



wwPDB EM Model Validation Summary Report ⓘ

Apr 8, 2020 – 03:37 PM EDT

PDB ID : 6PYT
EMDB ID : EMD-20526
Title : CryoEM Structure of Pyocin R2 - precontracted - trunk
Authors : Ge, P.; Avaylon, J.; Scholl, D.; Shneider, M.M.; Browning, C.; Buth, S.A.; Plattner, M.; Ding, K.; Leiman, P.G.; Miller, J.F.; Zhou, Z.H.
Deposited on : 2019-07-30
Resolution : 2.90 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

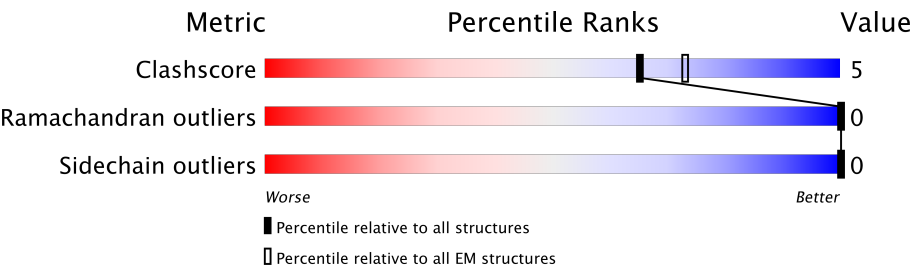
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

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 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	a	167	100%
1	b	167	100%
1	c	167	100%
1	d	167	100%
1	e	167	100%
1	f	167	100%
1	m	167	100%
1	n	167	100%
1	o	167	100%

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Mol	Chain	Length	Quality of chain
1	p	167	 100%
1	q	167	 100%
1	r	167	 100%
2	A	386	 89% 11%
2	B	386	 89% 11%
2	C	386	 90% 10%
2	D	386	 90% 10%
2	E	386	 89% 10%
2	F	386	 90% 10%
2	M	386	 90% 10%
2	N	386	 89% 11%
2	O	386	 89% 11%
2	P	386	 89% 11%
2	Q	386	 90% 10%
2	R	386	 89% 10%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 49920 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 Pyocin tube PA0623.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		
1	a	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		
1	n	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		
1	o	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		
1	p	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		
1	q	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		
1	r	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		
1	b	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		
1	c	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		
1	d	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		
1	e	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		
1	f	167	Total	C	N	O	S	0	0
			1263	800	215	243	5		

- Molecule 2 is a protein called Pyocin sheath PA0622.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
2	A	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
2	N	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
2	P	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
2	Q	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
2	R	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
2	B	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
2	C	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
2	D	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
2	E	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		
2	F	385	Total	C	N	O	S	0	0
			2897	1825	506	558	8		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Pyocin tube PA0623

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Pyocin tube PA0623

Chain a:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Pyocin tube PA0623

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Pyocin tube PA0623

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Pyocin tube PA0623

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Pyocin tube PA0623

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Pyocin tube PA0623

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Pyocin tube PA0623

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Pyocin tube PA0623

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Pyocin tube PA0623

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Pyocin tube PA0623

Chain e:  100%

There are no outlier residues recorded for this chain.

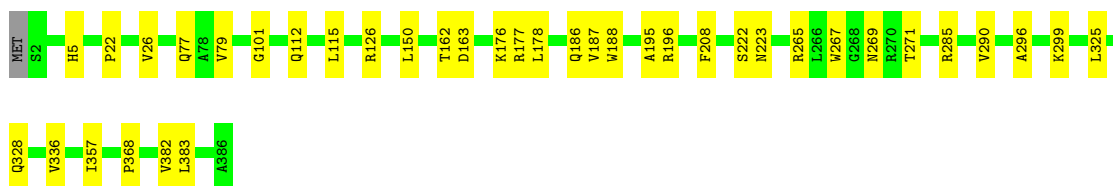
- Molecule 1: Pyocin tube PA0623

Chain f:  100%

There are no outlier residues recorded for this chain.

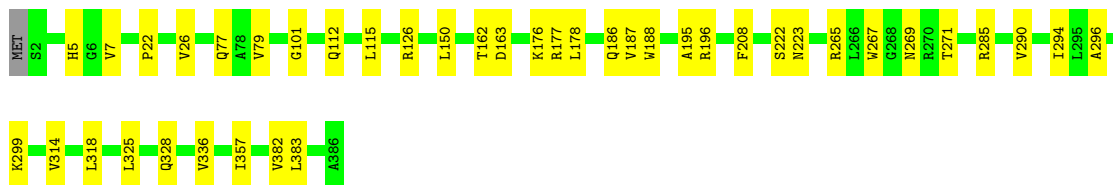
- Molecule 2: Pyocin sheath PA0622

Chain M:  90% 10%



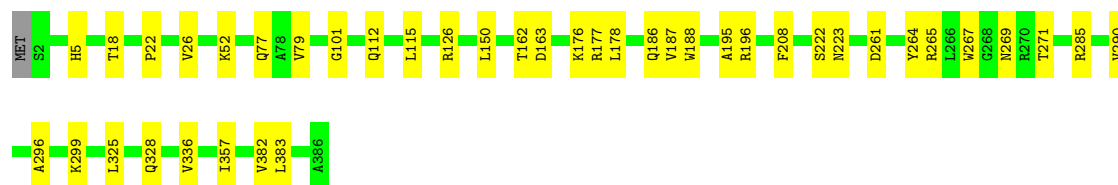
- Molecule 2: Pyocin sheath PA0622

Chain A:  89% 11%



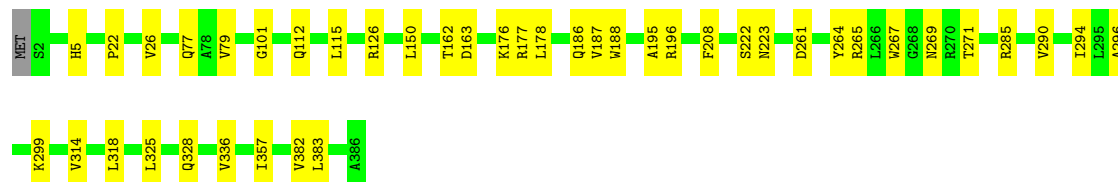
- Molecule 2: Pyocin sheath PA0622

Chain N:  89% 11%



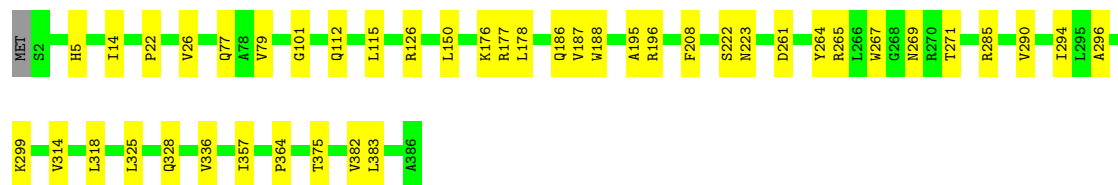
- Molecule 2: Pyocin sheath PA0622

Chain O:
89% 11%



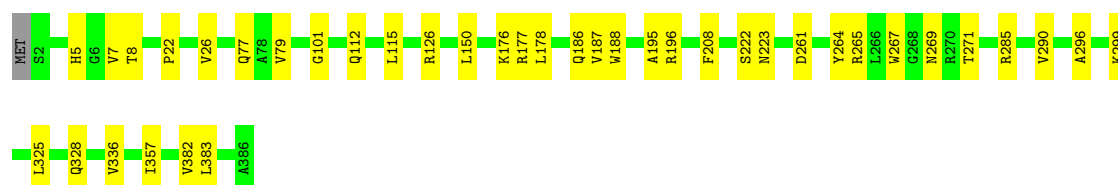
- Molecule 2: Pyocin sheath PA0622

Chain P:
89% 11%



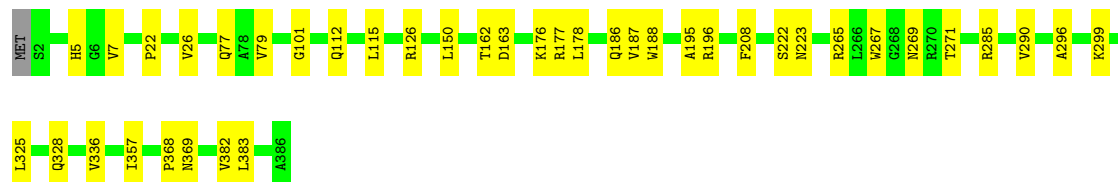
- Molecule 2: Pyocin sheath PA0622

Chain Q:
90% 10%



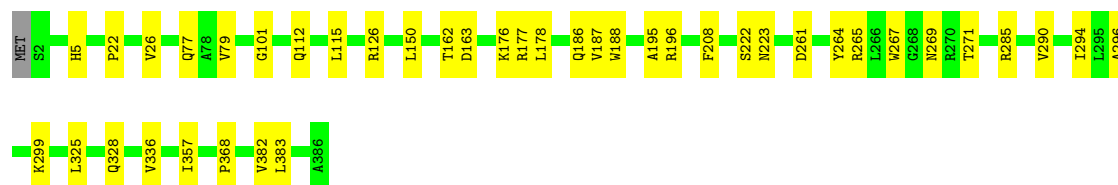
- Molecule 2: Pyocin sheath PA0622

Chain R:
89% 10%



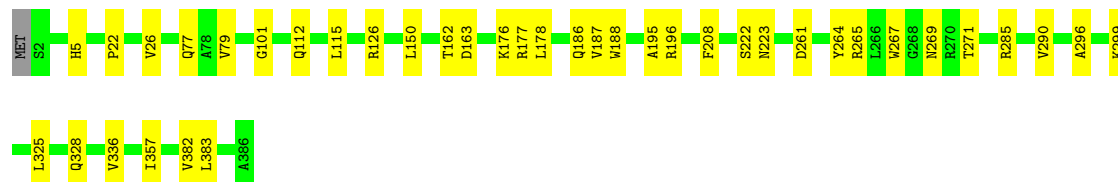
- Molecule 2: Pyocin sheath PA0622

Chain B:
89% 11%



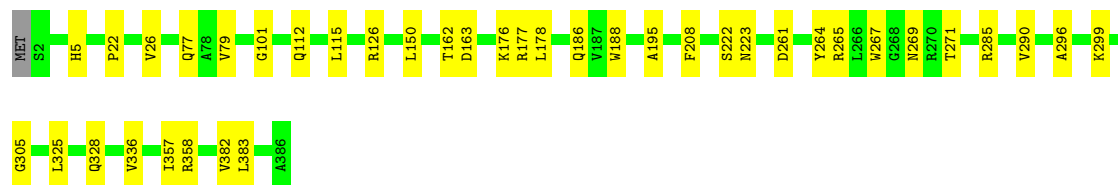
• Molecule 2: Pyocin sheath PA0622

Chain C: 90% 10%



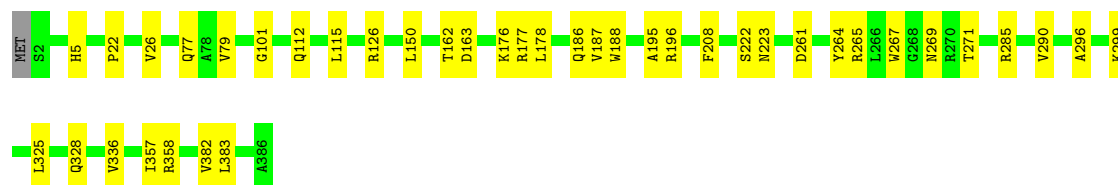
• Molecule 2: Pyocin sheath PA0622

Chain D: 90% 10%



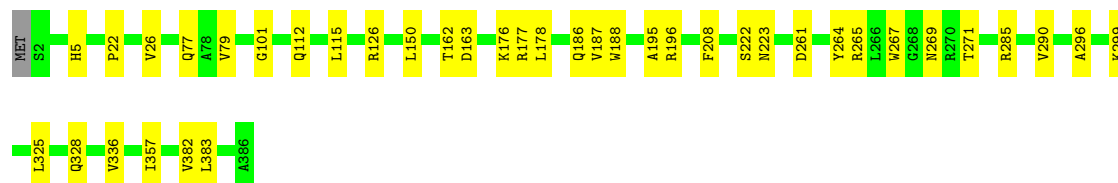
• Molecule 2: Pyocin sheath PA0622

Chain E: 89% 10%



• Molecule 2: Pyocin sheath PA0622

Chain F: 90% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=18.30°, rise=39.46 Å, axial sym=C6	Depositor
Number of segments used	15487	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.48	0/1285	0.66	0/1734
1	b	0.48	0/1285	0.66	0/1734
1	c	0.48	0/1285	0.66	0/1734
1	d	0.48	0/1285	0.66	0/1734
1	e	0.48	0/1285	0.66	0/1734
1	f	0.48	0/1285	0.66	0/1734
1	m	0.48	0/1285	0.66	0/1734
1	n	0.48	0/1285	0.66	0/1734
1	o	0.48	0/1285	0.66	0/1734
1	p	0.48	0/1285	0.66	0/1734
1	q	0.48	0/1285	0.66	0/1734
1	r	0.48	0/1285	0.66	0/1734
2	A	0.40	0/2955	0.59	0/4027
2	B	0.40	0/2955	0.59	0/4027
2	C	0.40	0/2955	0.59	0/4027
2	D	0.40	0/2955	0.59	0/4027
2	E	0.40	0/2955	0.59	0/4027
2	F	0.40	0/2955	0.59	0/4027
2	M	0.40	0/2955	0.59	0/4027
2	N	0.40	0/2955	0.59	0/4027
2	O	0.40	0/2955	0.59	0/4027
2	P	0.40	0/2955	0.59	0/4027
2	Q	0.40	0/2955	0.59	0/4027
2	R	0.40	0/2955	0.59	0/4027
All	All	0.43	0/50880	0.61	0/69132

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	a	1263	0	1255	0	0
1	b	1263	0	1255	0	0
1	c	1263	0	1255	0	0
1	d	1263	0	1255	0	0
1	e	1263	0	1255	0	0
1	f	1263	0	1255	0	0
1	m	1263	0	1255	0	0
1	n	1263	0	1255	0	0
1	o	1263	0	1255	0	0
1	p	1263	0	1255	0	0
1	q	1263	0	1255	0	0
1	r	1263	0	1255	0	0
2	A	2897	0	2855	25	0
2	B	2897	0	2855	25	0
2	C	2897	0	2855	23	0
2	D	2897	0	2855	25	0
2	E	2897	0	2855	24	0
2	F	2897	0	2855	23	0
2	M	2897	0	2855	23	0
2	N	2897	0	2855	24	0
2	O	2897	0	2855	25	0
2	P	2897	0	2855	28	0
2	Q	2897	0	2855	24	0
2	R	2897	0	2855	25	0
All	All	49920	0	49320	274	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 5.

The worst 5 of 274 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)
2:P:5:HIS:NE2	2:Q:267:TRP:O	2.31	0.63
2:R:176:LYS:HE3	2:R:177:ARG:HE	1.67	0.59
2:C:222:SER:HB2	2:C:269:ASN:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:176:LYS:HE3	2:M:177:ARG:HE	1.67	0.59
2:O:222:SER:HB2	2:O:269:ASN:HB3	1.85	0.59

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	a	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
1	b	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
1	c	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
1	d	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
1	e	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
1	f	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
1	m	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
1	n	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
1	o	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
1	p	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
1	q	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
1	r	165/167 (99%)	147 (89%)	18 (11%)	0	100	100
2	A	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
2	B	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
2	C	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
2	D	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
2	E	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
2	F	383/386 (99%)	349 (91%)	34 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
2	N	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
2	O	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
2	P	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
2	Q	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
2	R	383/386 (99%)	349 (91%)	34 (9%)	0	100	100
All	All	6576/6636 (99%)	5952 (90%)	624 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	a	130/130 (100%)	130 (100%)	0	100	100
1	b	130/130 (100%)	130 (100%)	0	100	100
1	c	130/130 (100%)	130 (100%)	0	100	100
1	d	130/130 (100%)	130 (100%)	0	100	100
1	e	130/130 (100%)	130 (100%)	0	100	100
1	f	130/130 (100%)	130 (100%)	0	100	100
1	m	130/130 (100%)	130 (100%)	0	100	100
1	n	130/130 (100%)	130 (100%)	0	100	100
1	o	130/130 (100%)	130 (100%)	0	100	100
1	p	130/130 (100%)	130 (100%)	0	100	100
1	q	130/130 (100%)	130 (100%)	0	100	100
1	r	130/130 (100%)	130 (100%)	0	100	100
2	A	297/298 (100%)	297 (100%)	0	100	100
2	B	297/298 (100%)	297 (100%)	0	100	100
2	C	297/298 (100%)	297 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	297/298 (100%)	297 (100%)	0	100	100
2	E	297/298 (100%)	297 (100%)	0	100	100
2	F	297/298 (100%)	297 (100%)	0	100	100
2	M	297/298 (100%)	297 (100%)	0	100	100
2	N	297/298 (100%)	297 (100%)	0	100	100
2	O	297/298 (100%)	297 (100%)	0	100	100
2	P	297/298 (100%)	297 (100%)	0	100	100
2	Q	297/298 (100%)	297 (100%)	0	100	100
2	R	297/298 (100%)	297 (100%)	0	100	100
All	All	5124/5136 (100%)	5124 (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. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	328	GLN
2	C	328	GLN
1	o	78	GLN
2	Q	328	GLN
2	R	328	GLN

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 [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.