

# wwPDB EM Validation Summary Report (i)

Nov 19, 2022 - 07:10 pm GMT

AVENI
4 V DIN
EMD-1799
tRNA translocation on the 70S ribosome: the post- translocational transloca-
tion intermediate TI(POST)
Ratje, A.H.; Loerke, J.; Mikolajka, A.; Bruenner, M.; Hildebrand, P.W.;
Starosta, A.L.; Doenhoefer, A.; Connell, S.R.; Fucini, P.; Mielke, T.; Whitford,
P.C.; Onuchic, J.N.; Yu, Y.; Sanbonmatsu, K.Y.; Hartmann, R.K.; Penczek,
P.A.; Wilson, D.N.; Spahn, C.M.T.
2010-10-21
7.60  Å(reported)
2WRJ, 2WRI

This is a wwPDB EM 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/EMValidationReportHelp 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:

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{MapQ}$	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 7.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	EM structures		
	(# Entries)	(#Entries)		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
Sidechain outliers	154315	3826		
RNA backbone	4643	859		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$  The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length		Quality of chain							
				97%							
1	AA	1522	• 22%	22% 58% 18%							
				91%							
2	AB	256	23%	14% 5% 9%							
			86%								
3	AC	239	24%	44%	14% 5% 14%						
				100%							
4	AD	209	30%	49%	16% 5%						
				93%							
5	AE	162	31%	44%	14% • 7%						

Continued on next page...

Validation Pipeline (wwPDB-VP) : 2.31.2



Mol	Chain	Length	Fugern	Quality of c	hain	
6	AF	101	33%	100%	)%	15% ·
	AC	150		99%		
(	AG	150	34%	48	3%	15% ••
8	AH	138	30%	5	7%	10% ·
9	AI	128	18%	59%	-	17% 5%•
10	AJ	105	11%	93% 54%	22%	6% 7%
11	AK	129	29%	92%	)	8% • 8%
12	AL	132	22%	94% 51%	1	5% 6% 6%
13	AM	126	18%	55%		19% 6% ·
14	AN	61	34%	98%	)	10% 10% •
15	AO	89	34%	99% 44%	)	19% ••
16	AP	88	11%	94% 66%		15% • 6%
17	AQ	105	25%	94% 56%		10% · 6%
18	AR	88	20%	80% 42%	15% •	20%
19	AS	93	8%	84% 49%	23%	• 16%
20	AT	106	18%	93% 48%	23%	5% 7%
21	AU	27	30%	89% 37%	19%	• 11%
22	AV	77	• 29%	99% 51%		19%
23	AX	11	9%	45%	45%	
24	AY	691	21%	96% 52%		20% • •
25	B0	85	40%	99%	41%	14% • •
26	B1	98	15%	95% 54%	2:	2% • 5%
27	B2	72	8%	99% 57%	29	% • •
28	B3	60	17%	98% 58%		15% 8% ·
29	B4	71	13%	80% 37% 15	% 15%	20%
30	B5	60	37%	98%		15% 10% ·



Mol	Chain	Length	Quality of chain								
31	B6	54	6% 37%	33%	179	% 7%					
32	B7	49	20%	98%	1	80/					
02		-15	20%	97%	1	070 • •					
33	B8	65	17%	58% 100%	11%	11% •					
34	B9	37	30%	43% 97%	22%	% 5%					
35	ВА	2915	• 24%		21%						
36	BB	122	16%	98% 66%		15% •					
37	BC	229	36%	100%		8% •					
38	BD	276	26%	100%	210						
00		210	2070	99%	21						
39	BE	206	19%	49% 99%	26%	•••					
40	BF	210	17%	21	.% ••						
41	BG	182	15%	55%	22%	7% •					
42	BH	180	17%	18%	• 8%						
43	BK	147	24%	189	<b>6</b> • 5%						
44	BL	121	5	15% ••	45%						
45	BN	140	210/	99%	210/						
40		140	21%	100%	21%	••					
46	BO	122	26%	55% 97%		17% •					
47	BP	150	16%	48%	25%	8% •					
48	BQ	141	23%	52%	18%	6%					
49	$\operatorname{BR}$	118	22%	53%	20	% • •					
50	BS	112	8%	88%	20% 7%	6 12%					
51	BT	146	1.20/	94%	210/	140/ 50/					
51		140	12%	21%	L4% 6%						
52	BU	118	20%	52% 100%	22%	5%•					
53	BV	101	21%	51%	22%	6%					
54	BW	113	19%	65%		12% •					
55	BX	96	23%	96%	2	0% •					
		- •	-								



Mol	Chain	Length		Quality of chain						
			96%							
56	BY	110	9%	58%	269	%	• •			
				89%						
57	BZ	206	20%	43%	19%	7%	11%			



# 2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 152777 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RRNA.

Mol	Chain	Residues		1	AltConf	Trace			
1	AA	1504	Total 32329	C 14390	N 5992	O 10444	Р 1503	0	0

• Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	234	Total 1900	C 1213	N 341	0 341	${ m S}{ m 5}$	0	0

• Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total 1612	C 1016	N 314	0 281	S 1	0	0

• Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	208	Total 1703	C 1066	N 339	0 291	${f S}7$	0	0

• Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
5	AE	150	Total 1146	С 724	N 217	O 201	${S \atop 4}$	0	0

• Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
6	AF	101	Total 843	C 531	N 155	0 154	${ m S} { m 3}$	0	0



• Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues		At	oms	AltConf	Trace		
7	AG	155	Total 1257	C 781	N 252	0 218	S 6	0	0

• Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues		At	oms	AltConf	Trace		
8	AH	138	Total 1116	C 705	N 215	0 193	${ m S} { m 3}$	0	0

• Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
9	AI	127	Total 1010	C 639	N 197	0 174	0	0

• Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
10	AJ	98	Total 794	C 499	N 156	0 138	S 1	0	0

• Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	AK	119	Total 885	C 549	N 168	0 165	${ m S} { m 3}$	0	0

• Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues		At	oms	AltConf	Trace		
12	AL	124	Total 970	C 611	N 195	0 163	S 1	0	0

• Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues		At	oms	AltConf	Trace		
13	AM	124	Total 987	C 611	N 205	O 169	${ m S} { m 2}$	0	0

• Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.



Mol	Chain	Residues		Ate	oms	AltConf	Trace		
14	AN	60	Total 492	C 312	N 104	0 72	$\frac{S}{4}$	0	0

• Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	AO	88	Total 734	C 459	N 147	0 126	${S \over 2}$	0	0

• Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues		At	oms			AltConf	Trace
16	AP	83	Total 700	C 443	N 139	0 117	S 1	0	0

• Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
17	AQ	99	Total 823	C 528	N 151	0 142	${ m S} { m 2}$	0	0

• Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
18	AR	70	Total 574	C 367	N 112	O 95	0	0

• Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	AS	78	Total 629	C 403	N 114	0 110	${ m S} { m 2}$	0	0

• Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues		At	oms			AltConf	Trace
20	AT	99	Total 763	C 470	N 162	0 129	${S \over 2}$	0	0

• Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.



Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
21	AU	24	Total 208	C 128	N 50	O 30	0	0

• Molecule 22 is a RNA chain called TRNA.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
22	AV	77	Total 1640	C 732	N 297	O 535	Р 76	0	0

• Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues		Ate	$\mathbf{oms}$		AltConf	Trace	
23	AX	11	Total 230	C 105	N 41	0 74	Р 10	0	0

• Molecule 24 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues		At	AltConf	Trace			
24	AY	666	Total 5214	C 3316	N 892	0 988	S 18	0	0

• Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	B0	84	Total 662	C 410	N 140	0 111	S 1	0	0

• Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues		At	oms	AltConf	Trace		
26	B1	93	Total 731	C 460	N 145	0 125	S 1	0	0

• Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues		At	oms			AltConf	Trace
27	B2	71	Total 598	C 370	N 121	O 106	S 1	0	0

• Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.



Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
28	B3	59	Total 467	C 298	N 90	0 78	S 1	0	0

• Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
29	B4	57	Total 450	C 285	N 77	O 83	${ m S}{ m 5}$	0	0

• Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
30	B5	59	Total 459	C 288	N 90	O 76	${f S}{5}$	0	0

• Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues		Atc	$\mathbf{ms}$			AltConf	Trace
21	R6	50	Total	С	Ν	Ο	S	0	0
	D0	50	433	270	88	71	4	0	0

• Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
32	B7	48	Total 418	C 257	N 104	O 55	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
33	B8	63	Total	С	N	0	S	0	0
			507	326	101	78	2		

• Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues		Atc	$\mathbf{ms}$			AltConf	Trace
34	B9	37	Total 307	C 188	N 68	O 47	${f S}{4}$	0	0

• Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.



Mol	Chain	Residues			Atoms			AltConf	Trace
35	BA	2901	Total 62474	C 27806	N 11681	O 20087	Р 2900	0	0

• Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues		A	AltConf	Trace			
36	BB	119	Total 2551	C 1136	N 471	O 826	Р 118	0	0

• Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues		At	oms			AltConf	Trace
37	BC	228	Total 1742	C 1101	N 319	0 319	${ m S} { m 3}$	0	0

• Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues		Ate	AltConf	Trace			
38	BD	275	Total 2145	C 1353	N 428	0 361	${ m S} { m 3}$	0	0

• Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues		At	oms			AltConf	Trace
39	BE	204	Total 1563	C 988	N 299	0 270	S 6	0	0

• Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues		At	oms			AltConf	Trace
40	BF	207	Total 1623	C 1035	N 303	0 282	${ m S} { m 3}$	0	0

• Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues		At	oms			AltConf	Trace
41	BG	181	Total 1474	C 942	N 268	O 260	$\begin{array}{c} \mathrm{S} \\ \mathrm{4} \end{array}$	0	0

• Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.



Mol	Chain	Residues		At	AltConf	Trace			
42	BH	166	Total 1268	C 803	N 237	0 227	S 1	0	0

• Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
43	BK	139	Total 1025	C 653	N 181	0 186	${f S}{5}$	0	0

• Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
44	BL	67	Total 477	C 301	N 81	O 95	0	0

• Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues		At	AltConf	Trace			
45	BN	138	Total 1104	C 712	N 206	0 182	S 4	0	0

• Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues		At	AltConf	Trace			
46	BO	122	Total 933	C 588	N 171	O 170	$\frac{S}{4}$	0	0

• Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues		At	AltConf	Trace			
47	BP	146	Total 1114	C 692	N 227	O 193	${S \over 2}$	0	0

• Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues		At	AltConf	Trace			
48	BQ	141	Total 1122	C 715	N 212	0 188	S 7	0	0

• Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.



Mol	Chain	Residues		Ato	ms	AltConf	Trace	
49	BR	117	Total 960	C 599	N 202	O 159	0	0

• Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
50	BS	98	Total 770	C 486	N 154	O 130	0	0

• Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues		At	AltConf	Trace			
51	BT	137	Total 1141	C 710	N 234	0 196	S 1	0	0

• Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues		At	AltConf	Trace			
52	BU	117	Total 958	C 604	N 202	0 151	S 1	0	0

• Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues		At	oms			AltConf	Trace
53	BV	101	Total 779	C 501	N 142	0 135	S 1	0	0

• Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues		At	oms			AltConf	Trace
54	BW	113	Total 896	C 563	N 176	0 155	${ m S} { m 2}$	0	0

• Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
55	BX	92	Total 725	C 471	N 131	O 123	0	0

• Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.



Mol	Chain	Residues		At	oms			AltConf	Trace
56	BY	106	Total 810	$\begin{array}{c} \mathrm{C} \\ 520 \end{array}$	N 154	0 131	${ m S}{ m 5}$	0	0

• Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues		At	oms			AltConf	Trace
57	BZ	184	Total 1467	C 936	N 261	O 268	${S \over 2}$	0	0

• Molecule 58 is FUSIDIC ACID (three-letter code: FUA) (formula:  $C_{31}H_{48}O_6$ ).



Mol	Chain	Residues	Atoms	AltConf
58	AY	1	Total         C         O           37         31         6	0

• Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).





Mol	Chain	Residues		Ate	oms			AltConf
50	۸V	1	Total	С	Ν	Ο	Р	0
- 39	AI	1	28	10	5	11	2	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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 RRNA





G557	(1558 A 550	USGO	U561	C562	A563		G566	G567	G568	G570	U571	A572	A573	A574 CE7E	G576	G577	C578	G579		U582	A583	G584	G585	C586	G587 G588	C589	C590	U591	G592	G594	G595	C596	U598	C599	C600		N603	G604	UGOS	G606	A 607	A609	G610	A611	C613	A614	C615 G616
G617	C618 1161 0		A621	A622	C623	G625	U626	G627	G628 G629	<b>G630</b>	G631	A632	G633	C634	U636	G637	G638	G 639	A 040	A642	C643	G644	C645	U646	C647	G649	G650	C651	0652 A653	G654	A655	C656	G658	U659	G660	G661 G662	4663	G664	A665	G666	G667	U669	G670	G671	G673	G674	A675
U677	U678	CG80	C681	G682	G683 A684	G685	U686	A687	G688	6690	G691	U692	G693	A694 A605	<b>A696</b>	U697	<b>G698</b>	C699	6/00	A702	G703	A704	U705	A706	C708	G100	G710	G711	A/12 G713	G714 •	A715	A716	G718	C719	C720	6721 A723	U723	G724	G725	C726	G727 A728	A729	G730	G731 G730	4733	G734	C735 C736
A737	C738	U740	6741	G742	U743	C745	A746	C747	C749	G750	U751	G752	A753	C754	C756	U757	G758	A759	6764 6764	CT62	G763	C764	G765	A766	A767 A768	G769	C770	G771	0773 C773	G774	G775	G776	G778	C779	A780	A781	CT83	C784	G785	G786	A787	U789	A790	G791	U793	A794	C795
C7.97	G798	C800	U801	A802	G803	C805	C806	A807	C808	C810	C811	C812	U813	A814 A815	A816	C817	G818	A819	0820	C822	G823	C824	G825	C826	1827 4828	G829	G830	U831	C832	C834	U835	G836 C927	G838	U839	C840	U841 C848	C849	U850	G851	G852	G853 G854	G855	C856	C857	4859 A859	A860	G861 C862
U863	A864	CB66	G867	C868	G869		A872	A873	G874	G876	C877	G878	C879	C880 C881	C882	C883	U884	G885	1000	<b>G</b> 888	<b>A</b> 889	<b>G</b> 890	U891	A892	C893 C894	G895	C896	C897		<b>A900</b>	A901	(902	C904	1905	9065	A907	<b>A909</b>	C910	U911	C912	A913 A914	A915	G916	G917	V919	U920	U921 G922
A923	C924	G926	G927	G928	(1929	C931	C932	<b>G933</b>	C934 4935	C936	A937	A938	G939	C940 C941	G942	U943	G944	G945	A340	C948	A949	U950	G951	U952	G953 G954	U955	U956	U957	A958 А959	0960	U961	C962	4964	A965	<b>G966</b>	C967	A969	C970	G971	C972	G973 A974	A975	G976	A977	C979	C980	U982
A983	C984	A986	G987	G988	C989	1991	U992	(993	A994 Caaf	A996	<b>7997</b>	6998	C999	01000	G1001A	G1002	G1003	A1004 A1005	C1006	C1007	C1008	G1009	G1010	G1011	G1013	A1014	A1015	A1016 G1017	C1018	C1019	U1020	G1021 G1022	G1023	G1024	U1025	C1027	C1028	C1029	C1030	C1030B	G1030C A1030D	G1031	G1032	G1033 G1034	A1035	G1036	C1037
C1 038	C1039		G1042	C1043	A1044	A1046	G1047	G1048	01049 G1050	C1051	U1052	G1053	C1 05 4	A1055 111056	G1057	G1058	C1059	C1060	19015	C1063	G1064	U1065	C1066	A1067	G1068		C1071	G1072	010/3 61074	C1075	C1076	G1077	G1079	A1080	G1081	G1082 111 083	G1084	U1085	U1086	G1087	G1088 G1089	U1090	U1091	A1092	G1094	U1 095	C1096 C1097
C1098	G1099	A1101	A1102	C1103	G1104	G1106	C1107	G1108	C1109 A1110		C1112	c1113	C1114	C1115	G1117	C1118	C1119	G1120	17110	A1123	G1124	U1125	U1126	G1127	C1128 C1129	A1130	G1131	C1132	G1133 G1134	U1135	U1136	C1137	G1139	C1140	C1141	G1142 C1143	G1144	C1145	A1146	C1147	01148	U1150	A1151	A1152	G1154	G1155	G1156
C1158	U1159 C1160	C1161	C1162	C1163	G1164 C1165	G1166	A1168	A1169	A1170	C1172	G1173	G1174	G1175	A1176 C1177	G1178	A1179	A1180	G1181	41102	G1184	G1185	G1186	G1187	A1188	C1189 G1190	A1191	C1192	G1193	U1194 C1195	U1196	G1197	G1198	C1200	A1201	G1202	C1203		G1206	G1207	C1208	C1209	U1211	U1212	A1213	G1214 G1215	G1216	C1217 C1218
U1219	G1220	G1222	C1223	G1224	A1225	A1227	C1228	A1229	C1230 G1231	U1232	G1233	C1234	U1235	A1236 C1237	A1238	A1239	U1240	G1241	C1 242	C1244	A1245	C1246	U1247	A1248	C1249 A1250	A1251	A1252	G1253	C1254 G1255	A1256	U1257	G1258	C1260	A1261	C1262	C1263	G1265	G1266	C1267	A1268	A1269	G1271	G1272	G1273	61274 A1275	G1276	C1277 • U1278 •
A1279	A1280	C1282	G1283	C1284	A1285	A1287	A1288	A1289	G1290 G1291	U1292	G1293	G1294	G1295	C1296	C1298	A1299	G1300	U1301	01302	G1304	G1305	A1306	U1307	U1308	61309 61310	G1311	G1312	U1313	C1314	G1316	C1317	A1318	C1320	C1321	C1322	61323 A1324	C1325	c1326	C1327	C1328	A1329	G1331	A1332	A1333	G1335	C1336	G1337 G1338













#### • Molecule 15: 30S RIBOSOMAL PROTEIN S15









ARG GLY ILE 164 165 166 A67 A67 A66 A66 A66 A66 A66 A66 A66 A	171 672 873 875 875 976 877 877 877 179 181 181 181 181 182 182 182 183 885	686 H87 V88 F90 F90 F90 E95 897 897 R96 S97 M98 R96 S97 N98 R96 S97 C101 L101 L101 C103	A104 1105 V106 V107 F108 F108 F109 F110 F115
V121 W122 R123 Q124 A125 E126 K127 Y128 K129 V120	PI31           R132           133           133           133           F133           A134           F135           A134           F135           A134           F135           A136           A134           F135           A136           A137           A137           A138           A137           A136           A138           A143           A144	L146 H147 L146 V149 V149 T150 T152 M153 Q154 Q154 C152 C158 C158 A160 C158 A160 C158 V162	VI83           M164           Q165           L166           P187           P172           P173           P173           P173           P174           P173           P174           P175           P176           P177           V180           V180
L131 R132 M183 K184 A185 A185 T187 Y186 Y186 Y188 G189 M190	bibit bibibit bibibit bibibit bibibibi	Y205 P207 P207 P207 P207 P208 P210 P211 P212 P217 P215 P217 P217 P218 P228 P222	F223 D224 E226 R226 R226 M228 K230 Y231 L232 C233 C233 C233 C233 C233 C233 C233
E241 1242 V243 A244 A245 A245 R246 R248 C248 C249 C249	1251 1252 1255 1255 1255 1255 1255 1255	N265 N266 K267 C269 Q269 Q270 Q270 L271 L273 L273 L273 L275 V276 V276 V276 V276 V277 P281 P280 P280	P283 1285 1285 P287 P287 P289 R290 <b>C291</b> P293 P293 P293 P293 P294 P293 P294 P295 P295 P295 P296 P296 P296 P296 P296 P296 P296 P296
I301 H302 P303 P304 P305 P305 R306 R307 P308 R310 A310	A311 L312 F314 F314 F314 M317 A316 P320 P320 F320 V321 C323 R321 F320 F320	L325 F327 F326 F328 R328 V330 V330 V330 F333 C333 C333 F35 C333 C333 C333 C333	N343 T344 T345 K345 R347 R345 R347 R345 R347 R345 R351 R351 R351 L355 L355 R353 R353 R353 R354 R353 R353 R356 R356 R356 R356 R356 R356
N1361 H1362 R1363 R264 E364 E365 E365 E365 E366 E366 E366 E366 E366	A371 6372 1373 1374 1375 0375 0375 0375 0379 0378 1380 K381 E382 1384	1385 0386 0386 1388 1388 1388 1388 0391 0391 1389 1395 1395 1395 1395 1395 1395 1395 139	E403 P404 P405 P407 P407 P407 P411 P411 P412 P415 P415 P415 P415 P415 P415 P415 P415 P415 P415 P415 P415 P415 P417 P412 P417
Q421           E422           K423           L424           A429           A429	1431 1432 1432 1435 1435 1436 1436 1437 1437 1442 1443 1443 1443	RM445           1446           0447           0447           0447           0447           0446           1446           1451           1451           1451           1451           1451           1451           1451           1451           1455           0455           1455           1455           1455           1455           1455           1455           1455           1455           1456           1457           1458           1458           1459           1461           1461	V463 P464 P465 P465 P465 P467 P467 P470 P475 P475 P475 P475 P475 P475 P476 P476 P476 P476 P476 P476 P476 P480
V481 A482 Y483 R484 E485 E485 I487 T486 R489 R489 R489	V491 V491 0492 E494 E495 E495 F495 F495 F495 F498 R499 R499 G500 G500 G500 G500	6505 9506 9507 9507 6608 8509 9511 1512 8513 8513 9515 9515 9515 8520 8520 6520	F523 E524 F526 V526 N526 A528 A528 C531 C531 C531 C531 C532 C531 C532 C532 C532 C532 C532 C532 C532 C532
A541 V542 V542 Q543 C545 C545 C545 C545 C545 C545 C545 C	q551         q551           8552         6553           6553         6553           P556         1555           P559         9557           P559         9563           P559         9564           P559         1563           P559         1563           P559         1563           P559         1563           P559         1563           P559         1563           P569         1563           P569         1563           P569         1563           P569         1563	V565 1566 15667 15667 15669 1569 15670 1577 1572 1577 1577 1577 1577 1577 1577	K583 I564 6865 6865 6866 6587 8688 8589 8589 8589 8593 8595 8595 8595 85
1601 1602 1602 1605 1605 M606 N606 V608 V608 V608	T611           7612           7612           7613           7616           7616           7616           7616           7618           7618           7618           7618           7618           7618           7618           7618           7618           7618           7618           7618           7618           7620           7621           7622           7623           7623           7623           7623           7623           7623           7623           7623           7623	MGSE           A6226           R627           R627           R629           Q630           Q633           G633           G633           R634           R635           G633           G633           G633           G634           G635           G638           G638           G638           G638           G638           G638           G638           G638           G638           G641           V642	I 643           R644           A 645           F 644           V 647           P648           E651           R652           F655           G654           P655           P656           P656           P658           P658           P658           P658           P658           P658           P658
X 660 X			
• Molecule 25: 50 Chain B0:	40%	111N L27 199% 41% 14%	
MET A.2 H3 K4 K5 C4 C4 C3 C3 C3 C3 C3 C3 C4 C4 C4 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5	R1           N12           013           014           015           016           016           017           018           019           016           017           018           019           010           011           012           013           014           015           016           121           121           121           121           123           123           124           125           125           121           121           122           123           123           124           125           125           125           125           125           125           125           125           125           125           126           127           128           129           120      <	425 426 426 428 428 430 431 433 433 433 433 433 433 440 440	143       144       144       144       144       144       144       144       145       145       145       156       158
A61 L62 V63 D64 G65 V67 E68 F69 F69	PT1           R72           R72           G73           R72           R72           G73           R72           R72           R72           R72           R72           R72           R73           R74           R74           R74           R74           R77           R82           R82           R82           R82           R82		

WORLDWIDE PROTEIN DATA BANK







0         C51.0         C61.0         A54.0         C51.7         C51.7 <thc1.7< th="">         C51.7         C51.7</thc1.7<>	A575         A613         6452         6392         033           U576         A514         C453         C393         C393         C393           0577         A515         A615         A644         C453         C393         C393
1         1	AE75         A513         C452         C392           U576         A514         C453         C393           C577         A515         A454         C453
R         CISIG         Cuells         Alary         Al	A575         A513         A513         A513         C452         C38           U576         A514         A514         A545         A53         C38         C38 <td< th=""></td<>
8         CS16         C455         A394           0         C517         A457         C395           0         C517         A457         C397           0         C513         A457         C397           0         C513         A457         C397           0         C523         C461         A401           0         C523         C461         A401           0         C523         C461         A402           0         C523         C461         A402           0         C523         C461         A402           0         C523         C465         A402           0         C524         C465         C403           0         C533         C465         C403           0         C534         C465         C403           0         C534         C465         C413           0         C534         C465         C413           0         C534         C435         C413           0         C534         C435         C413           0         C534         C435         C413           0         C534         C435 </th <th>AF75         A513         G452           U576         A514         C453           G577         A515         A464</th>	AF75         A513         G452           U576         A514         C453           G577         A515         A464
	A575 A513 A575 A513 C4 U576 A514 C4 C4 C4 A515 A515 A515 A515
73         C516         C465           73         C517         C465           74         C514         C465           75         C513         C465           75         C513         C465           75         C514         C465           75         C523         C465           75         C531         A477           75         C531         A477           75         C531         A477           75         C532         C465           74         C543         C465           74         C543         C465           74         C543	A575 A513 A513 A514 A514 A515 A515 A515 A515 A515 A515
18         C516         0           19         0         0           11         0         0           12         0         0           13         0         0           14         0         0           15         0         0           16         0         0           16         0         0           16         0         0           16         0         0           16         0         0           16         0         0           16         0         0           17         0         0           18         0         0           19         0         0           11         0         0           11         0         0           11         0         0           11         0         0           11         0         0           11         0         0           11         0         0           11         0         0           11         0         0           12 <t< th=""><th>A A B575 A A B576 A B B576 A B B576 A B B577 A B5777 A B5777 B577 A B577 B577</th></t<>	A A B575 A A B576 A B B576 A B B576 A B B577 A B5777 A B5777 B577 A B577 B577
78     C515       79     C517       80     U519       81     U519       85     G522       86     U519       86     U523       86     U523       86     U523       86     U524       86     U523       86     U524       86     U523       86     U524       86     U554       86     U556       86     U566	A575 U576 G577
8、 5、 5、 5、 5、 8、 8、 5、 5、 8、 8、 5、 5、 5、 5 × 5 × 5 × 5 × 5 × 5 × 5 × 5	•••
2 2 2 3 4 8 8 5 5 8 8 7 7 7 8 8 9 5 7 9 9 7 7 9 8 8 9 5 7 9 9 9 7 7 9 8 8 7 9 7 9 9 7 9 7 9 7 9	
A5 A5 A5 A5 A5 A5 A5 A5 A5 A5	C635 C635
9635           4637           4637           4637           9636           9641           6441           6442           4643           4644           4645           4645           4644           4644           4644           4644           4644           4644           4644           4644           4644           4644           4644           4644           4644           4644           4644           4644           46541           46642	
G674           A675           A675           A676           A677           A676           A676           A677           A677           A676           A677           A677           A676           A679           C679           G680           G683           G683           G684           A685           G699           G699           G690           G701           G702           G703           G704           G705           G717           G711           G711           G711           G711           G712           G714           G715           G716           G717           G723           G726           G728	C731 C732 G733
••••••	
A734           A735           A735           C7367           C7377           C7387           C7387           C7397           C7397           C749           C756           C756 <t< th=""><th>C791 G792 A793</th></t<>	C791 G792 A793
•••••••••••••••••••••••••••••••••••••••	<b>**</b>
C7 94 C7 95 C7 95 C7 95 C7 95 C7 95 C7 95 C7 95 C7 96 C7 95 C8 05 C8 05 C	U851 G852 G853
4 º o v o v o v o v o v o o v o v o o v o o v o v o v o o o v o v o o o v o o o v o o o v o o o o v o o o o o o	0 8 4
1         2	C91. U91. C91.
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	73 74 75
0     0 <th>A9 G9 C9</th>	A9 G9 C9
775 777 777 888 888 888 888 888 888 888	032 033 034



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U1035	G1036	G1 037	G1039	C1040	C1041	C1043	G1044	A1045	A1046	G1047	A1 048	A1050	G1051	C1052	C1053	A1054	G1055	G1056	A1 057	G1058	11 060	111 06 1	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1059	G1071	C1072	A1073	G1074	C1075	A1077	U1078	C1079	C1080		U1083	A1084	A1085	A1086	G1087	A1 088	060 11	G1091	C1092	G1093	U1094
A1095	A1096	01097 A1098	G1099	C1100	U1101	A1103	C1104	U1105	G1106	G1107	01108 C1108	G1110	A1111	G1112	U1113	G1114	G1115	C1116	G1117	C1118 C1110	G1120	C1121	G1122	C1123	C1124	G1125	A1126	A1127	A1128	A1129	G1131	A1132	U1 133	C1135	G1136 C1137	G1138	G1139	C1140	U1141	01142 A1142A	A1143	G1144	C1145	C1146	C114/	G1 149	C1150	G1151	C1152	C1153	G1154
A1155	A1156	G1157 C1158	U1159	G1160	C1161	G1163	G1164	U1165	C1166	U1167	G1168 C1169	G1170	G1171	G1173	A1174	U1175	G1176	A1177	C1178	C1179 C1180	C1181	A1182	G1183	G1184	C1185	G1186	G1187	U1188	A1189	G1190 G1191	G1192	G1193	A1194	G1195	C1196 C1107	U1198	U1199	C1200	C1201	C1202 G1203	A1204	U1205	G1206	C1207	C1208	G1209		G1212	A1213	A1214	G1215
G1216	C1217	C1218 G1219	A1220	C1 22 1	C1221	G1223	C1224	G1225	A1226	G1 227	G1229	C1230	G1231	G1232	C1233	U1234	G1235	01.230 11.027	61 23 R	G1239	U1240	A1241	A1242	G1243	G1244	G1245	A1246	A1247	01240	G1250	C1251	G1252	A1253	A1254 11755	G1256	C1257	C1258	G1259	G1 261	A1262	U1263	G1264	A1265	G1266	01.207	A1 269	C1270	G1271	A1272	U1273	A1274
A1275	A1276	G1277	G1279	G1280	G1281	G1283	A1284	G1285	A1286	A1287	01288	C1290	C1291	U1292	C1293	U1294	C1295	G1296	C1297	C1298	U1300	A1301	A1302	G1303	C1304	C1305	C1306	A1307	A1308	G1309	G1311	U1312	U1313	C1314	C1315	A1317	C1318	G1319	C1320	A1321	U1323	G1324	G1325	U1326	C1327	G1328	01329	A1331	G1332	C1333	G1334
U1335	A1336	G1338	G1339	U1340	U1341	G1343	G1344	C1345	G1346	G1347	61348 A 1340	C1350	C1351	U1352	A1353	A1354	G1355	G1356	U1357	61358	A1360	G1361	C1362	C1363	G1364	A1365	A1366	A1367	G1368	G1369	G1371	U1372	A1373	G1374	C1375	G1377	A1378	A1379	G1380	G1387	C1383	A1384	G1385	C1386	C1387	G1388	G1389	U1391	A1392	A1393	U1394
A1395	U1396	01397 C1398	C1399	G1400	G1401	C1403	C1404	U1405	U1406	C1407	C1408	G1410	C1411	A1412	G1413	G1414	U1415	G1416	C1417	61418	11420	G1421	G1422	G1423	G1424	G1425	G1426	A1427	C1428	G1429 C1430	U1431	C1432	U1433	A1434	G1435 C1436	C1437	U1438	A1439	G1440	G1441 C1442	G1443	G1444	A1445	C1445A	C1440	G1441	A1449	G1450	C1450A	C1451	A ZOLTH
U1453	G1455	G1456	C1458	G1459	A1460 C1461	C1462	C1463	C1464	G1465	G1466	C146/	A1469	G1470	A1471	A1472	G1473	C1474	G1475	C1476	A14//	G1479	G1480	U1481	G1482	G1484	G1485	A1486	G1487	G1488	01489	G1491	G1492	C1493	A1494	A1495	A1497	C1498	C1499	G1500	C1501	U1503	C1504	C1505	C1506	A1507	A1508	C1509	A1509B	G1510		TICTO
C1513	U1514	G1516	G1517	U1518	G1519 C1500	U1523	G1524	G1525	G1526	G1527	A1528 A1528A	G1529	C1530	C1531	C1532	G1533	U1534	A1535	C1530	G1538	G1539	U1540	G1541	A1542	C1543	A1544	A1545	C1546 C1 E 4 Z	C154/	C1549	C1550	C1551	G1552	A1553 A1554	G1555	C1556	C1557	A1558	G1560	G1561	A1562	G1563	C1564	C1565	A1500	A1 30 /	A1569	A1570	A1571	A1572	G1573
C1574	C1575	01576 C1577	U1578	A1579	A1580	C1582	A1583	C1584	A1586	A1587	C1588	U1590	G1591	C1592	G1593	G1594	G1595	A1596	A1597	C1598	C1033	G1601	U1602	A1603	C1604	C1605	G1606	C1607	A1608	A1609	C1611	C1612	G1613	A1614	C1615		A1618	G1619	G1620	01621 61622	G1623	G1624	C1625	G1626	G1627	G1628	01629 61630	C1631	A1631A	A1632	G1633
A1634	G1635	C1636	C1638	U1639	C1640	G1642	G1643	C1644	G1645	C1646	G164/ C1648	G1649	G1650	G1651	A1652	G1653	A1654	A1655	C1656	C165/	01050	C1660	G1661	C1662	c1663	A1664	A1665	G1666	G1667	A1668	C1670	U1671	C1672	U1673	G1674 C1675	A1676	A1677	G1678	U1679	01680	G1682	C1683	C1684	C1685	C1686	G1687	01688	A1690	<b>C1691</b>	U1692	U1693
C1694	G1695	G1696 G1697	A1698	G1699	A1700	G1702	G1703	G1704	G1705	U1706	G1 /0/	U1709	C1710	C1711	c1712	U1713	G1714	G1717	G1718	61/19	G1721	41722	U1739	G1740	A1741	G1742	C1743	C1744	C1745	G1746	G1747	G1747A	G1748 A1740	G1750	C1751	C1752	G1753	01755 41755	G1756	U1757	G1758	A1759	A1760	41762	G1763	G1764	C1765	U1766	C1767	01768	



•	•	•	• •		•	••			•				•			•	•		•	•	••		•	•		•		••			••			•		•	•	•		•		•	••			•	•
G1770	C1771	G1772	A1773	01/75 01775	G1776	U1777	U1/79	A1780	C1781	C1782	A1784	A1785	A1786	A1787	A1789	C1790	A1791	G1792 C1793	U1794	C1795	U1796	C1797	G1799	C1800	G1801	A1802	C1804	U1805	C1806 G1807	U1808	A1809	G1811	A1812	G1813	G1814 41815	G1816	G1817	U1818	A1819 11820	A1821	G1822	G1823	G1824	61825 G1826	C1827	G1828	A1829
C1830	G1831	C1832	U1833	0183 <del>4</del> G1835	C1836	C1837	C1838 G1839	G1840	U1841	G1842	C1843 C1844	G1845	G1846	A1847	G1849	G1850	U1851	C1852	A1854	G1855	G1856	G1857	A1859	G1860	G1861	G1863	U1864	G1865	C1866 A1876	A1877	G1878	C1879	C1881	C1882	G1883	A1885	C1886	C1887	G1888 A1889	A1890	G1891	C1892	C1893	C1894	G1896	G1897	U1898
G1899	A1900	A1901	C1902	G1904	C1905	G1906	G1907	C1909	G1910	U1911	A1912 A1913	<mark>C1914</mark>	U1915	A1916	A1918	A1919	C1920	G1921 G1922	U1923	C1924	C1925	01926	A1928	G1929	G1930	A1932	G1933	C1934	61935	A1937	A1938	01939	C1941	C1942	U1943	G1945	U1946	C1947	G1948	G1950	U1951	A1952	A1953	61954 111955	U1956	C1957	C1958
G1959	A1960	C1961	C1962	G1964	C1965	A1966	G1968	A1969	A1970	A1971	G1973	C1974	G1975	U1976		C1979	G1980		C1983	G1984	G1985	A1986 G1987	C1988	G1989	C1990	G1992	U1993	C1994	01995 C1996	G1997	G1998	C1999	A2001	G2002	G2003	A2005	C2006	C2007	C2008	G2010	U2011	G2012	A2013	A2014	U2016	U2017	G2018
A2019	A2020	C2021	U2022	G2024	c2025	C2026	U2028	G2029	A2030	A2031	G2032 A2033	U2034	G2035	C2036	G2038	C2039	C2040	02041 42042	C2043	C2044	C2045	G2046	G2048	G2049	C2050	G2052	G2053	A2054	G2056	A2057	A2058	A2059	G2061	A2062	C2063	C2065	C2066	G2067	U2068	G2070	A2071	G2072	C2073	U20/4	U2076	A2077	C2078
62021	G2080	C2081	A2082	C2084	C2085	U2086	G2088	U2089	G2090	U2091	02092 (2093	G2094	C2095	U2096	U2098	U2099	G2100		C2103	G2104	C2105	G2106 C2107	C2108	U2109	G2110	G2112	U2113	A2114	G2115 G2116	A2117	U2118	A2119	G2121	U2122	G2123	G2125	A2126	G2127	C2128	U2130	G2131	U2132	G2133	A2134 A2135	c2136	C2137	C2138
C2139	C2140	G2141	C2142	U2144	C2145	C2146	G214/ G2148	G2149	U2150	G2151	G2152	G2154	G2155	G2156	A2158	G2159	G2160	C2161	C2163	C2164	G2165	G2166	G2168	A2169	A2170	U2172	A2173	C2174	C2175	C2177	C2178	C2179 112180	G2181	G2182	C2183	C2185	G2186	G2187	C2188	G2190	G2191	G2192	G2193	G2194 C2195	C2196	U2197	A2198
A 21.99	C2200	C2201	C2202	C2205	G2206	G2207	N2218	G2219	<mark>G2220</mark>	G2221	G2223	G2224	A2225	C2226	G2228	C2229	G2230	C2231	U2233	G2234	G2235	C2236	G2238	G2239	C2240	G2242	U2243	U2244	02245 G2246	A2247	C2248	02249 62250	G2251	G2252	G2253	G2255	G2256	U2257	C2258	C2260	c2261	U2262	C2263	0.2264	A2266	A2267	A2268
A2269	G2270	G2271	U2272	A2213 A2274	C2275	G2276	A2278	G2279	G2280	C2281	G2283	C2284	C2285	A2286	A2201 A2288	G2289	G2290	U2291	C2293	C2294	C2295	U2296 C22947	A2298	G2299	G2300	G2302	G2303	G2304	A2305 C2306	G2307	G2308	A2309 A2310	A2311	U2312	C2313	G2315	C2316	C2317	G2318 G2319	A2320	G2321	A2322	G2323	C2324 G2325	C2326	A2327	A2328
62329	G2330	G2331	U2332	G2334	A2335	A2336	G2331 G2338	G2339	G2340	G2341	C2342 C2343	U2344	G2345	A2346	U2348	G2349	C2350	62351	G2353	G2354	C2355	C2356	G2358	C2359	A2360	G2362	C2363	C2364	G2365	G2367	C2368	A2369	G2371	G2372	G2373	G2375	A2376	A2377	A2378	C2380	C2381	<mark>G2382</mark>	G2383	G2384 C2385	<mark>C2386</mark>	U2387	A2388
62389	U2390	G2391	A2392	C2394	C2395	G2396	U2398	G2399	G2400	U2401	C2403	C2404	G2405	U2406	U2408	G2409	G2410	A2411	G2413	G2414	G2415	C2416	A2418	U2419	C2420	A2422	U2423	C2424	A2425 A2426	C2427	G2428	62429 42430	U2431	A2432	A2433	A2435	G2436	U2437	U2438	C2440	C2441	C2442	C2443	G2444 G2445	G2446	G2447	A2448
112,449	A2450	A2451	C2452	G2454	G2455	C2456	02458	A2459	U2460	C2461	U2462 C2463	C2464	C2465	C2466	G2468	A2469	G2470	C2471	U2473	C2474	C2475	A2476	A2478	G2479	C2480	G2482	C2483	G2484	G2486	G2487	A2488	G2489	U2491	U2492	U2493	G2495	C2496	A2497	C2498	U2500	C2501	G2502	A2503	02504 G2505	U2506	C2507	G2508
G2509	C2510	U2511	C2512	u2514	C2515	G2516	C251/ A2518	U2519	C2520	C2521	02522 G2523	G2524	G2525	G2526	U2528	G2529	A2530	A2531	A2533	A2534	G2535	G2536	C2538	C2539	C2540	A2542	G2543	G2544	02546	U2547	G2548	G2549 C2550	C2551	U2552	G2553	U2555	C2556	G2557	C2558	c2560	A2561	U2562	U2563	A2565	A2566	G2567	C2568















## V121 L122

#### • Molecule 47: 50S RIBOSOMAL PROTEIN L15











# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	65520	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	11.899	Depositor
Minimum map value	-4.902	Depositor
Average map value	0.213	Depositor
Map value standard deviation	0.884	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	378, 378, 378	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles $(^{\circ})$	90, 90, 90	wwPDB
Pixel spacing (Å)	1.26, 1.26, 1.26	Depositor



# 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: FUA, GDP

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	2.73	2519/36190~(7.0%)	2.44	3195/56486~(5.7%)	
2	AB	1.36	3/1935~(0.2%)	1.50	19/2609~(0.7%)	
3	AC	1.44	1/1636~(0.1%)	1.59	20/2205~(0.9%)	
4	AD	1.38	0/1733	1.56	26/2318~(1.1%)	
5	AE	1.45	1/1162~(0.1%)	1.44	9/1564~(0.6%)	
6	AF	1.39	0/856	1.57	12/1154~(1.0%)	
7	AG	1.34	1/1276~(0.1%)	1.51	12/1709~(0.7%)	
8	AH	1.41	1/1136~(0.1%)	1.60	15/1527~(1.0%)	
9	AI	1.48	4/1029~(0.4%)	2.08	17/1379~(1.2%)	
10	AJ	1.33	0/807	1.53	8/1085~(0.7%)	
11	AK	1.40	1/900~(0.1%)	1.50	6/1213~(0.5%)	
12	AL	1.42	1/986~(0.1%)	1.58	13/1320~(1.0%)	
13	AM	1.33	0/998	1.68	17/1336~(1.3%)	
14	AN	1.52	1/501~(0.2%)	1.72	9/664~(1.4%)	
15	AO	1.36	1/745~(0.1%)	1.58	9/992~(0.9%)	
16	AP	1.47	1/716~(0.1%)	1.59	11/963~(1.1%)	
17	AQ	1.43	1/836~(0.1%)	1.57	11/1117~(1.0%)	
18	AR	1.41	1/579~(0.2%)	1.56	12/768~(1.6%)	
19	AS	1.30	0/642	1.50	6/865~(0.7%)	
20	AT	1.32	0/765	1.53	10/1007~(1.0%)	
21	AU	1.50	1/212~(0.5%)	1.82	8/277~(2.9%)	
22	AV	2.70	127/1832~(6.9%)	2.42	155/2855~(5.4%)	
23	AX	2.50	14/257~(5.4%)	2.35	20/398~(5.0%)	
24	AY	1.35	3/5312~(0.1%)	1.53	54/7193~(0.8%)	
25	B0	1.32	0/671	1.75	11/892~(1.2%)	
26	B1	1.34	1/738~(0.1%)	1.58	9/981~(0.9%)	
27	B2	1.32	2/600~(0.3%)	1.60	9/793~(1.1%)	
28	B3	1.42	0/472	1.51	5/634 (0.8%)	
29	B4	1.28	0/460	1.67	9/621~(1.4%)	
30	B5	1.26	0/473	1.57	6/639~(0.9%)	
31	B6	1.29	0/440	1.71	$9/586\ \overline{(1.5\%)}$	
32	B7	1.37	0/426	1.76	9/561~(1.6%)	



Mal	Chain	Chain Bond lengths		Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
33	B8	1.35	0/515	1.68	7/679~(1.0%)	
34	B9	1.36	1/310~(0.3%)	1.54	3/407~(0.7%)	
35	BA	2.69	4845/69972~(6.9%)	2.42	5972/109237~(5.5%)	
36	BB	2.63	174/2853~(6.1%)	2.36	226/4451~(5.1%)	
37	BC	1.32	1/1774~(0.1%)	1.51	18/2391~(0.8%)	
38	BD	1.40	5/2195~(0.2%)	1.62	27/2955~(0.9%)	
39	BE	1.37	3/1596~(0.2%)	1.52	17/2153~(0.8%)	
40	BF	1.36	1/1658~(0.1%)	1.64	27/2244~(1.2%)	
41	BG	1.34	1/1499~(0.1%)	1.97	24/2016~(1.2%)	
42	BH	1.32	4/1292~(0.3%)	1.50	11/1744~(0.6%)	
43	BK	1.27	1/1044~(0.1%)	1.39	8/1416~(0.6%)	
44	BL	1.08	0/478	1.54	3/640~(0.5%)	
45	BN	1.34	2/1131~(0.2%)	1.52	11/1525~(0.7%)	
46	BO	1.40	2/943~(0.2%)	1.55	9/1269~(0.7%)	
47	BP	1.38	1/1131~(0.1%)	1.64	20/1504~(1.3%)	
48	BQ	1.43	3/1143~(0.3%)	1.59	18/1527~(1.2%)	
49	BR	1.35	2/974~(0.2%)	1.57	14/1302~(1.1%)	
50	BS	1.36	1/778~(0.1%)	1.71	13/1036~(1.3%)	
51	BT	1.32	0/1155	1.77	33/1542~(2.1%)	
52	BU	1.35	1/975~(0.1%)	1.59	18/1297~(1.4%)	
53	BV	1.27	0/790	1.55	9/1057~(0.9%)	
54	BW	1.33	0/907	1.59	11/1216~(0.9%)	
55	BX	1.37	0/739	1.39	5/993~(0.5%)	
56	BY	1.29	0/823	1.43	4/1098~(0.4%)	
57	BZ	1.41	$2\overline{/1499}~(0.1\%)$	1.54	16/2035~(0.8%)	
All	All	2.35	7735/165495~(4.7%)	2.21	$1026\overline{5}/246445~(4.2\%)$	

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	111
2	AB	0	10
3	AC	0	1
4	AD	0	14
5	AE	0	3
6	AF	0	5
7	AG	0	11
8	AH	0	8
9	AI	0	9



Mol	Chain	#Chirality outliers	#Planarity outliers
10	AJ	0	3
11	AK	0	3
12	AL	0	3
13	AM	0	6
14	AN	0	3
15	AO	0	2
16	AP	0	2
18	AR	0	1
20	AT	0	7
21	AU	0	1
22	AV	0	4
23	AX	0	2
24	AY	0	19
25	B0	0	3
26	B1	0	3
27	B2	0	5
28	B3	0	4
29	B4	0	1
30	B5	0	1
31	B6	0	3
32	B7	0	2
33	B8	0	3
35	BA	2	161
36	BB	0	2
37	BC	0	7
38	BD	0	8
39	BE	0	6
40	BF	0	4
41	BG	0	4
42	BH	0	5
43	BK	0	5
44	BL	0	3
45	BN	0	5
46	BO	0	4
47	BP	0	6
48	BQ	0	4
49	BR	0	3
50	BS	0	3
51	BT	0	10
52	BU	0	4
53	BV	0	3
54	BW	0	5



Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
55	BX	0	1
56	BY	0	2
57	BZ	0	6
All	All	3	514

The worst 5 of 7735 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1696	G	N7-C5	-15.22	1.30	1.39
1	AA	607	А	N7-C5	-14.64	1.30	1.39
35	BA	406	G	N7-C5	-14.28	1.30	1.39
1	AA	1144	G	C8-N7	-14.17	1.22	1.30
1	AA	1129	С	N3-C4	-13.63	1.24	1.33

The worst 5 of 10265 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
41	BG	112	PRO	O-C-N	-44.90	50.85	122.70
9	AI	53	VAL	O-C-N	-38.46	61.16	122.70
9	AI	104	ARG	O-C-N	-29.23	75.94	122.70
41	BG	112	PRO	CA-C-N	20.32	161.90	117.20
1	AA	1463	С	C6-N1-C2	18.92	127.87	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	575	G	C3'
35	BA	1799	G	C3'
35	BA	1992	G	C3'

5 of 514 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	21	G	Sidechain
1	AA	37	U	Sidechain
1	AA	39	G	Sidechain
1	AA	5	U	Sidechain



### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16035	1572	0
2	AB	1900	0	1951	268	0
3	AC	1612	0	1677	202	0
4	AD	1703	0	1767	195	0
5	AE	1146	0	1207	147	0
6	AF	843	0	857	95	0
7	AG	1257	0	1296	109	0
8	AH	1116	0	1177	98	0
9	AI	1010	0	1037	148	0
10	AJ	794	0	840	178	0
11	AK	885	0	904	79	0
12	AL	970	0	1057	149	0
13	AM	987	0	1059	140	0
14	AN	492	0	533	56	0
15	AO	734	0	771	71	0
16	AP	700	0	720	91	0
17	AQ	823	0	891	71	0
18	AR	574	0	644	92	0
19	AS	629	0	652	142	0
20	AT	763	0	861	124	0
21	AU	208	0	221	15	0
22	AV	1640	0	820	93	0
23	AX	230	0	119	17	0
24	AY	5214	0	5288	759	0
25	B0	662	0	688	86	0
26	B1	731	0	808	132	0
27	B2	598	0	653	123	0
28	B3	467	0	523	75	0
29	B4	450	0	449	101	0
30	B5	459	0	480	97	0
31	B6	433	0	461	177	0
32	B7	418	0	467	45	0
33	B8	507	0	576	112	0
34	B9	307	0	338	41	0
35	BA	62474	0	31032	3259	0
36	BB	2551	0	1278	166	0
37	BC	1742	0	1798	183	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	2145	0	2234	311	0
39	BE	1563	0	1629	273	0
40	BF	1623	0	1677	288	0
41	BG	1474	0	1535	278	0
42	BH	1268	0	1337	209	0
43	BK	1025	0	1066	184	0
44	BL	477	0	509	17	0
45	BN	1104	0	1180	154	0
46	BO	933	0	996	116	0
47	BP	1114	0	1187	270	0
48	BQ	1122	0	1179	151	0
49	BR	960	0	1021	157	0
50	BS	770	0	832	177	0
51	BT	1141	0	1202	266	0
52	BU	958	0	1015	166	0
53	BV	779	0	852	142	0
54	BW	896	0	953	123	0
55	BX	725	0	778	97	0
56	BY	810	0	901	174	0
57	BZ	1467	0	1492	249	0
58	AY	37	0	46	17	0
59	AY	28	0	12	6	0
All	All	152777	0	105568	12274	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

The worst 5 of 12274 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:252:ASP:CB	24:AY:254:LYS:HE3	1.55	1.36
37:BC:118:PRO:HA	37:BC:121:MET:CG	1.60	1.31
53:BV:18:LEU:HD22	53:BV:19:LYS:N	1.45	1.30
1:AA:1158:C:C5'	2:AB:133:LYS:HE2	1.62	1.28
53:BV:18:LEU:CD2	53:BV:19:LYS:H	1.50	1.25

There are no symmetry-related clashes.



## 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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
2	AB	232/256~(91%)	149 (64%)	49 (21%)	34~(15%)	0	3
3	AC	204/239~(85%)	129 (63%)	56~(28%)	19 (9%)	0	10
4	AD	206/209~(99%)	138 (67%)	49 (24%)	19  (9%)	1	11
5	AE	148/162~(91%)	113 (76%)	25~(17%)	10 (7%)	1	15
6	AF	99/101~(98%)	77 (78%)	18 (18%)	4 (4%)	3	23
7	AG	153/156~(98%)	108 (71%)	35~(23%)	10 (6%)	1	16
8	AH	136/138~(99%)	110 (81%)	23~(17%)	3(2%)	6	35
9	AI	125/128~(98%)	85 (68%)	24 (19%)	16 (13%)	0	5
10	AJ	96/105~(91%)	60 (62%)	23 (24%)	13 (14%)	0	4
11	AK	117/129~(91%)	91 (78%)	21 (18%)	5 (4%)	2	22
12	AL	122/132~(92%)	82 (67%)	23~(19%)	17 (14%)	0	4
13	AM	122/126~(97%)	73 (60%)	26 (21%)	23 (19%)	0	2
14	AN	58/61~(95%)	49 (84%)	5 (9%)	4 (7%)	1	15
15	AO	86/89~(97%)	55 (64%)	24 (28%)	7 (8%)	1	12
16	AP	81/88~(92%)	56 (69%)	19 (24%)	6 (7%)	1	13
17	AQ	97/105~(92%)	78~(80%)	15~(16%)	4 (4%)	3	22
18	AR	68/88~(77%)	49 (72%)	15 (22%)	4 (6%)	1	17
19	AS	76/93~(82%)	37 (49%)	21 (28%)	18 (24%)	0	1
20	AT	97/106~(92%)	49 (50%)	31 (32%)	17 (18%)	0	2
21	AU	22/27~(82%)	13 (59%)	8 (36%)	1 (4%)	2	22
24	AY	662/691~(96%)	440 (66%)	137 (21%)	85 (13%)	0	5
25	B0	82/85~(96%)	66 (80%)	13 (16%)	3 (4%)	3	24
26	B1	91/98~(93%)	65 (71%)	16 (18%)	10 (11%)	0	7
27	B2	69/72~(96%)	32 (46%)	24 (35%)	13 (19%)	0	2
28	B3	57/60~(95%)	41 (72%)	11 (19%)	5 (9%)	1	11



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
29	B4	55/71~(78%)	28~(51%)	12 (22%)	15~(27%)	0	0
30	B5	57/60~(95%)	36~(63%)	11~(19%)	10 (18%)	0	2
31	B6	48/54~(89%)	23~(48%)	11 (23%)	14 (29%)	0	0
32	B7	46/49~(94%)	38~(83%)	5 (11%)	3~(6%)	1	16
33	B8	61/65~(94%)	34~(56%)	16 (26%)	11 (18%)	0	2
34	B9	35/37~(95%)	21 (60%)	9 (26%)	5(14%)	0	4
37	BC	226/229~(99%)	161 (71%)	55 (24%)	10 (4%)	2	22
38	BD	273/276~(99%)	192 (70%)	47 (17%)	34 (12%)	0	5
39	BE	202/206~(98%)	120 (59%)	49 (24%)	33 (16%)	0	3
40	BF	205/210~(98%)	141 (69%)	37 (18%)	27 (13%)	0	4
41	BG	179/182~(98%)	113 (63%)	41 (23%)	25 (14%)	0	4
42	BH	164/180~(91%)	85 (52%)	43 (26%)	36 (22%)	0	1
43	BK	137/147~(93%)	87 (64%)	41 (30%)	9(7%)	1	15
44	BL	65/121~(54%)	57 (88%)	8 (12%)	0	100	100
45	BN	136/140~(97%)	90 (66%)	28 (21%)	18 (13%)	0	4
46	BO	120/122~(98%)	95~(79%)	16 (13%)	9 (8%)	1	13
47	BP	144/150~(96%)	78 (54%)	40 (28%)	26 (18%)	0	2
48	BQ	139/141~(99%)	103 (74%)	23 (16%)	13 (9%)	0	10
49	BR	115/118 (98%)	80 (70%)	20 (17%)	15 (13%)	0	5
50	BS	96/112~(86%)	46 (48%)	30 (31%)	20 (21%)	0	2
51	BT	135/146~(92%)	76 (56%)	32 (24%)	27 (20%)	0	2
52	BU	115/118 (98%)	75~(65%)	27 (24%)	13 (11%)	0	7
53	BV	99/101~(98%)	71 (72%)	11 (11%)	17 (17%)	0	3
54	BW	111/113 (98%)	78 (70%)	22 (20%)	11 (10%)	0	9
55	BX	90/96~(94%)	58 (64%)	24 (27%)	8 (9%)	1	11
56	BY	104/110~(94%)	50 (48%)	30 (29%)	24 (23%)	0	1
57	BZ	182/206~(88%)	113 (62%)	41 (22%)	28 (15%)	0	3
All	All	6645/7104~(94%)	4394 (66%)	1440 (22%)	811 (12%)	1	5

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5 of 811 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	20	GLU
	<i>a</i>	1	

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	Jerre Person Per						
Mol	Chain	$\mathbf{Res}$	Type				
2	AB	195	ASP				
2	AB	233	SER				
2	AB	239	VAL				
3	AC	12	LEU				

### 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 PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	P	erce	entiles
2	AB	202/220~(92%)	177 (88%)	25~(12%)		4	19
3	AC	160/188~(85%)	134 (84%)	26 (16%)		2	13
4	AD	180/181~(99%)	162 (90%)	18 (10%)		7	26
5	AE	115/123~(94%)	100 (87%)	15 (13%)		4	18
6	AF	90/90~(100%)	81 (90%)	9 (10%)		7	26
7	AG	126/127~(99%)	116 (92%)	10 (8%)		12	35
8	AH	119/119~(100%)	105 (88%)	14 (12%)		5	20
9	AI	98/99~(99%)	88 (90%)	10 (10%)		7	25
10	AJ	88/92~(96%)	73~(83%)	15 (17%)		2	12
11	AK	90/99~(91%)	85 (94%)	5~(6%)		21	46
12	AL	104/109~(95%)	90~(86%)	14 (14%)		4	17
13	AM	99/101~(98%)	87~(88%)	12 (12%)		5	20
14	AN	49/50~(98%)	45 (92%)	4 (8%)		11	34
15	AO	79/80~(99%)	69~(87%)	10~(13%)		4	18
16	AP	72/74~(97%)	67~(93%)	5(7%)		15	40
17	AQ	94/97~(97%)	82 (87%)	12 (13%)		4	18
18	AR	61/77~(79%)	58~(95%)	3~(5%)		25	50
19	AS	69/80~(86%)	57 (83%)	12 (17%)		2	11
20	AT	76/82~(93%)	67 (88%)	9 (12%)		5	20
21	AU	$1\overline{9/22}~(86\%)$	19 (100%)	0	1	.00	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	$\mathbf{entiles}$
24	AY	563/582~(97%)	478 (85%)	85 (15%)	3	14
25	B0	66/67~(98%)	58~(88%)	8 (12%)	5	20
26	B1	78/83~(94%)	61~(78%)	17~(22%)	1	6
27	B2	66/67~(98%)	58 (88%)	8 (12%)	5	20
28	B3	51/52~(98%)	44 (86%)	7~(14%)	3	17
29	B4	51/63~(81%)	34 (67%)	17 (33%)	0	2
30	B5	51/52~(98%)	45 (88%)	6 (12%)	5	20
31	B6	49/52~(94%)	35 (71%)	14 (29%)	0	2
32	B7	41/42~(98%)	36 (88%)	5 (12%)	5	20
33	B8	53/55~(96%)	45 (85%)	8 (15%)	3	14
34	B9	34/34~(100%)	29 (85%)	5 (15%)	3	15
37	BC	180/181 (99%)	166 (92%)	14 (8%)	12	36
38	BD	217/218~(100%)	179 (82%)	38 (18%)	2	11
39	BE	165/166~(99%)	135 (82%)	30 (18%)	1	10
40	BF	165/166~(99%)	151 (92%)	14 (8%)	10	33
41	BG	155/156~(99%)	121 (78%)	34 (22%)	1	5
42	BH	136/148~(92%)	124 (91%)	12 (9%)	10	31
43	BK	104/111~(94%)	88 (85%)	16 (15%)	2	14
44	BL	46/85~(54%)	43 (94%)	3~(6%)	17	42
45	BN	117/119~(98%)	98 (84%)	19~(16%)	2	13
46	BO	100/100~(100%)	90 (90%)	10 (10%)	7	26
47	BP	112/116~(97%)	89 (80%)	23 (20%)	1	7
48	BQ	111/111 (100%)	94 (85%)	17 (15%)	2	14
49	BR	100/101~(99%)	85 (85%)	15~(15%)	3	15
50	BS	77/88~(88%)	67 (87%)	10 (13%)	4	18
51	BT	120/127~(94%)	97 (81%)	23~(19%)	1	8
52	BU	92/94~(98%)	84 (91%)	8 (9%)	10	31
53	BV	82/82 (100%)	71 (87%)	11 (13%)	4	17
54	BW	91/92~(99%)	82 (90%)	9 (10%)	8	26
55	BX	$74/78~(9\overline{5\%})$	62 (84%)	12 (16%)	2	13
56	BY	87/91~(96%)	75 (86%)	12 (14%)	3	17



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
57	ΒZ	162/179~(90%)	133~(82%)	29~(18%)	2 10
All	All	5586/5868~(95%)	4819 (86%)	767 (14%)	7 17

5 of 767 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	BE	22	PRO
45	BN	26	LEU
39	BE	94	GLU
39	BE	18	ASP
41	BG	80	PHE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 173 such side chains are listed below:

Mol	Chain	Res	Type
40	BF	133	ASN
49	BR	3	HIS
41	BG	27	ASN
45	BN	101	HIS
51	BT	55	ASN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522~(98%)	277~(18%)	43 (2%)
22	AV	76/77~(98%)	16 (21%)	0
23	AX	10/11~(90%)	4 (40%)	0
35	BA	2900/2915~(99%)	637~(21%)	77~(2%)
36	BB	118/122~(96%)	25 (21%)	0
All	All	$4607/4647 \ (99\%)$	959~(20%)	120 (2%)

5 of 959 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	А
1	AA	33	А



5 of 120 RNA pucker outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
35	BA	603	А
35	BA	2690	С
35	BA	1210	А
35	BA	2689	U
35	BA	2849	U

### 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)

2 ligands are 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).

Mal	Mal Type Chain Dec I		Tinle	Bond lengths			Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
59	GDP	AY	702	-	24,30,30	2.06	6 (25%)	30,47,47	1.83	7 (23%)
58	FUA	AY	701	-	39,40,40	2.24	14 (35%)	49,64,64	1.87	13 (26%)

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
59	GDP	AY	702	-	-	3/12/32/32	0/3/3/3
58	FUA	AY	701	-	-	5/15/92/92	0/4/4/4



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AY	702	GDP	C5-C6	-6.09	1.35	1.47
58	AY	701	FUA	C14-C8	-4.93	1.50	1.59
58	AY	701	FUA	C29-C22	4.78	1.54	1.47
58	AY	701	FUA	C23-C22	-4.73	1.39	1.51
58	AY	701	FUA	C23-C24	-4.57	1.38	1.53

The worst 5 of 20 bond length outliers are listed below:

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
59	AY	702	GDP	C2-N1-C6	-4.23	117.31	125.10
58	AY	701	FUA	C13-C12-C11	-4.16	106.07	111.90
59	AY	702	GDP	PA-O3A-PB	-4.11	118.74	132.83
58	AY	701	FUA	C6-C5-C10	3.84	116.44	111.65
58	AY	701	FUA	C21-C14-C8	-3.75	108.81	112.27

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AY	701	FUA	C13-C17-C22-C29
58	AY	701	FUA	C17-C22-C23-C24
58	AY	701	FUA	C29-C22-C23-C24
59	AY	702	GDP	C5'-O5'-PA-O3A
58	AY	701	FUA	O3-C31-O2-C16

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AY	702	GDP	6	0
58	AY	701	FUA	17	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



any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1799. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

### 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150



The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices (i)

#### 6.3.1 Primary map



X Index: 153

Y Index: 174

Z Index: 160

The images above show the largest variance slices of the map in three orthogonal directions.

### 6.4 Orthogonal surface views (i)

#### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



## 7.2 Volume estimate (i)



The volume at the recommended contour level is  $1886 \text{ nm}^3$ ; this corresponds to an approximate mass of 1703 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



## 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.132  ${\rm \AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1799 and PDB model 4V5N. Per-residue inclusion information can be found in section 3 on page 16.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



### 9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

#### 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).



## 9.4 Atom inclusion (i)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	-0.0010
AA	0.0000	-0.0010
AB	0.0000	0.0000
AC	0.0000	0.0000
AD	0.0000	0.0000
AE	0.0000	0.0000
AF	0.0000	-0.0220
AG	0.0000	0.0000
AH	0.0000	0.0000
AI	0.0000	0.0000
AJ	0.0000	0.0000
AK	0.0000	0.0000
AL	0.0000	0.0000
AM	0.0000	0.0000
AN	0.0000	0.0000
AO	0.0000	0.0000
AP	0.0000	0.0000
AQ	0.0000	-0.0060
AR	0.0000	0.0000
AS	0.0000	0.0000
AT	0.0000	-0.0140
AU	0.0000	0.0000
AV	0.0000	0.0000
AX	0.0000	0.0000
AY	0.0000	0.0000
B0	0.0000	0.0000
B1	0.0000	0.0000
B2	0.0000	0.0000
B3	0.0000	0.0000
B4	0.0000	0.0000
B5	0.0000	0.0000
B6	0.0000	0.0000
B7	0.0000	0.0040
B8	0.0000	0.0000
B9	0.0000	0.0000



Chain	Atom inclusion	Q-score
BA	0.0000	-0.0020
BB	0.0000	0.0000
BC	0.0000	0.0000
BD	0.0000	-0.0140
BE	0.0000	0.0000
BF	0.0000	0.0000
BG	0.0000	0.0000
BH	0.0000	0.0000
BK	0.0000	0.0000
BL	0.0000	0.0000
BN	0.0000	0.0000
BO	0.0000	0.0000
BP	0.0000	0.0000
BQ	0.0000	0.0000
BR	0.0000	0.0000
BS	0.0000	0.0000
BT	0.0000	0.0000
BU	0.0000	0.0000
BV	0.0000	0.0000
BW	0.0000	0.0000
BX	0.0000	-0.0100
BY	0.0000	0.0000
BZ	0.0000	0.0000

