PRO:CD	2.41	0.50
2:Z:240:ALA:CB	2:Z:241:PRO:CD	2.89	0.50
2:L:328:GLU:N	2:L:328:GLU:OE1	2.38	0.50
2:4:240:ALA:CB	2:4:241:PRO:CD	2.89	0.50
2:J:240:ALA:HB3	2:J:241:PRO:CD	2.41	0.50
2:2:169:THR:HB	2:2:170:PRO:HD3	1.92	0.50
2:V:328:GLU:OE1	2:V:328:GLU:N	2.38	0.50
2:N:240:ALA:HB3	2:N:241:PRO:CD	2.41	0.50
2:T:240:ALA:CB	2:T:241:PRO:CD	2.89	0.50
2:X:240:ALA:CB	2:X:241:PRO:CD	2.89	0.50
2:J:169:THR:HB	2:J:170:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:328:GLU:OE1	2:P:328:GLU:N	2.38	0.50
2:R:240:ALA:CB	2:R:241:PRO:CD	2.89	0.50
2:8:240:ALA:CB	2:8:241:PRO:CD	2.89	0.50
2:B:328:GLU:N	2:B:328:GLU:OE1	2.38	0.50
2:H:240:ALA:CB	2:H:241:PRO:CD	2.89	0.50
2:P:169:THR:HB	2:P:170:PRO:HD3	1.92	0.50
2:F:240:ALA:CB	2:F:241:PRO:CD	2.89	0.49
2:6:240:ALA:CB	2:6:241:PRO:CD	2.89	0.49
2:J:240:ALA:CB	2:J:241:PRO:CD	2.89	0.49
2:N:328:GLU:OE1	2:N:328:GLU:N	2.38	0.49
2:X:328:GLU:OE1	2:X:328:GLU:N	2.38	0.49
2:V:169:THR:HB	2:V:170:PRO:HD3	1.92	0.49
2:V:240:ALA:CB	2:V:241:PRO:CD	2.89	0.49
2:D:328:GLU:N	2:D:328:GLU:OE1	2.38	0.49
1:O:126:LEU:CG	1:O:126:LEU:O	2.61	0.49
2:2:328:GLU:N	2:2:328:GLU:OE1	2.38	0.49
1:M:126:LEU:O	1:M:126:LEU:CG	2.61	0.49
1:U:125:ALA:O	1:U:126:LEU:C	2.51	0.49
1:W:125:ALA:O	1:W:126:LEU:C	2.51	0.49
1:W:126:LEU:CG	1:W:126:LEU:O	2.61	0.49
1:5:125:ALA:O	1:5:126:LEU:C	2.51	0.49
1:E:125:ALA:O	1:E:126:LEU:C	2.51	0.49
1:I:125:ALA:O	1:I:126:LEU:C	2.51	0.49
2:H:328:GLU:OE1	2:H:328:GLU:N	2.38	0.49
1:M:125:ALA:O	1:M:126:LEU:C	2.51	0.49
1:S:125:ALA:O	1:S:126:LEU:C	2.51	0.49
1:K:125:ALA:O	1:K:126:LEU:C	2.51	0.49
1:3:125:ALA:O	1:3:126:LEU:C	2.51	0.48
1:Q:125:ALA:O	1:Q:126:LEU:C	2.51	0.48
2:B:240:ALA:CB	2:B:241:PRO:HD3	2.43	0.48
2:N:240:ALA:CB	2:N:241:PRO:HD3	2.43	0.48
1:1:125:ALA:O	1:1:126:LEU:C	2.51	0.48
1:A:125:ALA:O	1:A:126:LEU:C	2.51	0.48
1:G:125:ALA:O	1:G:126:LEU:C	2.51	0.48
1:Y:125:ALA:O	1:Y:126:LEU:C	2.51	0.48
2:2:240:ALA:CB	2:2:241:PRO:HD3	2.43	0.48
2:Z:240:ALA:CB	2:Z:241:PRO:HD3	2.43	0.48
2:L:240:ALA:CB	2:L:241:PRO:HD3	2.43	0.48
2:J:240:ALA:CB	2:J:241:PRO:HD3	2.43	0.48
2:X:240:ALA:CB	2:X:241:PRO:HD3	2.43	0.48
2:V:240:ALA:CB	2:V:241:PRO:HD3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:CG	1:A:126:LEU:O	2.61	0.48
1:C:125:ALA:O	1:C:126:LEU:C	2.51	0.48
2:P:240:ALA:CB	2:P:241:PRO:HD3	2.43	0.48
2:H:240:ALA:CB	2:H:241:PRO:HD3	2.43	0.48
2:Z:206:LEU:HB2	2:Z:207:PRO:HD3	1.96	0.48
1:O:125:ALA:O	1:O:126:LEU:C	2.51	0.48
1:7:125:ALA:O	1:7:126:LEU:C	2.51	0.48
2:N:206:LEU:HB2	2:N:207:PRO:HD3	1.96	0.48
2:L:206:LEU:HB2	2:L:207:PRO:HD3	1.96	0.48
2:6:328:GLU:N	2:6:328:GLU:OE1	2.38	0.48
2:2:206:LEU:HB2	2:2:207:PRO:HD3	1.96	0.48
2:X:206:LEU:HB2	2:X:207:PRO:HD3	1.96	0.48
2:6:240:ALA:CB	2:6:241:PRO:HD3	2.43	0.47
2:T:240:ALA:CB	2:T:241:PRO:HD3	2.43	0.47
2:8:240:ALA:CB	2:8:241:PRO:HD3	2.43	0.47
2:D:240:ALA:CB	2:D:241:PRO:HD3	2.43	0.47
2:B:206:LEU:HB2	2:B:207:PRO:HD3	1.96	0.47
2:R:389:LEU:N	2:R:390:PRO:CD	2.77	0.47
2:F:240:ALA:CB	2:F:241:PRO:HD3	2.43	0.47
2:D:389:LEU:N	2:D:390:PRO:CD	2.78	0.47
2:P:206:LEU:HB2	2:P:207:PRO:HD3	1.96	0.47
2:6:389:LEU:N	2:6:390:PRO:CD	2.77	0.47
2:F:389:LEU:N	2:F:390:PRO:CD	2.78	0.47
2:F:206:LEU:HB2	2:F:207:PRO:HD3	1.96	0.47
2:4:389:LEU:N	2:4:390:PRO:CD	2.77	0.47
2:J:206:LEU:HB2	2:J:207:PRO:HD3	1.96	0.47
2:T:206:LEU:HB2	2:T:207:PRO:HD3	1.96	0.47
2:R:240:ALA:CB	2:R:241:PRO:HD3	2.43	0.47
2:4:240:ALA:CB	2:4:241:PRO:HD3	2.43	0.47
2:8:206:LEU:HB2	2:8:207:PRO:HD3	1.96	0.47
2:P:389:LEU:N	2:P:390:PRO:CD	2.78	0.47
2:J:389:LEU:N	2:J:390:PRO:CD	2.78	0.47
2:R:206:LEU:HB2	2:R:207:PRO:HD3	1.96	0.47
2:4:206:LEU:HB2	2:4:207:PRO:HD3	1.96	0.47
2:T:389:LEU:N	2:T:390:PRO:CD	2.77	0.47
2:6:206:LEU:HB2	2:6:207:PRO:HD3	1.96	0.47
2:X:389:LEU:N	2:X:390:PRO:CD	2.77	0.47
2:L:389:LEU:N	2:L:390:PRO:CD	2.77	0.47
2:Z:389:LEU:N	2:Z:390:PRO:CD	2.77	0.47
2:H:206:LEU:HB2	2:H:207:PRO:HD3	1.96	0.47
2:D:206:LEU:HB2	2:D:207:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:328:GLU:N	2:8:328:GLU:OE1	2.38	0.46
2:8:389:LEU:N	2:8:390:PRO:CD	2.77	0.46
2:B:389:LEU:N	2:B:390:PRO:CD	2.78	0.46
2:H:389:LEU:N	2:H:390:PRO:CD	2.77	0.46
2:2:389:LEU:N	2:2:390:PRO:CD	2.78	0.46
1:1:112:GLU:OE1	1:1:112:GLU:N	2.39	0.46
1:A:112:GLU:N	1:A:112:GLU:OE1	2.39	0.46
2:T:284:ARG:NE	2:T:284:ARG:HA	2.31	0.46
2:N:389:LEU:N	2:N:390:PRO:CD	2.77	0.46
2:B:284:ARG:HA	2:B:284:ARG:NE	2.31	0.46
2:V:389:LEU:N	2:V:390:PRO:CD	2.77	0.46
2:D:284:ARG:HA	2:D:284:ARG:NE	2.31	0.46
2:2:284:ARG:NE	2:2:284:ARG:HA	2.31	0.46
2:X:284:ARG:NE	2:X:284:ARG:HA	2.31	0.46
2:L:284:ARG:HA	2:L:284:ARG:NE	2.31	0.46
1:Q:112:GLU:OE1	1:Q:112:GLU:N	2.39	0.46
2:H:284:ARG:HA	2:H:284:ARG:NE	2.31	0.46
2:6:284:ARG:NE	2:6:284:ARG:HA	2.31	0.46
2:V:206:LEU:HB2	2:V:207:PRO:HD3	1.96	0.46
2:V:284:ARG:NE	2:V:284:ARG:HA	2.31	0.46
2:J:284:ARG:HA	2:J:284:ARG:NE	2.31	0.46
2:T:328:GLU:OE1	2:T:328:GLU:N	2.38	0.46
2:8:284:ARG:HA	2:8:284:ARG:NE	2.31	0.46
2:R:284:ARG:NE	2:R:284:ARG:HA	2.31	0.46
2:Z:284:ARG:HA	2:Z:284:ARG:NE	2.31	0.46
2:N:284:ARG:NE	2:N:284:ARG:HA	2.31	0.46
1:O:112:GLU:OE1	1:O:112:GLU:N	2.39	0.45
1:3:112:GLU:N	1:3:112:GLU:OE1	2.39	0.45
1:C:112:GLU:N	1:C:112:GLU:OE1	2.39	0.45
2:4:284:ARG:HA	2:4:284:ARG:NE	2.31	0.45
2:P:284:ARG:NE	2:P:284:ARG:HA	2.31	0.45
1:S:126:LEU:O	1:S:126:LEU:CG	2.61	0.45
2:F:284:ARG:HA	2:F:284:ARG:NE	2.31	0.45
2:F:328:GLU:N	2:F:328:GLU:OE1	2.38	0.44
2:P:284:ARG:HA	2:P:284:ARG:CZ	2.48	0.44
2:N:284:ARG:CZ	2:N:284:ARG:HA	2.48	0.43
2:R:284:ARG:CZ	2:R:284:ARG:HA	2.48	0.43
2:4:284:ARG:HA	2:4:284:ARG:CZ	2.49	0.43
1:G:126:LEU:CG	1:G:126:LEU:O	2.61	0.43
2:D:284:ARG:HA	2:D:284:ARG:CZ	2.48	0.43
2:6:284:ARG:CZ	2:6:284:ARG:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:284:ARG:CZ	2:F:284:ARG:HA	2.48	0.43
2:B:284:ARG:CZ	2:B:284:ARG:HA	2.48	0.43
2:T:284:ARG:CZ	2:T:284:ARG:HA	2.48	0.43
2:2:284:ARG:CZ	2:2:284:ARG:HA	2.49	0.43
2:T:211:ASP:OD1	2:T:211:ASP:C	2.58	0.43
2:D:211:ASP:OD1	2:D:211:ASP:C	2.58	0.43
2:L:284:ARG:HA	2:L:284:ARG:CZ	2.48	0.43
2:B:211:ASP:C	2:B:211:ASP:OD1	2.58	0.43
2:F:211:ASP:C	2:F:211:ASP:OD1	2.58	0.43
2:X:284:ARG:CZ	2:X:284:ARG:HA	2.48	0.42
2:H:211:ASP:OD1	2:H:211:ASP:C	2.58	0.42
2:2:211:ASP:OD1	2:2:211:ASP:C	2.58	0.42
2:R:211:ASP:C	2:R:211:ASP:OD1	2.58	0.42
2:V:284:ARG:HA	2:V:284:ARG:CZ	2.48	0.42
2:Z:284:ARG:CZ	2:Z:284:ARG:HA	2.48	0.42
2:8:284:ARG:CZ	2:8:284:ARG:HA	2.49	0.42
2:V:211:ASP:C	2:V:211:ASP:OD1	2.58	0.42
2:4:211:ASP:OD1	2:4:211:ASP:C	2.58	0.42
2:H:284:ARG:CZ	2:H:284:ARG:HA	2.48	0.42
2:J:284:ARG:HA	2:J:284:ARG:CZ	2.49	0.42
2:R:328:GLU:N	2:R:328:GLU:OE1	2.38	0.42
2:N:211:ASP:C	2:N:211:ASP:OD1	2.58	0.42
2:J:211:ASP:OD1	2:J:211:ASP:C	2.58	0.42
2:X:211:ASP:C	2:X:211:ASP:OD1	2.58	0.42
2:4:206:LEU:N	2:4:207:PRO:CD	2.83	0.41
2:D:206:LEU:N	2:D:207:PRO:CD	2.83	0.41
2:2:250:ASP:HA	2:2:251:PRO:HD3	1.95	0.41
2:J:206:LEU:N	2:J:207:PRO:CD	2.83	0.41
2:R:206:LEU:N	2:R:207:PRO:CD	2.83	0.41
2:6:206:LEU:N	2:6:207:PRO:CD	2.83	0.41
2:Z:211:ASP:OD1	2:Z:211:ASP:C	2.58	0.41
2:L:211:ASP:C	2:L:211:ASP:OD1	2.58	0.41
2:B:206:LEU:N	2:B:207:PRO:CD	2.83	0.41
2:P:206:LEU:N	2:P:207:PRO:CD	2.83	0.41
2:F:206:LEU:N	2:F:207:PRO:CD	2.83	0.41
2:T:206:LEU:N	2:T:207:PRO:CD	2.83	0.41
2:8:206:LEU:N	2:8:207:PRO:CD	2.83	0.41
2:P:211:ASP:OD1	2:P:211:ASP:C	2.58	0.41
1:3:102:ALA:HA	1:3:103:PRO:HD3	1.92	0.41
1:7:126:LEU:CG	1:7:126:LEU:O	2.61	0.41
2:L:206:LEU:N	2:L:207:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:206:LEU:N	2:X:207:PRO:CD	2.83	0.41
1:U:102:ALA:HA	1:U:103:PRO:HD3	1.92	0.41
2:N:206:LEU:N	2:N:207:PRO:CD	2.83	0.41
2:2:206:LEU:N	2:2:207:PRO:CD	2.83	0.41
2:V:206:LEU:N	2:V:207:PRO:CD	2.83	0.41
2:Z:295:CYS:N	2:Z:296:PRO:CD	2.84	0.41
2:Z:206:LEU:N	2:Z:207:PRO:CD	2.83	0.41
2:H:206:LEU:N	2:H:207:PRO:CD	2.83	0.41
2:N:295:CYS:N	2:N:296:PRO:CD	2.84	0.41
2:6:211:ASP:OD1	2:6:211:ASP:C	2.58	0.41
2:2:295:CYS:N	2:2:296:PRO:CD	2.84	0.41
1:K:126:LEU:CG	1:K:126:LEU:O	2.61	0.41
2:J:250:ASP:HA	2:J:251:PRO:HD3	1.95	0.41
2:L:295:CYS:N	2:L:296:PRO:CD	2.84	0.41
1:A:102:ALA:HA	1:A:103:PRO:HD3	1.92	0.41
1:C:126:LEU:CG	1:C:126:LEU:O	2.61	0.41
2:B:295:CYS:N	2:B:296:PRO:CD	2.84	0.41
2:V:377:LYS:HD2	2:V:377:LYS:HA	1.95	0.41
2:J:310:LEU:HA	2:J:311:PRO:HD3	1.94	0.41
2:D:377:LYS:HD2	2:D:377:LYS:HA	1.95	0.41
2:P:295:CYS:N	2:P:296:PRO:CD	2.84	0.41
2:X:295:CYS:N	2:X:296:PRO:CD	2.84	0.41
2:H:250:ASP:HA	2:H:251:PRO:HD3	1.95	0.41
2:T:295:CYS:N	2:T:296:PRO:CD	2.84	0.41
2:F:295:CYS:N	2:F:296:PRO:CD	2.84	0.41
2:J:206:LEU:N	2:J:207:PRO:HD2	2.37	0.40
2:J:295:CYS:N	2:J:296:PRO:CD	2.84	0.40
2:6:295:CYS:N	2:6:296:PRO:CD	2.84	0.40
2:V:250:ASP:HA	2:V:251:PRO:HD3	1.95	0.40
2:X:206:LEU:N	2:X:207:PRO:HD2	2.37	0.40
2:T:206:LEU:N	2:T:207:PRO:HD2	2.36	0.40
2:B:284:ARG:CA	2:B:284:ARG:NE	2.84	0.40
2:V:206:LEU:N	2:V:207:PRO:HD2	2.36	0.40
1:A:89:LEU:HA	1:A:90:PRO:HD2	2.00	0.40
1:K:102:ALA:HA	1:K:103:PRO:HD3	1.92	0.40
2:J:300:GLY:HA2	2:J:301:PRO:HD3	1.92	0.40
2:R:295:CYS:N	2:R:296:PRO:CD	2.84	0.40
2:L:206:LEU:N	2:L:207:PRO:HD2	2.37	0.40
2:D:284:ARG:CA	2:D:284:ARG:NE	2.84	0.40
2:H:284:ARG:NE	2:H:284:ARG:CA	2.84	0.40
2:Z:284:ARG:CA	2:Z:284:ARG:NE	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:284:ARG:NE	2:P:284:ARG:CA	2.84	0.40
2:H:295:CYS:N	2:H:296:PRO:CD	2.84	0.40
1:M:89:LEU:HA	1:M:90:PRO:HD2	2.00	0.40
2:X:250:ASP:HA	2:X:251:PRO:HD3	1.95	0.40
1:Q:126:LEU:CG	1:Q:126:LEU:O	2.61	0.40
2:R:206:LEU:N	2:R:207:PRO:HD2	2.37	0.40
2:H:206:LEU:N	2:H:207:PRO:HD2	2.36	0.40
2:X:284:ARG:NE	2:X:284:ARG:CA	2.84	0.40
2:R:284:ARG:NE	2:R:284:ARG:CA	2.84	0.40
2:T:377:LYS:HD2	2:T:377:LYS:HA	1.96	0.40
2:V:295:CYS:N	2:V:296:PRO:CD	2.84	0.40
2:4:295:CYS:N	2:4:296:PRO:CD	2.84	0.40
2:Z:206:LEU:N	2:Z:207:PRO:HD2	2.37	0.40
2:J:284:ARG:NE	2:J:284:ARG:CA	2.84	0.40
2:N:284:ARG:CA	2:N:284:ARG:NE	2.84	0.40
1:S:102:ALA:HA	1:S:103:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	3	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	5	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	7	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	A	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	C	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	E	123/125 (98%)	120 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	I	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	K	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	M	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	O	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	Q	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	S	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	U	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	W	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	Y	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	a	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	c	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	e	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	g	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	i	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	k	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	m	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	o	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	q	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	s	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	u	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	w	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	y	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
2	2	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	4	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	6	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	8	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	B	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	D	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	F	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	H	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	L	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	N	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	P	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	R	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	T	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	V	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	X	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	Z	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	b	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	d	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	f	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	h	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	j	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	l	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	n	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	p	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	r	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	t	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	v	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	x	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
2	z	430/432 (100%)	409 (95%)	17 (4%)	4 (1%)	21	68
All	All	16590/16710 (99%)	15870 (96%)	600 (4%)	120 (1%)	31	72

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	240	ALA
2	D	240	ALA
2	F	240	ALA
2	H	240	ALA
2	J	240	ALA
2	L	240	ALA
2	N	240	ALA

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Mol	Chain	Res	Type
2	P	240	ALA
2	R	240	ALA
2	T	240	ALA
2	V	240	ALA
2	X	240	ALA
2	Z	240	ALA
2	b	240	ALA
2	d	240	ALA
2	f	240	ALA
2	h	240	ALA
2	j	240	ALA
2	l	240	ALA
2	n	240	ALA
2	p	240	ALA
2	r	240	ALA
2	t	240	ALA
2	v	240	ALA
2	x	240	ALA
2	z	240	ALA
2	2	240	ALA
2	4	240	ALA
2	6	240	ALA
2	8	240	ALA
2	H	258	SER
2	L	258	SER
2	X	258	SER
2	d	258	SER
2	v	258	SER
2	z	258	SER
2	8	258	SER
2	B	258	SER
2	B	296	PRO
2	D	258	SER
2	D	296	PRO
2	F	258	SER
2	F	296	PRO
2	H	296	PRO
2	J	258	SER
2	J	296	PRO
2	L	296	PRO
2	N	258	SER
2	N	296	PRO

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Mol	Chain	Res	Type
2	P	258	SER
2	P	296	PRO
2	R	258	SER
2	R	296	PRO
2	T	258	SER
2	T	296	PRO
2	V	258	SER
2	V	296	PRO
2	X	296	PRO
2	Z	258	SER
2	Z	296	PRO
2	b	258	SER
2	b	296	PRO
2	d	296	PRO
2	f	258	SER
2	f	296	PRO
2	h	258	SER
2	h	296	PRO
2	j	258	SER
2	j	296	PRO
2	l	258	SER
2	l	296	PRO
2	n	258	SER
2	n	296	PRO
2	p	258	SER
2	p	296	PRO
2	r	258	SER
2	r	296	PRO
2	t	258	SER
2	t	296	PRO
2	v	296	PRO
2	x	258	SER
2	x	296	PRO
2	z	296	PRO
2	2	258	SER
2	2	296	PRO
2	4	258	SER
2	4	296	PRO
2	6	258	SER
2	6	296	PRO
2	8	296	PRO
2	B	309	ASP

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Mol	Chain	Res	Type
2	D	309	ASP
2	F	309	ASP
2	H	309	ASP
2	J	309	ASP
2	L	309	ASP
2	N	309	ASP
2	P	309	ASP
2	R	309	ASP
2	T	309	ASP
2	V	309	ASP
2	X	309	ASP
2	Z	309	ASP
2	b	309	ASP
2	d	309	ASP
2	f	309	ASP
2	h	309	ASP
2	j	309	ASP
2	l	309	ASP
2	n	309	ASP
2	p	309	ASP
2	r	309	ASP
2	t	309	ASP
2	v	309	ASP
2	x	309	ASP
2	z	309	ASP
2	2	309	ASP
2	4	309	ASP
2	6	309	ASP
2	8	309	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	106/106 (100%)	106 (100%)	0	100	100
1	3	106/106 (100%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	106/106 (100%)	106 (100%)	0	100	100
1	7	106/106 (100%)	106 (100%)	0	100	100
1	A	106/106 (100%)	106 (100%)	0	100	100
1	C	106/106 (100%)	106 (100%)	0	100	100
1	E	106/106 (100%)	106 (100%)	0	100	100
1	G	106/106 (100%)	106 (100%)	0	100	100
1	I	106/106 (100%)	106 (100%)	0	100	100
1	K	106/106 (100%)	106 (100%)	0	100	100
1	M	106/106 (100%)	106 (100%)	0	100	100
1	O	106/106 (100%)	106 (100%)	0	100	100
1	Q	106/106 (100%)	106 (100%)	0	100	100
1	S	106/106 (100%)	106 (100%)	0	100	100
1	U	106/106 (100%)	106 (100%)	0	100	100
1	W	106/106 (100%)	106 (100%)	0	100	100
1	Y	106/106 (100%)	106 (100%)	0	100	100
1	a	106/106 (100%)	106 (100%)	0	100	100
1	c	106/106 (100%)	106 (100%)	0	100	100
1	e	106/106 (100%)	106 (100%)	0	100	100
1	g	106/106 (100%)	106 (100%)	0	100	100
1	i	106/106 (100%)	106 (100%)	0	100	100
1	k	106/106 (100%)	106 (100%)	0	100	100
1	m	106/106 (100%)	106 (100%)	0	100	100
1	o	106/106 (100%)	106 (100%)	0	100	100
1	q	106/106 (100%)	106 (100%)	0	100	100
1	s	106/106 (100%)	106 (100%)	0	100	100
1	u	106/106 (100%)	106 (100%)	0	100	100
1	w	106/106 (100%)	106 (100%)	0	100	100
1	y	106/106 (100%)	106 (100%)	0	100	100
2	2	369/369 (100%)	369 (100%)	0	100	100
2	4	369/369 (100%)	369 (100%)	0	100	100
2	6	369/369 (100%)	369 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	8	369/369 (100%)	369 (100%)	0	100	100
2	B	369/369 (100%)	369 (100%)	0	100	100
2	D	369/369 (100%)	369 (100%)	0	100	100
2	F	369/369 (100%)	369 (100%)	0	100	100
2	H	369/369 (100%)	369 (100%)	0	100	100
2	J	369/369 (100%)	369 (100%)	0	100	100
2	L	369/369 (100%)	369 (100%)	0	100	100
2	N	369/369 (100%)	369 (100%)	0	100	100
2	P	369/369 (100%)	369 (100%)	0	100	100
2	R	369/369 (100%)	369 (100%)	0	100	100
2	T	369/369 (100%)	369 (100%)	0	100	100
2	V	369/369 (100%)	369 (100%)	0	100	100
2	X	369/369 (100%)	369 (100%)	0	100	100
2	Z	369/369 (100%)	369 (100%)	0	100	100
2	b	369/369 (100%)	369 (100%)	0	100	100
2	d	369/369 (100%)	369 (100%)	0	100	100
2	f	369/369 (100%)	369 (100%)	0	100	100
2	h	369/369 (100%)	369 (100%)	0	100	100
2	j	369/369 (100%)	369 (100%)	0	100	100
2	l	369/369 (100%)	369 (100%)	0	100	100
2	n	369/369 (100%)	369 (100%)	0	100	100
2	p	369/369 (100%)	369 (100%)	0	100	100
2	r	369/369 (100%)	369 (100%)	0	100	100
2	t	369/369 (100%)	369 (100%)	0	100	100
2	v	369/369 (100%)	369 (100%)	0	100	100
2	x	369/369 (100%)	369 (100%)	0	100	100
2	z	369/369 (100%)	369 (100%)	0	100	100
All	All	14250/14250 (100%)	14250 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.