



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:43 PM BST

PDB ID : 2WW9  
EMDB ID: : EMD-1651  
Title : Cryo-EM structure of the active yeast Ssh1 complex bound to the yeast 80S ribosome  
Authors : Becker, T.; Mandon, E.; Bhushan, S.; Jarasch, A.; Armache, J.P.; Funes, S.; Jossinet, F.; Gumbart, J.; Mielke, T.; Berninghausen, O.; Schulten, K.; Westhof, E.; Gilmore, R.; Beckmann, R.  
Deposited on : 2009-10-22  
Resolution : 8.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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) : trunk27241

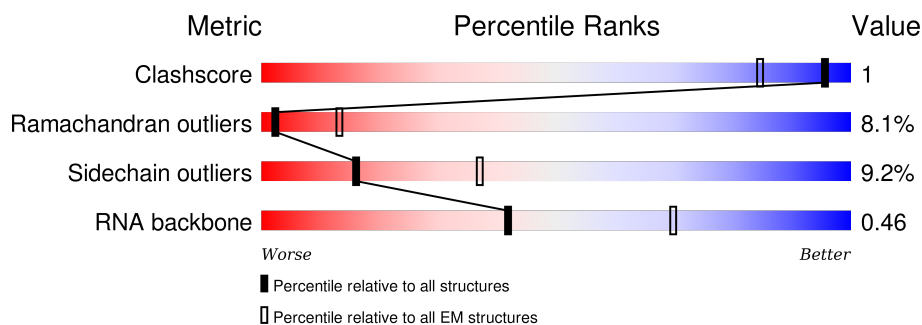
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.60 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
RNA backbone	3027	244

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	490	86% 11% .
2	B	80	68% 5% . 25%
3	C	87	22% .. 76%
4	D	63	. 43% 48% 8%
5	E	34	65% 35%
6	F	25	92% 8%
7	G	18	94% 6%
8	H	362	50% 16% 7% . 26%

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Mol	Chain	Length	Quality of chain
9	I	184	<div><div></div><div>65%12%5%•17%</div></div>
10	J	189	<div><div></div><div>27%•72%</div></div>
11	K	142	<div><div></div><div>50%6%•42%</div></div>
12	L	127	<div><div></div><div>74%21%••</div></div>
13	M	113	<div><div></div><div>61%9%••26%</div></div>
14	N	120	<div><div></div><div>44%8%••43%</div></div>
15	O	51	<div><div></div><div>43%20%10%27%</div></div>

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 14301 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 SEC SIXTY-ONE PROTEIN HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	490	Total	C	N	O	S	0	0
			3770	2487	603	671	9		

- Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN SSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	60	Total	C	N	O	S	0	0
			472	318	76	77	1		

- Molecule 3 is a protein called PROTEIN TRANSPORT PROTEIN SEB2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	21	Total	C	N	O	0	0
			162	112	24	26		

- Molecule 4 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	63	Total	C	N	O	P	0	0
			1347	603	245	436	63		

- Molecule 5 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	34	Total	C	N	O	P	0	0
			740	332	148	226	34		

- Molecule 6 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	25	Total	C	N	O	P	0	0
			536	239	99	173	25		

- Molecule 7 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	18	Total	C	N	O	P	0	0
			379	169	64	128	18		

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN L4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	269	Total	C	N	O	S	0	0
			2039	1281	391	363	4		

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	153	Total	C	N	O	S	0	0
			1212	756	236	219	1		

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	53	Total	C	N	O	S	0	0
			410	254	83	72	1		

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	83	Total	C	N	O	S	0	0
			663	424	111	126	2		

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	127	Total	C	N	O	S	0	0
			1002	630	193	178	1		

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	84	Total	C	N	O	S	0	0
			706	447	140	118	1		

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	69	Total	C	N	O	S	0	0
			547	345	101	99	2		

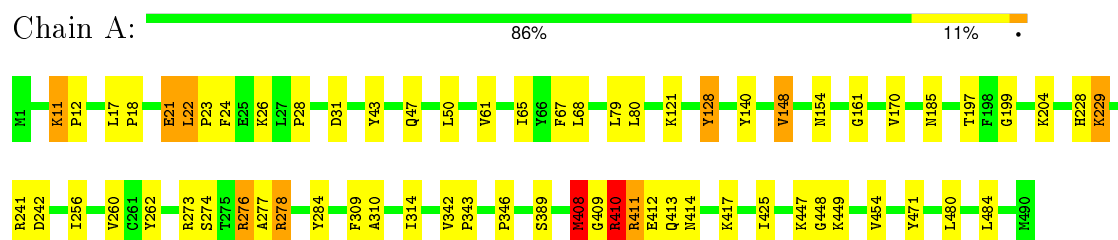
- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	37	Total	C	N	O	S	0	0
			316	200	66	48	2		

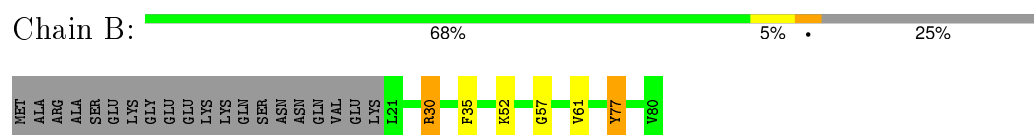
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

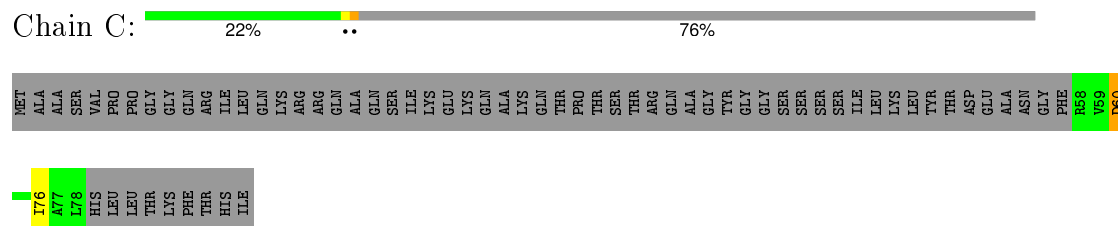
- Molecule 1: SEC SIXTY-ONE PROTEIN HOMOLOG



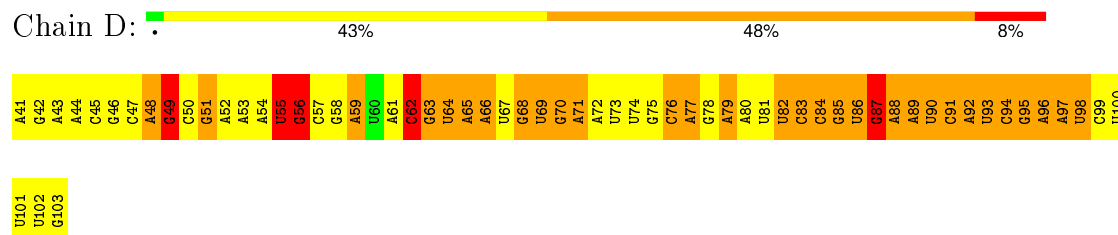
- Molecule 2: PROTEIN TRANSPORT PROTEIN SSS1



- Molecule 3: PROTEIN TRANSPORT PROTEIN SEB2



- Molecule 4: 25S RRNA



- Molecule 5: 25S RRNA

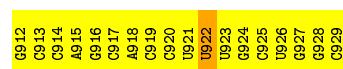




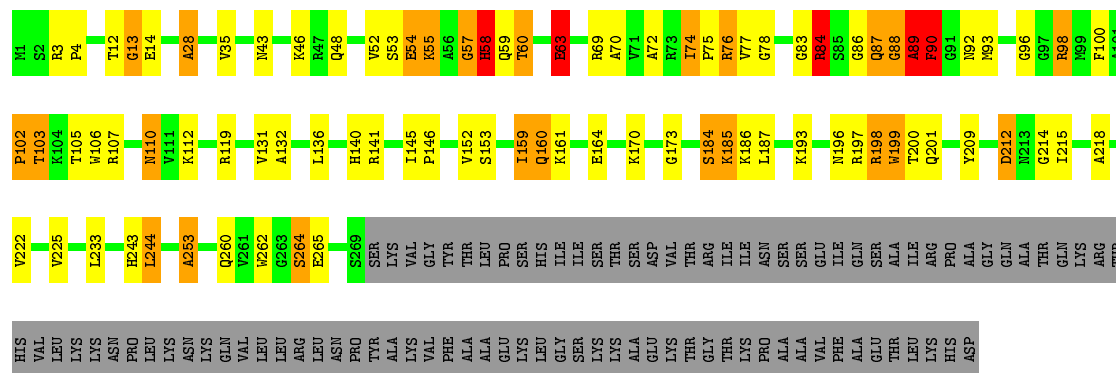
• Molecule 6: 25S RRNA



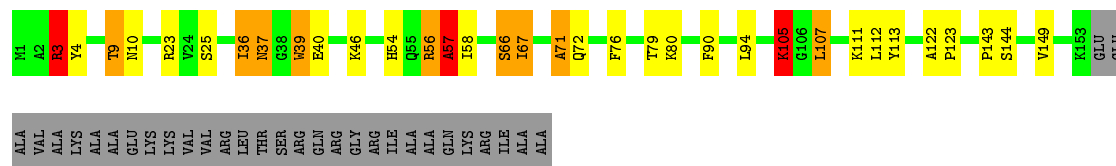
• Molecule 7: 25S RRNA



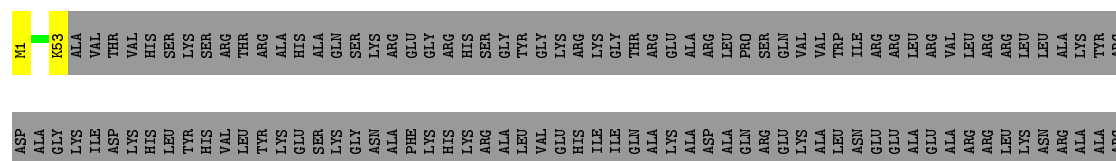
• Molecule 8: 60S RIBOSOMAL PROTEIN L4-B



• Molecule 9: 60S RIBOSOMAL PROTEIN L17-A



• Molecule 10: 60S RIBOSOMAL PROTEIN L19





ASP  
ARG  
ALA  
ARG  
ALA  
GLN  
ARG  
VAL  
ALA  
GLU  
LYS  
ARG  
ASP  
ALA  
LEU  
LEU  
LEU  
GLU  
ASP  
ALA

• Molecule 11: 60S RIBOSOMAL PROTEIN L25

Chain K:  50% 6% 42%

MET  
ALA  
PRO  
SER  
ALA  
LYS  
ALA  
THR  
ALA  
ALA  
LYS  
LYS  
VAL  
VAL  
LYS  
GLY  
THR  
ASN  
GLY  
LYS  
LYS  
ALA  
LEU  
LYS  
VAL  
ARG  
THR  
SER  
ALA  
THR  
PHE  
ARG  
LEU  
PRO  
LYS  
THR  
LEU  
LYS  
LEU  
ALA  
ARG  
ALA  
PRO  
LYS  
TYR  
ALA  
SER  
LYS  
ALA  
VAL  
PRO  
HIS  
TYR  
ASN  
ARG  
L57  
V62

Q65  
E70  
K74  
K100  
V105  
K109  
V110  
N111  
N117  
Y123  
D131  
I139  
GLY  
TYR  
ILE

• Molecule 12: 60S RIBOSOMAL PROTEIN L26-A

Chain L:  74% 21% . .

M1  
L6  
D11  
S10  
D11  
A22  
P23  
S24  
R28  
S36  
K37  
I45  
K46  
R52  
V56  
L57  
K63  
K64  
K77  
F78  
K84  
V85  
T86  
K87  
E88  
K89  
V95  
P96  
I97  
I106  
T107  
K108  
L111  
R121  
K122  
K125  
L126  
E127

• Molecule 13: 60S RIBOSOMAL PROTEIN L31-A

Chain M:  61% 9% . . 26%

MET  
ALA  
GLY  
LEU  
LYS  
ASP  
VAL  
VAL  
T9  
L20  
S24  
F25  
K26  
K38  
D47  
L51  
R62  
V67  
R77  
K78  
R79  
E82  
K86  
F90  
S91  
Y92  
VAL  
GLU  
PRO  
VAL  
LEU  
VAL  
VAL  
SER  
ALA  
LYS  
GLY  
LEU  
GLN  
THR  
VAL  
VAL  
GLU  
ASP  
ALA

• Molecule 14: 60S RIBOSOMAL PROTEIN L35

Chain N:  44% 8% . . 43%

M1  
A2  
G3  
V4  
K5  
L9  
S13  
K14  
K32  
V33  
Q34  
K35  
L36  
S37  
R38  
P39  
S40  
L41  
I44  
R67  
Q68  
L69  
TYR  
LYS  
GLY  
LYS  
LYS  
TYR  
GLN  
PRO  
LYS  
ASP  
LEU  
ARG  
ALA  
LYS  
LYS  
THR  
ARG  
ALA  
LEU  
ARG  
ALA  
LEU  
THR  
LYS  
PHE  
GLU  
SER  
GLN  
VAL  
THR  
GLU

LYS  
GLN  
ARG  
LYS  
LYS  
GLN  
ILE  
ALA  
PHE  
PRO  
GLN  
ARG  
LYS  
TYR  
ALA  
ILE  
LYS  
ALA

• Molecule 15: 60S RIBOSOMAL PROTEIN L39

Chain O:  43% 20% 10% 27%

M1  
R5  
S6  
F7  
K17  
K18  
Q19  
N20  
R21  
P22  
L23  
P24  
Q25  
W26  
T31  
N32  
R33  
T34  
R35  
R36  
Y37  
ASN  
ALA  
LYS  
ARG  
ARG  
ASN  
TRP  
ARG  
ARG  
THR  
LYS  
MET  
ASN  
ILE

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO163	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	0.90	0/3848	1.07	8/5234 (0.2%)
10	J	1.02	0/412	0.95	0/551
11	K	0.91	0/670	1.08	2/903 (0.2%)
12	L	1.01	0/1013	1.25	3/1351 (0.2%)
13	M	1.11	0/719	1.26	7/959 (0.7%)
14	N	1.07	1/549 (0.2%)	1.40	9/733 (1.2%)
15	O	1.11	0/321	1.41	4/426 (0.9%)
2	B	0.89	0/481	1.00	2/648 (0.3%)
3	C	0.95	0/164	0.88	0/222
4	D	1.62	0/1508	2.62	185/2348 (7.9%)
5	E	1.59	0/833	2.65	109/1298 (8.4%)
6	F	1.60	0/599	2.43	71/932 (7.6%)
7	G	1.54	0/421	2.30	50/653 (7.7%)
8	H	0.99	0/2079	1.39	30/2817 (1.1%)
9	I	1.04	0/1235	1.37	17/1662 (1.0%)
All	All	1.15	1/14852 (0.0%)	1.66	497/20737 (2.4%)

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
11	K	0	2
12	L	0	6
14	N	0	3
15	O	0	5
2	B	0	1
4	D	0	7
5	E	0	2
6	F	0	1
8	H	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	2
All	All	0	45

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	69	LEU	C-O	-12.03	1.00	1.23

The worst 5 of 497 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	532	A	P-O3'-C3'	18.10	141.42	119.70
4	D	69	U	P-O3'-C3'	14.78	137.43	119.70
6	F	1661	A	N1-C6-N6	14.08	127.05	118.60
4	D	53	A	N1-C6-N6	14.06	127.04	118.60
4	D	93	U	P-O3'-C3'	13.80	136.26	119.70

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	TYR	Sidechain
1	A	17	LEU	Peptide
1	A	21	GLU	Peptide
1	A	262	TYR	Sidechain
1	A	43	TYR	Sidechain

## 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	3770	0	3941	11	0
2	B	472	0	519	1	0
3	C	162	0	177	0	0
4	D	1347	0	678	0	0
5	E	740	0	369	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	536	0	272	0	0
7	G	379	0	195	0	0
8	H	2039	0	2106	13	0
9	I	1212	0	1231	5	0
10	J	410	0	452	0	0
11	K	663	0	699	1	0
12	L	1002	0	1093	1	0
13	M	706	0	741	0	0
14	N	547	0	613	4	0
15	O	316	0	349	0	0
All	All	14301	0	13435	37	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 1.

The worst 5 of 37 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)
11:K:100:LYS:HA	11:K:105:VAL:HG22	1.81	0.63
5:E:539:U:H3	5:E:546:G:H1	1.51	0.57
1:A:228:HIS:CG	1:A:229:LYS:H	2.23	0.57
1:A:65:ILE:HD12	1:A:68:LEU:HD12	1.88	0.54
12:L:56:VAL:HG22	12:L:106:ILE:HG22	1.89	0.53

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	488/490 (100%)	428 (88%)	41 (8%)	19 (4%)	<b>4</b> <b>36</b>
2	B	58/80 (72%)	57 (98%)	1 (2%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	19/87 (22%)	17 (90%)	1 (5%)	1 (5%)	2	29
8	H	267/362 (74%)	186 (70%)	38 (14%)	43 (16%)	0	5
9	I	151/184 (82%)	113 (75%)	24 (16%)	14 (9%)	1	16
10	J	51/189 (27%)	46 (90%)	5 (10%)	0	100	100
11	K	81/142 (57%)	71 (88%)	7 (9%)	3 (4%)	4	38
12	L	125/127 (98%)	101 (81%)	8 (6%)	16 (13%)	0	8
13	M	82/113 (73%)	64 (78%)	11 (13%)	7 (8%)	1	18
14	N	67/120 (56%)	60 (90%)	2 (3%)	5 (8%)	1	21
15	O	35/51 (69%)	25 (71%)	2 (6%)	8 (23%)	0	2
All	All	1424/1945 (73%)	1168 (82%)	140 (10%)	116 (8%)	2	19

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
1	A	148	VAL
1	A	274	SER
1	A	276	ARG
1	A	410	ARG

### 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	412/412 (100%)	387 (94%)	25 (6%)	23	60
2	B	50/67 (75%)	46 (92%)	4 (8%)	15	50
3	C	19/73 (26%)	17 (90%)	2 (10%)	8	36
8	H	209/288 (73%)	182 (87%)	27 (13%)	5	28
9	I	124/146 (85%)	109 (88%)	15 (12%)	6	31
10	J	44/154 (29%)	42 (96%)	2 (4%)	34	69
11	K	74/118 (63%)	67 (90%)	7 (10%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	110/110 (100%)	96 (87%)	14 (13%)	5	29
13	M	74/97 (76%)	65 (88%)	9 (12%)	6	31
14	N	62/105 (59%)	59 (95%)	3 (5%)	31	67
15	O	33/46 (72%)	29 (88%)	4 (12%)	6	31
All	All	1211/1616 (75%)	1099 (91%)	112 (9%)	16	43

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	193	LYS
9	I	66	SER
13	M	82	GLU
8	H	201	GLN
8	H	244	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	ASN
12	L	42	GLN
8	H	213	ASN
1	A	403	GLN
8	H	43	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	62/63 (98%)	27 (43%)	10 (16%)
5	E	33/34 (97%)	7 (21%)	2 (6%)
6	F	24/25 (96%)	1 (4%)	0
7	G	17/18 (94%)	1 (5%)	0
All	All	136/140 (97%)	36 (26%)	12 (8%)

5 of 36 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	48	A
4	D	49	G

*Continued on next page...*

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Mol	Chain	Res	Type
4	D	51	G
4	D	56	G
4	D	59	A

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	69	U
4	D	89	A
4	D	96	A
4	D	65	A
4	D	93	U

#### 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.