

wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 10:49 AM EST

PDB ID	:	4V6Y
EMDB ID	:	EMD-1716
Title	:	E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in classic pre-translocation
		state (pre1a)
Authors	:	Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.;
		Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on	:	2013-10-14
Resolution	:	12.00 Å(reported)
Based on initial models	:	2HGP, 2WRI, 2K4C, 3I1O

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	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 12.00 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
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	
			45%	
1	AB	220	93%	7%
			32%	
2	AC	208	92%	7%
			44%	
3	AD	206	87%	12%
			42%	
4	AE	152	89%	11% •
			63%	
5	AF	101	87%	13%
			55%	
6	AG	152	88%	12%
			22%	
7	AH	130	91%	8% •



Mol	Chain	Length	Quality of chain	
8	AI	128	47%	18%
		120	43%	10%
9	AJ	100	84%	16%
10	AK	118	40%	11%
			54%	
11	AL	124	85%	15% •
12	AM	115	<u> </u>	1494
12	11111	110	28%	1470 •
13	AN	101	86%	12% ••
14	AO	89	87%	12%
	110	00	23%	
15	AP	81	84%	16%
16		82	46%	00/
10	ng	02	53%	9% •
17	AR	57	93%	7%
10	٨C	01	42%	
10	AS	01	89%	11%
19	AT	86	90%	10%
20	ΔΤΙ	52	34%	
20	AU		<u> </u>	26% 8%
21	AA	1533	15% 56%	24% 5%
00	Δ 1	76	53%	222/
		10	60%	
23	A2	15	20% 40% 20%	20%
0.4	4.0		39%	
24	A3	((17% 55% 51%	18% 10%
25	BC	273	91%	8%
			35%	
26	BD	209	89%	11%
27	BE	201	89%	10%
			37%	
28	BF	179	89%	11% •
29	BG	177	92%	7% ••
	יות	140	87%	
30	BH	149	94%	5% •
31	BI	142	94%	5% •
	D.	4.12	32%	
32	BJ	142	91%	8% •

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Mol	Chain	Length	Quality of chain	
33	BK	123	53%	10%
24	рī	144	51%	
- 04	DL	144	39%	14% •
35	BM	136	88%	12%
36	BN	121	88%	12%
37	ВО	117	30%	10% •
38	BP	115	37%	16% •
39	BO	118	41%	14%
00	54	110	51%	1470 •••
40	BR	103	89%	10% •
41	BS	110	48% 92%	8%
42	BT	94	91%	7% •
43	BU	104	47%	8% ••
	BV	94	44%	E0/
		54	45%	2%
45	BW	80	68%	12%
46	BX	79	84%	10% • •
47	BY	63	50% 90%	10%
48	ΒZ	59	29% 	7% ••
40	PO	57	58%	
49	D0	57	40%	11% ·
50	B1	52	88%	12%
51	B2	46	76%	22% •
52	B3	65	58%	12% •
53	B4	38	39%	8% •
54	BA	2903	31%	24%
		2000	27%	27/0 •
55	BB	118	15% 59% 89%	19% 5% •
56	B5	234	88%	6% • 5%

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2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 147653 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	AB	220	Total 1708	C 1083	N 306	0 312	S 7	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
AB	7	ACE	-	acetylation	UNP P0A7V0	
AB	226	NH2	-	amidation	UNP P0A7V0	

• Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	AC	207	Total 1625	C 1028	N 306	O 288	${ m S} { m 3}$	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	207	NH2	-	amidation	UNP P0A7V3

• Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms				AltConf	Trace	
3	AD	205	Total 1643	C 1026	N 315	0 298	$\frac{S}{4}$	0	0

• Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	152	Total 1109	C 689	N 212	O 202	S 6	0	1

There are 2 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	acetylation	UNP P0A7W1
AE	159	NH2	-	amidation	UNP P0A7W1

• Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	101	Total 818	C 515	N 149	0 148	S 6	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	101	NH2	-	amidation	UNP P02358

• Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	152	Total 1178	C 732	N 227	0 215	${S \atop 4}$	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	acetylation	UNP P02359
AG	152	NH2	-	amidation	UNP P02359

• Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AH	129	Total 979	C 616	N 173	0 184	${f S}{f 6}$	0	0

• Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AI	128	Total 1025	C 636	N 206	0 180	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	2	ACE	-	acetylation	UNP P0A7X3



• Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AJ	100	Total 790	C 495	N 151	0 143	S 1	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	acetylation	UNP P0A7R5
AJ	103	NH2	-	amidation	UNP P0A7R5

• Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	118	Total 880	C 542	N 174	0 161	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	11	ACE	-	acetylation	UNP P0A7R9

• Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	AL	123	Total 955	C 590	N 196	0 165	$\frac{S}{4}$	0	0

• Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues		At	oms			AltConf	Trace
12	AM	114	Total 877	C 541	N 178	0 155	${ m S} { m 3}$	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AM	114	NH2	-	amidation	UNP P0A7S9

• Molecule 13 is a protein called 30S ribosomal protein S14.



Mol	Chain	Residues		At	oms			AltConf	Trace
13	AN	100	Total 805	C 499	N 164	O 139	${ m S} { m 3}$	0	0

• Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues		At	oms			AltConf	Trace
14	AO	88	Total 714	C 439	N 144	O 130	S 1	0	0

• Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues		At	oms			AltConf	Trace
15	AP	81	Total 639	C 400	N 127	0 111	S 1	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	81	NH2	-	amidation	UNP P0A7T3

• Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues		At	oms			AltConf	Trace
16	AQ	82	Total 652	C 413	N 122	0 114	${ m S} { m 3}$	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	acetylation	UNP P0AG63
AQ	83	NH2	-	amidation	UNP P0AG63

• Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues		Aton	ıs		AltConf	Trace
17	AR	57	Total 459	C 290	N 87	O 82	0	1

There are 2 discrepancies between the modelled and reference sequences:

AR 18 ACE - acetylation UNP P0A7T7	Chain	Residue	Modelled	Actual	Comment	Reference
	AR	18	ACE	-	acetylation	UNP P0A7T7



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Chain	Residue	Modelled	Actual	Comment	Reference
AR	74	NH2	-	amidation	UNP P0A7T7

• Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AS	81	Total 641	C 410	N 121	0 108	${ m S} { m 2}$	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	acetylation	UNP P0A7U3
AS	81	NH2	-	amidation	UNP P0A7U3

• Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	АТ	86	Total	С	Ν	Ο	S	0	0
		00	668	413	137	115	3	Ŭ	Ŭ

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	1	ACE	-	acetylation	UNP P0A7U7

• Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AU	53	Total 429	C 267	N 87	0 74	S 1	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	acetylation	UNP P68679
AU	54	NH2	-	amidation	UNP P68679

• Molecule 21 is a RNA chain called 16S ribosomal RNA.



Mol	Chain	Residues		1	AltConf	Trace			
21	AA	1530	Total 32828	C 14642	N 6024	O 10633	Р 1529	0	0

• Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A1	76	Total 1627	C 728	N 292	0 531	Р 75	S 1	0	0

• Molecule 23 is a RNA chain called 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	15	Total 309	C 140	N 46	0 109	Р 14	0	0

• Molecule 24 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A3	77	Total 1642	С 734	N 297	0 534	Р 76	S 1	0	0

• Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BC	272	Total 2083	C 1288	N 424	0 364	S 7	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	272	NH2	-	amidation	UNP P60422

• Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues		At	oms	AltConf	Trace		
26	BD	209	Total 1565	C 979	N 288	0 294	$\frac{S}{4}$	0	0

• Molecule 27 is a protein called 50S ribosomal protein L2.



Mol	Chain	Residues		At	oms	AltConf	Trace		
27	BE	201	Total 1552	C 974	N 283	O 290	${ m S}{ m 5}$	0	0

• Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
28	BF	178	Total 1420	C 905	N 251	O 258	S 6	0	0

• Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	BG	176	Total 1323	C 832	N 243	0 246	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
30	BH	149	Total 1111	C 699	N 197	0 214	S 1	0	0

• Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms	AltConf	Trace		
31	BI	141	Total 1032	C 651	N 179	0 196	S 6	0	0

• Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
32	BJ	142	Total 1129	С 714	N 212	O 199	$\frac{S}{4}$	0	0

• Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	123	Total 939	C 587	N 181	0 165	S 6	0	1

There is a discrepancy between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
BK	123	NH2	-	amidation	UNP P0ADY3

• Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	oms	AltConf	Trace		
34	BL	143	Total 1045	C 649	N 206	0 189	S 1	0	0

• Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms	AltConf	Trace		
35	BM	136	Total 1074	C 686	N 205	0 177	S 6	0	0

• Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
36	BN	121	Total 961	C 593	N 197	0 166	${f S}{5}$	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	121	NH2	-	amidation	UNP P0AG44

• Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
37	ВО	116	Total 892	C 552	N 178	O 162	0	0

• Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BP	114	Total 917	C 574	N 179	0 163	S 1	0	0

• Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
39	BQ	117	Total 947	C 604	N 192	O 151	0	0



• Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BR	103	Total 816	C 516	N 153	0 145	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		At	AltConf	Trace			
41	BS	110	Total 857	C 532	N 166	0 156	${ m S} { m 3}$	0	0

• Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BT	94	Total 739	C 466	N 140	0 131	${S \atop 2}$	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	94	NH2	-	amidation	UNP P0ADZ0

• Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
43	BU	103	Total 780	C 492	N 147	0 141	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	103	NH2	-	amidation	UNP P60624

• Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		At	AltConf	Trace			
44	BV	94	Total 753	C 479	N 137	0 134	${ m S} { m 3}$	0	0

• Molecule 45 is a protein called 50S ribosomal protein L24.



Mol	Chain	Residues	Atoms					AltConf	Trace
45	BW	80	Total 599	C 369	N 120	0 109	S 1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	5	ACE	-	acetylation	UNP P0A7L8

• Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	77	Total 625	C 388	N 129	0 106	${ m S} { m 2}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BX	-1	ACE	-	acetylation	UNP P0A7M2

• Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BY	63	Total 509	C 313	N 99	O 95	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
18	BZ	58	Total	С	Ν	Ο	S	0	0
40	40 DZ	58	449	281	87	79	2	0	0

• Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B0	56	Total 444	C 269	N 94	O 80	S 1	0	0

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

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
50	B1	52	Total 413	C 265	N 76	О 72	0	1



There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	2	ACE	-	acetylation	UNP P0A7N9
B1	53	NH2	-	amidation	UNP P0A7N9

• Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B2	46	Total 377	C 228	N 90	O 57	${ m S} { m 2}$	0	0

• Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B3	64	Total 504	C 323	N 105	0 74	${S \over 2}$	0	0

• Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	R/	38	Total	С	Ν	Ο	S	0	0
- 55	00 D4	00	302	185	65	48	4	0	0

• Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues			AltConf	Trace			
54	BA	2903	Total 62317	C 27801	N 11467	O 20147	Р 2902	0	0

• Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues		At	toms			AltConf	Trace
55	BB	117	Total 2504	C 1116	N 459	0 813	Р 116	0	0

• Molecule 56 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues		At	oms			AltConf	Trace
56	B5	223	Total 1658	C 1038	N 302	0 312	S 6	0	0

• Molecule 57 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).





Mol	Chain	Residues	A	AltConf			
57	A1	1	Total 7	$\begin{array}{c} \mathrm{C} \\ 5 \end{array}$	N 1	0 1	0

• Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues			AltConf			
58	BA	1	Total	С	Ν	0	\mathbf{S}	0
00	DA	Ĩ	10	6	1	2	1	



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: 30S ribosomal protein S2





• Molecule 4: 30S ribosomal protein S5











• Molecule 19: 30S ribosomal protein S20











• Molecule 25: 50S ribosomal protein L35





Chain BF:

WORLDWIDE PPDB PROTEIN DATA BANK 11%

89%





• Molecule 32: 50S ribosomal protein L9







• Molecule 41: 50S ribosomal protein L20





PROTEIN DATA BANK



• Molecule 52: 50S ribosomal protein L33











			••	••	Þ	٠	•	•	٠		٠	•	٠		-	•				٠						_	•	•	٠	_				• •		••	•			٠	••	Þ
U1352	A1353	G1355	G1356	C1357	G1358 A1359	G1360	G1361	C1363	G1364	A1365 A1366	A1367	<mark>G1368</mark>	G1369	C13/0 G1371	U1372	A1373	G1374	C1376	G1377	U1379	G1380	G1381 G1382	A1383	A1304 A1385	C1386 A1387	G1388	G1389 II1390	U1391	A1392 A1393	U1394	N1 396	U1397 C1398	C1399	U1400	61401	01402 A1403	C1404	U1405 U1406	G1407	01409 01409	G1410	U1411
U1412	A1413	C1414 111415	G1416	C1417 G1418	A1419	A1420 G1421	G1422	G1426	A1427	61429	G1430	A1431	A1433	A1434 G1435	G1436	C1437	U1438	A1439 U1440	G1441	U1442	U1443 G1444	G1445	C1446 C1447	G1448	G1450	C1451	61452 A1453	C1454	G1455 G1456	U1457 11458	G1459	U1460 C1461	C1462	C1463 G1464	G1465	<mark>U1466</mark> U1467	U1468	A1469 A1470	G1471 C1472	G1473		
U1474	G1475	01476 A1477		C1480	G1482	G1483	U1484 111 ABE	U1486	U1487	C1488	C1489	A1490 G1491	G1492	C1493 A1494	A1495	A1496 U1497	C1498	C1 499	A1502	A1503	A1505	U1506	C1507	A1509	G1510	G1511 C1512	U1513	G1514	A1515 • G1516	G1517 C1518	G1519	U1520	A1522	U1523	G1524	C1526	G1527	A1528 G1529	G1530	A1532	C1533	01534 A1535
C1536	G1537	G1538	U1539	G1540	U1542	G1543 A1544	A1545	G1546 C1547	A1548	A1549	C1550	A1552	A1553	G1555	C1556	C1557	C1558	U1559	C1561	U1562 U1563	C1564	C1565 A1566	G1567	A1569	A1570 A1571	A1572	G1573	C1574 C1575	U1576	U1578	A1579 A1580	G1581 61580	A1583	U1584	C1585	61587	G1588 111 580	A1590	A1591 C1592	A1593	01594 C1595	•
A1596	A1597	A1598	U1599	G1601	U1602 A1603	C1604	C1605 C1606	C1607	A1609	A1610		G1613	A1614	C1615		A1618	G1619 G1620	07010	U1624	C1625	G1627	G1628	01023 A1630	G1631 A1632	G1633	A1635 A1635	U1636 A1637	C1638	C1639 A1640	A1641	G1642 G1643	C1644	G1645	C1646	U1648	G1649 A1650	G1651	A1652 G1653	A1654 A1655	C1656	U1657	
C1658	G1659	G1660	G1661 111662	G1663	A1664 A1665	G1666 G1667	A1668	A1669 C1670	U1671	A1672 G1673	G1674	C1675 A1676	A1677	A1678	A1679	G1681	G1682	U1683	G1684	C1685 C1686		A1689 A1690	C1691 111692		G1696	A1698	G1699	A1700 A1701	G1702	C1704	C1 706	G1707	C1708	01709	A1711	U1712 A1713	U1714	G1715 U1716	A1717	G1718 G1719	U1720	
G1721	A1722	G1723	G1724 U1725	C1726	C1728	U1729	CI 730	C1732	G1733 G1734	A1735	01736 G1737	G1738	A1739 G1740	C1741	01742 G1743	A1744	A1745	A1746	01/4/ C1748	A1749	01751 U1751	C1752	G1753 A1754	A1755 C1756	A1757	01758 A1759	C1760 C1761	A1762	G1763	U1765	61766	C1768	01769 G1770	C1771	A1//2 A1773	C1774 111775			U1778	A1780		
U1781	U1782	A1783 A1784	A1785	A1786 A1787	C1788 A1760	C1790	A1791	G1793	A1794	C1795 U1796	G1797	01798 G1799	C1800	A1801 A1802	A1803	C1804	A1005 C1806	G1807 A1808	A1809	A1810 G1811	U1812	G1813 G1814	A1815	C1816	G1817	A1819	U1820 A1821	C1822 C1823		G1826 U1827	G1828	A1829 C1830	G1831	C1832 C1833	U1834	G1835 C1836	C1837	G1840	U1841	G1842		
C1843	C1844	G1845	G1846	A1847	A1848 G1849	G1850 U1851	U1852	A1853 A1854	U1855	U1856	41857 A1858	U1859	G1861	G1862	01864	U1865	A1866	G1867 C1868	G1869	C18/0 A1871	A1872	G1873 C1874	G1875	A18/6 A1877	G1878		C1881	U1882 U1883	G1884 A1995	01886	C1 887 G1 888	A1889 A1890	G1891	C1892 C1893	C1894	C1895 C1896	G1897	U1898 A1899	A1900	C1902		
G1903	G1904 C1005	C1 906	G1907	C1 908	C1909 G1910	U1911 A1912	A1913	C1914	A1916	U1917	A1918	A1919	C1 920		C1924	C1925	A1927	A1928 G1929	G1930	01931 A1932	G1933	G1935	A1936	A193/ A1938	U1939 U1940	C1941	01943 U1943	U1944	01946 U1946	C1947	G1950 111 051	A1952	A1953 G1954	<mark>U1955</mark>	U1956	C1958	G1959	A1960 C1961	C1962 U1963	G1964		
C1965	A1966	C1967	61968	A1970	01971 G1972	G1973 C1974	G1975	U1976 A1977	A1978	U1979	G1980	A1981 U1982	G1983		C1986	A1987	G1988 G1989	C1990	01991	U1993	C1994	U1995	C1997	A1998	C1999	C2001	G2002	A2003 G2004	A2005 C2006	U2007	A2009	G2010	U2011	A2013	A2014	A2015	U2017	G2018	A2019 A2020	C2021	02023 C2023	G2024
C2025		62020	A2030	A2031 G2032	A2033	G2035	C2036 A2037	G2038	U2039	A2042	C2043	C2044 C2045	G2046	C2047	G2048		A2051	A2052 G2053	A2054	C2055	G2056	42058	A2059	A2060	A2062	C2063 C2064	C2065	C2066	U2068	G2069	A2071	C2073	U2074	U2076 U2076	A2077	U2079	A2080	U2081	G2083	c2084	U2085 U2086	
G2087	A2088	A2090	C2091 112092	G2093	A2094 A2095	C2096	A2097 U2098	U2099	G2100 A2101	G2102	C2104 C2104	20107	4210/ A2108	U2109 C2110		G2112	U2113 A2114	62115	G2116 A2117	U2118	A2119	G2121	U2122 G2123	G2124	G2125 A2126	G2127	G2128	C2129		U2132	G2133	A2135	G2136	U2137 G2138	U2 139	G2140	G2141	A2142 C2143	G2144 C2145	C2146	47 14 l	











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14235	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose $(e^-/\text{\AA}^2)$	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	162740	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	198.725	Depositor
Minimum map value	-116.714	Depositor
Average map value	-0.391	Depositor
Map value standard deviation	21.414	Depositor
Recommended contour level	30.0	Depositor
Map size (Å)	359.04, 359.04, 359.04	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.87, 1.87, 1.87	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: NH2, OMC, ACE, FME, 7MG, H2U, PSU, 5MU, 4SU, CM0, 6MZ

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	I	Bond lengths		Bond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	AB	0.72	0/1736	1.11	13/2340~(0.6%)
2	AC	0.76	0/1651	1.17	14/2225~(0.6%)
3	AD	0.76	0/1665	1.23	21/2227~(0.9%)
4	AE	0.70	0/1119	1.12	11/1506~(0.7%)
5	AF	0.79	0/835	1.15	7/1128~(0.6%)
6	AG	0.77	0/1188	1.24	16/1593~(1.0%)
7	AH	0.74	0/989	1.11	7/1326~(0.5%)
8	AI	0.85	0/1035	1.33	20/1377~(1.5%)
9	AJ	0.78	0/797	1.39	16/1079~(1.5%)
10	AK	0.80	0/894	1.27	12/1207~(1.0%)
11	AL	0.80	0/969	1.25	13/1300~(1.0%)
12	AM	0.82	0/884	1.29	13/1181~(1.1%)
13	AN	0.82	0/817	1.25	9/1088~(0.8%)
14	AO	0.77	0/722	1.18	6/964~(0.6%)
15	AP	0.82	0/648	1.42	14/870~(1.6%)
16	AQ	0.71	0/658	1.18	8/883~(0.9%)
17	AR	0.77	0/463	1.19	5/623~(0.8%)
18	AS	0.80	0/653	1.23	7/879~(0.8%)
19	AT	0.75	0/672	1.18	7/890~(0.8%)
20	AU	0.87	0/431	1.59	8/572~(1.4%)
21	AA	1.88	441/36759~(1.2%)	2.29	2411/57346~(4.2%)
22	A1	1.89	18/1668~(1.1%)	2.23	102/2595~(3.9%)
23	A2	1.67	1/343~(0.3%)	2.18	19/531~(3.6%)
24	A3	1.93	26/1722~(1.5%)	2.27	102/2685~(3.8%)
25	BC	0.79	0/2121	1.28	19/2852~(0.7%)
26	BD	0.72	0/1586	1.23	12/2134~(0.6%)
27	BE	0.71	0/1571	1.17	11/2113~(0.5%)
28	BF	0.77	0/1444	1.18	13/1937~(0.7%)
29	BG	0.72	0/1343	1.16	7/1816~(0.4%)
30	BH	0.67	0/1122	1.14	6/1515~(0.4%)
31	BI	0.69	0/1046	1.11	$7/1410\ (0.5\%)$
32	BJ	0.74	$0/1\overline{152}$	1.23	9/1551~(0.6%)



Mol	Chain	I	Bond lengths		Bond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
33	BK	0.76	0/947	1.23	11/1268~(0.9%)
34	BL	0.76	0/1054	1.28	14/1403~(1.0%)
35	BM	0.79	0/1093	1.27	11/1460~(0.8%)
36	BN	0.80	0/973	1.26	12/1301~(0.9%)
37	BO	0.80	0/902	1.28	10/1209~(0.8%)
38	BP	0.77	0/929	1.26	9/1242~(0.7%)
39	BQ	0.80	0/960	1.37	17/1278~(1.3%)
40	BR	0.73	0/829	1.22	9/1107~(0.8%)
41	BS	0.71	0/864	1.18	7/1156~(0.6%)
42	BT	0.73	0/744	1.19	5/994~(0.5%)
43	BU	0.70	0/787	1.17	6/1051~(0.6%)
44	BV	0.72	0/766	1.12	5/1025~(0.5%)
45	BW	0.73	0/604	1.25	4/799~(0.5%)
46	BX	0.82	0/635	1.47	14/848~(1.7%)
47	BY	0.70	0/510	1.22	5/677~(0.7%)
48	ΒZ	0.73	0/453	1.27	4/605~(0.7%)
49	B0	0.78	0/450	1.25	4/599~(0.7%)
50	B1	0.75	0/417	1.10	3/556~(0.5%)
51	B2	0.91	0/380	1.45	8/498~(1.6%)
52	B3	0.73	0/513	1.24	6/676~(0.9%)
53	B4	0.72	0/303	1.25	3/397~(0.8%)
54	BA	1.74	$6\overline{67}/69796~(1.0\%)$	2.28	$47\overline{47/108888}$ (4.4%)
55	BB	1.83	58/2800~(2.1%)	2.30	198/4367~(4.5%)
56	B5	0.68	0/1673	1.14	10/2255~(0.4%)
All	All	1.56	1211/160085~(0.8%)	2.06	8067/239402~(3.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AD	0	1
4	AE	0	1
13	AN	0	1
14	AO	0	1
21	AA	0	342
22	A1	0	13
23	A2	0	5
24	A3	0	19
46	BX	0	1
54	BA	0	646



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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	23
56	B5	0	1
All	All	0	1054

The worst 5 of 1211 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2048	G	C2-N2	-6.80	1.27	1.34
24	A3	75	С	N3-C4	-6.76	1.29	1.33
21	AA	1063	С	C4-N4	-6.70	1.27	1.33
23	A2	80	С	C4-N4	-6.68	1.27	1.33
55	BB	113	С	C4-N4	-6.68	1.27	1.33

The worst 5 of 8067 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
55	BB	34	A	N1-C6-N6	-13.76	110.34	118.60
54	BA	323	С	O4'-C1'-N1	13.51	119.01	108.20
54	BA	547	А	O4'-C1'-N9	12.98	118.58	108.20
54	BA	1943	U	O4'-C1'-N1	12.88	118.50	108.20
54	BA	1340	U	O4'-C1'-N1	12.80	118.44	108.20

There are no chirality outliers.

5 of 1054 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	5	U	Sidechain
3	AD	44	LYS	Peptide
4	AE	148	SER	Peptide
13	AN	69	ARG	Sidechain
14	AO	68	TYR	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	AB	1708	0	1736	0	0



	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	H(addod)	Clashos	Symm_Clashos
		1695		1600	Clashes	Symm-Clashes
	AC AD	1020	0	1099	0	0
3	AD AE	1045	0	1/10	0	0
4	AE	010	0	1132	1	0
		010	0	000	1	0
	AG	070	0	1234	0	0
(АП	979	0	1054	1	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
10	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	1	0
21	AA	32828	0	16011	4	0
22	A1	1627	0	802	0	0
23	A2	309	0	156	0	0
24	A3	1642	0	811	2	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	1	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	1	0
33	BK	939	0	1012	1	0
34	BL	1045	0	1117	2	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	1	0
38	BP	917	0	965	1	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	753	0	780	0	0
45	BW	599	0	614	1	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	1	0
52	B3	504	0	574	3	0
53	B4	302	0	343	0	0
54	BA	62317	0	30495	12	0
55	BB	2504	0	1187	0	0
56	B5	1658	0	1751	1	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	98156	28	0

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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 0.

The worst 5 of 28 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
34:BL:64:PHE:CE2	52:B3:24:LYS:HE2	2.40	0.56
20:AU:30:GLU:H	20:AU:31:VAL:HG22	1.72	0.54
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.30	0.49
56:B5:19:LYS:HE3	56:B5:21:TYR:CE2	2.46	0.49
52:B3:2:LYS:HE3	54:BA:242:G:C8	2.51	0.45

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	Perce	entiles
1	AB	218/220~(99%)	199 (91%)	17 (8%)	2(1%)	17	57
2	AC	205/208~(99%)	187 (91%)	15 (7%)	3~(2%)	10	46
3	AD	203/206~(98%)	184 (91%)	14 (7%)	5(2%)	5	32
4	AE	150/152~(99%)	132 (88%)	14 (9%)	4(3%)	5	31
5	AF	99/101~(98%)	88 (89%)	8 (8%)	3~(3%)	4	28
6	AG	150/152~(99%)	136 (91%)	11 (7%)	3(2%)	7	38
7	AH	127/130~(98%)	116 (91%)	8 (6%)	3 (2%)	6	33
8	AI	126/128 (98%)	113 (90%)	7 (6%)	6(5%)	2	21
9	AJ	98/100~(98%)	90 (92%)	4 (4%)	4 (4%)	3	23
10	AK	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	17	57
11	AL	121/124 (98%)	108 (89%)	7 (6%)	6(5%)	2	20
12	AM	112/115~(97%)	100 (89%)	9 (8%)	3 (3%)	5	31
13	AN	98/101~(97%)	83 (85%)	12 (12%)	3 (3%)	4	27
14	AO	86/89~(97%)	76 (88%)	8 (9%)	2(2%)	6	34
15	AP	79/81~(98%)	67 (85%)	8 (10%)	4 (5%)	2	19
16	AQ	80/82~(98%)	75 (94%)	3 (4%)	2(2%)	5	32
17	AR	55/57~(96%)	51 (93%)	4 (7%)	0	100	100
18	AS	79/81~(98%)	75 (95%)	3 (4%)	1 (1%)	12	48
19	AT	84/86~(98%)	76 (90%)	7 (8%)	1 (1%)	13	50
20	AU	51/53~(96%)	32 (63%)	9 (18%)	10 (20%)	0	2
25	BC	270/273~(99%)	246 (91%)	18 (7%)	6(2%)	6	35
26	BD	207/209~(99%)	177 (86%)	19 (9%)	11 (5%)	2	19
27	BE	199/201~(99%)	179 (90%)	11 (6%)	9 (4%)	2	22
28	BF	176/179~(98%)	150 (85%)	20 (11%)	6 (3%)	3	26
29	BG	174/177~(98%)	156 (90%)	15 (9%)	3 (2%)	9	42
30	BH	147/149~(99%)	133 (90%)	12 (8%)	2 (1%)	11	46
31	BI	139/142~(98%)	130 (94%)	7 (5%)	2 (1%)	11	46
32	BJ	140/142~(99%)	122 (87%)	15 (11%)	3 (2%)	7	36
33	BK	121/123~(98%)	112 (93%)	9 (7%)	0	100	100
34	BL	141/144 (98%)	127 (90%)	10 (7%)	4 (3%)	5	30
35	BM	134/136~(98%)	118 (88%)	11 (8%)	5(4%)	3	24
36	BN	119/121~(98%)	107 (90%)	10 (8%)	2 (2%)	9	42



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
37	BO	114/117~(97%)	106 (93%)	7 (6%)	1 (1%)	17	57
38	BP	112/115~(97%)	94 (84%)	11 (10%)	7~(6%)	1	17
39	BQ	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	5	31
40	BR	101/103~(98%)	91 (90%)	8 (8%)	2(2%)	7	38
41	BS	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	17	57
42	BT	92/94~(98%)	71 (77%)	17 (18%)	4 (4%)	2	22
43	BU	101/104 (97%)	88 (87%)	10 (10%)	3 (3%)	4	28
44	BV	92/94~(98%)	90~(98%)	2 (2%)	0	100	100
45	BW	78/80~(98%)	60 (77%)	15 (19%)	3 (4%)	3	24
46	BX	75/79~(95%)	64 (85%)	9 (12%)	2(3%)	5	31
47	BY	61/63~(97%)	53~(87%)	7 (12%)	1 (2%)	9	44
48	BZ	56/59~(95%)	51 (91%)	4 (7%)	1 (2%)	8	40
49	B0	54/57~(95%)	45 (83%)	6 (11%)	3~(6%)	2	19
50	B1	50/52~(96%)	47 (94%)	1 (2%)	2(4%)	3	23
51	B2	44/46~(96%)	43~(98%)	1 (2%)	0	100	100
52	B3	62/65~(95%)	59~(95%)	2(3%)	1 (2%)	9	44
53	B4	36/38~(95%)	31 (86%)	3 (8%)	2(6%)	2	19
56	B5	221/234 (94%)	207 (94%)	12 (5%)	2 (1%)	17	57
All	All	5876/6008~(98%)	5263 (90%)	456 (8%)	157 (3%)	8	31

Continued from previous page...

5 of 157 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	149	PRO
6	AG	11	ILE
6	AG	56	SER
8	AI	110	VAL
9	AJ	57	VAL

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 sidechain conformation was



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	AB	180/180~(100%)	177 (98%)	3 (2%)	60	78
2	AC	170/171~(99%)	170 (100%)	0	100	100
3	AD	172/173~(99%)	169 (98%)	3 (2%)	60	78
4	AE	113/113 (100%)	111 (98%)	2 (2%)	59	77
5	AF	87/87~(100%)	85 (98%)	2 (2%)	50	70
6	AG	123/123~(100%)	121 (98%)	2 (2%)	62	79
7	AH	104/105~(99%)	104 (100%)	0	100	100
8	AI	105/105~(100%)	102 (97%)	3 (3%)	42	64
9	AJ	86/86~(100%)	86 (100%)	0	100	100
10	AK	90/90~(100%)	89 (99%)	1 (1%)	73	84
11	AL	103/104 (99%)	102 (99%)	1 (1%)	76	86
12	AM	91/92~(99%)	91 (100%)	0	100	100
13	AN	83/84~(99%)	82 (99%)	1 (1%)	71	83
14	AO	76/77~(99%)	74 (97%)	2 (3%)	46	66
15	AP	65/65~(100%)	65 (100%)	0	100	100
16	AQ	74/74~(100%)	73~(99%)	1 (1%)	67	80
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70~(100%)	69~(99%)	1 (1%)	67	80
19	AT	65/65~(100%)	64 (98%)	1 (2%)	65	80
20	AU	44/44 (100%)	41 (93%)	3 (7%)	16	41
25	BC	216/217~(100%)	213 (99%)	3 (1%)	67	80
26	BD	164/164~(100%)	160 (98%)	4 (2%)	49	69
27	BE	165/165~(100%)	162 (98%)	3 (2%)	59	77
28	BF	149/150~(99%)	147 (99%)	2 (1%)	69	81
29	BG	137/138~(99%)	134 (98%)	3 (2%)	52	71
30	BH	114/114 (100%)	112 (98%)	2 (2%)	59	77
31	BI	109/110~(99%)	108 (99%)	1 (1%)	78	87
32	BJ	$1\overline{16/116}\ (100\%)$	115 (99%)	1 (1%)	78	87
33	BK	103/103~(100%)	103 (100%)	0	100	100
34	BL	102/103~(99%)	100 (98%)	2 (2%)	55	74
35	BM	109/109~(100%)	107 (98%)	2 (2%)	59	77

analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
36	BN	100/100~(100%)	99~(99%)	1 (1%)	76	86
37	BO	86/87~(99%)	86 (100%)	0	100	100
38	BP	99/100~(99%)	97~(98%)	2 (2%)	55	74
39	BQ	89/90~(99%)	88~(99%)	1 (1%)	73	84
40	BR	84/84~(100%)	82~(98%)	2(2%)	49	69
41	BS	93/93~(100%)	92~(99%)	1 (1%)	73	84
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84~(99%)	82~(99%)	1 (1%)	71	83
44	BV	78/78~(100%)	78 (100%)	0	100	100
45	BW	59/59~(100%)	57~(97%)	2(3%)	37	60
46	BX	67/68~(98%)	67~(100%)	0	100	100
47	BY	55/55~(100%)	55~(100%)	0	100	100
48	ΒZ	48/49~(98%)	47 (98%)	1 (2%)	53	72
49	B0	47/48~(98%)	47 (100%)	0	100	100
50	B1	45/45~(100%)	44 (98%)	1 (2%)	52	71
51	B2	38/38~(100%)	35~(92%)	3 (8%)	12	35
52	B3	51/52~(98%)	51 (100%)	0	100	100
53	B4	34/34~(100%)	33~(97%)	1 (3%)	42	64
56	B5	$17\overline{3}/181~(96\%)$	170 (98%)	3 (2%)	60	78
All	All	4842/4870 (99%)	4774 (99%)	68 (1%)	68	80

Continued from previous page...

 $5~{\rm of}~68$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
45	BW	23	LYS
48	ΒZ	37	ARG
56	B5	12	ARG
20	AU	20	ARG
20	AU	18	PHE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such side chains are listed below:

Mol	Chain	Res	Type
44	BV	88	HIS



Continued from previous page...

Mol	Chain	Res	Type
45	BW	56	HIS
46	BX	31	ASN
10	AK	100	ASN
4	AE	96	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533~(99%)	264 (17%)	77~(5%)
22	A1	74/76~(97%)	14 (18%)	6 (8%)
23	A2	14/15~(93%)	5~(35%)	2(14%)
24	A3	76/77~(98%)	14 (18%)	7 (9%)
54	BA	2902/2903~(99%)	451 (15%)	146~(5%)
55	BB	116/118~(98%)	12 (10%)	3(2%)
All	All	4711/4722~(99%)	760 (16%)	241~(5%)

5 of 760 RNA backbone outliers are listed below:

Mol	Chain	\mathbf{Res}	\mathbf{Type}	
21	AA	6	G	
21	AA	7	А	
21	AA	8	А	
21	AA	9	G	
21	AA	13	U	

5 of 241 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	449	А
54	BA	2563	U
54	BA	1236	G
54	BA	2531	А
54	BA	2858	С

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

11 non-standard protein/DNA/RNA residues 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	Tuno	Chain	Dog	Tink	Bo	ond leng	$_{\rm ths}$	Bond angles		
	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
22	4SU	A1	7	22	18,21,22	1.45	2 (11%)	26,30,33	1.05	1 (3%)
22	5MU	A1	54	22	19,22,23	0.85	0	28,32,35	1.53	4 (14%)
22	7MG	A1	46	22	22,26,27	5.20	1 (4%)	29,39,42	1.48	2 (6%)
24	PSU	A3	56	24	18,21,22	1.12	2 (11%)	22,30,33	1.44	3 (13%)
22	PSU	A1	55	22	18,21,22	1.02	1 (5%)	22,30,33	1.08	1 (4%)
24	4SU	A3	8	24	18,21,22	1.43	1 (5%)	26,30,33	0.77	1 (3%)
24	OMC	A3	33	24	19,22,23	0.91	0	26,31,34	0.96	1 (3%)
24	5MU	A3	55	24	19,22,23	0.87	0	28,32,35	1.66	5 (17%)
22	6MZ	A1	37	22	18,25,26	1.16	2 (11%)	16,36,39	1.57	2 (12%)
22	CM0	A1	34	22,23	22,26,27	1.55	1 (4%)	28,37,40	1.14	2 (7%)
24	H2U	A3	21	24	18,21,22	1.42	3 (16%)	21,30,33	1.08	2 (9%)

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
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3
24	PSU	A3	56	24	-	0/7/25/26	0/2/2/2
22	PSU	A1	55	22	-	2/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/7/25/26	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	CM0	A1	34	22,23	-	2/12/30/31	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
22	A1	46	7MG	C8-N9	-24.09	1.32	1.46
22	A1	34	CM0	O5-C5	-5.83	1.23	1.36



Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)				
24	A3	8	4SU	C5-C4	-4.94	1.36	1.42				
22	A1	7	4SU	C5-C4	-4.90	1.36	1.42				
24	A3	21	H2U	C2-N3	-3.69	1.31	1.38				

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The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
22	A1	46	7MG	N9-C8-N7	6.20	112.24	103.38
22	A1	37	6MZ	C9-N6-C6	4.97	127.15	122.87
24	A3	55	5MU	C5M-C5-C6	-4.33	117.06	122.85
22	A1	54	5MU	C5M-C5-C6	-3.95	117.57	122.85
24	A3	56	PSU	C6-C5-C4	3.95	120.96	118.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	34	CM0	O5-C7-C8-O9
22	A1	34	CM0	O5-C7-C8-O8
22	A1	55	PSU	O4'-C1'-C5-C4
22	A1	55	PSU	O4'-C1'-C5-C6
22	A1	46	7MG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



Mol ′	Type	Chain	Dec	Link	B	ond leng	Bond angles			
MOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
57	VAL	A1	101	22,58	4,6,7	0.78	0	6,7,9	1.19	1 (16%)
58	FME	BA	3001	57	8,9,10	0.49	0	7,9,11	1.29	2 (28%)

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).

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
57	VAL	A1	101	22,58	-	4/5/6/8	-
58	FME	BA	3001	57	-	0/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
57	A1	101	VAL	O-C-CA	-2.61	117.93	124.78
58	BA	3001	FME	C-CA-N	2.24	113.78	109.73
58	BA	3001	FME	O-C-CA	-2.13	119.20	124.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A1	101	VAL	N-CA-CB-CG2
57	A1	101	VAL	C-CA-CB-CG1
57	A1	101	VAL	C-CA-CB-CG2
57	A1	101	VAL	N-CA-CB-CG1

There are no ring outliers.

No monomer is involved in short contacts.

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-1716. 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: 96



Y Index: 96



Z Index: 96



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: 97

Y Index: 104

Z Index: 91

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 30.0. 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 2406 $\rm nm^3;$ this corresponds to an approximate mass of 2173 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 0.083 ${\rm \AA^{-1}}$



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-1716 and PDB model 4V6Y. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 30.0 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 (30.0).



9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 58% 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 (30.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5809	0.0180
A1	0.4192	-0.0110
A2	0.4078	-0.0330
A3	0.5177	0.0450
AA	0.6384	0.0190
AB	0.4785	0.0280
AC	0.6124	0.0150
AD	0.5094	-0.0070
AE	0.5488	0.0080
AF	0.3601	0.0060
AG	0.4307	0.0070
AH	0.7115	0.0430
AI	0.4730	-0.0040
AJ	0.5602	-0.0110
AK	0.5731	0.0230
AL	0.4137	-0.0070
AM	0.4438	0.0150
AN	0.6809	0.0190
AO	0.5087	0.0310
AP	0.6823	0.0440
AQ	0.5228	0.0340
AR	0.4692	0.0080
AS	0.5449	0.0160
AT	0.5951	0.0300
AU	0.6284	0.0620
B0	0.3528	-0.0110
B1	0.5891	0.0570
B2	0.3380	-0.0510
B3	0.3910	-0.0420
B4	0.5719	0.0110
B5	0.0570	-0.0090
BA	0.6258	0.0230
BB	0.6953	0.0270
BC	0.4427	-0.0250
BD	0.6047	0.0180



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Chain	Atom inclusion	Q-score
BE	0.4967	0.0200
BF	0.5647	0.0200
BG	0.4603	-0.0100
BH	0.1378	-0.0170
BI	0.0323	0.0000
BJ	0.5936	0.0040
BK	0.4420	0.0060
BL	0.3996	0.0080
BM	0.5537	0.0130
BN	0.4756	-0.0090
BO	0.6744	0.0450
BP	0.5845	0.0210
BQ	0.5551	-0.0030
BR	0.4956	0.0310
BS	0.4438	0.0030
BT	0.5173	0.0120
BU	0.4688	0.0280
BV	0.5745	0.0250
BW	0.5412	-0.0020
BX	0.2862	-0.0370
BY	0.3984	0.0120
BZ	0.6499	0.0530

