

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 07:09 AM EDT

PDB ID	:	4V8A
Title	:	The structure of thermorubin in complex with the 70S ribosome from Thermus
		thermophilus.
Authors	:	Bulkley, D.; Johnson, F.A.; Steitz, T.A.
Deposited on	:	2011-12-05
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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
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	AA	2915	36%	43%	15% • •			
1	BA	2915	3% 45%	34%	15% • •			
2	AB	122	27%	52%	16% · ·			
2	BB	122	49%	35%	13% ••			



Mol	Chain	Length	Quality of chain			
3	AD	276	64%	28%	7%	
3	BD	276	% 6 4%	29%	6%	
4	AE	206	48%	43%	8% •	
4	BE	206	60%	29%	10% •	
5	AF	205	.% 5 6%	36%	7% •	
5	BF	205	60%	32%	6% •	
6	AG	182	29% 47%	45%	7% •	
6	BG	182	4%	46%	5% ••	
7	AH	180	21%	47%	6% ·	
7	BH	180	61%	33%	•••	
8	AI	148	43%	40%	14% ••	
8	BI	148	.% 51%	30%	16% ••	
9	AN	140	.% 44%	44%	11% •	
9	BN	140	54%	40%	6% •	
10	AO	122	60%	37%	•	
10	BO	122	67%	30%	•	
11	AP	150	3% 60%	31%	7% •	
11	BP	150	64%	27%	7% •	
12	AQ	141	% 55%	36%	9%	
12	BQ	141	56%	33%	11%	
13	AR	118	50%	38%	12%	
13	BR	118	57%	32%	11%	
14	AS	112	45%	43%	11% •	
14	BS	112	44%	46%	9% •	
15	AT	146	% 47%	38%	5% 10%	



Mol	Chain	Length	Quality of chain				
15	BT	146	.% 	55%	3.	2%	• 10%
16	AU	118		62%		34%	••
16	BU	118		70%		22%	6% •
17	AV	101	.% 	61%		31%	7% •
17	BV	101		67%		27%	5%•
18	AW	113		60%		34%	5%•
18	BW	113		70%		24%	5%•
19	AX	96		70%		26%	••
19	BX	96		64%		30%	5%•
20	AY	110	6%	55%		37%	5%••
20	BY	110	.% •	65%		28%	
21	AZ	206	3%	55%		36%	•••
21	BZ	206		62%		28%	6% •
22	A0	85	2%	55%	31	•	11%
22	B0	85		62%		22% •	11%
23	A1	98	2%	61%		31%	7% •
23	B1	98	.% 	63%		30%	6% •
24	A2	72	.% 	54%		36%	7% •
24	B2	72		60%		32%	6% •
25	A3	60	8%	55%		35%	8% •
25	B3	60		75%		20%	•••
26	A4	71	28%	27%	10%	35%	
26	B4	71	32%	23%	8% •	35%	
27	A5	60		53%	35	5%	10% •
27	B5	60		67%		23%	7% ••



Chain Length Quality of chain Mol 6% 28A65444% 43% 9% . . 28B654• 50% 39% 9% 8% 29A749 . . 53% 43% 2% 29B74933% 57% 8% • • • 30 A86554% 42% 30 B86566% 29% • • 12% CA31 152129% 53% 14% •• 12% DA • • 31 152131% 51% 14% 5% CB 3225638% 40% 11% 11% 12% DB 3225638% 42% 9% 11% 19% 33 CC23954% 28% 5% 14% 14% DC 33 23947% 33% 6% 14% 5% 34 CD 20948% 41% 9% • 5% DD 3420951% 40% 8% 2% CE 3516241% 42% 8% 9% • 3% 35DE 16244% 40% 6% • 9% 5% CF 36 101 57% 35% 7% • <u>3%</u> \mathbf{DF} 36 1017% •• 60% 31% 49% CG37 1568% •• 57% 33% 48% • •• DG 3715652% 42% 3% 38CH13857% 8% • 35% DH 3813852% 37% 10% • 39% CI 1283952% 38% 9% • 55% DI 1283953% 37% 8% • 41% CJ40 10528% 9% • 9% 54%



Mol	Chain		Qual	ity of chain	
			44%		
40	DJ	105	43%	38%	10% 9%
41	CK	129	56%	29%	• 12%
41	DK	129	51%	33%	• 12%
42	CL	132	53%	53% 31%	
42	DL	132	% • 53%	33%	6% 8%
43	СМ	126	40% 50%	32%	9% 10%
43	DM	126	43%	35%	12% • 10%
44	CN	61	25%	51%	15% •
44	DN	61	34%	34%	13% ••
45	CO	89	49%	39%	10% •
45	DO	89	<u>6%</u> 54%	36%	9% •
46	CP	88	47%	34%	13% 7%
46	DP	88	44%	45%	• 7%
47	CQ	105	2% 5 4%	35%	5% 6%
47	DQ	105	^{3%} 64%	25%	6% 6%
48	CR	88	51%	23% ••	23%
48	DR	88	^{3%} 53%	22% •	23%
49	CS	93	47%	34% 10%	• 16%
49	DS	93	56% 39%	42%	• 16%
50	CT	106	40%	42%	8% • 9%
50	DT	106	9%	34%	•• 9%
51	CU	27	44%	26%	7% 15%
51	DU	27	48%	30%	7% 15%

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
52	T8B	AA	3001	-	-	Х	-
52	T8B	BA	3001	-	-	Х	-



2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 279316 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1		2827	Total	С	Ν	Ο	Р	0	0	0
1	лл	2021	60900	27102	11403	19569	2826	0	0	U
1	ВΛ	2827	Total	С	Ν	Ο	Р	0	0	0
	DA	2021	60900	27102	11403	19569	2826		0	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	272A	G	U	CONFLICT	GB AP008226.1
BA	272A	G	U	CONFLICT	GB AP008226.1

• Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	AB	120	Total	С	Ν	0	Р	0	0	0
	nD	120	2574	1146	476	833	119	0	0	Ŭ
9	BB	120	Total	С	Ν	0	Р	0	0	0
		120	2574	1146	476	833	119	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	120	G	А	CONFLICT	GB AP008226.1
BB	120	G	А	CONFLICT	GB AP008226.1

• Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
3		275	Total	С	Ν	0	S	0	0	0
5	AD	215	2136	1349	423	361	3	0	0	0
2	ВD	275	Total	С	Ν	0	S	0	0	0
5		215	2136	1349	423	361	3	0	0	0



• Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	٨F	204	Total	С	Ν	0	S	0	0	0
4	AL	204	1555	982	297	270	6	0	0	0
4	DE	204	Total	С	Ν	0	S	0	0	0
4	DE	204	1555	982	297	270	6	0	0	0

• Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	٨F	202	Total	С	Ν	0	S	0	0	1
5	AF	203	1576	1005	297	272	2	0	0	
5	PE	202	Total	С	Ν	0	S	0	0	1
5	ЛС	203	1576	1005	297	272	2	0	U	

• Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	AC	181	Total	С	Ν	Ο	S	0	0	0
0	ЛО	101	1368	879	242	244	3	0	0	0
6	BC	181	Total	С	Ν	0	S	0	0	0
0	DG	101	1368	879	242	244	3	0		U

• Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	лн	174	Total	С	Ν	0	\mathbf{S}	0	0	0
1	АП	114	1317	837	243	236	1	0	0	0
7	рц	174	Total	С	Ν	0	S	0	0	0
		1/4	1317	837	243	236	1			U

• Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	ΔΤ	145	Total	С	Ν	0	S	0	0	0
0	AI	140	1046	674	180	191	1	0	0	0
0	BI	1.45	Total	С	Ν	0	S	0	0	0
0	DI	140	1046	674	180	191	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	110	GLU	ASP	CONFLICT	UNP Q5SLQ1



Chain	Residue	Modelled	Actual	Comment	Reference
BI	110	GLU	ASP	CONFLICT	UNP Q5SLQ1

• Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	AN	140	Total	С	Ν	0	S	0	0	0
9	AN	140	1112	717	207	184	4	0	0	0
0	DN	140	Total	С	Ν	0	S	0	0	0
9	DN	140	1112	717	207	184	4	0	0	0

• Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	AO	122	Total	С	N	0	S	0	0	0
			923	583	168	168	4	Ŭ		Ŭ
10	BO	199	Total	С	Ν	0	\mathbf{S}	0	0	0
10	DO	122	923	583	168	168	4	0	0	0

• Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
11		1.47	Total	С	Ν	0	S	0	0	0
	AI	141	1119	695	227	194	3	0	0	0
11	PD	1.47	Total	С	Ν	0	S	0	0	0
	DF	147	1119	695	227	194	3	0	0	0

• Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
19		1.41	Total	С	Ν	Ο	S	0	0	0
12	лų	141	1122	715	212	188	7	0	0	0
10	BO	1.41	Total	С	Ν	Ο	S	0	0	0
12	DQ	141	1122	715	212	188	7	0	0	0

• Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
12	٨B	118	Total	С	Ν	0	S	0	0	0
10	лц	110	968	604	203	160	1	0	0	0
12	PD	110	Total	С	Ν	0	S	0	0	0
10	DR	110	968	604	203	160	1			U



• Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
14	19	110	Total	С	Ν	Ο	0	0	0
14	AS	110	865	544	172	149	0	0	0
14	PC	110	Total	С	Ν	Ο	0	0	0
14	Do	110	865	544	172	149	0	0	0

• Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
15	۸T	121	Total	С	Ν	0	S	0	0	0
1.0	AI	101	1063	666	213	183	1	0	0	0
15	РТ	121	Total	С	Ν	0	S	0	0	0
1.5	DI	101	1063	666	213	183	1	0	0	0

• Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
16	AU	116	Total	С	Ν	Ο	S	0	0	0
10	110	110	959	608	201	149	1	0	0	0
16	BII	116	Total	С	Ν	0	\mathbf{S}	0	0	0
10	DU	110	959	608	201	149	1	0	0	0

• Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
17	AV	101	Total	С	Ν	0	S	0	0	0
11	ΛV	101	771	495	140	135	1	0	0	0
17	BV	101	Total	С	Ν	0	S	0	0	0
11	DV	101	771	495	140	135	1	0	0	0

• Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
18		119	Total	С	Ν	0	S	0	0	0
10	ΔΨ	112	881	554	172	153	2	0	0	0
10	BW	119	Total	С	Ν	0	\mathbf{S}	0	0	0
10	DW	112	881	554	172	153	2	0	0	U

• Molecule 19 is a protein called 50S ribosomal protein L23.



Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
10	٨v	05	Total	С	Ν	Ο	\mathbf{S}	0	0	0
19	ЛЛ	90	742	483	134	124	1	0	0	0
10	PV	05	Total	С	Ν	0	S	0	0	0
19	DA	90	742	483	134	124	1	0	0	0

• Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20		107	Total	С	Ν	0	S	0	0	0
20	AI	107	785	503	145	131	6	0	0	0
20	DV	107	Total	С	Ν	0	S	0	0	0
20	DI	107	785	503	145	131	6	0	0	0

• Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
21	AZ	198	Total 1522	C 972	N 269	O 279	${S \over 2}$	0	0	0
21	BZ	198	Total 1522	C 972	N 269	0 279	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0

• Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
	10	76	Total	С	Ν	0	S	0	0	0
	AU	70	594	368	125	100	1	0	0	0
	B0	76	Total	С	Ν	0	S	0	0	0
	D0	10	594	368	125	100	1			U

• Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
- 0.2	Δ.1	07	Total	С	Ν	0	S	0	0	0
20	AI	91	745	469	144	131	1	0	0	0
- 12	P1	07	Total	С	Ν	0	S	0	0	0
20		91	745	469	144	131	1		0	U

• Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
24	A2	70	Total 588	$\begin{array}{c} \mathrm{C} \\ 365 \end{array}$	N 118	O 103	${ m S} { m 2}$	0	0	0



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
24	B2	70	Total 588	$\begin{array}{c} \mathrm{C} \\ 365 \end{array}$	N 118	O 103	${ m S} { m 2}$	0	0	0

• Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		Aton	ns		ZeroOcc	AltConf	Trace
25	Λ3	50	Total	С	Ν	0	0	0	0
20	AJ		458	293	87	78	0	0	0
25	D3	50	Total	С	Ν	0	0	0	0
20	60	- 59	458	293	87	78		U	

• Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
26	Δ.4	46	Total	С	Ν	Ο	S	0	0	0
20	A4	40	349	223	57	64	5	0	0	0
26	P/	46	Total	С	Ν	Ο	S	0	0	0
20	D4	40	349	223	57	64	5		0	U

• Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
97	Δ.5	50	Total	С	Ν	0	S	0	0	0
21	AJ		455	286	90	74	5	0	0	0
97	DE	50	Total	С	Ν	Ο	S	0	0	0
21	D0		455	286	90	74	5	0	0	0

• Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
28	16	53	Total	С	Ν	Ο	S	0	0	0
20	A0		449	278	90	77	4	0	0	0
20	P6	52	Total	С	Ν	0	S	0	0	0
20	DU		449	278	90	77	4	0	0	0

• Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	Δ7	18	Total	С	Ν	0	S	0	0	0
29	AI	40	418	257	104	55	2	0	0	0
20	B7	18	Total	С	Ν	0	S	0	0	0
29	Dí	40	418	257	104	55	2	0	0	0



• Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
30	18	64	Total	С	Ν	Ο	\mathbf{S}	0	0	0
30	ЛО	04	509	326	99	82	2	0	0	0
20	D0	64	Total	С	Ν	Ο	S	0	0	0
30	Do	04	509	326	99	82	2	0	0	0

• Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues		1	Atoms			ZeroOcc	AltConf	Trace
31	CA	1498	Total 32208	C 14334	N 5974	O 10402	Р 1498	0	0	0
31	DA	1498	Total 32208	C 14334	N 5974	O 10402	Р 1498	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	?	-	U	DELETION	GB AP008226.1
DA	?	-	U	DELETION	GB AP008226.1

• Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	CB	220	Total	С	Ν	Ο	S	0	0	0
32	CD	229	1777	1134	318	320	5	0	0	0
20	DB	220	Total	С	Ν	0	S	0	0	0
52		229	1777	1134	318	320	5	0	0	U

• Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
22	CC	206	Total	С	Ν	Ο	S	0	0	0
- 55		200	1450	906	279	264	1	0	0	0
22	DC	206	Total	С	Ν	Ο	S	0	0	0
ാ	DC	200	1450	906	279	264	1	0		U

• Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
34	CD	208	Total 1520	C 960	N 283	0 272	${f S}{5}$	0	0	0



Continued from previous page...

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
34	DD	208	Total 1520	C 960	N 283	O 272	${ m S}{ m 5}$	0	0	0

• Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues		Atoms					AltConf	Trace
35	CF	148	Total	С	Ν	0	S	0	0	0
- 55	UL	140	1105	699	204	198	4	0	0	0
25	DF	148	Total	С	Ν	0	S	0	0	0
- 55		140	1105	699	204	198	4	0	0	0

• Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
26	CE	100	Total	С	Ν	0	S	0	0	0
- 30	Or	100	781	495	137	146	3	0	0	0
26	DE	100	Total	С	Ν	0	S	0	0	0
- 50		100	781	495	137	146	3	0		U

• Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues		Atoms					AltConf	Trace
37	CG	155	Total 1167	C 727	N 224	O 210	S 6	0	0	0
37	DG	155	Total 1167	C 727	N 224	O 210	S 6	0	0	0

• Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
38	СН	138	Total	С	Ν	0	S	0	0	0
00		100	1045	665	188	190	2	0	0	0
20	חם	128	Total	С	Ν	0	S	0	0	0
00		130	1045	665	188	190	2			U

• Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues		Ato	\mathbf{ms}		ZeroOcc	AltConf	Trace
30	CI	195	Total	С	Ν	Ο	0	0	0
- 39		120	852	533	163	156	0	0	0
20	ות	195	Total	С	Ν	Ο	0	0	0
- 39		120	852	533	163	156	0	0	0



There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	58	ARG	HIS	CONFLICT	UNP P80374
DI	58	ARG	HIS	CONFLICT	UNP P80374

• Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
40	CI	06	Total	С	Ν	Ο	0	0	0
40 0.1	90	659	408	131	120	0	0		
40	DI	06	Total	С	Ν	Ο	0	0	0
40	DJ	90	659	408	131	120		0	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	75	LEU	ILE	CONFLICT	UNP Q5SHN7
DJ	75	LEU	ILE	CONFLICT	UNP Q5SHN7

• Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
41	CK	114	Total	С	Ν	0	S	0	0	0
41	UN	114	828	516	155	154	3	0	0	0
41	DK	114	Total	С	Ν	0	S	0	0	0
41	DK	114	828	516	155	154	3	0	0	0

• Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
42	CI	199	Total	С	Ν	0	S	0	0	0
42		122	909	570	179	159	1	0	0	0
49	וח	199	Total	С	Ν	0	\mathbf{S}	0	0	0
42		122	909	570	179	159	1	0	0	0

• Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
12	CM	114	Total	С	Ν	0	S	0	0	0
40	UM	114	801	494	164	142	1	0	0	0
12	DM	114	Total	С	Ν	0	S	0	0	0
40	DIVI	114	801	494	164	142	1	0	0	0



• Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
44	CN	60	Total	С	Ν	Ο	S	0	0	0
	UN	00	478	303	99	72	4	0	0	0
4.4	DN	60	Total	С	Ν	Ο	S	0	0	0
44	DN	00	478	303	99	72	4	0	0	0

• Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
45	CO	88	Total	С	Ν	Ο	S	0	0	0
		88	724	453	143	126	2	0	0	0
45	DO	<u> </u>	Total	С	Ν	0	S	0	0	0
		00	724	453	143	126	2			U

• Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
46	CP	82	Total	С	Ν	Ο	S	0	0	0
		02	651	416	123	111	1	0	0	0
46	פת	80	Total	С	Ν	Ο	\mathbf{S}	0	0	0
40		02	651	416	123	111	1	0	0	0

• Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
47	CO	00	Total	С	Ν	0	\mathbf{S}	0	0	0
	UQ	99	823	528	151	142	2	0	0	0
47	DO	00	Total	С	Ν	0	S	0	0	0
47	DQ	99	823	528	151	142	2	0	0	0

• Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues		Aton	ns		ZeroOcc	AltConf	Trace
48	CB	68	Total	С	Ν	0	0	0	0
	ΟR	08	514	329	98	87	0	0	0
48	лр	68	Total	С	Ν	0	0	0	0
	DR	00	514	329	98	87	0	U	0

• Molecule 49 is a protein called 30S ribosomal protein S19.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
49	CS	78	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	Co	10	544	342	105	95	2	0	0	0
49	DS	79	Total	С	Ν	0	S	0	0	0
	Do	10	544	342	105	95	2	0	0	0

• Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
50	СТ	06	Total	С	Ν	0	S	0	0	0
	U1	90	708	435	151	120	2	0	0	0
50	рт	06	Total	С	Ν	0	S	0	0	0
50		90	708	435	151	120	2	0	0	U

• Molecule 51 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues		Aton	ıs		ZeroOcc	AltConf	Trace
51	CU	23	Total 199	C 122	N 48	O 29	0	0	0
51	DU	23	Total 199	C 122	N 48	O 29	0	0	0

• Molecule 52 is Thermorubin (three-letter code: T8B) (formula: $C_{32}H_{24}O_{12}$).



Mol	Chain	Residues	At	\mathbf{oms}		ZeroOcc	AltConf
52	АА	1	Total 44	C 32	0 12	0	0



Mol	Chain	Residues	At	\mathbf{oms}		ZeroOcc	AltConf
52	ВА	1	Total 44	C 32	O 12	0	0

• Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	АА	2	Total Mg 2 2	0	0
53	ВА	2	Total Mg 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: 23S ribosomal RNA







C1710	C1/11 C1712	-	U1720	A1722	U1739	41741 A1741	G1742	C1743	G1746	-	G1753	01/34 A1755	G1756	01757		C1761	A1762 G1763	G1764	C1765	01766 C1767		A1773	01774 01775	-	01779 41780	C1781	C1782 A1783	A1784	A1785	A1787	C1788	C1790	A1791	C1793	U1794	C1795 U1796	C1797	01798	C1800	G1801 A1802	A1803 C1804
U1805	G1814	A1815	G1816 C1817	U1818	A1819	07010	G1823	C1826	C1827	G1828	A1829	01833	U1834	G1835 C1836	C1837	C1838	G1839 G1840		C1844	41847	A1848	G1849	G1850	A1853	A1854 C1855		G1858	G1863	A1 07.6	A1877	G1878	C1882	G1883 A1 884	500 TV	A1889	A1890 G1891	C1892	C1 800	A1900	G1906	A1913
C1914	01915 A1916	<mark>U1917</mark>	A1918 A1919	C1920		A192/ A1928	G1929	G1930 111931		C1934	G1935	A1930 A1937	A 1938	U1939	C1941	C1942	U1946	C1947	G1948	II1955	00010	C1962	01963 G1964	C1965	A1966 C1967	G1968	A1969 A1970	A1971	A1972	C1974	G1975 111076	A1977		A1981	C1982	A 1986	G1987	111001	G1992	U1993 C1994	G1997
G1998	CIAAA	C2007	<u>63010</u>	U2010	G2012	A2013 A2014	A2015	U2016 112017	G2018	A2019	A2020	U2021	G2023	G2024	G2027	U2028	G2029 A2030	A2031	G2032	A2033	G2035	C2036	C2040	U2041	A2042 C2043		G2049 C2060	A2051	G2052	C2055	G2056	A2058 A2058	A2059	G2061	A2062	C2063 C2064	C2065	C2066 C2067	U2068	G2069 G2070	A2071
U2074	9/020	C2078	U2079	C2081	A2082	C2084	C2085	U2086	G2094	C2095	U2096	U2098	U2099	G2100	U2102	C2103	G2104 • C2105 •	G2106	C2107	C2108	G2110	C2111	02112 02113	A2114	G2115 C2116	A2117	U2118	G2120	G2121	G2123	G2124	A2126	G2127	U2130	G2131	02132 62133	A2134	A2135	C2137	C2138 C2139 C	C2140 G2141
C2142	U2144	C2145	C2146	G2148	G2149	G2151	G2152	G2153	G2155	G2156	G2157	G2159	G2160	C2161	C2163	C2164	G2165 G2166	U2167	G2168	A2169	A2171	U2172	A2173 C2174	C2175	A2176	C2178	C2179	G2181	20101	C2185	G2186	C2188	U2189	G2 19 1	G2192	G2193	A2198	A2199	C2201	C2202 U2203	<mark>C2205</mark> G2206
G2207	A2208 U2218	G2219	6000	G2224	A2225	42227 A2227	G2228	C2229	U2233	G2234	G2235	G2237	G2238	G2239 C2240	A2241	G2242	U2243 U2244		A2247	C2248 117249	G2250	G2251	G2253 G2253		G2256 1100577		C2261	C2263	C2264	A2268	A2269	U2272	A2273	C2275	<mark>G2276</mark>	G2277 A2278	G2279	G2280	G2282	C2283 C2284	C2285 A2286
A2287	A2288 G2289	G2290	U2291 77797	C2293 C2293	C2294	U2296	C2297	A2298 C22399	G2300	C2301	G2302	G2304	A2305	C2306	G2308	A2309	A2310 A2311	U2312	C2313	C2314 C2315	C2316	C2317	G2318 G2319	A2320	62321 47322	G2323	C2324 67375	C2326	A2327	62329	G2330 C7331	TOCZE	G2334	A2335 A2336	G2337	G2338	C2342	C2343	62345	A2346 C2347	U2348 G2349
C2350	62351 A2352	G2353	G2354 C7355	C2356	U2357	G2359 C2359	A2360	A2361 C9369	C2363	C2364	G2365	62367 G2367		G2371	A2376	A2377	A2378 G2379	C2380	C2381	G2382 G2383	G2384	C2385	02386 02387	A2388	G2389 117390	G2391	A2392 A7303	C2394	C2395	06070	G2399	00575	C2403	G2405	U2406	G2407 U2408	G2409	G2410 A2411	TTLOU	G2414 G2415	C2416
U2419	G2420 G2421	A2422	U2423	A2425	A2426	G2428	G2429	A2430 112431	A2432	A2433	A2434	A2430	U2438	A2439	C2441		G2445 G2446	G2447	A2448	02449 47450	002.74	A2453	G2454 G2455	C2456	112469	C2463	C2464	00470	G2468	G2470	C2471	U2473	C2474	A2476	C2477	G2481	G2482	C2483	G2485	G2486 G2487	A2488 G2489
G2490	U2493	G2494	G2495	62490 A2497	C2498	U2500	C2501	62502 42503	U2504	G2505	U2506	G2508		C2512	U2514	C2515	G2516 C2517	A2518	U2519	C2520 C2521	U2522	G2523	G2524 G2525	G2526	(10 CO	A2530	A2531	G2535	G2536 117537	C2538	C2539	A2542	G2543 C2543	11075	G2550	C2551 112552	G2553	U2554	C2558	C2559 C2560	A2561 U2562
U2563	A2565 A2565	A2566	G2567	00000	A2572	G2574	C2575	G2576 A2577	G2578		G2582	U2584	U2585	C2586 A7587	0074	A2590	C2591 G2592	U2593	C2594	0.0507	A2598	G2599	A2600 C2601	A	G2603 112604	U2605	C2606	G2608	U2609 69610	U2611	C2612	U2615	C2616 C7617	G2618	C2619	C2620	G2627	C2628	G2630	G2631	G2638 A2639
G2640	62641	<mark>G2645</mark>	C2646 112647	17070	C2658	42059 A2660	G2661	A2662 G2663		C2667	C 06 70	C/075	G2677	C2678	C2680	C2681	U2682 C2683	U2684	G2685	G2686 112687	U2688	U2689	C2690	A2693	G2694 Средб	U2696	G2697 117698	C2699	C2700	C2703	20202		C2710	U2712	A2712A	A2713 G2714		A2721	C2723	U2726	G2727 U2728
G2729	G2730 G2731	G2732	A2733	62735	G2736	42131 A2738	U2739	A2740 A2741	C2742	C2743	G2744	U2746	G2747	A2748	A2750	G2751	C2752	C2755	U2756	A2757 A7758	G2759	C2760	62/61	A2764	A2765	C2767	C2768	00120	A2776	A2778	A7701	G2782	G2783	C2785	U2786	C2787 C2788	C2789	A2790	G2792	G2793 C2794	C C









U847 G848 A849

84

6831

G855	C856		0000 G859	U860	A861	G862	A863	6864 706F		A870	-	A878	G879	G880	1001 (1887	G883	C884	C885	C886	A88/	6880	A890	G892	C893	C894	4896	C897	C898	A899	A900	COD	C903	-	A910	A911	C912		C916
G944	A945	0340	G948	C949		A953	G954	CS55	49.57 A9.57	U958	<u>A959</u>	A960	C961		C9 10	G974	C975	G975A		(A/8)	A983		6987	A988	(1989 0000	1001	C992	G993	C994	C995	1997	C998	<u>6660</u>	A1000	A1001	G1002	G1003	C1005
A1027	A1028	111022	00010	G1037	C1038	G1039	C1040	C1041	G1043	G1044	A1045	A1046	G1047	A1048	0.1049 A 1050	G1051	C1052	U	A	9 0	2 4	: 13	C	n	þ	5 5	0	U	U	A	5	Ä	Ð	U	A	5	00	Þ (
U	5	0 <	A	U	А	5	с :	- t	41106	U	U	G	G1107	01108	G1110	A1111	G1112	U1113	G1114	G1115 C1116	01110	G1125	A1126		A1129	01130 61131		C1135	G1136	00110	C1140	U1141	U1142	A1142A	A1143		G1149	01150
A1177	C1178		C1180 C1181	A1182	G1183	G1184	C1185	G1186	U1188	A1189	G1190	G1191	G1192	G1193	G1195		C1201	C1202	G1203	A1204	G1209	A1210	U1211	G1212		01210	A1220		G1223	C1224	41226	G1227	-	G1231		G1236		61239 111240
A1262	U1263	4120 4	A1205 G1266	U1267	A1268	A1269	C1270	61271	01273 01273	A1274	A1275		A1278	G1279	111 28.2	G1283	-	A1286		C1289	C1 29 1	U1292	C1293	U1294	C1295	21 202	G1299	U1300	A1301	900 PD	01307	A1308	G1309	G1310	G1311	U1312	01313 04244	C1314
U1340	U1341	A1342	G1344 G1344	-	A1349	C1350	C1351	114967	G1358	A1359	A1360		G1364	A1365	A1367	G1368	G1369	C1370	G1371	013/2		A1378	A1379	G1380	00015	01384	G1385	C1386		U1394	CACTW	G1400	G1401	C1402	C1403	C1404	U1405	01406 C1407
G1426	A1427	C1428	G1430	U1431	C1432	U1433	A1434	10110		A1445	-	G1448	A1449	G1450	111453	G1455	-	G1459	A1460	G1401	C1467		A1471		G1475	01410 01477	G1478	G1479	G1480	U1481	70515	A1486	G1487	G1488	U1489	A1490	G1491	G1492 C1493
G1510		11014 41010	C1516	G1517	U1518	G1519		G1529 G1520	C1531	C1532	IJ	U	A	C 61537	G1538	G1539	<mark>U1540</mark>	G1541	A1542	41545	C1546	C1547	C1548		A1558	600TB	A1566	A1567	G1568	A1569	A1571		C1577	U1578	A1579	A1580	G1581	01582 41583
A1614	1	11010	G1622	-	C1625	G1626		G1633	G1635	C1636	A1637	C1638	U1639	C1640	G1642		G1647	C1648	G1649	G1651	A1652	G1653	A1654	A1655	C1656	C1057		A1665	G1666	G1667	A1000	C1670	U1671	C1672	U1673	G1674	C1675	A10/0
A1700	A1701	20/19	C1711	C1712		G1719	01720	12110	01739	G1740	A1741	G1742	C1743	01710	04/15	G1753	C1754	A1755	G1756	01/5/ 61768	A1759	A1760	C1761	A1762	G1763	#0/TP	G172	A1773	C1774	111 1770	01//9 01780	C1781	C1782	A1783	A1784	A1785	A1786	C1 790
C1806	0	A 1010		G1814	A1815	G1816	G1817	01818	U1820		G1823	G1824	A1825	G1826 C1807	61828	A1829		U1833	U1834	G1836	C1837	C1838	G1839	G1840	01012	C TOTO	G1846	A1847		A1854	00010	G1858	-	A1876	A1877	G1878	000	C1883

	A1009	U1012	C1013	111010	A1020	A1021	G1022	G1024	G1025	U1026	A1027	A1028	U1033		G1037	C1038	G1039	C1040	G1042	C1043	G1044	A1045	A1046 C1047	A1048	C1049	A1050	G1051 C1052	0	А	5	5 A	U	5	οD	IJ	5	ວ ະ	• D	A	5	Å	4 U	U	۹ J	50	0 0
5 1	υυ	0	D	n v	A	А	ლ <	4 D	U	ß	C I	5	P A	A	U	A	5 5	ב נ	0 0	A1106	υ	n	G 107	U1108	C1109	G1110	A1111 G1112	U1113	G1114	G1115 C1116		G1125	A1126	A1129	U1130	G1131	1110	G1135 G1136		G1139	C1140	01141 U1142	A1142A	A1143	G1149	C1150
00110	G1154 A1155		U1165	C1166	G1169	G1170	G1171 C1173	A1174	U1175	G1176	A1177	C1178	C1180	C1181	A1182	G1183	G1184	C1185 C1186	G1187	U1188	A1189	G1190	G1191 C1100	G1193	A1194	G1195	C1001	C1202	G1203	A1204	G1209	A1210	U1211	21219	C1218	G1219	A1220	G1223	C1224	G1225	A1226		G1231	<u>61736</u>	00770	G1239
1171V	A1242	05710	A1247	C1 75 7	A1253	A1254	U1255 C1256	C1257	C1258		A1262	01263	A1265	G1266	U1267	A1268	A1269	C1270	A1272	U1273	A1274	A1275	A1078	G1279		U1282	G1283	A1286		C1289	C1290	U1292	C1293	01294 C1295	-	C1298	61.299	A1301		C1306	A1307	G1309	G1310	G1311 11312	01312 01313	C1314
170T0	G1325	01320 C1327	G1328	01329	A1331	G1332	C1333	G1337	G1338	G1339	U1340	01341	61343	G1344		A1349	C1350		U1357	G1358	A1359	A1360	C1364	A1365	A1366	A1367	G1368 G1369	C1370	G1371	U1372	CICTN	A1378	A1379	61380	C1383	A1384	G1385	00010	U1394	A1395		G1401	C1402	C1403	01405 U1405	U1406
00410		61413 G1413		G1416	G1418 G1418	A1419	U1420	G1422	-	G1425	G1426	A1427	G1429	C1430	U1431	C1432	U1433	A 14-04	C1437		A1445	-	G1448 A1440	G1450		U1453	G1455	G1459	A1460	G1461	C1467		A1471	G1475	C1476	A1477	G1478	G14/9 G1480	U1481	G1482	A 1 1 0 C	G1487	G1488	U1489	A1490 G1491	G1492
121TV	A1495	M1497		01503 71504	C1505	C1506	A1507	C1509	A1509A	A1509B	G1510		G1515	C1516	G1517	U1518	G1519	C1500	C1530	C1531	C1532	5	0 4	4 D	G1537	G1538	G1539 111540	G1541	A1542	4 1 L L	A 1343 C1546	C1547	C1548	A1558	G1559	4	A1566	61568	A1569	A1570		C1577	U1578	A1579	A1560 G1581	C1582
400T0	A1586 A1586	C1588		C1598	U1602		A1608	A1603 A1610	-	G1613	A1614	C1617		G1622		C1625	G1626	C1632	A1634	G1635	C1636	A1637	C1638 111639	C1640	A1641	G1642	G1647	C1648	G1649	G1650	A1652	G1653	A1654	A1655 C1656	C1657	C1658	A 1 C C C	G1666	G1667	A1668	A1669	U1671	C1672	U1673	G1675	A1676
0/010	01679 111.620		C1685	C1686 C1687	U1688	A1689	01 60 6	G1697	A1698	G1699	A1700	A1701	20110	C1711	C1712		G1719 11700	07/T0	A1722	U1739	G1740	A1741	G1 742		G1746		G1753 C1754	A1755	G1756	01757	41759 A1759	A1760	C1761	A1 /62 G1763	<mark>G1764</mark>		61772	C1774		U1779	A1780	C1782	A1783	A1784	A1786 A1786	
TCITY	G1792	01794 U1794	C1795	01796 C1797	U1798	G1799	C1800	A1802	A1803		C1806	A 1010	G1811		G1814	A1815	G1816 61815	0101/	A1819	U1820	-	G1823	G1824 A1825	G1826	C1827	G1828	A1829	U1833	U1834	G1835	C1837	C1838	G1839	G1840	C1843	0	G1846 A10.47	TOTA	A1854	G1855	1000	00015	A1876	A1877	O/OTD	C1882
100TV	A1885	C1887	G1888	A1889 A1890		C1895	G1896 71007	01898 01898	G1899	A1900	A1901	C1902	COGTO	G1906	<mark>G1907</mark>	C1908		A1910	U1915	A1916	U1917	A1918	A1919		C1925	U1926	A1927 A1928	G1929	G1930	U1931	G1935	A1936	A1937	A1938	G1948	G1949	G1950	A1952	A1953	G1954	U1955 114056	C1957	C1958	G1959	U1963	G1964
10610	G1968 A1969	A1970 A1970	A1971	A1972	C1979	<mark>G1980</mark>	A1981	C1983	-	C1990	U1991	G1992		G1997	G1998	C1999	20002		G2009		G2012	A2013	A2014	U2016		A2020	C2021	G2023	G2024		02029 G2029	A2030	A2031	G2032 A2033	U2034	G2035	C2036	G2038		A2042	C2043	C2050	A2051	G2052 C2053	42053 A2054	C2055





• Molecule 2: 5S ribosomal RNA





• Molecule 4: 50S ribosomal protein L3





















• Molecule 18: 50S ribosomal protein L22



Chain AW:	60%	34%	5%•
M1 E2 K4 K4 A7 A7 Y9 Y10 K11	R15 R15 V17 V17 V16 L19 L23 S28 S28 S28 S28 S28 R37 V50 V50 V50 V50 V50 V50 V50 V50 V50 V50	D67 V71 Y75 V76 D77 E78	K83 L86 P87 R88 R90 G91 R92
A93 D94 195 K97 K98 K98 R99 T100 T100	1104 1106 1107 1107 1107 1107		
• Molecule 18	3:50S ribosomal protein L22		
Chain BW:	70%	24%	5%•
• Molecule 19	2 50S ribosomal protein L23	K83 R84 U85 L86 L86 L86 K97 K97 K98 R99	1106 1107 6112 118
Chain AX:	70%	26%	
M K2 P11 V12 L13 K16 A17 Y17	A19 G20 G20 C20 K25 K33 K34 K34 K34 K34 K40 K40 K40 K40 K40 K40 K40 K40 K40 K4	G71 R76 K77 K78 K78 A84 A84 A84 G94	L196
• Molecule 19	0:50S ribosomal protein L23		
Chain BX:	64%	30%	5%•
M1 K2 K2 X5 V5 V7 V12 V12	R15 K16 K16 K16 K16 W29 W31 K33 K33 K33 K33 K33 K33 K33 K33 K53 K55 K55	667 K72 K72 K78 A78 A78 A78 A78 A78 A78 A78 A78 A78 A	982 192 193 115 115
• Molecule 20): 50S ribosomal protein L24		
Chain AY:	55%	37%	5% • •
M1 K2 K4 M5 H6 K8 K8 K9 K9 K9 K9 K9 K9	D11 112 112 112 123 125 125 125 123 123 123 123 123 123 123 123 123 123	P00 L67 H68 A69 S70 K71 V72 R73 P74 P74	C76 P77 C79 C79 C79 C80 K81 K81 K81 K84 V85
R86 F89 L90 R91 R94 K94 K94 K95 F89 K95	R97 798 C998 C100 C100 C100 C100 C100 C100 C100 C10		
• Molecule 20): 50S ribosomal protein L24		
Chain BY:	65%	28%	
M1 M5 K3 K23 K23 K28	Y35 E40 G41 V42 V42 K47 A48 K47 A48 K47 A48 A69 C58 A69 S70 K71 K73 K73 K73 K73 K73 K73 K73 K73 K73 K73	R84 V85 R86 R87 L90 L90 R91 R93 C93	K94 R97 C99 A100 K101 C102
D107 THR GLU GLU			





• Molecule 23: 50S ribosomal protein L28


















D #	o D	G3	U4 U5	GG	G7 A8	69	A10	119	014	G15	A16 1117	C18	C19	020 G 21	G22	C23	0.24 C25	A26	A32	A33 C34	G35	C36 U37	G 38	6.59	G44	U45 G46	C47	C48	A51		G57	C58 A59	A60	G61	<mark>G64</mark>	UG5	066 067	G68	G70	C71 C72
G7.6	G77	G78	679 G	n	n	n	A	C91	C92	G93	036	698	000	C100 A101	G102	C103	G104 G105	C106	G108	A109	G111	G112 G113	U114	6115 A116	G117	U118 A119	A120	C121 G122	C123	A1 30	C131	A134		C137	0015	G142	A143 G144	G145	G147 G147	G148 A149
C150	C153	C154	C155	G157	G158 C150	A160	A161	A162 C163	U164	C165	G166 G167	G168	C169	0170 A171	A172	U173	C175 C175	C176	C178			C186 C187	C188	C189B	C189C	C189D U189E	U189F	G189G G189H		U189K C189T	U190	G191 U192	C193	C194	A130 A196	A197	G198 G199	G200		U203 U204
G216 C217		C219	G220 C221	U222	U223	C225		0229 G230	G231	G232	C233 C234	C235	G236	C23/ C238	U239	C240	C241 C242	A243	0245 C245	A246 C247		G251 U252	U253	G255 G255	U256	G257	A262	A263	G266	C267	C269	A270 C271	C272	A273	C277	G278	A279 C280	G281	G284	G285
G289	6292	G293	U294 C295	U296	G297 A 208	G299	A300	G302	A303	U304	C308	6309	G310	C311	G316		A321 C322	U323	A325	G326 A377	C328	A329 C330	G331	6333 6333	C334	C335 C336	C337	A338 C339	U340	C341 C342	U343	A344	<mark>G346</mark>	G347	4349 A349	G 350	G351 C352	A353	G354 C355	<mark>1359</mark>
A360	G362	A363	A364 U365	C366	U367	<mark>C369</mark>	C370	G372	A373	A374	0376 G376	G377		6380 C381	A382	A383	6384	G388	C390	G391 C307		A397 C398	G399	C4 00	U405	G406	G409	G410 A411	A412	G413 A414	A415 A415	G416 C417	C418	11404	0421 C422	G423	G424 G425	G426	0427 G428	U429 A430
A431	6433	U434	C435 C436	U437	G438 4430	A441	C442	C443 C444	G445	G446	G4447 A448		A452	A453	C456	C457	G460	A461		6473 6474	G475	G476 A477	C479	C483	G484	G485 U486	A487	C488 C489	G490	6491 6492	7040	A496 U498		C501	CE03	C504	G505	A509	A510 C511	U512 C513
C514	G517	C518	C519 A520	G521	C522 A523	0704	G527	G529	G530	U531	A532 A533	U534		6538 4539	G540	G541	G543 C543	G544 G545	G546	A547 C548	C549	US52	A553	C224	A559	U560 U561	C562	A563 C564	US65	G566 G567	G568	C569 G570	U571	A572	A574	G575	G576 G577	C578	G5/9 U580	A583
G584 C514	G586 G517	C518	C590 C519 U591 A520	G521	C596 C522	Ceoo	C601 G527	A60.2 U603 G529	G604 G530	U605 U531	G606 A532 A607 A533	A608 U534		C612 G538 C613 A539	G540	G616 G541	G617 G542 C618 C543	0544 CEDO	A621 G546	A622 A547 C623 G548	C624 C549	G625 U626 U552	G627 A553	G629 C554	G630 A559	G631 U560 A632 U561	G633 C562	C634 A563 C635 C564	U565	G638 G566 C630 C567	G568	A642 C569 C543 C570	U571	A653 A572	C656 A574	G657 G575	G658 G576 U659 G577	G660 C578	G662 U580	A663 G664 A583
A665 G584 C514	G667 C586 G517	G668 C518	U669 C590 C519 G670 U591 A520	G671 G521	U672 C596 C522 C673 A573	G674 C600	A675 C601 G527	A676 A602 C528 C529 U677 U603 G529	G604 G530	C680 U605 U531	C681 G606 A532 G682 A607 A533	G683 A608 U534	A684	G685 C612 G538 II686 C613 A539	A687 G540	G688 G616 G541	C689 G617 G542 G690 C618 C543	G691 U619 G544	A621 G546	A695 A622 A547 A696 C633 C548	U697 C624 C549	G698 G625 C699 U626 U552	G627 A553	C/ 0/ G628 C554 C7 08 G629	G709 G630 A559	G710 G631 U560 A632 U561	G713 G633 C562	G714 C634 A563 A715 G635 C564	A716 U565	C717 G638 G566 C718 G630 G567	C719 G568	C720 A642 C569 G721 C643 G570 ●	A722 U571	U723 A653 A572	G7 25 C656 A574	C7.26 G657 G575	G7.27 G658 G576 A7.28 U659 G577	A729 G660 C578	G/30 G001 G5/9 G731 G662 U580	4663 G734 G664 A583
C735 A665 G584 C514	A737 G667 C586 G517	C738 G668 C518 C518	C C C C C C C C C C C C C C C C C C C	G742 G671 G521	U743 U672 C596 C522 C744 C673 A523	C745 G674 C600	A746 A675 C601 G527	C/4/ A6/6 A60/2 C528 C748 U677 U603 G529	C749 G604 G530	G750 C680 U605 U531	4753 C681 G606 A532 4753 G682 A607 A533	C754 G683 A608 U534	G755 A684	C/56 G685 C612 G538 11757 11686 C613 A539	G758 A687 G540	G616 G541 G541 G541 G541 G541 G541 G541 G541	G/63 C689 G61/ G542 C764 G690 C618 C543	G765 G691 U619 G544	G769 A621 G546	A695 A622 A547 A777 A696 C623 C548	G778 U697 C624 C549	C779 G698 G625 A780 C699 U626 U552	A781 G627 A553	A/82 C/0/ G628 C554 C783 C708 G629	C784 G709 G630 A559	G785 G710 G631 U560 G786 A632 U561	A787 G713 G633 C562	U788 G714 C634 A563 11789 A715 G635 C564	A790 A716 U565	G791 C717 G638 G566 A702 C718 C633 C667	U793 C719 G568	A794 C720 A642 C569 6721 C643 6570 ●	C797 A722 U571	G798 U723 A653 A572	G133 G124 G124 G125 C656 A513 A513	U801 C726 G657 G575	A802 G727 G658 G576 G803 A728 11659 G577	U804 A729 G660 C578	C805 G730 G601 G579 G579 U580	C810 A663 A683 C811 G734 G664 A683
C812 C735 A665 C584 C514	0013 0/30 0000 0000 0000 A000 A014 A737 0667 0586 0517	A815 C738 G668 C518	A816 U669 C590 C519 C817 G741 G670 U591 A520	G818 G742 G671 G521	A819 U743 U672 C596 C522 T1820 C744 C673 A523	G821 C745 G674 C600	A746 A675 C601 G527	G826 C/4/ A676 A602 C528 C826 C748 U677 U603 G529	U827 C749 G604 G530	A828 G750 C680 U605 U531	G829 C681 G606 A532 4753 G682 A607 A533	C832 C754 G683 A608 U534	U833 G755 A684	C834 C756 G685 C612 G538 1835 11757 11686 C613 A539	G836 G758 A687 G540	G837 G688 G616 G541	G838 G613 C689 G617 G542 U839 C764 G690 C618 C543	C840 G765 G691 U619 G544	C348 G769 A621 G546	4695 A622 A547 4696 C633 C548	G852 G778 U697 C624 C549	G853 C779 G698 G625 U522 G854 A780 C699 U526 U552	G855 A781 G627 A553	C857 C708 C629 C504	G858 C784 G709 G630 A559	A859 G785 G710 G631 U560 A860 G786 A632 U561	A787 G713 G633 C562	U863 U788 G714 C634 A563 A864 U789 A715 G635 C564	A865 A790 A716 U565	C866 G791 C717 G638 G566 C867 A700 C718 G638 G567	C368 U793 C719 C568	G869 A794 C720 A642 C569 UB70 G721 G721 G570 6	U871 C797 A722 U571	A872 G798 U723 A653 A572	4872 G874 G800 G725 C656 A574	C875 U801 C726 G657 G575	4802 G727 G658 G576 G578 G576 G577 G658 G577	C879 U804 A729 G660 C578	C805 G731 G662 U580 C883 G731 G662 U580	UB84 C810 A 663 A 663 A 6885 C811 C734 C664 A 583
C812 C735 A665 C584 C514	4009 0013 0130 0000 0000 0000 0000 0000 0	U891 A815 C738 G668 C518	A892 A816 U669 C590 C519 C993 C817 G741 G670 U591 A520	G894 G818 G742 G671 G521	G895 A819 U743 U672 C596 C522 11820 774.4 6573 6573 6573	C899 G821 C745 G674 C600	A900 A746 A675 C601 C527	A301 G825 C/4/ A0/6 A002 C528 G826 C748 U677 U603 G529	G903 U827 C749 G604 G530	C904 A828 C750 C680 U605 U531	0905 0829 0581 0506 A532 A753 0582 A607 A533	A908 C832 C754 G683 A608 U534	U833 G755 A684	A913 C834 C/56 G685 C612 G538 4914 II835 I1757 II686 C613 4539	G836 G758 A687 G540	G917 G837 G688 G616 G541	U920 U839 G/63 C689 G61/ G542 U920 U839 C764 G690 C618 C543	U921 C840 G765 G691 U619 G544	4923 C848 G769 A621 G546 C546	10076 1351 1377 1606 152 1547	G927 G852 G778 U697 C624 C549	G928 G853 C779 G698 G625 G929 G854 A780 C699 U626	C930 G855 A781 G627 A553	C931 C936 A / 82 C / 0/ G628 C554 C932 C857 C783 C708 G629	G933 G858 C784 G709 G630 A559	C934 A859 G785 G710 G631 U560 A935 A860 G786 A32 U561	C936 • A787 G713 G633 C562	A937 U863 U788 G714 C634 A563 A938 A864 U789 A715 G635 C564	(2939 A865 A790 A716 U565	C940 C866 G791 C717 G638 G566 C041 C867 170 C638 G566	Cont <th< th=""><th>U943 G869 A794 C720 A642 C569 G944 U870 G721 C643 G570 O</th><th>G945 U871 C797 A722 U571</th><th>A946 A872 G798 U723 A653 A572</th><th>6341 8013 6139 01 24 8013 C948 6874 6800 6725 6656 A574</th><th>A949 C875 U801 C726 G657 G575</th><th>4802 G727 G658 G576 1952 1952 1955 1952 1952 1952 1952 1952</th><th>C353 C879 U804 A729 G660 C578</th><th>G994 C805 G1/30 G601 G5/9 U965 C883 G7/31 G662 U580</th><th>U956 U884 C810 A63 U957 0688 C811 C734 C644 A533</th></th<>	U943 G869 A794 C720 A642 C569 G944 U870 G721 C643 G570 O	G945 U871 C797 A722 U571	A946 A872 G798 U723 A653 A572	6341 8013 6139 01 24 8013 C948 6874 6800 6725 6656 A574	A949 C875 U801 C726 G657 G575	4802 G727 G658 G576 1952 1952 1955 1952 1952 1952 1952 1952	C353 C879 U804 A729 G660 C578	G994 C805 G1/30 G601 G5/9 U965 C883 G7/31 G662 U580	U956 U884 C810 A63 U957 0688 C811 C734 C644 A533









• Molecule 32: 30S ribosomal protein S2



PRO ALA VAL ARG VAL LYS LYS GLU GLU

 \bullet Molecule 34: 30S ribosomal protein S4

































4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	209.37Å 445.46Å 619.56Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution(A)	49.29 - 3.20	Depositor
Resolution (A)	49.43 - 2.90	EDS
% Data completeness	100.0 (49.29-3.20)	Depositor
(in resolution range)	99.7 (49.43-2.90)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.13 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX	Depositor
P. P.	0.228 , 0.273	Depositor
n, n_{free}	0.228 , 0.273	DCC
R_{free} test set	63228 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	75.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.29, 70.6	EDS
L-test for $twinning^2$	$ < L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	279316	wwPDB-VP
Average B, all atoms $(Å^2)$	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: MG, T8B

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).

Mal	Chain	B	ond lengths		Bond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	AA	0.82	17/68203~(0.0%)	1.30	624/106459~(0.6%)
1	BA	1.20	70/68203~(0.1%)	1.37	800/106459~(0.8%)
2	AB	0.94	0/2879	1.25	21/4492~(0.5%)
2	BB	0.88	0/2879	1.26	21/4492~(0.5%)
3	AD	0.54	0/2186	0.75	2/2944~(0.1%)
3	BD	0.67	0/2186	0.81	4/2944~(0.1%)
4	AE	0.55	0/1588	0.76	0/2145
4	BE	0.72	0/1588	0.83	1/2145~(0.0%)
5	AF	0.51	0/1609	0.70	0/2177
5	BF	0.73	0/1609	0.77	0/2177
6	AG	0.61	0/1393	0.66	0/1892
6	BG	0.46	0/1393	0.64	0/1892
7	AH	0.58	0/1343	0.68	1/1820~(0.1%)
7	BH	0.59	0/1343	0.70	0/1820
8	AI	0.63	1/1061~(0.1%)	0.78	0/1451
8	BI	0.50	0/1061	0.74	0/1451
9	AN	0.52	0/1139	0.72	0/1538
9	BN	0.74	0/1139	0.78	0/1538
10	AO	0.50	0/933	0.72	1/1257~(0.1%)
10	BO	0.67	0/933	0.74	0/1257
11	AP	0.50	0/1135	0.75	1/1510~(0.1%)
11	BP	0.64	0/1135	0.81	2/1510~(0.1%)
12	AQ	0.53	0/1143	0.74	0/1527
12	BQ	0.64	0/1143	0.74	0/1527
13	AR	0.51	0/982	0.74	0/1312
13	BR	0.69	0/982	0.82	1/1312~(0.1%)
14	AS	0.64	0/875	0.79	0/1168
14	BS	0.53	0/875	0.79	1/1168~(0.1%)
15	AT	0.52	0/1077	0.73	0/1444
15	BT	0.61	0/1077	0.79	1/1444~(0.1%)
16	AU	0.56	0/977	0.69	0/1301
16	BU	0.88	$\overline{1/977}~(0.1\%)$	0.81	1/1301~(0.1%)



Mol Chain		В	ond lengths		Bond angles
NIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
17	AV	0.58	0/782	0.67	0/1049
17	BV	0.70	0/782	0.77	0/1049
18	AW	0.56	0/891	0.75	0/1197
18	BW	0.82	0/891	0.80	0/1197
19	AX	0.55	0/756	0.77	1/1016 (0.1%)
19	BX	0.66	0/756	0.76	1/1016~(0.1%)
20	AY	0.50	0/798	0.77	0/1073
20	BY	0.61	0/798	0.80	1/1073~(0.1%)
21	AZ	0.57	0/1555	0.68	0/2118
21	BZ	0.49	0/1555	0.71	0/2118
22	A0	0.50	0/602	0.69	0/804
22	B0	0.66	0/602	0.77	0/804
23	A1	0.51	0/752	0.72	0/1003
23	B1	0.62	0/752	0.76	0/1003
24	A2	0.59	0/590	0.68	0/781
24	B2	0.60	0/590	0.74	0/781
25	A3	0.45	0/463	0.69	0/623
25	B3	0.65	0/463	0.74	0/623
26	A4	0.65	0/358	0.74	0/487
26	B4	0.56	0/358	0.74	1/487~(0.2%)
27	A5	0.67	1/469~(0.2%)	0.83	2/634~(0.3%)
27	B5	0.79	0/469	0.88	0/634
28	A6	0.59	0/456	0.70	0/609
28	B6	0.68	0/456	0.74	0/609
29	A7	0.57	0/426	0.75	0/561
29	B7	0.78	0/426	0.84	0/561
30	A8	0.50	0/516	0.73	0/679
30	B8	0.70	0/516	0.82	0/679
31	CA	0.80	10/36054~(0.0%)	1.18	176/56272~(0.3%)
31	DA	0.77	7/36054~(0.0%)	1.19	211/56272~(0.4%)
32	CB	0.51	0/1811	0.69	0/2452
32	DB	0.56	0/1811	0.69	0/2452
33	CC	0.56	0/1474	0.65	0/2003
33	DC	0.58	0/1474	0.65	0/2003
34	CD	0.53	0/1550	0.72	3/2106 (0.1%)
34	DD	0.84	$2/1550 \ (0.1\%)$	0.78	4/2106 (0.2%)
35	CE	0.49	0/1121	0.70	1/1517 (0.1%)
35	DE	0.52	0/1121	0.72	1/1517 (0.1%)
36	CF	0.49	0/794	0.64	0/1082
36	DF	0.49	0/794	0.67	1/1082 (0.1%)
37	CG	0.57	0/1186	0.65	0/1603
37	DG	0.56	0/1186	0.62	0/1603
38	CH	0.44	0/1065	0.67	0/1445



N <i>T</i> 1	Chain	E	Bond lengths		Bond angles
Mol	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
38	DH	0.44	0/1065	0.64	0/1445
39	CI	0.62	0/867	0.71	0/1180
39	DI	0.62	0/867	0.69	0/1180
40	CJ	0.60	0/672	0.74	1/919~(0.1%)
40	DJ	0.60	0/672	0.70	1/919~(0.1%)
41	CK	0.47	0/843	0.71	0/1144
41	DK	0.47	0/843	0.67	0/1144
42	CL	0.44	0/925	0.67	0/1251
42	DL	0.46	0/925	0.69	0/1251
43	CM	0.67	0/811	0.72	0/1103
43	DM	0.63	0/811	0.73	1/1103~(0.1%)
44	CN	0.60	0/487	0.68	0/649
44	DN	0.59	0/487	0.74	0/649
45	СО	0.49	0/735	0.64	0/981
45	DO	0.47	0/735	0.61	0/981
46	CP	0.51	0/667	0.70	0/905
46	DP	0.43	0/667	0.65	0/905
47	CQ	0.46	0/836	0.68	0/1117
47	DQ	0.47	0/836	0.66	0/1117
48	CR	0.43	0/519	0.64	0/699
48	DR	0.50	0/519	0.67	0/699
49	CS	0.69	0/558	0.88	1/759~(0.1%)
49	DS	0.76	1/558~(0.2%)	0.87	3/759~(0.4%)
50	CT	0.47	0/710	0.72	0/940
50	DT	0.42	0/710	0.68	0/940
51	CU	0.64	0/203	0.67	0/266
51	DU	0.59	0/203	0.70	0/266
All	All	0.86	110/303650~(0.0%)	1.16	1892/454928~(0.4%)

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
26	A4	0	1
34	CD	0	1
34	DD	0	1
42	CL	0	1
42	DL	0	1
All	All	0	5

The worst 5 of 110 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
34	DD	12	CYS	CB-SG	19.94	2.16	1.82
34	DD	26	CYS	CB-SG	15.79	2.09	1.82
31	DA	1492	А	C6-N6	-12.21	1.24	1.33
31	CA	1492	А	C2-N3	12.12	1.44	1.33
31	CA	1493	А	N9-C4	-11.96	1.30	1.37

The worst 5 of 1892 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
31	DA	1492	A	C6-N1-C2	-28.45	101.53	118.60
31	DA	1492	А	C5-C6-N1	26.41	130.90	117.70
31	CA	1492	А	C8-N9-C4	-21.05	97.38	105.80
1	BA	1332	G	C2-N3-C4	-19.65	102.08	111.90
1	BA	1332	G	N3-C4-C5	17.99	137.59	128.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A4	42	PHE	Peptide
34	CD	11	LEU	Peptide
42	CL	26	ALA	Peptide
34	DD	11	LEU	Peptide
42	DL	26	ALA	Peptide

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	AA	60900	0	30712	1406	0
1	BA	60900	0	30712	1060	0
2	AB	2574	0	1306	87	0
2	BB	2574	0	1306	35	0
3	AD	2136	0	2218	77	0
3	BD	2136	0	2218	81	0
4	AE	1555	0	1607	81	0
4	BE	1555	0	1607	54	0
5	AF	1576	0	1616	57	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BF	1576	0	1616	59	0
6	AG	1368	0	1324	70	0
6	BG	1368	0	1324	61	0
7	AH	1317	0	1376	66	0
7	BH	1317	0	1376	33	0
8	AI	1046	0	1067	55	2
8	BI	1046	0	1067	47	0
9	AN	1112	0	1180	60	0
9	BN	1112	0	1180	34	0
10	AO	923	0	981	28	0
10	BO	923	0	981	23	0
11	AP	1119	0	1186	38	0
11	BP	1119	0	1186	40	0
12	AQ	1122	0	1179	43	0
12	BQ	1122	0	1179	47	0
13	AR	968	0	1033	43	0
13	BR	968	0	1033	33	0
14	AS	865	0	905	62	0
14	BS	865	0	905	54	0
15	AT	1063	0	1103	48	0
15	BT	1063	0	1103	37	0
16	AU	959	0	1019	31	0
16	BU	959	0	1019	20	0
17	AV	771	0	830	22	0
17	BV	771	0	830	15	0
18	AW	881	0	935	25	0
18	BW	881	0	935	24	0
19	AX	742	0	799	22	0
19	BX	742	0	799	23	0
20	AY	785	0	832	36	0
20	BY	785	0	832	30	0
21	AZ	1522	0	1511	56	0
21	ΒZ	1522	0	1511	47	0
22	A0	594	0	604	27	0
22	B0	594	0	604	21	0
23	A1	745	0	804	26	0
23	B1	745	0	804	26	0
24	A2	588	0	643	31	0
24	B2	588	0	643	18	0
25	A3	458	0	503	22	0
25	B3	458	0	503	6	0
26	A4	349	0	340	22	0



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Mol	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
26	B4	349	0	340	16	0
27	A5	455	0	476	25	0
27	B5	455	0	476	18	0
28	A6	449	0	464	19	0
$\frac{-3}{28}$	B6	449	0	466	17	0
29	A7	418	0	467	18	0
29	B7	418	0	467	14	0
30	A8	509	0	565	23	0
30	B8	509	0	565	20	0
31	CA	32208	0	16256	921	2
31	DA	32208	0	16254	923	0
32	CB	1777	0	1747	100	0
32	DB	1777	0	1747	95	0
33	CC	1450	0	1314	45	0
33	DC	1450	0	1314	58	0
34	CD	1520	0	1407	73	0
34	DD	1520	0	1406	85	0
35	CE	1105	0	1130	48	0
35	DE	1105	0	1130	54	0
36	CF	781	0	741	25	0
36	DF	781	0	741	29	0
37	CG	1167	0	1108	39	0
37	DG	1167	0	1108	46	0
38	СН	1045	0	1033	45	0
38	DH	1045	0	1033	53	0
39	CI	852	0	742	43	0
39	DI	852	0	742	52	0
40	CJ	659	0	552	31	0
40	DJ	659	0	552	37	0
41	CK	828	0	822	24	0
41	DK	828	0	822	32	0
42	CL	909	0	927	43	0
42	DL	909	0	927	38	0
43	CM	801	0	743	33	0
43	DM	801	0	743	37	0
44	CN	478	0	498	33	0
44	DN	478	0	497	30	0
45	CO	724	0	749	32	0
45	DO	724	0	749	27	0
46	CP	651	0	638	33	0
46	DP	651	0	638	28	0
47	CQ	823	0	891	33	0
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WORLDWIDE PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	DQ	823	0	891	22	0
48	CR	514	0	530	19	0
48	DR	514	0	530	17	0
49	CS	544	0	457	21	0
49	DS	544	0	457	26	0
50	CT	708	0	764	37	0
50	DT	708	0	764	26	0
51	CU	199	0	208	8	0
51	DU	199	0	208	6	0
52	AA	44	0	20	31	0
52	BA	44	0	20	23	0
53	AA	2	0	0	0	0
53	BA	2	0	0	0	0
All	All	279316	0	185722	7170	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 16.

The worst 5 of 7170 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)
52:AA:3001:T8B:C13	31:DA:1492:A:H5"	1.47	1.41
34:DD:26:CYS:SG	34:DD:26:CYS:CB	2.09	1.41
34:DD:12:CYS:SG	34:DD:12:CYS:CB	2.16	1.34
52:AA:3001:T8B:H13	52:AA:3001:T8B:C22	1.58	1.33
52:BA:3001:T8B:H13	52:BA:3001:T8B:C22	1.58	1.32

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)
8:AI:89:TYR:O	31:CA:357:G:O2'[2_654]	2.11	0.09
8:AI:91:SER:OG	31:CA:368:U:OP2[2_654]	2.12	0.08



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	Perc	entiles
3	AD	273/276~(99%)	240 (88%)	27~(10%)	6 (2%)	6	35
3	BD	273/276~(99%)	246 (90%)	23~(8%)	4 (2%)	10	44
4	AE	202/206~(98%)	177 (88%)	18~(9%)	7~(4%)	3	24
4	BE	202/206~(98%)	174 (86%)	21~(10%)	7 (4%)	3	24
5	AF	198/205~(97%)	168 (85%)	25~(13%)	5 (2%)	5	32
5	BF	198/205~(97%)	170 (86%)	21~(11%)	7 (4%)	3	24
6	AG	179/182~(98%)	136 (76%)	33~(18%)	10 (6%)	2	14
6	BG	179/182~(98%)	135~(75%)	30~(17%)	14 (8%)	1	6
7	AH	172/180~(96%)	143 (83%)	21~(12%)	8 (5%)	2	17
7	BH	172/180~(96%)	144 (84%)	22~(13%)	6 (4%)	3	24
8	AI	143/148~(97%)	103 (72%)	28~(20%)	12 (8%)	1	5
8	BI	143/148~(97%)	109 (76%)	24~(17%)	10 (7%)	1	8
9	AN	138/140~(99%)	113 (82%)	16~(12%)	9 (6%)	1	10
9	BN	138/140~(99%)	119 (86%)	13 (9%)	6 (4%)	2	20
10	AO	120/122~(98%)	108 (90%)	8 (7%)	4 (3%)	4	25
10	BO	120/122~(98%)	109 (91%)	7~(6%)	4(3%)	4	25
11	AP	143/150~(95%)	117 (82%)	18 (13%)	8 (6%)	2	14
11	BP	143/150~(95%)	126 (88%)	12 (8%)	5 (4%)	3	24
12	AQ	139/141~(99%)	126 (91%)	9~(6%)	4 (3%)	4	28
12	BQ	139/141~(99%)	126 (91%)	9~(6%)	4 (3%)	4	28
13	AR	116/118~(98%)	95 (82%)	16 (14%)	5 (4%)	2	20
13	BR	$\overline{116/118}\ (98\%)$	108 (93%)	7~(6%)	1 (1%)	17	56
14	AS	$\overline{108/112}\ (96\%)$	84 (78%)	21 (19%)	3 (3%)	5	29
14	BS	108/112~(96%)	93 (86%)	12 (11%)	3 (3%)	5	29
15	AT	129/146~(88%)	109 (84%)	16 (12%)	4 (3%)	4	26
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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
15	BT	129/146~(88%)	116 (90%)	12 (9%)	1 (1%)	19	58
16	AU	114/118~(97%)	104 (91%)	10~(9%)	0	100	100
16	BU	114/118~(97%)	111 (97%)	3~(3%)	0	100	100
17	AV	99/101~(98%)	89 (90%)	8 (8%)	2 (2%)	7	38
17	BV	99/101~(98%)	89 (90%)	9~(9%)	1 (1%)	15	54
18	AW	110/113~(97%)	101 (92%)	8 (7%)	1 (1%)	17	56
18	BW	110/113~(97%)	104 (94%)	6~(6%)	0	100	100
19	AX	93/96~(97%)	82 (88%)	9 (10%)	2 (2%)	6	35
19	BX	93/96~(97%)	82 (88%)	9 (10%)	2 (2%)	6	35
20	AY	105/110~(96%)	90 (86%)	10 (10%)	5 (5%)	2	17
20	BY	105/110~(96%)	88 (84%)	13 (12%)	4 (4%)	3	22
21	AZ	196/206~(95%)	153 (78%)	32 (16%)	11 (6%)	2	14
21	BZ	196/206~(95%)	158 (81%)	31 (16%)	7 (4%)	3	23
22	A0	74/85~(87%)	67 (90%)	6 (8%)	1 (1%)	11	46
22	B0	74/85~(87%)	67 (90%)	6 (8%)	1 (1%)	11	46
23	A1	95/98~(97%)	88 (93%)	5 (5%)	2 (2%)	7	37
23	B1	95/98~(97%)	86 (90%)	6~(6%)	3 (3%)	4	26
24	A2	68/72~(94%)	59 (87%)	8 (12%)	1 (2%)	10	44
24	B2	68/72~(94%)	63 (93%)	5 (7%)	0	100	100
25	A3	57/60~(95%)	54 (95%)	3~(5%)	0	100	100
25	B3	57/60~(95%)	54 (95%)	2 (4%)	1 (2%)	8	41
26	A4	44/71~(62%)	30 (68%)	10 (23%)	4 (9%)	1	3
26	B4	44/71~(62%)	30 (68%)	10 (23%)	4 (9%)	1	3
27	A5	57/60~(95%)	50 (88%)	6 (10%)	1 (2%)	8	41
27	B5	57/60~(95%)	49 (86%)	6 (10%)	2 (4%)	3	24
28	A6	51/54~(94%)	46 (90%)	4 (8%)	1 (2%)	7	38
28	B6	51/54~(94%)	47 (92%)	4 (8%)	0	100	100
29	A7	46/49~(94%)	41 (89%)	4 (9%)	1 (2%)	6	35
29	B7	46/49~(94%)	42 (91%)	3 (6%)	1 (2%)	6	35
30	A8	62/65~(95%)	48 (77%)	13 (21%)	1 (2%)	9	43
30	B8	62/65~(95%)	57 (92%)	5 (8%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	$\mathbf{entiles}$
32	CB	227/256~(89%)	171 (75%)	36~(16%)	20 (9%)	1	4
32	DB	227/256~(89%)	173 (76%)	39~(17%)	15 (7%)	1	9
33	CC	204/239~(85%)	163 (80%)	30~(15%)	11 (5%)	2	14
33	DC	204/239~(85%)	144 (71%)	42 (21%)	18 (9%)	1	4
34	CD	206/209~(99%)	154 (75%)	40 (19%)	12 (6%)	1	13
34	DD	206/209~(99%)	152 (74%)	47 (23%)	7 (3%)	3	24
35	CE	146/162~(90%)	112 (77%)	23~(16%)	11 (8%)	1	7
35	DE	146/162~(90%)	116 (80%)	25 (17%)	5 (3%)	3	24
36	CF	98/101~(97%)	87 (89%)	8 (8%)	3 (3%)	4	26
36	DF	98/101~(97%)	85 (87%)	9 (9%)	4 (4%)	3	21
37	CG	153/156~(98%)	127 (83%)	16 (10%)	10 (6%)	1	10
37	DG	153/156~(98%)	129 (84%)	18 (12%)	6 (4%)	3	22
38	CH	136/138~(99%)	116 (85%)	18 (13%)	2 (2%)	10	44
38	DH	136/138~(99%)	118 (87%)	13 (10%)	5 (4%)	3	22
39	CI	123/128~(96%)	93 (76%)	20 (16%)	10 (8%)	1	5
39	DI	123/128~(96%)	94 (76%)	21 (17%)	8 (6%)	1	10
40	CJ	94/105~(90%)	66 (70%)	19 (20%)	9 (10%)	0	3
40	DJ	94/105~(90%)	74 (79%)	14 (15%)	6 (6%)	1	10
41	CK	112/129~(87%)	96 (86%)	12~(11%)	4 (4%)	3	23
41	DK	112/129~(87%)	90 (80%)	19~(17%)	3(3%)	5	30
42	CL	120/132~(91%)	98 (82%)	17~(14%)	5 (4%)	3	20
42	DL	120/132~(91%)	100 (83%)	15~(12%)	5 (4%)	3	20
43	CM	112/126~(89%)	84 (75%)	18~(16%)	10 (9%)	1	4
43	DM	112/126~(89%)	80 (71%)	20~(18%)	12 (11%)	0	2
44	CN	58/61~(95%)	43 (74%)	10 (17%)	5 (9%)	1	4
44	DN	58/61~(95%)	48 (83%)	7 (12%)	3 (5%)	2	15
45	CO	86/89~(97%)	71 (83%)	12 (14%)	3 (4%)	3	24
45	DO	$86/\overline{89~(97\%)}$	68 (79%)	16 (19%)	2(2%)	6	34
46	CP	80/88 (91%)	50 (62%)	23 (29%)	7 (9%)	1	4
46	DP	80/88~(91%)	52 (65%)	25 (31%)	3 (4%)	3	22
47	CQ	97/105~(92%)	84 (87%)	8 (8%)	5(5%)	2	15



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
47	DQ	97/105~(92%)	81 (84%)	13~(13%)	3(3%)	4	26
48	CR	66/88~(75%)	55~(83%)	10 (15%)	1 (2%)	10	44
48	DR	66/88~(75%)	60 (91%)	6~(9%)	0	100	100
49	CS	76/93~(82%)	48 (63%)	17~(22%)	11 (14%)	0	1
49	DS	76/93~(82%)	54 (71%)	17~(22%)	5(7%)	1	9
50	CT	94/106~(89%)	73 (78%)	13 (14%)	8 (8%)	1	4
50	DT	94/106~(89%)	72 (77%)	15~(16%)	7 (7%)	1	7
51	CU	21/27~(78%)	18 (86%)	3~(14%)	0	100	100
51	DU	21/27~(78%)	16 (76%)	3 (14%)	2 (10%)	0	3
All	All	11280/12044 (94%)	9338 (83%)	1460 (13%)	482 (4%)	2	20

5 of 482 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	239	ARG
3	AD	275	LYS
5	AF	60	SER
6	AG	14	GLU
6	AG	78	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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
3	AD	215/218~(99%)	185 (86%)	30 (14%)	3 16
3	BD	215/218~(99%)	189 (88%)	26 (12%)	5 22
4	AE	163/166~(98%)	139 (85%)	24~(15%)	3 14
4	BE	163/166~(98%)	134 (82%)	29~(18%)	2 9
5	AF	158/162~(98%)	133 (84%)	25~(16%)	2 12
5	BF	158/162~(98%)	138 (87%)	20 (13%)	4 20
6	AG	128/156~(82%)	110 (86%)	18 (14%)	3 16



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Mol	Chain	Analysed	Rotameric	Outliers	P	erce	entiles
6	BG	128/156~(82%)	114 (89%)	14 (11%)		6	26
7	AH	141/148~(95%)	125 (89%)	16 (11%)		6	25
7	BH	141/148~(95%)	124 (88%)	17 (12%)		5	22
8	AI	102/124~(82%)	76 (74%)	26~(26%)		0	2
8	BI	102/124 (82%)	76 (74%)	26~(26%)		0	2
9	AN	117/119~(98%)	94 (80%)	23~(20%)		1	7
9	BN	117/119~(98%)	91 (78%)	26~(22%)		1	4
10	AO	98/100~(98%)	89 (91%)	9 (9%)		9	33
10	BO	98/100~(98%)	89 (91%)	9~(9%)		9	33
11	AP	113/116~(97%)	96 (85%)	17 (15%)		3	14
11	BP	113/116~(97%)	97~(86%)	16 (14%)		3	15
12	AQ	111/111 (100%)	94 (85%)	17 (15%)		2	13
12	BQ	111/111 (100%)	94 (85%)	17 (15%)		2	13
13	AR	101/101 (100%)	80 (79%)	21 (21%)		1	6
13	BR	101/101 (100%)	79 (78%)	22~(22%)		1	5
14	AS	84/88~(96%)	67 (80%)	17 (20%)		1	6
14	BS	84/88~(96%)	72 (86%)	12 (14%)		3	15
15	AT	110/127~(87%)	99 (90%)	11 (10%)		7	30
15	BT	110/127~(87%)	100 (91%)	10 (9%)		9	34
16	AU	93/94~(99%)	83 (89%)	10 (11%)		6	27
16	BU	93/94~(99%)	77 (83%)	16 (17%)		2	10
17	AV	80/82~(98%)	63 (79%)	17 (21%)		1	5
17	BV	80/82~(98%)	63 (79%)	17 (21%)		1	5
18	AW	89/92~(97%)	75 (84%)	14 (16%)		2	12
18	BW	89/92~(97%)	78 (88%)	11 (12%)		4	21
19	AX	75/78~(96%)	67 (89%)	8 (11%)		6	27
19	BX	75/78~(96%)	66 (88%)	9 (12%)		5	22
20	AY	80/91 (88%)	70 (88%)	10 (12%)		4	21
20	BY	80/91 (88%)	72 (90%)	8 (10%)		7	30
21	AZ	159/179~(89%)	139 (87%)	20 (13%)		4	21
21	BZ	159/179~(89%)	137 (86%)	22 (14%)		3	16



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Mol	Chain	Analysed	Rotameric	Outliers	Perc	entiles
22	A0	59/67~(88%)	52 (88%)	7~(12%)	5	22
22	B0	59/67~(88%)	52 (88%)	7~(12%)	5	22
23	A1	78/83~(94%)	68~(87%)	10~(13%)	4	20
23	B1	78/83~(94%)	70 (90%)	8 (10%)	7	29
24	A2	65/67~(97%)	56~(86%)	9 (14%)	3	16
24	B2	65/67~(97%)	57 (88%)	8 (12%)	4	21
25	A3	49/52~(94%)	43 (88%)	6(12%)	5	22
25	B3	49/52~(94%)	43 (88%)	6~(12%)	5	22
26	A4	39/63~(62%)	32~(82%)	7~(18%)	2	9
26	B4	39/63~(62%)	30 (77%)	9~(23%)	1	3
27	A5	50/52~(96%)	43 (86%)	7(14%)	3	16
27	B5	50/52~(96%)	43 (86%)	7 (14%)	3	16
28	A6	50/52~(96%)	40 (80%)	10 (20%)	1	6
28	B6	50/52~(96%)	41 (82%)	9~(18%)	1	9
29	A7	41/42~(98%)	35~(85%)	6~(15%)	3	15
29	B7	41/42~(98%)	32 (78%)	9~(22%)	1	5
30	A8	52/55~(94%)	45 (86%)	7~(14%)	4	18
30	B8	52/55~(94%)	47 (90%)	5~(10%)	8	32
32	CB	177/220~(80%)	141 (80%)	36~(20%)	1	6
32	DB	177/220~(80%)	142 (80%)	35~(20%)	1	7
33	CC	114/188~(61%)	95~(83%)	19~(17%)	2	10
33	DC	114/188~(61%)	96 (84%)	18 (16%)	2	12
34	CD	139/181~(77%)	117 (84%)	22~(16%)	2	12
34	DD	139/181~(77%)	120 (86%)	19~(14%)	3	17
35	CE	108/123~(88%)	86 (80%)	22~(20%)	1	6
35	DE	108/123~(88%)	88 (82%)	20~(18%)	1	8
36	CF	77/90~(86%)	65~(84%)	12~(16%)	2	12
36	DF	77/90~(86%)	65 (84%)	12 (16%)	2	12
37	CG	$\overline{104/127}~(82\%)$	86 (83%)	18 (17%)	2	10
37	DG	104/127~(82%)	88 (85%)	16 (15%)	2	13
38	СН	103/119~(87%)	85 (82%)	18 (18%)	2	9



4	V	8	А	
4	V	8	А	

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
38	DH	103/119~(87%)	84 (82%)	19 (18%)	1	8
39	CI	62/99~(63%)	53 (86%)	9 (14%)	3	15
39	DI	62/99~(63%)	54 (87%)	8 (13%)	4	19
40	CJ	52/92~(56%)	42 (81%)	10 (19%)	1	8
40	DJ	52/92~(56%)	41 (79%)	11 (21%)	1	5
41	CK	81/99~(82%)	69~(85%)	12 (15%)	3	14
41	DK	81/99~(82%)	71 (88%)	10 (12%)	4	21
42	CL	92/109~(84%)	81 (88%)	11 (12%)	5	22
42	DL	92/109~(84%)	83 (90%)	9 (10%)	8	31
43	CM	63/101~(62%)	49 (78%)	14 (22%)	1	4
43	DM	63/101~(62%)	49 (78%)	14 (22%)	1	4
44	CN	46/50~(92%)	35 (76%)	11 (24%)	0	3
44	DN	46/50~(92%)	33 (72%)	13 (28%)	0	1
45	СО	77/80~(96%)	65 (84%)	12 (16%)	2	12
45	DO	77/80~(96%)	66 (86%)	11 (14%)	3	15
46	CP	63/74~(85%)	49 (78%)	14 (22%)	1	4
46	DP	63/74~(85%)	53 (84%)	10 (16%)	2	12
47	CQ	94/97~(97%)	90 (96%)	4 (4%)	29	64
47	DQ	94/97~(97%)	84 (89%)	10 (11%)	6	27
48	CR	49/77~(64%)	44 (90%)	5 (10%)	7	29
48	DR	49/77~(64%)	46 (94%)	3 (6%)	18	54
49	CS	42/80~(52%)	25 (60%)	17 (40%)	0	0
49	DS	42/80~(52%)	36 (86%)	6 (14%)	3	15
50	CT	65/82~(79%)	53 (82%)	12 (18%)	1	8
50	DT	65/82~(79%)	57 (88%)	8 (12%)	4	21
51	CU	18/22~(82%)	16 (89%)	2 (11%)	6	25
51	DU	18/22~(82%)	14 (78%)	4 (22%)	1	4
All	All	8652/9990 (87%)	7319 (85%)	1333 (15%)	2	13

5 of 1333 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	CH	19	VAL
	<i>a</i>	7	



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Mol	Chain	Res	Type
34	DD	158	ILE
40	CJ	16	LEU
37	CG	146	GLU
47	CQ	60	ILE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such side chains are listed below:

Mol	Chain	Res	Type
13	BR	13	HIS
40	DJ	13	HIS
35	CE	78	HIS
39	DI	124	GLN
45	DO	28	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2819/2915~(96%)	581 (20%)	59(2%)
1	BA	2819/2915~(96%)	586 (20%)	60~(2%)
2	AB	119/122~(97%)	25 (21%)	0
2	BB	119/122~(97%)	21~(17%)	0
31	CA	1496/1521~(98%)	339~(22%)	31 (2%)
31	DA	1496/1521~(98%)	341 (22%)	27~(1%)
All	All	8868/9116 (97%)	1893 (21%)	177 (1%)

5 of 1893 RNA backbone outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	AA	10	G
1	AA	14	А
1	AA	15	G
1	AA	34	С
1	AA	45	С

5 of 177 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	BA	2689	U
31	CA	1165	С
31	CA	60	А



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type
31	CA	428	G
31	DA	60	А

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	Chain	Chain	Chain	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
IVIOI	туре	Unam	Res	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
52	T8B	BA	3001	53	48,48,48	0.99	2 (4%)	63,71,71	1.22	8 (12%)			
52	T8B	AA	3001	53	48,48,48	0.99	2 (4%)	63,71,71	1.22	8 (12%)			

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
52	T8B	BA	3001	53	-	1/26/26/26	0/5/5/5
52	T8B	AA	3001	53	-	1/26/26/26	0/5/5/5

All (4) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
52	AA	3001	T8B	O11-C26	3.09	1.38	1.32
52	BA	3001	T8B	O11-C26	3.08	1.38	1.32
52	BA	3001	T8B	C25-C24	2.28	1.50	1.43
52	AA	3001	T8B	C25-C24	2.27	1.50	1.43

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
52	BA	3001	T8B	C21-C23-C24	-4.15	120.19	125.03
52	AA	3001	T8B	C21-C23-C24	-4.14	120.21	125.03
52	BA	3001	T8B	O5-C14-O6	3.13	120.29	116.44
52	AA	3001	T8B	O5-C14-O6	3.13	120.29	116.44
52	BA	3001	T8B	O11-C26-C25	2.76	124.96	121.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	AA	3001	T8B	C21-C23-C24-C25
52	BA	3001	T8B	C21-C23-C24-C25

There are no ring outliers.

2 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	BA	3001	T8B	23	0
52	AA	3001	T8B	31	0

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 sufficient must be highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	AA	2827/2915~(96%)	0.03	117 (4%) 37 24	46, 70, 113, 128	0
1	BA	2827/2915~(96%)	0.08	73 (2%) 56 40	27, 56, 110, 126	0
2	AB	120/122~(98%)	0.03	4 (3%) 46 30	68, 95, 108, 111	0
2	BB	120/122~(98%)	-0.24	0 100 100	46, 80, 95, 103	0
3	AD	275/276~(99%)	-0.15	0 100 100	45, 67, 82, 103	0
3	BD	275/276~(99%)	-0.16	2 (0%) 87 81	36, 59, 78, 103	0
4	AE	204/206~(99%)	-0.10	1 (0%) 91 86	47, 72, 87, 98	0
4	BE	204/206~(99%)	-0.18	0 100 100	33, 60, 81, 96	0
5	AF	203/205~(99%)	-0.34	2 (0%) 82 72	44, 77, 95, 112	0
5	BF	203/205~(99%)	-0.23	0 100 100	26, 64, 90, 110	0
6	AG	181/182~(99%)	1.35	52 (28%) 0 0	89, 106, 114, 116	0
6	BG	181/182~(99%)	0.10	8 (4%) 34 21	81, 101, 110, 118	0
7	AH	174/180~(96%)	0.91	37 (21%) 0 1	80, 93, 101, 108	0
7	BH	174/180~(96%)	-0.16	0 100 100	63, 78, 91, 98	0
8	AI	145/148~(97%)	0.59	21 (14%) 2 1	72, 104, 116, 123	0
8	BI	145/148~(97%)	-0.10	1 (0%) 87 81	68, 90, 98, 100	0
9	AN	140/140~(100%)	-0.08	1 (0%) 87 81	58,73,90,94	0
9	BN	140/140~(100%)	-0.19	0 100 100	38, 57, 82, 85	0
10	AO	122/122~(100%)	-0.33	0 100 100	56, 73, 85, 91	0
10	BO	122/122~(100%)	-0.22	0 100 100	43, 64, 82, 89	0
11	AP	147/150~(98%)	-0.01	4 (2%) 54 39	47, 81, 96, 105	0
11	BP	147/150 (98%)	-0.17	0 100 100	$28, 68, \overline{91, 100}$	0
12	AQ	141/141 (100%)	-0.04	1 (0%) 87 81	60, 78, 91, 97	0
12	BQ	$14\overline{1/141}\ (100\%)$	-0.09	0 100 100	44,65,78,88	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
13	AR	118/118~(100%)	-0.18	0 100 100	47,66,78,88	0
13	BR	118/118~(100%)	-0.19	0 100 100	35, 53, 69, 86	0
14	AS	110/112~(98%)	0.53	13 (11%) 4 2	74, 91, 102, 109	0
14	BS	110/112~(98%)	-0.13	0 100 100	58, 79, 93, 100	0
15	AT	131/146~(89%)	-0.22	1 (0%) 86 78	66, 76, 99, 109	0
15	BT	131/146~(89%)	-0.27	1 (0%) 86 78	55, 68, 91, 102	0
16	AU	116/118~(98%)	-0.05	0 100 100	53, 70, 84, 89	0
16	BU	116/118~(98%)	-0.15	0 100 100	34, 50, 70, 84	0
17	AV	101/101 (100%)	-0.19	1 (0%) 82 72	48, 79, 93, 103	0
17	BV	101/101 (100%)	-0.31	0 100 100	31, 61, 81, 95	0
18	AW	112/113~(99%)	-0.24	0 100 100	50, 59, 80, 104	0
18	BW	112/113~(99%)	-0.31	0 100 100	36, 45, 75, 106	0
19	AX	95/96~(98%)	-0.08	0 100 100	54, 71, 89, 93	0
19	BX	95/96~(98%)	-0.17	0 100 100	33, 59, 83, 91	0
20	AY	107/110~(97%)	0.15	7 (6%) 18 11	71, 81, 94, 105	0
20	BY	107/110~(97%)	-0.24	1 (0%) 84 75	56, 71, 89, 103	0
21	AZ	198/206~(96%)	0.01	7 (3%) 44 28	80, 92, 103, 108	0
21	BZ	198/206~(96%)	-0.35	0 100 100	64, 82, 97, 103	0
22	A0	76/85~(89%)	0.24	2 (2%) 56 40	59, 74, 84, 89	0
22	B0	76/85~(89%)	-0.24	0 100 100	46, 60, 74, 82	0
23	A1	97/98~(98%)	0.12	2 (2%) 63 49	54, 71, 94, 99	0
23	B1	97/98~(98%)	-0.08	1 (1%) 82 72	42,65,91,95	0
24	A2	70/72~(97%)	-0.05	1 (1%) 75 63	65, 81, 92, 101	0
24	B2	70/72~(97%)	-0.13	0 100 100	52, 70, 85, 102	0
25	A3	59/60~(98%)	0.46	5 (8%) 10 6	63, 74, 92, 101	0
25	B3	59/60~(98%)	-0.16	0 100 100	43, 56, 84, 94	0
26	A4	46/71~(64%)	0.54	7 (15%) 2 1	101, 109, 113, 119	0
26	B4	46/71~(64%)	0.26	6 (13%) 3 2	98, 107, 113, 118	0
27	A5	59/60~(98%)	-0.35	0 100 100	46, 64, 78, 91	0
27	B5	59/60~(98%)	-0.19	0 100 100	28, 52, 71, 89	0
28	A6	53/54~(98%)	0.14	3 (5%) 23 13	62, 76, 87, 89	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
28	B6	53/54~(98%)	-0.10	0 100 100	52,66,77,85	0
29	A7	48/49~(97%)	0.14	4 (8%) 11 6	43, 54, 79, 99	0
29	B7	48/49~(97%)	-0.00	1 (2%) 63 49	29, 44, 73, 89	0
30	A8	64/65~(98%)	0.13	0 100 100	60,68,76,85	0
30	B8	64/65~(98%)	0.13	0 100 100	45, 56, 65, 79	0
31	CA	1498/1521~(98%)	0.57	190 (12%) 3 2	59, 99, 120, 126	0
31	DA	1498/1521~(98%)	0.52	180 (12%) 4 2	65, 99, 120, 128	0
32	CB	229/256~(89%)	0.12	14 (6%) 21 12	93, 103, 111, 117	0
32	DB	229/256~(89%)	0.65	32 (13%) 2 1	95, 105, 112, 115	0
33	CC	206/239~(86%)	1.00	45 (21%) 0 0	92, 106, 112, 115	0
33	DC	206/239~(86%)	0.87	33 (16%) 1 1	97, 108, 115, 120	0
34	CD	208/209~(99%)	0.03	10 (4%) 30 18	85, 98, 108, 114	0
34	DD	208/209~(99%)	0.02	10 (4%) 30 18	87, 97, 107, 123	0
35	CE	148/162~(91%)	-0.14	4 (2%) 54 39	74, 93, 103, 110	0
35	DE	148/162~(91%)	0.10	5 (3%) 45 29	84, 96, 104, 110	0
36	CF	100/101~(99%)	-0.07	5 (5%) 28 16	80, 92, 101, 107	0
36	DF	100/101~(99%)	-0.14	3 (3%) 50 34	84, 93, 103, 110	0
37	CG	155/156~(99%)	2.14	77~(49%) 0 0	99, 109, 115, 120	0
37	DG	155/156~(99%)	2.07	75~(48%) 0 0	97, 109, 115, 119	0
38	CH	138/138~(100%)	0.05	4 (2%) 51 36	82, 94, 101, 104	0
38	DH	138/138 (100%)	-0.09	3 (2%) 62 48	86, 96, 102, 106	0
39	CI	125/128~(97%)	1.89	50 (40%) 0 0	97, 111, 117, 120	0
39	DI	125/128~(97%)	2.77	71~(56%) 0 0	100, 112, 118, 120	0
40	CJ	96/105~(91%)	2.13	43 (44%) 0 0	100, 109, 115, 117	0
40	DJ	96/105~(91%)	1.91	46 (47%) 0 0	97, 110, 115, 119	0
41	CK	114/129~(88%)	-0.12	1 (0%) 84 75	72, 93, 101, 105	0
41	DK	114/129~(88%)	0.22	4 (3%) 44 28	75, 95, 103, 107	0
42	CL	122/132 (92%)	-0.23	0 100 100	72, 85, 96, 100	0
42	DL	122/132 (92%)	-0.15	1 (0%) 86 78	77, 87, 96, 105	0
43	CM	114/126 (90%)	2.13	51 (44%) 0 0	102, 111, 118, 126	0
43	DM	$\overline{114/126}~(90\%)$	1.76	44 (38%) 0 0	101, 109, 115, 117	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(A^2)$	Q<0.9
44	CN	60/61~(98%)	1.19	15~(25%) 0 0	99, 108, 116, 118	0
44	DN	60/61~(98%)	1.59	21 (35%) 0 0	103, 111, 116, 122	0
45	CO	88/89~(98%)	0.02	2 (2%) 60 47	72, 91, 101, 107	0
45	DO	88/89~(98%)	0.18	5 (5%) 23 13	81, 93, 103, 107	0
46	CP	82/88~(93%)	0.62	6 (7%) 15 9	88, 96, 106, 112	0
46	DP	82/88~(93%)	0.43	3 (3%) 41 26	86, 94, 103, 111	0
47	CQ	99/105~(94%)	0.04	2 (2%) 65 51	78, 90, 98, 102	0
47	DQ	99/105~(94%)	0.17	3 (3%) 50 34	79, 92, 100, 103	0
48	CR	68/88~(77%)	0.15	9 (13%) 3 2	80, 91, 102, 103	0
48	DR	68/88~(77%)	0.21	3 (4%) 34 21	85, 93, 104, 106	0
49	CS	78/93~(83%)	2.61	44 (56%) 0 0	107, 111, 117, 123	0
49	DS	78/93~(83%)	2.84	52~(66%) 0 0	91, 112, 117, 119	0
50	CT	96/106~(90%)	0.18	3 (3%) 49 32	84, 93, 99, 102	0
50	DT	96/106~(90%)	0.69	10 (10%) 6 4	82, 92, 100, 101	0
51	CU	23/27~(85%)	2.89	12 (52%) 0 0	106, 112, 117, 119	0
51	DU	23/27~(85%)	2.65	13 (56%) 0 0	104, 109, 112, 113	0
All	All	20372/21160 (96%)	0.26	1591 (7%) 13 7	26, 84, 115, 128	0

The worst 5 of 1591 RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
39	CI	30	GLY	12.5
49	CS	40	ILE	12.5
43	CM	85	GLY	12.2
31	CA	1353	G	11.0
31	CA	1286	А	10.7

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, 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
52	T8B	AA	3001	44/44	0.85	0.28	20,20,20,20	0
53	MG	BA	3002	1/1	0.85	0.15	30,30,30,30	0
52	T8B	BA	3001	44/44	0.89	0.34	20,20,20,20	0
53	MG	BA	3003	1/1	0.94	0.16	30,30,30,30	0
53	MG	AA	3002	1/1	0.95	0.20	30,30,30,30	0
53	MG	AA	3003	1/1	0.98	0.17	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.

