

wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 - 10:08 am BST

PDB ID	:	4V9I
Title	:	Crystal structure of thermus thermophilus 70S in complex with tRNAs and
		mRNA containing a pseudouridine in a stop codon
Authors	:	Fernandez, I.S.; Ng, C.L.; Kelley, A.C.; Guowei, W.; Yu, Y.T.; Ramakrishnan,
		V.
Deposited on	:	2013-04-04
Resolution	:	3.30 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 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	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



Motrio	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1149(3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182(3.34-3.26)
RSRZ outliers	127900	1115(3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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 on 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	1504	4% 51%	39%	10%				
1	CA	1504	<u>6%</u> 52%	39%	9%				
2	AB	234	5%	32%	•				
2	СВ	234	65%	30%	5%				



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Mol	Chain	Length	Quality of chain		
	AC	00.0	2%		
3	AC	206	64%	30%	••
3	CC	206	62%	34%	· ·
			3%		
4	AD	208	63%	31%	5% •
4	CD	20.8	% •	2021	50/
	UD	200	61%	33%	5% •
5	AE	150	67%	27%	6%
F	CE	150	3%		
	<u> </u>	100	63%	33%	•
6	AF	101	72%	26%	•
	<u> </u>	101	2%		
6	CF	101	73%	25%	•
7	AG	155	75%	21%	
			9%		
7	CG	155	81%	17%	ό •
8	AH	138	69%	30%	
		100	2%		•
8	CH	138	75%	22%	•
0	AT	197	6%	000/	20/
- 3		121		20%	6%
9	CI	127	68%	29%	•
10	АТ	0.0	12%		
10	AJ	98	55%	36%	8% •
10	CJ	98	58%	34%	7% •
			3%		
11	AK	119	61%	36%	•
11	CK	119	72%	25%	<u> </u>
	~		6%		
12	AL	124	68%	29%	• •
19	CL	19/	6% 6004	260/	E04
		124	10%	20%0	3% •
13	AM	124	60%	31%	9%
10	CM	104	24%		
13		124	67%	27%	6%
14	AN	60	62%	33%	5%
			12%		
14	CN	60	65%	28%	7%
15	AO	88	б <u>6</u> %	27%	6% •



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Mol	Chain	Length	Quality of chain					
15	СО	88	2% 6 9%	24%	7%			
16	AP	83	^{2%} 64%	33%	•			
16	CP	83	65%	25%	8% •			
17	AQ	99	68%	28%				
17	CQ	99	^{2%} 76%	2:	1% •			
18	AR	70	% • 69%	26%				
18	CR	70	3%	26%	•			
19	AS	78	8%	40%	9% •			
19	CS	78	65%	28%	6%			
20	AT	99	4% 68%	24%	8%			
20	CT	99	^{2%}	21%	5%			
21	AU	24	58%	38%	· ·			
21	CU	24	58%	330%				
21	AV	77	% •	2204	1604			
22	CV	77	10%	240/	10%			
- <u>2</u> 2 - <u>2</u> 2		76	43%	54%0	10%			
20	AW	10	37% 42% 58%		20% •			
23	CW	76	47% 40%	41%	12%			
24	AY	75	5% 37% 52% 52%	47%	11%			
24	CY	75	5% 37%	47%	11%			
25	AX	7	43%	57%				
26	BA	2915	42% 37%	15	5% • •			
26	DA	2915	45% 3	8%	13% • •			
27	BB	119	49%	33%	18% •			
27	DB	119	47%	43%	10%			
28	BC	206	58% 65%	23%	• 8%			



	Onam	Length	Quant		
29	BD	271	46%	40%	11% •
29	DD	271	55%	35%	7% •
30	BE	204	% 50%	37%	11% •
30	DE	20.4	2%	2004	
00		204	2%	39%	9%
31	BF	207	3% 3%	31%	12% •
31	DF	207	57%	36%	7%
32	BG	181	58%	32%	8% •
32	DG	181	54%	41%	6%
33	BH	159	52%	33%	11% •
33	DH	159	73%	19%	6% •
34	BI	145	%	2704	6%
24		145	3%	2175	070
		140	49%	34%	5%
35	BJ	130	78% 67%		19% •
35	DJ	130	76%	18	% 5%
36	BN	138	43%	42%	13% •
36	DN	138	2% 5 6%	30%	12% •
37	ВО	122	64%	34%	<mark>.</mark>
37	DO	122	67%	30%	•
38	BP	146	2%	2006 2506	806
20	מת	146	3%	2370 2370	070
30		140	34% %	42% 19	9% 5%
39	BQ	141	62% 2%	30%	8%
39	DQ	141	72%	23%	· •
40	BR	117	49%	40%	9% •
40	DR	117	46%	48%	6%
41	BS	98	40%	40%	17% •

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Mol

Chain Length Quality of chain 3% DS 98 4156% 33% 8% • 4% BT4213736% 42% 20% • 4% 42DT 13739% 41% . 18% ΒU 4311732% 56% 9% . 4% 43DU 11762% 30% 8% % 44 ΒV 10149% 6% 32% 14% 11% DV 44 10151% 35% 11% • % BW451135% • 54% 40% 4% DW 4511363% 30% 6% • BX469266% 25% 9% DX 469264% 26% 8% • 10% BY1004729% 42% 23% 6% 13% 47DY 100• 39% 41% 17% 31% BZ48 17676% 20% • 38% DZ 17648 70% 27% • 49B084 61% 36% • 8% 49D0. 84 62% 37% 3% B1509361% 33% 5% 2% 50D193. . 59% 34% 3% B2517151% 35% 13% . % 51D2716% • 73% 20% 3% 52 B35953% 44% • 8% 52D35973% 25% • 3% B4305347% 43% 7%• 7% D4533060% 37% .

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Mol	Chain	Length		Quality of chain							
54	B5	59	5%		41%	1	5% •				
54	D5	59	5%	59%	22%	15	•				
55	B6	44	5% 7%	55%		27%	11%				
55	D6	44	2% 11%	55%	_	30%	5%				
56	B7	48	2%	63%		35%	•				
56	D7	48	2%	58%		38%	•				
57	B8	63	30%		49%	179	/0 •				
57	D8	63	3%		44%		• 6%				
58	B9	36	47%	6	42%		8% •				
58	D9	36	11%	75%		19%	6%				
59	CX	4	25%	25%		50%					
60		106		73%		010/					
60	DC	196		73%		21%					

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	PSU	AX	19	-	-	Х	-



2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 295724 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues		I	Atoms		ZeroOcc	AltConf	Trace	
1		AA 1504	Total	С	Ν	Ο	Р	0	0	0
L T			32329	14390	5992	10444	1503	0	0	U
1		1504	Total	С	Ν	Ο	Р	0	0	0
	1504	32329	14390	5992	10444	1503	0	0	0	

• Molecule 2 is a protein called 30S Ribosomal protein S2.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
2	AB	234	Total	С	Ν	Ο	S	0	0	0
	AD	234	1901	1213	341	342	5	0	0	
0	CB	CB 234	Total	С	Ν	Ο	S	0	0	0
	СВ		1901	1213	341	342	5	0	0	0

• Molecule 3 is a protein called 30S Ribosomal protein S3.

Mo	l Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
3		206	Total	С	Ν	Ο	S	0	0	0
J	AU	200	1613	1016	314	282	1	0	0	0
2	CC	206	Total	С	Ν	Ο	S	0	0	0
1 3		200	1613	1016	314	282	1	0	0	0

• Molecule 4 is a protein called 30S Ribosomal protein S4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4		208	Total	С	Ν	Ο	\mathbf{S}	0	0	0
4	AD	208	1703	1066	339	291	7	0	0	0
4	CD	208	Total	С	Ν	Ο	S	0	0	0
4	CD	208	1703	1066	339	291	7	0	0	0

• Molecule 5 is a protein called 30S Ribosomal protein S5.



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	AE	150	Total 1147	С 724	N 217	O 202	S 4	0	0	0
5	CE	150	Total 1147	C 724	N 217	O 202	$\frac{S}{4}$	0	0	0

• Molecule 6 is a protein called 30S Ribosomal protein S6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6		101	Total	С	Ν	Ο	S	0	0	0
0	Аг	101	843	531	155	154	3	0	0	0
6	CF	101	Total	С	Ν	0	S	0	0	0
0	UL	101	843	531	155	154	3	0	0	0

• Molecule 7 is a protein called 30S Ribosomal protein S7.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	AG	155	Total 1257	C 781	N 252	O 218	${f S}{f 6}$	0	0	0
7	CG	155	Total 1257	C 781	$rac{N}{252}$	O 218	S 6	0	0	0

• Molecule 8 is a protein called 30S Ribosomal protein S8.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	лц	128	Total	С	Ν	Ο	\mathbf{S}	0	0	0
0	AII	130	1116	705	215	193	3	0	0	0
0	СН	128	Total	С	Ν	Ο	S	0	0	0
0		130	1116	705	215	193	3	0	0	0

• Molecule 9 is a protein called 30S Ribosomal protein S9.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
0	ΔŢ	197	Total	С	Ν	Ο	0	0	0
9	AI 12	127	1011	639	198	174	0	0	0
0	CI	197	Total	С	Ν	Ο	0	0	0
9		127	1011	639	198	174	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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



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 $\bullet\,$ Molecule 10 is a protein called 30S Ribosomal protein S10.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	AT	08	Total	С	Ν	Ο	S	0	0	0
10	AJ	90	795	499	156	139	1		0	0
10	CI	0.8	Total	С	Ν	Ο	S	0	0	0
10	UJ UJ	90	795	499	156	139	1	0	0	0

• Molecule 11 is a protein called 30S Ribosomal protein S11.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
11	AK	110	Total	С	Ν	Ο	S	0	0	0
		119	885	549	168	165	3	0	0	0
11	CK	110	Total	С	Ν	0	S	0	0	0
		119	885	549	168	165	3			U

• Molecule 12 is a protein called 30S Ribosomal protein S12.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
19	ΔT	194	Total	С	Ν	Ο	S	0	0	0
	12 AL	124	971	611	195	164	1	0	0	0
19	CI	194	Total	С	Ν	Ο	S	0	0	0
12		124	971	611	195	164	1	0	0	0

• Molecule 13 is a protein called 30S Ribosomal protein S13.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
12	АМ	194	Total	С	Ν	Ο	\mathbf{S}	0	0	0
10		124	988	611	205	170	2	0	0	0
12	CM	194	Total	С	Ν	Ο	S	0	0	0
10	UM	124	988	611	205	170	2	0	0	0

• Molecule 14 is a protein called 30S Ribosomal protein S14.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
14	AN	60	Total	С	Ν	Ο	\mathbf{S}	0	0	Ο
14		00	492	312	104	72	4	0	0	
14	CN	60	Total	С	Ν	Ο	\mathbf{S}	0	0	0
		00	492	312	104	72	4	0	U	0

• Molecule 15 is a protein called 30S Ribosomal protein S15.



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
15		88	Total	С	Ν	Ο	S	0	0	Ο
	АО	00	734	459	147	126	2	0	0	0
15	CO	88	Total	С	Ν	Ο	S	0	0	Ο
		88	734	459	147	126	2	0	0	0

• Molecule 16 is a protein called 30S Ribosomal protein S16.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
16	٨D	0.2	Total	С	Ν	Ο	\mathbf{S}	0	0	0
10	AI	00	701	443	139	118	1	0	0	0
16	CD	0.2	Total	С	Ν	0	S	0	0	0
10		00	701	443	139	118	1		0	U

• Molecule 17 is a protein called 30S Ribosomal protein S17.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
17	AQ	99	Total 824	C 528	N 151	О 143	${ m S} { m 2}$	0	0	0
17	CQ	99	Total 824	C 528	N 151	0 143	S 2	0	0	0

• Molecule 18 is a protein called 30S Ribosomal protein S18.

Mol	Chain	Residues		Ator	\mathbf{ns}		ZeroOcc	AltConf	Trace
18	AR	70	Total	С	Ν	Ο	0	0	0
10	АЦ	10	574	367	112	95	0	0	0
18	CB	70	Total	С	Ν	0	0	0	0
10		10	574	367	112	95	0		

• Molecule 19 is a protein called 30S Ribosomal protein S19.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	٨٩	79	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	AB	10	630	403	114	111	2	0	0	0
10	CC	79	Total	С	Ν	0	S	0	0	0
	05	10	630	403	114	111	2	0	0	0

• Molecule 20 is a protein called 30S Ribosomal protein S20.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	AT	99	Total 763	$\begin{array}{c} \mathrm{C} \\ 470 \end{array}$	N 162	O 129	${ m S} { m 2}$	0	0	0



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	CT	99	Total 763	C 470	N 162	O 129	${ m S} { m 2}$	0	0	0

• Molecule 21 is a protein called 30S Ribosomal protein THX.

Mol	Chain	Residues		Aton	ıs		ZeroOcc	AltConf	Trace
91	ATI	94	Total	С	Ν	Ο	0	0	0
	AU	24	209	128	50	31	0	0	0
01	CU	24	Total	С	Ν	0	0	0	0
		24	209	128	50	31	0	0	0

• Molecule 22 is a RNA chain called P-SITE tRNA.

Mol	Chain	Residues		\mathbf{A}	toms			ZeroOcc	AltConf	Trace
- 22	AV	77	Total	С	Ν	Ο	Р	0	0	0
	AV		1640	732	297	535	76	0	0	0
- 22	CV	77	Total	С	Ν	0	Р	0	0	0
			1640	732	297	535	76			U

• Molecule 23 is a RNA chain called E-SITE tRNA.

Mol	Chain	Residues		\mathbf{A}	toms			ZeroOcc	AltConf	Trace
23	AW	76	Total 1619	С 723	N 290	O 531	Р 75	0	0	0
23	CW	76	Total 1619	С 723	N 290	O 531	Р 75	0	0	0

• Molecule 24 is a RNA chain called A-SITE tRNA.

Mol	Chain	Residues		\mathbf{A}	toms			ZeroOcc	AltConf	Trace
24	AV	75	Total	С	Ν	Ο	Р	0	0	0
24	AI	10	1619	722	309	514	74	0	0	0
24	CV	75	Total	С	Ν	0	Р	0	0	0
24	UI	10	1619	722	309	514	74	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	?	-	С	DELETION	GB 443419838
CY	?	-	С	DELETION	GB 443419838

• Molecule 25 is a RNA chain called mRNA.



Mol	Chain	Residues		\mathbf{At}	\mathbf{oms}			ZeroOcc	AltConf	Trace
25	ΛV	7	Total	С	Ν	Ο	Р	0	0	0
20			151	68	29	47	7			U

• Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues			Atoms			ZeroOcc	AltConf	Trace
26	BA	2807	Total 60459	C 26907	N 11311	O 19435	Р 2806	0	0	0
26	DA	2807	Total 60459	C 26907	N 11311	O 19435	Р 2806	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1151	А	G	CONFLICT	GB 55771382
DA	1151	А	G	CONFLICT	GB 55771382

• Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues		\mathbf{A}	toms			ZeroOcc	AltConf	Trace
27	BB	119	Total 2551	C 1136	N 471	O 826	Р 118	0	0	0
27	DB	119	Total 2551	C 1136	N 471	O 826	Р 118	0	0	0

• Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues		Ato	\mathbf{ms}		ZeroOcc	AltConf	Trace
28	BC	190	Total 1157	C 706	N 220	O 231	0	0	0

• Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
20	дд	971	Total	С	Ν	Ο	\mathbf{S}	0	0	0
		271	2105	1329	416	357	3	0	0	0
20	מת	971	Total	С	Ν	0	S	0	0	0
		271	2105	1329	416	357	3	0	0	0

• Molecule 30 is a protein called 50S ribosomal protein L3.



Mol	Chain	Residues		\mathbf{At}	\mathbf{oms}			ZeroOcc	AltConf	Trace
20	DF	20.4	Total	С	Ν	Ο	S	0	0	0
50	DE	204	1564	988	299	271	6	0	0	0
20	ΠF	20.4	Total	С	Ν	Ο	S	0	0	0
30	DĽ	204	1564	988	299	271	6	0	0	0

• Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
21	BE	207	Total	С	Ν	Ο	S	0	0	0
101	Dr	207	1624	1035	303	283	3	0	0	0
91	DE	207	Total	С	Ν	Ο	S	0	0	0
101		207	1624	1035	303	283	3	0	0	0

• Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
32	BG	181	Total 1474	C 942	N 268	O 260	S 4	0	0	0
32	DG	181	Total 1474	C 942	N 268	O 260	S 4	0	0	0

• Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
22	рц	150	Total	С	Ν	Ο	\mathbf{S}	0	0	0
00	DII	109	1223	773	228	221	1	0	0	0
22	рц	150	Total	С	Ν	Ο	S	0	0	0
00		109	1223	773	228	221	1	0	0	0

• Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
24	BI	145	Total	С	Ν	Ο	\mathbf{S}	0	0	0
04	DI	140	1132	723	200	208	1	0	0	0
24	ות	145	Total	С	Ν	0	S	0	0	0
04		140	1132	723	200	208	1	0	0	0

• Molecule 35 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
35	BJ	130	Total 651	C 390	N 130	O 131	0	0	0



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Mol	Chain	Residues		Ato	\mathbf{ms}		ZeroOcc	AltConf	Trace
35	DJ	130	Total 651	m C m 390	N 130	О 131	0	0	0

• Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
26	BN	128	Total	С	Ν	Ο	S	0	0	0
- 50	DN	130	1105	712	206	183	4	0	0	0
26	DN	128	Total	С	Ν	Ο	S	0	0	0
- 50		130	1105	712	206	183	4	0	0	0

• Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
27	BO	199	Total	С	Ν	Ο	\mathbf{S}	0	0	0
51	DO	122	933	588	171	170	4	0	0	0
27	DO	199	Total	С	Ν	0	S	0	0	0
51		122	933	588	171	170	4	0	0	0

• Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
38	BD	146	Total	С	Ν	Ο	S	0	0	0
00		140	1114	692	227	193	2	0	0	0
90	סת	146	Total	С	Ν	Ο	S	0	0	0
30		140	1114	692	227	193	2			U

• Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
39	BQ	141	Total 1122	C 715	N 212	O 188	S 7	0	0	0
39	DQ	141	Total 1122	C 715	N 212	0 188	S 7	0	0	0

• Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
40	BB	117	Total	С	Ν	Ο	0	0	0
40	DR		960	599	202	159	0	0	0
40	סח	117	Total	С	Ν	Ο	0	0	0
40	DR		960	599	202	159	0	0	0



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• Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
41	BC	08	Total	С	Ν	Ο	0	0	0
41		90	771	486	154	131	0	0	0
41	חפ	08	Total	С	Ν	Ο	0	0	0
1 41	60	30	771	486	154	131		0	

• Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
49	вт	127	Total	С	Ν	Ο	S	0	0	0
42	DI	197	1142	710	234	197	1	0	0	0
49	рт	127	Total	С	Ν	0	S	0	0	0
42		197	1142	710	234	197	1	0	0	0

• Molecule 43 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
/3	BII	117	Total	С	Ν	Ο	S	0	0	0
40	DU	111	958	604	202	151	1	0	0	0
12	рц	117	Total	С	Ν	Ο	S	0	0	0
40	D0		958	604	202	151	1	0		0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	32	ALA	PHE	CONFLICT	UNP P60491
DU	32	ALA	PHE	CONFLICT	UNP P60491

• Molecule 44 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		Atoms					AltConf	Trace
44	BV	101	Total	С	Ν	Ο	\mathbf{S}	0	0	0
44	DV	101	779	501	142	135	1	0	0	0
44	DV	101	Total	С	Ν	Ο	\mathbf{S}	0	0	0
44		101	779	501	142	135	1	0	U	U

• Molecule 45 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BW	113	Total 896	$ m C \ 563$	N 176	O 155	${ m S} { m 2}$	0	0	0



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	DW	113	Total 896	C 563	N 176	O 155	${ m S} 2$	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	113	ALA	LYS	CONFLICT	UNP Q5SHP3
DW	113	ALA	LYS	CONFLICT	UNP Q5SHP3

• Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
46	РV	0.2	Total	С	Ν	Ο	0	0	0
40 DA	92	726	471	131	124	0	0	0	
46	DV	0.2	Total	С	Ν	Ο	0	0	0
40 DA	DA	\mathcal{P}_{Λ} 92	726	471	131	124	0	0	U

• Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BV	100	Total	С	Ν	Ο	S	0	0	0
41	DI	100	776	500	148	124	4	0	0	0
47	DV	100	Total	С	Ν	Ο	S	0	0	0
41		100	776	500	148	124	4	0	0	0

• Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
48	BZ	176	Total 1404	C 897	N 252	O 253	${ m S} { m 2}$	0	0	0
48	DZ	176	Total 1404	C 897	N 252	O 253	S 2	0	0	0

• Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
40	BU	8.4	Total	С	Ν	Ο	\mathbf{S}	0	0	0
49	BU 84	04	662	410	140	111	1	0	0	0
40	DO	Q /	Total	С	Ν	0	S	0	0	0
49	DU	04	662	410	140	111	1	0	0	0

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



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	R1	03	Total	С	Ν	Ο	\mathbf{S}	0	0	0
00	DI	90	734	460	147	126	1	0	0	0
50	D1	0.3	Total	С	Ν	Ο	S	0	0	0
- 50		90	734	460	147	126	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	ARG	LYS	CONFLICT	UNP P60494
D1	81	ARG	LYS	CONFLICT	UNP P60494

• Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
51	Bu	71	Total	С	Ν	Ο	S	0	0	0
51	D2		598	370	121	106	1	0	0	0
51	D9	71	Total	С	Ν	Ο	S	0	0	0
51			598	370	121	106	1	0	0	0

• Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
50	D3	50	Total	С	Ν	Ο	\mathbf{S}	0	0	0
02	D0		468	298	90	79	1	0	0	0
50	D3	50	Total	С	Ν	Ο	S	0	0	0
02	100		468	298	90	79	1		0	0

• Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
52	P/	20	Total	С	Ν	Ο	S	0	0	0
00	D4		226	142	36	44	4	0	0	0
59	D4	20	Total	С	Ν	Ο	S	0	0	0
00		50	226	142	36	44	4			

• Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
54	R5	50	Total	С	Ν	Ο	S	0	0	0
04	D0	09	459	288	90	76	5	0	0	0
54	D5	50	Total	С	Ν	Ο	S	0	0	0
04	D0	09	459	288	90	76	5	0	0	0



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• Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
55	B6	4.4	Total	С	Ν	Ο	\mathbf{S}	0	0	0
00	DU	44	381	235	77	65	4	0	0	0
55	De	4.4	Total	С	Ν	Ο	S	0	0	0
00		44	381	235	77	65	4		U	

• Molecule 56 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
56	B7	48	Total	С	Ν	Ο	\mathbf{S}	0	0	0
50	Di	40	419	257	104	56	2	0	0	0
56	D7	18	Total	С	Ν	Ο	\mathbf{S}	0	0	0
00		40	419	257	104	56	2	0	U	

• Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
57	B8	63	Total	С	Ν	Ο	S	0	0	0
01	DO	00	508	326	101	79	2	0	0	0
57	D8	63	Total	С	Ν	Ο	S	0	0	0
57	Do	0.5	508	326	101	79	2	0	0	0

• Molecule 58 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
58	B0	36	Total	С	Ν	Ο	S	0	0	0
00	D9		299	183	67	46	3	0	0	0
59	D0	26	Total	С	Ν	Ο	S	0	0	0
00	D9	- 50	299	183	67	46	3	0	0	0

• Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues		\mathbf{At}	\mathbf{oms}			ZeroOcc	AltConf	Trace
59	CX	4	Total 85	C 38	N 14	O 29	Р 4	0	0	0

• Molecule 60 is a protein called 50S Ribosomal protein L1.

Mol	Chain	Residues		Ato	\mathbf{ms}		ZeroOcc	AltConf	Trace
60	DC	190	Total 1157	C 706	N 220	О 231	0	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: 16S ribosomal RNA















• Molecule 6: 30S Ribosomal protein S6









• Molecule 9: 30S Ribosomal protein S9





• Molecule 9: 30S Ribosomal protein S9



• Molecule 10: 30S Ribosomal protein S10





• Molecule 10: 30S Ribosomal protein S10









• Molecule 16: 30S Ribosomal protein S16 Chain CP: 65% 25% 8% V5. E5. • Molecule 17: 30S Ribosomal protein S17 Chain AQ: 68% 28% L31 Y32 G33 K34 V35 • Molecule 17: 30S Ribosomal protein S17 Chain CQ: 76% 21% • Molecule 18: 30S Ribosomal protein S18 Chain AR: 69% 26% D33 Y34 R35 R35 F43 F43 L44 C44 E46 E46 E46 F47 T47 R54 T56 G57 C57 • Molecule 18: 30S Ribosomal protein S18 Chain CR: 70% 26% • Molecule 19: 30S Ribosomal protein S19 Chain AS: 49% 40% 9% Y80 R81 • Molecule 19: 30S Ribosomal protein S19 35% Chain CS: 65% 28% 6%













5 5		D 13	5 0	- D I	o ∎ i	9 ¥	¥	9 0	¥	5 5	G	A U	C		n	n ·	A A	A	ე ა	1 13	Þ	50	5	D A	Å	∩ ¥	5	ם ני	р.	C Þ	Ω	A1151	U1153	C1154 C1155	A1156	G1157 11158	G1159	61160	<mark>C1163</mark>
G1167		61170 A1171	A1172 A1173	A1174 11175	61176 61176	A1177 U1178	C1179	G1180 G1181	G1182	G1183 C1184	U1185	U1186 A1187	A1188	G1189	C1197	C1198	G1199 A1200	A1201	G1202	U1204		6 T 2 0 3	U1212	G1215	G1216	6121/ A1218	U1219	61220 A1221	C1222	C1223	G1228	C1229	G1231	U1232	G1234	G1235	A1238	61239	C1245
A1 248	01249	<mark>C1252</mark>	G1253 A1254	U1255		C1261	A1264	C1266 C1266	C1267	G1268 C1269	G1270	41271 61272		01279 61280	G1281	A1282	61283 61284	U1285	A1286 A1287		G1290	A1291 A1292	G1293	01294 G1295	C1296	61297 A1298	A1299	01301 G1301	C1302	G1305	C1306	A1307	G1309	A1310	U1312	A1313 A1314	C1315	61316 A1317	<mark>U1318</mark>
A1319 A1320	04044	A1323 G1324	G1325 G1326	A1 200	G1330	A1331 A1332	U1333	U1337	C1338	01339 C1340		01345 A1346	A1347	C1351	A1352	A1353	61304	01357	U1358 C1350		C1363	61365 C1365	A1366	61370	U1371	C13/2	A1376	G13//	G1383	61384	A1 <mark>3</mark> 87	00010	61391 61391	G1392	A1394	C1395 C1306	U1397	G1401	U1402
G1403 A1404	A1405	G1406	A1410 A1411	A1412	G1414	C1415	C1421	61422 A1423	A1424	G1425	A1429	G1430 C1431		01436	U1439	A1440	01441 01442	C1443	C1448	C1449	U1450 114454	01451 C1452	C1453	A1457	G1458	01460 U1460	G1461	C 1402	U1465	A1472	C1473	G1474	U1476		U1483	A1484 G1485		61488 61489	A1490
C1404	A1495	G1496 C1497	C1498 A1499	U1500		C1504 G1505	A1506	61907	C1513	G1516	A1517	A1518	G1521	C1522 41523	G1524	G1525	61526 U1527	G1528	61529 61530		A1535	G 1537	C1538	A1539 A1540	A1541	01542 C1543	C1544	61546 C1546	C1547	01548 C1549	C1550	C1551 A1657	A1553	C1554	A1556	G1557 C1558	U1559	G1564	<mark>U1565</mark>
61 570		A1574 G1575	C1576 C1577	C1578	n .	G A	5 5	უ ლ	'n	A G	C1589	A1591 A1591		C1595	A1600	1001	A1604 G1605		A1612 A1613	G1614	A1615	A1010 A1617	A1618	G1619 C1620	C1621	01622 C1623	U1624	A1626		C1630 A1631	A1632	C1633	01035 01635	G1636	G1638	G1639 G1640		C1643 C1644	<mark>C1645</mark>
G1646 111647	A1648	C1649 C1650	G1651 C1652	A1653 A165A	A1655	C1656	A1661	C1662 A1663		C1670 G1671		A1683 C1684	U1685	C1686 A1687	G1688	G1689	G1691	C1692	G1693 C1694		A1698	A1700	A1701	C1702 C1703	C1704	q0/I0	G1713	C1716	U1717	G1720		G1724 111725	01726 U1726	G1727	C1729	C1730	01734		01 <mark>7</mark> 39
C1740	G1742	G1743 A1744	G1745 A1746	A1747	617 49	G1763	01764	61/65 A1766	U1767	G1768 A1769	<mark>61770</mark>	C1771 C1772		G1775 G1776	G1777	G1778	G1780		G1783 C1784		A1789	A1792	G1793	6179 4	C1801	61802 A1803	C1804	01805 61806	U1807	01808 01809	A1810	C1811	A1814	A1815 A1816	A1817	C1818 A1810	C1820	12.91W	01 <mark>8</mark> 24
808	G1829	C1830 G1831	A1832 A1833	A1020	CODTW	A1842 G1843	G1844	A1845 G1846	G1847	01848 A1849	U1850	A1851 G1852	G1853	G1854 41855	G1856	C1857	61858 A1859	C1860	C1865		C1868	G1870	U1871	G1872 C1873	C1874	61875 61876	A1877	A18/8 G1879		61887 61888	A1889	114 80.4	G1895	C1896	A1898	G1899	C1901	C1903	<mark>61904</mark>
A1905 A1006	C1907	61908 61909	A1910 A1911	1101R	G1917	G1918 U1919	<mark>G1920</mark>	A1921 A1922	C1923	61924	<mark>61927</mark>	61928 C1929	C1930	61931 11932	A1933	A1934	01936 U1936	A1937	U1938 A1030	A1940	C1941	61943	U1944	C1945 C1946	U1947	A1948 A1949	G1950	61951 U1952	A1953	61954 C1955	G1956	A1957	A1959	111067	C1968	A1073	A1974	CVELD U1976	<mark>U1977</mark>
C1083	U1984	61985	C1988 G1989	A1990	A1992	A1993	<mark>G2001</mark>	A2002 C2003		G2008 C2009	<mark>G</mark> 2010	C2011 U2012	G2013	02014 C2015		G2018	61029	<mark>C2029</mark>	G2030 G2031		A2034	A2035 A2036	U2037	02038 G2039	A2040	A2041 C2042	U2043	G2045	C2046	C2047 G2048	U2049	G2050 A2051	A2052	G2053 A2054	U2055	G2056 C2057	G2058	U2062	<mark>A2063</mark>
C2064	G2070	C2071 A2072	G2073 G2074	A2075	G2077	A2078	A2081	G2082 A2083	C2084	C2085 C2086	<mark>C2087</mark>	G2088 U2089	G2090	62091 42092	g2093		U2096 U2097	A2098	C2099	A2 103	G2104	C2106 C2106	U2107	G2108	U2113	62114 62115	C2116	0211/ C2118	U2119	02120 G2121	G2122	U2123	62125	C2126		G2131	G2133	U2134	<mark>G2136</mark>
G2137	U2139	A2140 G2141	G2142 • U2143 •	G2144 C2144	G2146	A2147 G2148	C2149	U2151	<mark>G2152</mark>	02153 62154	A2 155	A2156 C2157		C2 160	<mark>C2164</mark>	U2165	C2167	G2168	G2169 C2170		G2174	G2176	G2 177	G2178 A2179	G 2180	G2181 C2182	G2183	C2184 C2185	G2186	6218/	A2192	U2193	C2195	C2196	C2198	C2199	U2201	G2202 G2203	<mark>C2204</mark>





A260	0264 C265	C266	G268	0209 0270	U271 G272	0273 C274	C275	<mark>G276</mark> G277		6282 6283	U284	6286 6286	U D	G289 G289	<mark>6290</mark>	C294	U295 0206	6297 6297	<mark>G298</mark> A	104	A C302	C303 G304	CTOV	6313	6318	<mark>C319</mark> C320	<mark>6321</mark>	A322 A323	G327		6330 6331	<mark>6332</mark> A333	A334 G335	C336 A337	
C342 A343	6344 1345	6346 6347		6350 U351	<mark>G352</mark> A353	A354 A355	G356	C357	C360	6361 U362	Loop Loop	6365 C366		0374 6374	6375		6379	A380 U381	113.85	G386	A387 G388	<mark>(389</mark> (390	U391 A207	C393	C394	A397 G398		6412 0413	G414 G415	A416	<mark>6417</mark> C418	C419 A420	U421 6422	U431	G432
G433 G434	C435 G436	6437 4437	C439	0	<mark>6444</mark> C445	C446 U447	A448	A449	A454	A455 G456	U L L L	0459 0460		00F 0	C469	6471 6471	A472 11473	04/3 A474	C480	C481	A482 G483	<mark>6</mark> 488	U489	G492	G 493 G 494	<u>A495</u> <u>A496</u>	A497	6498 6499	U500	A504	4505 6506	A507 A508	G515	4516 6517	G518
<mark>G519</mark> G520	6524	A525 A525	A527	0528 A529	6532	0533 0534	U535	6536 A537		G545 G546	C547	0549 0549	A550	4552 A552	4553 2554	C555	A556		6563 C564	C565	C567	5 5	A570 A571	G572	G575	U576	6581	6583	U584 G585		0590 0591	G592 A593	A594 (595	C596 A597	U598
G599 A600	(1000) (1600)	C603	G605	A608	C609 U610	C611	<mark>6620</mark>	6621 6622	<mark>C623</mark>	<mark>G624</mark> A625	6626	0627 0628	U629	<mark>6632</mark>	0633	G635	U636	063 <i>8</i> 6638	A639 G640	6641	0642 6643	G644 A645	G646	60 [±] / C648	G649 U650	A651 G652		4655	A661 G662	0663	C664	A667 A668	C669 A670	G671	C674
G675 C676	A	: 15 C) ლ (., .,	00	5 0	Å	ი ი	D I	• •	00	ວບ	5 5	₽ C	A	6702	U703	C7 05 C7 05	G706 C707	G708	G7 10 C7 10	G7 15	A7 16 C7 17	CT 18	C7 19 G7 20	A721 A722	A7 23	C/ 24	G727 G728		A731 G732	A735	G736 C737	G7 46	G7 47
A752	G753 C754	U755	G763	A/04	A768 G769	U770 G771	G772	A773 G774	G775	C776	<mark>6779</mark>	A780 A781	C782	G784 G784	G785 11786	G787		6791 A792	U793 G794		A797 A798	<mark>C799</mark> C800	C801	U803	C804	4807 U808	G809	A810 G811	G816	G817	C818 U819	<mark>4820</mark> G821	G822	<mark>G826</mark> A827	A828
<mark>4829</mark> 4830	6831 C832	U833 4834	A835	C830 C837	<mark>G838</mark> A839	6840 C841		A848	G851	0852 U853	4050	U859 U859	<mark>C860</mark>	<mark>0863</mark>	G864 4865	A866	A867	U873	U874 4875	G876	G877 G878	U879 C880	A881	G883	<mark>C884</mark> U885	<mark>(888</mark>		6891 C892	U893 G894	<u>A895</u>		<mark>C903</mark> U904	6905 U906	A907	A912
A916		P COV	G925	G 928	(<u>1929</u> (1930	<mark>C931</mark> C932	A933	C934 C935	A936	G 937 C938	C939	0940 A941	C942	C943 A944	A945	C948	C949	0952	C953 4954	A955	<mark>C959</mark>	<mark>C960</mark> G961	A962	6964 G964	6965 6966	0967 0968		G973 G973	0974 0975	G976	A977 G978	U981	<mark>6982</mark>	A985 G986	1987
<mark>G988</mark> A989	(9990 1990	<mark>6992</mark>	<mark>6996</mark>	U1002	A1003 A1004	C1005 G1006	U1007	C1008 C1009	G1010	U1013	C1014	A1017	G1018	C1021	61022	A1025	A1026	G1027 A1028	61032		C1036 C1037	G1038 C1039	C1040	61042	C1043 U1044	A1045 A1046	G1047	G1048 C1049	C1050 C1051		A1054 A1055	G1056 U1057	C1058 U1059	G1060	U1064
A1065 A1066	G1067 111068	G1069 G1070	11071		G1075 G1076	A1077	C1083	G1084 C1085	C1086	61087 C1088	G1089	A1090 A1091	G1092	C1094	A1095	C1097	C1098	4 U	G	1 15 1	.9 D	DU	55	20	U A	G A	Å	5 0	A D	יס	A C	טכ	C C	n	Ā
A A	G	101) (5 5	U A	A U	Ā	5 5	Ū	D 4	0:	U A1151	G1152	C1154	G1155 A1156	G1157	U1158	G1159 G1160	C1161 C1162	C1163	G1167	C1168	A1173	A11/7 U1175	G1176	C1179 G1180	G1181	61182 61183	C1184 U1185	U1186	A1187 A1188	G1189	61194 C1195	C1198	G1199
A1200 A1201	61205	C1206	G1208	61209 U1210	C1211 U1212	<mark>61213</mark>	G1216	G1217 A1218	U1219	61220 41221	C1222	C1223	A1226	01232	A1233	G1239	100FJ	C1244	01249	C1252	61253 A1254	<mark>U1255</mark> G1256	A1257	61259	61260 C1261	<mark>C1262</mark> G1263	A1264	C1265	<mark>C1269</mark>	61272	A1286	A1287 G1288	G1289 G1290	A1291 A1292	G1293
U129 4 G1295	C1296 C1297	A1298	G1301	C1302	<mark>G1309</mark> A1310	61311 U1312	A1313	A1314 C1315	G1316	A1317 U1318		A1323 G1324	G1325	61326 U1327	61328 41320	G1330	A1331	A1332 U1333	C1334 C1335	C1336	01337 C1338	U1345	A1346 A1347	61348	C1351	A1352 A1353	G1354	61300	U1358 C1359		G1364 C1365	A1366 A1367	G1370	U1371 C1372	G1373
U1374 C1375	A1376 C1377	C1378 C1378	U1380	A1381 G1382	G1383	61392 61393	A1394	A1399	G1400	61401 U1402	G1403	A1404 A1405		61409 A1410	C1413	G1414 G1414	C1415	C1420	C1421 G1422	A1423	A1424 G1425	A1429	G1430		01436	U1439 A1440	U1441	01442 C1443	C1447	C1448	C1449 U1450	<mark>U1451</mark> C1452	C1453 C1454	G1455 C1456	A1457

wwPDB	X-ray	Structure	Validation	Summary	Report

G1458	G1461	C1462	G1463	01465	G1466	6146/	G1470	G1471 A1472	C1473	G1474	C14/5 U1476	C1477	U1478	A14/A	C1482	6.1488	G 1489	A1490 C1491		G1494	61496 G1496	C1497	01730 A1499	U1500	C1504	61505 A1506	G 1507	C1513	A1517		G1521 C1522	A1523	G1524 G1525	G1526	U1527 G1528	G1529 01520	A1531	G1532 G1533	U1534 A1535
G1536	G1537 C1538	A1539	A1540 A1541	01542	C1543	01544 61545	C1546	C1547 U1548	C1549	C1550	A1553	C1554	A1555	61557	C1558	01559 C1560	U1561	G1562 C1563	G 1564	U1565	61567 61567	01870		A1574	C1576	C1578	G1579	Ă	ე ლ	5 5	5	9 5	A C1589	A1590	A1591 C1592	C1593	C1595	C1596 C1597	<mark>G1598</mark> A1599
A1600	G1601	A1604	G1605	61607 61607	A1608	61609	A1612	A1613 G1614	A1615	A1616	C1621	U1622	C1623	01024 A1625		01628	C1630	A1631 A1632	C1633	000 50	G1637	G1638 C1630	6015	C1643	U1647	A1048	C1652 A1653	A1654	A1655 C1656		A1659 C1660	A1661	C1662 A1663		G1667	C1670	TIOTS	01685 01686	A1687 G1688
G1689	C1690 G1691	C1692	G1693 71604	61695		A1698 G1699	A1700	A1701 C1702	C1703	C1704		C1709	01110	61/12 61/13		61720 C1721	A1722	A1723 G1724	01725	01726	G1/2/ G1728	C1729	01734	A1735	C1740	G1742	G1743 A1744	<mark>G1745</mark>	A1746 A1747		01755 C1756		G1763 U1764	G1765	A1766 U1767	G1768	G1770	C1771 C1772	C1773 C1774
G1775	G1776 G1777	G1778	A1779		G1783	G1786	U1787	G1788 A1789		A1792	61/93 61794		C1797		G1802	A1803	G1806	01807 01808	U1809	A1810	C1811 C1812	A1813 A1814	A1017 A1815	A1816 A1817	C1818	C1820	A1821	01824	C1825 U1826	C1827	01828 G1829	C1830	G1831 A1832	A1833	C1834 U1835	110 12	OF OF P	A1849 U1850	A1851
G1854	A1855 G1856	C1857	G1858 11 050	ACOTH	U1863	01864 G1865	C1866	C1867 C1868	G1869		C1873 C1874	G1875	G1876	A16// A1878	G1879	A1883		G1887 G1888	A1889		01894 G1895	C1896 A1807	A1097 A1898	G1899	C1901	C1902 C1903	G1904 A1905	A1906	C1907 C1908	G1909	A1910	C1914	C1915 C1916	G1917	G1920	A1921	C1923	G1927	<mark>G1928</mark> C1929
C1930	A1933	A1934	C1935	A1937		61943 U1944	C1945	C1946 U1947	A1948	A1949	61951 61951		C1955	41957	A1958	A1959 U1960	U1961	C1962 C1963		U1967	CTAOR	A1973	G 1975	U1976	C1983	01984 G1985	C1986 A1987	C1988	G1989 A1990	A1991	A1992 A1993	G 1994	C1995	<mark>G2001</mark>	A2002 C2003	C2004	92009	G2008 C2009	<mark>G2010</mark> C2011
U2012	G2013 U2014	C2015		G2019	C2020	62021	C2027	02028 02029	G 2030	G2031	02032 62033	A2034	A2035	42030 U2037		A2041 C2042	U2043	62044	C2047	G2048	A2052	62053 AD054	N2055 U2055	G2056 C2057	G2058	G2060	C2061	A2063	C2064	C2071	A2072	C2076	G2077 A2078	A2079	A2080 A2081	G2082	A2003 C2084	C2085 C2086	C2087 G2088
U2089	G2090 G2091		C2094 11000E	U2096		02100 G2101		02107 (22108	G2109	U2110	11129	G2114	G2115	U2117	C2118	U2120 U2120	G2121	G2122 U2123	C2124	G2125	C2129	U2130	C2132	G2133	A2135	62130 G2137	A2138	A2140	G2141	U2143	G2146	A2147	G2148 C2149 ●	C2150	U2151 • (2152 •	U2153	42155 A2155	A2156 C2157	C2158 C2159
C2160	C2161 G2162	C2163	C2164	G2168	G2169		G2174	G2175 G2176	G2177	G2178	62180	G2181	C2182	C2184	C2185	62186	G2 189	A2190 A2191	A2 192	U2193	C2 195	C2 196	C2198	C2199	U2201	62203 62203	90661	G2207	G2208 C2209	U2210	62211 62212	G2213	G2214 G2215	C2216	C2217 U2218	A2219 10000	G2221	<mark>(2222)</mark> (2223	U222 4 C2225
G2226	G2227	U2229	G2230	62232 62232	G2233	G2235	A2236	C2237	<mark>G2241</mark>	C2242	02243	C2247	G2248	62250		62253 U2254	U2255	02256 (2257	A2258	(2259	02260 G2261	G2262	00775	G2 <mark>266</mark>	U2273	A2277	112283	A2284	A2285 C2286	G2287	G2288 A2289	G2290	G2291 C2292	G 2293	C2294	A2297	A2 299	G2300 G2301	<mark>U2302</mark> C2303
-	A2309 G2310		G2313	G2315	A2316	62318	G2319	A2320 A2321	A2322	U2323	02324	02327	C2328	G2330 G2330	A2331	62332	<mark>G2336</mark>	C2337 A2338	A2339		62342	G2345 A7346	A2347	<u>63551</u>	62352 62352	02354 02354	40357	<mark>C2358</mark>	U2359 G2360	C2361	C2367		A2371 A2372		A2380	62 <mark>384</mark> 0386		A2388 A2389	G2394
G2395	C2396 C2397	U2398		62402	A2403	62405 C2405	C2406	62407 62408	U2409	G2410	C2413	C2414	C2415	62410 U2417		62420 62421	A2422	G2425	G2426	C2427	U2430	C2431	42 43 3 A2 43 3	U2434	A2436	62 <u>440</u>	A2441 112442	A2443	A2444 A2445	A2 446	U2449	A2450	C2451 C2452	C2453	A2459	U2460	A2 46 2	C2463	<mark>G2</mark> 466 C2467
U2468	G2469 A2470	U2471	C2472	02474 C2474	C2475	0.2476	G2479	A2480 G2481	C2482	CO A DE	C2485	A2487	C2488	62490 62490	C2491	G2492 G2493	C2494	G2495 G2496	G2497	G2498	A2499 G2500	G2501 117507	70070	C2509	C2512	62013 A2514	U2515 G2516	U2517	C2518 G2519		U2522	G2527	C2528 A2529		G2535	U2539	42040 A2541	A2542	<mark>G2547</mark> U2548








 \bullet Molecule 29: 50S ribosomal protein L2



 \bullet Molecule 29: 50S ribosomal protein L2















 \bullet Molecule 34: 50S ribosomal protein L9



 \bullet Molecule 37: 50S ribosomal protein L14





 \bullet Molecule 37: 50S ribosomal protein L14



E120 V121 L122

 \bullet Molecule 38: 50S ribosomal protein L15













R 11 R 11 R 11 R 11 R 11 R 13 R 13 R 13 R 13 R 13 R 25 R

 \bullet Molecule 41: 50S ribosomal protein L18



• Molecule 42: 50S ribosomal protein L19



• Molecule 42: 50S ribosomal protein L19





• Molecule 43: 50S ribosomal protein L20



• Molecule 43: 50S ribosomal protein L20









V105 E109 G112 A113

• Molecule 46: 50S ribosomal protein L23





E178

 \bullet Molecule 48: 50S ribosomal protein L25







• Molecule 54: 50S ribosomal protein L32



Chain D5:	5%	59%	22%	15% •
A2 H4 P5 V6 R15 R15	D17 A18 R19	C33 C33 K40 P41 P41 P47 C445 C46 C46 C46 C46 C46 C46 C46 C46 C46 C46		
• Molecule	55:	50S ribosomal protein L33		
Chain B6:	5% 7%	55%	27%	11%
19 111 111 114 114 114 115 116 116 116	K17 R18 R19	M20 421 123 123 123 123 123 130 133 130 133 133 133 133 133 133 13	H46 1147 1147 1149 1149 1150 1150 1151 1150 1152	
• Molecule	55:	50S ribosomal protein L33		
Chain D6:	2% 11	% 55%	30%	6 5%
19 111 114 114 114 114 114 116 116	K17 R18 R19	M20 M22 M21 M22 M24 M26 M26 M26 M25 M26 M26 M26 M26 M26 M23 M23 M23 M23 M23 M23 M23 M23 M23 M23	H46 147 148 149 H49 E51 V52 V52	
• Molecule	56:	50S ribosomal protein L34		
Chain B7:	2%	63%	35%	
M1 P7 N8 R9 R10 K11 R12	H16 G17	F18 R21 R21 R39 R39 R39 R44 A45 R44 R45 R45 R45 R45		
• Molecule	56:	50S ribosomal protein L34		
Chain D7:	2%	58%	38%	•
M1 K2 V5 W5 N8 N8	RJO K11 K11	N12 N23 T24 C27 C27 C27 N23 N23 N23 N23 N30 N40 N40 N41 N41 N45 N45 N45 N46 N46 N46 N46 N46 N46 N46 N46 N46 N46		
• Molecule	57:	50S ribosomal protein L35		
Chain B8:		30% 49%		17% •
P2 M4 K5 K5 K8 K8 K8 K8	A10 K11 K12	N13 N14 N14 N16 N16 N22 N22 N23 N24 N25 N25 N25 N25 N25 N25 N25 N25 N25 N25	K44 K47 R46 R46 F48 F48 F48 F48 L50 L50 L50 A51 K52 F53	E56 R57 R57 L60 L61 L61 L62 P63 Y64
• Molecule	57:	50S ribosomal protein L35		
Chain D8:	3%	46%	44%	• 6%
<mark>≅≅≇≌≇⊨≊8</mark> ● Molecule	e 58:	<mark>첫월</mark> 위 <mark>응용</mark> 호호 알 울 분원일발원월 58 <mark>8</mark> 28 전 28 <mark>5</mark> 50S ribosomal protein L36	F 448 V 449 A 51 A 51 F 53 F 53 B 54 A 55 A 55 A 55 A 55 A 55 A 55 A 55 A	164 164 163 163 164



Chain B9:	47%		42%	8% •
K2 V3 R4 K8 K8 K14 C14 C14 V16 V16	418 R119 V25 V25 E28 E28 F30 F30	H32 H32 Q36 G37 G37		
• Molecule 58: 5	0S ribosomal p	rotein L36		
Chain D9:	_	75%		19% 6%
K2 45 110 110 117 117 117 117	R18 126 126 132 132 132 132 132			
• Molecule 59: m	nRNA			
Chain CX:	25% 25%	25%	50%	Ó
A16 U17 018 U19				
• Molecule 60: 5	0S Ribosomal p	orotein L1		
Chain DC:		73% 72%		21% • • •
K18 V19 Y22 T22 T22 T22 T22 T22 T22 T22 T22 L22 VAL	LU LEU ALA A35 A35 R36 F37 F37 F37 F37 F37 F37 F37 F33 F33 F33	H44 A45 K46 L47 G48 P51 R52 R52	D55 Q56 N37 N57 N58 R59 Q60 T61 Y62 V62 V62 V62 V62 V62 V62 V62 V62 V62 V	G67 Q71 V72 N73 N73 L75 A76 A76 A76 A76 C79 G80 B85 A86
				••••
E87 E88 A89 A91 C92 C94 C94 C95 C95 C95 C95 C95 C95 C95 C95 C95 C95	199 1100 1100 1100 1100 1100 1100 1100	4110 4119 4120 4121 4123 4124 4125 4126 4126 4126 4126	A128 A129 A130 A131 A133 A133 A133 A133 A140 A141 A141	A142 A144 A144 A146 A146 A146 A149 A154 A154 A155 A155 A155 A155 A155 A155
<u> </u>	0 0 0 0 1 0 0 0 0 0 0 0 0	1 0 0 7 9 9 9 6 6 9 9 9	7 0 0 7 0 0 4 0 0 0 1 0 0 4	<u>ល្ល ០ ។ ៧ ៧ ។ ៧ ០ ৮ ០ ០ ។</u>
A15 A15 A16 A16 A16 A16 A16 A16 A16 A16 A16 A16	A17 A17 A17 A17 A17 A17 A17 A17 A17 A17	A10 A13 A13 A13 A13 A13 A13 A13 A13 A13 A13	A19 A19 A19 A19 A19 A19 A19 A19 A19 A19	A20 A21 A21 A21 A21 A21 A21 A21 A22 A22 A22
A223				



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	209.92Å 449.90Å 624.90Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{Bosolution} \left(\overset{\wedge}{\mathbf{A}} \right)$	39.57 - 3.30	Depositor
Resolution (A)	39.57 - 3.30	EDS
% Data completeness	95.6(39.57 - 3.30)	Depositor
(in resolution range)	$95.6\ (39.57 - 3.30)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.81 (at 3.32 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0031	Depositor
D D.	0.225 , 0.279	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.230 , 0.279	DCC
R_{free} test set	41956 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	63.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.28 , 66.5	EDS
L-test for $twinning^2$	$ < L >=0.37, < L^2>=0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	295724	wwPDB-VP
Average B, all atoms $(Å^2)$	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.64% 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.



 $^{^1 {\}rm Intensities}$ 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: PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bond lengths		Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AA	0.42	4/36190~(0.0%)	0.75	26/56486~(0.0%)	
1	CA	0.40	1/36190~(0.0%)	0.73	17/56486~(0.0%)	
2	AB	0.43	0/1936	0.67	0/2609	
2	CB	0.44	0/1936	0.64	0/2609	
3	AC	0.49	0/1637	0.71	0/2205	
3	CC	0.44	0/1637	0.67	0/2205	
4	AD	0.54	0/1733	0.84	4/2318~(0.2%)	
4	CD	0.52	0/1733	0.77	1/2318~(0.0%)	
5	AE	0.45	0/1163	0.76	0/1564	
5	CE	0.46	0/1163	0.72	0/1564	
6	AF	0.49	0/856	0.77	1/1154~(0.1%)	
6	CF	0.48	0/856	0.75	0/1154	
7	AG	0.43	0/1276	0.65	0/1709	
7	CG	0.40	0/1276	0.64	0/1709	
8	AH	0.47	0/1136	0.72	0/1527	
8	CH	0.45	0/1136	0.69	0/1527	
9	AI	0.48	0/1029	0.71	0/1378	
9	CI	0.42	0/1029	0.68	0/1378	
10	AJ	0.47	0/808	0.76	0/1085	
10	CJ	0.46	0/808	0.68	0/1085	
11	AK	0.49	0/900	0.71	0/1213	
11	CK	0.45	0/900	0.70	0/1213	
12	AL	0.55	0/987	0.81	0/1320	
12	CL	0.50	0/987	0.77	0/1320	
13	AM	0.45	0/999	0.78	0/1336	
13	CM	0.43	0/999	0.68	0/1336	
14	AN	0.50	0/501	0.88	1/664~(0.2%)	
14	CN	0.46	0/501	0.74	0/664	
15	AO	0.46	0/745	0.70	0/992	
15	CO	0.40	0/745	0.64	0/992	
16	AP	0.47	0/717	0.74	0/963	
16	CP	0.50	0/717	0.78	1/963~(0.1%)	



N.T. 1		Bond lengths		Bond angles		
IVI01	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
17	AQ	0.44	0/837	0.70	0/1117	
17	CQ	0.46	0/837	0.72	0/1117	
18	AR	0.47	0/579	0.79	0/768	
18	CR	0.47	0/579	0.69	0/768	
19	AS	0.47	0/643	0.68	0/865	
19	CS	0.43	0/643	0.61	0/865	
20	AT	0.45	0/765	0.70	0/1007	
20	CT	0.43	0/765	0.71	0/1007	
21	AU	0.52	0/213	0.71	0/277	
21	CU	0.53	0/213	0.68	0/277	
22	AV	0.40	0/1832	0.75	1/2855~(0.0%)	
22	CV	0.38	0/1832	0.72	0/2855	
23	AW	0.29	0/1809	0.68	2/2819~(0.1%)	
23	CW	0.27	0/1809	0.70	1/2819~(0.0%)	
24	AY	0.86	17/1815~(0.9%)	0.94	1/2833~(0.0%)	
24	CY	0.86	17/1815~(0.9%)	0.94	1/2833~(0.0%)	
25	AX	0.31	0/147	0.72	0/227	
26	BA	0.57	22/67709~(0.0%)	0.91	196/105690~(0.2%)	
26	DA	0.45	5/67709~(0.0%)	0.80	93/105690~(0.1%)	
27	BB	0.45	0/2853	0.81	3/4451~(0.1%)	
27	DB	0.35	0/2853	0.72	0/4451	
28	BC	0.46	0/1160	0.59	0/1584	
29	BD	0.71	0/2155	0.95	1/2905~(0.0%)	
29	DD	0.60	0/2155	0.85	0/2905	
30	BE	0.70	1/1597~(0.1%)	0.91	1/2153~(0.0%)	
30	DE	0.56	1/1597~(0.1%)	0.83	2/2153~(0.1%)	
31	BF	0.68	0/1659	0.88	1/2244~(0.0%)	
31	DF	0.52	0/1659	0.75	0/2244	
32	BG	0.49	0/1499	0.74	0/2016	
32	DG	0.44	0/1499	0.67	0/2016	
33	BH	0.64	1/1246~(0.1%)	0.88	2/1682~(0.1%)	
33	DH	0.47	0/1246	0.67	1/1682~(0.1%)	
34	BI	0.48	0/1147	0.75	1/1551~(0.1%)	
34	DI	0.47	0/1147	0.72	0/1551	
35	BJ	0.51	0/650	$0.5\overline{5}$	0/907	
35	DJ	0.44	$0/\overline{650}$	0.53	0/907	
36	BN	0.70	$0/113\overline{2}$	0.96	0/1525	
36	DN	0.49	0/1132	0.77	0/1525	
37	BO	0.57	0/943	0.81	0/1269	
37	DO	0.53	0/943	0.78	0/1269	
38	BP	$0.7\overline{1}$	$0/113\overline{1}$	1.09	$3/1504 \ (0.2\%)$	
38	DP	0.57	0/1131	0.98	2/1504~(0.1%)	
39	BQ	0.58	0/1143	0.85	1/1527~(0.1%)	



7.7.1	Bond lengths		ond lengths	Bond angles		
IVI01	Chain	RMSZ	$ \tilde{Z} >5$	RMSZ	# Z > 5	
39	DQ	0.46	0/1143	0.68	0/1527	
40	BR	0.70	0/974	0.98	1/1302~(0.1%)	
40	DR	0.54	0/974	0.87	0/1302	
41	BS	0.60	0/779	0.98	0/1036	
41	DS	0.48	0/779	0.79	0/1036	
42	BT	0.59	0/1156	0.97	1/1542~(0.1%)	
42	DT	0.58	0/1156	0.95	0/1542	
43	BU	0.76	0/975	0.98	1/1297~(0.1%)	
43	DU	0.50	0/975	0.75	0/1297	
44	BV	0.69	0/790	1.03	4/1057~(0.4%)	
44	DV	0.47	0/790	0.76	0/1057	
45	BW	0.65	0/907	0.95	1/1216~(0.1%)	
45	DW	0.52	0/907	0.77	0/1216	
46	BX	0.67	0/740	0.94	1/993~(0.1%)	
46	DX	0.52	0/740	0.74	0/993	
47	BY	0.68	0/789	0.99	3/1051~(0.3%)	
47	DY	0.53	0/789	0.83	0/1051	
48	ΒZ	0.49	0/1436	0.72	0/1949	
48	DZ	0.44	0/1436	0.66	0/1949	
49	B0	0.61	0/671	0.85	0/892	
49	D0	0.51	0/671	0.76	0/892	
50	B1	0.62	0/741	0.84	0/984	
50	D1	0.53	0/741	0.84	1/984~(0.1%)	
51	B2	0.57	0/600	0.86	0/793	
51	D2	0.48	0/600	0.79	0/793	
52	B3	0.55	0/473	0.87	0/634	
52	D3	0.44	0/473	0.70	0/634	
53	B4	0.53	0/229	0.79	0/309	
53	D4	0.49	0/229	0.75	0/309	
54	B5	0.73	0/473	1.08	0/639	
54	D5	0.57	0/473	0.88	0/639	
55	B6	0.96	1/388~(0.3%)	2.06	4/518~(0.8%)	
55	D6	0.83	0/388	1.06	2/518~(0.4%)	
56	B7	0.73	0/427	0.96	0/561	
56	D7	0.58	0/427	0.85	0/561	
57	B8	0.75	0/516	1.12	2/679~(0.3%)	
57	D8	0.54	0/516	0.88	1/679~(0.1%)	
58	B9	0.69	0/302	1.00	2/397~(0.5%)	
58	D9	0.45	0/302	0.73	0/397	
59	CX	0.52	0/94	0.72	0/144	
60	DC	0.48	0/1160	0.55	0/1584	
All	All	0.50	70/321233~(0.0%)	0.81	$388/480213 \ (0.1\%)$	



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	AA	1	0
1	CA	1	0
2	AB	0	1
13	AM	0	1
13	CM	0	1
23	AW	1	0
23	CW	1	0
26	BA	22	0
26	DA	20	0
29	BD	0	3
29	DD	0	2
30	BE	0	2
30	DE	0	1
33	BH	0	1
38	BP	0	10
38	DP	0	4
40	BR	0	2
40	DR	0	1
41	BS	0	1
42	BT	0	3
43	BU	0	3
44	BV	0	2
47	BY	0	1
55	B6	0	1
55	D6	0	1
57	B8	0	1
All	All	46	42

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	B6	47	THR	C-N	8.32	1.53	1.34
24	AY	50	G	C1'-N9	-6.96	1.37	1.46
24	CY	50	G	C1'-N9	-6.95	1.37	1.46
26	BA	1816	А	O3'-P	6.86	1.69	1.61
24	CY	66	G	C1'-N9	-6.73	1.37	1.46

The worst 5 of 388 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
55	B6	45	LYS	O-C-N	-30.98	73.14	122.70
55	B6	45	LYS	CA-C-N	22.24	166.13	117.20
26	BA	2513	G	O5'-P-OP1	-13.46	93.59	105.70
26	BA	1850	U	O5'-P-OP1	-12.67	94.30	105.70
26	BA	1955	С	C2'-C3'-O3'	12.16	136.24	109.50

5 of 46 chirality outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atom
1	AA	412	A	C1'
23	AW	47	U	C1'
26	BA	98	G	C1'
26	BA	497	A	C3'
26	BA	715	G	C4',C3',C1'

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	23	ARG	Peptide
13	AM	69	GLU	Peptide
29	BD	224	ALA	Peptide
29	BD	244	ARG	Peptide
29	BD	36	PRO	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	32329	0	16318	494	1
1	CA	32329	0	16318	469	0
2	AB	1901	0	1951	42	0
2	CB	1901	0	1951	43	0
3	AC	1613	0	1677	43	0
3	CC	1613	0	1677	46	0
4	AD	1703	0	1763	64	0
4	CD	1703	0	1763	50	0
5	AE	1147	0	1207	44	0
5	CE	1147	0	1207	35	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AF	843	0	857	14	0
6	CF	843	0	857	18	0
7	AG	1257	0	1296	20	0
7	CG	1257	0	1296	12	0
8	AH	1116	0	1177	28	0
8	CH	1116	0	1177	17	0
9	AI	1011	0	1043	31	0
9	CI	1011	0	1043	27	0
10	AJ	795	0	840	36	0
10	CJ	795	0	840	36	0
11	AK	885	0	904	31	0
11	CK	885	0	904	17	0
12	AL	971	0	1057	16	0
12	CL	971	0	1057	19	0
13	AM	988	0	1059	35	0
13	CM	988	0	1059	26	0
14	AN	492	0	529	14	0
14	CN	492	0	529	21	0
15	AO	734	0	771	17	0
15	CO	734	0	771	21	0
16	AP	701	0	720	22	0
16	CP	701	0	720	17	0
17	AQ	824	0	891	23	0
17	CQ	824	0	891	13	0
18	AR	574	0	644	16	0
18	CR	574	0	644	16	0
19	AS	630	0	652	30	0
19	CS	630	0	652	12	0
20	AT	763	0	861	26	0
20	CT	763	0	861	14	0
21	AU	209	0	221	4	0
21	CU	209	0	221	3	0
22	AV	1640	0	837	29	0
22	CV	1640	0	837	27	0
23	AW	1619	0	822	58	0
23	CW	1619	0	822	21	0
24	AY	1619	0	792	222	0
24	CY	1619	0	792	241	0
25	AX	151	0	76	15	0
26	BA	60459	0	30488	1163	0
26	DA	60459	0	30487	1024	0
27	BB	2551	0	1295	38	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	DB	2551	0	1295	35	0
28	BC	1157	0	1160	27	0
29	BD	2105	0	2182	126	0
29	DD	2105	0	2182	89	0
30	BE	1564	0	1629	97	0
30	DE	1564	0	1629	66	0
31	BF	1624	0	1677	72	0
31	DF	1624	0	1677	63	0
32	BG	1474	0	1535	53	0
32	DG	1474	0	1535	49	0
33	BH	1223	0	1282	48	0
33	DH	1223	0	1282	22	0
34	BI	1132	0	1218	30	0
34	DI	1132	0	1218	29	1
35	BJ	651	0	649	10	0
35	DJ	651	0	649	14	0
36	BN	1105	0	1180	62	0
36	DN	1105	0	1180	42	0
37	BO	933	0	996	33	0
37	DO	933	0	996	30	0
38	BP	1114	0	1187	141	0
38	DP	1114	0	1187	82	0
39	BQ	1122	0	1179	35	0
39	DQ	1122	0	1179	31	0
40	BR	960	0	1021	47	0
40	DR	960	0	1021	46	0
41	BS	771	0	832	46	0
41	DS	771	0	832	33	0
42	BT	1142	0	1202	92	0
42	DT	1142	0	1202	72	0
43	BU	958	0	1018	57	0
43	DU	958	0	1018	52	0
44	BV	779	0	852	54	0
44	DV	779	0	852	39	0
45	BW	896	0	956	40	0
45	DW	896	0	956	23	0
46	BX	726	0	778	26	0
46	DX	726	0	778	20	0
47	BY	776	0	868	79	0
47	DY	776	0	870	45	0
48	BZ	1404	0	1432	20	0
48	DZ	1404	0	1432	34	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	B0	662	0	688	18	0
49	D0	662	0	688	20	0
50	B1	734	0	808	22	0
50	D1	734	0	808	21	0
51	B2	598	0	653	24	0
51	D2	598	0	653	13	0
52	B3	468	0	523	20	0
52	D3	468	0	523	12	0
53	B4	226	0	229	8	0
53	D4	226	0	229	4	0
54	B5	459	0	477	48	0
54	D5	459	0	478	21	0
55	B6	381	0	390	52	0
55	D6	381	0	391	30	0
56	B7	419	0	467	12	0
56	D7	419	0	467	15	0
57	B8	508	0	576	58	0
57	D8	508	0	576	33	0
58	B9	299	0	324	19	0
58	D9	299	0	324	7	0
59	CX	85	0	43	7	0
60	DC	1157	0	1160	22	0
All	All	295724	0	201402	6566	1

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 13.

The worst 5 of 6566 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)
24:AY:10:C:H41	24:AY:45:G:N2	1.03	1.51
24:CY:7:A:N1	24:CY:66:G:N2	1.61	1.48
24:AY:7:A:N1	24:AY:66:G:N2	1.61	1.46
24:CY:10:C:H41	24:CY:45:G:N2	1.03	1.46
24:CY:9:G:H21	24:CY:11:C:N4	1.02	1.45

All (1) 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)	
1:AA:358:U:OP1	$34:DI:87:LYS:NZ[4_455]$	2.03	0.17	

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	Perce	entiles
2	AB	232/234~(99%)	170 (73%)	51~(22%)	11 (5%)	2	14
2	CB	232/234~(99%)	181 (78%)	41 (18%)	10 (4%)	2	16
3	AC	204/206~(99%)	150 (74%)	40 (20%)	14 (7%)	1	8
3	CC	204/206~(99%)	159 (78%)	32~(16%)	13~(6%)	1	9
4	AD	206/208~(99%)	155 (75%)	37~(18%)	14 (7%)	1	8
4	CD	206/208~(99%)	160 (78%)	36~(18%)	10 (5%)	2	14
5	AE	148/150~(99%)	129 (87%)	15~(10%)	4 (3%)	5	26
5	CE	148/150~(99%)	130 (88%)	16 (11%)	2 (1%)	11	38
6	AF	99/101~(98%)	89 (90%)	7(7%)	3 (3%)	4	24
6	CF	99/101~(98%)	88 (89%)	9 (9%)	2 (2%)	7	32
7	AG	153/155~(99%)	133 (87%)	18 (12%)	2 (1%)	12	40
7	CG	153/155~(99%)	130 (85%)	18~(12%)	5 (3%)	4	22
8	AH	136/138~(99%)	119 (88%)	14~(10%)	3(2%)	6	30
8	CH	136/138~(99%)	115 (85%)	18~(13%)	3~(2%)	6	30
9	AI	125/127~(98%)	96 (77%)	25~(20%)	4 (3%)	4	22
9	CI	125/127~(98%)	101 (81%)	21~(17%)	3 (2%)	6	28
10	AJ	96/98~(98%)	76 (79%)	17~(18%)	3 (3%)	4	23
10	CJ	96/98~(98%)	73 (76%)	18 (19%)	5 (5%)	2	13
11	AK	117/119~(98%)	96 (82%)	19 (16%)	2 (2%)	9	35
11	CK	117/119~(98%)	102 (87%)	12 (10%)	3 (3%)	5	27
12	AL	122/124 (98%)	95 (78%)	18 (15%)	9 (7%)	1	7



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
12	CL	122/124~(98%)	95 (78%)	20~(16%)	7 (6%)	1	11
13	AM	122/124~(98%)	87 (71%)	23~(19%)	12 (10%)	0	3
13	CM	122/124~(98%)	90 (74%)	23~(19%)	9 (7%)	1	7
14	AN	58/60~(97%)	43 (74%)	11 (19%)	4 (7%)	1	8
14	CN	58/60~(97%)	46 (79%)	8 (14%)	4 (7%)	1	8
15	AO	86/88~(98%)	62 (72%)	19(22%)	5 (6%)	1	11
15	CO	86/88~(98%)	71 (83%)	10 (12%)	5 (6%)	1	11
16	AP	81/83~(98%)	68 (84%)	13~(16%)	0	100	100
16	CP	81/83~(98%)	64 (79%)	12 (15%)	5 (6%)	1	10
17	AQ	97/99~(98%)	85 (88%)	8 (8%)	4 (4%)	3	17
17	CQ	97/99~(98%)	89 (92%)	5(5%)	3 (3%)	4	23
18	AR	68/70~(97%)	55 (81%)	8 (12%)	5 (7%)	1	7
18	CR	68/70~(97%)	58 (85%)	6 (9%)	4 (6%)	1	10
19	AS	76/78~(97%)	57 (75%)	11 (14%)	8 (10%)	0	3
19	CS	76/78~(97%)	64 (84%)	8 (10%)	4 (5%)	2	12
20	AT	97/99~(98%)	71 (73%)	22~(23%)	4 (4%)	3	17
20	CT	97/99~(98%)	72 (74%)	21 (22%)	4 (4%)	3	17
21	AU	22/24~(92%)	13 (59%)	7(32%)	2 (9%)	1	4
21	CU	22/24~(92%)	17 (77%)	4 (18%)	1 (4%)	2	15
28	BC	182/206~(88%)	111 (61%)	50 (28%)	21 (12%)	0	2
29	BD	269/271~(99%)	214 (80%)	34~(13%)	21 (8%)	1	6
29	DD	269/271~(99%)	217 (81%)	31~(12%)	21 (8%)	1	6
30	BE	202/204~(99%)	138 (68%)	47 (23%)	17 (8%)	1	5
30	DE	202/204~(99%)	152 (75%)	35~(17%)	15 (7%)	1	7
31	BF	205/207~(99%)	163 (80%)	28 (14%)	14 (7%)	1	8
31	DF	205/207~(99%)	163 (80%)	28 (14%)	14 (7%)	1	8
32	BG	$\overline{179/181}\ (99\%)$	140 (78%)	27~(15%)	12 (7%)	1	8
32	DG	179/181~(99%)	137~(76%)	31 (17%)	11 (6%)	1	10
33	BH	157/159~(99%)	113 (72%)	24 (15%)	20 (13%)	0	1
33	DH	157/159~(99%)	116 (74%)	25(16%)	16 (10%)	0	3
34	BI	$143/\overline{145}~(99\%)$	107 (75%)	29(20%)	7(5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
34	DI	143/145~(99%)	110 (77%)	25~(18%)	8 (6%)	2	11
35	BJ	128/130~(98%)	70 (55%)	42 (33%)	16 (12%)	0	1
35	DJ	128/130~(98%)	72~(56%)	42~(33%)	14 (11%)	0	2
36	BN	136/138~(99%)	100 (74%)	25~(18%)	11 (8%)	1	6
36	DN	136/138~(99%)	108 (79%)	15~(11%)	13~(10%)	0	4
37	BO	120/122~(98%)	106 (88%)	12~(10%)	2 (2%)	9	35
37	DO	120/122~(98%)	106 (88%)	13~(11%)	1 (1%)	19	51
38	BP	144/146~(99%)	82 (57%)	37~(26%)	25 (17%)	0	1
38	DP	144/146~(99%)	87 (60%)	28~(19%)	29 (20%)	0	0
39	BQ	139/141~(99%)	109 (78%)	25~(18%)	5 (4%)	3	20
39	DQ	139/141~(99%)	116 (84%)	19~(14%)	4(3%)	4	24
40	BR	115/117~(98%)	93 (81%)	16 (14%)	6 (5%)	2	13
40	DR	115/117~(98%)	92 (80%)	17 (15%)	6 (5%)	2	13
41	BS	96/98~(98%)	58 (60%)	22~(23%)	16 (17%)	0	1
41	DS	96/98~(98%)	63~(66%)	20~(21%)	13 (14%)	0	1
42	BT	135/137~(98%)	95 (70%)	23~(17%)	17 (13%)	0	1
42	DT	135/137~(98%)	89 (66%)	30~(22%)	16 (12%)	0	2
43	BU	115/117~(98%)	90 (78%)	19~(16%)	6 (5%)	2	13
43	DU	115/117~(98%)	92~(80%)	19~(16%)	4 (4%)	3	21
44	BV	99/101~(98%)	74 (75%)	14~(14%)	11 (11%)	0	2
44	DV	99/101~(98%)	72 (73%)	17~(17%)	10 (10%)	0	3
45	BW	111/113~(98%)	92~(83%)	16~(14%)	3 (3%)	5	26
45	DW	111/113~(98%)	96 (86%)	7~(6%)	8 (7%)	1	7
46	BX	90/92~(98%)	80 (89%)	7 (8%)	3 (3%)	4	22
46	DX	90/92~(98%)	75~(83%)	8 (9%)	7 (8%)	1	6
47	BY	98/100~(98%)	53 (54%)	22~(22%)	23 (24%)	0	0
47	DY	98/100~(98%)	$60 \ (61\%)$	$19 \ (19\%)$	19 (19%)	0	1
48	BZ	174/176~(99%)	141 (81%)	26 (15%)	7 (4%)	3	18
48	DZ	174/176~(99%)	130 (75%)	33 (19%)	11 (6%)	1	9
49	B0	82/84~(98%)	75 (92%)	6 (7%)	1 (1%)	13	42
49	D0	82/84 (98%)	72 (88%)	9 (11%)	1 (1%)	13	42



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
50	B1	91/93~(98%)	76 (84%)	12~(13%)	3~(3%)	4	22
50	D1	91/93~(98%)	74 (81%)	10~(11%)	7 (8%)	1	6
51	B2	69/71~(97%)	53 (77%)	10~(14%)	6 (9%)	1	5
51	D2	69/71~(97%)	54 (78%)	11~(16%)	4 (6%)	1	11
52	B3	57/59~(97%)	51 (90%)	5~(9%)	1 (2%)	8	35
52	D3	57/59~(97%)	53~(93%)	3~(5%)	1 (2%)	8	35
53	B4	28/30~(93%)	21 (75%)	4 (14%)	3~(11%)	0	3
53	D4	28/30~(93%)	20 (71%)	5~(18%)	3~(11%)	0	3
54	B5	57/59~(97%)	43~(75%)	9~(16%)	5~(9%)	1	5
54	D5	57/59~(97%)	48 (84%)	4~(7%)	5~(9%)	1	5
55	B6	42/44~(96%)	21~(50%)	8 (19%)	13~(31%)	0	0
55	D6	42/44~(96%)	23~(55%)	7~(17%)	12 (29%)	0	0
56	B7	46/48~(96%)	45~(98%)	1 (2%)	0	100	100
56	D7	46/48~(96%)	45~(98%)	0	1 (2%)	6	30
57	B8	61/63~(97%)	44 (72%)	10~(16%)	7(12%)	0	2
57	D8	61/63~(97%)	47 (77%)	8 (13%)	6~(10%)	0	3
58	B9	34/36~(94%)	32 (94%)	2~(6%)	0	100	100
58	D9	34/36~(94%)	33 (97%)	1 (3%)	0	100	100
60	DC	182/196~(93%)	115 (63%)	47 (26%)	20 (11%)	0	2
All	All	$11\overline{898/12136}~(98\%)$	9181 (77%)	1900 (16%)	817 (7%)	1	8

5 of 817 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	106	LYS
2	AB	165	VAL
3	AC	12	LEU
3	AC	20	SER
3	AC	47	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
2	AB	202/202~(100%)	185~(92%)	$17 \ (8\%)$	11	35
2	CB	202/202~(100%)	181 (90%)	21~(10%)	7	25
3	AC	160/160~(100%)	142 (89%)	18~(11%)	6	22
3	CC	160/160~(100%)	145 (91%)	15~(9%)	8	30
4	AD	180/180~(100%)	160 (89%)	20 (11%)	6	23
4	CD	180/180~(100%)	160 (89%)	20 (11%)	6	23
5	AE	115/115~(100%)	104 (90%)	11 (10%)	8	29
5	CE	115/115~(100%)	101 (88%)	14 (12%)	5	20
6	AF	90/90~(100%)	82 (91%)	8 (9%)	9	32
6	CF	90/90~(100%)	85 (94%)	5~(6%)	21	52
7	AG	126/126~(100%)	115 (91%)	11 (9%)	10	34
7	CG	126/126~(100%)	115 (91%)	11 (9%)	10	34
8	AH	119/119~(100%)	108 (91%)	11 (9%)	9	31
8	CH	119/119~(100%)	107 (90%)	12~(10%)	7	27
9	AI	98/98~(100%)	88 (90%)	10~(10%)	7	27
9	CI	98/98~(100%)	89 (91%)	9~(9%)	9	31
10	AJ	88/88 (100%)	76 (86%)	12~(14%)	3	16
10	СJ	88/88 (100%)	79 (90%)	9~(10%)	7	27
11	AK	90/90~(100%)	82 (91%)	8 (9%)	9	32
11	CK	90/90~(100%)	84 (93%)	6 (7%)	16	45
12	AL	104/104~(100%)	88 (85%)	16~(15%)	2	12
12	CL	104/104~(100%)	90 (86%)	14 (14%)	4	16
13	AM	99/99~(100%)	88 (89%)	11 (11%)	6	23
13	CM	99/99~(100%)	88 (89%)	11 (11%)	6	23
14	AN	49/49~(100%)	43 (88%)	6 (12%)	5	20
14	CN	49/49~(100%)	44 (90%)	5(10%)	7	27
15	AO	79/79~(100%)	73 (92%)	6 (8%)	13	39
15	СО	79/79~(100%)	76 (96%)	3~(4%)	33	62
16	AP	72/72~(100%)	65~(90%)	7~(10%)	8	29
16	CP	72/72~(100%)	62 (86%)	10 (14%)	3	16

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	Perce	\mathbf{n} tiles
17	AQ	94/94~(100%)	88~(94%)	6~(6%)	17	46
17	CQ	94/94~(100%)	89~(95%)	5~(5%)	22	53
18	AR	61/61~(100%)	54 (88%)	7~(12%)	5	22
18	CR	61/61~(100%)	59 (97%)	2(3%)	38	66
19	AS	69/69~(100%)	56 (81%)	13~(19%)	1	6
19	\mathbf{CS}	69/69~(100%)	58 (84%)	11~(16%)	2	11
20	AT	76/76~(100%)	68~(90%)	8 (10%)	7	25
20	CT	76/76~(100%)	67~(88%)	9~(12%)	5	21
21	AU	19/19~(100%)	15 (79%)	4 (21%)	1	4
21	CU	19/19~(100%)	17 (90%)	2(10%)	7	25
28	BC	61/66~(92%)	55~(90%)	6 (10%)	8	29
29	BD	213/213~(100%)	180 (84%)	33~(16%)	2	12
29	DD	213/213~(100%)	176 (83%)	37~(17%)	2	8
30	BE	165/165~(100%)	134 (81%)	31 (19%)	1	6
30	DE	165/165~(100%)	139 (84%)	26~(16%)	2	11
31	BF	165/165~(100%)	138 (84%)	27~(16%)	2	10
31	DF	165/165~(100%)	149 (90%)	16~(10%)	8	29
32	BG	155/155~(100%)	128 (83%)	27~(17%)	2	8
32	DG	155/155~(100%)	137 (88%)	18 (12%)	5	22
33	BH	132/132~(100%)	106 (80%)	26~(20%)	1	5
33	DH	132/132~(100%)	120 (91%)	12 (9%)	9	31
34	BI	122/122~(100%)	110 (90%)	12~(10%)	8	29
34	DI	122/122~(100%)	111 (91%)	$11 \ (9\%)$	9	32
36	BN	117/117~(100%)	90 (77%)	27~(23%)	1	3
36	DN	117/117~(100%)	94 (80%)	23~(20%)	1	5
37	BO	100/100~(100%)	92~(92%)	8 (8%)	12	37
37	DO	100/100~(100%)	93~(93%)	7(7%)	15	43
38	BP	$112/\overline{112}\;(100\%)$	83 (74%)	29(26%)	0	2
38	DP	112/112~(100%)	86 (77%)	26~(23%)	1	3
39	BQ	$111/\overline{111}\ (100\%)$	97(87%)	14(13%)	4	19
39	$\overline{\mathrm{DQ}}$	$111/111 \ (\overline{100\%})$	101 (91%)	10 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	BR	100/100~(100%)	85~(85%)	15~(15%)	3 13
40	DR	100/100~(100%)	85~(85%)	15~(15%)	3 13
41	BS	77/77~(100%)	60 (78%)	17~(22%)	1 3
41	DS	77/77~(100%)	67 (87%)	10~(13%)	4 17
42	BT	120/120~(100%)	98~(82%)	22~(18%)	1 7
42	DT	120/120~(100%)	93 (78%)	27~(22%)	1 3
43	BU	92/92~(100%)	78~(85%)	14~(15%)	3 13
43	DU	92/92~(100%)	82~(89%)	10~(11%)	6 24
44	BV	82/82~(100%)	60~(73%)	22~(27%)	0 1
44	DV	82/82~(100%)	65~(79%)	17~(21%)	1 4
45	BW	91/91~(100%)	81~(89%)	10~(11%)	6 24
45	DW	91/91~(100%)	80~(88%)	11~(12%)	5 20
46	BX	74/74~(100%)	67~(90%)	7~(10%)	8 29
46	DX	74/74~(100%)	65~(88%)	9~(12%)	5 20
47	BY	84/84~(100%)	65~(77%)	19~(23%)	1 3
47	DY	84/84~(100%)	67~(80%)	17~(20%)	1 5
48	ΒZ	155/155~(100%)	141 (91%)	14 (9%)	9 32
48	DZ	155/155~(100%)	148 (96%)	7~(4%)	27 58
49	B0	66/66~(100%)	55~(83%)	11 (17%)	2 10
49	D0	66/66~(100%)	60 (91%)	6 (9%)	9 31
50	B1	78/78~(100%)	68 (87%)	10~(13%)	4 18
50	D1	78/78~(100%)	62~(80%)	16 (20%)	1 4
51	B2	66/66~(100%)	51 (77%)	15~(23%)	1 3
51	D2	66/66~(100%)	60 (91%)	6 (9%)	9 31
52	B3	51/51~(100%)	47 (92%)	4 (8%)	12 38
52	D3	51/51~(100%)	48 (94%)	3 (6%)	19 49
53	B4	27/27~(100%)	22 (82%)	5 (18%)	1 7
53	D4	27/27~(100%)	24 (89%)	3 (11%)	6 23
54	B5	51/51~(100%)	39 (76%)	12 (24%)	1 3
54	D5	51/51~(100%)	41 (80%)	10 (20%)	1 5
55	B6	43/43~(100%)	33 (77%)	10 (23%)	1 3



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	D6	43/43~(100%)	36~(84%)	7~(16%)	2 10
56	B7	41/41~(100%)	35~(85%)	6~(15%)	3 14
56	D7	41/41~(100%)	32~(78%)	9~(22%)	1 3
57	B8	53/53~(100%)	41 (77%)	12~(23%)	1 3
57	D8	53/53~(100%)	43~(81%)	10~(19%)	1 6
58	B9	33/33~(100%)	26 (79%)	7~(21%)	1 4
58	D9	33/33~(100%)	30~(91%)	3~(9%)	9 31
60	DC	61/66~(92%)	$56 \ (92\%)$	5(8%)	11 36
All	All	9654/9664~(100%)	8391 (87%)	1263 $(13%)$	4 17

5 of 1263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BY	79	CYS
3	CC	34	LEU
47	DY	8	LYS
48	ΒZ	125	LEU
54	B5	35	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
42	BT	38	ASN
56	B7	8	ASN
46	DX	41	ASN
42	BT	84	GLN
48	BZ	73	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504~(99%)	300~(19%)	43 (2%)
1	CA	1504/1504~(100%)	296~(19%)	53 (3%)
22	AV	76/77~(98%)	18 (23%)	4(5%)
22	CV	76/77~(98%)	22 (28%)	1 (1%)
23	AW	75/76~(98%)	22~(29%)	2(2%)
23	CW	75/76~(98%)	19~(25%)	2(2%)



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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	AY	74/75~(98%)	38~(51%)	4 (5%)
24	CY	74/75~(98%)	38~(51%)	4 (5%)
25	AX	6/7~(85%)	3~(50%)	1 (16%)
26	BA	2800/2915~(96%)	779~(27%)	151 (5%)
26	DA	2799/2915~(96%)	754 (26%)	122~(4%)
27	BB	118/119~(99%)	36~(30%)	4(3%)
27	DB	118/119~(99%)	27~(22%)	4(3%)
59	CX	3/4~(75%)	2~(66%)	0
All	All	9301/9543~(97%)	2354~(25%)	395~(4%)

5 of 2354 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	22	G

5 of 395 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2416	G
1	CA	262	G
26	DA	2236	А
26	BA	2469	G
26	BA	2812	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bo Counts	ond leng RMSZ	# Z >2	B Counts	ond ang RMSZ	cles $ \# Z > 2$
N/L-1	т	<u></u>	D	т. 1	Bo	ond leng	\mathbf{ths}	В	ond ang	les
Mol	Type	Chain	Res	Link	Bo Counts	ond leng RMSZ	# Z >2	B Counts	ond ang RMSZ	# Z > 2

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
25	PSU	AX	19	24,25	-	2/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
25	AX	19	PSU	C5-C1'	-5.61	1.47	1.52
25	AX	19	PSU	C4-N3	2.67	1.37	1.33
25	AX	19	PSU	C2-N1	2.59	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
25	AX	19	PSU	N1-C2-N3	-17.54	114.49	128.43
25	AX	19	PSU	C4-N3-C2	14.55	127.42	115.14
25	AX	19	PSU	C5-C4-N3	-8.30	114.67	125.36
25	AX	19	PSU	C6-N1-C2	2.65	119.73	115.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	AX	19	PSU	O4'-C4'-C5'-O5'
25	AX	19	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	AX	19	PSU	7	0



5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
60	DC	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DC	110:ALA	С	119:ALA	Ν	13.98
1	DC	136:ALA	С	139:ALA	Ν	11.93



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	$ $ $<$ $\mathbf{RSRZ}>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	AA	1504/1504~(100%)	0.11	60 (3%) 38 36	23,77,165,393	0
1	CA	1504/1504~(100%)	0.26	95 (6%) 20 20	38,86,188,312	0
2	AB	234/234~(100%)	0.26	12 (5%) 28 26	66, 113, 158, 196	0
2	CB	234/234~(100%)	0.67	34 (14%) 2 2	85, 139, 177, 216	0
3	AC	206/206~(100%)	-0.05	5 (2%) 59 56	64, 96, 134, 183	0
3	CC	206/206~(100%)	0.87	30 (14%) 2 2	90, 130, 182, 221	0
4	AD	208/208~(100%)	0.12	7 (3%) 45 43	55,91,126,174	0
4	CD	208/208~(100%)	-0.08	3 (1%) 75 75	49, 79, 108, 139	0
5	AE	150/150~(100%)	-0.02	0 100 100	47, 76, 104, 125	0
5	CE	150/150~(100%)	0.14	4 (2%) 54 52	58,88,126,148	0
6	AF	101/101~(100%)	-0.21	0 100 100	52,80,108,124	0
6	CF	101/101~(100%)	-0.08	2 (1%) 65 64	52,82,116,139	0
7	AG	155/155~(100%)	-0.01	7 (4%) 33 32	61,97,137,156	0
7	CG	155/155~(100%)	0.58	14 (9%) 9 9	82,119,157,175	0
8	AH	138/138~(100%)	-0.20	0 100 100	50,81,105,135	0
8	CH	138/138~(100%)	-0.02	3 (2%) 62 60	59,95,119,146	0
9	AI	127/127~(100%)	0.32	8 (6%) 20 20	58,112,146,230	0
9	CI	127/127~(100%)	1.17	32~(25%) 0 0	94,136,180,235	0
10	AJ	98/98~(100%)	0.72	12 (12%) 4 3	67,119,160,187	0
10	CJ	98/98~(100%)	1.36	26~(26%) 0 0	94,158,190,226	0
11	AK	$119/119\ (100\%)$	-0.01	4 (3%) 45 43	45, 79, 108, 165	0
11	CK	119/119~(100%)	0.48	11 (9%) 9 9	55, 95, 132, 161	0
12	AL	124/124~(100%)	0.03	8 (6%) 18 18	47, 71, 105, 155	0
12	CL	124/124~(100%)	0.14	8 (6%) 18 18	$50,81,115,12\overline{4}$	0



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Mol	Chain	Analysed	<RSRZ $>$	# RSRZ > 2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
13	AM	124/124~(100%)	0.70	13 (10%) 6 6	68, 112, 153, 231	0
13	CM	124/124~(100%)	1.50	30~(24%) 0 0	101, 153, 200, 218	0
14	AN	60/60~(100%)	0.07	0 100 100	55,85,135,155	0
14	CN	60/60~(100%)	0.86	7 (11%) 4 4	104, 137, 160, 182	0
15	AO	88/88~(100%)	0.02	1 (1%) 80 81	48,80,111,130	0
15	CO	88/88 (100%)	0.02	2 (2%) 60 59	55, 87, 117, 139	0
16	AP	83/83 (100%)	0.20	2 (2%) 59 56	65, 92, 125, 149	0
16	CP	83/83 (100%)	-0.11	0 100 100	51, 73, 112, 139	0
17	AQ	99/99~(100%)	0.12	0 100 100	51, 90, 112, 117	0
17	CQ	99/99~(100%)	0.02	2 (2%) 65 64	63, 87, 115, 126	0
18	AR	70/70~(100%)	-0.10	1 (1%) 75 75	48, 76, 108, 138	0
18	CR	70/70~(100%)	0.06	2 (2%) 51 50	61, 91, 126, 149	0
19	AS	78/78~(100%)	0.38	6 (7%) 13 12	72,114,165,189	0
19	CS	78/78~(100%)	1.54	27 (34%) 0 0	111, 160, 209, 221	0
20	AT	99/99~(100%)	0.24	4 (4%) 38 36	67,102,150,169	0
20	CT	99/99~(100%)	0.05	2 (2%) 65 64	49, 96, 135, 150	0
21	AU	24/24~(100%)	0.34	0 100 100	74, 92, 117, 119	0
21	CU	24/24~(100%)	2.84	14 (58%) 0 0	105, 141, 205, 253	0
22	AV	77/77~(100%)	-0.08	1 (1%) 77 77	34,78,122,187	0
22	CV	77/77~(100%)	0.40	8 (10%) 6 6	41, 107, 162, 175	0
23	AW	76/76~(100%)	1.93	33~(43%) 0 0	37,183,225,269	0
23	CW	76/76~(100%)	2.60	44 (57%) 0 0	59, 192, 268, 296	0
24	AY	75/75~(100%)	1.76	30~(40%) 0 0	37,107,188,213	0
24	CY	75/75~(100%)	2.48	39~(52%) 0 0	37,107,188,213	0
25	AX	6/7~(85%)	0.13	0 100 100	50,53,106,116	0
26	BA	2807/2915~(96%)	-0.20	75 (2%) 54 52	9,38,151,312	0
26	DA	2807/2915~(96%)	0.01	114 (4%) 37 35	24,64,168,297	0
27	BB	$\overline{119/119}~(100\%)$	-0.25	0 100 100	$\overline{32, 60, 91, 118}$	0
27	DB	119/119~(100%)	0.42	8 (6%) 17 17	71, 112, 151, 191	0
28	BC	$\overline{190/206}~(92\%)$	3.56	120~(63%) 0 0	108, 181, 242, 295	0
29	BD	271/271~(100%)	-0.45	0 100 100	18, 36, 76, 122	0


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Mol	Chain	Analysed	$<$ RSRZ $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathbf{\AA}^2)$	$Q{<}0.9$
29	DD	271/271~(100%)	-0.26	1 (0%) 92 93	23, 56, 91, 127	0
30	BE	204/204~(100%)	-0.28	2 (0%) 82 82	18, 48, 92, 134	0
30	DE	204/204~(100%)	-0.13	5 (2%) 57 54	28,65,120,165	0
31	$_{ m BF}$	207/207~(100%)	-0.29	4 (1%) 66 65	17, 48, 133, 191	0
31	DF	207/207~(100%)	0.04	7 (3%) 45 43	31,87,149,214	0
32	BG	181/181~(100%)	0.03	5 (2%) 53 51	56, 82, 129, 172	0
32	DG	181/181~(100%)	0.49	14 (7%) 13 12	82, 128, 167, 210	0
33	BH	159/159~(100%)	-0.10	5 (3%) 49 48	32, 68, 118, 181	0
33	DH	159/159~(100%)	0.91	35 (22%) 0 1	70, 128, 180, 235	0
34	BI	145/145~(100%)	-0.04	1 (0%) 87 88	44, 95, 123, 159	0
34	DI	145/145~(100%)	0.26	5 (3%) 45 43	48, 101, 137, 159	0
35	BJ	130/130~(100%)	2.98	64 (49%) 0 0	120, 164, 275, 373	0
35	DJ	130/130~(100%)	3.50	87 (66%) 0 0	122, 193, 233, 284	0
36	BN	138/138~(100%)	-0.32	3 (2%) 62 60	24, 46, 95, 129	0
36	DN	138/138~(100%)	-0.01	3 (2%) 62 60	54, 90, 120, 133	0
37	BO	122/122~(100%)	-0.48	0 100 100	26, 49, 75, 91	0
37	DO	122/122~(100%)	-0.35	0 100 100	39,64,85,92	0
38	BP	146/146~(100%)	-0.08	3 (2%) 63 62	21,65,115,159	0
38	DP	146/146~(100%)	0.29	5 (3%) 45 43	39,92,134,174	0
39	BQ	141/141~(100%)	-0.34	2 (1%) 75 75	27, 51, 85, 188	0
39	DQ	141/141~(100%)	0.14	3 (2%) 63 62	58, 92, 125, 161	0
40	BR	117/117~(100%)	-0.36	0 100 100	21, 42, 78, 93	0
40	DR	117/117~(100%)	-0.14	1 (0%) 84 84	40,65,100,131	0
41	BS	98/98~(100%)	-0.06	1 (1%) 82 82	35,64,105,136	0
41	DS	98/98~(100%)	0.34	3 (3%) 49 48	72,110,151,181	0
42	BT	137/137~(100%)	-0.13	5 (3%) 42 40	34,64,139,181	0
42	DT	$\overline{137/137}\;(100\%)$	0.01	6 (4%) 34 33	43, 77, 135, 170	0
43	BU	117/117~(100%)	-0.43	0 100 100	15, 37, 73, 98	0
43	DU	117/117~(100%)	0.10	5 (4%) 35 34	40,80,135,155	0
44	BV	101/101~(100%)	-0.32	1 (0%) 82 82	24, 51, 85, 119	0
44	DV	101/101~(100%)	0.58	11 (10%) 5 5	61,110,143,183	0

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Mol	Chain	Analysed	<RSRZ $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
45	BW	113/113~(100%)	-0.35	1 (0%) 84 84	25, 37, 75, 137	0
45	DW	113/113~(100%)	0.01	4 (3%) 44 42	49,66,103,147	0
46	BX	92/92~(100%)	-0.45	0 100 100	25,44,73,82	0
46	DX	92/92~(100%)	-0.11	0 100 100	43, 77, 98, 114	0
47	BY	100/100~(100%)	0.25	10 (10%) 7 7	34,66,163,201	0
47	DY	100/100~(100%)	0.66	13 (13%) 3 3	56, 100, 175, 209	0
48	BZ	176/176~(100%)	1.75	54 (30%) 0 0	43, 119, 275, 309	0
48	DZ	176/176~(100%)	2.37	66 (37%) 0 0	92, 149, 299, 353	0
49	B0	84/84 (100%)	-0.15	0 100 100	25, 43, 78, 110	0
49	D0	84/84 (100%)	0.51	7 (8%) 11 11	58, 84, 105, 128	0
50	B1	93/93~(100%)	-0.17	3 (3%) 47 46	26, 48, 94, 131	0
50	D1	93/93~(100%)	-0.04	2 (2%) 62 60	39,63,111,153	0
51	B2	71/71~(100%)	-0.01	2 (2%) 53 51	34,61,101,164	0
51	D2	71/71~(100%)	-0.01	1 (1%) 75 75	60, 90, 131, 150	0
52	B3	59/59~(100%)	-0.16	2 (3%) 45 43	29, 48, 92, 149	0
52	D3	59/59~(100%)	0.56	5 (8%) 10 10	65, 101, 135, 253	0
53	B4	30/30~(100%)	0.00	1 (3%) 46 44	69,116,141,154	0
53	D4	30/30~(100%)	0.83	2 (6%) 17 17	121, 142, 163, 173	0
54	B5	59/59~(100%)	0.05	3 (5%) 28 26	21, 42, 139, 213	0
54	D5	59/59~(100%)	-0.06	3 (5%) 28 26	42, 67, 130, 179	0
55	B6	44/44~(100%)	0.12	2 (4%) 33 32	30,60,93,118	0
55	D6	44/44~(100%)	0.54	1 (2%) 60 59	51, 90, 113, 121	0
56	B7	48/48 (100%)	-0.31	1 (2%) 63 62	20, 30, 63, 124	0
56	D7	48/48 (100%)	-0.19	1 (2%) 63 62	31, 49, 80, 98	0
57	B8	63/63~(100%)	-0.26	0 100 100	30, 44, 64, 129	0
57	D8	63/63~(100%)	-0.01	2 (3%) 47 46	50, 77, 112, 154	0
58	B9	36/36~(100%)	-0.03	0 100 100	34, 49, 63, 78	0
58	D9	36/36~(100%)	0.58	4 (11%) 5 5	63, 91, 115, 125	0
59	CX	4/4 (100%)	0.37	1 (25%) 0 0	70,87,90,158	0
60	DC	190/196~(96%)	3.98	143 (75%) 0 0	109, 188, 240, 265	0
All	All	21440/21679~(98%)	0.24	1591 (7%) 14 14	9,77,180,393	0



Mol	Chain	\mathbf{Res}	Type	RSRZ
35	ВJ	52	ALA	25.7
48	DZ	172	ALA	20.9
35	BJ	51	ALA	20.7
26	DA	2812	G	20.5
48	DZ	151	HIS	15.8

The worst 5 of 1591 RSRZ outliers are listed below:

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
25	PSU	AX	19	20/21	0.93	0.15	$83,\!95,\!104,\!110$	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

