



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 14, 2018 – 09:00 PM EST

PDB ID : 6ESF
EMDB ID: : EMD-3947
Title : Nucleosome : Class 1
Authors : Bilokapic, S.; Halic, M.
Deposited on : 2017-10-20
Resolution : 3.70 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
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-20030736

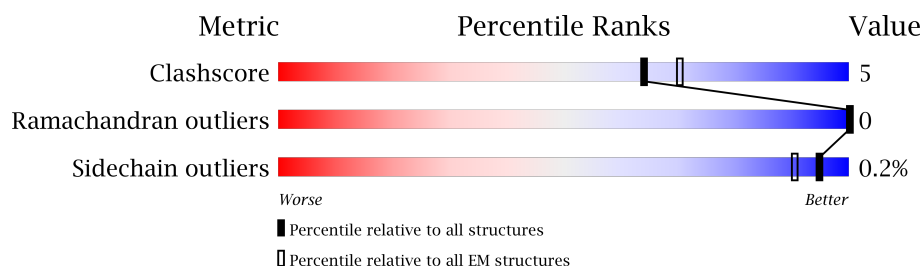
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	135	55% 18% 27%
1	E	135	59% 14% 27%
2	B	102	67% 16% 18%
2	F	102	69% 15% 17%
3	C	129	67% 13% 19%
3	G	129	68% 13% 19%
4	D	122	66% 11% 23%
4	H	122	66% 11% 23%
5	I	147	84% 16%

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Mol	Chain	Length	Quality of chain
6	J	147	 <div>90%10%</div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12091 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
			811	512	157	139	3		
1	E	98	Total	C	N	O	S	0	0
			807	509	156	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	variant	UNP P84233
E	102	ALA	GLY	variant	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	84	Total	C	N	O	S	0	0
			678	428	135	114	1		
2	F	85	Total	C	N	O	S	0	0
			683	430	136	116	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	104	Total	C	N	O	0	0
			804	507	157	140		
3	G	105	Total	C	N	O	0	0
			811	511	158	142		

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	94	Total	C	N	O	S	0	0
			735	463	132	138	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	94	Total	C	N	O	S	0	0
			735	463	132	138	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	variant	UNP P02281
H	29	THR	SER	variant	UNP P02281

- Molecule 5 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	147	Total	C	N	O	P	0	0
			3031	1434	570	880	147		

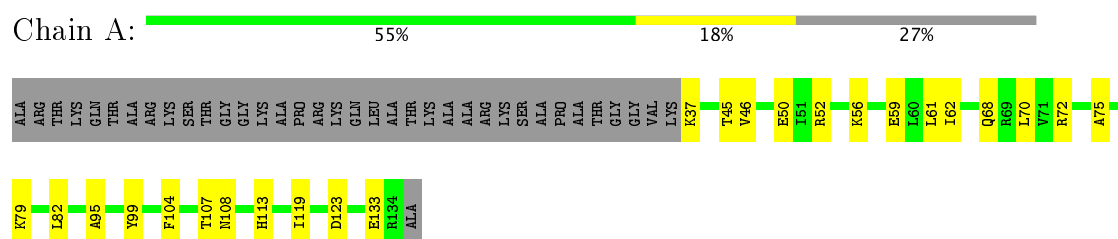
- Molecule 6 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	147	Total	C	N	O	P	0	0
			2996	1423	542	884	147		

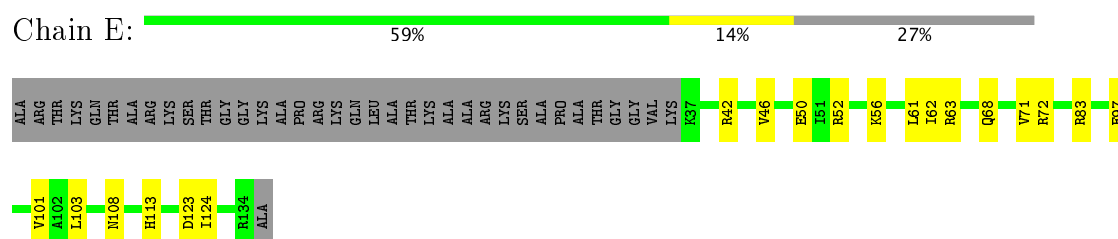
3 Residue-property plots

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.

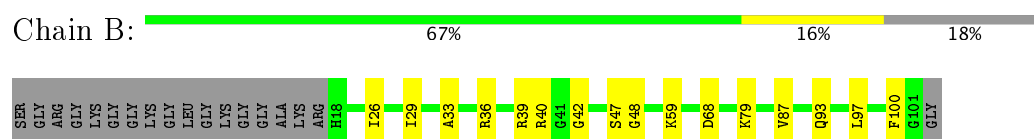
- Molecule 1: Histone H3.2



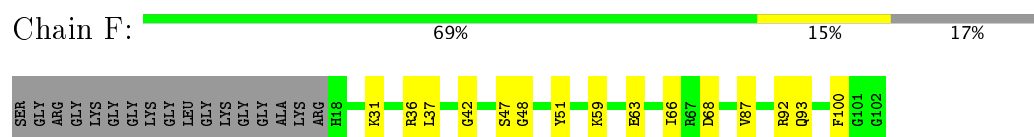
- Molecule 1: Histone H3.2



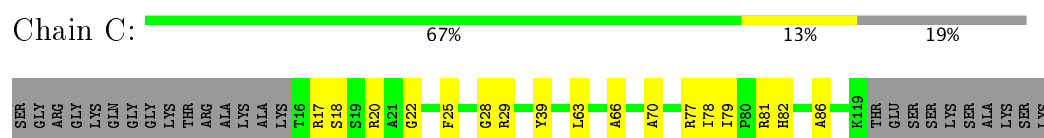
- Molecule 2: Histone H4



- Molecule 2: Histone H4



- Molecule 3: Histone H2A



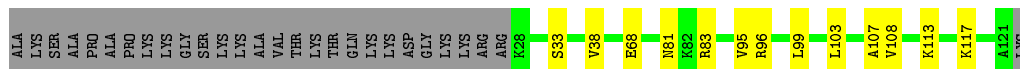
- Molecule 3: Histone H2A

Chain G:  68% 13% 19%



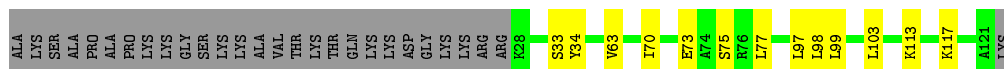
- Molecule 4: Histone H2B 1.1

Chain D:  66% 11% 23%




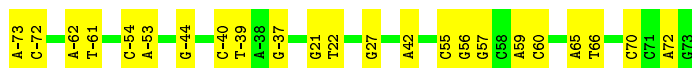
- Molecule 4: Histone H2B 1.1

Chain H:  66% 11% 23%




- Molecule 5: DNA (147-MER)

Chain I:  84% 16%



- Molecule 6: DNA (147-MER)

Chain J:  90% 10%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	55000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	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 ⓘ

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	0.40	0/823	0.60	0/1104
1	E	0.40	0/819	0.60	0/1100
2	B	0.39	0/686	0.60	0/918
2	F	0.41	0/691	0.55	0/923
3	C	0.40	0/814	0.61	0/1099
3	G	0.38	0/821	0.61	0/1109
4	D	0.42	0/746	0.56	0/1004
4	H	0.41	0/746	0.56	0/1004
5	I	0.86	0/3404	1.05	1/5256 (0.0%)
6	J	0.85	0/3356	1.03	0/5173
All	All	0.68	0/12906	0.87	1/18690 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	42	DA	O4'-C1'-N9	5.18	111.63	108.00

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	811	0	853	20	0
1	E	807	0	842	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	678	0	726	12	0
2	F	683	0	729	10	0
3	C	804	0	859	16	0
3	G	811	0	866	12	0
4	D	735	0	760	9	0
4	H	735	0	760	12	0
5	I	3031	0	1649	15	0
6	J	2996	0	1651	10	0
All	All	12091	0	9695	100	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.

All (100) 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:68:GLN:HE21	1:A:72:ARG:HH21	1.30	0.79
1:E:52:ARG:O	1:E:56:LYS:HB2	1.86	0.75
1:E:68:GLN:HE21	1:E:72:ARG:HH21	1.33	0.75
1:E:46:VAL:O	1:E:50:GLU:HB2	1.93	0.67
1:A:62:ILE:HG22	2:B:33:ALA:HB1	1.78	0.65
3:C:28:GLY:HA3	5:I:44:DG:H3'	1.81	0.63
1:A:108:ASN:ND2	2:B:42:GLY:O	2.32	0.62
3:G:82:HIS:O	3:G:86:ALA:HB2	2.00	0.62
3:C:66:ALA:O	3:C:70:ALA:HB2	1.99	0.62
3:G:66:ALA:O	3:G:70:ALA:HB2	2.00	0.60
1:E:108:ASN:ND2	2:F:42:GLY:O	2.34	0.60
6:J:61:DA:H2''	6:J:62:DT:H2'	1.84	0.60
1:A:70:LEU:HD22	2:B:29:ILE:HD11	1.86	0.58
3:C:17:ARG:HG2	3:C:20:ARG:HD2	1.84	0.58
3:G:29:ARG:NH1	4:H:33:SER:O	2.37	0.57
4:H:99:LEU:HD12	4:H:103:LEU:HB3	1.87	0.56
1:E:42:ARG:NH1	6:J:71:DT:OP2	2.37	0.56
1:A:104:PHE:HA	1:A:107:THR:HG22	1.88	0.56
3:G:82:HIS:O	3:G:86:ALA:CB	2.53	0.56
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.31	0.55
3:C:82:HIS:O	3:C:86:ALA:CB	2.55	0.55
3:C:82:HIS:O	3:C:86:ALA:HB2	2.06	0.55
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.32	0.55
1:A:79:LYS:HD3	1:A:82:LEU:HD21	1.90	0.54
1:E:97:GLU:O	1:E:101:VAL:HB	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:59:DA:H2''	5:I:60:DC:H2'	1.91	0.53
4:H:113:LYS:O	4:H:117:LYS:HB2	2.08	0.53
4:D:113:LYS:O	4:D:117:LYS:CB	2.57	0.53
3:C:79:ILE:HG13	3:C:81:ARG:H	1.74	0.53
1:E:62:ILE:HD11	2:F:37:LEU:HD11	1.91	0.53
2:F:92:ARG:HH12	4:H:97:LEU:HD22	1.73	0.53
4:D:113:LYS:O	4:D:117:LYS:HB2	2.09	0.52
5:I:-37:DG:O6	6:J:36:DC:N4	2.42	0.52
3:G:73:ASN:HB2	3:G:82:HIS:HE2	1.74	0.52
1:A:46:VAL:O	1:A:50:GLU:HB3	2.09	0.52
3:C:29:ARG:NH1	4:D:33:SER:O	2.42	0.52
1:A:50:GLU:OE1	2:B:39:ARG:NH1	2.44	0.51
3:C:39:TYR:OH	4:D:68:GLU:OE1	2.28	0.51
2:F:87:VAL:HG21	2:F:100:PHE:HB2	1.93	0.51
3:G:27:VAL:O	3:G:31:HIS:HB2	2.11	0.51
2:B:87:VAL:HG21	2:B:100:PHE:HB2	1.93	0.50
1:E:61:LEU:O	2:F:36:ARG:NH2	2.39	0.50
3:C:66:ALA:O	3:C:70:ALA:CB	2.58	0.50
1:A:99:TYR:OH	1:A:133:GLU:OE2	2.28	0.50
1:A:52:ARG:O	1:A:56:LYS:HB2	2.11	0.50
3:G:17:ARG:HG2	3:G:20:ARG:HD2	1.94	0.50
3:C:18:SER:O	3:C:22:GLY:N	2.44	0.50
1:A:37:LYS:NZ	5:I:72:DA:OP1	2.38	0.49
2:F:47:SER:OG	2:F:48:GLY:N	2.45	0.49
5:I:65:DA:H1'	5:I:66:DT:H5'	1.94	0.49
3:C:77:ARG:HH11	5:I:-54:DC:H5'	1.77	0.48
1:A:46:VAL:O	1:A:50:GLU:CB	2.62	0.48
2:B:47:SER:OG	2:B:48:GLY:N	2.46	0.48
1:E:103:LEU:HD21	1:E:124:ILE:HG23	1.96	0.47
6:J:-69:DA:H2''	6:J:-68:DG:H2'	1.95	0.47
1:A:61:LEU:HD12	2:B:36:ARG:HE	1.80	0.47
4:H:113:LYS:O	4:H:117:LYS:CB	2.63	0.47
3:C:18:SER:OG	3:C:25:PHE:O	2.33	0.46
3:C:77:ARG:HH21	6:J:58:DG:H5'	1.79	0.46
3:C:78:ILE:HG23	3:C:82:HIS:HB2	1.97	0.46
1:A:59:GLU:O	2:B:40:ARG:NH2	2.42	0.46
3:G:39:TYR:HD1	4:H:75:SER:HB2	1.81	0.46
1:E:46:VAL:O	1:E:50:GLU:CB	2.62	0.46
3:G:55:LEU:HD23	4:H:63:VAL:HG13	1.98	0.46
4:H:70:ILE:HG23	4:H:98:LEU:HD12	1.97	0.46
2:B:68:ASP:OD2	2:B:93:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-57:DC:H4'	6:J:-56:DC:H5'	1.98	0.45
4:H:33:SER:OG	4:H:34:TYR:N	2.50	0.44
5:I:-54:DC:H2''	5:I:-53:DA:C8	2.52	0.44
3:G:77:ARG:HH22	5:I:57:DG:H4'	1.83	0.44
4:H:73:GLU:O	4:H:77:LEU:CB	2.66	0.44
5:I:21:DG:H2'	5:I:22:DT:H71	1.99	0.44
2:F:59:LYS:NZ	2:F:63:GLU:OE2	2.42	0.43
2:F:68:ASP:OD2	2:F:93:GLN:NE2	2.51	0.43
2:B:79:LYS:N	6:J:28:DG:OP1	2.49	0.43
1:E:83:ARG:NH1	5:I:27:DG:OP1	2.52	0.43
5:I:-62:DA:H2'	5:I:-61:DT:H71	1.98	0.43
1:A:75:ALA:HB1	1:A:82:LEU:HD12	2.00	0.43
1:E:71:VAL:HG13	2:F:66:ILE:HD11	2.01	0.43
1:A:45:THR:OG1	5:I:70:DC:OP1	2.32	0.43
3:G:58:LEU:HD21	4:H:99:LEU:HD11	2.01	0.42
2:B:26:ILE:HD12	2:B:59:LYS:HD3	2.01	0.42
4:D:103:LEU:O	4:D:107:ALA:HB2	2.20	0.42
4:D:81:ASN:HB3	4:D:83:ARG:HH11	1.85	0.42
5:I:-73:DA:H2''	5:I:-72:DC:C5	2.54	0.42
1:A:107:THR:HG23	1:A:119:ILE:HD12	2.02	0.41
3:C:63:LEU:HD11	4:D:38:VAL:HG13	2.02	0.41
1:E:61:LEU:HA	1:E:63:ARG:HH21	1.85	0.41
6:J:-27:DC:H4'	6:J:-26:DT:H5'	2.00	0.41
5:I:55:DC:H2''	5:I:56:DG:N7	2.36	0.41
5:I:-40:DC:H2'	5:I:-39:DT:C6	2.55	0.41
3:G:60:ALA:O	3:G:64:GLU:HB2	2.21	0.41
3:C:70:ALA:HA	3:C:82:HIS:CD2	2.55	0.41
4:H:73:GLU:O	4:H:77:LEU:HB2	2.21	0.41
4:D:96:ARG:HG3	4:D:108:VAL:HG21	2.03	0.41
6:J:1:DT:H6	6:J:1:DT:H2'	1.75	0.40
1:A:95:ALA:HB2	2:B:97:LEU:HD22	2.03	0.40
4:D:95:VAL:HG13	4:D:99:LEU:HD12	2.03	0.40
6:J:-23:DC:H2''	6:J:-22:DA:H8	1.86	0.40
2:F:31:LYS:HG3	2:F:51:TYR:CE1	2.57	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	A	96/135 (71%)	92 (96%)	4 (4%)	0	100	100
1	E	96/135 (71%)	93 (97%)	3 (3%)	0	100	100
2	B	82/102 (80%)	79 (96%)	3 (4%)	0	100	100
2	F	83/102 (81%)	79 (95%)	4 (5%)	0	100	100
3	C	102/129 (79%)	96 (94%)	6 (6%)	0	100	100
3	G	103/129 (80%)	99 (96%)	4 (4%)	0	100	100
4	D	92/122 (75%)	90 (98%)	2 (2%)	0	100	100
4	H	92/122 (75%)	85 (92%)	7 (8%)	0	100	100
All	All	746/976 (76%)	713 (96%)	33 (4%)	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	86/110 (78%)	86 (100%)	0	100	100
1	E	85/110 (77%)	85 (100%)	0	100	100
2	B	70/78 (90%)	70 (100%)	0	100	100
2	F	70/78 (90%)	70 (100%)	0	100	100
3	C	83/101 (82%)	83 (100%)	0	100	100
3	G	84/101 (83%)	83 (99%)	1 (1%)	75	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	80/102 (78%)	80 (100%)	0	100	100
4	H	80/102 (78%)	80 (100%)	0	100	100
All	All	638/782 (82%)	637 (100%)	1 (0%)	95	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	25	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	68	GLN
2	B	25	ASN
4	D	46	HIS
4	D	81	ASN
1	E	68	GLN
2	F	25	ASN
4	H	46	HIS
4	H	81	ASN

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.