



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:04 PM GMT

PDB ID : 1IBM  
Title : STRUCTURE OF THE THERMUS THERMOPHILUS 30S RIBOSOMAL SUBUNIT IN COMPLEX WITH A MESSENGER RNA FRAGMENT AND COGNATE TRANSFER RNA ANTICODON STEM-LOOP BOUND AT THE A SITE  
Authors : Ogle, J.M.; Brodersen, D.E.; Clemons Jr., W.M.; Tarry, M.J.; Carter, A.P.; Ramakrishnan, V.  
Deposited on : 2001-03-28  
Resolution : 3.31 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

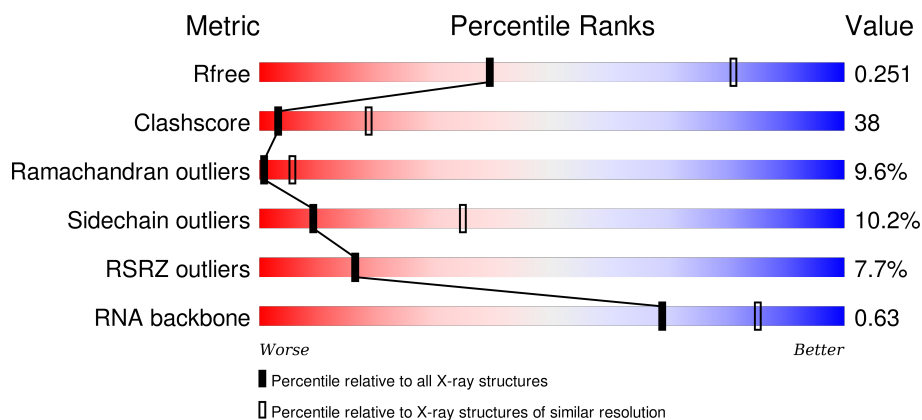
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.31 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.



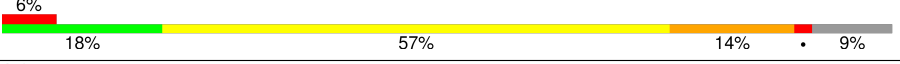
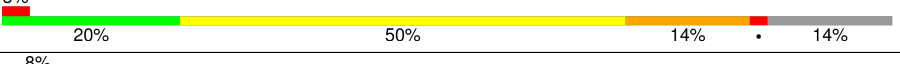
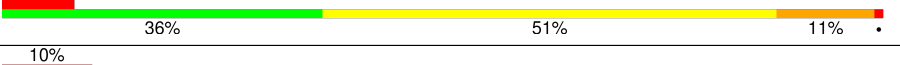
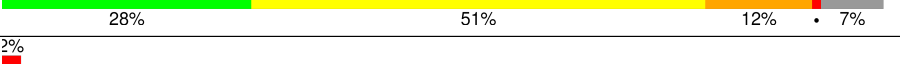
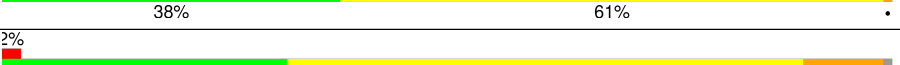
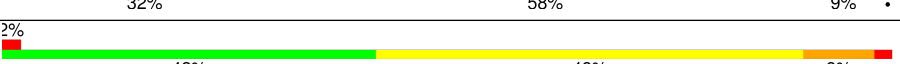
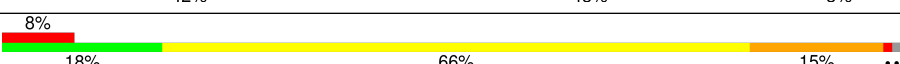
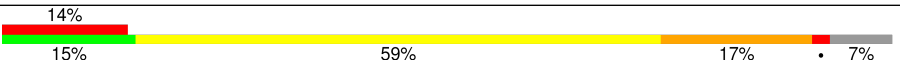
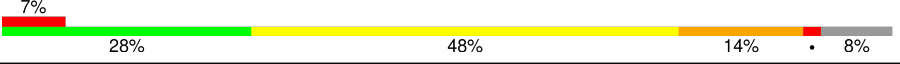
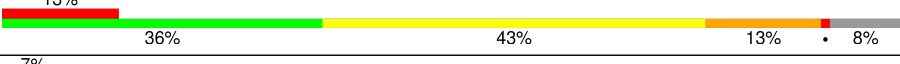
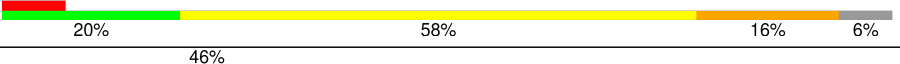
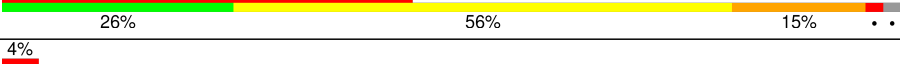

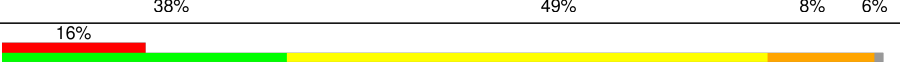
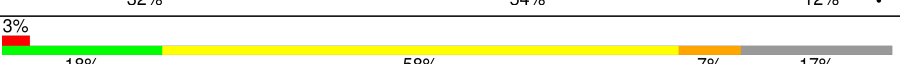
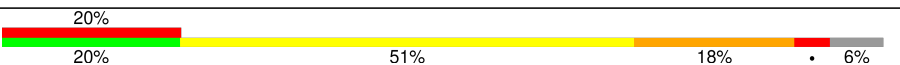

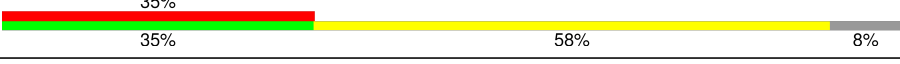

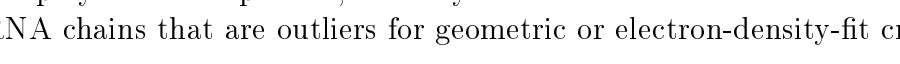
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)
RNA backbone	2183	1002 (3.84-2.80)

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	1522	<div> <div>4%</div> <div>27%</div> <div>59%</div> <div>11%</div> <div>••</div> </div>
2	X	6	<div> <div>67%</div> <div>67%</div> <div>33%</div> </div>
3	Y	15	<div> <div>20%</div> <div>33%</div> <div>27%</div> <div>7%</div> <div>7%</div> <div>27%</div> </div>
4	Z	4	<div> <div>25%</div> <div>50%</div> <div>25%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
5	B	256	
6	C	239	
7	D	209	
8	E	162	
9	F	101	
10	G	156	
11	H	138	
12	I	128	
13	J	105	
14	K	129	
15	L	135	
16	M	126	
17	N	61	
18	O	89	
19	P	88	
20	Q	105	
21	R	88	
22	S	93	
23	T	106	
24	V	26	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1561	-	-	-	X
25	MG	A	1574	-	-	-	X
25	MG	A	1593	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1611	-	-	-	X
25	MG	A	1628	-	-	-	X
25	MG	A	1646	-	-	-	X

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52160 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 RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32391	14418	6002	10465	1506			

- Molecule 2 is a RNA chain called P-SITE MESSENGER RNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	6	Total	C	N	O	P	0	0	0
			117	54	14	44	5			

- Molecule 3 is a RNA chain called ANTICODON STEM-LOOP OF PHENYLALANINE TRANSFER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	11	Total	C	N	O	P	0	0	0
			233	106	44	73	10			

- Molecule 4 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Z	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	I	127	Total	C	N	O		0	0	0
			1011	639	198	174				

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	?	-	PHE	CONFLICT/DELETION	GB 12056104
P	?	-	HIS	CONFLICT/DELETION	GB 12056104
P	?	-	TYR	CONFLICT/DELETION	GB 12056104

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	R	73	Total	C	N	O	S	0	0	0
			597	380	118	99				

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	S	87	Total	C	N	O	S	0	0	0
			697	444	130	121	2			

- Molecule 23 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 24 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	24	Total	C	N	O		0	0	0
			208	128	50	30				

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	H	1	Total	Mg	0	0
			1	1		
25	A	118	Total	Mg	0	0
			118	118		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	D	1	Total	Mg	0	0
			1	1		

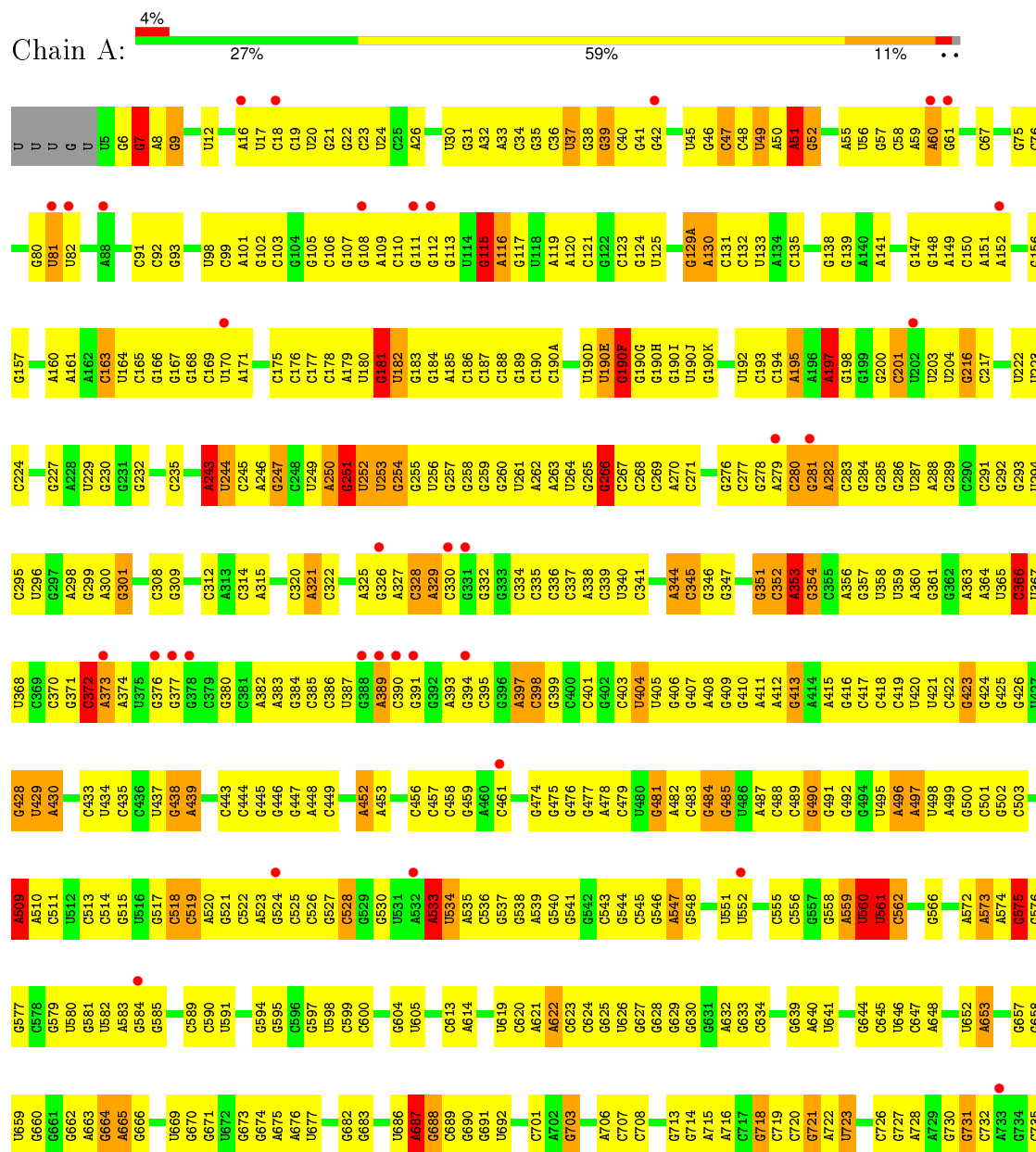
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total	Zn	0	0
			1	1		
26	N	1	Total	Zn	0	0
			1	1		

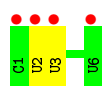
### 3 Residue-property plots

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 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.

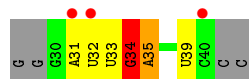
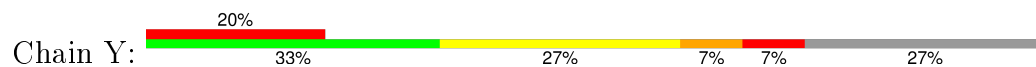
#### • Molecule 1: 16S RIBOSOMAL RNA







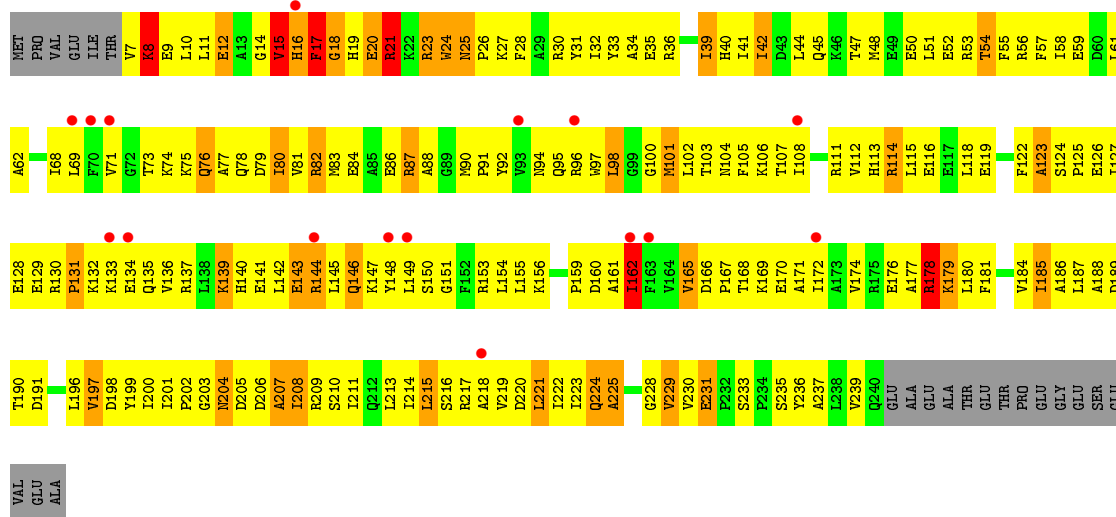
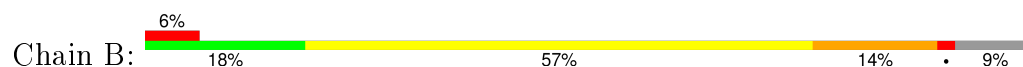
- Molecule 3: ANTICODON STEM-LOOP OF PHENYLALANINE TRANSFER RNA



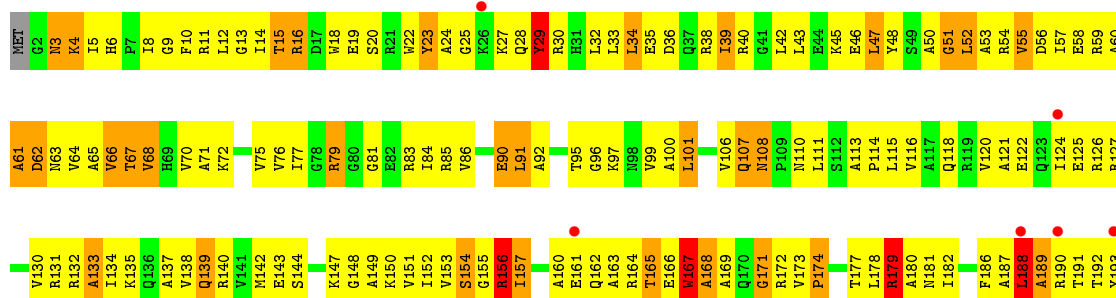
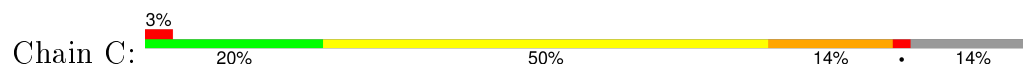
- Molecule 4: A-SITE MESSENGER RNA FRAGMENT



- Molecule 5: 30S RIBOSOMAL PROTEIN S2



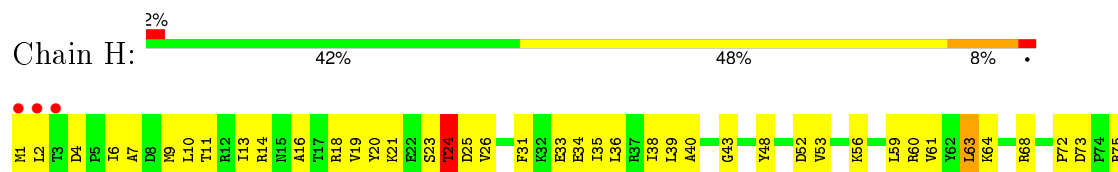
- Molecule 6: 30S RIBOSOMAL PROTEIN S3



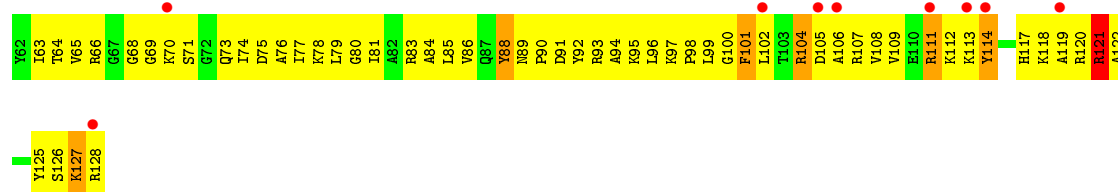
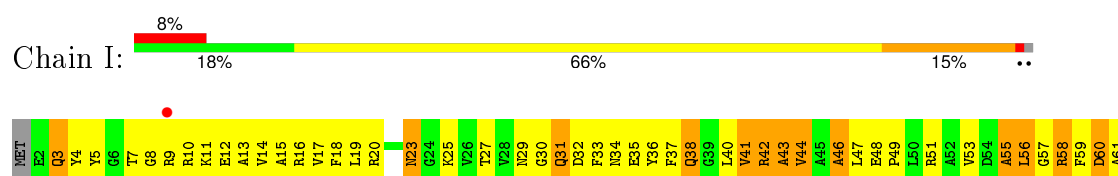




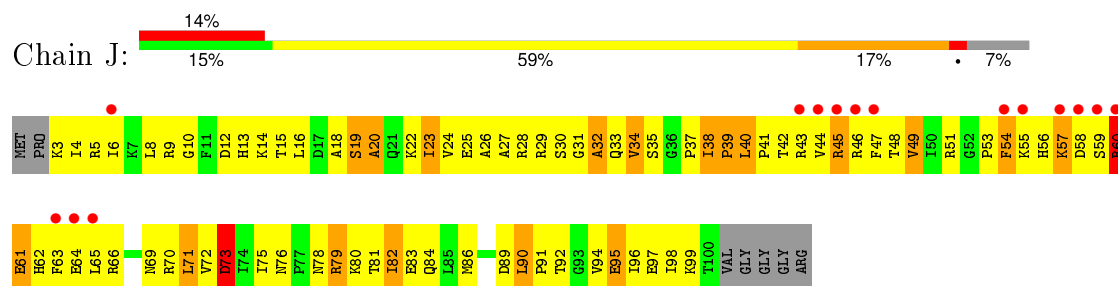
• Molecule 11: 30S RIBOSOMAL PROTEIN S8



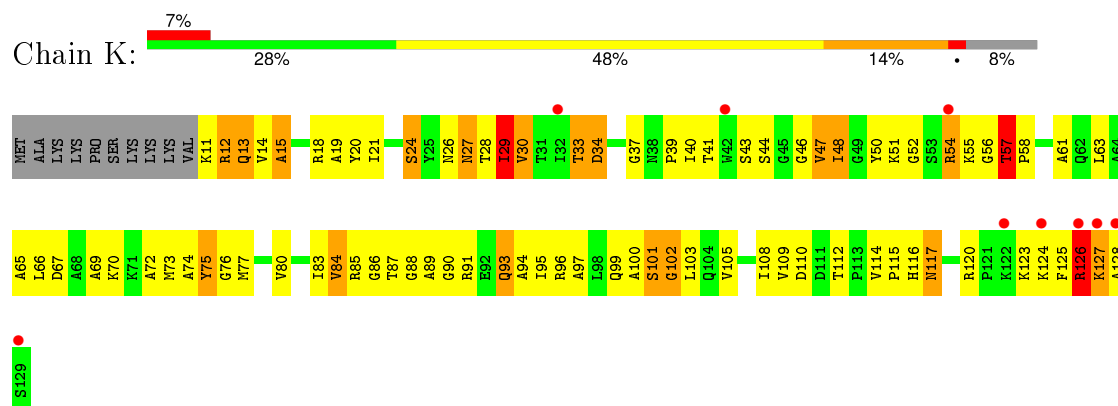
• Molecule 12: 30S RIBOSOMAL PROTEIN S9



• Molecule 13: 30S RIBOSOMAL PROTEIN S10



• Molecule 14: 30S RIBOSOMAL PROTEIN S11









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.57Å 401.57Å 176.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	316.23 – 3.31 200.79 – 3.31	Depositor EDS
% Data completeness (in resolution range)	90.6 (316.23-3.31) 90.6 (200.79-3.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.231 , 0.286 0.209 , 0.251	Depositor DCC
$R_{free}$ test set	9648 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.8	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 83.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 191960 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.73	EDS
Total number of atoms	52160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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: ZN, MG

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	0.57	0/36259	0.74	36/56593 (0.1%)
2	X	0.58	0/128	0.76	0/196
3	Y	0.33	0/261	0.76	1/405 (0.2%)
4	Z	0.46	0/84	0.81	0/128
5	B	0.34	0/1935	0.66	0/2609
6	C	0.36	0/1636	0.65	0/2205
7	D	0.39	0/1733	0.65	0/2318
8	E	0.46	0/1162	0.79	0/1564
9	F	0.32	0/856	0.61	0/1154
10	G	0.34	0/1276	0.61	0/1709
11	H	0.45	0/1136	0.75	0/1527
12	I	0.34	0/1029	0.67	0/1378
13	J	0.35	0/805	0.67	1/1082 (0.1%)
14	K	0.40	0/900	0.67	0/1213
15	L	0.43	0/986	0.74	0/1320
16	M	0.36	0/947	0.67	0/1270
17	N	0.41	0/501	0.76	0/664
18	O	0.39	0/745	0.62	0/992
19	P	0.46	0/716	0.77	1/963 (0.1%)
20	Q	0.48	0/870	0.76	0/1159
21	R	0.37	0/603	0.67	0/799
22	S	0.35	0/712	0.71	1/956 (0.1%)
23	T	0.39	0/765	0.71	0/1007
24	V	0.45	0/212	0.67	0/277
All	All	0.51	0/56257	0.73	40/83488 (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
1	A	1	29

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	G	C2'-C3'-O3'	9.30	129.96	109.50
1	A	559	A	C2'-C3'-O3'	8.99	129.29	109.50
1	A	575	G	C2'-C3'-O3'	8.98	129.25	109.50
1	A	366	C	C2'-C3'-O3'	8.93	129.15	109.50
1	A	243	A	C2'-C3'-O3'	8.21	127.56	109.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	366	C	C3'

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190(F)	G	Sidechain
1	A	197	A	Sidechain
1	A	24	U	Sidechain
1	A	249	U	Sidechain
1	A	37	U	Sidechain

## 5.2 Too-close contacts [i](#)

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	32391	0	16349	1272	0
2	X	117	0	64	3	0
3	Y	233	0	120	11	0
4	Z	77	0	42	4	0
5	B	1900	0	1951	279	0
6	C	1612	0	1677	245	0
7	D	1703	0	1764	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	1146	0	1207	124	0
9	F	843	0	857	84	0
10	G	1257	0	1296	124	0
11	H	1116	0	1177	103	0
12	I	1011	0	1043	158	0
13	J	792	0	835	145	0
14	K	885	0	904	88	0
15	L	970	0	1057	119	0
16	M	937	0	995	121	0
17	N	492	0	529	77	0
18	O	734	0	771	60	0
19	P	700	0	720	54	0
20	Q	857	0	930	99	0
21	R	597	0	668	81	0
22	S	697	0	723	120	0
23	T	763	0	861	82	0
24	V	208	0	221	13	0
25	A	118	0	0	0	0
25	D	1	0	0	0	0
25	H	1	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52160	0	36761	3359	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 38.

The worst 5 of 3359 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:1397:C:OP2	8:E:24:ARG:NH2	1.62	1.27
5:B:84:GLU:HB3	5:B:219:VAL:HG21	1.25	1.18
6:C:14:ILE:HG22	6:C:15:THR:H	1.12	1.15
1:A:1443:G:H5''	1:A:1446:A:H5'	1.31	1.11
7:D:36:ARG:H	7:D:37:PRO:HD3	0.95	1.11

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 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	
5	B	232/256 (91%)	143 (62%)	59 (25%)	30 (13%)	0	2
6	C	204/239 (85%)	125 (61%)	49 (24%)	30 (15%)	0	1
7	D	206/209 (99%)	139 (68%)	49 (24%)	18 (9%)	1	7
8	E	148/162 (91%)	114 (77%)	24 (16%)	10 (7%)	1	12
9	F	99/101 (98%)	81 (82%)	17 (17%)	1 (1%)	19	59
10	G	153/156 (98%)	104 (68%)	37 (24%)	12 (8%)	1	9
11	H	136/138 (99%)	112 (82%)	19 (14%)	5 (4%)	4	28
12	I	125/128 (98%)	85 (68%)	25 (20%)	15 (12%)	0	3
13	J	96/105 (91%)	58 (60%)	23 (24%)	15 (16%)	0	1
14	K	117/129 (91%)	84 (72%)	18 (15%)	15 (13%)	0	2
15	L	122/135 (90%)	84 (69%)	24 (20%)	14 (12%)	0	3
16	M	116/126 (92%)	74 (64%)	28 (24%)	14 (12%)	0	2
17	N	58/61 (95%)	38 (66%)	14 (24%)	6 (10%)	1	4
18	O	86/89 (97%)	58 (67%)	23 (27%)	5 (6%)	2	16
19	P	81/88 (92%)	59 (73%)	20 (25%)	2 (2%)	7	38
20	Q	102/105 (97%)	83 (81%)	12 (12%)	7 (7%)	1	12
21	R	71/88 (81%)	50 (70%)	17 (24%)	4 (6%)	2	17
22	S	85/93 (91%)	55 (65%)	17 (20%)	13 (15%)	0	1
23	T	97/106 (92%)	57 (59%)	30 (31%)	10 (10%)	1	4
24	V	22/26 (85%)	16 (73%)	6 (27%)	0	100	100
All	All	2356/2540 (93%)	1619 (69%)	511 (22%)	226 (10%)	1	5

5 of 226 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	16	HIS

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Mol	Chain	Res	Type
5	B	17	PHE
5	B	20	GLU
5	B	21	ARG
5	B	24	TRP

### 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 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	
5	B	202/220 (92%)	177 (88%)	25 (12%)	6	25
6	C	160/188 (85%)	143 (89%)	17 (11%)	8	32
7	D	180/181 (99%)	161 (89%)	19 (11%)	8	32
8	E	115/123 (94%)	100 (87%)	15 (13%)	5	22
9	F	90/90 (100%)	88 (98%)	2 (2%)	60	84
10	G	126/127 (99%)	119 (94%)	7 (6%)	26	65
11	H	119/119 (100%)	103 (87%)	16 (13%)	5	21
12	I	98/99 (99%)	89 (91%)	9 (9%)	11	40
13	J	87/92 (95%)	78 (90%)	9 (10%)	9	34
14	K	90/99 (91%)	77 (86%)	13 (14%)	4	18
15	L	104/111 (94%)	96 (92%)	8 (8%)	16	51
16	M	94/101 (93%)	82 (87%)	12 (13%)	5	23
17	N	49/50 (98%)	44 (90%)	5 (10%)	9	35
18	O	79/80 (99%)	70 (89%)	9 (11%)	7	29
19	P	72/74 (97%)	68 (94%)	4 (6%)	26	65
20	Q	96/97 (99%)	88 (92%)	8 (8%)	14	47
21	R	64/77 (83%)	60 (94%)	4 (6%)	22	60
22	S	75/80 (94%)	62 (83%)	13 (17%)	2	11
23	T	76/82 (93%)	69 (91%)	7 (9%)	11	40
24	V	19/21 (90%)	18 (95%)	1 (5%)	28	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1995/2111 (94%)	1792 (90%)	203 (10%)	9 35

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	H	85	ARG
13	J	49	VAL
22	S	32	LYS
11	H	105	ARG
12	I	38	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
9	F	94	GLN
11	H	82	HIS
22	S	14	HIS
9	F	100	ASN
10	G	51	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	201 (13%)	70 (4%)
2	X	5/6 (83%)	0	0
3	Y	10/15 (66%)	2 (20%)	1 (10%)
4	Z	3/4 (75%)	1 (33%)	0
All	All	1524/1547 (98%)	204 (13%)	71 (4%)

5 of 204 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 71 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	559	A
1	A	819	A
1	A	1347	G
1	A	560	U
1	A	748	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](#)

Of 122 ligands modelled in this entry, 122 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	1507/1522 (99%)	0.58	60 (3%) 42 40	16, 53, 140, 201	0
2	X	6/6 (100%)	5.18	4 (66%) 0 0	59, 71, 178, 201	0
3	Y	11/15 (73%)	1.63	3 (27%) 1 1	66, 90, 182, 190	0
4	Z	4/4 (100%)	1.44	1 (25%) 1 1	71, 77, 89, 119	0
5	B	234/256 (91%)	0.30	16 (6%) 20 20	19, 87, 173, 201	0
6	C	206/239 (86%)	0.14	7 (3%) 49 48	22, 80, 160, 201	0
7	D	208/209 (99%)	0.53	17 (8%) 14 14	17, 60, 145, 180	0
8	E	150/162 (92%)	0.62	16 (10%) 8 7	17, 48, 107, 201	0
9	F	101/101 (100%)	0.08	2 (1%) 68 67	35, 88, 148, 185	0
10	G	155/156 (99%)	-0.03	3 (1%) 70 69	27, 70, 150, 201	0
11	H	138/138 (100%)	0.35	3 (2%) 65 65	5, 39, 108, 136	0
12	I	127/128 (99%)	0.47	10 (7%) 15 15	19, 82, 144, 184	0
13	J	98/105 (93%)	0.54	15 (15%) 3 3	30, 107, 188, 201	0
14	K	119/129 (92%)	0.59	9 (7%) 17 17	12, 54, 130, 201	0
15	L	124/135 (91%)	0.75	17 (13%) 4 4	16, 57, 144, 187	0
16	M	118/126 (93%)	0.59	9 (7%) 17 17	32, 70, 144, 170	0
17	N	60/61 (98%)	1.95	28 (46%) 0 0	39, 70, 140, 201	0
18	O	88/89 (98%)	0.43	4 (4%) 37 35	7, 56, 145, 201	0
19	P	83/88 (94%)	0.97	16 (19%) 2 2	10, 41, 101, 150	0
20	Q	104/105 (99%)	0.99	17 (16%) 2 2	10, 43, 157, 201	0
21	R	73/88 (82%)	0.52	3 (4%) 41 39	32, 66, 166, 201	0
22	S	87/93 (93%)	0.99	19 (21%) 1 1	54, 99, 176, 201	0
23	T	99/106 (93%)	0.94	15 (15%) 3 3	15, 50, 123, 156	0
24	V	24/26 (92%)	1.69	9 (37%) 0 1	26, 59, 128, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3924/4087 (96%)	0.57	303 (7%)	16 16	5, 60, 152, 201	0

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	K	129	SER	25.6
14	K	128	ALA	18.3
2	X	2	U	14.0
18	O	89	GLY	11.8
22	S	3	ARG	10.9

## 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(Å <sup>2</sup> )	Q<0.9
25	MG	A	1628	1/1	0.72	0.56	19.64	27,27,27,27	1
25	MG	A	1646	1/1	0.93	0.75	12.45	27,27,27,27	0
25	MG	A	1561	1/1	0.88	0.28	7.52	27,27,27,27	0
25	MG	A	1574	1/1	0.94	0.28	4.17	27,27,27,27	0
25	MG	A	1611	1/1	0.96	0.16	2.56	27,27,27,27	0
25	MG	A	1593	1/1	0.95	0.23	2.38	27,27,27,27	0
26	ZN	D	506	1/1	0.98	0.34	1.15	27,27,27,27	0
25	MG	A	211	1/1	0.88	0.29	0.99	27,27,27,27	0
25	MG	A	1568	1/1	0.96	0.31	0.62	27,27,27,27	0
25	MG	A	1606	1/1	0.77	0.23	0.52	27,27,27,27	1
25	MG	A	1589	1/1	0.94	0.28	0.48	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1560	1/1	0.96	0.27	0.38	27,27,27,27	0
25	MG	A	1612	1/1	0.87	0.34	-0.11	27,27,27,27	0
25	MG	A	1551	1/1	0.95	0.28	-0.19	27,27,27,27	0
25	MG	A	1597	1/1	0.94	0.20	-0.52	27,27,27,27	0
25	MG	A	1567	1/1	0.94	0.21	-0.95	27,27,27,27	1
25	MG	A	1632	1/1	0.99	0.32	-0.97	27,27,27,27	0
25	MG	A	1601	1/1	0.97	0.21	-1.01	27,27,27,27	0
26	ZN	N	507	1/1	0.99	0.14	-1.04	27,27,27,27	1
25	MG	A	1599	1/1	0.94	0.19	-1.05	27,27,27,27	0
25	MG	A	1573	1/1	0.93	0.26	-1.09	27,27,27,27	0
25	MG	A	1617	1/1	0.96	0.22	-1.21	27,27,27,27	0
25	MG	A	1627	1/1	0.88	0.16	-1.22	27,27,27,27	0
25	MG	A	1594	1/1	0.90	0.22	-1.26	27,27,27,27	0
25	MG	A	1626	1/1	0.83	0.14	-1.32	27,27,27,27	1
25	MG	A	1645	1/1	0.90	0.18	-1.32	27,27,27,27	0
25	MG	A	1609	1/1	0.96	0.24	-1.53	27,27,27,27	0
25	MG	A	1656	1/1	0.76	0.17	-1.68	27,27,27,27	0
25	MG	A	1558	1/1	0.84	0.20	-1.82	27,27,27,27	0
25	MG	A	1555	1/1	0.98	0.26	-1.94	27,27,27,27	0
25	MG	A	1582	1/1	0.96	0.17	-1.98	27,27,27,27	0
25	MG	A	1587	1/1	0.94	0.19	-1.98	27,27,27,27	0
25	MG	A	1598	1/1	0.97	0.18	-2.22	27,27,27,27	0
25	MG	D	215	1/1	0.85	0.13	-2.53	27,27,27,27	0
25	MG	A	1576	1/1	0.95	0.16	-2.77	27,27,27,27	0
25	MG	A	1643	1/1	0.90	0.16	-2.82	27,27,27,27	1
25	MG	A	210	1/1	0.87	0.14	-3.57	27,27,27,27	1
25	MG	A	1564	1/1	0.93	0.13	-3.85	27,27,27,27	0
25	MG	A	1586	1/1	0.97	0.15	-3.93	27,27,27,27	0
25	MG	A	1629	1/1	0.92	0.13	-4.24	27,27,27,27	0
25	MG	A	1648	1/1	0.99	0.08	-4.44	27,27,27,27	0
25	MG	A	1605	1/1	0.88	0.12	-4.52	27,27,27,27	0
25	MG	A	1545	1/1	0.92	0.09	-4.56	27,27,27,27	0
25	MG	A	1654	1/1	0.85	0.06	-4.87	27,27,27,27	1
25	MG	A	1595	1/1	0.93	0.07	-6.81	27,27,27,27	0
25	MG	A	1563	1/1	0.94	0.20	-	27,27,27,27	0
25	MG	A	1569	1/1	0.91	0.34	-	27,27,27,27	0
25	MG	A	1600	1/1	0.98	0.06	-	27,27,27,27	0
25	MG	A	1603	1/1	0.91	0.24	-	27,27,27,27	0
25	MG	A	1590	1/1	0.89	0.20	-	27,27,27,27	0
25	MG	A	1584	1/1	0.85	0.24	-	27,27,27,27	0
25	MG	A	1625	1/1	0.87	0.21	-	27,27,27,27	0
25	MG	A	1610	1/1	0.92	0.27	-	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1591	1/1	0.97	0.33	-	27,27,27,27	0
25	MG	A	1548	1/1	0.89	0.30	-	27,27,27,27	1
25	MG	A	1546	1/1	0.98	0.32	-	27,27,27,27	0
25	MG	A	1634	1/1	0.91	0.15	-	27,27,27,27	0
25	MG	A	86	1/1	0.95	0.28	-	27,27,27,27	0
25	MG	A	1639	1/1	0.88	0.27	-	27,27,27,27	1
25	MG	A	214	1/1	0.83	0.19	-	27,27,27,27	1
25	MG	A	1614	1/1	0.97	0.20	-	27,27,27,27	0
25	MG	A	1613	1/1	0.93	0.34	-	27,27,27,27	0
25	MG	A	1575	1/1	0.92	0.32	-	27,27,27,27	0
25	MG	A	1607	1/1	0.69	0.24	-	27,27,27,27	1
25	MG	A	1604	1/1	0.95	0.10	-	27,27,27,27	0
25	MG	A	1559	1/1	0.94	0.26	-	27,27,27,27	0
25	MG	A	1649	1/1	0.89	0.14	-	27,27,27,27	1
25	MG	A	1572	1/1	0.97	0.11	-	27,27,27,27	0
25	MG	A	1647	1/1	0.88	0.15	-	27,27,27,27	0
25	MG	A	1655	1/1	0.56	0.26	-	27,27,27,27	1
25	MG	A	1550	1/1	0.97	0.34	-	27,27,27,27	0
25	MG	A	1631	1/1	0.94	0.31	-	27,27,27,27	0
25	MG	A	1596	1/1	0.95	0.40	-	27,27,27,27	0
25	MG	A	1642	1/1	0.95	0.24	-	27,27,27,27	1
25	MG	A	1552	1/1	0.96	0.34	-	27,27,27,27	0
25	MG	A	1651	1/1	0.60	0.12	-	27,27,27,27	0
25	MG	A	1641	1/1	0.66	0.28	-	27,27,27,27	1
25	MG	A	1602	1/1	0.94	0.17	-	27,27,27,27	0
25	MG	A	87	1/1	0.82	0.41	-	27,27,27,27	1
25	MG	A	1557	1/1	0.98	0.26	-	27,27,27,27	0
25	MG	A	1636	1/1	0.75	0.15	-	27,27,27,27	1
25	MG	A	1640	1/1	0.47	0.28	-	27,27,27,27	1
25	MG	A	1578	1/1	0.97	0.24	-	27,27,27,27	0
25	MG	A	1592	1/1	0.94	0.38	-	27,27,27,27	0
25	MG	A	1571	1/1	0.95	0.26	-	27,27,27,27	0
25	MG	A	1653	1/1	0.87	0.19	-	27,27,27,27	1
25	MG	A	1619	1/1	0.94	0.27	-	27,27,27,27	0
25	MG	A	1622	1/1	0.78	0.34	-	27,27,27,27	0
25	MG	A	1615	1/1	0.88	0.25	-	27,27,27,27	0
25	MG	A	1547	1/1	0.77	0.15	-	27,27,27,27	0
25	MG	A	1620	1/1	0.77	0.32	-	27,27,27,27	1
25	MG	A	1638	1/1	0.89	0.18	-	27,27,27,27	0
25	MG	A	1633	1/1	0.93	0.32	-	27,27,27,27	0
25	MG	A	1580	1/1	0.95	0.23	-	27,27,27,27	0
25	MG	A	1650	1/1	0.90	0.27	-	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1618	1/1	0.88	0.15	-	27,27,27,27	1
25	MG	A	1562	1/1	0.86	0.14	-	27,27,27,27	1
25	MG	A	1566	1/1	0.94	0.19	-	27,27,27,27	0
25	MG	A	1553	1/1	0.97	0.39	-	27,27,27,27	0
25	MG	A	1624	1/1	0.70	0.29	-	27,27,27,27	1
25	MG	A	1621	1/1	0.87	0.23	-	27,27,27,27	0
25	MG	A	1608	1/1	0.93	0.09	-	27,27,27,27	0
25	MG	A	1585	1/1	0.90	0.32	-	27,27,27,27	0
25	MG	A	1623	1/1	0.87	0.14	-	27,27,27,27	0
25	MG	A	71	1/1	0.96	0.37	-	27,27,27,27	0
25	MG	A	1556	1/1	0.86	0.43	-	27,27,27,27	0
25	MG	A	1565	1/1	0.95	0.36	-	27,27,27,27	0
25	MG	A	1616	1/1	0.89	0.10	-	27,27,27,27	0
25	MG	A	1652	1/1	0.89	0.10	-	27,27,27,27	0
25	MG	A	1644	1/1	0.89	0.25	-	27,27,27,27	1
25	MG	A	1554	1/1	0.98	0.23	-	27,27,27,27	0
25	MG	A	1549	1/1	0.97	0.33	-	27,27,27,27	0
25	MG	A	1583	1/1	0.97	0.16	-	27,27,27,27	0
25	MG	A	1588	1/1	0.94	0.17	-	27,27,27,27	0
25	MG	A	1637	1/1	0.77	0.12	-	27,27,27,27	1
25	MG	A	1581	1/1	0.95	0.16	-	27,27,27,27	0
25	MG	H	213	1/1	0.95	0.15	-	27,27,27,27	0
25	MG	A	1635	1/1	0.92	0.15	-	27,27,27,27	0
25	MG	A	1577	1/1	0.91	0.14	-	27,27,27,27	0
25	MG	A	1579	1/1	0.54	0.31	-	27,27,27,27	1
25	MG	A	1630	1/1	0.98	0.30	-	27,27,27,27	0
25	MG	A	1570	1/1	0.90	0.31	-	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.