



wwPDB EM Map/Model Validation Report ⓘ

Jul 18, 2016 – 06:28 PM EDT

PDB ID : 5JZH
EMDB ID: : EMD-8185
Title : Cryo-EM structure of aerolysin prepore
Authors : Iacovache, I.; Zuber, B.
Deposited on : 2016-05-16
Resolution : 3.90 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) : rb-20027790

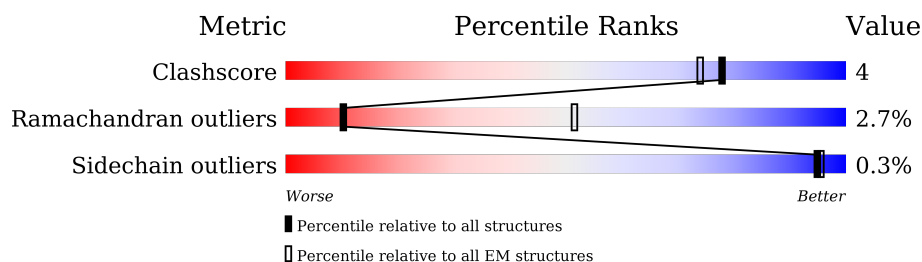
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	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	A	424	89% 10% .
1	B	424	88% 11% .
1	C	424	88% 11% .
1	D	424	90% 9% .
1	E	424	89% 9% .
1	F	424	88% 10% .
1	G	424	90% 9% .
1	H	424	88% 10% .
1	I	424	90% 9% .

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Mol	Chain	Length	Quality of chain
1	J	424	<div><div></div><div>88%</div><div>10%</div><div></div></div>
1	K	424	<div><div></div><div>89%</div><div>9%</div><div></div></div>
1	L	424	<div><div></div><div>90%</div><div>9%</div><div></div></div>
1	M	424	<div><div></div><div>88%</div><div>10%</div><div></div></div>
1	N	424	<div><div></div><div>88%</div><div>10%</div><div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 90790 atoms, of which 44226 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 Aerolysin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	B	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	C	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	D	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	E	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	F	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	G	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	H	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	I	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	J	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	K	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	L	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	M	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		
1	N	424	Total	C	H	N	O	S	0	0
			6485	2100	3159	574	643	9		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	GLY	TYR	engineered mutation	UNP P09167
B	221	GLY	TYR	engineered mutation	UNP P09167

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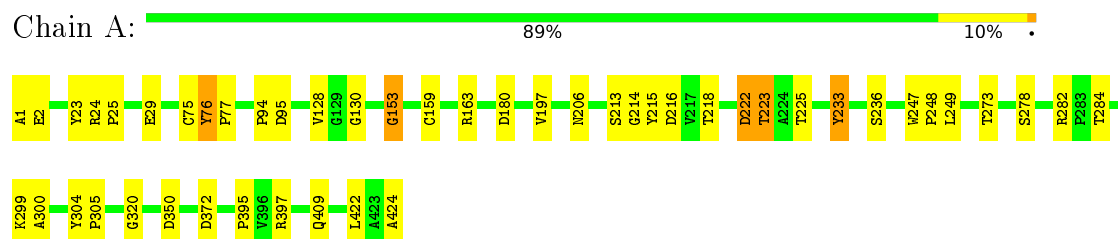
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Chain	Residue	Modelled	Actual	Comment	Reference
C	221	GLY	TYR	engineered mutation	UNP P09167
D	221	GLY	TYR	engineered mutation	UNP P09167
E	221	GLY	TYR	engineered mutation	UNP P09167
F	221	GLY	TYR	engineered mutation	UNP P09167
G	221	GLY	TYR	engineered mutation	UNP P09167
H	221	GLY	TYR	engineered mutation	UNP P09167
I	221	GLY	TYR	engineered mutation	UNP P09167
J	221	GLY	TYR	engineered mutation	UNP P09167
K	221	GLY	TYR	engineered mutation	UNP P09167
L	221	GLY	TYR	engineered mutation	UNP P09167
M	221	GLY	TYR	engineered mutation	UNP P09167
N	221	GLY	TYR	engineered mutation	UNP P09167

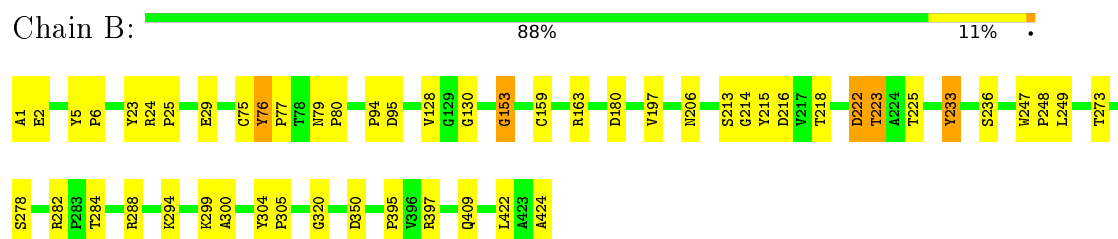
3 Residue-property plots [i](#)

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.

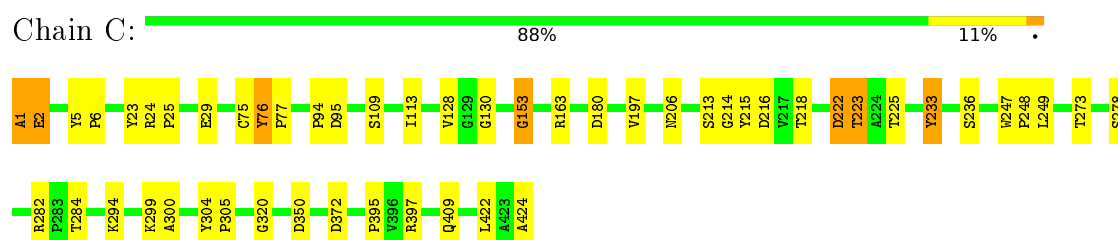
- Molecule 1: Aerolysin



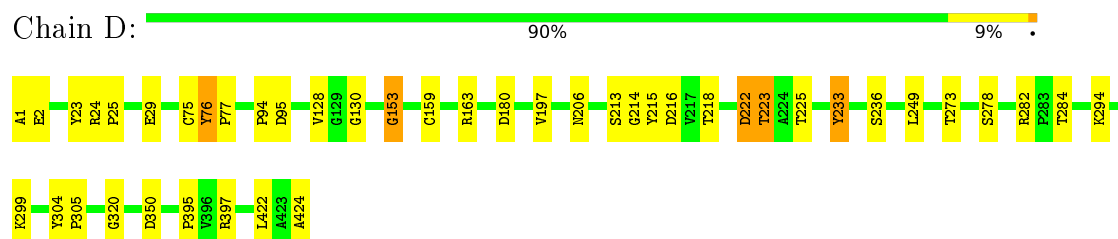
- Molecule 1: Aerolysin




- Molecule 1: Aerolysin

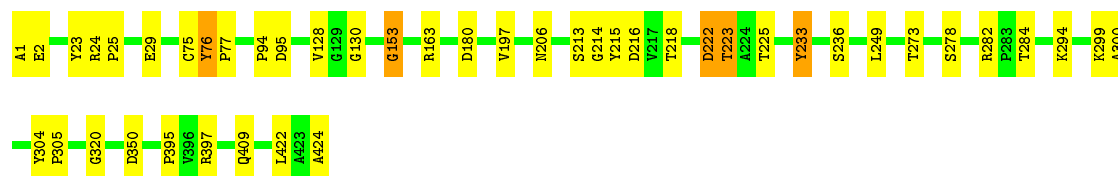


- Molecule 1: Aerolysin




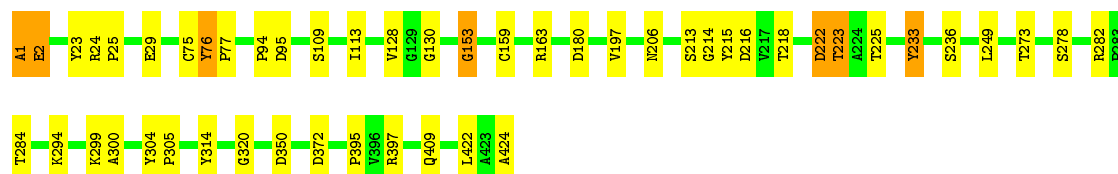
- Molecule 1: Aerolysin

Chain E:  89% 9% .



• Molecule 1: Aerolysin

Chain F:  88% 10% .



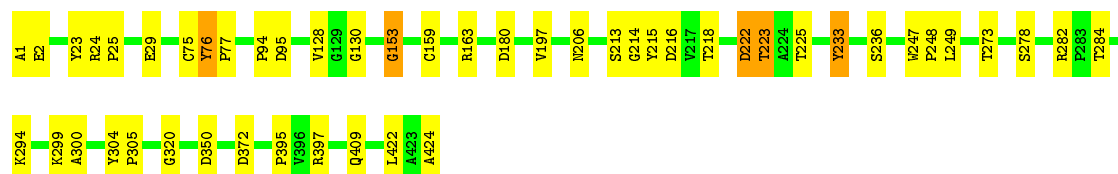
• Molecule 1: Aerolysin

Chain G:  90% 9% .




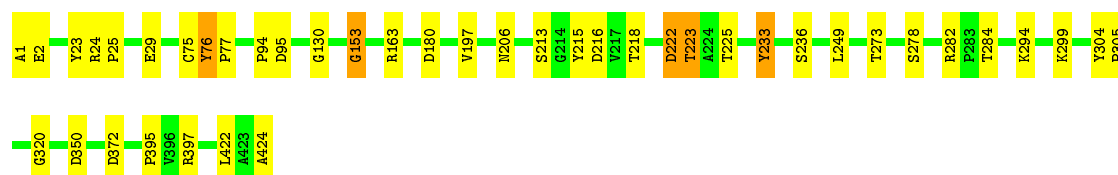
• Molecule 1: Aerolysin

Chain H:  88% 10% .




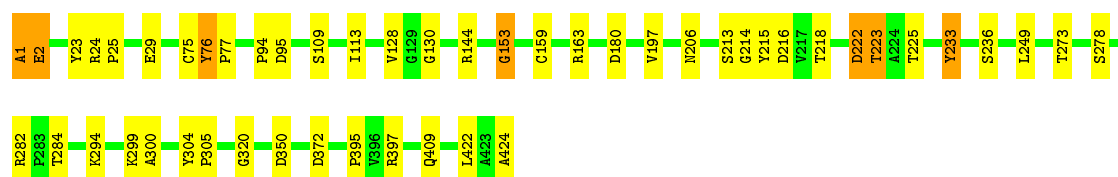
• Molecule 1: Aerolysin

Chain I:  90% 9% .



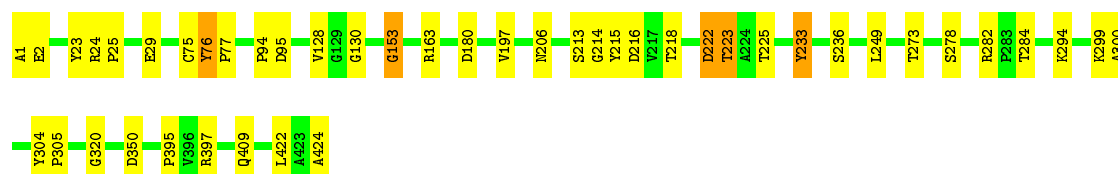
• Molecule 1: Aerolysin

Chain J:  88% 10% .



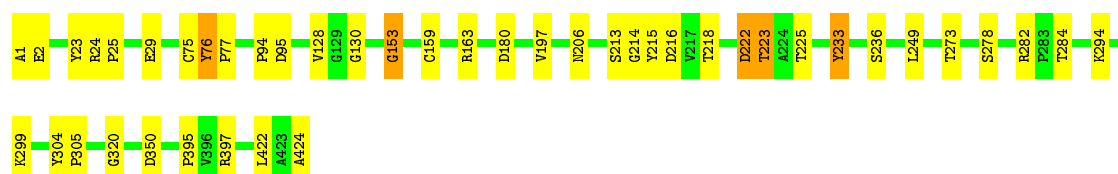
- Molecule 1: Aerolysin

Chain K: 89% 9%



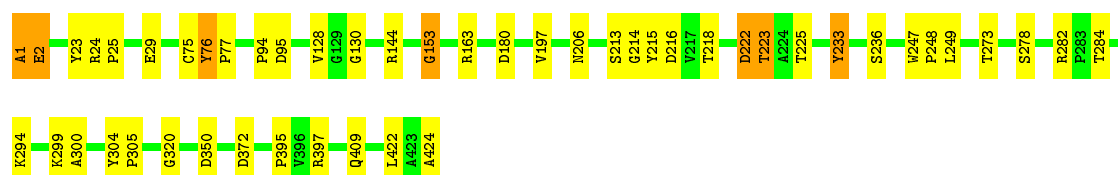
- Molecule 1: Aerolysin

Chain L: 90% 9%



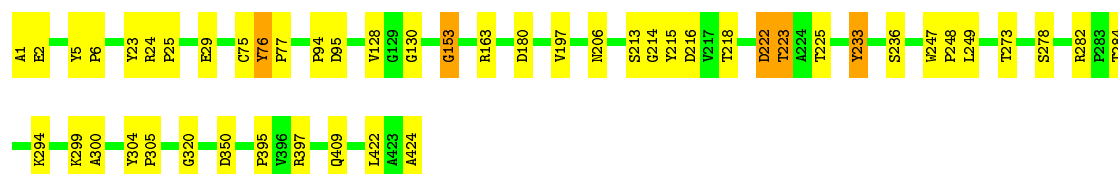
- Molecule 1: Aerolysin

Chain M: 88% 10%



- Molecule 1: Aerolysin

Chain N: 88% 10%



4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	42962	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	A	0.82	2/3421 (0.1%)	1.03	6/4669 (0.1%)
1	B	0.82	2/3421 (0.1%)	1.03	7/4669 (0.1%)
1	C	0.82	2/3421 (0.1%)	1.03	6/4669 (0.1%)
1	D	0.82	2/3421 (0.1%)	1.03	6/4669 (0.1%)
1	E	0.82	2/3421 (0.1%)	1.03	6/4669 (0.1%)
1	F	0.82	2/3421 (0.1%)	1.03	7/4669 (0.1%)
1	G	0.82	2/3421 (0.1%)	1.03	6/4669 (0.1%)
1	H	0.82	2/3421 (0.1%)	1.03	6/4669 (0.1%)
1	I	0.82	2/3421 (0.1%)	1.03	6/4669 (0.1%)
1	J	0.82	2/3421 (0.1%)	1.03	7/4669 (0.1%)
1	K	0.82	2/3421 (0.1%)	1.03	6/4669 (0.1%)
1	L	0.82	2/3421 (0.1%)	1.03	6/4669 (0.1%)
1	M	0.82	2/3421 (0.1%)	1.03	7/4669 (0.1%)
1	N	0.82	2/3421 (0.1%)	1.03	6/4669 (0.1%)
All	All	0.82	28/47894 (0.1%)	1.03	88/65366 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	9
1	C	0	9
1	D	0	9
1	E	0	9
1	F	0	9
1	G	0	9
1	H	0	9
1	I	0	9
1	J	0	9
1	K	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	9
1	M	0	9
1	N	0	9
All	All	0	126

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	424	ALA	C-OXT	-12.09	1.00	1.23
1	C	424	ALA	C-O	-12.07	1.00	1.23
1	E	424	ALA	C-O	-12.07	1.00	1.23
1	K	424	ALA	C-O	-12.07	1.00	1.23
1	H	424	ALA	C-OXT	-12.07	1.00	1.23

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	TYR	O-C-N	-32.49	59.36	121.10
1	F	76	TYR	O-C-N	-32.47	59.40	121.10
1	H	76	TYR	O-C-N	-32.46	59.42	121.10
1	J	76	TYR	O-C-N	-32.46	59.42	121.10
1	B	76	TYR	O-C-N	-32.46	59.43	121.10

There are no chirality outliers.

5 of 126 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Mainchain,Peptide
1	A	222	ASP	Mainchain,Peptide
1	A	320	GLY	Mainchain,Peptide
1	A	422	LEU	Mainchain
1	A	76	TYR	Mainchain

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	3326	3159	3159	26	0
1	B	3326	3159	3159	27	0
1	C	3326	3159	3159	29	0
1	D	3326	3159	3159	23	0
1	E	3326	3159	3159	24	0
1	F	3326	3159	3159	26	0
1	G	3326	3159	3159	24	0
1	H	3326	3159	3159	26	0
1	I	3326	3159	3159	22	0
1	J	3326	3159	3159	26	0
1	K	3326	3159	3159	24	0
1	L	3326	3159	3159	23	0
1	M	3326	3159	3159	27	0
1	N	3326	3159	3159	26	0
All	All	46564	44226	44226	326	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 4.

The worst 5 of 326 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:F:222:ASP:HA	1:F:223:THR:HB	1.85	0.58
1:J:222:ASP:HA	1:J:223:THR:HB	1.85	0.58
1:G:222:ASP:HA	1:G:223:THR:HB	1.85	0.58
1:M:222:ASP:HA	1:M:223:THR:HB	1.85	0.58
1:C:222:ASP:HA	1:C:223:THR:HB	1.85	0.58

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	A	422/424 (100%)	371 (88%)	39 (9%)	12 (3%)	6	46
1	B	422/424 (100%)	371 (88%)	39 (9%)	12 (3%)	6	46
1	C	422/424 (100%)	371 (88%)	40 (10%)	11 (3%)	7	47
1	D	422/424 (100%)	371 (88%)	39 (9%)	12 (3%)	6	46
1	E	422/424 (100%)	371 (88%)	40 (10%)	11 (3%)	7	47
1	F	422/424 (100%)	371 (88%)	39 (9%)	12 (3%)	6	46
1	G	422/424 (100%)	371 (88%)	40 (10%)	11 (3%)	7	47
1	H	422/424 (100%)	371 (88%)	39 (9%)	12 (3%)	6	46
1	I	422/424 (100%)	371 (88%)	40 (10%)	11 (3%)	7	47
1	J	422/424 (100%)	371 (88%)	39 (9%)	12 (3%)	6	46
1	K	422/424 (100%)	371 (88%)	40 (10%)	11 (3%)	7	47
1	L	422/424 (100%)	371 (88%)	39 (9%)	12 (3%)	6	46
1	M	422/424 (100%)	371 (88%)	40 (10%)	11 (3%)	7	47
1	N	422/424 (100%)	371 (88%)	40 (10%)	11 (3%)	7	47
All	All	5908/5936 (100%)	5194 (88%)	553 (9%)	161 (3%)	10	46

5 of 161 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	PRO
1	B	77	PRO
1	C	77	PRO
1	D	77	PRO
1	E	77	PRO

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	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	B	355/355 (100%)	354 (100%)	1 (0%)	94	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	D	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	E	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	F	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	G	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	H	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	I	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	J	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	K	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	L	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	M	355/355 (100%)	354 (100%)	1 (0%)	94	97
1	N	355/355 (100%)	354 (100%)	1 (0%)	94	97
All	All	4970/4970 (100%)	4956 (100%)	14 (0%)	95	97

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	233	TYR
1	H	233	TYR
1	L	233	TYR
1	F	233	TYR
1	K	233	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 [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.