



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 10, 2019 – 05:24 PM EST

PDB ID : 6OSJ  
EMDB ID: : EMD-20183  
Title : Cryo-EM structure of the N-terminally acetylated full length alpha-synuclein  
fibrils (Ac1-140)  
Authors : Xiaodan, N.; Ryan, P.M.; Jiansen, J.; Jennifer, C.L.  
Deposited on : 2019-05-01  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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) : 2.4

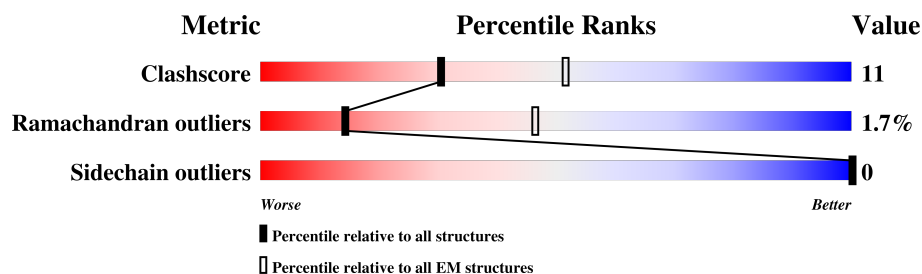
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*










The reported resolution of this entry is 2.80 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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  $\geq 3$ , 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	140	
1	B	140	
1	C	140	
1	D	140	
1	E	140	
1	F	140	
1	G	140	
1	H	140	
1	I	140	

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Mol	Chain	Length	Quality of chain
1	J	140	<div><div></div><div></div><div></div><div>36%</div><div>8%</div><div>56%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4210 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 Alpha-synuclein.

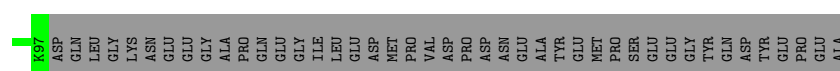
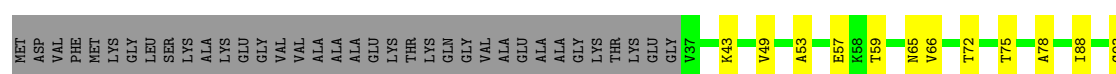
Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	61	Total	C	N	O	0	0
			421	265	73	83		
1	B	61	Total	C	N	O	0	0
			421	265	73	83		
1	C	61	Total	C	N	O	0	0
			421	265	73	83		
1	D	61	Total	C	N	O	0	0
			421	265	73	83		
1	E	61	Total	C	N	O	0	0
			421	265	73	83		
1	F	61	Total	C	N	O	0	0
			421	265	73	83		
1	G	61	Total	C	N	O	0	0
			421	265	73	83		
1	H	61	Total	C	N	O	0	0
			421	265	73	83		
1	I	61	Total	C	N	O	0	0
			421	265	73	83		
1	J	61	Total	C	N	O	0	0
			421	265	73	83		

### 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 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.

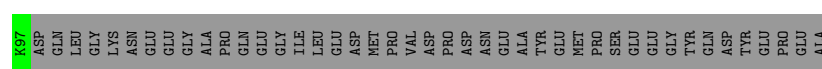
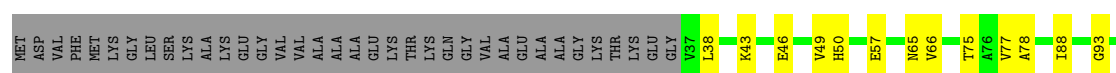
- Molecule 1: Alpha-synuclein

Chain A:



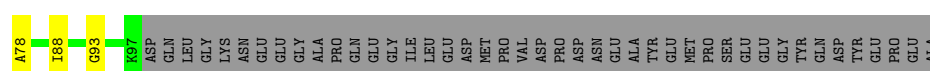
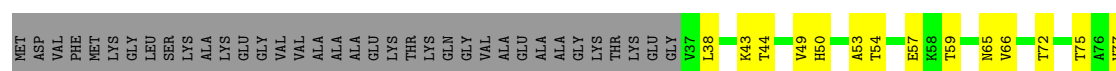
- Molecule 1: Alpha-synuclein

Chain B:



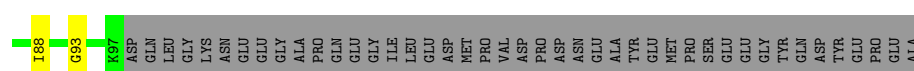
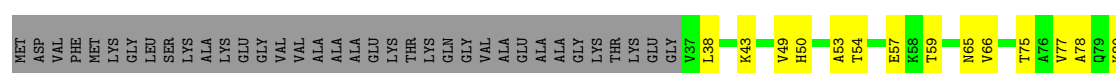
- Molecule 1: Alpha-synuclein

Chain C:




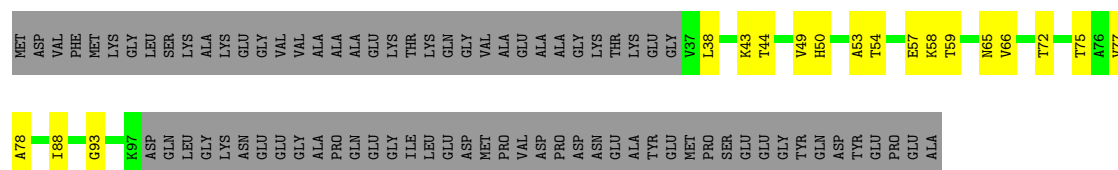
- Molecule 1: Alpha-synuclein

Chain D:




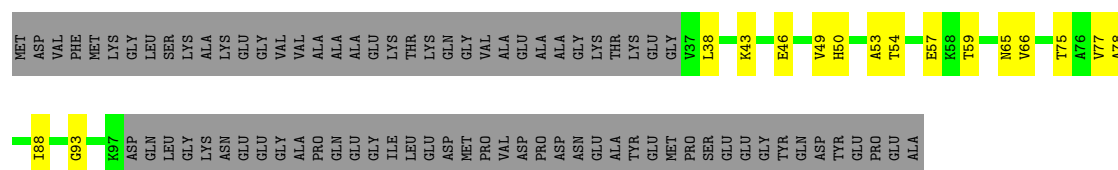
- Molecule 1: Alpha-synuclein

Chain E:  31% 13% 56%




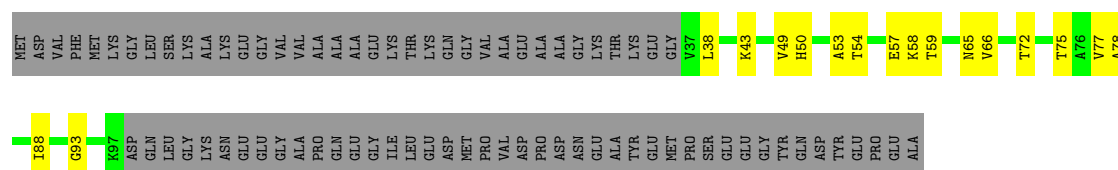
- Molecule 1: Alpha-synuclein

Chain F:  32% 11% 56%




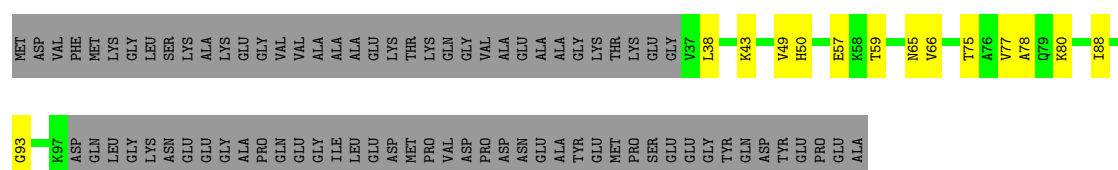
- Molecule 1: Alpha-synuclein

Chain G:  31% 12% 56%




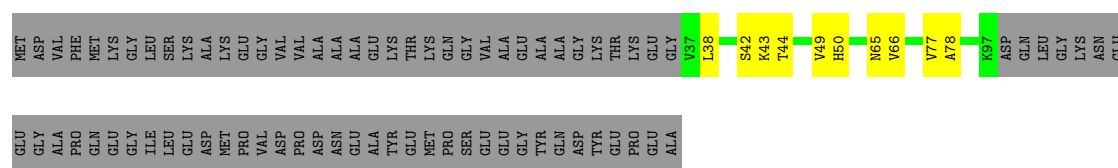
- Molecule 1: Alpha-synuclein

Chain H:  34% 10% 56%




- Molecule 1: Alpha-synuclein

Chain I:  36% 7% 56%



- Molecule 1: Alpha-synuclein

Chain J:  36% 8% 56%

MET	ASP	VAL	PHE	MET	LYS	GLY	LEU	SER	LYS	ALA	LYS	GLU	GLY	VAL	VAL	ALA	ALA	GLU	LYS	THR	LYS	GLN	GLY	VAL	ALA	GLU	ALA	ALA	GLY	LYS	THR	LYS	GLY	GLY	V37	L38	K43	V49	H50	T59	N65	V66	T75	A76	V77	A78	G93	K97	ASP	GLN	LEU						
GLY	LYS	ASN	GLU	GLU	GLY	ALA	PRO	GLN	GLU	GLY	ILE	LEU	GLU	ASP	MET	PRO	VAL	ASP	PRO	ASP	ASN	GLU	ALA	TYR	GLU	MET	PRO	SER	GLU	GLU	GLY	TYR	GLN	ASP	TYR	GLU	PRO	GLU	ALA	GLY	V37	L38	K43	V49	H50	T59	N65	V66	T75	A76	V77	A78	G93	K97	ASP	GLN	LEU

## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=179.643°, rise=2.4 Å, axial sym=C1	Depositor
Number of segments used	12132	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.3	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.53	0/423	0.68	0/572
1	B	0.53	0/423	0.68	0/572
1	C	0.53	0/423	0.68	0/572
1	D	0.53	0/423	0.68	0/572
1	E	0.53	0/423	0.68	0/572
1	F	0.53	0/423	0.68	0/572
1	G	0.53	0/423	0.68	0/572
1	H	0.53	0/423	0.68	0/572
1	I	0.54	0/423	0.68	0/572
1	J	0.53	0/423	0.68	0/572
All	All	0.53	0/4230	0.68	0/5720

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 [i](#)

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	421	0	447	10	0
1	B	421	0	447	11	0
1	C	421	0	447	21	0
1	D	421	0	447	22	0
1	E	421	0	447	26	0
1	F	421	0	447	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	421	0	447	22	0
1	H	421	0	447	21	0
1	I	421	0	447	8	0
1	J	421	0	447	10	0
All	All	4210	0	4470	93	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 11.

All (93) 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:57:GLU:OE2	1:G:50:HIS:ND1	2.23	0.66
1:E:88:ILE:HG21	1:G:77:VAL:HG21	1.77	0.65
1:H:57:GLU:OE2	1:I:50:HIS:ND1	2.26	0.63
1:B:57:GLU:OE2	1:C:50:HIS:ND1	2.26	0.62
1:C:88:ILE:HG21	1:E:77:VAL:HG21	1.81	0.62
1:A:88:ILE:HG21	1:C:77:VAL:HG21	1.81	0.62
1:D:57:GLU:OE2	1:E:50:HIS:ND1	2.26	0.62
1:D:88:ILE:HG21	1:F:77:VAL:HG21	1.83	0.61
1:H:88:ILE:HG21	1:J:77:VAL:HG21	1.83	0.61
1:B:88:ILE:HG21	1:D:77:VAL:HG21	1.83	0.61
1:F:88:ILE:HG21	1:H:77:VAL:HG21	1.83	0.61
1:G:88:ILE:HG21	1:I:77:VAL:HG21	1.85	0.58
1:E:59:THR:HB	1:G:59:THR:O	2.03	0.58
1:E:49:VAL:HA	1:G:49:VAL:O	2.05	0.56
1:E:57:GLU:OE1	1:G:57:GLU:HG2	2.05	0.56
1:E:75:THR:HA	1:G:75:THR:O	2.05	0.56
1:D:59:THR:HB	1:F:59:THR:O	2.06	0.55
1:C:49:VAL:HA	1:E:49:VAL:O	2.06	0.55
1:C:50:HIS:CD2	1:E:50:HIS:HB2	2.42	0.54
1:A:59:THR:HB	1:C:59:THR:O	2.08	0.54
1:B:38:LEU:HD13	1:D:38:LEU:HD23	1.91	0.53
1:B:78:ALA:HA	1:D:78:ALA:O	2.09	0.53
1:F:78:ALA:HA	1:H:78:ALA:O	2.09	0.52
1:E:50:HIS:CD2	1:G:50:HIS:HB2	2.45	0.52
1:H:78:ALA:HA	1:J:78:ALA:O	2.10	0.52
1:F:38:LEU:HD13	1:H:38:LEU:HD23	1.93	0.51
1:E:53:ALA:O	1:G:53:ALA:HA	2.10	0.51
1:A:75:THR:HA	1:C:75:THR:O	2.11	0.51
1:H:59:THR:HB	1:J:59:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:THR:HA	1:F:75:THR:O	2.12	0.50
1:E:54:THR:HG22	1:G:54:THR:OG1	2.12	0.50
1:E:78:ALA:HA	1:G:78:ALA:O	2.11	0.50
1:D:49:VAL:HA	1:F:49:VAL:O	2.12	0.50
1:D:78:ALA:HA	1:F:78:ALA:O	2.12	0.50
1:A:93:GLY:HA3	1:C:93:GLY:O	2.13	0.48
1:D:57:GLU:OE1	1:F:57:GLU:HG2	2.13	0.48
1:H:49:VAL:HA	1:J:49:VAL:O	2.14	0.48
1:A:57:GLU:OE1	1:C:57:GLU:HG2	2.14	0.48
1:E:72:THR:HA	1:G:72:THR:O	2.14	0.47
1:E:93:GLY:HA3	1:G:93:GLY:O	2.14	0.47
1:D:50:HIS:CD2	1:F:50:HIS:HB2	2.49	0.47
1:C:59:THR:HB	1:E:59:THR:O	2.14	0.47
1:B:75:THR:HA	1:D:75:THR:O	2.14	0.47
1:B:46:GLU:HB3	1:D:80:LYS:HD3	1.97	0.47
1:H:50:HIS:CD2	1:J:50:HIS:HB2	2.50	0.47
1:C:78:ALA:HA	1:E:78:ALA:O	2.14	0.46
1:H:93:GLY:HA3	1:J:93:GLY:O	2.15	0.46
1:H:75:THR:HA	1:J:75:THR:O	2.15	0.46
1:C:75:THR:HA	1:E:75:THR:O	2.15	0.46
1:B:49:VAL:HA	1:D:49:VAL:O	2.17	0.46
1:F:49:VAL:HA	1:H:49:VAL:O	2.16	0.46
1:D:65:ASN:OD1	1:D:66:VAL:N	2.49	0.45
1:H:65:ASN:OD1	1:H:66:VAL:N	2.49	0.45
1:B:65:ASN:OD1	1:B:66:VAL:N	2.49	0.45
1:F:65:ASN:OD1	1:F:66:VAL:N	2.49	0.45
1:F:75:THR:HA	1:H:75:THR:O	2.16	0.45
1:G:49:VAL:HA	1:I:49:VAL:O	2.16	0.45
1:J:65:ASN:OD1	1:J:66:VAL:N	2.49	0.45
1:E:77:VAL:HG13	1:G:77:VAL:HG23	1.98	0.45
1:I:65:ASN:OD1	1:I:66:VAL:N	2.49	0.45
1:F:50:HIS:CE1	1:G:57:GLU:OE2	2.69	0.45
1:A:72:THR:HA	1:C:72:THR:O	2.16	0.45
1:E:58:LYS:HA	1:G:58:LYS:O	2.16	0.45
1:G:65:ASN:OD1	1:G:66:VAL:N	2.49	0.45
1:A:49:VAL:HA	1:C:49:VAL:O	2.16	0.45
1:A:65:ASN:OD1	1:A:66:VAL:N	2.49	0.45
1:B:77:VAL:HG13	1:D:77:VAL:HG23	1.98	0.45
1:C:65:ASN:OD1	1:C:66:VAL:N	2.49	0.45
1:F:46:GLU:HB3	1:H:80:LYS:HD3	1.99	0.45
1:C:44:THR:HG23	1:E:44:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:ASN:OD1	1:E:66:VAL:N	2.49	0.44
1:F:93:GLY:HA3	1:H:93:GLY:O	2.16	0.44
1:H:77:VAL:HG13	1:J:77:VAL:HG23	1.98	0.44
1:F:77:VAL:HG13	1:H:77:VAL:HG23	1.99	0.44
1:A:53:ALA:O	1:C:53:ALA:HA	2.18	0.44
1:C:38:LEU:HD13	1:E:38:LEU:HB3	2.00	0.43
1:D:77:VAL:HG13	1:F:77:VAL:HG23	1.99	0.43
1:A:78:ALA:HA	1:C:78:ALA:O	2.17	0.43
1:C:54:THR:HG22	1:E:54:THR:OG1	2.19	0.43
1:B:93:GLY:HA3	1:D:93:GLY:O	2.18	0.42
1:D:93:GLY:HA3	1:F:93:GLY:O	2.19	0.42
1:G:38:LEU:HD13	1:I:38:LEU:HD23	2.00	0.42
1:H:38:LEU:HD13	1:J:38:LEU:HD23	2.01	0.42
1:F:50:HIS:CD2	1:H:50:HIS:HB2	2.55	0.41
1:D:53:ALA:O	1:F:53:ALA:HA	2.20	0.41
1:E:72:THR:OG1	1:G:72:THR:HG23	2.20	0.41
1:G:78:ALA:HA	1:I:78:ALA:O	2.19	0.41
1:G:50:HIS:CD2	1:I:50:HIS:HB2	2.56	0.41
1:B:50:HIS:CD2	1:D:50:HIS:HB2	2.56	0.41
1:D:54:THR:HG22	1:F:54:THR:OG1	2.20	0.41
1:I:42:SER:O	1:I:44:THR:OG1	2.33	0.41
1:C:77:VAL:HG13	1:E:77:VAL:HG23	2.03	0.40
1:F:59:THR:HB	1:H:59:THR:O	2.22	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	A	59/140 (42%)	47 (80%)	11 (19%)	1 (2%)	10	32
1	B	59/140 (42%)	47 (80%)	11 (19%)	1 (2%)	10	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	59/140 (42%)	47 (80%)	11 (19%)	1 (2%)	10	32
1	D	59/140 (42%)	47 (80%)	11 (19%)	1 (2%)	10	32
1	E	59/140 (42%)	47 (80%)	11 (19%)	1 (2%)	10	32
1	F	59/140 (42%)	47 (80%)	11 (19%)	1 (2%)	10	32
1	G	59/140 (42%)	47 (80%)	11 (19%)	1 (2%)	10	32
1	H	59/140 (42%)	47 (80%)	11 (19%)	1 (2%)	10	32
1	I	59/140 (42%)	47 (80%)	11 (19%)	1 (2%)	10	32
1	J	59/140 (42%)	47 (80%)	11 (19%)	1 (2%)	10	32
All	All	590/1400 (42%)	470 (80%)	110 (19%)	10 (2%)	14	32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	B	43	LYS
1	C	43	LYS
1	D	43	LYS
1	E	43	LYS
1	F	43	LYS
1	G	43	LYS
1	H	43	LYS
1	I	43	LYS
1	J	43	LYS

### 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	43/103 (42%)	43 (100%)	0	100	100
1	B	43/103 (42%)	43 (100%)	0	100	100
1	C	43/103 (42%)	43 (100%)	0	100	100
1	D	43/103 (42%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	43/103 (42%)	43 (100%)	0	100	100
1	F	43/103 (42%)	43 (100%)	0	100	100
1	G	43/103 (42%)	43 (100%)	0	100	100
1	H	43/103 (42%)	43 (100%)	0	100	100
1	I	43/103 (42%)	43 (100%)	0	100	100
1	J	43/103 (42%)	43 (100%)	0	100	100
All	All	430/1030 (42%)	430 (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 ⓘ

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.