wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:04 PM GMT

PDB ID	:	1N33
Title	:	Structure of the Thermus thermophilus 30S ribosomal subunit bound to codon and near-cognate transfer rna anticodon stem-loop mismatched at the second codon position at the a site with paromomycin
Authors	:	Ogle, J.M.; Murphy IV, F.V.; Tarry, M.J.; Ramakrishnan, V.
Deposited on	:	2002-10-25
Resolution	:	3.35 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

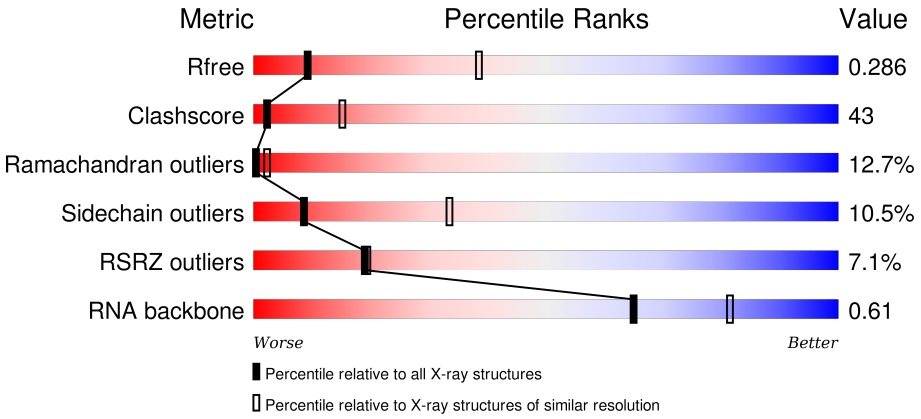
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.35 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)
RNA backbone	2183	1016 (3.92-2.80)

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 >=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 <=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	6% 25% 60% 13%
2	Y	17	18% 24% 24% 35%
3	Z	6	17% 50% 17% 33%
4	B	256	11% 16% 54% 18% 9%

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Mol	Chain	Length	Quality of chain
5	C	239	4% 18% 49% 18% 14%
6	D	208	10% 27% 59% 14%
7	E	161	31% 48% 12% 7%
8	F	101	15% 37% 51% 11%
9	G	155	3% 29% 58% 12%
10	H	138	% 25% 59% 14%
11	I	128	12% 19% 59% 20%
12	J	104	25% 11% 55% 27% 6%
13	K	129	6% 32% 51% 9% 8%
14	L	135	5% 25% 51% 16% 8%
15	M	126	6% 23% 56% 14% 6%
16	N	60	7% 17% 63% 18%
17	O	88	5% 33% 59% 8%
18	P	88	5% 18% 64% 11% 6%
19	Q	104	8% 16% 67% 14%
20	R	88	5% 13% 60% 9% 17%
21	S	92	17% 24% 47% 15% 13%
22	T	106	4% 18% 59% 15% 7%
23	V	26	12% 12% 69% 12% 8%

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	1546	-	-	-	X
25	MG	A	1551	-	-	-	X
25	MG	A	1555	-	-	-	X
25	MG	A	1558	-	-	-	X
25	MG	A	1560	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1582	-	-	-	X
25	MG	A	1584	-	-	-	X
25	MG	A	1587	-	-	-	X
25	MG	A	1588	-	-	-	X
25	MG	A	1592	-	-	-	X
25	MG	A	1597	-	-	-	X
25	MG	A	1629	-	-	-	X
25	MG	A	211	-	-	-	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52140 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	1513	Total	C	N	O	P	22	0	0
			32508	14472	6016	10509	1511			

- Molecule 2 is a RNA chain called ANTICODON STEM-LOOP OF SER TRANSFER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	11	Total	C	N	O	P	0	0	0
			235	106	45	74	10			

- Molecule 3 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	25	ASP	GLU	CONFLICT	UNP P24319
H	37	ARG	LYS	CONFLICT	UNP P24319
H	52	ASP	GLU	CONFLICT	UNP P24319
H	61	VAL	ILE	CONFLICT	UNP P24319
H	62	TYR	HIS	CONFLICT	UNP P24319
H	81	HIS	LYS	CONFLICT	UNP P24319
H	88	LYS	ARG	CONFLICT	UNP P24319
H	115	SER	PRO	CONFLICT	UNP P24319

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	LYS	ARG	CONFLICT	UNP P24321
Q	53	LEU	VAL	CONFLICT	UNP P24321
Q	62	SER	ALA	CONFLICT	UNP P24321
Q	79	SER	GLU	CONFLICT	UNP P24321
Q	82	MET	LEU	CONFLICT	UNP P24321
Q	90	ILE	VAL	CONFLICT	UNP P24321
Q	96	GLN	ALA	CONFLICT	UNP P24321

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

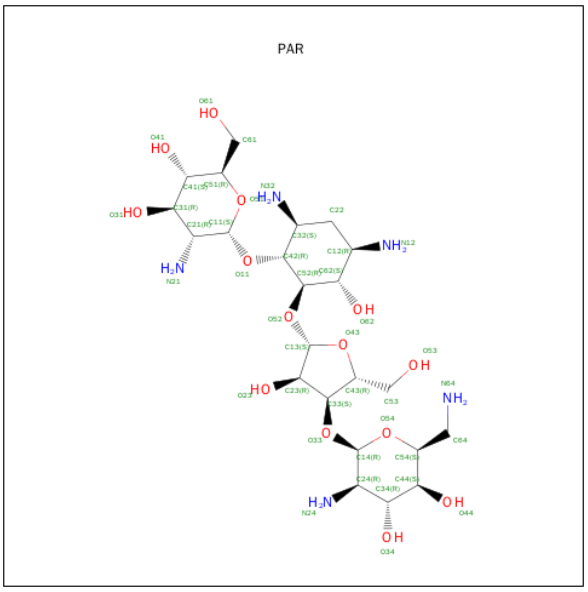
- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

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

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

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C N O 42 23 5 14	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	Z	2	Total Mg 2 2	0	0
25	A	103	Total Mg 103 103	0	0
25	Y	1	Total Mg 1 1	0	0

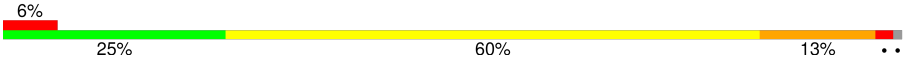
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

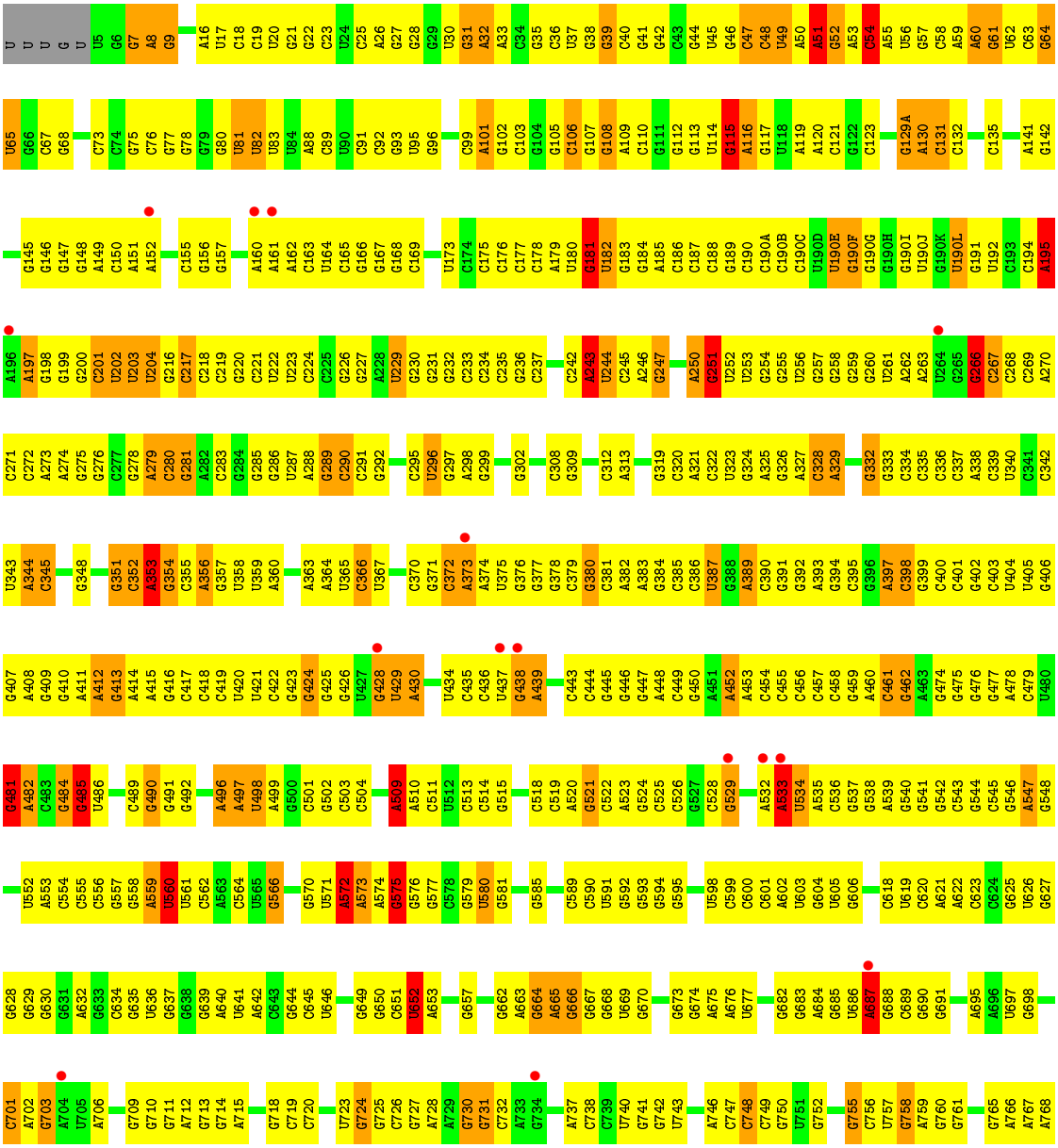
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	D	1	Total Zn 1 1	0	0
26	N	1	Total Zn 1 1	0	0

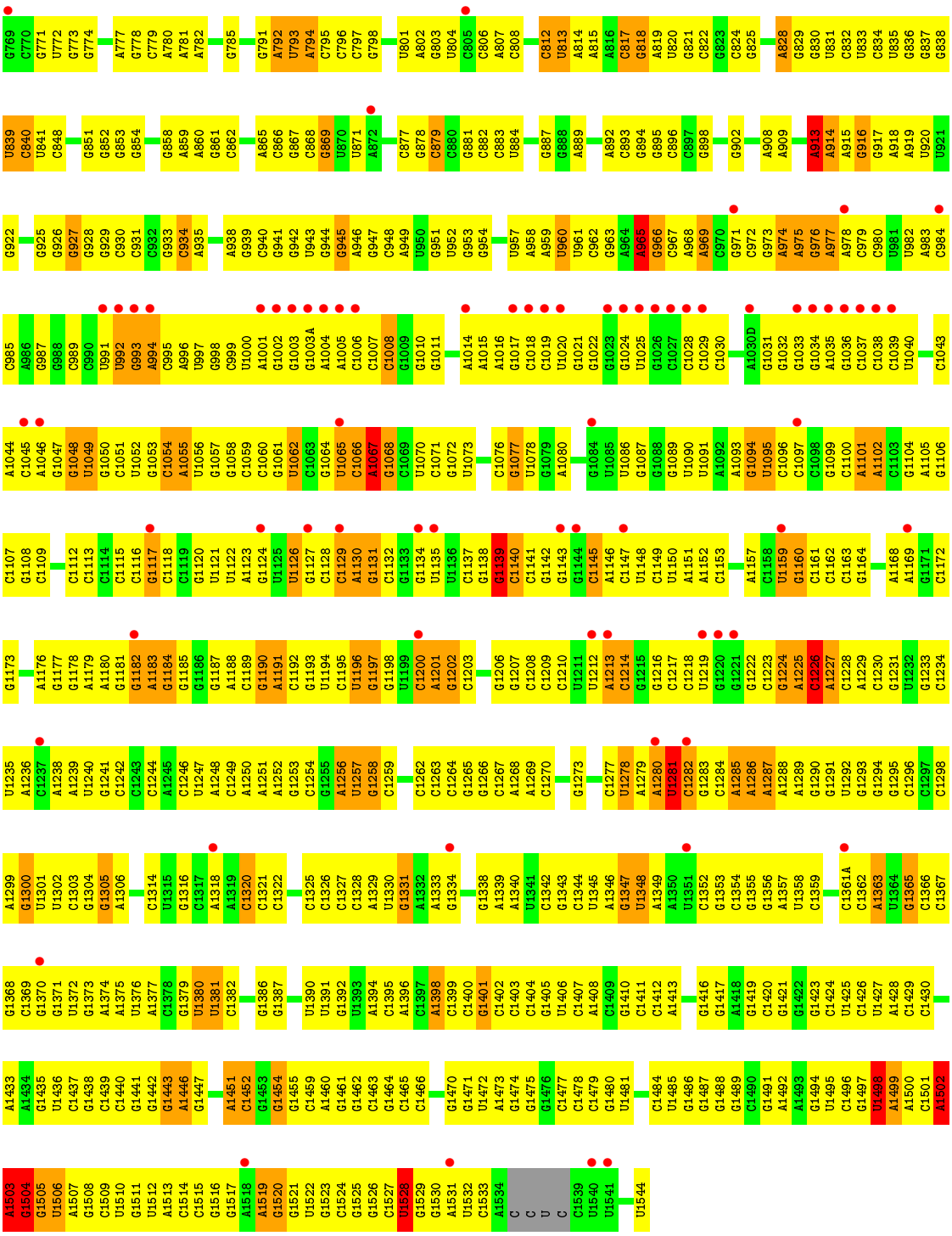
3 Residue-property plots (i)

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: 16S RIBOSOMAL RNA

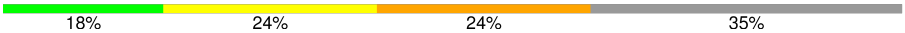
Chain A: 

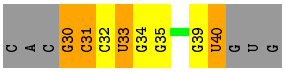




• Molecule 2: ANTICODON STEM-LOOP OF SER TRANSFER RNA

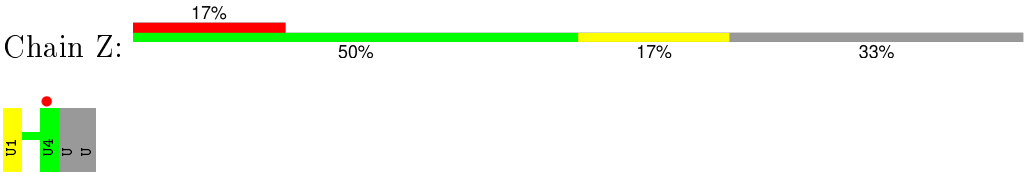
Chain Y:





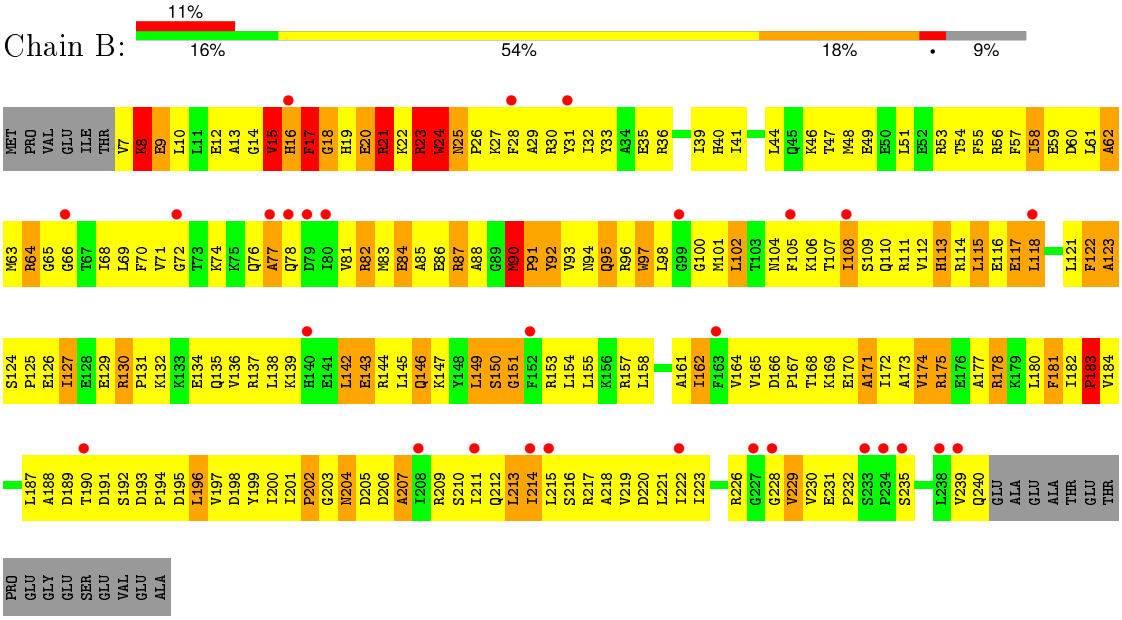
• Molecule 3: A-SITE MESSENGER RNA FRAGMENT

Chain Z:



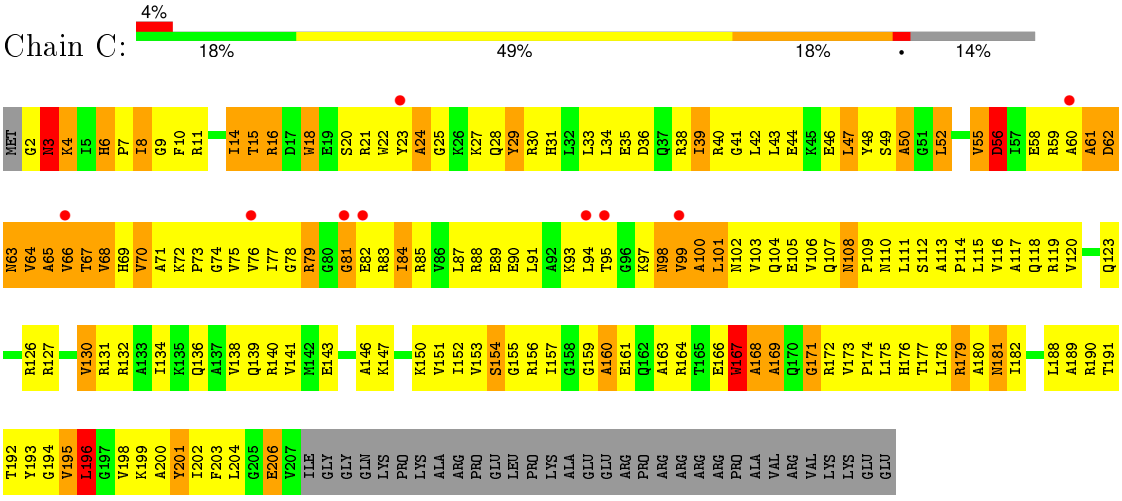
• Molecule 4: 30S RIBOSOMAL PROTEIN S2

Chain B:



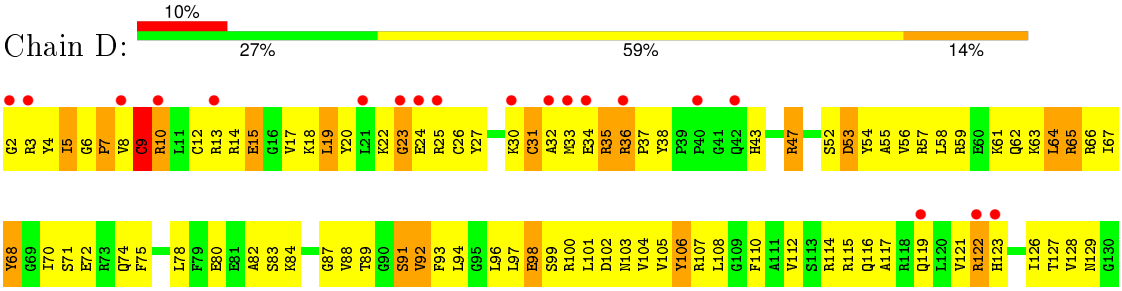
• Molecule 5: 30S RIBOSOMAL PROTEIN S3

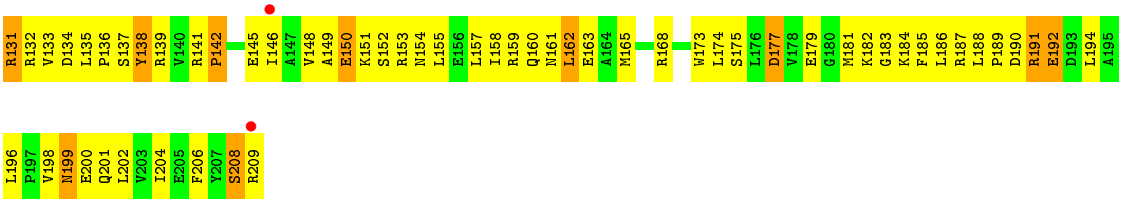
Chain C:



• Molecule 6: 30S RIBOSOMAL PROTEIN S4

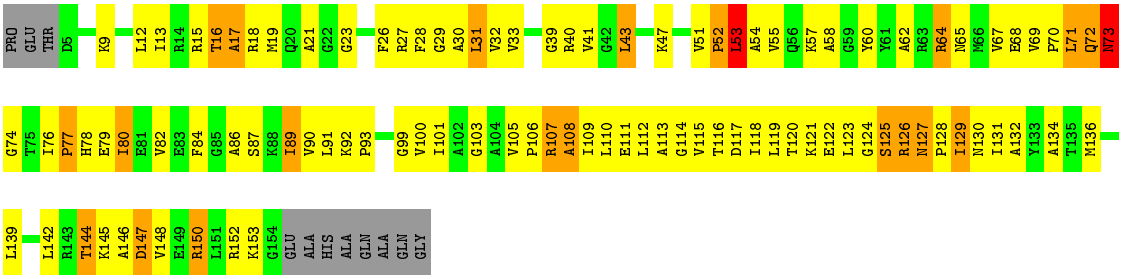
Chain D:





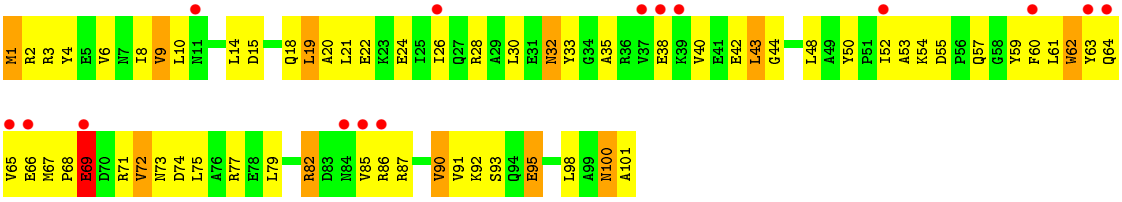
- Molecule 7: 30S RIBOSOMAL PROTEIN S5

Chain E:



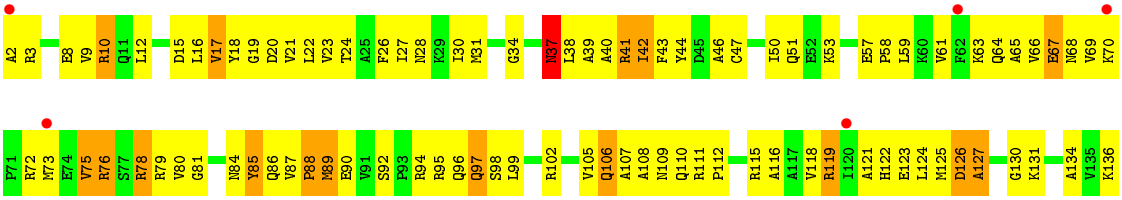
- Molecule 8: 30S RIBOSOMAL PROTEIN S6

Chain F:



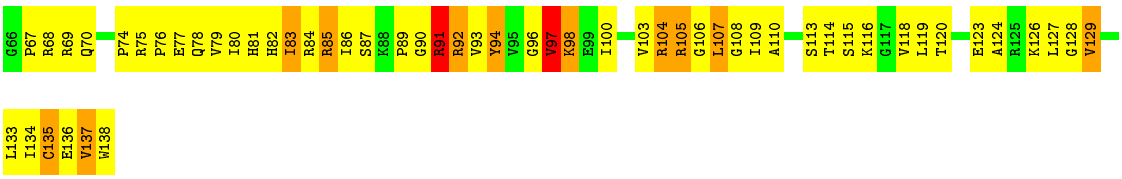
- Molecule 9: 30S RIBOSOMAL PROTEIN S7

Chain G:

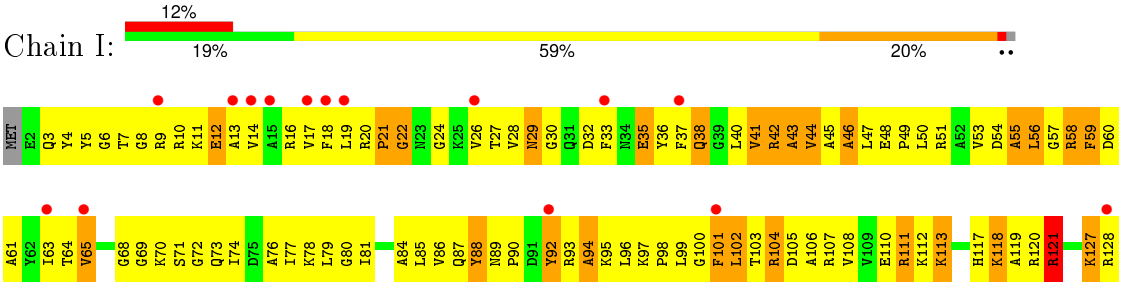


- Molecule 10: 30S RIBOSOMAL PROTEIN S8

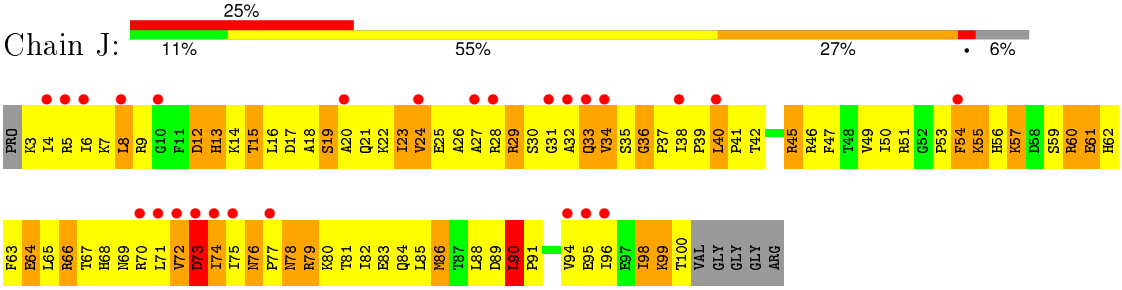
Chain H:



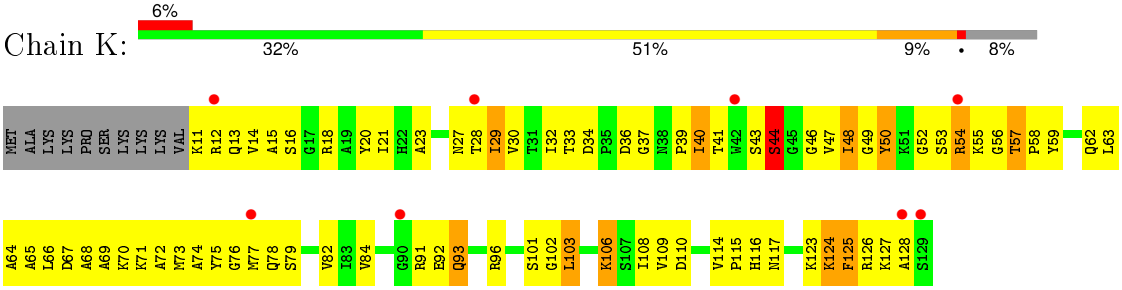
• Molecule 11: 30S RIBOSOMAL PROTEIN S9



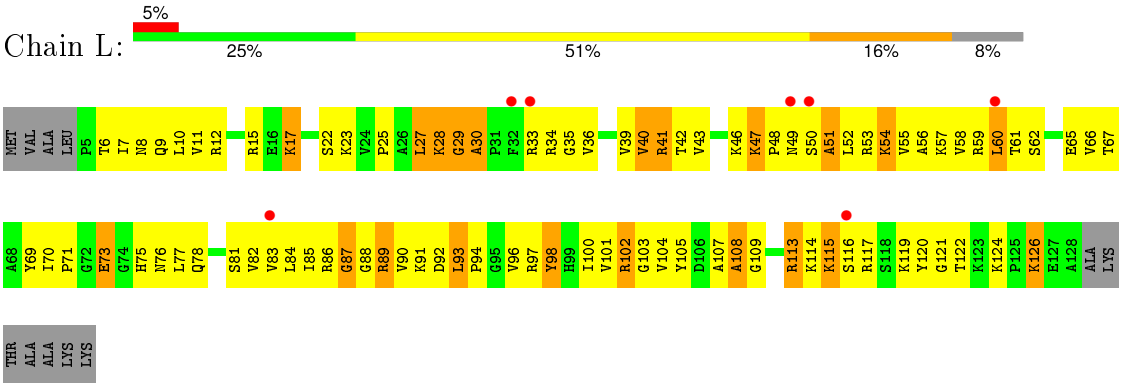
• Molecule 12: 30S RIBOSOMAL PROTEIN S10



• Molecule 13: 30S RIBOSOMAL PROTEIN S11

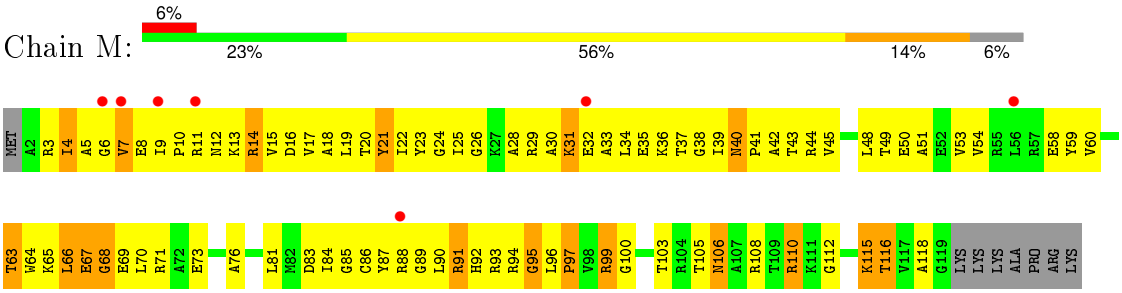


• Molecule 14: 30S RIBOSOMAL PROTEIN S12



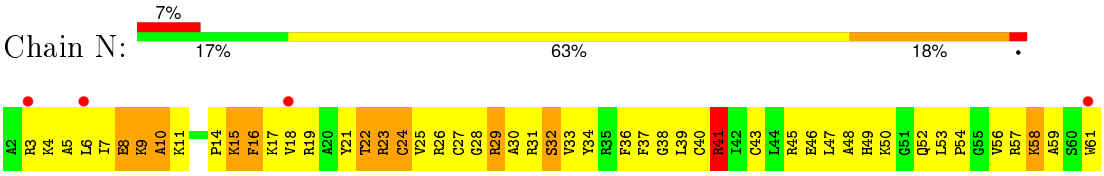
• Molecule 15: 30S RIBOSOMAL PROTEIN S13

Chain M:



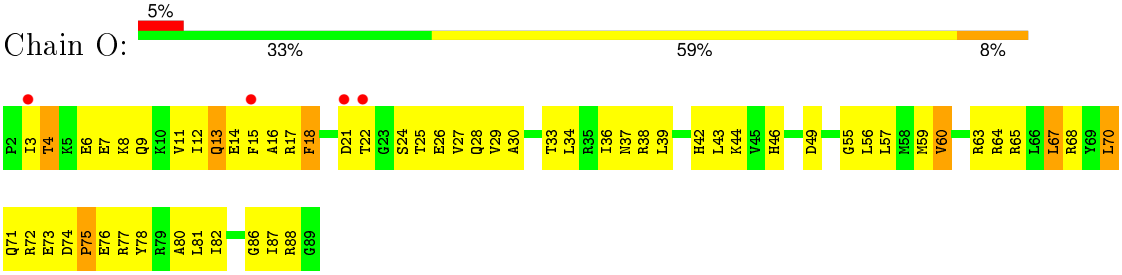
- Molecule 16: 30S RIBOSOMAL PROTEIN S14

Chain N:



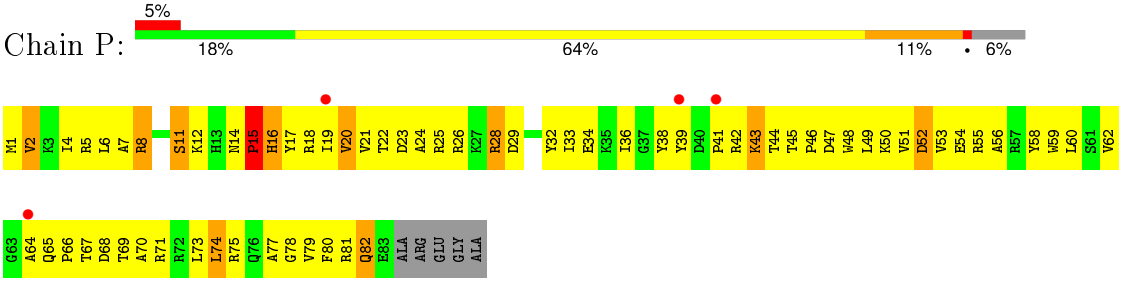
- Molecule 17: 30S RIBOSOMAL PROTEIN S15

Chain O:



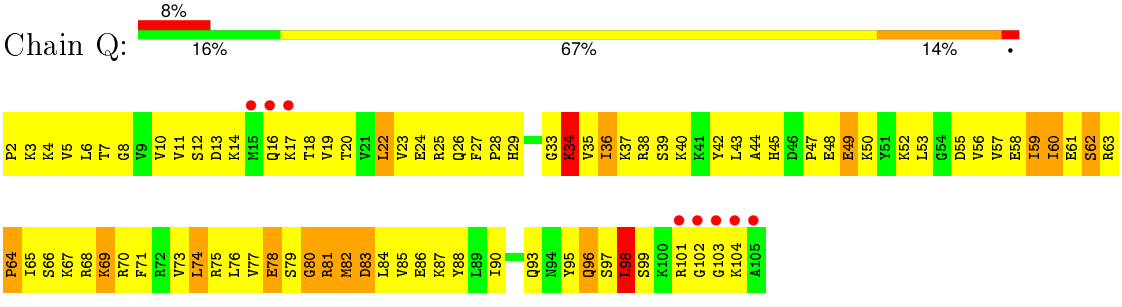
- Molecule 18: 30S RIBOSOMAL PROTEIN S16

Chain P:



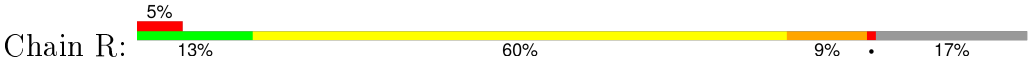
- Molecule 19: 30S RIBOSOMAL PROTEIN S17

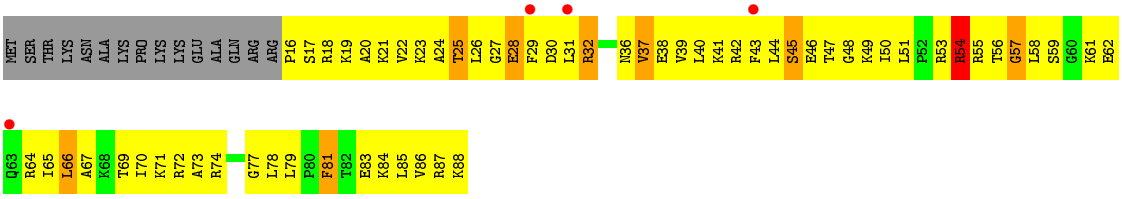
Chain Q:



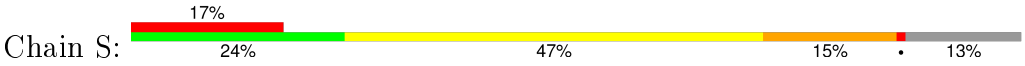
- Molecule 20: 30S RIBOSOMAL PROTEIN S18

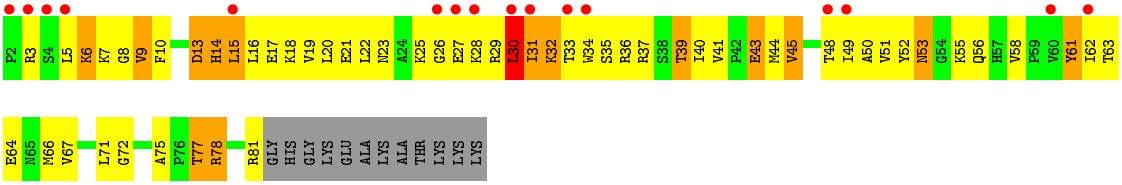
Chain R:



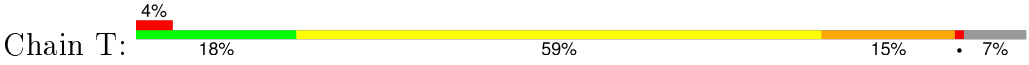


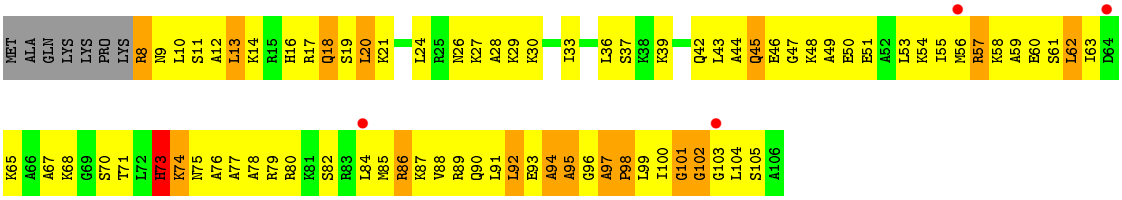
• Molecule 21: 30S RIBOSOMAL PROTEIN S19



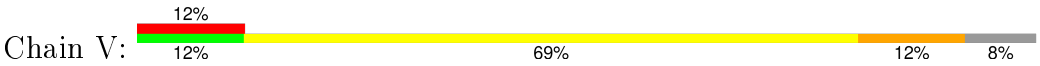


• Molecule 22: 30S RIBOSOMAL PROTEIN S20





• Molecule 23: 30S RIBOSOMAL PROTEIN THX



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.60Å 401.60Å 176.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.54 – 3.35 74.58 – 3.35	Depositor EDS
% Data completeness (in resolution range)	88.6 (74.54-3.35) 88.6 (74.58-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.284 0.235 , 0.286	Depositor DCC
R_{free} test set	9128 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	104.3	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 136.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 181372 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	52140	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, PSU

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	0.58	1/36387 (0.0%)	0.76	33/56789 (0.1%)
2	Y	0.59	0/241	0.92	2/375 (0.5%)
3	Z	0.48	0/84	0.78	0/128
4	B	0.36	0/1935	0.66	0/2609
5	C	0.38	0/1636	0.65	0/2205
6	D	0.42	0/1733	0.68	0/2318
7	E	0.48	0/1162	0.77	0/1564
8	F	0.37	0/856	0.66	0/1154
9	G	0.35	0/1276	0.60	0/1709
10	H	0.53	0/1136	0.83	1/1527 (0.1%)
11	I	0.35	0/1029	0.64	0/1378
12	J	0.38	0/805	0.71	1/1082 (0.1%)
13	K	0.41	0/900	0.69	0/1213
14	L	0.44	0/986	0.79	0/1320
15	M	0.35	0/947	0.61	0/1270
16	N	0.39	0/501	0.66	0/664
17	O	0.41	0/745	0.63	0/992
18	P	0.53	0/716	0.84	0/963
19	Q	0.55	0/870	0.80	0/1159
20	R	0.39	0/603	0.68	0/799
21	S	0.35	0/661	0.68	0/890
22	T	0.45	0/765	0.81	2/1007 (0.2%)
23	V	0.37	0/212	0.59	0/277
All	All	0.53	1/56186 (0.0%)	0.74	39/83392 (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	3	46
10	H	0	1
All	All	3	47

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	758	G	C5-C6	-5.26	1.37	1.42

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243	A	C2'-C3'-O3'	10.26	132.07	109.50
1	A	366	C	C2'-C3'-O3'	8.95	129.19	109.50
1	A	1498	U	C2'-C3'-O3'	8.91	129.10	109.50
1	A	1528	U	C2'-C3'-O3'	8.77	128.80	109.50
1	A	181	G	C2'-C3'-O3'	8.66	128.56	109.50

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	243	A	C3'
1	A	1504	G	C3'
1	A	1528	U	C3'

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	C	Sidechain
1	A	115	G	Sidechain
1	A	190(L)	U	Sidechain
1	A	51	A	Sidechain
1	A	54	C	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	32508	0	16414	1353	0
2	Y	235	0	121	11	0
3	Z	77	0	42	1	0
4	B	1900	0	1951	303	0
5	C	1612	0	1677	285	0
6	D	1703	0	1764	212	0
7	E	1146	0	1207	129	0
8	F	843	0	857	94	0
9	G	1257	0	1296	132	0
10	H	1116	0	1177	143	0
11	I	1011	0	1043	177	0
12	J	792	0	835	169	2
13	K	885	0	904	103	0
14	L	970	0	1057	138	0
15	M	937	0	995	121	0
16	N	492	0	531	89	0
17	O	734	0	771	78	0
18	P	700	0	720	86	0
19	Q	857	0	930	130	0
20	R	597	0	668	93	0
21	S	647	0	673	94	0
22	T	763	0	861	96	0
23	V	208	0	221	37	0
24	A	42	0	45	4	0
25	A	103	0	0	0	0
25	Y	1	0	0	0	0
25	Z	2	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52140	0	36760	3828	2

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 43.

The worst 5 of 3828 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)
6:D:36:ARG:H	6:D:37:PRO:HD3	1.05	1.11
1:A:1443:G:H5"	1:A:1446:A:H5"	1.28	1.09
1:A:1356:G:H2'	1:A:1357:A:C8	1.90	1.06
6:D:63:LYS:HD2	6:D:198:VAL:HG23	1.34	1.06
1:A:1250:A:H4'	11:I:68:GLY:H	1.18	1.05

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:79:ARG:NH1	12:J:79:ARG:NH1[8_665]	1.67	0.53
12:J:80:LYS:NZ	12:J:80:LYS:NZ[8_665]	1.96	0.24

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
4	B	232/256 (91%)	132 (57%)	57 (25%)	43 (18%)	0 1
5	C	204/239 (85%)	115 (56%)	46 (22%)	43 (21%)	0 1
6	D	206/208 (99%)	145 (70%)	46 (22%)	15 (7%)	1 11
7	E	148/161 (92%)	115 (78%)	20 (14%)	13 (9%)	1 7
8	F	99/101 (98%)	73 (74%)	21 (21%)	5 (5%)	2 21
9	G	153/155 (99%)	93 (61%)	39 (26%)	21 (14%)	0 2
10	H	136/138 (99%)	102 (75%)	24 (18%)	10 (7%)	1 11
11	I	125/128 (98%)	70 (56%)	37 (30%)	18 (14%)	0 1
12	J	96/104 (92%)	54 (56%)	22 (23%)	20 (21%)	0 1
13	K	117/129 (91%)	77 (66%)	29 (25%)	11 (9%)	1 6
14	L	122/135 (90%)	81 (66%)	23 (19%)	18 (15%)	0 1
15	M	116/126 (92%)	63 (54%)	35 (30%)	18 (16%)	0 1
16	N	58/60 (97%)	34 (59%)	14 (24%)	10 (17%)	0 1
17	O	86/88 (98%)	57 (66%)	26 (30%)	3 (4%)	4 32
18	P	81/88 (92%)	52 (64%)	24 (30%)	5 (6%)	2 15
19	Q	102/104 (98%)	81 (79%)	11 (11%)	10 (10%)	1 5
20	R	71/88 (81%)	47 (66%)	14 (20%)	10 (14%)	0 2
21	S	78/92 (85%)	46 (59%)	21 (27%)	11 (14%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
22	T	97/106 (92%)	51 (53%)	33 (34%)	13 (13%)	0 2
23	V	22/26 (85%)	16 (73%)	4 (18%)	2 (9%)	1 6
All	All	2349/2532 (93%)	1504 (64%)	546 (23%)	299 (13%)	0 2

5 of 299 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	8	LYS
4	B	9	GLU
4	B	15	VAL
4	B	16	HIS
4	B	21	ARG

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
4	B	202/220 (92%)	177 (88%)	25 (12%)	6 24
5	C	160/188 (85%)	149 (93%)	11 (7%)	19 58
6	D	180/180 (100%)	160 (89%)	20 (11%)	8 30
7	E	115/122 (94%)	101 (88%)	14 (12%)	6 25
8	F	90/90 (100%)	81 (90%)	9 (10%)	9 36
9	G	126/126 (100%)	118 (94%)	8 (6%)	22 61
10	H	119/119 (100%)	101 (85%)	18 (15%)	3 17
11	I	98/99 (99%)	86 (88%)	12 (12%)	6 25
12	J	87/91 (96%)	73 (84%)	14 (16%)	3 14
13	K	90/99 (91%)	83 (92%)	7 (8%)	16 51
14	L	104/111 (94%)	91 (88%)	13 (12%)	6 24
15	M	94/101 (93%)	88 (94%)	6 (6%)	22 60
16	N	49/49 (100%)	44 (90%)	5 (10%)	9 35
17	O	79/79 (100%)	73 (92%)	6 (8%)	16 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	P	72/74 (97%)	62 (86%)	10 (14%)	4 20
19	Q	96/96 (100%)	86 (90%)	10 (10%)	9 34
20	R	64/77 (83%)	61 (95%)	3 (5%)	32 71
21	S	71/79 (90%)	63 (89%)	8 (11%)	7 29
22	T	76/82 (93%)	67 (88%)	9 (12%)	6 27
23	V	19/21 (90%)	18 (95%)	1 (5%)	28 66
All	All	1991/2103 (95%)	1782 (90%)	209 (10%)	8 33

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	H	56	LYS
11	I	127	LYS
21	S	25	LYS
10	H	91	ARG
11	I	38	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
8	F	100	ASN
9	G	106	GLN
21	S	23	ASN
9	G	37	ASN
9	G	122	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	206 (13%)	66 (4%)
2	Y	10/17 (58%)	2 (20%)	0
3	Z	3/6 (50%)	0	0
All	All	1524/1545 (98%)	208 (13%)	66 (4%)

5 of 208 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A

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

5 of 66 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	509	A
1	A	812	C
1	A	1380	U
1	A	533	A
1	A	687	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
2	PSU	Y	40	2	13,21,22	2.13	4 (30%)	18,30,33	6.00	6 (33%)

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
2	PSU	Y	40	2	-	0/7/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	40	PSU	O4'-C1'	-2.61	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	40	PSU	C6-N1	2.72	1.40	1.34
2	Y	40	PSU	O3'-C3'	3.58	1.51	1.43
2	Y	40	PSU	C4-N3	5.17	1.42	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	40	PSU	N1-C2-N3	-20.68	115.14	128.33
2	Y	40	PSU	C4'-O4'-C1'	-3.22	106.29	109.58
2	Y	40	PSU	O4'-C4'-C3'	-2.07	100.98	105.15
2	Y	40	PSU	O2'-C2'-C1'	-2.04	107.33	111.83
2	Y	40	PSU	C6-N1-C2	3.37	120.88	115.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	40	PSU	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 109 ligands modelled in this entry, 108 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
24	PAR	A	1545	-	45,45,45	2.06	14 (31%)	59,67,67	1.00	2 (3%)

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
24	PAR	A	1545	-	-	0/18/94/94	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	O33-C33	2.01	1.48	1.43
24	A	1545	PAR	C14-C24	2.05	1.56	1.52
24	A	1545	PAR	C21-N21	2.10	1.50	1.47
24	A	1545	PAR	O51-C51	2.29	1.50	1.44
24	A	1545	PAR	C23-C33	2.36	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1545	PAR	O54-C54-C64	2.39	110.77	106.10
24	A	1545	PAR	O11-C11-C21	2.56	112.71	107.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1545	PAR	4	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

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^{th} 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^2)	Q<0.9
1	A	1512/1522 (99%)	0.63	87 (5%) 26 26	25, 86, 178, 198	0
2	Y	10/17 (58%)	0.43	0 100 100	91, 117, 190, 194	0
3	Z	4/6 (66%)	0.61	1 (25%) 1 1	87, 92, 96, 197	0
4	B	234/256 (91%)	0.51	29 (12%) 5 5	22, 132, 191, 198	0
5	C	206/239 (86%)	0.23	9 (4%) 38 37	55, 126, 183, 198	0
6	D	208/208 (100%)	0.39	21 (10%) 9 9	16, 91, 157, 197	0
7	E	150/161 (93%)	-0.07	0 100 100	31, 83, 138, 198	0
8	F	101/101 (100%)	0.66	15 (14%) 3 3	56, 117, 174, 194	0
9	G	155/155 (100%)	0.23	5 (3%) 51 51	64, 127, 175, 198	0
10	H	138/138 (100%)	-0.11	1 (0%) 89 89	4, 65, 145, 197	0
11	I	127/128 (99%)	0.63	15 (11%) 6 6	57, 140, 187, 198	0
12	J	98/104 (94%)	1.18	26 (26%) 1 1	51, 146, 197, 198	0
13	K	119/129 (92%)	0.39	8 (6%) 21 21	48, 99, 169, 198	0
14	L	124/135 (91%)	0.32	7 (5%) 28 27	37, 88, 157, 181	0
15	M	118/126 (93%)	0.37	7 (5%) 26 25	60, 120, 175, 196	0
16	N	60/60 (100%)	0.56	4 (6%) 21 21	60, 117, 174, 198	0
17	O	88/88 (100%)	0.22	4 (4%) 37 36	21, 83, 147, 198	0
18	P	83/88 (94%)	0.12	4 (4%) 34 34	10, 62, 121, 172	0
19	Q	104/104 (100%)	0.33	8 (7%) 16 17	14, 75, 157, 198	0
20	R	73/88 (82%)	0.50	4 (5%) 29 28	46, 99, 178, 194	0
21	S	80/92 (86%)	1.07	16 (20%) 1 1	74, 138, 191, 198	0
22	T	99/106 (93%)	0.05	4 (4%) 42 41	24, 70, 136, 186	0
23	V	24/26 (92%)	0.85	3 (12%) 5 5	44, 122, 183, 198	0
All	All	3915/4077 (96%)	0.47	278 (7%) 19 19	4, 98, 179, 198	0

The worst 5 of 278 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	J	10	GLY	9.3
21	S	3	ARG	9.0
6	D	23	GLY	8.0
21	S	2	PRO	6.7
16	N	3	ARG	6.6

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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^2)	Q<0.9
2	PSU	Y	40	20/21	0.95	0.32	-	25,25,25,25	0

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^{th} 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^2)	Q<0.9
25	MG	A	211	1/1	0.85	0.87	74.91	34,34,34,34	1
25	MG	A	1560	1/1	0.97	0.54	19.53	34,34,34,34	0
25	MG	A	1558	1/1	0.96	0.47	11.76	34,34,34,34	0
25	MG	A	1629	1/1	0.97	0.49	11.67	34,34,34,34	0
25	MG	A	1555	1/1	0.97	0.55	10.59	34,34,34,34	0
25	MG	A	1588	1/1	0.94	0.54	8.67	34,34,34,34	0
25	MG	A	1546	1/1	0.96	0.39	7.90	34,34,34,34	0
25	MG	A	1587	1/1	0.97	0.41	6.91	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1551	1/1	0.97	0.42	4.53	34,34,34,34	0
25	MG	A	1592	1/1	0.93	0.30	2.44	34,34,34,34	0
25	MG	A	1582	1/1	0.98	0.28	2.04	34,34,34,34	0
25	MG	A	1584	1/1	0.94	0.31	2.04	34,34,34,34	0
25	MG	A	210	1/1	0.80	0.26	1.66	34,34,34,34	1
25	MG	A	1572	1/1	0.89	0.25	1.19	34,34,34,34	0
25	MG	A	1597	1/1	0.63	0.47	1.08	25,25,25,25	1
25	MG	A	1569	1/1	0.96	0.38	0.65	34,34,34,34	0
24	PAR	A	1545	42/42	0.93	0.25	0.47	30,30,30,30	0
25	MG	A	493	1/1	0.95	0.26	-0.04	34,34,34,34	1
25	MG	A	1623	1/1	0.92	0.30	-0.12	34,34,34,34	1
25	MG	A	1570	1/1	0.98	0.24	-0.37	34,34,34,34	0
25	MG	A	1578	1/1	0.98	0.26	-0.66	34,34,34,34	0
26	ZN	D	306	1/1	0.98	0.23	-0.81	34,34,34,34	0
25	MG	A	1600	1/1	0.98	0.19	-0.87	34,34,34,34	1
26	ZN	N	307	1/1	0.99	0.19	-0.92	34,34,34,34	1
25	MG	A	1586	1/1	0.94	0.17	-0.96	34,34,34,34	0
25	MG	A	1591	1/1	0.94	0.21	-1.02	34,34,34,34	0
25	MG	A	1590	1/1	0.97	0.21	-1.03	34,34,34,34	0
25	MG	A	1602	1/1	0.95	0.16	-1.04	34,34,34,34	1
25	MG	A	1593	1/1	0.94	0.21	-1.06	34,34,34,34	0
25	MG	Z	400	1/1	0.97	0.10	-2.29	34,34,34,34	1
25	MG	A	1561	1/1	0.94	0.14	-2.51	34,34,34,34	1
25	MG	A	1619	1/1	0.91	0.12	-2.61	34,34,34,34	1
25	MG	A	1598	1/1	0.90	0.15	-2.95	34,34,34,34	0
25	MG	A	1552	1/1	0.97	0.42	-	34,34,34,34	0
25	MG	A	1625	1/1	0.98	0.26	-	34,34,34,34	0
25	MG	A	1606	1/1	0.59	0.45	-	34,34,34,34	1
25	MG	A	473	1/1	0.95	0.37	-	34,34,34,34	1
25	MG	A	214	1/1	0.92	0.23	-	34,34,34,34	1
25	MG	A	466	1/1	0.85	0.26	-	34,34,34,34	1
25	MG	A	1614	1/1	0.91	0.30	-	34,34,34,34	1
25	MG	Z	501	1/1	0.97	0.25	-	34,34,34,34	1
25	MG	A	1618	1/1	0.62	0.65	-	34,34,34,34	1
25	MG	A	1632	1/1	0.86	0.29	-	34,34,34,34	1
25	MG	A	1553	1/1	0.97	0.28	-	34,34,34,34	0
25	MG	A	1567	1/1	0.93	0.35	-	34,34,34,34	0
25	MG	A	1615	1/1	0.91	0.28	-	34,34,34,34	1
25	MG	A	1580	1/1	0.81	0.66	-	34,34,34,34	0
25	MG	A	1605	1/1	0.92	0.27	-	34,34,34,34	0
25	MG	A	1589	1/1	0.91	0.42	-	34,34,34,34	0
25	MG	A	1634	1/1	0.93	0.59	-	34,34,34,34	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1565	1/1	0.88	0.62	-	34,34,34,34	1
25	MG	A	471	1/1	0.94	0.59	-	34,34,34,34	1
25	MG	A	1550	1/1	0.83	0.17	-	34,34,34,34	1
25	MG	Y	500	1/1	0.96	0.28	-	25,25,25,25	1
25	MG	A	1627	1/1	0.91	0.24	-	34,34,34,34	1
25	MG	A	1624	1/1	0.85	0.45	-	34,34,34,34	0
25	MG	A	1583	1/1	0.95	0.24	-	34,34,34,34	0
25	MG	A	1557	1/1	0.94	0.38	-	34,34,34,34	0
25	MG	A	1548	1/1	0.61	1.36	-	34,34,34,34	1
25	MG	A	467	1/1	0.98	0.14	-	34,34,34,34	0
25	MG	A	1577	1/1	0.94	0.23	-	34,34,34,34	1
25	MG	A	1612	1/1	0.81	0.39	-	34,34,34,34	0
25	MG	A	1616	1/1	0.89	0.23	-	34,34,34,34	1
25	MG	A	86	1/1	0.98	0.32	-	34,34,34,34	0
25	MG	A	1622	1/1	0.83	0.61	-	34,34,34,34	1
25	MG	A	1630	1/1	0.96	0.82	-	34,34,34,34	0
25	MG	A	1559	1/1	0.95	0.76	-	34,34,34,34	0
25	MG	A	1566	1/1	0.92	0.54	-	34,34,34,34	0
25	MG	A	1549	1/1	0.89	0.39	-	34,34,34,34	0
25	MG	A	1633	1/1	0.92	0.82	-	34,34,34,34	1
25	MG	A	1607	1/1	0.72	1.22	-	34,34,34,34	1
25	MG	A	71	1/1	0.81	0.30	-	34,34,34,34	0
25	MG	A	1575	1/1	0.67	0.35	-	34,34,34,34	1
25	MG	A	1585	1/1	0.69	0.55	-	34,34,34,34	1
25	MG	A	1628	1/1	0.94	0.35	-	34,34,34,34	0
25	MG	A	1595	1/1	0.76	0.37	-	34,34,34,34	1
25	MG	A	1599	1/1	0.88	0.20	-	34,34,34,34	0
25	MG	A	470	1/1	0.92	0.55	-	34,34,34,34	0
25	MG	A	1603	1/1	0.93	0.52	-	34,34,34,34	1
25	MG	A	1631	1/1	0.98	0.13	-	34,34,34,34	1
25	MG	A	1604	1/1	0.87	0.77	-	34,34,34,34	0
25	MG	A	1568	1/1	0.96	0.26	-	34,34,34,34	0
25	MG	A	1596	1/1	0.97	0.20	-	34,34,34,34	1
25	MG	A	1626	1/1	0.86	0.35	-	34,34,34,34	1
25	MG	A	1574	1/1	0.99	0.40	-	34,34,34,34	0
25	MG	A	1547	1/1	0.97	0.57	-	34,34,34,34	0
25	MG	A	1609	1/1	0.77	0.31	-	34,34,34,34	1
25	MG	A	1620	1/1	0.82	0.30	-	34,34,34,34	1
25	MG	A	1571	1/1	0.94	0.25	-	34,34,34,34	0
25	MG	A	1581	1/1	0.93	0.75	-	34,34,34,34	0
25	MG	A	1576	1/1	0.95	0.42	-	34,34,34,34	1
25	MG	A	1608	1/1	0.90	0.50	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1613	1/1	0.92	0.35	-	34,34,34,34	0
25	MG	A	1579	1/1	0.96	0.26	-	34,34,34,34	0
25	MG	A	1617	1/1	0.94	0.49	-	34,34,34,34	0
25	MG	A	87	1/1	0.81	0.31	-	34,34,34,34	0
25	MG	A	1594	1/1	0.78	0.20	-	34,34,34,34	0
25	MG	A	1621	1/1	0.87	0.47	-	34,34,34,34	1
25	MG	A	1564	1/1	0.91	0.44	-	34,34,34,34	0
25	MG	A	1610	1/1	0.85	0.20	-	34,34,34,34	0
25	MG	A	1573	1/1	0.94	0.30	-	34,34,34,34	0
25	MG	A	1563	1/1	0.97	0.63	-	34,34,34,34	0
25	MG	A	1554	1/1	0.98	0.24	-	34,34,34,34	0
25	MG	A	1601	1/1	0.83	0.15	-	34,34,34,34	1
25	MG	A	1562	1/1	0.82	0.42	-	34,34,34,34	0
25	MG	A	1611	1/1	0.95	0.32	-	34,34,34,34	0
25	MG	A	441	1/1	0.72	0.31	-	34,34,34,34	1
25	MG	A	469	1/1	0.94	0.19	-	34,34,34,34	1
25	MG	A	1556	1/1	0.89	0.53	-	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.