



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:57 AM GMT

PDB ID : 3NMU  
Title : Crystal Structure of substrate-bound halfmer box C/D RNP  
Authors : Li, H.; Xue, S.; Wang, R.  
Deposited on : 2010-06-22  
Resolution : 2.73 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
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/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

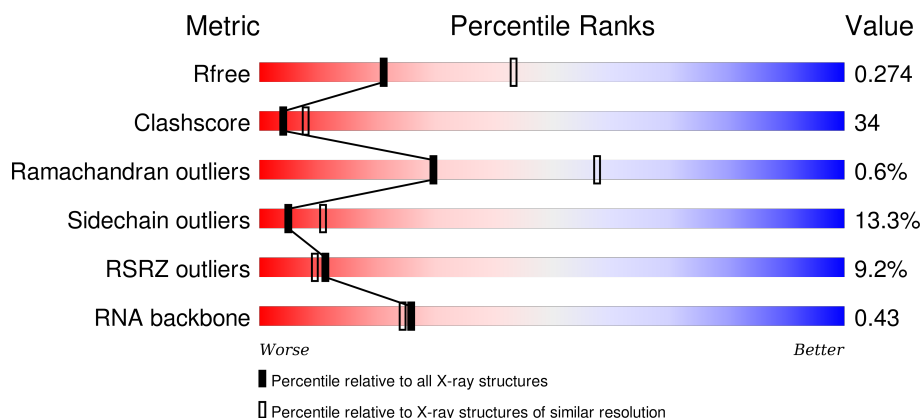
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)
RNA backbone	2183	1004 (3.10-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	379	<div> <div>12%</div> <div>46%</div> <div>43%</div> <div>7%</div> <div>• •</div> </div>
1	B	379	<div> <div>8%</div> <div>43%</div> <div>46%</div> <div>8%</div> <div>•</div> </div>
2	C	129	<div> <div>29%</div> <div>30%</div> <div>55%</div> <div>9%</div> <div>6%</div> </div>
2	G	129	<div> <div>5%</div> <div>40%</div> <div>47%</div> <div>6%</div> <div>• 6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	34	<div><div></div><div>21%50%26%</div><div></div></div>
3	E	34	<div><div></div><div>18%24%59%15%</div><div></div></div>
4	F	234	<div><div></div><div>56%33%8%</div><div></div></div>
4	J	234	<div><div></div><div>3%50%40%7%</div><div></div></div>
5	I	13	<div><div></div><div>15%85%15%</div><div></div></div>
5	K	13	<div><div></div><div>23%15%62%15%8%</div><div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13531 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 NOP5/NOP56 related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2981	1903	518	553	7			
1	B	366	Total	C	N	O	S	0	0	0
			2981	1903	518	553	7			

- Molecule 2 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	121	Total	C	N	O	S	0	0	0
			926	591	153	179	3			
2	G	121	Total	C	N	O	S	0	0	0
			926	591	153	179	3			

- Molecule 3 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	34	Total	C	N	O	P	0	0	0
			732	326	136	236	34			
3	E	34	Total	C	N	O	P	0	0	0
			732	326	136	236	34			

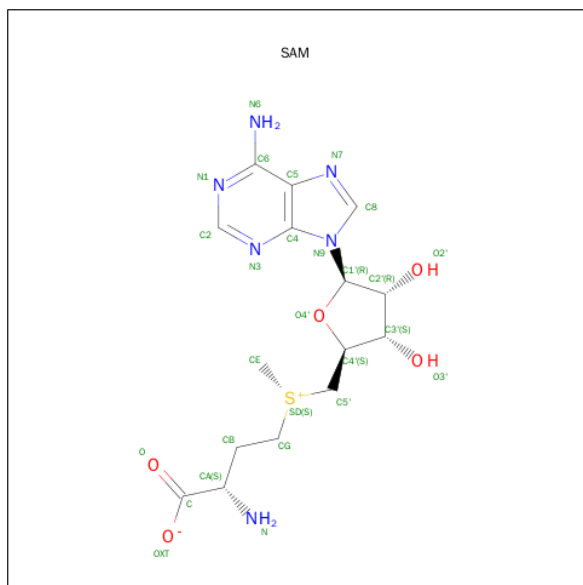
- Molecule 4 is a protein called Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	227	Total	C	N	O	S	0	0	0
			1822	1174	312	334	2			
4	J	227	Total	C	N	O	S	0	0	0
			1822	1174	312	334	2			

- Molecule 5 is a RNA chain called RNA (5'-R(\*GP\*AP\*GP\*CP\*UP\*UP\*CP\*AP\*AP\*CP\*GP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	13	Total	C	N	O	P	0	0	0
			275	124	51	88	12			
5	K	12	Total	C	N	O	P	0	0	0
			255	114	46	83	12			

- Molecule 6 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula:  $C_{15}H_{22}N_6O_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	N	O	S	0	0
			26	15	6	4	1		
6	J	1	Total	C	N	O	S	0	0
			26	15	6	4	1		

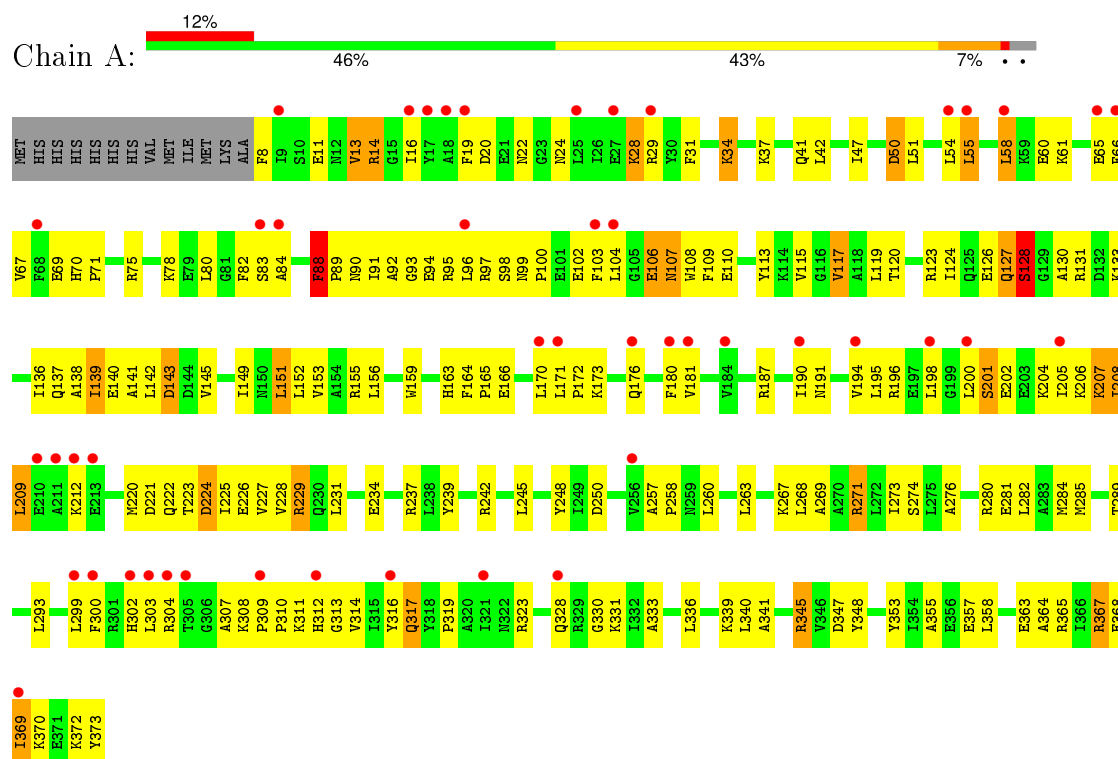
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total	O	0	0
			7	7		
7	B	5	Total	O	0	0
			5	5		
7	C	2	Total	O	0	0
			2	2		
7	F	8	Total	O	0	0
			8	8		
7	G	2	Total	O	0	0
			2	2		
7	J	3	Total	O	0	0
			3	3		

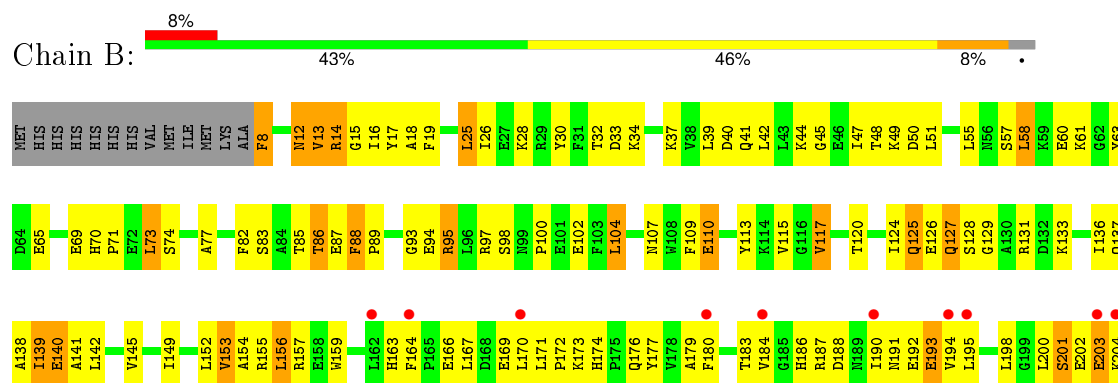
### 3 Residue-property plots [i](#)

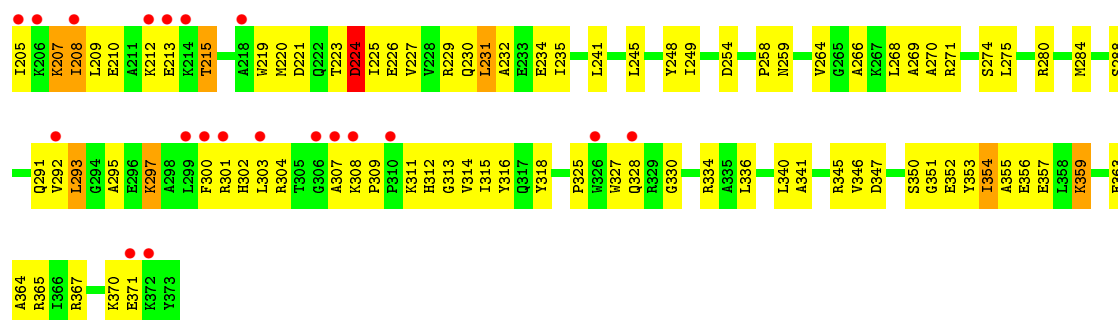
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: NOP5/NOP56 related protein

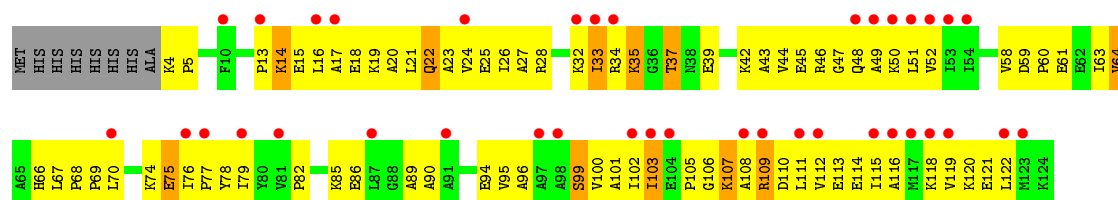


#### • Molecule 1: NOP5/NOP56 related protein

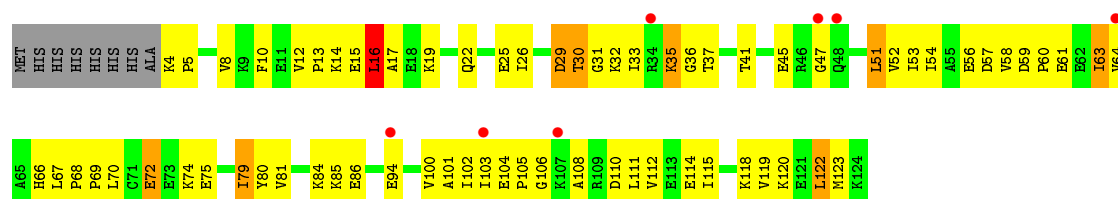




• Molecule 2: 50S ribosomal protein L7Ae



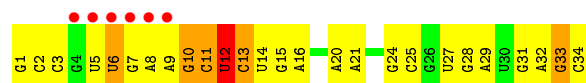
• Molecule 2: 50S ribosomal protein L7Ae



• Molecule 3: RNA (34-MER)

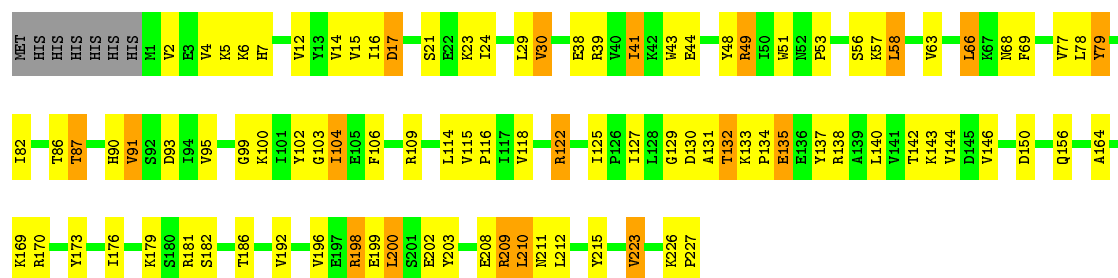


• Molecule 3: RNA (34-MER)

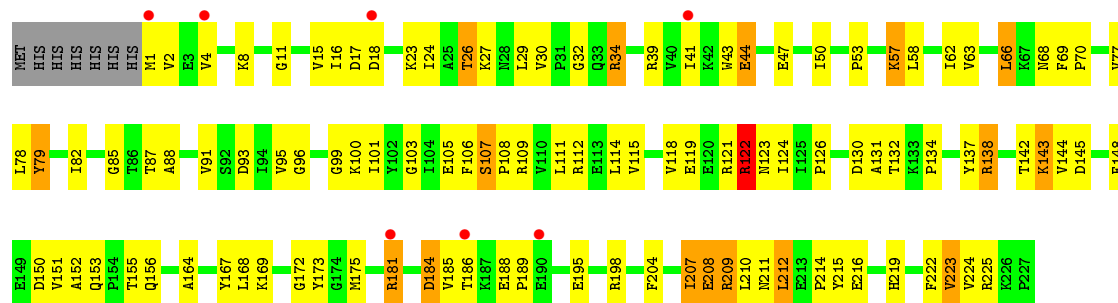


• Molecule 4: Fibrillar-like rRNA/tRNA 2'-O-methyltransferase

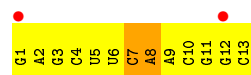
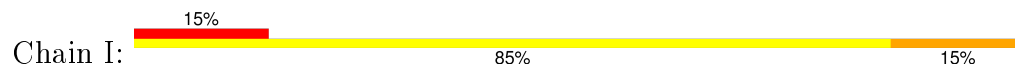




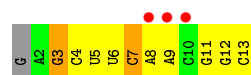
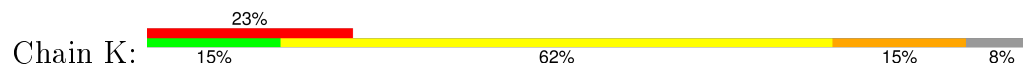
- Molecule 4: Fibrillar-like rRNA/tRNA 2'-O-methyltransferase



- Molecule 5: RNA (5'-R(\*GP\*AP\*GP\*CP\*UP\*UP\*CP\*AP\*AP\*CP\*GP\*GP\*C)-3')



- Molecule 5: RNA (5'-R(\*GP\*AP\*GP\*CP\*UP\*UP\*CP\*AP\*AP\*CP\*GP\*GP\*C)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	293.51Å 94.05Å 96.81Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	33.57 – 2.73 49.08 – 2.73	Depositor EDS
% Data completeness (in resolution range)	79.6 (33.57-2.73) 79.0 (49.08-2.73)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_589)	Depositor
R, $R_{free}$	0.222 , 0.284 0.207 , 0.274	Depositor DCC
$R_{free}$ test set	1788 reflections (3.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.4	Xtriage
Anisotropy	0.828	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 61445 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13531	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAM

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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.50	0/3036	0.73	2/4085 (0.0%)
1	B	0.56	0/3036	0.76	3/4085 (0.1%)
2	C	0.44	0/938	0.65	0/1264
2	G	0.45	0/938	0.62	0/1264
3	D	0.48	0/819	0.99	1/1276 (0.1%)
3	E	0.47	0/819	1.00	2/1276 (0.2%)
4	F	0.57	0/1861	0.76	2/2515 (0.1%)
4	J	0.58	0/1861	0.79	0/2515
5	I	0.42	0/307	0.88	0/477
5	K	0.37	0/284	0.81	0/440
All	All	0.52	0/13899	0.78	10/19197 (0.1%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	12	U	C2-N1-C1'	7.50	126.69	117.70
1	B	142	LEU	CA-CB-CG	7.42	132.36	115.30
1	B	26	ILE	CB-CA-C	-6.22	99.16	111.60
1	A	88	PHE	C-N-CD	6.11	141.24	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	PHE	C-N-CA	-5.99	96.83	122.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	SER	Peptide
1	B	213	GLU	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	2981	0	3022	225	0
1	B	2981	0	3022	247	0
2	C	926	0	977	106	0
2	G	926	0	977	64	0
3	D	732	0	369	48	0
3	E	732	0	369	47	0
4	F	1822	0	1869	78	0
4	J	1822	0	1869	116	0
5	I	275	0	143	23	0
5	K	255	0	131	16	0
6	F	26	0	22	0	0
6	J	26	0	22	8	0
7	A	7	0	0	1	0
7	B	5	0	0	0	0
7	C	2	0	0	0	0
7	F	8	0	0	1	0
7	G	2	0	0	0	0
7	J	3	0	0	1	0
All	All	13531	0	12792	892	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 34.

The worst 5 of 892 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:187:ARG:CG	1:A:212:LYS:HZ1	1.54	1.20
4:F:209:ARG:HG3	4:F:209:ARG:HH11	1.05	1.17
1:A:187:ARG:HB2	1:A:212:LYS:HE2	1.30	1.14
1:A:187:ARG:HB2	1:A:212:LYS:CE	1.82	1.08
1:A:187:ARG:HG3	1:A:212:LYS:HZ1	1.13	1.08

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 X-ray entries followed by that with respect to entries of similar resolution.

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	364/379 (96%)	330 (91%)	30 (8%)	4 (1%)	17	41
1	B	364/379 (96%)	326 (90%)	37 (10%)	1 (0%)	46	74
2	C	119/129 (92%)	102 (86%)	16 (13%)	1 (1%)	24	50
2	G	119/129 (92%)	104 (87%)	14 (12%)	1 (1%)	24	50
4	F	225/234 (96%)	218 (97%)	7 (3%)	0	100	100
4	J	225/234 (96%)	206 (92%)	17 (8%)	2 (1%)	21	47
All	All	1416/1484 (95%)	1286 (91%)	121 (8%)	9 (1%)	30	58

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	122	ARG
1	A	208	ILE
1	B	208	ILE
4	J	208	GLU
1	A	128	SER

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	312/324 (96%)	270 (86%)	42 (14%)	5	10
1	B	312/324 (96%)	264 (85%)	48 (15%)	3	8
2	C	98/105 (93%)	85 (87%)	13 (13%)	5	11
2	G	98/105 (93%)	86 (88%)	12 (12%)	6	13
4	F	197/204 (97%)	171 (87%)	26 (13%)	5	11
4	J	197/204 (97%)	177 (90%)	20 (10%)	9	20
All	All	1214/1266 (96%)	1053 (87%)	161 (13%)	5	11

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	193	GLU
2	C	14	LYS
4	J	66	LEU
1	B	203	GLU
1	B	293	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	174	HIS
1	B	186	HIS
2	C	48	GLN
1	B	163	HIS
1	B	328	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	33/34 (97%)	11 (33%)	1 (3%)
3	E	33/34 (97%)	7 (21%)	1 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	I	12/13 (92%)	2 (16%)	0
5	K	11/13 (84%)	3 (27%)	0
All	All	89/94 (94%)	23 (25%)	2 (2%)

5 of 23 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	D	11	C
3	D	12	U
3	D	13	C
3	D	18	C
3	D	19	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	11	C
3	E	11	C

## 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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SAM	F	228	-	22,28,29	1.23	3 (13%)	18,40,42	3.01	5 (27%)
6	SAM	J	228	-	22,28,29	1.04	1 (4%)	18,40,42	3.51	3 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SAM	F	228	-	-	0/8/31/33	0/3/3/3
6	SAM	J	228	-	-	0/8/31/33	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	228	SAM	C2-N1	2.19	1.38	1.33
6	F	228	SAM	C2-N3	2.79	1.37	1.32
6	J	228	SAM	C2-N3	2.87	1.37	1.32
6	F	228	SAM	O4'-C1'	3.51	1.45	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	228	SAM	N3-C2-N1	-14.34	117.92	128.89
6	F	228	SAM	N3-C2-N1	-11.36	120.19	128.89
6	F	228	SAM	C4-C5-N7	-2.28	107.38	109.48
6	J	228	SAM	C1'-N9-C4	-2.06	123.83	126.94
6	J	228	SAM	C4-C5-N7	-2.01	107.63	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	228	SAM	8	0

## 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.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	366/379 (96%)	0.76	47 (12%) 5 4	61, 83, 116, 157	0
1	B	366/379 (96%)	0.64	30 (8%) 14 12	52, 78, 113, 136	0
2	C	121/129 (93%)	1.55	38 (31%) 1 0	88, 132, 160, 167	0
2	G	121/129 (93%)	0.81	7 (5%) 26 26	83, 108, 132, 143	0
3	D	34/34 (100%)	-0.14	0 100 100	93, 125, 214, 217	0
3	E	34/34 (100%)	0.65	6 (17%) 2 1	103, 129, 212, 215	0
4	F	227/234 (97%)	0.17	0 100 100	55, 69, 91, 112	0
4	J	227/234 (97%)	0.40	7 (3%) 52 53	52, 70, 112, 140	0
5	I	13/13 (100%)	1.65	2 (15%) 3 2	167, 192, 219, 221	0
5	K	12/13 (92%)	1.13	3 (25%) 1 1	176, 191, 213, 214	0
All	All	1521/1578 (96%)	0.64	140 (9%) 11 9	52, 82, 148, 221	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	108	ALA	9.8
5	I	1	G	8.1
2	C	48	GLN	7.7
2	C	111	LEU	5.6
1	A	66	PHE	5.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SAM	J	228	26/27	0.94	0.25	0.89	54,70,105,108	0
6	SAM	F	228	26/27	0.92	0.19	-0.45	52,69,102,106	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.