



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

May 29, 2017 – 03:03 PM EDT

PDB ID : 5X0X
EMDB ID: : EMD-6699
Title : Complex of Snf2-Nucleosome complex with Snf2 bound to position +6 of the nucleosome
Authors : Li, M.; Liu, X.; Xia, X.; Chen, Z.; Li, X.
Deposited on : 2017-01-23
Resolution : 3.97 Å(reported)

This is a wwPDB/EMDatabank EM Map/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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

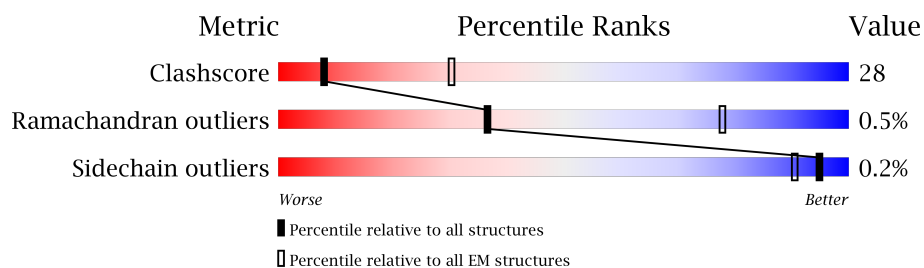
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.97 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	136	49% 23% 28%
1	E	136	51% 18% 30%
2	B	103	46% 34% 20%
2	F	103	51% 32% 17%
3	C	130	60% 22% 18%
3	G	130	62% 20% 18%
4	D	125	65% 10% 26%
4	H	125	62% 13% 26%
5	I	167	10% 76% 13%

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Mol	Chain	Length	Quality of chain
6	J	167	<div><div></div><div>14%73%13%</div></div>
7	O	735	<div><div></div><div>30%49%21%</div></div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16748 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			800	505	153	139	3		
1	E	95	Total	C	N	O	S	0	0
			778	491	148	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	82	Total	C	N	O	S	0	0
			653	413	127	112	1		
2	F	86	Total	C	N	O	S	0	0
			672	424	130	117	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			811	510	158	143		
3	G	107	Total	C	N	O	0	0
			815	513	159	143		

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	see sequence details	UNP P02281

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Chain	Residue	Modelled	Actual	Comment	Reference
H	29	THR	SER	see sequence details	UNP P02281

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

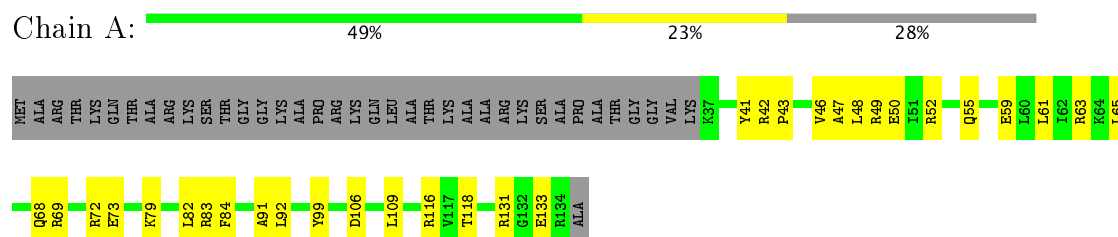
- Molecule 7 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	583	Total	C	N	O	S	0	0
			4789	3045	846	881	17		

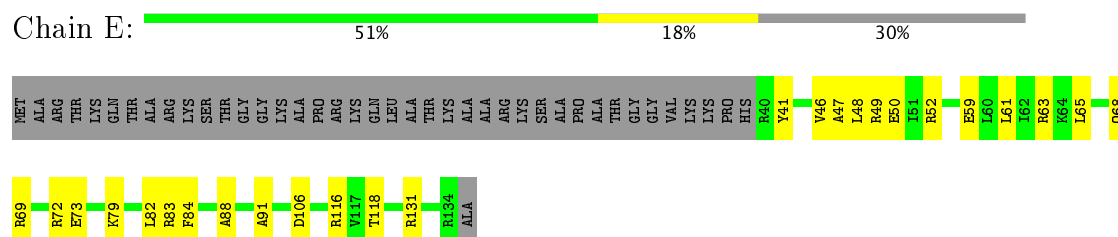
3 Residue-property plots [i](#)

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.

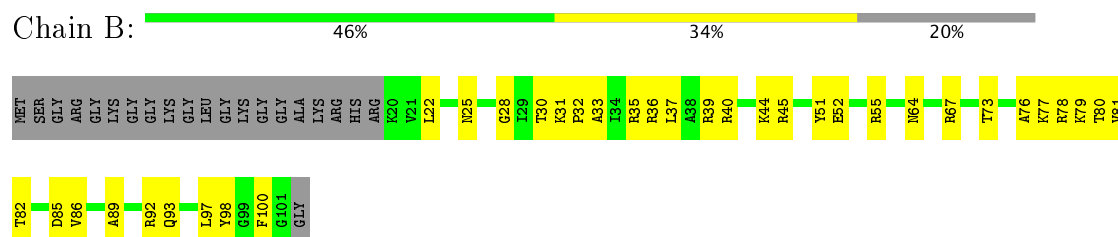
• Molecule 1: Histone H3.2



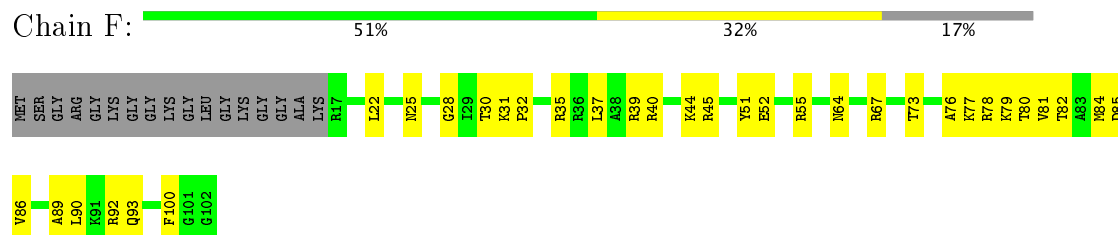
• Molecule 1: Histone H3.2



• Molecule 2: Histone H4

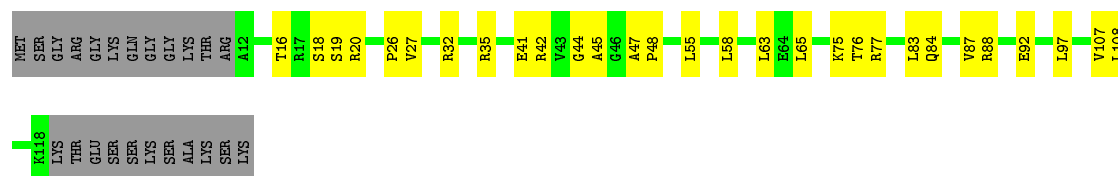


• Molecule 2: Histone H4



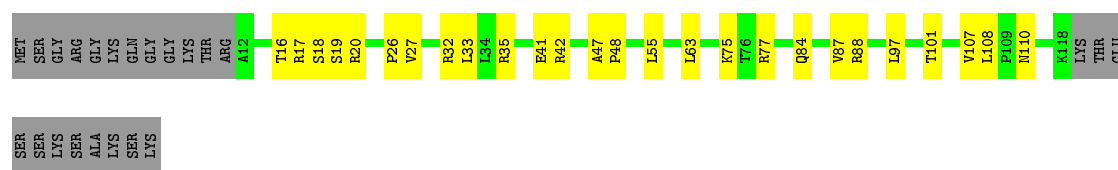
• Molecule 3: Histone H2A

Chain C:  60% 22% 18%



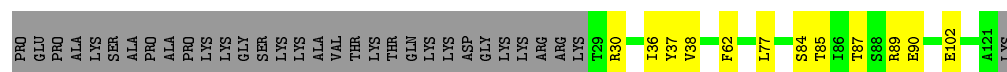
• Molecule 3: Histone H2A

Chain G:  62% 20% 18%



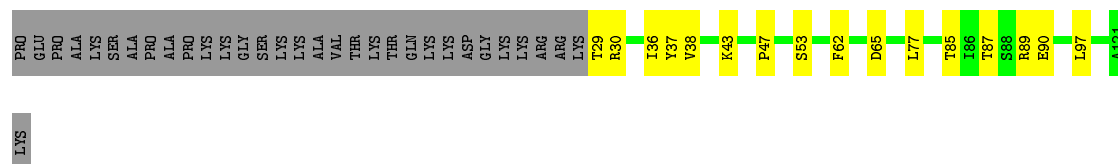
• Molecule 4: Histone H2B 1.1

Chain D:  65% 10% 26%



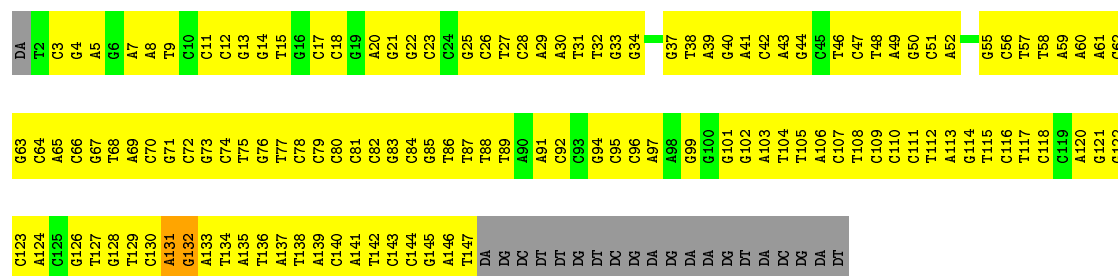
• Molecule 4: Histone H2B 1.1

Chain H:  62% 13% 26%



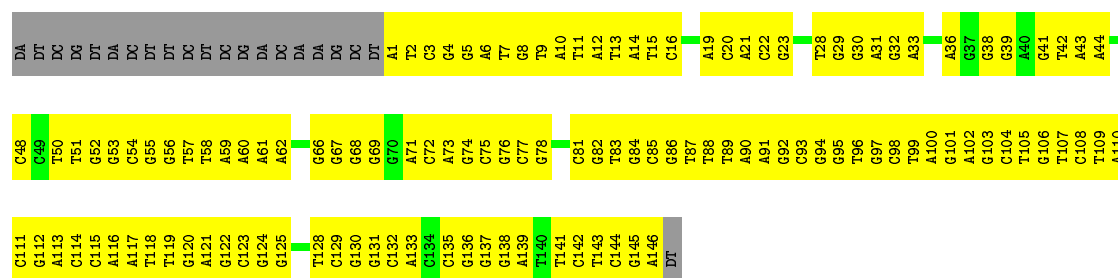
• Molecule 5: DNA (167-MER)

Chain I:  10% 76% 13%

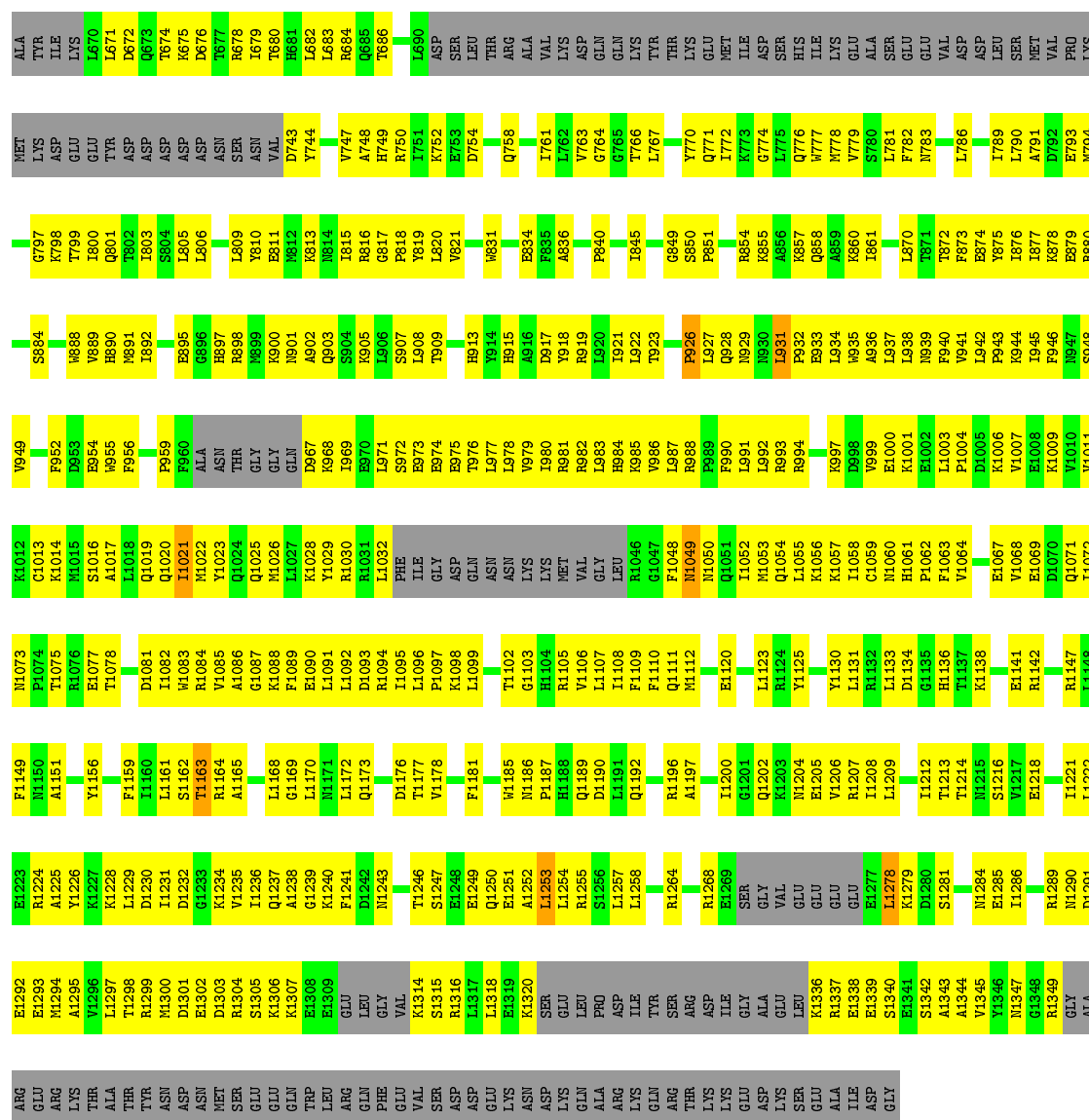


• Molecule 6: DNA (167-MER)

Chain J:  14% 73% 13%



- Molecule 7: Transcription regulatory protein SNF2



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	90725	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	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	0.57	0/812	0.57	0/1091
1	E	0.58	0/788	0.58	0/1057
2	B	0.67	0/660	0.62	0/885
2	F	0.67	0/680	0.62	0/912
3	C	0.56	0/821	0.59	0/1112
3	G	0.56	0/825	0.59	0/1116
4	D	0.63	0/729	0.59	0/985
4	H	0.63	0/737	0.59	0/993
5	I	1.16	0/3333	1.02	2/5137 (0.0%)
6	J	1.14	0/3381	0.99	1/5221 (0.0%)
7	O	0.36	0/4864	0.56	2/6536 (0.0%)
All	All	0.82	0/17630	0.79	5/25045 (0.0%)

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
7	O	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	132	DG	O4'-C4'-C3'	-6.02	102.09	104.50
7	O	959	PRO	N-CA-CB	5.92	110.40	103.30
7	O	1253	LEU	CA-CB-CG	-5.76	102.04	115.30
5	I	131	DA	O4'-C4'-C3'	-5.14	102.44	104.50
6	J	36	DA	O4'-C4'-C3'	-5.07	102.47	104.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	O	915	HIS	Peptide
7	O	926	PRO	Peptide
7	O	931	LEU	Peptide

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	800	0	829	33	0
1	E	778	0	813	27	0
2	B	653	0	695	34	0
2	F	672	0	698	32	0
3	C	811	0	849	30	0
3	G	815	0	860	22	0
4	D	718	0	725	11	0
4	H	726	0	747	16	0
5	I	2975	0	1639	201	0
6	J	3011	0	1639	191	0
7	O	4789	0	4882	380	0
All	All	16748	0	14376	854	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 28.

The worst 5 of 854 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)
7:O:1301:ASP:O	7:O:1305:SER:HB2	1.54	1.08
7:O:749:HIS:HB3	7:O:752:LYS:HD3	1.53	0.90
5:I:74:DC:N3	6:J:74:DG:N1	2.19	0.90
5:I:11:DC:O2	6:J:137:DG:N2	2.05	0.89
5:I:110:DC:O2	6:J:38:DG:N2	2.06	0.89

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	96/136 (71%)	87 (91%)	9 (9%)	0	100	100
1	E	93/136 (68%)	84 (90%)	9 (10%)	0	100	100
2	B	80/103 (78%)	77 (96%)	3 (4%)	0	100	100
2	F	84/103 (82%)	81 (96%)	3 (4%)	0	100	100
3	C	105/130 (81%)	100 (95%)	4 (4%)	1 (1%)	18	61
3	G	105/130 (81%)	100 (95%)	4 (4%)	1 (1%)	18	61
4	D	91/125 (73%)	83 (91%)	8 (9%)	0	100	100
4	H	91/125 (73%)	83 (91%)	8 (9%)	0	100	100
7	O	569/735 (77%)	494 (87%)	71 (12%)	4 (1%)	25	68
All	All	1314/1723 (76%)	1189 (90%)	119 (9%)	6 (0%)	37	73

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	O	954	GLU
7	O	1021	ILE
7	O	1163	THR
7	O	1049	ASN
3	C	87	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/111 (76%)	84 (100%)	0	100	100
1	E	82/111 (74%)	82 (100%)	0	100	100
2	B	67/79 (85%)	67 (100%)	0	100	100
2	F	67/79 (85%)	67 (100%)	0	100	100
3	C	81/102 (79%)	81 (100%)	0	100	100
3	G	82/102 (80%)	82 (100%)	0	100	100
4	D	77/105 (73%)	77 (100%)	0	100	100
4	H	79/105 (75%)	79 (100%)	0	100	100
7	O	526/667 (79%)	524 (100%)	2 (0%)	93	96
All	All	1145/1461 (78%)	1143 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	O	820	LEU
7	O	1278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	81	ASN
7	O	801	GLN
7	O	1188	HIS
4	H	44	GLN
7	O	1202	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.