wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 05:57 AM EDT

PDB ID	:	2UXD
Title	:	Crystal structure of an extended tRNA anticodon stem loop in complex with its cognate mRNA CGGG in the context of the Thermus thermophilus 30S subunit.
Authors	:	Dunham, C.M.; Selmer, M.; Phelps, S.S.; Kelley, A.C.; Suzuki, T.; Joseph, S.; Ramakrishnan, V.
Deposited on	:	2007-03-28
Resolution	:	3.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

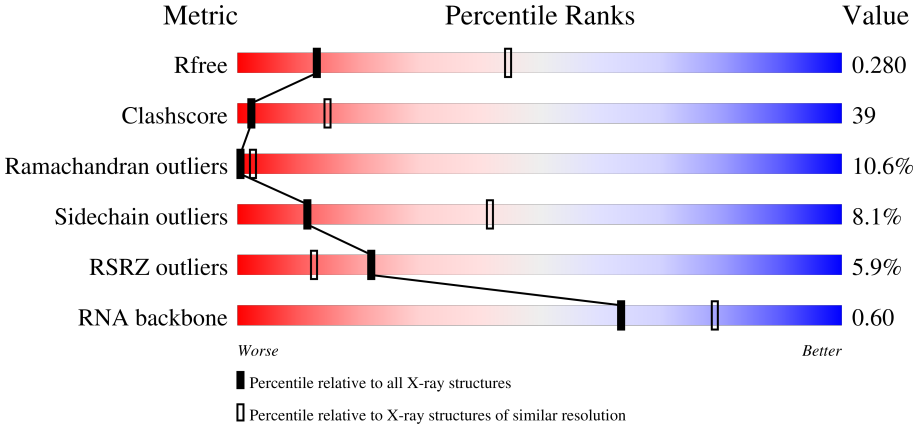
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	1523	7%; 28%, 54%, 13%, • •
2	B	256	5%; 22%, 57%, 11%, • 8%
3	C	239	10%; 18%, 52%, 15%, • 13%
4	D	209	5%; 32%, 55%, 11%, •

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Mol	Chain	Length	Quality of chain
5	E	162	30% 51% 10% • 7%
6	F	101	3% 40% 51% 9%
7	G	156	4% 30% 55% 14% •
8	H	138	40% 47% 12% •
9	I	128	6% 30% 59% 10% •
10	J	105	13% 21% 56% 17% 6%
11	K	129	2% 36% 45% 11% • 8%
12	L	135	% 22% 56% 15% 7%
13	M	126	10% 27% 55% 17% •
14	N	61	5% 33% 49% 16% •
15	O	89	% 44% 49% 6% •
16	P	88	% 43% 43% 8% • 5%
17	Q	105	3% 32% 59% 6% • •
18	R	88	5% 27% 45% 10% 17%
19	S	93	10% 16% 59% 12% 13%
20	T	106	6% 29% 52% 11% • 7%
21	V	27	4% 22% 63% 7% 7%
22	X	4	50% 50%
23	Y	18	6% 11% 11% 22% 56%

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	G	3002	-	-	-	X
25	MG	G	3004	-	-	-	X
25	MG	G	3005	-	-	-	X
25	MG	G	3007	-	-	-	X
25	MG	G	3017	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	G	3018	-	-	-	X
25	MG	G	3023	-	-	-	X
25	MG	G	3030	-	-	-	X
25	MG	G	3035	-	-	-	X
25	MG	G	3036	-	-	-	X
25	MG	G	3037	-	-	-	X
25	MG	G	3040	-	-	-	X
25	MG	G	3042	-	-	-	X
25	MG	G	3047	-	-	-	X
25	MG	G	3048	-	-	-	X
25	MG	G	3049	-	-	-	X
25	MG	G	3050	-	-	-	X
25	MG	G	3054	-	-	-	X
25	MG	G	3057	-	-	-	X
25	MG	G	3061	-	-	-	X
25	MG	G	3064	-	-	-	X
25	MG	G	3067	-	-	-	X
26	K	G	3075	-	-	-	X
26	K	G	3077	-	-	-	X

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 51468 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
			Total	C	N	O	P			
1	A	1484	31852	14194	5901	10285	1472	0	0	0

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	235	1901	1213	342	341	5	0	0	1

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	1613	1016	315	281	1	0	0	1

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	151	1147	724	218	201	4	0	0	1

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	99	793	498	157	137	1	0	0	1

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	125	971	611	196	163	1	0	0	1

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	125	997	617	207	171	2	0	0	0

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	84	701	443	140	117	1	0	0	1

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	81	648	414	120	112	2	0	0	1

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	T	99	762	469	162	129	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	41	VAL	ILE	conflict	UNP P80380

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	V	25	209	128	51	30	0	0	1

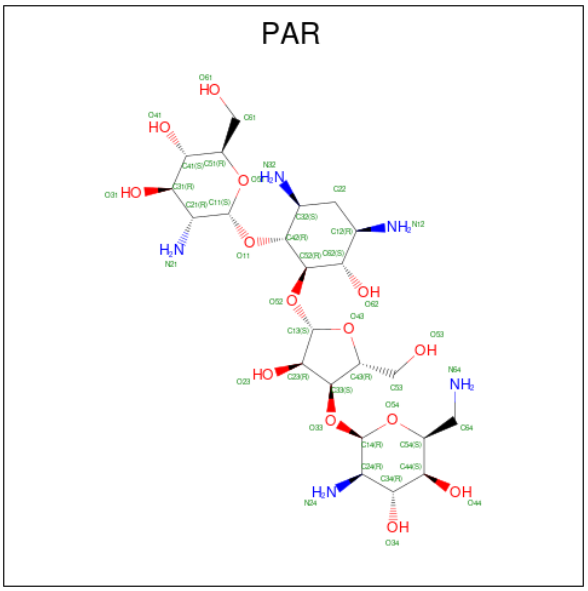
- Molecule 22 is a RNA chain called ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON CCCG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	X	4	90	39	18	29	4	0	0	0

- Molecule 23 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT CGGG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	Y	8	167	75	28	56	8	0	0	0

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
25	G	70	70	70	0	0

- Molecule 26 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
26	G	8	8	8	0	0

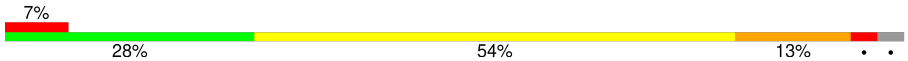
- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

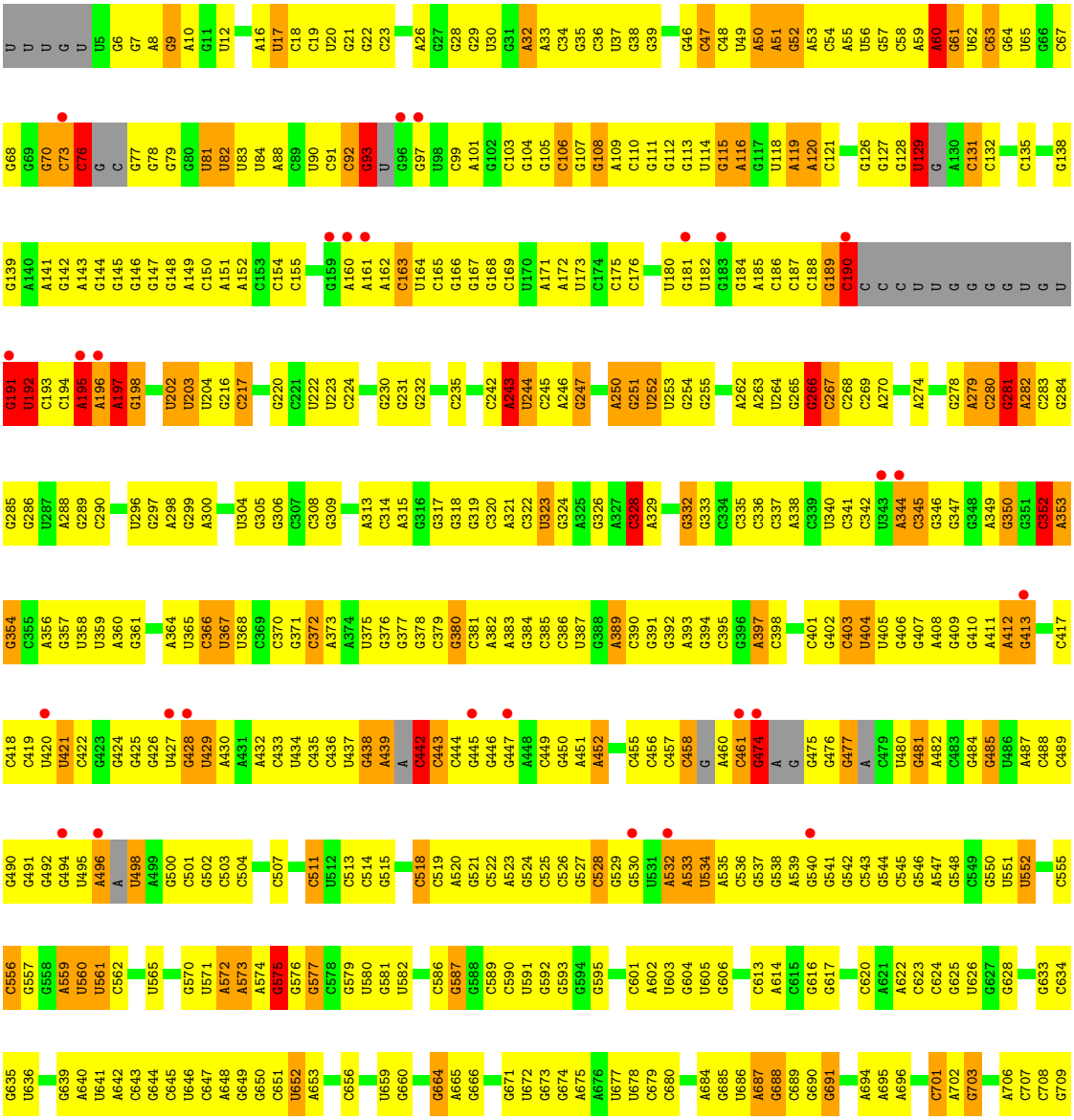
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
27	G	2	2	2	0	0

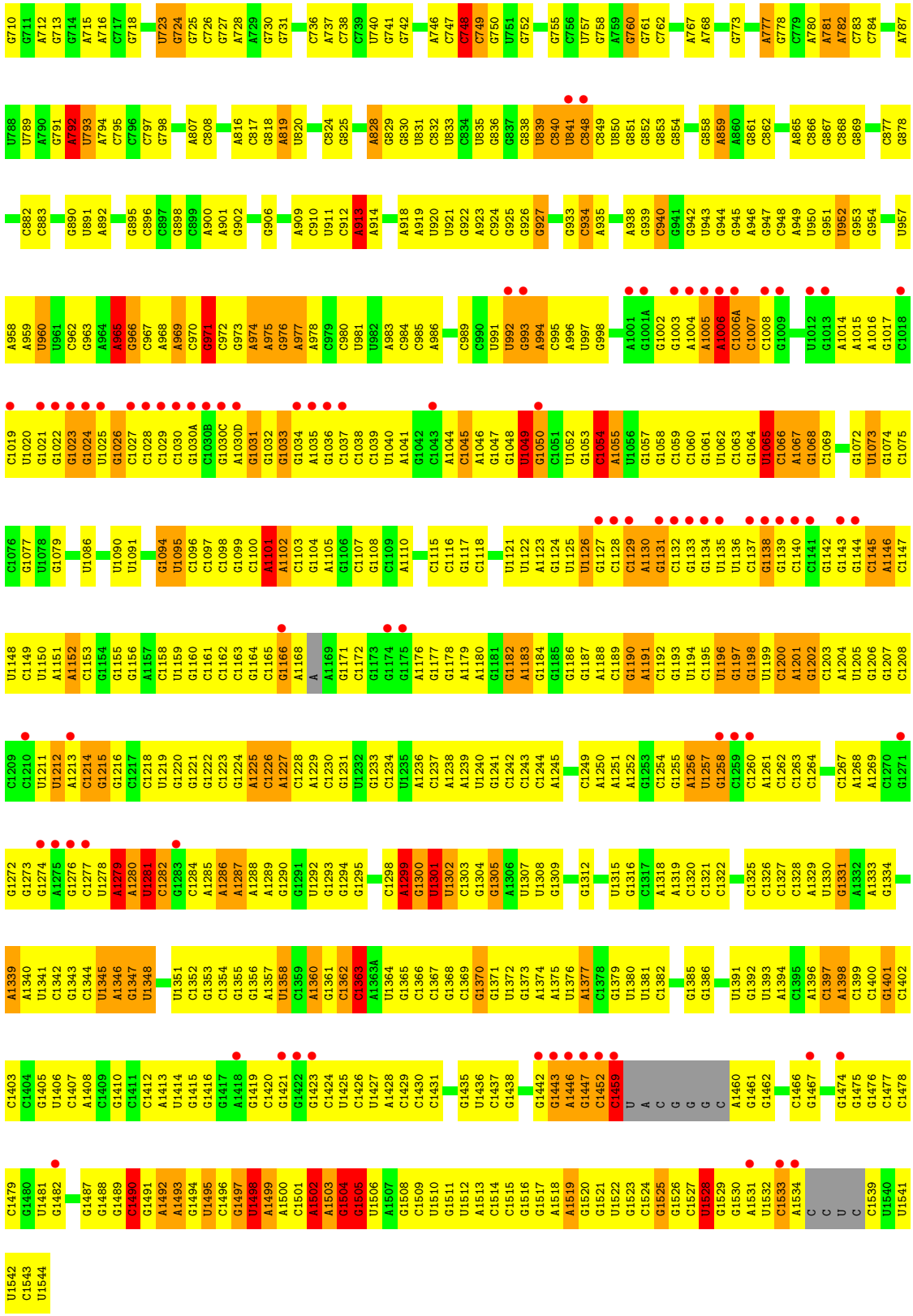
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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

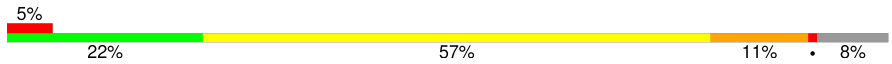
Chain A: 

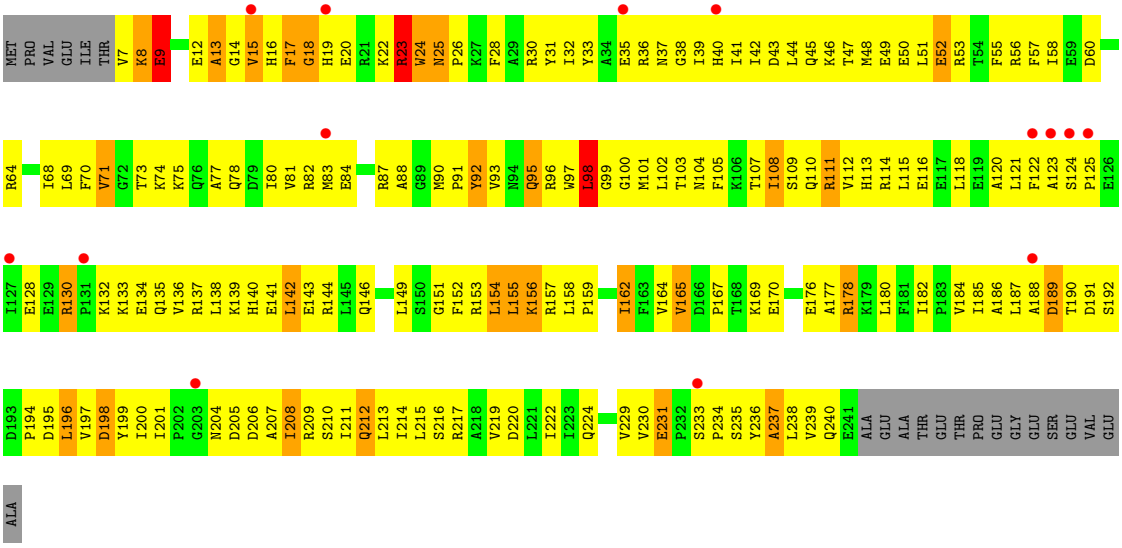




- Molecule 2: RIBOSOMAL PROTEIN S2

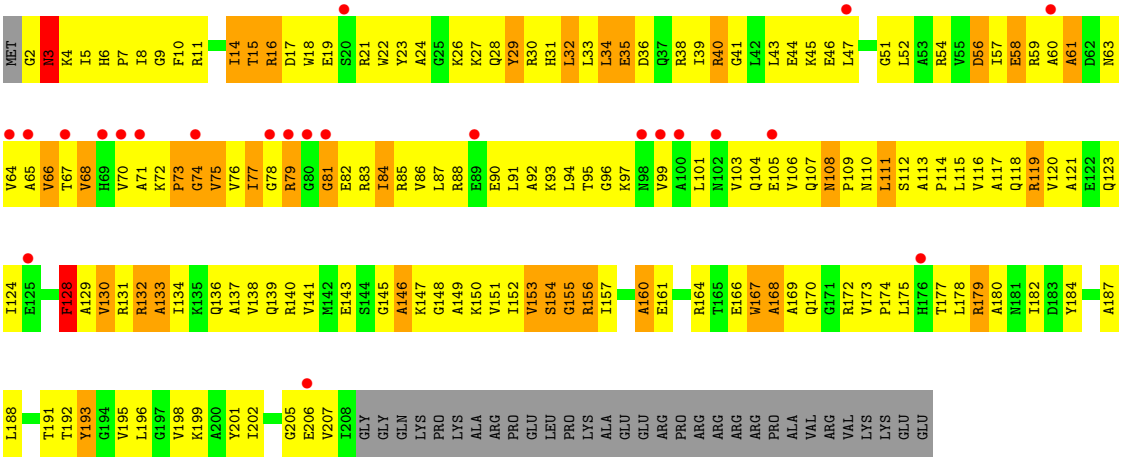
Chain B:





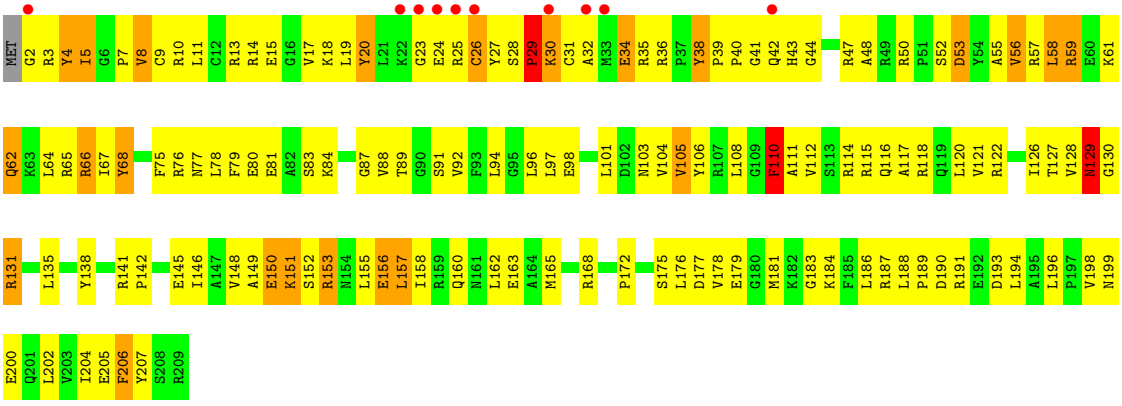
• Molecule 3: RIBOSOMAL PROTEIN S3

Chain C:



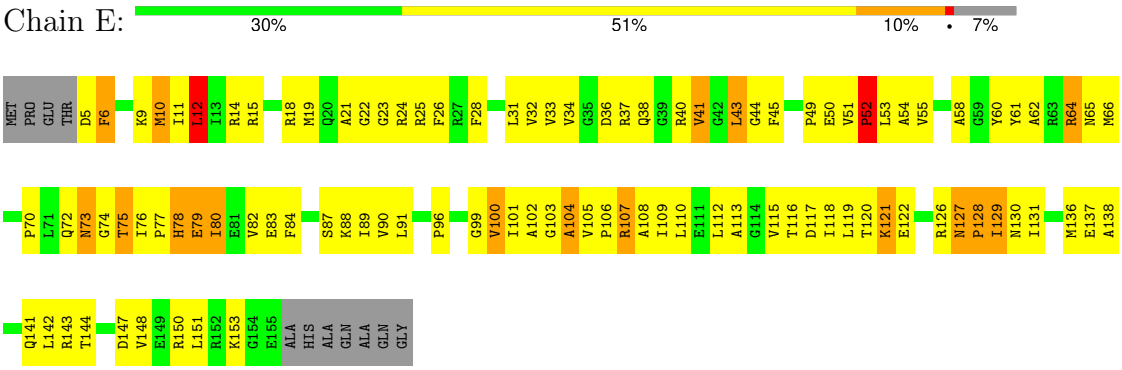
• Molecule 4: RIBOSOMAL PROTEIN S4

Chain D:



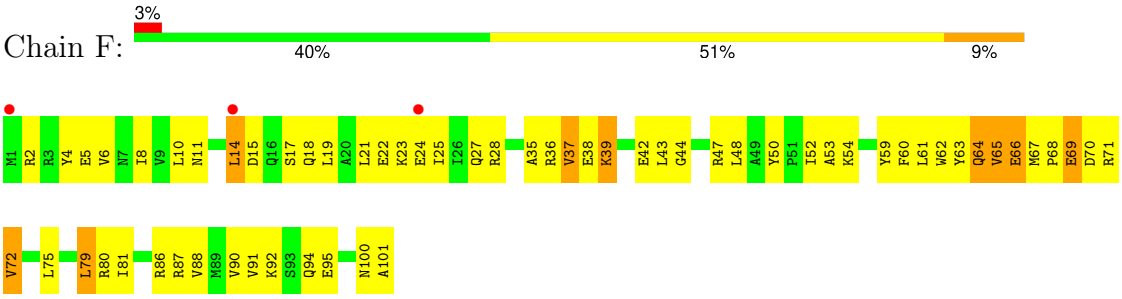
- Molecule 5: RIBOSOMAL PROTEIN S5

Chain E:



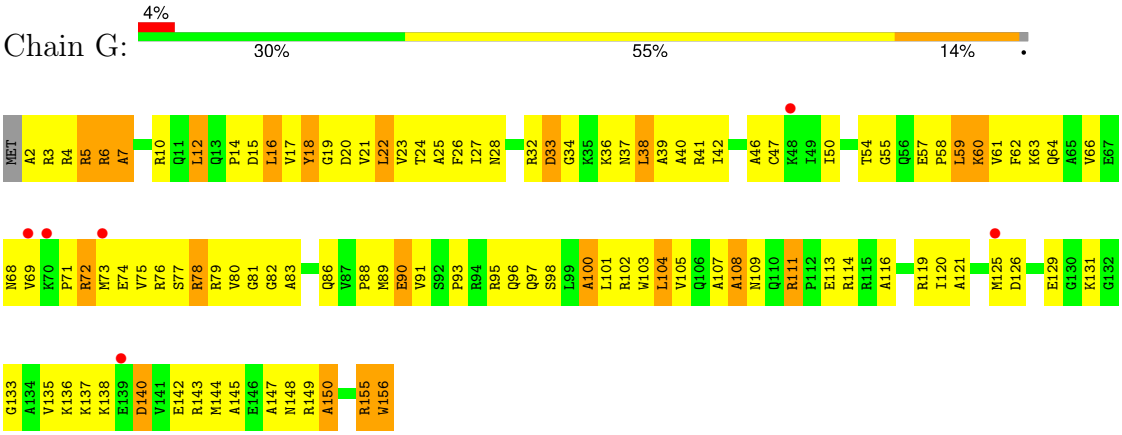
- Molecule 6: RIBOSOMAL PROTEIN S6

Chain F:



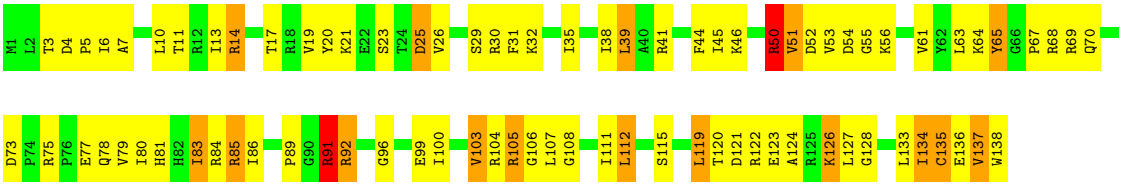
- Molecule 7: RIBOSOMAL PROTEIN S7

Chain G:



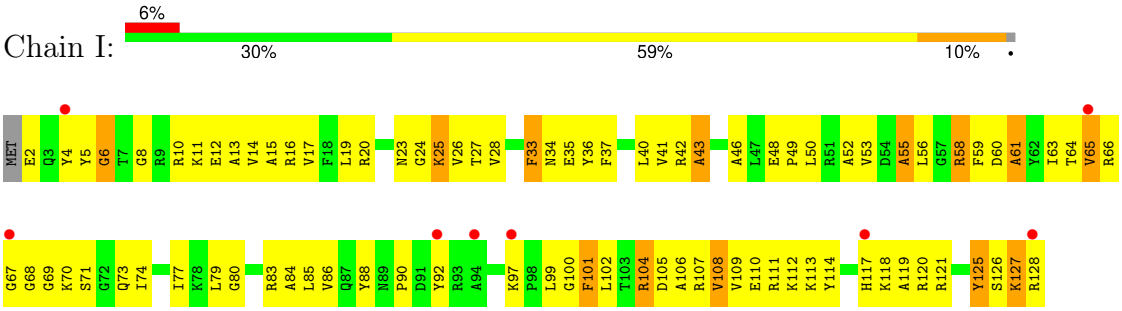
- Molecule 8: RIBOSOMAL PROTEIN S8

Chain H:



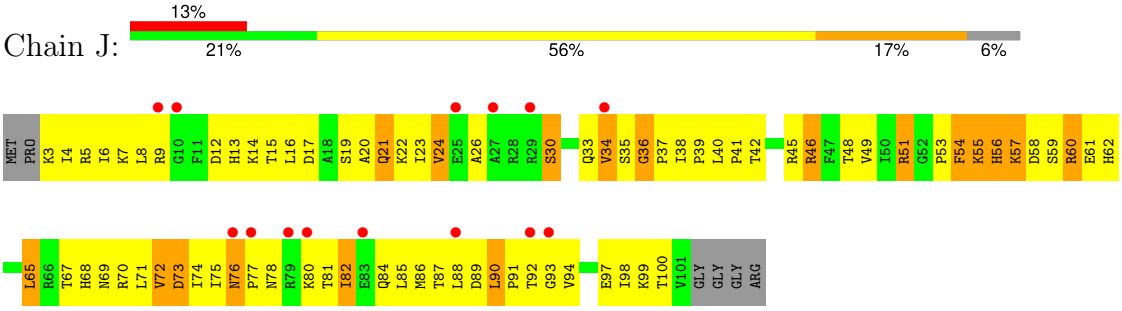
- Molecule 9: RIBOSOMAL PROTEIN S9

Chain I:



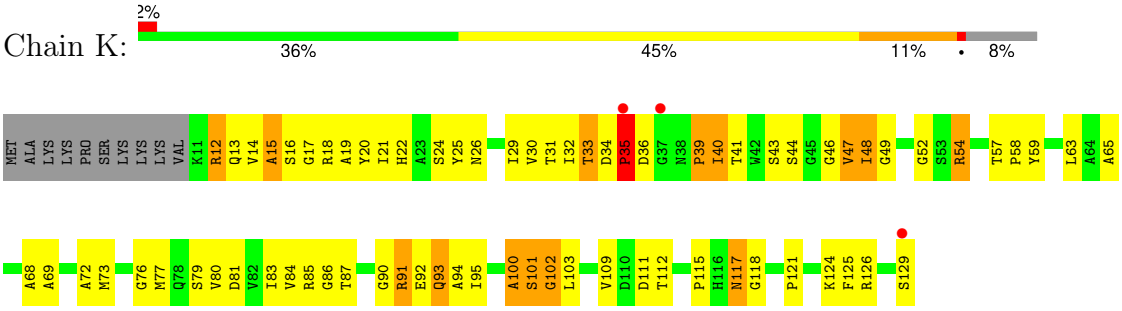
• Molecule 10: RIBOSOMAL PROTEIN S10

Chain J:



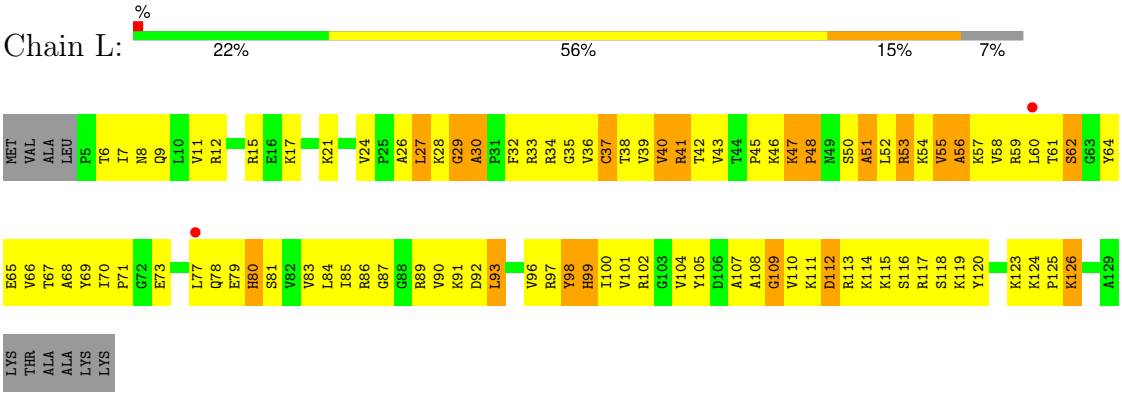
• Molecule 11: RIBOSOMAL PROTEIN S11

Chain K:



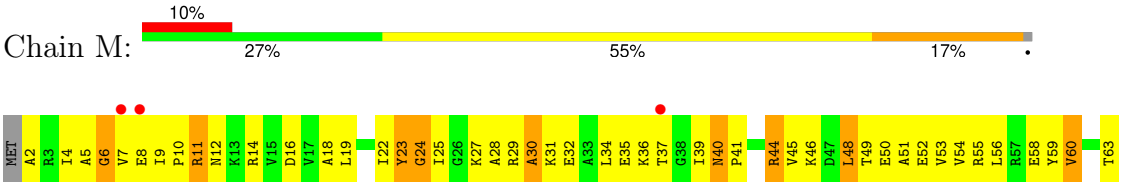
• Molecule 12: RIBOSOMAL PROTEIN S12

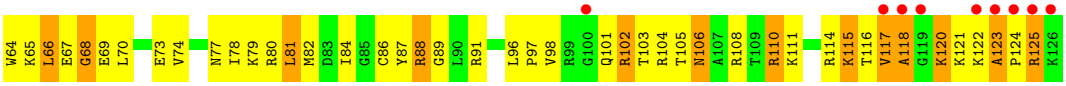
Chain L:



• Molecule 13: RIBOSOMAL PROTEIN S13

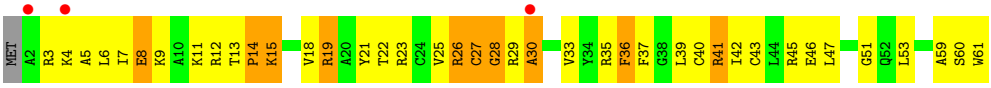
Chain M:





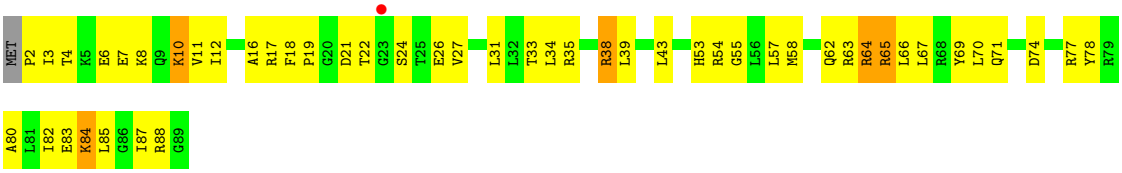
• Molecule 14: RIBOSOMAL PROTEIN S14

Chain N:



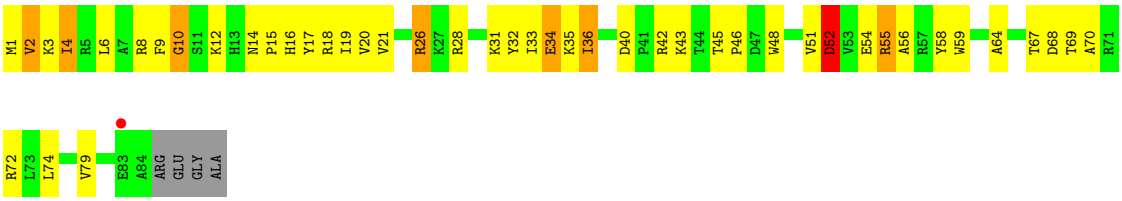
• Molecule 15: RIBOSOMAL PROTEIN S15

Chain O:



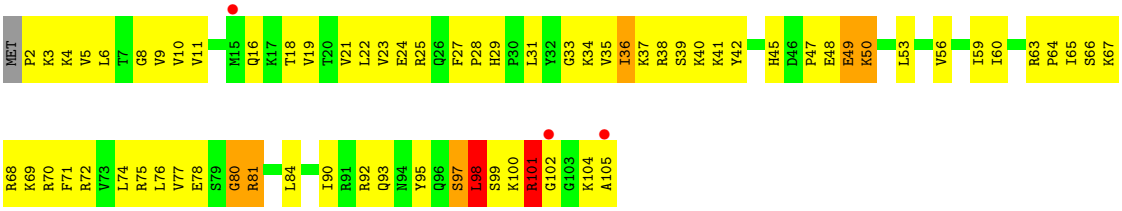
• Molecule 16: RIBOSOMAL PROTEIN S16

Chain P:



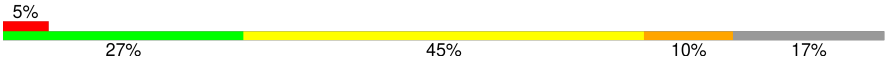
• Molecule 17: RIBOSOMAL PROTEIN S17

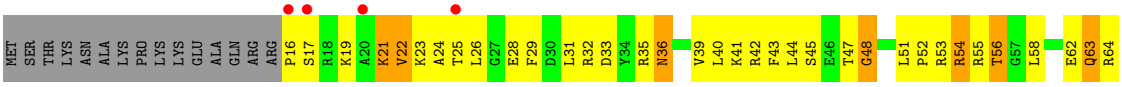
Chain Q:



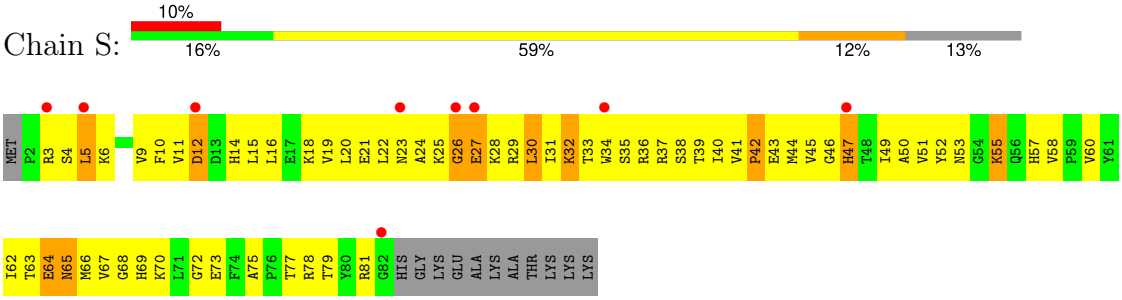
• Molecule 18: RIBOSOMAL PROTEIN S18

Chain R:

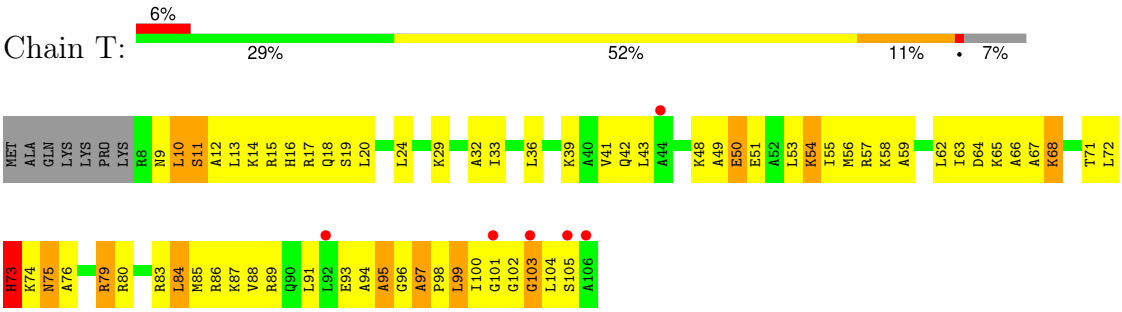




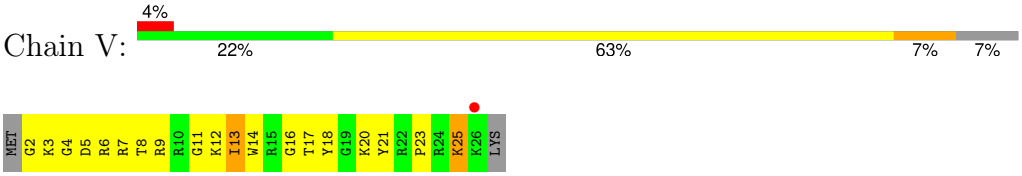
• Molecule 19: RIBOSOMAL PROTEIN S19



• Molecule 20: RIBOSOMAL PROTEIN S20

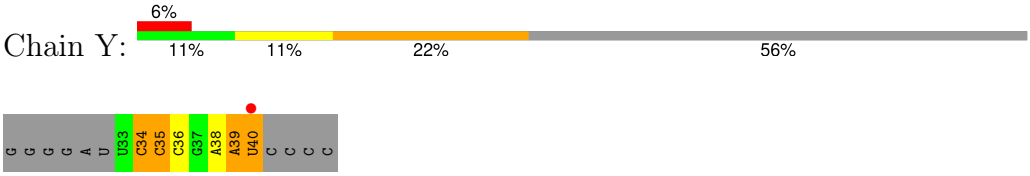


• Molecule 21: RIBOSOMAL PROTEIN THX



• Molecule 22: ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON CCCG

• Molecule 23: A-SITE MESSENGER RNA FRAGMENT CGGG



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.90Å 401.90Å 174.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 3.20 49.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.38-3.20) 98.2 (49.38-2.80)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.282 0.238 , 0.280	Depositor DCC
R_{free} test set	17219 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	89.1	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 85.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	51468	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: K, PAR, MG, ZN

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	0.62	16/35645 (0.0%)	0.77	53/55610 (0.1%)
2	B	0.37	0/1936	0.62	0/2611
3	C	0.34	0/1637	0.58	0/2207
4	D	0.36	0/1733	0.60	0/2318
5	E	0.49	0/1163	0.75	1/1566 (0.1%)
6	F	0.32	0/856	0.58	0/1154
7	G	0.31	0/1276	0.58	0/1709
8	H	0.49	0/1136	0.76	1/1527 (0.1%)
9	I	0.33	0/1029	0.56	0/1378
10	J	0.35	0/806	0.60	0/1084
11	K	0.40	0/900	0.69	0/1213
12	L	0.42	0/987	0.71	0/1322
13	M	0.32	0/1008	0.62	0/1347
14	N	0.33	0/501	0.60	0/664
15	O	0.37	0/745	0.59	0/992
16	P	0.47	0/717	0.79	1/965 (0.1%)
17	Q	0.46	0/870	0.76	0/1159
18	R	0.35	0/603	0.63	0/799
19	S	0.32	0/662	0.58	0/892
20	T	0.41	0/764	0.70	0/1006
21	V	0.52	0/213	0.71	0/279
22	X	0.98	1/100 (1.0%)	0.93	0/153
23	Y	0.59	0/185	0.84	0/285
All	All	0.55	17/55472 (0.0%)	0.73	56/82240 (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	8	57

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	496	A	C3'-O3'	7.89	1.53	1.42
1	A	190	C	C3'-O3'	7.73	1.52	1.42
22	X	1	C	OP3-P	-7.35	1.52	1.61
1	A	129	U	C3'-O3'	7.24	1.52	1.42
1	A	73	C	C3'-O3'	7.07	1.52	1.42

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	575	G	C2'-C3'-O3'	10.78	133.22	109.50
1	A	190	C	N1-C1'-C2'	10.38	127.49	114.00
1	A	1498	U	C2'-C3'-O3'	9.97	131.43	109.50
1	A	748	C	C2'-C3'-O3'	9.67	130.78	109.50
1	A	129	U	C2'-C3'-O3'	9.59	130.60	109.50

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	115	G	C3'
1	A	129	U	C3'
1	A	281	G	C3'
1	A	748	C	C3'
1	A	1006	A	C1'

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	C	Sidechain
1	A	128	G	Sidechain
1	A	17	U	Sidechain
1	A	70	G	Sidechain
1	A	93	G	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	31852	0	16122	1389	0
2	B	1901	0	1951	247	0
3	C	1613	0	1677	261	0
4	D	1703	0	1764	178	0
5	E	1147	0	1207	112	0
6	F	843	0	857	75	0
7	G	1257	0	1296	141	0
8	H	1116	0	1177	114	0
9	I	1011	0	1043	134	0
10	J	793	0	835	145	0
11	K	885	0	904	87	0
12	L	971	0	1057	154	0
13	M	997	0	1072	115	0
14	N	492	0	531	66	0
15	O	734	0	771	65	0
16	P	701	0	720	58	0
17	Q	857	0	930	83	0
18	R	597	0	666	60	0
19	S	648	0	673	93	0
20	T	762	0	859	84	0
21	V	209	0	221	19	0
22	X	90	0	45	11	0
23	Y	167	0	87	14	0
24	A	42	0	45	0	0
25	G	70	0	0	0	0
26	G	8	0	0	0	0
27	G	2	0	0	0	0
All	All	51468	0	36510	3377	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 39.

The worst 5 of 3377 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:189:G:H2'	1:A:190:C:C6	1.68	1.27
3:C:27:LYS:HA	3:C:30:ARG:HH12	1.09	1.13
10:J:38:ILE:HD11	10:J:71:LEU:HB2	1.20	1.11
1:A:1305:G:H22	1:A:1331:G:H2'	1.02	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1356:G:H2'	1:A:1357:A:C8	1.88	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	
2	B	233/256 (91%)	149 (64%)	60 (26%)	24 (10%)	0	3
3	C	205/239 (86%)	119 (58%)	53 (26%)	33 (16%)	0	0
4	D	206/209 (99%)	131 (64%)	54 (26%)	21 (10%)	0	3
5	E	149/162 (92%)	124 (83%)	15 (10%)	10 (7%)	1	9
6	F	99/101 (98%)	73 (74%)	19 (19%)	7 (7%)	1	8
7	G	153/156 (98%)	100 (65%)	35 (23%)	18 (12%)	0	2
8	H	136/138 (99%)	107 (79%)	19 (14%)	10 (7%)	1	7
9	I	125/128 (98%)	78 (62%)	34 (27%)	13 (10%)	0	3
10	J	97/105 (92%)	53 (55%)	29 (30%)	15 (16%)	0	1
11	K	117/129 (91%)	85 (73%)	18 (15%)	14 (12%)	0	2
12	L	123/135 (91%)	92 (75%)	16 (13%)	15 (12%)	0	2
13	M	123/126 (98%)	89 (72%)	21 (17%)	13 (11%)	0	2
14	N	58/61 (95%)	33 (57%)	19 (33%)	6 (10%)	0	3
15	O	86/89 (97%)	60 (70%)	23 (27%)	3 (4%)	3	24
16	P	82/88 (93%)	62 (76%)	16 (20%)	4 (5%)	2	17
17	Q	102/105 (97%)	82 (80%)	10 (10%)	10 (10%)	0	3
18	R	71/88 (81%)	49 (69%)	15 (21%)	7 (10%)	0	3
19	S	79/93 (85%)	50 (63%)	15 (19%)	14 (18%)	0	0
20	T	97/106 (92%)	67 (69%)	19 (20%)	11 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	V	23/27 (85%)	18 (78%)	2 (9%)	3 (13%)	0 1
All	All	2364/2541 (93%)	1621 (69%)	492 (21%)	251 (11%)	0 2

5 of 251 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	17	PHE
2	B	23	ARG
2	B	95	GLN
2	B	98	LEU

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
2	B	202/220 (92%)	182 (90%)	20 (10%)	8 30
3	C	160/188 (85%)	151 (94%)	9 (6%)	21 57
4	D	180/181 (99%)	165 (92%)	15 (8%)	11 40
5	E	115/123 (94%)	98 (85%)	17 (15%)	3 14
6	F	90/90 (100%)	84 (93%)	6 (7%)	16 50
7	G	126/127 (99%)	115 (91%)	11 (9%)	10 37
8	H	119/119 (100%)	104 (87%)	15 (13%)	4 21
9	I	98/99 (99%)	94 (96%)	4 (4%)	30 66
10	J	87/92 (95%)	80 (92%)	7 (8%)	12 42
11	K	90/99 (91%)	85 (94%)	5 (6%)	21 57
12	L	104/111 (94%)	96 (92%)	8 (8%)	13 44
13	M	100/101 (99%)	90 (90%)	10 (10%)	7 30
14	N	49/50 (98%)	44 (90%)	5 (10%)	7 29
15	O	79/80 (99%)	74 (94%)	5 (6%)	18 52
16	P	72/74 (97%)	68 (94%)	4 (6%)	21 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	96/97 (99%)	90 (94%)	6 (6%)	18	52
18	R	64/77 (83%)	60 (94%)	4 (6%)	18	52
19	S	71/80 (89%)	69 (97%)	2 (3%)	43	74
20	T	76/82 (93%)	68 (90%)	8 (10%)	7	28
21	V	19/22 (86%)	19 (100%)	0	100	100
All	All	1997/2112 (95%)	1836 (92%)	161 (8%)	11	42

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

Mol	Chain	Res	Type
12	L	99	HIS
17	Q	38	ARG
13	M	44	ARG
14	N	27	CYS
18	R	87	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	106	GLN
12	L	49	ASN
19	S	23	ASN
8	H	78	GLN
10	J	84	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1472/1523 (96%)	218 (14%)	66 (4%)
22	X	3/4 (75%)	1 (33%)	0
23	Y	7/18 (38%)	4 (57%)	0
All	All	1482/1545 (95%)	223 (15%)	66 (4%)

5 of 223 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G

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Mol	Chain	Res	Type
1	A	32	A
1	A	39	G
1	A	47	C

5 of 66 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1347	G
1	A	1452	C
1	A	1528	U
1	A	484	G
1	A	442	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 81 ligands modelled in this entry, 80 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	3001	-	44,45,45	1.40	7 (15%)	63,67,67	1.20	7 (11%)

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	3001	-	-	1/18/94/94	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	3001	PAR	C52-C42	3.56	1.59	1.52
24	A	3001	PAR	O54-C14	2.80	1.49	1.41
24	A	3001	PAR	C11-C21	2.77	1.57	1.52
24	A	3001	PAR	C31-C21	2.59	1.56	1.53
24	A	3001	PAR	O51-C11	2.20	1.47	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	3001	PAR	O33-C14-C24	3.52	113.84	108.08
24	A	3001	PAR	O54-C54-C64	3.41	112.62	106.07
24	A	3001	PAR	C14-O54-C54	3.10	119.78	113.72
24	A	3001	PAR	O11-C11-C21	2.99	112.97	108.08
24	A	3001	PAR	O52-C13-O43	-2.64	108.67	111.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

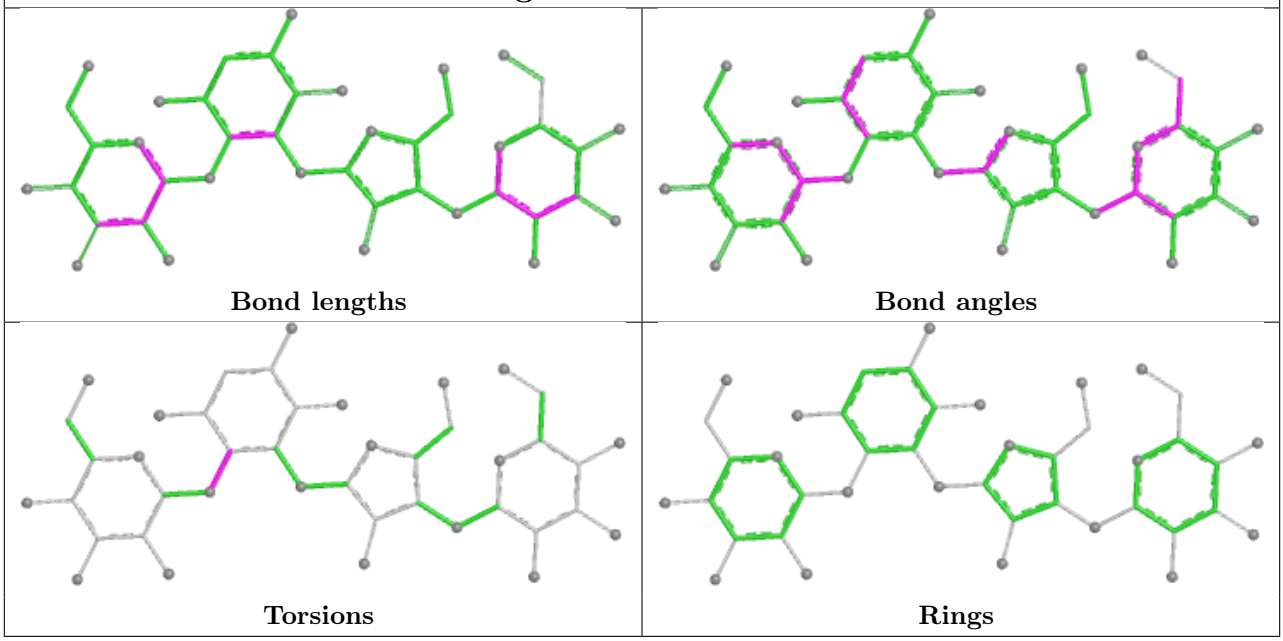
Mol	Chain	Res	Type	Atoms
24	A	3001	PAR	C52-C42-O11-C11

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PAR A 3001



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, 95th 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	1484/1523 (97%)	0.78	108 (7%)	15	9	40, 86, 171, 201	0
2	B	235/256 (91%)	0.20	14 (5%)	21	12	50, 117, 152, 155	0
3	C	207/239 (86%)	0.45	23 (11%)	5	3	61, 123, 153, 155	0
4	D	208/209 (99%)	0.13	10 (4%)	30	18	57, 101, 143, 155	0
5	E	151/162 (93%)	-0.19	0	100	100	43, 76, 119, 149	0
6	F	101/101 (100%)	0.33	3 (2%)	50	34	64, 116, 146, 151	0
7	G	155/156 (99%)	0.26	6 (3%)	39	25	63, 121, 153, 155	0
8	H	138/138 (100%)	-0.20	0	100	100	39, 67, 111, 132	0
9	I	127/128 (99%)	0.36	8 (6%)	20	11	54, 123, 155, 155	0
10	J	99/105 (94%)	0.95	14 (14%)	2	2	70, 139, 155, 155	0
11	K	119/129 (92%)	0.09	3 (2%)	57	43	44, 89, 134, 148	0
12	L	125/135 (92%)	0.15	2 (1%)	72	59	38, 96, 137, 155	0
13	M	125/126 (99%)	0.59	12 (9%)	8	4	68, 108, 144, 155	0
14	N	60/61 (98%)	0.29	3 (5%)	28	16	74, 116, 145, 155	0
15	O	88/89 (98%)	-0.03	1 (1%)	80	69	49, 88, 136, 145	0
16	P	84/88 (95%)	0.05	1 (1%)	79	67	46, 75, 109, 154	0
17	Q	104/105 (99%)	0.02	3 (2%)	51	36	47, 76, 132, 155	0
18	R	73/88 (82%)	0.10	4 (5%)	25	14	52, 95, 141, 155	0
19	S	81/93 (87%)	0.56	9 (11%)	5	3	95, 136, 154, 155	0
20	T	99/106 (93%)	0.29	6 (6%)	21	12	51, 84, 139, 155	0
21	V	25/27 (92%)	0.57	1 (4%)	38	25	63, 89, 132, 152	0
22	X	4/4 (100%)	0.48	0	100	100	102, 111, 115, 128	0
23	Y	8/18 (44%)	1.16	1 (12%)	3	2	104, 144, 155, 155	0
All	All	3900/4086 (95%)	0.44	232 (5%)	22	13	38, 96, 154, 201	0

The worst 5 of 232 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	125	ARG	8.6
1	A	1447	G	7.9
4	D	25	ARG	7.9
1	A	1166	G	6.9
1	A	1452	C	6.8

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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
25	MG	G	3002	1/1	0.06	1.42	84,84,84,84	1
25	MG	G	3023	1/1	0.37	1.17	84,84,84,84	0
25	MG	G	3061	1/1	0.43	0.66	84,84,84,84	0
25	MG	G	3004	1/1	0.44	0.49	84,84,84,84	0
25	MG	G	3050	1/1	0.46	0.84	84,84,84,84	0
25	MG	G	3030	1/1	0.46	0.81	84,84,84,84	0
25	MG	G	3059	1/1	0.56	0.38	84,84,84,84	0
25	MG	G	3048	1/1	0.63	0.64	84,84,84,84	0
25	MG	G	3064	1/1	0.63	0.45	84,84,84,84	0
25	MG	G	3067	1/1	0.64	0.73	84,84,84,84	0
25	MG	G	3049	1/1	0.67	1.02	84,84,84,84	0
25	MG	G	3069	1/1	0.67	0.27	84,84,84,84	0
25	MG	G	3071	1/1	0.67	0.35	84,84,84,84	0
26	K	G	3077	1/1	0.69	0.87	84,84,84,84	1
26	K	G	3078	1/1	0.69	0.29	84,84,84,84	1
25	MG	G	3018	1/1	0.70	0.71	84,84,84,84	0
25	MG	G	3036	1/1	0.71	0.76	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	G	3046	1/1	0.72	0.24	84,84,84,84	0
25	MG	G	3042	1/1	0.73	1.27	84,84,84,84	0
25	MG	G	3057	1/1	0.73	1.29	84,84,84,84	0
26	K	G	3075	1/1	0.74	0.54	84,84,84,84	1
25	MG	G	3040	1/1	0.75	0.98	84,84,84,84	0
25	MG	G	3007	1/1	0.75	1.19	84,84,84,84	0
25	MG	G	3035	1/1	0.76	0.50	84,84,84,84	0
25	MG	G	3054	1/1	0.76	0.43	84,84,84,84	0
25	MG	G	3037	1/1	0.77	0.54	84,84,84,84	0
25	MG	G	3005	1/1	0.78	1.02	84,84,84,84	0
25	MG	G	3047	1/1	0.78	0.75	84,84,84,84	0
25	MG	G	3017	1/1	0.79	0.45	84,84,84,84	0
25	MG	G	3058	1/1	0.80	0.60	84,84,84,84	0
25	MG	G	3010	1/1	0.80	1.13	84,84,84,84	0
25	MG	G	3070	1/1	0.83	0.28	84,84,84,84	0
25	MG	G	3041	1/1	0.83	0.57	84,84,84,84	0
25	MG	G	3060	1/1	0.83	0.52	84,84,84,84	0
25	MG	G	3068	1/1	0.83	0.69	84,84,84,84	0
25	MG	G	3034	1/1	0.83	0.47	84,84,84,84	0
25	MG	G	3066	1/1	0.84	0.64	84,84,84,84	0
25	MG	G	3033	1/1	0.84	1.15	84,84,84,84	0
25	MG	G	3020	1/1	0.84	0.74	84,84,84,84	0
25	MG	G	3044	1/1	0.85	1.05	84,84,84,84	0
25	MG	G	3031	1/1	0.85	0.28	84,84,84,84	0
26	K	G	3074	1/1	0.85	0.44	84,84,84,84	1
25	MG	G	3014	1/1	0.85	1.18	84,84,84,84	0
25	MG	G	3006	1/1	0.85	0.71	84,84,84,84	0
25	MG	G	3062	1/1	0.85	0.70	84,84,84,84	0
26	K	G	3072	1/1	0.86	0.24	84,84,84,84	0
25	MG	G	3063	1/1	0.86	0.72	84,84,84,84	0
25	MG	G	3003	1/1	0.86	0.59	84,84,84,84	0
25	MG	G	3053	1/1	0.86	0.83	84,84,84,84	0
25	MG	G	3013	1/1	0.86	0.77	84,84,84,84	0
25	MG	G	3026	1/1	0.87	1.15	84,84,84,84	0
25	MG	G	3027	1/1	0.87	0.51	84,84,84,84	0
25	MG	G	3043	1/1	0.87	0.86	84,84,84,84	0
26	K	G	3076	1/1	0.88	0.13	84,84,84,84	0
26	K	G	3079	1/1	0.88	0.20	84,84,84,84	1
25	MG	G	3052	1/1	0.89	0.67	84,84,84,84	0
25	MG	G	3045	1/1	0.89	0.62	84,84,84,84	0
24	PAR	A	3001	42/42	0.89	0.28	84,84,84,84	0
25	MG	G	3028	1/1	0.89	0.97	84,84,84,84	0

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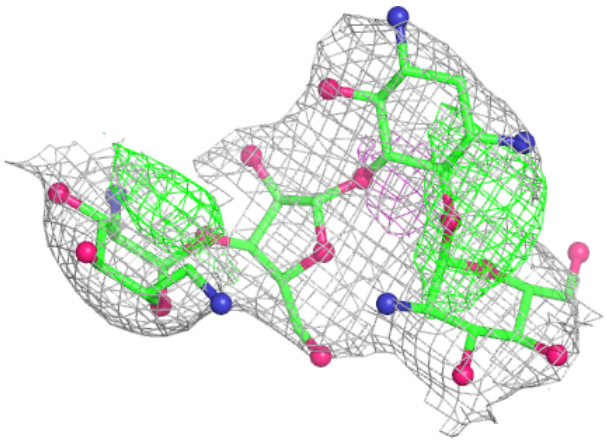
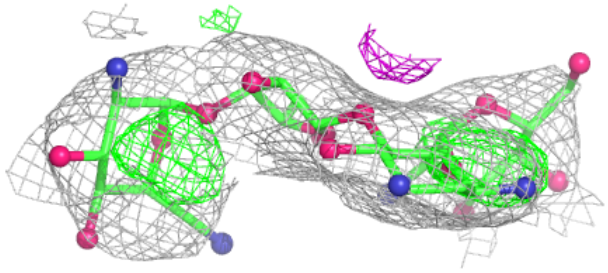
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	G	3056	1/1	0.90	0.64	84,84,84,84	0
25	MG	G	3025	1/1	0.90	0.65	84,84,84,84	0
25	MG	G	3024	1/1	0.91	0.73	84,84,84,84	0
25	MG	G	3029	1/1	0.91	1.17	84,84,84,84	0
25	MG	G	3009	1/1	0.91	0.15	84,84,84,84	0
25	MG	G	3065	1/1	0.92	0.13	84,84,84,84	0
25	MG	G	3015	1/1	0.92	0.61	84,84,84,84	0
25	MG	G	3016	1/1	0.93	0.69	84,84,84,84	0
26	K	G	3073	1/1	0.93	0.42	84,84,84,84	1
25	MG	G	3019	1/1	0.94	1.09	84,84,84,84	0
25	MG	G	3008	1/1	0.94	0.08	84,84,84,84	0
25	MG	G	3012	1/1	0.94	0.70	84,84,84,84	0
25	MG	G	3055	1/1	0.94	0.36	84,84,84,84	0
25	MG	G	3021	1/1	0.95	0.28	84,84,84,84	0
25	MG	G	3011	1/1	0.95	0.36	84,84,84,84	0
25	MG	G	3039	1/1	0.96	0.70	84,84,84,84	0
25	MG	G	3038	1/1	0.96	0.13	84,84,84,84	0
27	ZN	G	3080	1/1	0.96	0.26	84,84,84,84	1
25	MG	G	3051	1/1	0.97	0.63	84,84,84,84	0
25	MG	G	3022	1/1	0.98	0.39	84,84,84,84	0
25	MG	G	3032	1/1	0.98	1.23	84,84,84,84	0
27	ZN	G	3081	1/1	0.98	0.18	84,84,84,84	0

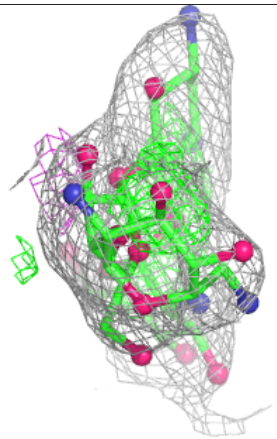
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR A 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.