



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:36 AM GMT

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 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/ValidationPDFNotes.html>

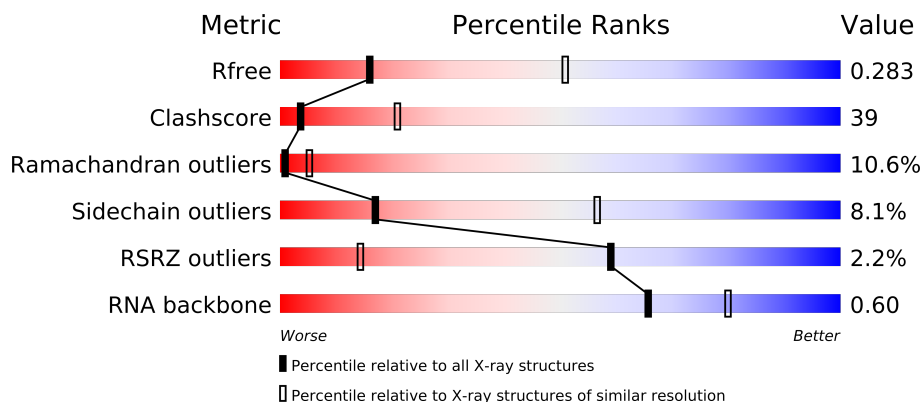
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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.




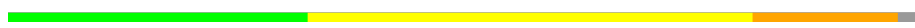


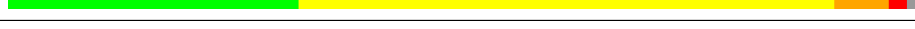

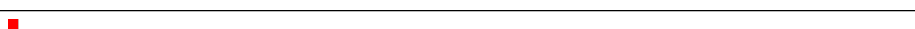
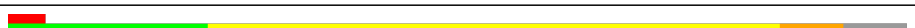



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1523	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	X	4	
23	Y	18	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 51470 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1484	Total	C	N	O	P	0	0	0
			31853	14194	5901	10286	1472			

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

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

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
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

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

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
18	R	73	Total	C	N	O		0	0	0
			597	380	118	99				

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

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
21	V	25	Total	C	N	O	0	0	1
			209	128	51	30			

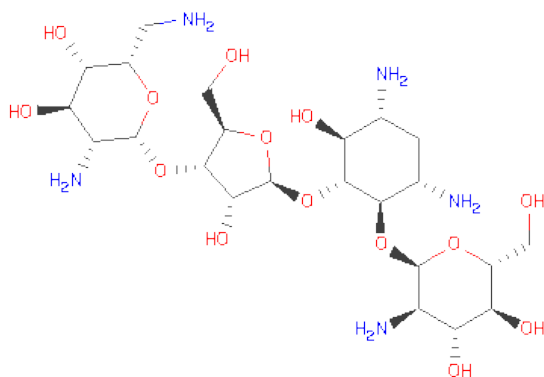
- Molecule 22 is a RNA chain called ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON CCCG.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	8	Total	C	N	O	P	0	0	0
			168	75	28	57	8			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

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

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

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

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

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

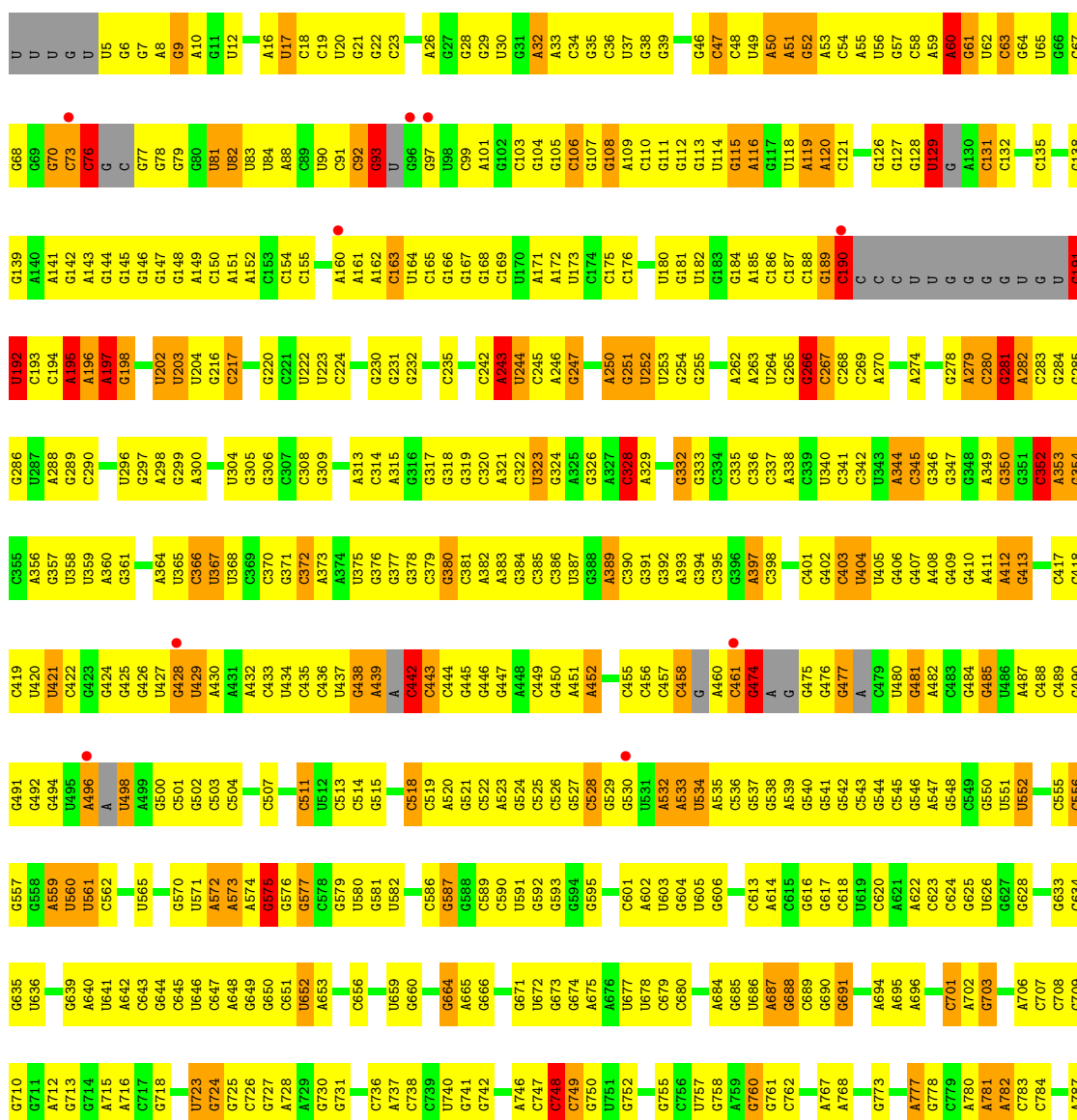
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	G	2	Total	Zn	0	0
			2	2		

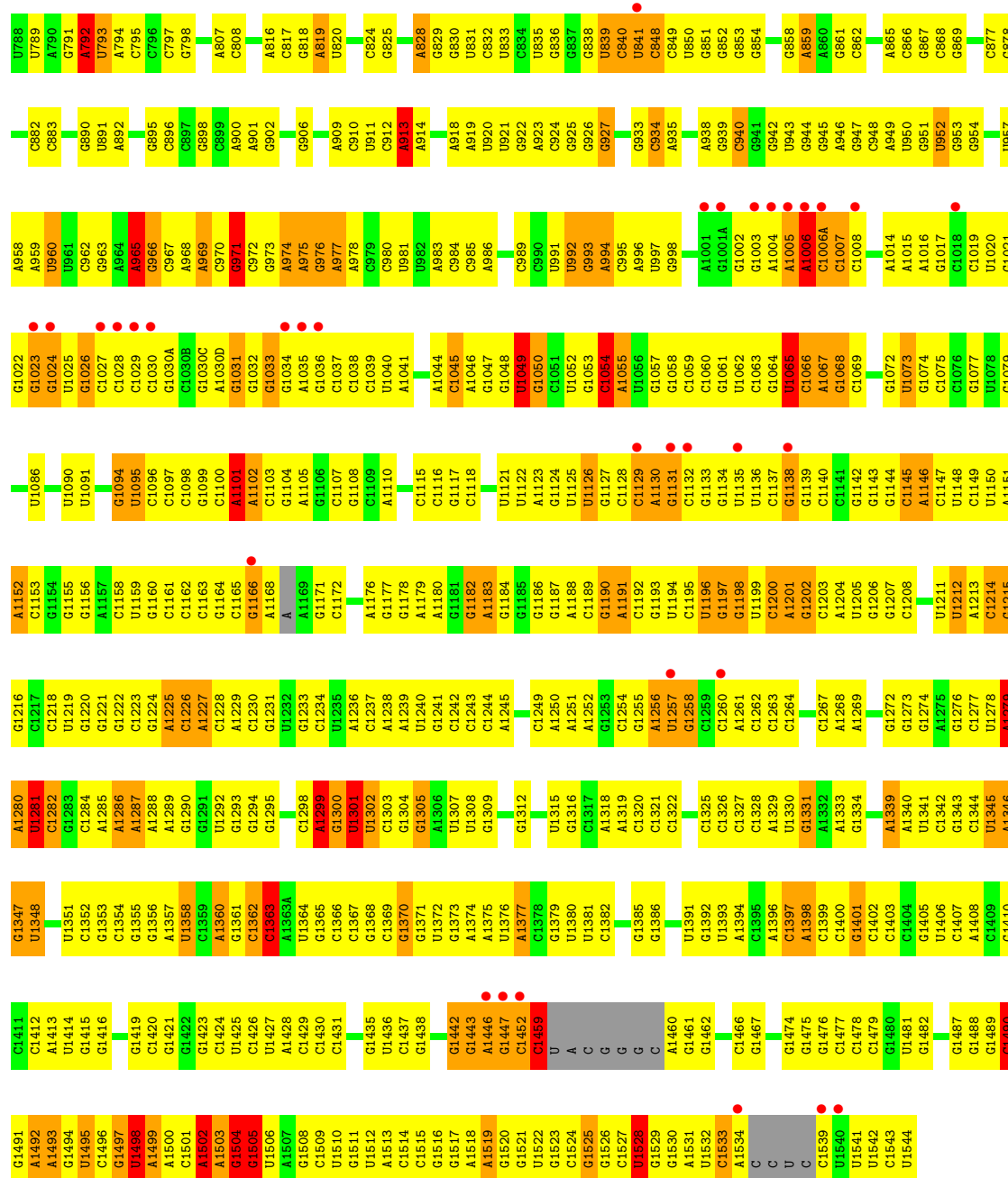
3 Residue-property plots

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

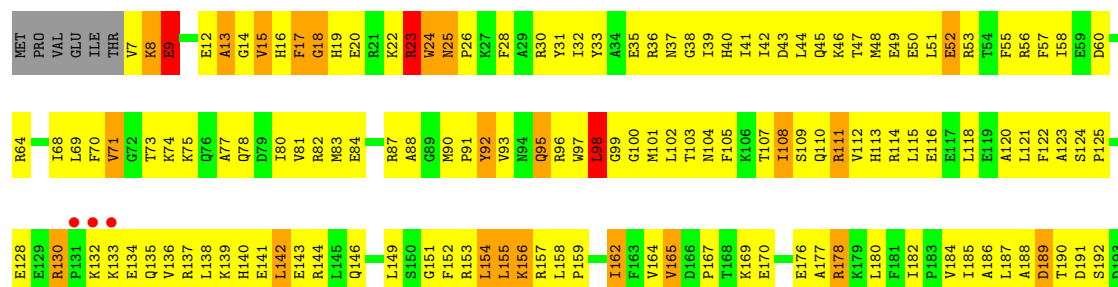
Chain A: 





• Molecule 2: RIBOSOMAL PROTEIN S2

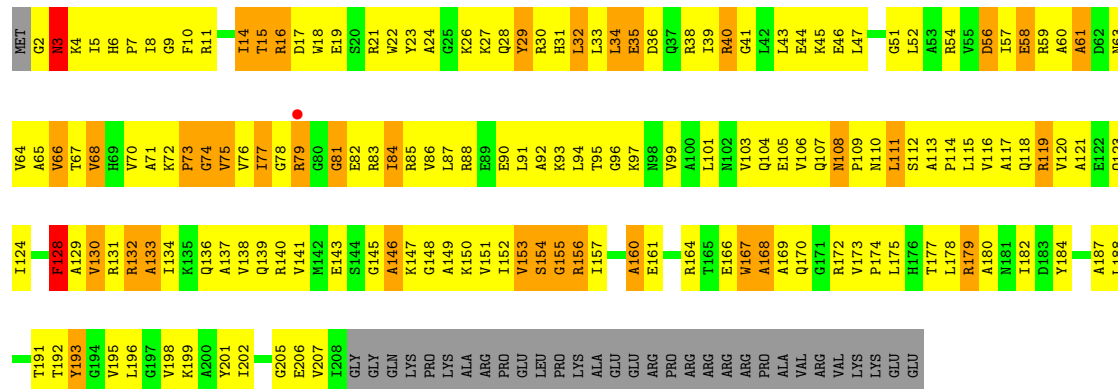
Chain B:





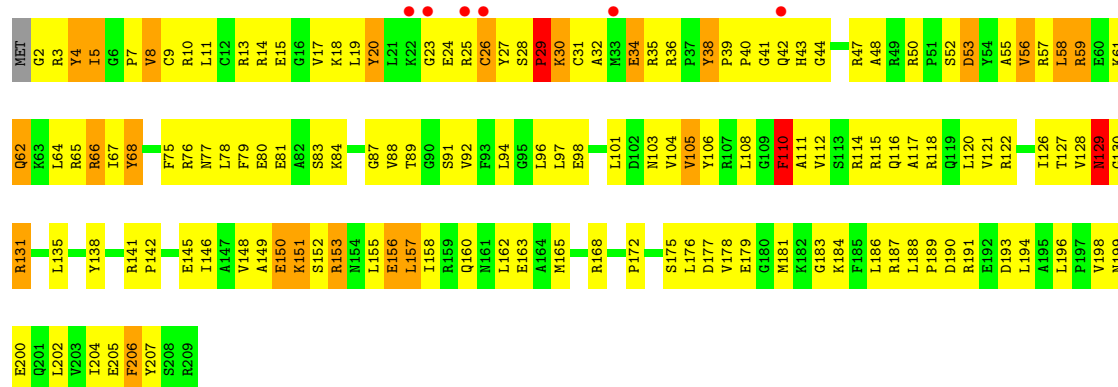
• Molecule 3: RIBOSOMAL PROTEIN S3

Chain C:



• Molecule 4: RIBOSOMAL PROTEIN S4

Chain D:



• Molecule 5: RIBOSOMAL PROTEIN S5

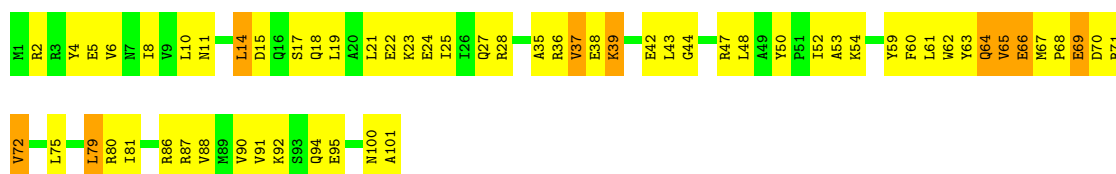
Chain E:



• Molecule 6: RIBOSOMAL PROTEIN S6

Chain F:





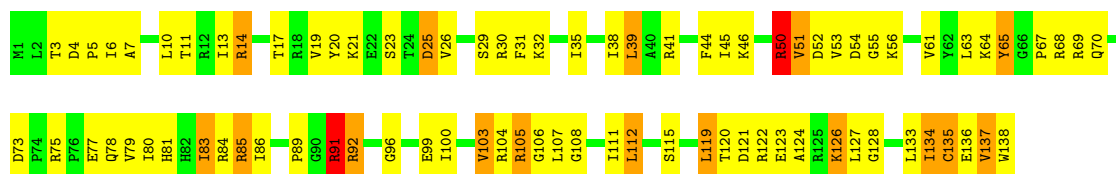
• Molecule 7: RIBOSOMAL PROTEIN S7

Chain G:



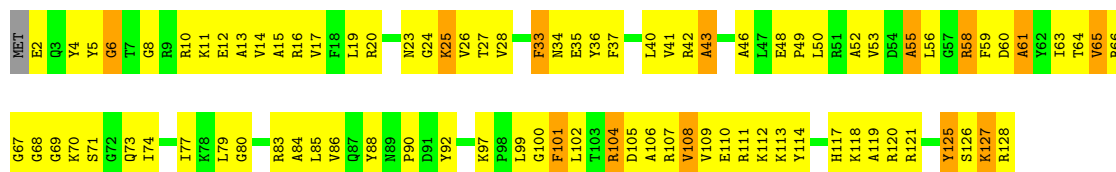
• Molecule 8: RIBOSOMAL PROTEIN S8

Chain H:



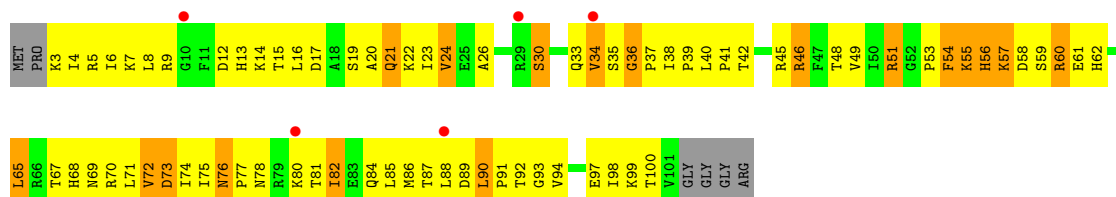
• Molecule 9: RIBOSOMAL PROTEIN S9

Chain I:



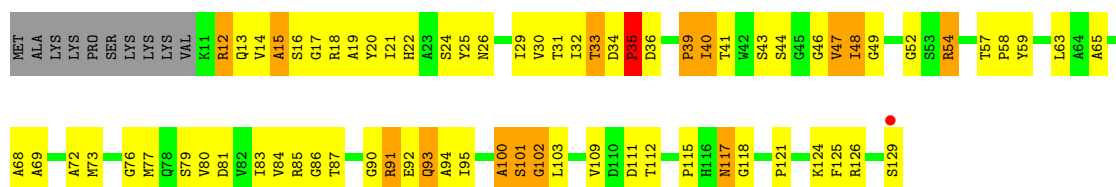
• Molecule 10: RIBOSOMAL PROTEIN S10

Chain J:



• Molecule 11: RIBOSOMAL PROTEIN S11

Chain K:



• Molecule 12: RIBOSOMAL PROTEIN S12

Chain L:



• Molecule 13: RIBOSOMAL PROTEIN S13

Chain M:



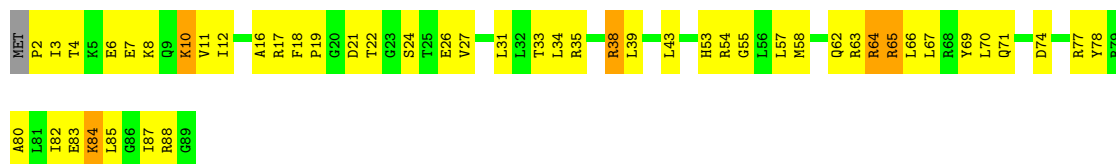
• Molecule 14: RIBOSOMAL PROTEIN S14

Chain N:



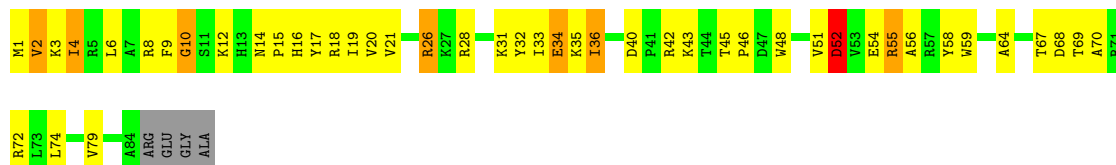
• Molecule 15: RIBOSOMAL PROTEIN S15

Chain O:



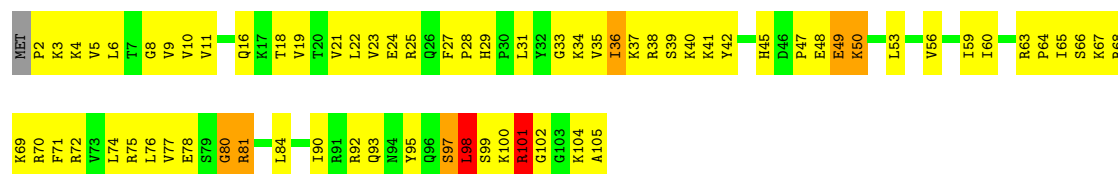
• Molecule 16: RIBOSOMAL PROTEIN S16

Chain P:



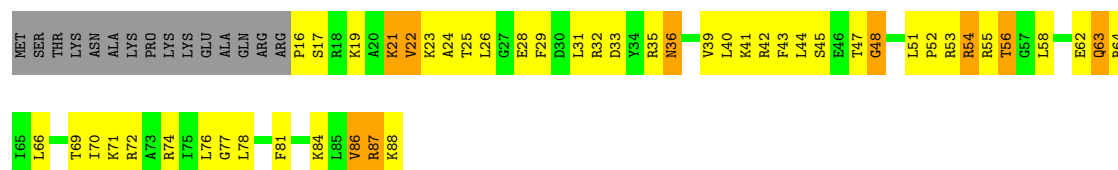
- Molecule 17: RIBOSOMAL PROTEIN S17

Chain Q:



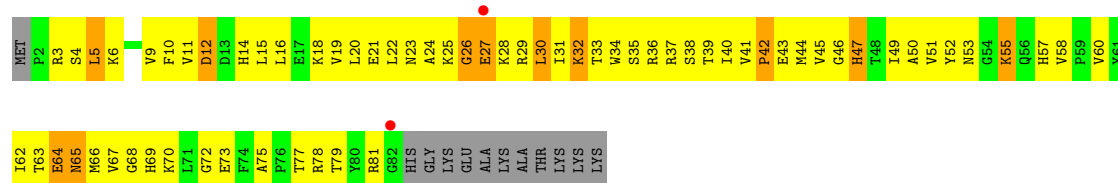
- Molecule 18: RIBOSOMAL PROTEIN S18

Chain R:



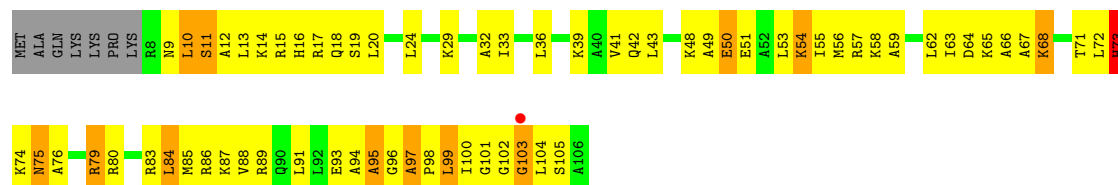
- Molecule 19: RIBOSOMAL PROTEIN S19

Chain S:



- Molecule 20: RIBOSOMAL PROTEIN S20

Chain T:



- Molecule 21: RIBOSOMAL PROTEIN THX

Chain V:



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

Chain X:



- Molecule 23: A-SITE MESSENGER RNA FRAGMENT CGGG

Chain Y: 

G	G	G	G	A	U	U33	C34	C35	C36	G37	A38	A39	U40	C	C	C

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.282 0.242 , 0.283	Depositor DCC
R_{free} test set	11550 reflections (5.31%)	DCC
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 , 75.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 339725 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	51470	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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, ZN, PAR, 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	0.62	17/35646 (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	0.79	1/186 (0.5%)	0.84	0/285
All	All	0.55	19/55474 (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 19 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
23	Y	33	U	OP3-P	-7.15	1.52	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	31853	0	16122	1390	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	168	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	51470	0	36510	3378	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

The worst 5 of 3378 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(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

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	
2	B	233/256 (91%)	149 (64%)	60 (26%)	24 (10%)	1	6
3	C	205/239 (86%)	119 (58%)	53 (26%)	33 (16%)	0	1
4	D	206/209 (99%)	131 (64%)	54 (26%)	21 (10%)	1	6
5	E	149/162 (92%)	124 (83%)	15 (10%)	10 (7%)	2	16
6	F	99/101 (98%)	73 (74%)	19 (19%)	7 (7%)	2	13
7	G	153/156 (98%)	100 (65%)	35 (23%)	18 (12%)	1	4
8	H	136/138 (99%)	107 (79%)	19 (14%)	10 (7%)	2	12
9	I	125/128 (98%)	78 (62%)	34 (27%)	13 (10%)	1	5
10	J	97/105 (92%)	53 (55%)	29 (30%)	15 (16%)	0	1
11	K	117/129 (91%)	85 (73%)	18 (15%)	14 (12%)	1	4
12	L	123/135 (91%)	92 (75%)	16 (13%)	15 (12%)	1	3
13	M	123/126 (98%)	89 (72%)	21 (17%)	13 (11%)	1	5
14	N	58/61 (95%)	33 (57%)	19 (33%)	6 (10%)	1	6
15	O	86/89 (97%)	60 (70%)	23 (27%)	3 (4%)	6	37
16	P	82/88 (93%)	62 (76%)	16 (20%)	4 (5%)	3	26
17	Q	102/105 (97%)	82 (80%)	10 (10%)	10 (10%)	1	7
18	R	71/88 (81%)	49 (69%)	15 (21%)	7 (10%)	1	7
19	S	79/93 (85%)	50 (63%)	15 (19%)	14 (18%)	0	1
20	T	97/106 (92%)	67 (69%)	19 (20%)	11 (11%)	1	4
21	V	23/27 (85%)	18 (78%)	2 (9%)	3 (13%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2364/2541 (93%)	1621 (69%)	492 (21%)	251 (11%)	1 5

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 ⓘ

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%)	11 42
3	C	160/188 (85%)	151 (94%)	9 (6%)	30 75
4	D	180/181 (99%)	165 (92%)	15 (8%)	16 55
5	E	115/123 (94%)	98 (85%)	17 (15%)	4 20
6	F	90/90 (100%)	84 (93%)	6 (7%)	23 66
7	G	126/127 (99%)	115 (91%)	11 (9%)	15 51
8	H	119/119 (100%)	104 (87%)	15 (13%)	7 30
9	I	98/99 (99%)	94 (96%)	4 (4%)	41 82
10	J	87/92 (95%)	80 (92%)	7 (8%)	17 57
11	K	90/99 (91%)	85 (94%)	5 (6%)	30 75
12	L	104/111 (94%)	96 (92%)	8 (8%)	18 59
13	M	100/101 (99%)	90 (90%)	10 (10%)	11 41
14	N	49/50 (98%)	44 (90%)	5 (10%)	11 40
15	O	79/80 (99%)	74 (94%)	5 (6%)	25 69
16	P	72/74 (97%)	68 (94%)	4 (6%)	30 75
17	Q	96/97 (99%)	90 (94%)	6 (6%)	25 69
18	R	64/77 (83%)	60 (94%)	4 (6%)	25 69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	S	71/80 (89%)	69 (97%)	2 (3%)	56 89
20	T	76/82 (93%)	68 (90%)	8 (10%)	10 39
21	V	19/22 (86%)	19 (100%)	0	100 100
All	All	1997/2112 (95%)	1836 (92%)	161 (8%)	17 56

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

Mol	Chain	Res	Type
7	G	97	GLN
8	H	92	ARG
18	R	54	ARG
7	G	113	GLU
8	H	26	VAL

Some 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	37	ASN
9	I	23	ASN
19	S	23	ASN
7	G	68	ASN
7	G	97	GLN

5.3.3 RNA ⓘ

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
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	701	C
1	A	1006	A
1	A	1490	C
1	A	748	C
1	A	965	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	45,45,45	1.76	8 (17%)	67,67,67	1.32	8 (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	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	3001	PAR	C22-C32	5.49	1.56	1.52
24	A	3001	PAR	C22-C12	4.72	1.55	1.52
24	A	3001	PAR	C52-C42	3.67	1.59	1.52
24	A	3001	PAR	O54-C14	2.81	1.49	1.41
24	A	3001	PAR	C11-C21	2.75	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	3001	PAR	O54-C54-C64	4.59	112.62	106.97
24	A	3001	PAR	O52-C13-C23	3.73	114.16	107.50
24	A	3001	PAR	C14-O54-C54	3.11	119.78	113.73
24	A	3001	PAR	O52-C13-O43	-2.97	108.67	111.51
24	A	3001	PAR	O33-C14-C24	2.91	113.84	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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%)	0.21	42 (2%)	50	11	40, 86, 171, 201	0
2	B	235/256 (91%)	-0.01	3 (1%)	74	24	50, 117, 152, 155	0
3	C	207/239 (86%)	0.04	1 (0%)	88	46	61, 123, 153, 155	0
4	D	208/209 (99%)	0.02	6 (2%)	49	10	57, 101, 143, 155	0
5	E	151/162 (93%)	-0.22	0	100	100	43, 76, 119, 149	0
6	F	101/101 (100%)	0.01	0	100	100	64, 116, 146, 151	0
7	G	155/156 (99%)	0.07	1 (0%)	86	41	63, 121, 153, 155	0
8	H	138/138 (100%)	-0.23	0	100	100	39, 67, 111, 132	0
9	I	127/128 (99%)	0.14	0	100	100	54, 123, 155, 155	0
10	J	99/105 (94%)	0.39	5 (5%)	27	5	70, 139, 155, 155	0
11	K	119/129 (92%)	-0.07	1 (0%)	83	35	44, 89, 134, 148	0
12	L	125/135 (92%)	-0.02	0	100	100	38, 96, 137, 155	0
13	M	125/126 (99%)	0.36	7 (5%)	24	5	68, 108, 144, 155	0
14	N	60/61 (98%)	0.13	0	100	100	74, 116, 145, 155	0
15	O	88/89 (98%)	-0.15	0	100	100	49, 88, 136, 145	0
16	P	84/88 (95%)	-0.10	0	100	100	46, 75, 109, 154	0
17	Q	104/105 (99%)	-0.11	0	100	100	47, 76, 132, 155	0
18	R	73/88 (82%)	-0.05	0	100	100	52, 95, 141, 155	0
19	S	81/93 (87%)	0.15	2 (2%)	54	12	95, 136, 154, 155	0
20	T	99/106 (93%)	0.02	1 (1%)	79	29	51, 84, 139, 155	0
21	V	25/27 (92%)	0.23	1 (4%)	36	7	63, 89, 132, 152	0
22	X	4/4 (100%)	0.15	0	100	100	102, 111, 115, 128	0
23	Y	8/18 (44%)	0.93	2 (25%)	1	1	104, 144, 155, 155	0
All	All	3900/4086 (95%)	0.09	72 (1%)	59	18	38, 96, 154, 201	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	125	ARG	7.8
1	A	1534	A	6.2
1	A	1452	C	6.1
13	M	122	LYS	5.8
13	M	124	PRO	5.8

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	G	3008	1/1	0.07	-	84,84,84,84	0
25	MG	G	3058	1/1	0.53	-	84,84,84,84	0
25	MG	G	3011	1/1	0.31	-	84,84,84,84	0
25	MG	G	3004	1/1	0.52	-	84,84,84,84	0
25	MG	G	3061	1/1	0.67	-	84,84,84,84	0
25	MG	G	3068	1/1	0.65	-	84,84,84,84	0
25	MG	G	3021	1/1	0.31	-	84,84,84,84	0
25	MG	G	3060	1/1	0.51	-	84,84,84,84	0
25	MG	G	3044	1/1	1.01	-	84,84,84,84	0
25	MG	G	3045	1/1	0.67	-	84,84,84,84	0
26	K	G	3078	1/1	0.25	-	84,84,84,84	1
25	MG	G	3022	1/1	0.56	-	84,84,84,84	0
25	MG	G	3065	1/1	0.11	-	84,84,84,84	0
25	MG	G	3035	1/1	0.52	-	84,84,84,84	0
25	MG	G	3054	1/1	0.42	-	84,84,84,84	0
25	MG	G	3046	1/1	0.25	-	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	G	3037	1/1	0.49	-	84,84,84,84	0
25	MG	G	3039	1/1	0.69	-	84,84,84,84	0
25	MG	G	3063	1/1	0.60	-	84,84,84,84	0
25	MG	G	3057	1/1	1.32	-	84,84,84,84	0
25	MG	G	3002	1/1	1.20	-	84,84,84,84	1
26	K	G	3076	1/1	0.11	-	84,84,84,84	0
25	MG	G	3038	1/1	0.13	-	84,84,84,84	0
25	MG	G	3010	1/1	1.11	-	84,84,84,84	0
25	MG	G	3015	1/1	0.58	-	84,84,84,84	0
25	MG	G	3056	1/1	0.68	-	84,84,84,84	0
25	MG	G	3019	1/1	1.05	-	84,84,84,84	0
25	MG	G	3009	1/1	0.15	-	84,84,84,84	0
25	MG	G	3013	1/1	0.76	-	84,84,84,84	0
25	MG	G	3028	1/1	0.95	-	84,84,84,84	0
25	MG	G	3005	1/1	1.01	-	84,84,84,84	0
25	MG	G	3055	1/1	0.36	-	84,84,84,84	0
25	MG	G	3069	1/1	0.31	-	84,84,84,84	0
26	K	G	3072	1/1	0.22	-	84,84,84,84	0
25	MG	G	3012	1/1	0.69	-	84,84,84,84	0
25	MG	G	3050	1/1	0.84	-	84,84,84,84	0
25	MG	G	3016	1/1	0.67	-	84,84,84,84	0
25	MG	G	3007	1/1	1.09	-	84,84,84,84	0
25	MG	G	3064	1/1	0.36	-	84,84,84,84	0
25	MG	G	3053	1/1	0.73	-	84,84,84,84	0
25	MG	G	3003	1/1	0.62	-	84,84,84,84	0
25	MG	G	3024	1/1	0.75	-	84,84,84,84	0
25	MG	G	3071	1/1	0.35	-	84,84,84,84	0
25	MG	G	3070	1/1	0.29	-	84,84,84,84	0
25	MG	G	3066	1/1	0.60	-	84,84,84,84	0
25	MG	G	3014	1/1	1.15	-	84,84,84,84	0
25	MG	G	3052	1/1	0.69	-	84,84,84,84	0
25	MG	G	3048	1/1	0.64	-	84,84,84,84	0
24	PAR	A	3001	42/42	0.26	-	84,84,84,84	0
25	MG	G	3049	1/1	1.02	-	84,84,84,84	0
25	MG	G	3017	1/1	0.47	-	84,84,84,84	0
25	MG	G	3029	1/1	1.16	-	84,84,84,84	0
26	K	G	3073	1/1	0.27	-	84,84,84,84	1
25	MG	G	3067	1/1	0.54	-	84,84,84,84	0
26	K	G	3074	1/1	0.33	-	84,84,84,84	1
25	MG	G	3034	1/1	0.47	-	84,84,84,84	0
25	MG	G	3051	1/1	0.56	-	84,84,84,84	0
25	MG	G	3018	1/1	0.71	-	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	G	3006	1/1	0.68	-	84,84,84,84	0
25	MG	G	3040	1/1	0.96	-	84,84,84,84	0
26	K	G	3077	1/1	0.72	-	84,84,84,84	1
25	MG	G	3059	1/1	0.39	-	84,84,84,84	0
26	K	G	3075	1/1	0.49	-	84,84,84,84	1
26	K	G	3079	1/1	0.13	-	84,84,84,84	1
25	MG	G	3025	1/1	0.66	-	84,84,84,84	0
25	MG	G	3020	1/1	0.74	-	84,84,84,84	0
25	MG	G	3041	1/1	0.53	-	84,84,84,84	0
25	MG	G	3062	1/1	0.58	-	84,84,84,84	0
25	MG	G	3036	1/1	0.65	-	84,84,84,84	0
25	MG	G	3031	1/1	0.25	-	84,84,84,84	0
25	MG	G	3026	1/1	1.11	-	84,84,84,84	0
25	MG	G	3030	1/1	0.78	-	84,84,84,84	0
27	ZN	G	3081	1/1	0.15	-	84,84,84,84	0
25	MG	G	3033	1/1	1.16	-	84,84,84,84	0
25	MG	G	3043	1/1	0.66	-	84,84,84,84	0
25	MG	G	3042	1/1	1.31	-	84,84,84,84	0
25	MG	G	3027	1/1	0.53	-	84,84,84,84	0
27	ZN	G	3080	1/1	0.25	-	84,84,84,84	1
25	MG	G	3047	1/1	0.71	-	84,84,84,84	0
25	MG	G	3023	1/1	1.14	-	84,84,84,84	0
25	MG	G	3032	1/1	1.19	-	84,84,84,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.