



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 14, 2018 – 10:18 PM EST

PDB ID : 6ESH
EMDB ID: : EMD-3949
Title : Nucleosome breathing : Class 3
Authors : Bilokapic, S.; Halic, M.
Deposited on : 2017-10-20
Resolution : 5.10 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

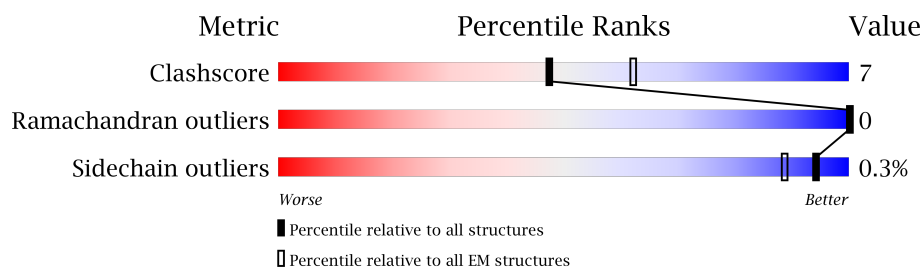
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.10 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	58% 15% 27%
1	E	135	59% 11% 30%
2	B	102	68% 12% 21%
2	F	102	60% 19% 22%
3	C	129	60% 18% 22%
3	G	129	64% 16% .. 19%
4	D	122	65% 10% 25%
4	H	122	58% 15% 27%
5	I	147	63% 29% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	J	147	<div><div></div><div>66%</div><div>24%</div><div>• 7%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11474 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	95	Total	C	N	O	S	0	0
			784	495	150	136	3		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			648	410	126	111	1		
2	F	80	Total	C	N	O	S	0	0
			641	405	125	110	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	100	Total	C	N	O	0	0
			771	484	151	136		
3	G	104	Total	C	N	O	0	0
			804	507	157	140		

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	91	Total	C	N	O	S	0	0
			708	447	125	134	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	89	Total	C	N	O	S	0	0
			690	436	122	130	2		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is a DNA chain called DNA (137-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	137	Total	C	N	O	P	0	0
			2822	1335	528	822	137		

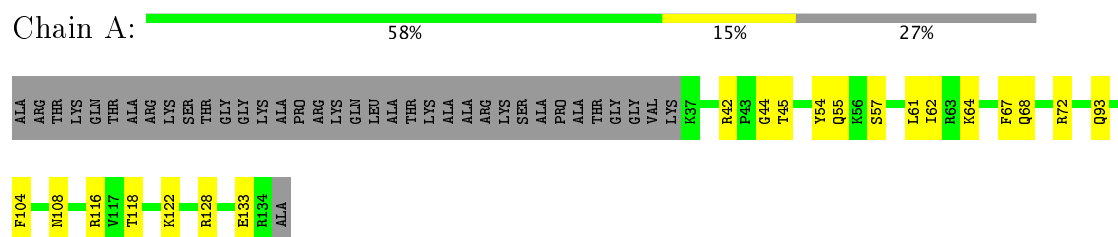
- Molecule 6 is a DNA chain called DNA (137-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	137	Total	C	N	O	P	0	0
			2795	1326	510	822	137		

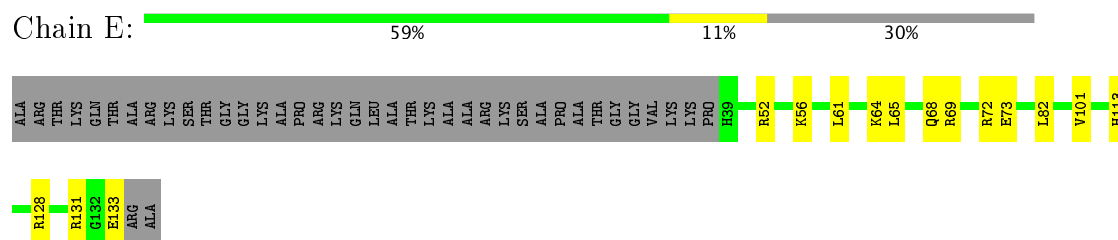
3 Residue-property plots

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.

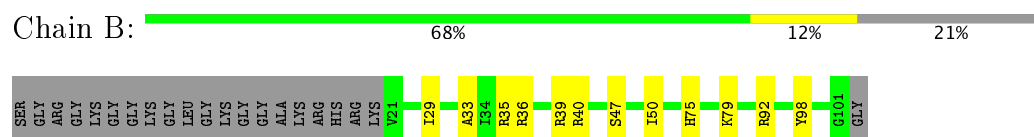
• Molecule 1: Histone H3.2



• Molecule 1: Histone H3.2



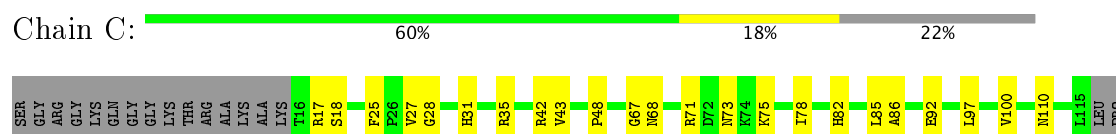
• Molecule 2: Histone H4



• Molecule 2: Histone H4



• Molecule 3: Histone H2A



LYS
LYS
THR
GLU
SER
SER
LYS
SER
LYS
ALA
LYS
SER
LYS
LYS

• Molecule 3: Histone H2A

Chain G: 64% 16% 19%

SER GLY ARG GLY LYS GLN GLY LYS THR ARG ALA LYS LYS T16 R17 S18 F25 P25 V27 G28 H31 R32 R35 Y39 P48 V54 N68 R71 D72 N73 R77 R81 R82 L85 A86 V87 R88 R89 L93 L102 K119 THR GLU SER

SER
LYS
SER
ALA
LYS
SER
LYS

• Molecule 4: Histone H2B 1.1

Chain D: 65% 10% 25%

ALA LYS SER ALA ALA PRO PRO LYS LYS GLY THR LYS VAL LYS THR GLN LYS LYS ASP GLY LYS ARG ARG LYS THR ARG K31 H46 I51 A55 I58 E73 T87 S88 R89 E90 L98 L99 L103 A104 A121 LYS

• Molecule 4: Histone H2B 1.1

Chain H: 58% 15% 27%

ALA LYS SER ALA ALA PRO PRO LYS LYS GLY SER LYS LYS VAL LYS THR GLN LYS LYS ASP GLY LYS ARG ARG LYS THR ARG LYS GLU S33 Y34 I58 D65 I70 A71 G72 E73 A74 S75 N81 R82 R83 R89 V95 R96 L97 L98 L99 L103

A107
A121
LYS

• Molecule 5: DNA (137-MER)

Chain I: 63% 29% 7%

DA DC DA DG DA DG DT DG DA T-63 A-62 T-59 C-58 T-57 G-56 G-51 T-50 A-43 A-38 G-37 G-36 G-35 A-34 G-33 C-28 C-27 C-26 G-21 T-17 T-16 A-15 A-12 G-6 G-5 G-4 A-3 C-2 A-1 G0 G4 T5 A6 C7 G8 T9 G10 G18

A26 G27 A28 T35 A36 C37 T45 C49 G50 T54 C55 G56 G57 C61 C70 G73

• Molecule 6: DNA (137-MER)

Chain J: 66% 24% 7%

G-73 T-72 G-71 G-70 G-61 G-60 T-59 G-58 C-57 C-56 G-55 A-54 G-53 C-46 A-45 A-44 G-40 T-39 T-36 A-35 G-34 T-28 T-6 A-5 G-2 G-1 C6 C7 C8 G9 T13 T14 T15 A16 A17 A24 G25 G26 G27 T34 C35 C36 C37 T38 C44 C45 A50

C51 G58 A63 DA DA DA DA DC DC DT

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	22000	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, 100	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), FEI FALCON II (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	0.31	0/823	0.54	0/1104
1	E	0.31	0/795	0.57	0/1067
2	B	0.32	0/655	0.58	0/878
2	F	0.31	0/648	0.58	0/868
3	C	0.30	0/780	0.61	1/1054 (0.1%)
3	G	0.31	0/814	0.66	2/1099 (0.2%)
4	D	0.31	0/719	0.52	0/969
4	H	0.34	0/701	0.60	1/946 (0.1%)
5	I	0.89	0/3168	1.13	14/4891 (0.3%)
6	J	0.88	0/3132	1.11	11/4828 (0.2%)
All	All	0.67	0/12235	0.92	29/17704 (0.2%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	26	DA	O4'-C1'-N9	-8.44	102.09	108.00
6	J	16	DA	O4'-C1'-N9	7.50	113.25	108.00
6	J	-28	DT	O4'-C1'-N1	-7.37	102.84	108.00
6	J	58	DG	O4'-C1'-N9	6.96	112.87	108.00
5	I	28	DA	O4'-C1'-N9	-6.70	103.31	108.00
6	J	13	DT	O4'-C1'-N1	-6.70	103.31	108.00
5	I	-28	DC	O4'-C1'-N1	-6.55	103.41	108.00
5	I	4	DG	O4'-C4'-C3'	-6.50	101.90	104.50
6	J	35	DC	O4'-C1'-N1	6.06	112.24	108.00
5	I	-12	DA	O4'-C1'-N9	-6.06	103.76	108.00
6	J	-58	DG	OP2-P-O3'	6.01	118.43	105.20
5	I	-35	DG	O4'-C1'-N9	-5.97	103.82	108.00
3	G	85	LEU	CA-CB-CG	5.91	128.88	115.30
6	J	-34	DG	O4'-C1'-N9	5.89	112.12	108.00
5	I	-21	DG	O4'-C1'-N9	5.88	112.12	108.00
4	H	103	LEU	CA-CB-CG	5.85	128.76	115.30
5	I	-15	DA	O4'-C1'-N9	-5.84	103.91	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	44	DC	O4'-C1'-N1	-5.78	103.95	108.00
5	I	57	DG	O4'-C1'-N9	-5.62	104.07	108.00
5	I	36	DA	OP2-P-O3'	5.61	117.54	105.20
5	I	-59	DT	OP1-P-O3'	5.51	117.33	105.20
6	J	-39	DT	P-O3'-C3'	5.32	126.08	119.70
6	J	-5	DA	O4'-C1'-N9	5.29	111.70	108.00
3	G	35	ARG	NE-CZ-NH1	-5.27	117.67	120.30
3	C	85	LEU	CA-CB-CG	5.24	127.35	115.30
6	J	-35	DA	O4'-C1'-N9	-5.18	104.38	108.00
5	I	61	DC	O4'-C1'-N1	5.09	111.57	108.00
5	I	36	DA	P-O3'-C3'	5.07	125.79	119.70
5	I	-62	DA	O4'-C1'-N9	-5.07	104.45	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	17	0
1	E	784	0	820	12	0
2	B	648	0	693	12	0
2	F	641	0	684	16	0
3	C	771	0	815	16	0
3	G	804	0	859	18	0
4	D	708	0	727	10	0
4	H	690	0	708	14	0
5	I	2822	0	1537	27	0
6	J	2795	0	1537	28	0
All	All	11474	0	9233	126	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 7.

All (126) 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:E:52:ARG:O	1:E:56:LYS:HB2	1.84	0.77
1:A:104:PHE:O	1:A:108:ASN:HB2	1.86	0.76
1:A:62:ILE:HA	2:B:36:ARG:HH21	1.61	0.66
1:E:68:GLN:HE21	1:E:72:ARG:HH21	1.46	0.64
5:I:45:DT:C4	6:J:-46:DC:N4	2.68	0.61
3:G:27:VAL:O	3:G:31:HIS:HB2	2.00	0.60
3:C:18:SER:OG	3:C:25:PHE:O	2.20	0.59
3:G:102:ILE:HB	4:H:58:ILE:HD12	1.87	0.57
2:F:77:LYS:HG3	4:H:89:ARG:HH22	1.70	0.56
3:G:68:ASN:OD1	3:G:71:ARG:NH2	2.38	0.56
3:G:32:ARG:NE	6:J:-44:DA:OP2	2.35	0.56
3:G:28:GLY:HA3	6:J:-44:DA:H3'	1.88	0.55
1:A:54:TYR:HB3	2:B:40:ARG:HE	1.71	0.55
2:F:75:HIS:O	4:H:89:ARG:NH2	2.40	0.55
3:G:27:VAL:HG13	3:G:48:PRO:HB2	1.88	0.55
5:I:-33:DG:N2	6:J:34:DT:O2	2.40	0.55
2:B:35:ARG:O	2:B:39:ARG:HB2	2.06	0.54
2:B:92:ARG:HH21	4:D:98:LEU:HD23	1.73	0.54
3:C:17:ARG:HH21	3:C:28:GLY:HA2	1.73	0.54
1:E:128:ARG:NE	1:E:133:GLU:OE1	2.40	0.54
1:E:72:ARG:NH1	1:E:82:LEU:O	2.40	0.54
2:F:37:LEU:O	2:F:41:GLY:N	2.39	0.54
3:C:42:ARG:HB2	6:J:38:DT:H4'	1.90	0.54
6:J:16:DA:H1'	6:J:17:DA:C8	2.43	0.53
6:J:26:DG:H2''	6:J:27:DG:C8	2.43	0.53
2:F:47:SER:HB3	2:F:50:ILE:HG12	1.91	0.53
3:G:31:HIS:CG	3:G:35:ARG:HH12	2.27	0.53
6:J:-6:DT:H2''	6:J:-5:DA:C8	2.44	0.53
4:H:73:GLU:HG3	4:H:98:LEU:HD21	1.91	0.53
3:G:17:ARG:HH21	3:G:28:GLY:HA2	1.74	0.53
5:I:70:DC:N4	6:J:-71:DG:O6	2.43	0.52
3:C:73:ASN:O	3:C:75:LYS:NZ	2.41	0.52
1:A:55:GLN:O	3:G:81:ARG:NH2	2.43	0.52
1:A:62:ILE:HG22	2:B:33:ALA:HB1	1.90	0.52
3:C:17:ARG:NE	5:I:-43:DA:OP1	2.42	0.52
3:C:35:ARG:HG2	3:C:43:VAL:HB	1.93	0.51
3:C:82:HIS:O	3:C:86:ALA:HB2	2.11	0.51
1:E:128:ARG:HB3	1:E:133:GLU:HB2	1.90	0.51
1:E:73:GLU:OE1	2:F:25:ASN:ND2	2.43	0.51
1:A:61:LEU:HD12	2:B:36:ARG:HD2	1.93	0.50
2:F:26:ILE:HG13	2:F:55:ARG:HD3	1.94	0.50
6:J:15:DT:H2''	6:J:16:DA:C8	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-28:DC:N4	6:J:27:DG:O6	2.45	0.50
2:B:75:HIS:O	4:D:89:ARG:NH1	2.44	0.49
2:F:38:ALA:O	2:F:42:GLY:N	2.45	0.49
3:G:18:SER:OG	3:G:25:PHE:O	2.23	0.49
4:D:87:THR:OG1	4:D:90:GLU:OE1	2.26	0.49
4:H:81:ASN:O	4:H:83:ARG:NH1	2.45	0.49
5:I:9:DT:H2"	5:I:10:DG:C8	2.48	0.49
2:F:38:ALA:HB1	2:F:43:VAL:HB	1.94	0.49
6:J:50:DA:H1'	6:J:51:DC:H5'	1.95	0.49
1:A:64:LYS:HD3	1:A:93:GLN:HE22	1.77	0.48
3:G:27:VAL:O	3:G:31:HIS:CB	2.61	0.48
3:G:54:VAL:HG22	4:H:107:ALA:HB1	1.94	0.48
2:F:55:ARG:O	2:F:59:LYS:HB2	2.14	0.48
2:B:98:TYR:OH	4:H:65:ASP:OD2	2.29	0.47
5:I:-27:DC:H2"	5:I:-26:DC:C5	2.49	0.47
5:I:-51:DG:H2'	5:I:-50:DT:H71	1.96	0.47
1:A:42:ARG:HG3	5:I:70:DC:H3'	1.97	0.47
1:A:67:PHE:HD1	2:B:29:ILE:HD11	1.80	0.47
3:C:31:HIS:CD2	3:C:35:ARG:HE	2.32	0.47
6:J:-2:DC:H2"	6:J:-1:DG:C8	2.50	0.47
1:E:128:ARG:HA	1:E:131:ARG:HB2	1.98	0.46
5:I:54:DT:H4'	5:I:55:DC:H5'	1.98	0.46
4:H:33:SER:OG	4:H:34:TYR:N	2.45	0.46
3:G:85:LEU:O	3:G:89:ASN:HB2	2.16	0.46
2:F:35:ARG:NH2	5:I:9:DT:OP2	2.49	0.46
1:A:116:ARG:HD3	5:I:-3:DA:H3'	1.98	0.45
5:I:36:DA:H1'	5:I:37:DC:H5'	1.98	0.45
5:I:5:DT:H2"	5:I:6:DA:C8	2.51	0.45
6:J:-61:DG:H2"	6:J:-60:DG:H5'	1.98	0.45
3:C:68:ASN:OD1	3:C:71:ARG:NH2	2.49	0.45
1:E:101:VAL:HG13	2:F:41:GLY:HA2	1.99	0.45
1:A:128:ARG:NE	1:A:133:GLU:OE1	2.49	0.45
6:J:-40:DG:H2'	6:J:-39:DT:C6	2.51	0.45
3:G:87:VAL:HG22	3:G:93:LEU:HD13	1.98	0.45
1:A:44:GLY:N	6:J:9:DG:OP1	2.46	0.45
4:D:99:LEU:HB2	4:D:104:ALA:HB2	1.99	0.44
4:D:55:ALA:HA	4:D:58:ILE:HG22	1.98	0.44
2:F:78:ARG:NH2	2:F:85:ASP:OD2	2.47	0.44
3:C:97:LEU:HD22	3:C:100:VAL:HG21	1.99	0.44
5:I:-38:DA:H2"	5:I:-37:DG:C8	2.53	0.44
5:I:35:DT:H2"	5:I:36:DA:C5	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-6:DG:H1'	5:I:-5:DG:H5'	1.98	0.44
3:G:39:TYR:O	4:H:75:SER:OG	2.24	0.44
4:D:73:GLU:HG3	4:D:98:LEU:HD21	1.99	0.44
5:I:-17:DT:O4	6:J:16:DA:N6	2.51	0.43
3:G:31:HIS:O	3:G:35:ARG:NH1	2.51	0.43
2:B:47:SER:HB3	2:B:50:ILE:HG12	1.99	0.43
2:F:45:ARG:HE	5:I:7:DC:H4'	1.84	0.43
2:B:79:LYS:HB2	6:J:27:DG:H5''	2.00	0.43
3:C:31:HIS:ND1	3:C:48:PRO:HG2	2.34	0.43
5:I:35:DT:O2	6:J:-34:DG:N2	2.51	0.43
1:A:68:GLN:HE21	1:A:72:ARG:HH21	1.66	0.43
3:G:73:ASN:HD22	3:G:82:HIS:CD2	2.37	0.42
2:F:92:ARG:NH1	4:H:97:LEU:O	2.50	0.42
5:I:49:DC:H2''	5:I:50:DG:C8	2.54	0.42
1:E:64:LYS:HZ1	5:I:18:DG:H3'	1.84	0.42
4:D:99:LEU:HB3	4:D:103:LEU:HG	2.01	0.42
4:H:70:ILE:O	4:H:74:ALA:HB3	2.19	0.42
4:H:71:ALA:O	4:H:75:SER:HB2	2.19	0.42
3:C:67:GLY:HA3	4:D:46:HIS:CD2	2.55	0.42
2:F:75:HIS:CD2	4:H:81:ASN:HD21	2.38	0.42
3:C:27:VAL:O	3:C:31:HIS:HB2	2.20	0.42
1:E:65:LEU:HB3	1:E:69:ARG:NH1	2.34	0.42
3:C:27:VAL:O	3:C:31:HIS:CB	2.68	0.42
5:I:7:DC:H2''	5:I:8:DG:C8	2.55	0.42
6:J:-57:DC:H2''	6:J:-56:DC:C5	2.55	0.41
3:C:78:ILE:HB	4:D:51:ILE:HD12	2.02	0.41
5:I:-37:DG:O6	6:J:36:DC:N4	2.52	0.41
1:E:61:LEU:O	2:F:36:ARG:NH2	2.47	0.41
1:A:122:LYS:HG3	1:E:113:HIS:HE1	1.84	0.41
1:A:116:ARG:NH1	1:A:118:THR:O	2.51	0.41
3:C:92:GLU:HB3	4:D:103:LEU:HD13	2.02	0.41
3:G:77:ARG:HD3	6:J:-54:DA:H5''	2.03	0.41
5:I:-57:DT:H2''	5:I:-56:DG:C8	2.55	0.41
6:J:6:DC:H2''	6:J:7:DC:C5	2.56	0.41
1:A:57:SER:OG	2:B:40:ARG:NH2	2.53	0.41
6:J:24:DA:C8	6:J:24:DA:H5'	2.55	0.41
6:J:-36:DT:H2''	6:J:-35:DA:C5	2.55	0.41
4:H:95:VAL:HG13	4:H:99:LEU:HD23	2.02	0.41
5:I:-1:DA:H2''	5:I:0:DG:H8	1.87	0.40
6:J:45:DC:H6	6:J:45:DC:H2'	1.73	0.40
1:A:45:THR:OG1	5:I:70:DC:OP1	2.38	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-54:DA:H2''	6:J:-53:DG:C8	2.57	0.40
6:J:-71:DG:H2''	6:J:-70:DG:C8	2.57	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	96/135 (71%)	90 (94%)	6 (6%)	0	100	100
1	E	93/135 (69%)	86 (92%)	7 (8%)	0	100	100
2	B	79/102 (78%)	76 (96%)	3 (4%)	0	100	100
2	F	78/102 (76%)	77 (99%)	1 (1%)	0	100	100
3	C	98/129 (76%)	94 (96%)	4 (4%)	0	100	100
3	G	102/129 (79%)	98 (96%)	4 (4%)	0	100	100
4	D	89/122 (73%)	88 (99%)	1 (1%)	0	100	100
4	H	87/122 (71%)	85 (98%)	2 (2%)	0	100	100
All	All	722/976 (74%)	694 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	86/110 (78%)	86 (100%)	0	100	100
1	E	83/110 (76%)	83 (100%)	0	100	100
2	B	67/78 (86%)	67 (100%)	0	100	100
2	F	66/78 (85%)	66 (100%)	0	100	100
3	C	79/101 (78%)	78 (99%)	1 (1%)	73	87
3	G	83/101 (82%)	82 (99%)	1 (1%)	75	88
4	D	77/102 (76%)	77 (100%)	0	100	100
4	H	75/102 (74%)	75 (100%)	0	100	100
All	All	616/782 (79%)	614 (100%)	2 (0%)	94	96

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

Mol	Chain	Res	Type
3	C	110	ASN
3	G	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
3	C	73	ASN
3	C	110	ASN
1	E	68	GLN
1	E	93	GLN
2	F	25	ASN
3	G	31	HIS
3	G	73	ASN
4	H	46	HIS
4	H	60	ASN
4	H	81	ASN

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.