

wwPDB EM Validation Summary Report (i)

Nov 28, 2022 – 09:57 AM EST

PDB ID	:	7LS2
EMDB ID	:	EMD-23501
Title	:	80S ribosome from mouse bound to eEF2 (Class I)
Authors	:	Loerch, S.; Smith, P.R.; Kunder, N.; Stanowick, A.D.; Lou, TF.; Campbell,
		Z.T.
Deposited on	:	2021-02-17
Resolution	:	3.10 Å(reported)

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. dev 43
Mogul	:	1.8.5 (274361), 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)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
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	
1	A1	270	● 82%	18%
2	B1	266	86%	14%
3	C1	192	98%	••
4	D1	214	96%	••
5	E1	178	95%	• •
6	F1	211	96%	••
7	G1	217	64% 36%	
8	H1	204	98%	•



Mol	Chain	Length	Quality of chain	
9	A2	4731	• 60% 17% • 22%	
10	B2	121	86% 13	
11	C2	156	8 1% 18%	.
12	D2	257	• 96%	•••
13	E2	403	98%	•
14	F2	419	► 87% • 1	12%
15	G2	297	99%	
16	H2	296	• 74% • 25%	
17	I2	203	98%	•••
18	J2	184	83% • 17	!%
19	K2	188	• 99%	
20	L2	196	92%	• 6%
21	M2	176	99%	
22	N2	160	98%	
23	02	128	• 79% 21%	
24	P2	140	•	8%
25	02	157	8% 69% · 30%	
26	R2	156	• 76% 24%	
27	S2	145	90%	8%
28	T2	136	• •	
20	12 U2	148	• • •	
30	V2	160	8%	
31	W2	115	· 11%0 • 21%0	
ം ച		110	×1% · 18%	C
<u>ರಿ/</u>		120	85% · 14	1%
აპ	Y 2	135	94%	• 5%

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Mol	Chain	Length	Quality of chain	
34	Z2	110	97%	••
35	a2	117	96%	• •
36	b2	123	98%	•
37	c2	105	96%	•••
38	d2	97	88% •	11%
39	e2	70	99%	·
40	f2	51	98%	•
41	g2	128	4 0% • 59%	
42	h2	25	96%	·
43	i2	106	92%	5% •
44	j2	92	95%	•••
45	k2	137	90%	• 9%
46	m2	1871	71% 21%	• 8%
47	n2	75	5% 68% 32%	
48	p2	264	81%	9%
49	q2	243	92%	• 7%
50	r2	263	98%	
51	w2	158	9%	· ·
52	z2	135	98%	
53	02	295	73% 27%	
54	s2	204	92%	7%
55	v2	165	58% • 41%	
56	x2	145	87%	10%
57	y2	146	98%	
58	A3	152	93%	• 5%



Mol	Chain	Length	Quality of chain
59	B3	145	95% ••
60	C3	119	8 5% • 14%
61	D3	83	100%
62	E3	143	98%
63	F3	115	83%
64	C3	69	16%
65	Ц9 Ц9	56	95%
00	115	30	95% · ·
66	13	317	96% ••
67	J3	293	75% • 24%
68	K3	249	90% · 9%
69	L3	194	93% • 5%
70	M3	132	92% 8%
71	N3	151	5% 99%
72	O3	151	• 87% • 11%
73	P3	130	98%
74	03	133	7%
75	- Q0 - D2	105	9770 ·
7.5	n.s	125	60% 40%
76	53	84	96%
77	Τ3	133	41% • 59%
78	U3	156	37% • 60%
79	m	858	97% ···
80	j	317	• 61% • 38%
81	k	165	<u>13%</u> 90% ·· 7%
82	А	386	7% 16% 84%
83	t	194	92% · 6%

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Mol	Chain	Length	Quality of chain	
84	u	208	7% 97%	
85	L1	217	29%	• 5%



2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 227130 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 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	222	Total 1851	C 1190	N 356	O 297	S 8	1	0

• Molecule 2 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	230	Total 1863	C 1188	N 359	0 312	$\frac{S}{4}$	1	0

• Molecule 3 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	190	Total 1519	C 956	N 284	0 273	S 6	0	0

• Molecule 4 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	208	Total 1690	C 1073	N 327	0 278	S 12	0	0

• Molecule 5 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
5	E1	174	Total 1397	C 880	N 260	O 251	S 6	0	0

• Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
6	F1	207	Total 1676	C 1048	N 344	O 280	${S \atop 4}$	0	0



• Molecule 7 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	G1	139	Total 1143	C 732	N 221	0 183	${ m S} 7$	0	0

• Molecule 8 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues		Ate	Atoms					
8	H1	203	Total 1701	C 1072	N 359	O 266	$\frac{S}{4}$	0	0	

• Molecule 9 is a RNA chain called 28S rRNA.

Mol	Chain	Residues			Atoms			AltConf	Trace
9	A2	3706	Total 79519	C 35463	N 14497	O 25854	Р 3705	0	0

• Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues		A	AltConf	Trace			
10	B2	120	Total 2558	C 1141	N 456	0 842	Р 119	0	0

• Molecule 11 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues		Α	toms			AltConf	Trace
11	C2	156	Total 3315	C 1481	N 585	O 1094	Р 155	0	0

• Molecule 12 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
12	D2	251	Total 1921	C 1204	N 393	0 318	S 6	0	0

• Molecule 13 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues		At	oms			AltConf	Trace
13	E2	402	Total 3238	C 2060	N 609	O 555	S 14	0	0

• Molecule 14 is a protein called 60S ribosomal protein L4.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	F2	367	Total 2928	C 1842	N 583	O 488	S 15	0	0

• Molecule 15 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues		At	AltConf	Trace			
15	G2	293	Total 2385	C 1506	N 440	0 425	S 14	0	0

• Molecule 16 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues		Ate	AltConf	Trace			
16	H2	221	Total 1789	C 1145	N 342	O 298	${S \atop 4}$	0	0

• Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I2	201	Total 1640	$\begin{array}{c} \mathrm{C} \\ 1055 \end{array}$	N 320	O 259	S 6	0	0

• Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
18	J2	153	Total 1242	C 777	N 241	O 215	S 9	0	0

• Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	K2	186	Total 1511	C 946	N 313	0 248	$\frac{S}{4}$	0	0

• Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
20	L2	184	Total 1542	C 955	N 332	0 246	S 9	0	0

• Molecule 21 is a protein called 60S ribosomal protein L18a.



Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
21	M2	175	Total 1450	C 924	N 283	O 233	S 10	0	0

• Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	N2	159	Total 1298	C 823	N 253	O 216	S 6	0	0

• Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues		At	oms	AltConf	Trace		
23	O2	101	Total 825	C 529	N 144	0 150	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 24 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues		At	oms	AltConf	Trace		
24	Ρ2	129	Total 969	C 613	N 182	O 169	${ m S}{ m 5}$	0	0

• Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues		At	oms	AltConf	Trace		
25	Q2	110	Total 895	C 563	N 180	0 148	$\frac{S}{4}$	0	0

• Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues		At	oms	AltConf	Trace		
26	R2	118	Total 967	C 618	N 181	O 167	S 1	0	0

• Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues		At	oms	AltConf	Trace		
27	S2	134	Total 1115	C 700	N 226	0 186	${ m S} { m 3}$	0	0

• Molecule 28 is a protein called 60S ribosomal protein L27.



Mol	Chain	Residues		At	oms	AltConf	Trace		
28	Τ2	135	Total 1107	С 714	N 208	O 182	${ m S} { m 3}$	0	0

• Molecule 29 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	U2	147	Total 1164	C 736	N 239	0 185	$\frac{S}{4}$	0	0

• Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	V2	117	Total 945	C 596	N 198	0 146	${ m S}{ m 5}$	0	0

• Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues		At	oms			AltConf	Trace
31	W2	94	Total 732	C 465	N 130	0 131	S 6	0	0

• Molecule 32 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues		At	oms			AltConf	Trace
32	X2	107	Total 888	C 560	N 171	0 155	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues		At	oms			AltConf	Trace
33	Y2	128	Total 1053	C 667	N 216	0 165	${ m S}{ m 5}$	0	0

• Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues		At	oms			AltConf	Trace
34	Z2	109	Total 876	C 555	N 174	0 143	$\begin{array}{c} \mathrm{S} \\ \mathrm{4} \end{array}$	0	0

• Molecule 35 is a protein called 60S ribosomal protein L34.



Mol	Chain	Residues		At	oms			AltConf	Trace
35	a2	114	Total 906	$\begin{array}{c} \mathrm{C} \\ 565 \end{array}$	N 187	0 148	S 6	0	0

• Molecule 36 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues		At	oms	AltConf	Trace		
36	b2	120	Total 1001	C 634	N 201	0 165	S 1	0	0

• Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues		At	oms	AltConf	Trace		
37	c2	102	Total 827	C 516	N 173	0 133	$\frac{S}{5}$	0	0

• Molecule 38 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues		At	oms			AltConf	Trace
38	d2	86	Total 705	C 434	N 155	0 111	${ m S}{ m 5}$	0	0

• Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues		At	oms			AltConf	Trace
39	e2	69	Total 568	C 365	N 103	O 99	S 1	0	0

• Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
40	fD	50	Total	С	Ν	Ο	S	0	0
40	12	- 50	444	281	98	64	1	0	0

• Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
41	g2	52	Total 430	C 267	N 90	O 67	S 6	0	0

• Molecule 42 is a protein called 60S ribosomal protein L41.



Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
42	h2	24	Total 230	C 139	N 62	O 26	${ m S} { m 3}$	0	0

• Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues		At	oms	AltConf	Trace		
43	i2	103	Total 842	C 528	N 172	0 136	S 6	0	0

• Molecule 44 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues		At	oms		AltConf	Trace	
44	j2	89	Total 694	C 436	N 133	0 118	${f S}7$	0	0

• Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues		At	oms			AltConf	Trace
45	k2	125	Total 1001	C 621	N 207	0 168	${ m S}{ m 5}$	0	0

• Molecule 46 is a RNA chain called 18S rRNA.

Mol	Chain	Residues		1	Atoms			AltConf	Trace
46	m2	1724	Total 36817	C 16440	N 6606	O 12048	Р 1723	0	0

• Molecule 47 is a RNA chain called tRNA.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
47	n2	75	Total 1604	С 717	N 298	0 515	Р 74	0	0

• Molecule 48 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues		At	oms			AltConf	Trace
48	p2	214	Total 1738	C 1103	N 310	0 311	S 14	0	0

• Molecule 49 is a protein called 40S ribosomal protein S3.



Mol	Chain	Residues		Ate	oms			AltConf	Trace
49	q2	226	Total 1756	C 1119	N 316	0 314	S 7	0	0

• Molecule 50 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues		Ate		AltConf	Trace		
50	r2	262	Total 2076	C 1324	N 386	O 358	S 8	0	0

• Molecule 51 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues		At	oms			AltConf	Trace
51	w2	153	Total 1247	C 793	N 234	0 214	S 6	0	0

• Molecule 52 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues		At	oms			AltConf	Trace
52	z2	134	Total 1080	C 678	N 201	0 197	${f S}$ 4	0	0

• Molecule 53 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
53	02	214	Total 1694	C 1077	N 297	0 312	S 8	0	0

• Molecule 54 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
54	s2	189	Total 1496	C 934	N 285	O 270	${ m S} 7$	0	0

• Molecule 55 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues		At	oms	AltConf	Trace		
55	v2	97	Total 819	С 534	N 147	0 133	${f S}{5}$	0	0

• Molecule 56 is a protein called 40S ribosomal protein S15.



Mol	Chain	Residues		At	oms			AltConf	Trace
56	x2	130	Total 1073	C 681	N 205	O 180	${ m S} 7$	0	0

• Molecule 57 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues		At	oms	AltConf	Trace		
57	y2	144	Total 1143	C 726	N 216	0 198	${ m S} { m 3}$	0	0

• Molecule 58 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues		At	oms		AltConf	Trace	
58	A3	144	Total 1190	C 746	N 241	O 202	S 1	0	0

• Molecule 59 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues		At	oms			AltConf	Trace
59	B3	141	Total 1104	C 691	N 215	0 196	${ m S} { m 2}$	0	0

• Molecule 60 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues		At	oms	AltConf	Trace		
60	C3	102	Total 807	C 507	N 153	0 143	$\frac{S}{4}$	0	0

• Molecule 61 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues		At	oms	AltConf	Trace		
61	D3	83	Total 638	C 392	N 119	0 122	${ m S}{ m 5}$	0	0

• Molecule 62 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues		At	oms			AltConf	Trace
62	E3	141	Total 1098	C 693	N 219	0 183	${ m S} { m 3}$	0	0

• Molecule 63 is a protein called 40S ribosomal protein S26.



Mol	Chain	Residues		At	oms	AltConf	Trace		
63	F3	100	Total 811	$\begin{array}{c} \mathrm{C} \\ 506 \end{array}$	N 169	O 131	${f S}{5}$	1	0

• Molecule 64 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
64	G3	64	Total 506	C 308	N 102	0 94	${ m S} { m 2}$	0	0

• Molecule 65 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
65	H3	54	Total 455	C 284	N 93	O 73	${ m S}{ m 5}$	0	0

• Molecule 66 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues		At		AltConf	Trace		
66	I3	313	Total 2436	C 1535	N 424	O 465	S 12	0	0

• Molecule 67 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues		At	oms			AltConf	Trace
67	J3	222	Total 1725	C 1116	N 298	O 302	S 9	0	0

• Molecule 68 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues		At	oms			AltConf	Trace
68	K3	227	Total 1840	C 1149	N 367	0 317	${f S}{7}$	0	0

• Molecule 69 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues		At	oms		AltConf	Trace	
69	L3	185	Total 1525	C 969	N 306	0 248	$\frac{S}{2}$	0	0

• Molecule 70 is a protein called 40S ribosomal protein S12.



Mol	Chain	Residues		At	oms		AltConf	Trace	
70	M3	122	Total 942	$\begin{array}{c} \mathrm{C} \\ 593 \end{array}$	N 164	O 177	S 8	0	0

• Molecule 71 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues		At	oms		AltConf	Trace	
71	N3	150	Total 1208	С 773	N 229	O 205	S 1	0	0

• Molecule 72 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	O3	134	Total 1002	C 612	N 197	0 187	S 6	0	0

• Molecule 73 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	P3	129	Total 1034	$\begin{array}{c} \mathrm{C} \\ 659 \end{array}$	N 193	O 176	S 6	0	0

• Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues		At	oms		AltConf	Trace	
74	Q3	129	Total 1049	C 662	N 206	0 176	${ m S}{ m 5}$	0	0

• Molecule 75 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues		At	oms			AltConf	Trace
75	R3	75	Total 598	C 382	N 111	0 104	S 1	0	0

• Molecule 76 is a protein called 40S ribosomal protein S27-like.

Mol	Chain	Residues		At	oms		AltConf	Trace	
76	S3	83	Total 652	C 409	N 121	0 115	S 7	0	0

• Molecule 77 is a protein called 40S ribosomal protein S30.



Mol	Chain	Residues	Atoms					AltConf	Trace
77	Т3	55	Total 438	C 271	N 95	0 71	S 1	0	0

• Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms				AltConf	Trace	
78	U3	62	Total 505	C 317	N 96	O 85	${ m S} 7$	0	0

• Molecule 79 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	m	851	Total 6649	С 4217	N 1146	0 1242	S 44	0	0

• Molecule 80 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms				AltConf	Trace	
80	j	196	Total 1507	C 959	N 263	0 276	S 9	0	0

• Molecule 81 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	k	153	Total 1159	C 721	N 218	0 217	${ m S} { m 3}$	0	0

• Molecule 82 is a protein called Isoform 3 of Plasminogen activator inhibitor 1 RNA-binding protein.

Mol	Chain	Residues		Ator	\mathbf{ns}	AltConf	Trace	
82	А	61	Total 486	C 289	N 94	O 103	0	0

• Molecule 83 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	t	183	Total 1477	C 944	N 270	O 262	S 1	0	0

• Molecule 84 is a protein called 40S ribosomal protein S8.



Mol	Chain	Residues	Atoms					AltConf	Trace
84	u	206	Total 1686	C 1058	N 332	O 291	${f S}{5}$	0	0

• Molecule 85 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms				AltConf	Trace	
85	L1	206	Total 1660	C 1061	N 300	O 291	S 8	0	0

• Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
86	d2	1	Total Zn 1 1	0
86	g2	1	Total Zn 1 1	0
86	i2	1	Total Zn 1 1	0
86	j2	1	Total Zn 1 1	0
86	F3	1	Total Zn 1 1	0
86	H3	1	Total Zn 1 1	0
86	U3	1	Total Zn 1 1	0

• Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
87	H3	1	Total Mg 1 1	0

• Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





Mol	Chain	Residues	Atoms					AltConf
00	m	1	Total	С	Ν	Ο	Р	0
00	88 III	1	28	10	5	11	2	0

• Molecule 89 is water.

Mol	Chain	Residues	Atoms	AltConf
89	B1	1	Total O 1 1	0
89	A2	1	Total O 1 1	0
89	m2	2	Total O 2 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: 60S ribosomal protein L7



• Molecule 6: 60	S ribosomal protein L13		
Chain F1:	96%		
MET A2 B5 V59 V59 H67	A136 X162 LYS LYS LYS		
• Molecule 7: 60	S ribosomal protein L14		
Chain G1:	64%	36	%
MET V2 P140 LYS LYS LYS ALA ALA ALA ALA ALA ALA	ALA TLE ALA ALA ALA ALA ALA ALA ALA ALA ALA A	1HK GLY GLY CLYS CLYS CLYS ALA GLN GLN ALA ALA ALA ALA ALA CLN GLN	ALA ALA ALA GLY GLN CLN CLN ALA ALA PRO PRO PRO ALA CLY GLY
GLN LYS GLY GLY GLN LYS PRO ALA GLN LYS ALA ALA PRO	ALA PRO LYS ALA ALA GLY LYS LYS ALA		
• Molecule 8: 60	S ribosomal protein L15		
Chain H1:	989	6	
MET G2 K140 R193 R204			
• Molecule 9: 28	8S rRNA		
Chain A2:	60%	17% •	22%
C1 C2 C2 C2 C2 C2 C2 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4	A59 A64 A65 A65 A65 A166 C104 A106 A106 A106 C109 C109 C109 C109 C109 C109 C109 C109	C112 C116 C116 C133 C133 C133 C133 C133 C133	U1 43 6144 6144 6145 6155 6164 0164 0164 0171 0171 0171
C178 C178 C183 C183 C188 C188 C188 C188 C188 C18	4197 4197 1200 1200 1200 1200 1200 1200 1200 120	2256 2257 2258 2258 2269 2265 2265 2265 2265 2265 2265 2265	A279 C297 U297 U315 U315 C326 A329 A329 C330 C330 C330
C340 C341 C345 C345 C345 C373 C373 C373 A396 C397	A338 (3395) (3395) (3396) (3410) (4411) (4412) (4413) (4413) (4413) (4413) (4413) (4413) (443) (443) (443) (443)	0450 0451 0453 0453 0453 0455 0455 0455 0457 0467 0481 0481	с С. <mark>1485</mark> С. <mark>1485</mark> С.487 С.486 С.489 С.489 С.491 С.492 С.491
U499 0 0500 0500 0501 0502 0503 0503 0505 0503 0503 0503 0503 0503 0503 0503 0503 0503 0503 0503 0503 0503 0503 0503 0503 0503 0503	81114 1911 000000000000000000000000000000	< ប ប ប ប ⊃ ប ប < ប ប ប o ប o t	
0000000000000000	с с с с с с с с с с с с с с с с с с с	4693 6694 6694 6704 6704 6711 715 6735 6735 6733 6733 6733	A1 40 C1 46 C1 46 C1 48 C1 48 C1 50 C1 48 C1 50 C1 50 C
◆ 24000000000000000000000000000000000000	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	U800 1800 1803 1803 1812 1813 1814 1814 1814 1814 1814 1814 1815 1815	624 (831 (834 (834 (833) (843) (843) (843) (843) (843) (843) (843)
	W P	ORLDWIDE ROTEIN DATA BANK	









MET A2 C3 R75 Y122	ALA ALA ALA ALA ALA ALA ALA ALA
THR GLU GLU LYS LYS PRO ALA ALA	
• Molecule 1	15: 60S ribosomal protein L5
Chain G2:	99%
MET G2 F3 ALA ALA GLU SER	
• Molecule 1	16: 60S ribosomal protein L6
Chain H2:	74% • 25%
MET ALA GLY GLU LYS ALA PRO ASP THR	LYS LYS LYS LYS LYS LYS LYS LYS LYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
LYS LYS LYS LYS GLU LYS VAL L9G	V201 D212 D212 LV25 PRO ARG ARG ARG ARG ARG ARG ARG CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
• Molecule 1	17: 60S ribosomal protein L13a
Chain I2:	98%
MET ALA E3 E3 E3 E3 E1 17 E1 17 E1 17 E1 E1 E1 E1 E1 E1 E1 E1 E1 E1 E1 E1 E1	
• Molecule 1	18: 60S ribosomal protein L17
Chain J2:	83% · 17%
MET V2 Q118 E154 GLN VAL	PRO PRO GLU GLU GLU GLU GLU CYS CLVS CLVS CLVS CLVS CLVS CLVS CLVS CLV
• Molecule 1	19: 60S ribosomal protein L18
Chain K2:	99%
MET GLY V3 D124 E175	
• Molecule 2	20: 60S ribosomal protein L19
Chain L2:	92% · 6%

R1 4 R2 R3 R17 A177	
\bullet Molecule 21: 60S ribosomal protein L18a	
Chain M2: 99%	
\bullet Molecule 22: 60S ribosomal protein L21	
Chain N2: 98%	
MET 122 13 14 16 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	
\bullet Molecule 23: 60S ribosomal protein L22	
Chain O2: 79% 21%	_
MET ALA ALA ALA LYS LYS LYS LYS LYS CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	
• Molecule 24: 60S ribosomal protein L23	
Chain P2: 91% · 8	9%
MET SER BIT GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY	
\bullet Molecule 25: 60S ribosomal protein L24	
Chain Q2: 69% · 30%	_
M1 M1 M25 G62 G62 G62 G62 G12 G12 G12 G12 G12 G12 G12 G1	PRO LYS LYS LYS LYS TLLE VAL LYS PRO VAL
LYS VAL ALA ARG ARG GLY GLY ARG ARG ARG	
\bullet Molecule 26: 60S ribosomal protein L23a	
Chain R2: 76% 24%	_
MET ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
WORLDWIDE PROTEIN DATA BANK	

• Molecule 27: 60S ribosomal protein L26	
Chain S2: 90%	• 8%
M N20 N20 N20 N21 N21 N21 N21 N21 N21 N21 N21 N21 N21	
• Molecule 28: 60S ribosomal protein L27	
Chain T2:	%
MET G 2 D 35 D 35 F 13 6 F 13 6	
• Molecule 29: 60S ribosomal protein L27a	
Chain U2:	% ••
NET P2 A148	
• Molecule 30: 60S ribosomal protein L29	
Chain V2: 71%	• 27%
MET A2 R25 R25 R75 R73 A74 A74 A74 P75 P75 P77 P77 P77 P77 P77 P77 P77 P77	VAL VAL CUNS THR ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
ALA PRO VAL LYS ALA PRO	
• Molecule 31: 60S ribosomal protein L30	
Chain W2: 81%	• 18%
MET VAL ALA ALA ALA ALA ALA ALA ALA ALA CIT SER M20 CLU CLU CLU CLU CLU CLU CLU CLU	
• Molecule 32: 60S ribosomal protein L31	
Chain X2: 85%	• 14%
MET PRO ALA ALA ALA ALA ALA CLY GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C	
• Molecule 33: 60S ribosomal protein L32	
Chain Y2: 94%	• 5%



 \bullet Molecule 34: 60S ribosomal protein L35a

Chain Z2:	97%	•••
MET S2 N91 110 1110		
• Molecule 35:	60S ribosomal protein L34	
Chain a2:	96%	
MET V2 N28 R54 ALA ALA LYS		
• Molecule 36:	60S ribosomal protein L35	
Chain b2:	98%	·
MET ALA LYS I4 D82 A123		
• Molecule 37:	60S ribosomal protein L36	
Chain c2:	96%	• •
MET A2 R29 LYS LYS ASP		
• Molecule 38:	60S ribosomal protein L37	
Chain d2:	88%	• 11%
MET T2 N57 N57 AR6 AR6 ALA ALA ALA ALA	ALA ALA SER SER SER SER	
• Molecule 39:	60S ribosomal protein L38	
Chain e2:	99%	
MET P2 K70		

• Molecule 40: 60S ribosomal protein L39



Chain f2:		98%		·
MET 32 G50 L51				
• Molecule 41:	Ubiquitin-60S ri	bosomal protein L4	40	
Chain g2:	40%	·	59%	_
MET GLN TLE PHE VAL LYS THR LEU CLY	THR ILLE THR LEU CLU CLU CLU CLU CLU CLU CLU CLU CLU CL	GLU ASN VAL LYS LYS ALA LYS GLN GLN GLU GLV GLU GLU FRO	PRO ASP GLN GLN GLN GLN TLE PHE ALA GLV CLV CLV CLV CLV CLV	ALT ARG THR LEU SER ASP TYR ASP
TLE CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	ARG ARG GLY GLY K128 K128 K128			
• Molecule 42:	60S ribosomal p	rotein L41		
Chain h2:		96%		·
M1 S24 LYS				
• Molecule 43:	60S ribosomal p	rotein L36a		
Chain i2:		92%	5	5% •
MET V2 H18 D42 B42 R57 C77	185 1996 1104 GIM PHE			
• Molecule 44:	60S ribosomal p	rotein L37a		
Chain j2:		95%		•••
MET ALA LYS R4 R4 R13 T16 D91				
• Molecule 45:	60S ribosomal p	rotein L28		
Chain k2:		90%	·	9%
MET S2 M108 M108 R119 LYS LYS LYS	ARG THR ARG PRO THR LYS SER SER			
• Molecule 46:	18S rRNA			
Chain m2:		71%	21%	• 8%





• Molecule 47:	tRNA	
Chain n2:	68%	32%
A2 09 010 011 012 013 013 014 016 016 016 016 016	(18 (19 (19 (19 (19 (19 (19 (19 (19 (19 (19	
• Molecule 48:	40S ribosomal protein S3a	
Chain p2:	81%	19%
MET ALA VAL CLY CLY CLY CLY ASN ASN LYS LEU LEU LEU CLYS	CLY CLYS CLYS CLYS CLYS CLYS LYS LYS CLYS C	THR GLY GLY C VAL ANG ANG ANG ANG ANG ANG AND PRO CUU PRO CUU SER SER SER SER
VAL		
• Molecule 49:	40S ribosomal protein S3	
Chain q2:	92%	• 7%
MET A2 V41 E47 E47 E81	Y167 P206 P206 CLY CLY PR0 PR0	
• Molecule 50:	40S ribosomal protein S4, X isoform	
Chain r2:	98%	
MET A2 D21 138 R39 B59 B59	1220 9261 8261 9263 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9	
• Molecule 51:	40S ribosomal protein S11	
Chain w2:	95%	
MET A2 14 14 124 V23 V23 L24	626 627 728 631 631 859 869 869 8119 6119 €130 8154 9154 9154 9154 0118 8153 8153 8153 8153 8153 8153 8154 916	
• Molecule 52:	40S ribosomal protein S17	
Chain z2:	98%	
MET Q2 Q2 B3 B3 B3 B3 B3 B3 B3 B3 B3 B3 B3 B3 B3		

 \bullet Molecule 53: 40S ribosomal protein SA



Chain o2:	• 73%		27%	
MET SER G3 E136 E208	E211 K212 E213 E213 E214 Q215 Q215 Q215 Q215 ALA ALA ALA ALA GLU GLU GLU GLU GLU	THAT THAT ALA PRO ALA PRO GLU PHE THAT ALA ALA GLN PRO	VAL VAL ALA ALA ALA ALP SER GLU VAL GLU VAL VAL VAL SER SER	VAL PRO ILE GLN GLN PHE
PRO THR GLU ASP TRP SER ALA GLN	PR0 ALA ALA ALA ALA GLU GLU PR0 PR0 PR0 ALA ALA ALA ALA ALA ALA ALA ALA ALA THR VAL TRP VAL TRP VAL	SER		
• Molecule	54: 40S ribosomal protein S5			
Chain s2:	10%	, D	7%	
MET THR GLU TRP GLU GLU ALA THR	PRO ALA VAL ALA ALA GLU GLU DI6 D16 D16 B36 C B36 C B36 C B36 C B36 C B36 C B36 C B36 C B36 C B36 C B36 C B36 C B36 C B36 C B16 C B17 C B17 C B17 C C C C C C C C C C C C C C C C C C C	D124	V134 R135 R136 D140 K182 R204	
• Molecule	55: 40S ribosomal protein S10)		
Chain v2:	• 58%	·	41%	
MET L2 Y12 E13 F16	VES VES VTO VTO VTO VTO VTO VTO VTO VTO VTO VTO	GLY GLU ARG ARG ARG ARG ARG PHE ARG GLY GLU ALA	ARC ARC TTRR TTRR TTRR ARC ARC SER ALA PRO FRO GLY	ALA ASP LYS LYS ALA GLU
ALA GLY ALA GLY GLY SER ALA THR GLU	PHE OLN PHE ARG CLY PHE CLY ARG CLY CLN CLN CLN CLN CLN CLN			
• Molecule	56: 40S ribosomal protein S15			
Chain x2:	• • 87%		• 10%	
MET ALA GLU VAL GLU GLN LYS K8	V37 178 H79 B82 B82 P131 C132 P131 C132 A137 SER ARG P1136 ARG P1137 L11E	LYS LYS		
• Molecule	57: 40S ribosomal protein S16	i		
Chain y2:	<u>.</u>	98%		
MET PRO S3 K4 L7	R146			
• Molecule	58: 40S ribosomal protein S18			
Chain A3:	• 93	3%	• 5%	
MET S2 K8 K8	112 R38 V98 C128 C128 C128 C128 C128 C128 C128 C12			
• Molecule	59: 40S ribosomal protein S19)		



Chain B3:	95%	
MET PRO CLY CLA M33 E44 M33 E44 G69 G69 G69 D118	HIS HIS	
• Molecule 60: 40S ribo	osomal protein S20	
Chain C3:	85%	• 14%
MET PHE PHE LYS LYS CLY GLY VAL VAL CLU CLU CLU CLU CLU	T68 E72 K75 A117 ALA ALA	
• Molecule 61: 40S ribo	osomal protein S21	
Chain D3:	100%	
There are no outlier res	sidues recorded for this chain.	
• Molecule 62: 40S ribo	osomal protein S23	
Chain E3:	98%	
MET C2 K25 L36 F105 R142		
• Molecule 63: 40S ribo	osomal protein S26	
Chain F3:	83%	• 13%
MET T2 K12 K12 C74 D60 C74 C74 R87 F100 AR0	PRO ALA GLY ALA ALA PRO PRO PRO PRO PRO PRO PRO	
• Molecule 64: 40S ribo	osomal protein S28	
Chain G3:	93%	7%
MET ASP ASP THR SER R5 V6 A12 C A12 S33 S33 S33 S33 S33 S33 S33 S33 S33 S3	E62 R65 R67 ARG ARG	
• Molecule 65: 40S ribo	osomal protein S29	
Chain H3:	95%	
MET G17 H12 Q16 D56		

• Molecule 66: Receptor of activated protein C kinase 1



Chain I3:	96%		
MET 12 12 12 12 12 12 15 16 16 16 16 16 16 16 16 16 16 16 16 16	11.32 12203 ← 2209 ← 12246 1276 ← 2279 ← 1297 1297 1297	GLY THR ARG	
• Molecule 67: 40S	S ribosomal protein S2		
Chain J3:	75%	• 24%	I
MET ALA ALA ASP ALA ALA ALA ALA ALA CLY CLY CLY PRU PRU	61.Y 61.Y 61.Y 61.Y 61.Y 61.Y 71.Y 71.Y 71.Y 71.Y 71.Y 71.Y 71.Y 7	GLY ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	ASP LYS E59
R117 + F236 F236 T262 T262 T278 N279 V280 V280	VAL ARG GLN GLN ALA ALA ALA ALA THR THR		
• Molecule 68: 40S	5 ribosomal protein S6		
Chain K3:	90%	• 9%	
MI G11 152 H70 H70 H70	R95 C100 C100 D120 D126 C100 D126 C127 C127 C127 C127 C127 C127 C127 C127 C120 C100 C122 C122	SER ARG ALGU ALR SER SER SER SER SER CLU SER CLU CSER LYS	
• Molecule 69: 40S	s ribosomal protein S9		
Chain L3:	93%	• 5%	ó
MET P2 V3 V3 N136 N136 N136 N136 N136 P122 P	C183 C184 A185 C186 ALA ASP ASP ASP CLU CLU CLU CLU CLU CLU CLU		
• Molecule 70: 40S	s ribosomal protein S12		
Chain M3:	92%	8%	-
MET ALA GLU GLU GLV GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	A32 A32 A32 A30 A50 A50 A57 A67 A67 A67 A67 A67 A67	194 194 194 194 194 194 194 194 194 194 194 194 194 194 194 194 194 195 194 195 101 101 112	K116 E117 S118 Q119 A120 K121 D122 V123 T124 E125 E125
Y127 F128 K129 K131 K132 K132			
• Molecule 71: 40S	S ribosomal protein S13		
Chain N3:	99%		
MET G2 S14 K76 K76 A148			



• Molecule 72:	40S ribosomal protein	n S14		
Chain O3:		87%		• 11%
MET ALA ARG ARG ARG LYS GLU LYS LYS LYS CLU CLY	GLU GLN VAL ILE SER LEU C18 C18 C18 C18 D138 K142 K142			
• Molecule 73:	40S ribosomal protein	n S15a		
Chain P3:		98%		
MET V2 R3 M4 D80 F104 F130				
• Molecule 74:	40S ribosomal protein	n S24		
Chain Q3:	-	97%		
MET N2 D3 K49 G66 G126	A127 G128 K129 PR0 LYS GLU			
• Molecule 75:	40S ribosomal protein	n S25		
Chain R3:	60%		409	6
MET PRO LYS ASP ASP ASP LYS LYS LYS LYS ASP	ALA GLY LYS LYS ALA LYS LYS ASP ASP ASP ASP ASP ASU ASU ASU ASU ASU ASU ASU ASU ASU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	GLY LYS ALA LYS LYS LYS LYS TRP TRP TRP CLYS GLY	LYS VAL R41 K60 E61 G115	GLY ASP ALA PRO PRO ALA GLU GLU ALA ALA
• Molecule 76:	40S ribosomal protein	n S27-like		
Chain S3:		96%		•••
MET P2 D6 L24 H84				
• Molecule 77:	40S ribosomal protein	n S30		
Chain T3:	41%	•	59%	
MET GLN CLN LEU VAL ALA ALA GLN GLN CLU LEU	THR LEU GLU GLU VAL VAL CLY GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN	VAL ALA ALA SER LEU GLU GLU GLY TLE ALA PRO GLU SSP	GLN VAL VAL VAL LEU LEU ALA GLY SER PRO	LEU GLU ASP GLU ALA ALA THR LEU GLY GLY CYS GLY
ALA LEU THR THR LEU GLU VAL ALA ALA ARG MET	LLEU GLY LLYS LLYS LLYS SS GLY F49 F49 K51 K51			

 \bullet Molecule 78: Ubiquitin-40S ribosomal protein S27a


Chain	U3:	5% 37%	·		60%	
MET GLN ILE PHE VAL	LYS THR LEU	THR GLY LYS LYS THR THR LEU GLU GLU PGLU	ASP THR TILE GLU GLU ASN VAL LYS ALA LYS TILE GLN	ASP LYS GLU GLY ILE PRO ASP GLN	GLN ARG ILEU ILEU ALA GLY GLN ILEU	GLU GLY GLY ARG THR LEU SER ASP TYR ASN
ILE GLN GLU SER	THR LEU HIS	LEU VAL LEU ARG ARG ARG ARG ALY ALA ALX ALX	LYS LYS LYS LYS SER TYR THR THR PRO LYS K90	H93 Y106 E110 N111 G112	R116 L117 R113 E125 C126 G127 F131	R138 N151 N151 L78 PRO GLU ASP L78
• Mole	ecule	79: Elongation	factor 2			
Chain	m:	<u>.</u>	97%	6		
MET VAL N2 F3	D6 H79	K41 K41 144 A45 A45 A48 A48 A48 A48 A48 A48	A50 451 E52 R54 A54 B57 B57	L76 L77 D122	K225 F235 ALA ALA ALA LYS GLY GLY G241	G261 R263 R263 R263 C372 E373 C406 R408 R408 R408
E439	G473 V474 D475	E509 E530 E539 E539 E539 E539 E539 E539 E539 E539	K666 669 663 H714 1745 L745	E771 9806 9817 E845	D855 K856 L857	
• Mole	ecule	80: 60S acidic	ibosomal protei	n P0		
Chain	j:		61%	·	38%	
MET PRO ARG GLU DS	N30	E70 B133 D100 L160 T198 Y199	PRO GLU VAL ALEU ALEU ALE GLU ALA ALA HIEU HIEU	SER ARG PHE LEU GLY VAL ARG ASN	VAL ALA SER SER VAL CYS CYS CYS CLS CLS CLY CLY TYR	PRO THR VAL ALA SER VAL PRO HIS SER TLE
ILE ASN GLY TYR LYS	ARG VAL LEU	ALA LEU LEU SER VAL CLU CLU THR THR THR PHE PHE PHE	THR GLU CYS CLYS CYAL CYS CYS CYS ALA ALA ALA ASP ASP	SEK ALA PHE ALA ALA ALA ALA ALA ALA	ALA ALA THR THR ALA ALA ALA ALA	ALA ALA ALA ALA ALA ALA ALA CLU SLUS LYS
GLU GLU GLU GLU	SER ASP GLU	ASP MET GLY PHE GLY LEU PHE ASP				
• Mole	ecule	81: 60S ribosor	nal protein L12			
Chain	k:	13%	90%			••• 7%
MET PRO LYS PHE	ASP PRO ASN	E9 V10 K11 H16 C17 T18 C17 C17 C17 C17 C17 C18 C20 C20 C20 C20 C20 C20 C20 C20 C20 C20	A24 P34 K40 K41 K48	L56 T63 T64 Q65 N66 R67	q70 P89 R92 R119 S120 €121	C1 41 143 143 143 144 144 144 144 1
PRO ALA SER						
• Mole	ecule	82: Isoform 3 c	f Plasminogen a	ctivator inhi	bitor 1 RNA-	binding protein
Chain	A:	7% 16%		84%		
MET PRO GLY HIS LEU	GLY GLU	PHE GLY CYS CYS CYS CYS CYS VAL THR ASL ASN ASN ASN ASN CJN	PHE ASP ASP GLU SER ASP PRC PHE GLU VAL LEU	LYS ALA ALA GLU GLU LYS LYS CLV GLU	ALLA GLY GLY GLY GLY GLY GLY GLY CLY	ALA LYS SER ALA ALA GLN GLN GLN
THR ASN SER ASN ALA	ALA GLY LYS	LEU LEU LYS CLYS GLU GLU ASP ASC LYS LYS	PRO LEU PRO PRO SER VAL ALA ALA ASP LYS	LTS GLU GLU GLU GLU FRO PRO PRO ALLA	LEU LYS LYS GLY GLY ARG ARG ARG VAL	ARG PRO ASP ALSP GLN CLEU CLEU GLN GLY ASP







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23297	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	30.264	Depositor
Minimum map value	-17.005	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	1.034	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	814.07996, 814.07996, 814.07996	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: 2MG, GDP, 6MZ, E6G, OMC, B8W, I4U, ZN, B8T, PSU, B9H, 4AC, MHG, P7G, A2M, 5MC, 1MA, OMG, B8Q, E7G, UR3, OMU, B8N, G7M, MG, DDE, MLZ, B9B

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	E	Bond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A1	0.26	0/1888	0.51	0/2516
2	B1	0.24	0/1898	0.50	0/2553
3	C1	0.25	0/1537	0.51	0/2065
4	D1	0.25	0/1728	0.51	0/2306
5	E1	0.25	0/1420	0.53	0/1899
6	F1	0.25	0/1707	0.54	0/2286
7	G1	0.26	0/1165	0.51	0/1558
8	H1	0.25	0/1746	0.54	0/2338
9	A2	0.24	0/86883	0.79	28/135484~(0.0%)
10	B2	0.23	0/2858	0.79	0/4455
11	C2	0.23	0/3679	0.79	0/5732
12	D2	0.26	0/1959	0.55	0/2627
13	E2	0.25	0/3305	0.50	0/4422
14	F2	0.25	0/2971	0.52	0/3987
15	G2	0.25	0/2431	0.49	0/3256
16	H2	0.25	0/1822	0.51	0/2443
17	I2	0.26	0/1670	0.50	0/2232
18	J2	0.25	0/1268	0.51	0/1700
19	K2	0.25	0/1535	0.57	0/2048
20	L2	0.23	0/1558	0.52	0/2059
21	M2	0.26	0/1490	0.53	0/2000
22	N2	0.25	0/1326	0.50	0/1769
23	O2	0.25	0/839	0.49	0/1126
24	P2	0.26	0/983	0.49	0/1319
25	Q2	0.26	0/909	0.51	0/1203
26	R2	0.25	0/984	0.51	0/1323
27	S2	0.24	0/1132	0.52	0/1504
28	Τ2	0.26	0/1130	0.49	0/1507
29	U2	0.25	0/1193	0.51	0/1593
30	V2	0.24	0/963	0.47	0/1275
31	W2	0.25	0/742	0.46	0/996



Mal	Chain	Bond	lengths	B	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
32	X2	0.24	0/903	0.53	0/1216
33	Y2	0.24	0/1071	0.51	0/1429
34	Z2	0.26	0/895	0.55	0/1198
35	a2	0.24	0/916	0.55	0/1221
36	b2	0.24	0/1009	0.51	0/1332
37	c2	0.24	0/838	0.53	0/1111
38	d2	0.25	0/720	0.57	0/952
39	e2	0.24	0/574	0.47	0/760
40	f2	0.24	0/454	0.54	0/599
41	g2	0.23	0/425	0.52	0/561
42	h2	0.23	0/231	0.67	0/294
43	i2	0.25	0/855	0.53	0/1128
44	j2	0.25	0/704	0.49	0/935
45	k2	0.24	0/1016	0.54	0/1363
46	m2	0.22	0/40772	0.79	12/63546~(0.0%)
47	n2	0.22	0/1795	0.80	0/2798
48	p2	0.24	0/1765	0.47	0/2362
49	q2	0.25	0/1784	0.50	0/2402
50	r2	0.25	0/2118	0.50	0/2849
51	w2	0.25	0/1268	0.53	0/1696
52	z2	0.23	0/1094	0.49	0/1469
53	o2	0.24	0/1731	0.48	0/2352
54	s2	0.23	0/1517	0.48	0/2038
55	v2	0.24	0/843	0.44	0/1137
56	x2	0.25	0/1094	0.51	0/1460
57	y2	0.25	0/1161	0.52	0/1553
58	A3	0.23	0/1208	0.55	0/1618
59	B3	0.24	0/1122	0.48	0/1503
60	C3	0.23	0/817	0.53	0/1097
61	D3	0.26	0/645	0.50	0/863
62	E3	0.25	0/1116	0.51	0/1490
63	F3	0.25	0/828	0.55	0/1109
64	G3	0.24	0/508	0.59	0/680
65	H3	0.25	0/466	0.51	0/618
66	I3	0.24	0/2493	0.50	0/3394
67	J3	0.25	0/1762	0.47	0/2382
68	K3	0.24	0/1863	0.53	0/2481
69	L3	0.24	0/1550	0.53	0/2069
70	M3	0.23	$\overline{0/952}$	0.42	0/1278
71	N3	0.23	0/1232	0.47	0/1656
72	O3	0.25	0/1015	0.53	0/1361
73	P3	0.25	0/1051	0.52	0/1406
74	Q3	0.24	0/1066	0.50	0/1415



Mol Chain		Bond	lengths	Bond angles		
MOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
75	R3	0.24	0/604	0.50	0/810	
76	S3	0.24	0/665	0.49	0/890	
77	Τ3	0.25	0/443	0.54	0/582	
78	U3	0.25	0/515	0.50	0/682	
79	m	0.25	0/6756	0.47	0/9122	
80	j	0.24	0/1530	0.46	0/2064	
81	k	0.23	0/1173	0.49	0/1581	
82	А	0.23	0/493	0.51	0/655	
83	t	0.25	0/1499	0.47	0/2007	
84	u	0.24	0/1715	0.52	0/2287	
85	L1	0.24	0/1686	0.49	0/2262	
All	All	0.24	0/241045	0.69	40/352704~(0.0%)	

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
46	m2	624	C	N3-C2-O2	-8.27	116.11	121.90
46	m2	1149	С	N3-C2-O2	-8.18	116.18	121.90
9	A2	260	С	N3-C2-O2	-7.97	116.32	121.90
9	A2	822	С	N3-C2-O2	-7.77	116.46	121.90
9	A2	1893	С	C2-N1-C1'	7.24	126.77	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	ntiles
1	A1	221/270~(82%)	214 (97%)	7 (3%)	0	100	100
2	B1	227/266~(85%)	220 (97%)	7 (3%)	0	100	100
3	C1	188/192~(98%)	185 (98%)	3 (2%)	0	100	100
4	D1	204/214~(95%)	201 (98%)	3 (2%)	0	100	100
5	E1	172/178~(97%)	167 (97%)	5 (3%)	0	100	100
6	F1	205/211~(97%)	194 (95%)	11 (5%)	0	100	100
7	G1	137/217~(63%)	133 (97%)	4 (3%)	0	100	100
8	H1	201/204~(98%)	198 (98%)	3 (2%)	0	100	100
12	D2	249/257~(97%)	234 (94%)	15 (6%)	0	100	100
13	E2	400/403~(99%)	397 (99%)	3 (1%)	0	100	100
14	F2	364/419~(87%)	359~(99%)	5 (1%)	0	100	100
15	G2	291/297~(98%)	284 (98%)	7 (2%)	0	100	100
16	H2	215/296~(73%)	208 (97%)	7 (3%)	0	100	100
17	I2	199/203~(98%)	195 (98%)	4 (2%)	0	100	100
18	J2	151/184~(82%)	146 (97%)	5 (3%)	0	100	100
19	K2	184/188~(98%)	181 (98%)	3 (2%)	0	100	100
20	L2	182/196~(93%)	181 (100%)	1 (0%)	0	100	100
21	M2	173/176~(98%)	166 (96%)	7 (4%)	0	100	100
22	N2	157/160~(98%)	155 (99%)	2 (1%)	0	100	100
23	O2	99/128~(77%)	97~(98%)	2 (2%)	0	100	100
24	P2	127/140~(91%)	125 (98%)	2 (2%)	0	100	100
25	Q2	106/157~(68%)	104 (98%)	2 (2%)	0	100	100
26	R2	116/156~(74%)	114 (98%)	2 (2%)	0	100	100
27	S2	132/145~(91%)	131 (99%)	1 (1%)	0	100	100
28	Τ2	133/136~(98%)	131 (98%)	2 (2%)	0	100	100
29	U2	145/148~(98%)	139 (96%)	6 (4%)	0	100	100
30	V2	115/160~(72%)	110 (96%)	5 (4%)	0	100	100
31	W2	92/115 (80%)	86 (94%)	6 (6%)	0	100	100
32	X2	105/125~(84%)	104 (99%)	1 (1%)	0	100	100
33	Y2	126/135~(93%)	125 (99%)	1 (1%)	0	100	100
34	Z2	107/110~(97%)	106 (99%)	1 (1%)	0	100	100
35	a2	112/117~(96%)	110 (98%)	2 (2%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
36	b2	118/123~(96%)	115 (98%)	3 (2%)	0	100	100
37	c2	100/105~(95%)	97 (97%)	3 (3%)	0	100	100
38	d2	84/97~(87%)	82 (98%)	2 (2%)	0	100	100
39	e2	67/70~(96%)	67 (100%)	0	0	100	100
40	f2	48/51~(94%)	45 (94%)	3 (6%)	0	100	100
41	g2	49/128~(38%)	48 (98%)	1 (2%)	0	100	100
42	h2	22/25~(88%)	22 (100%)	0	0	100	100
43	i2	101/106~(95%)	95 (94%)	6 (6%)	0	100	100
44	j2	87/92~(95%)	83 (95%)	4 (5%)	0	100	100
45	k2	123/137~(90%)	119 (97%)	4 (3%)	0	100	100
48	p2	212/264~(80%)	210 (99%)	2 (1%)	0	100	100
49	q2	224/243~(92%)	217 (97%)	7 (3%)	0	100	100
50	r2	260/263~(99%)	252 (97%)	8 (3%)	0	100	100
51	w2	151/158~(96%)	144 (95%)	7 (5%)	0	100	100
52	z2	132/135~(98%)	128 (97%)	4 (3%)	0	100	100
53	02	212/295~(72%)	211 (100%)	1 (0%)	0	100	100
54	s2	187/204~(92%)	182 (97%)	5 (3%)	0	100	100
55	v2	95/165~(58%)	93 (98%)	2 (2%)	0	100	100
56	x2	128/145~(88%)	124 (97%)	3 (2%)	1 (1%)	19	54
57	y2	142/146~(97%)	139 (98%)	3 (2%)	0	100	100
58	A3	142/152~(93%)	138 (97%)	4 (3%)	0	100	100
59	B3	139/145~(96%)	139 (100%)	0	0	100	100
60	C3	100/119~(84%)	97 (97%)	3 (3%)	0	100	100
61	D3	81/83~(98%)	80 (99%)	1 (1%)	0	100	100
62	E3	139/143~(97%)	135 (97%)	4 (3%)	0	100	100
63	F3	99/115~(86%)	98 (99%)	1 (1%)	0	100	100
64	G3	62/69~(90%)	61 (98%)	1 (2%)	0	100	100
65	H3	52/56~(93%)	50 (96%)	2 (4%)	0	100	100
66	I3	311/317~(98%)	295 (95%)	16 (5%)	0	100	100
67	J3	220/293~(75%)	217 (99%)	3 (1%)	0	100	100
68	K3	$\overline{225/249}~(90\%)$	223 (99%)	2 (1%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
69	L3	183/194~(94%)	181~(99%)	2(1%)	0	100	100
70	M3	120/132~(91%)	114 (95%)	6 (5%)	0	100	100
71	N3	148/151~(98%)	144 (97%)	4 (3%)	0	100	100
72	O3	132/151~(87%)	126 (96%)	6 (4%)	0	100	100
73	P3	127/130~(98%)	124 (98%)	3 (2%)	0	100	100
74	Q3	127/133~(96%)	122 (96%)	5 (4%)	0	100	100
75	R3	73/125~(58%)	73 (100%)	0	0	100	100
76	S3	81/84~(96%)	80~(99%)	1 (1%)	0	100	100
77	T3	53/133~(40%)	50 (94%)	3 (6%)	0	100	100
78	U3	60/156~(38%)	59~(98%)	1 (2%)	0	100	100
79	m	846/858~(99%)	823~(97%)	23 (3%)	0	100	100
80	j	194/317~(61%)	191 (98%)	3 (2%)	0	100	100
81	k	151/165~(92%)	144 (95%)	6 (4%)	1 (1%)	22	57
82	А	57/386~(15%)	57~(100%)	0	0	100	100
83	t	179/194~(92%)	174 (97%)	5 (3%)	0	100	100
84	u	204/208~(98%)	195 (96%)	9 (4%)	0	100	100
85	L1	204/217~(94%)	187 (92%)	16 (8%)	1 (0%)	29	64
All	All	12686/14730~(86%)	12350 (97%)	333 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
81	k	147	HIS
56	x2	108	LYS
85	L1	207	LYS

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 analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	A1	194/234~(83%)	194 (100%)	0	100	100
2	B1	198/223~(89%)	197 (100%)	1 (0%)	88	94
3	C1	169/171~(99%)	168 (99%)	1 (1%)	86	94
4	D1	177/180~(98%)	174 (98%)	3 (2%)	60	83
5	E1	147/149~(99%)	142 (97%)	5 (3%)	37	69
6	F1	174/178~(98%)	169 (97%)	5(3%)	42	72
7	G1	118/157~(75%)	118 (100%)	0	100	100
8	H1	171/172~(99%)	168 (98%)	3 (2%)	59	82
12	D2	193/199~(97%)	190 (98%)	3 (2%)	62	84
13	E2	347/348~(100%)	341 (98%)	6 (2%)	60	83
14	F2	307/347~(88%)	303 (99%)	4 (1%)	69	87
15	G2	245/249~(98%)	245 (100%)	0	100	100
16	H2	198/256~(77%)	196 (99%)	2 (1%)	76	90
17	I2	172/173~(99%)	169 (98%)	3 (2%)	60	83
18	J2	134/164~(82%)	133 (99%)	1 (1%)	84	93
19	K2	164/165~(99%)	164 (100%)	0	100	100
20	L2	163/175~(93%)	160 (98%)	3 (2%)	59	82
21	M2	155/156~(99%)	154 (99%)	1 (1%)	86	94
22	N2	138/139~(99%)	136 (99%)	2 (1%)	67	86
23	O2	91/114~(80%)	91 (100%)	0	100	100
24	P2	100/107~(94%)	99 (99%)	1 (1%)	76	90
25	Q2	90/126~(71%)	89 (99%)	1 (1%)	73	89
26	R2	106/133~(80%)	106 (100%)	0	100	100
27	S2	124/135~(92%)	121 (98%)	3 (2%)	49	76
28	Τ2	117/118~(99%)	117 (100%)	0	100	100
29	U2	120/121~(99%)	119 (99%)	1 (1%)	81	92
30	V2	98/124 (79%)	95 (97%)	3 (3%)	40	70
31	W2	79/97~(81%)	78 (99%)	1 (1%)	69	87
32	X2	98/110~(89%)	97~(99%)	1 (1%)	76	90
33	Y2	114/121~(94%)	113 (99%)	1 (1%)	78	91
34	Z2	88/89~(99%)	86 (98%)	2 (2%)	50	77
35	a2	98/100~(98%)	96 (98%)	2 (2%)	55	80



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
36	b2	108/110~(98%)	108 (100%)	0	100	100	
37	c2	86/90~(96%)	85~(99%)	1 (1%)	71	88	
38	d2	73/80~(91%)	72 (99%)	1 (1%)	67	86	
39	e2	64/65~(98%)	64 (100%)	0	100	100	
40	f2	47/48~(98%)	47 (100%)	0	100	100	
41	g2	47/115 (41%)	46 (98%)	1 (2%)	53	79	
42	h2	23/24~(96%)	23 (100%)	0	100	100	
43	i2	91/94~(97%)	86 (94%)	5 (6%)	21	53	
44	j2	73/75~(97%)	71 (97%)	2(3%)	44	74	
45	k2	109/121~(90%)	107 (98%)	2 (2%)	59	82	
48	p2	195/229~(85%)	195 (100%)	0	100	100	
49	q2	189/202~(94%)	186 (98%)	3 (2%)	62	84	
50	r2	224/225~(100%)	221 (99%)	3 (1%)	69	87	
51	w2	137/142~(96%)	134 (98%)	3 (2%)	52	78	
52	z2	120/121~(99%)	118 (98%)	2 (2%)	60	83	
53	o2	179/242~(74%)	179 (100%)	0	100	100	
54	s2	159/170~(94%)	158 (99%)	1 (1%)	86	94	
55	v2	88/136~(65%)	86 (98%)	2(2%)	50	77	
56	x2	116/130~(89%)	113 (97%)	3(3%)	46	74	
57	y2	119/121~(98%)	118 (99%)	1 (1%)	81	92	
58	A3	125/132~(95%)	123 (98%)	2 (2%)	62	84	
59	B3	112/115~(97%)	109 (97%)	3 (3%)	44	74	
60	C3	93/107~(87%)	92 (99%)	1 (1%)	73	89	
61	D3	67/67~(100%)	67 (100%)	0	100	100	
62	E3	113/115~(98%)	112 (99%)	1 (1%)	78	91	
63	F3	88/98~(90%)	84 (96%)	4 (4%)	27	60	
64	G3	57/62~(92%)	57 (100%)	0	100	100	
65	H3	48/49~(98%)	47 (98%)	1 (2%)	53	79	
66	I3	272/275~(99%)	264 (97%)	8 (3%)	42	72	
67	J3	188/224~(84%)	185 (98%)	3 (2%)	62	84	
68	K3	198/218~(91%)	195 (98%)	3 (2%)	65	85	



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
69	L3	161/168~(96%)	156~(97%)	5 (3%)	40	70	
70	M3	102/108~(94%)	102 (100%)	0	100	100	
71	N3	130/131~(99%)	130 (100%)	0	100	100	
72	O3	104/119~(87%)	101 (97%)	3(3%)	42	72	
73	P3	112/113~(99%)	111 (99%)	1 (1%)	78	91	
74	Q3	111/115~(96%)	111 (100%)	0	100	100	
75	R3	66/103~(64%)	66~(100%)	0	100	100	
76	S3	75/76~(99%)	73~(97%)	2(3%)	44	74	
77	T3	45/106~(42%)	44 (98%)	1 (2%)	52	78	
78	U3	55/140~(39%)	51 (93%)	4 (7%)	14	43	
79	m	725/729~(100%)	711~(98%)	14 (2%)	57	81	
80	j	164/255~(64%)	160 (98%)	4 (2%)	49	76	
81	k	126/137~(92%)	121 (96%)	5 (4%)	31	65	
82	А	52/304~(17%)	52~(100%)	0	100	100	
83	t	164/174~(94%)	160 (98%)	4 (2%)	49	76	
84	u	178/180~(99%)	$1\overline{74} (98\%)$	4 (2%)	52	78	
85	L1	187/197~(95%)	181 (97%)	6 (3%)	39	69	
All	All	11052/12487~(88%)	10884 (98%)	168 (2%)	66	85	

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
69	L3	3	VAL
79	m	745	LEU
69	L3	175	ARG
78	U3	138	ARG
81	k	70	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
67	J3	267	GLN
69	L3	111	GLN
74	Q3	94	HIS
73	P3	91	ASN



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Mol	Chain	Res	Type
61	D3	35	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B2	119/121~(98%)	16 (13%)	0
11	C2	155/156~(99%)	28 (18%)	2(1%)
46	m2	$1715/1871 \ (91\%)$	385~(22%)	0
47	n2	74/75~(98%)	24 (32%)	0
9	A2	3676/4731~(77%)	784 (21%)	13~(0%)
All	All	5739/6954~(82%)	1237~(21%)	15~(0%)

5 of 1237 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A2	2	G
9	A2	25	А
9	A2	39	А
9	A2	42	А
9	A2	48	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A2	2382	С
11	C2	59	А
9	A2	2430	G
11	C2	83	С
9	A2	4351	U

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

101 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).



Mol	Type	Chain	Bog	Link	В	ond leng	gths	Bond angles		
	туре	Chan	Ites		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	OMU	m2	116	46	19,22,23	3.00	8 (42%)	26,31,34	1.61	4 (15%)
9	B8T	A2	4135	9	19,22,23	<mark>3.26</mark>	8 (42%)	26,31,34	0.85	<mark>1 (3%)</mark>
9	UR3	A2	1668	9	19,22,23	<mark>3.19</mark>	7 (36%)	26,32,35	1.35	3 (11%)
9	6MZ	A2	3872	9	$18,\!25,\!26$	1.83	3 (16%)	16,36,39	1.86	2 (12%)
9	UR3	A2	4249	9	19,22,23	3.14	7 (36%)	26,32,35	1.27	<mark>3 (11%)</mark>
46	PSU	m2	614	46	18,21,22	4.33	6 (33%)	22,30,33	2.70	6 (27%)
9	A2M	A2	3523	9	18,25,26	2.67	10 (55%)	18,36,39	1.85	4 (22%)
9	PSU	A2	3385	9	18,21,22	4.35	6 (33%)	22,30,33	2.76	5 (22%)
9	B8W	A2	3837	9	18,26,27	<mark>6.03</mark>	9 (50%)	21,38,41	<mark>3.31</mark>	9 (42%)
9	5MC	A2	4099	9	18,22,23	3.56	7 (38%)	26,32,35	1.03	1 (3%)
9	OMU	A2	4272	9	19,22,23	3.00	8 (42%)	26,31,34	1.66	4 (15%)
9	PSU	A2	4280	9	18,21,22	4.37	6 (33%)	22,30,33	2.74	5 (22%)
9	A2M	A2	3379	9	18,25,26	2.63	9 (50%)	18,36,39	1.87	4 (22%)
9	PSU	A2	3420	9	18,21,22	4.35	6 (33%)	22,30,33	2.63	5 (22%)
9	G7M	A2	2277	9	20,26,27	3.97	9 (45%)	17,39,42	1.12	1 (5%)
9	A2M	A2	4223	9	18,25,26	2.64	9 (50%)	18,36,39	1.89	4 (22%)
9	OMC	A2	3357	9	19,22,23	3.02	8 (42%)	26,31,34	0.71	0
9	A2M	A2	3481	9	18,25,26	2.64	9 (50%)	18,36,39	1.89	4 (22%)
46	A2M	m2	1033	46	18,25,26	2.64	9 (50%)	18,36,39	1.84	4 (22%)
46	A2M	m2	27	46	18,25,26	2.65	10 (55%)	18,36,39	1.82	3 (16%)
46	UR3	m2	1832	46	19,22,23	3.15	7 (36%)	26,32,35	1.32	2 (7%)
9	PSU	A2	4183	9	18,21,22	4.37	6 (33%)	22,30,33	2.84	<mark>5 (22%)</mark>
9	OMU	A2	3958	9	19,22,23	2.98	8 (42%)	26,31,34	1.71	5 (19%)
46	PSU	m2	824	46	18,21,22	4.37	6 (33%)	22,30,33	2.72	5 (22%)
9	A2M	A2	1337	9	18,25,26	2.63	9 (50%)	18,36,39	1.83	4 (22%)
9	A2M	A2	1347	9	18,25,26	2.73	10 (55%)	18,36,39	1.92	4 (22%)
9	E7G	A2	1599	9	24,27,28	<mark>3.74</mark>	10 (41%)	30,40,43	2.23	10 (33%)
9	PSU	A2	4102	9	18,21,22	4.34	6 (33%)	22,30,33	2.73	5 (22%)
46	PSU	m2	1245	46	18,21,22	4.38	6 (33%)	22,30,33	2.71	<mark>5 (22%)</mark>
46	PSU	m2	1083	46	18,21,22	4.35	6 (33%)	22,30,33	2.76	5 (22%)
9	OMC	A2	4188	9	19,22,23	3.01	8 (42%)	26,31,34	0.79	0
9	OMG	A2	1852	9	18,26,27	2.58	8 (44%)	19,38,41	1.49	4 (21%)
9	A2M	A2	1140	9	18,25,26	2.67	10 (55%)	18,36,39	1.92	4 (22%)
9	OMG	A2	2528	9	18,26,27	2.61	8 (44%)	19,38,41	1.52	4 (21%)
9	PSU	A2	1395	9	18,21,22	4.37	7 (38%)	22,30,33	2.69	5 (22%)



Mal	Turne	Chain	Dec	Tink	В	ond leng	gths	Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
9	PSU	A2	4152	9	18,21,22	<mark>4.39</mark>	7 (38%)	22,30,33	2.81	<mark>5 (22%)</mark>
9	I4U	A2	3846	9	$21,\!24,\!25$	4.74	16 (76%)	27,34,37	1.08	1 (3%)
46	4AC	m2	1844	46	$21,\!24,\!25$	3.67	9 (42%)	29,34,37	1.10	<mark>3 (10%)</mark>
9	MHG	A2	4023	9	29,32,33	4.05	10 (34%)	34,46,49	2.55	12 (35%)
14	MLZ	F2	333	14	8,9,10	0.71	0	4,9,11	0.92	0
9	PSU	A2	4094	9	18,21,22	4.41	7 (38%)	22,30,33	2.75	<u>6 (27%)</u>
9	A2M	A2	2118	9	18,25,26	2.64	10 (55%)	18,36,39	1.81	4 (22%)
46	A2M	m2	670	46	$18,\!25,\!26$	2.69	10 (55%)	18,36,39	1.82	4 (22%)
9	OMG	A2	4275	9	$18,\!26,\!27$	2.60	8 (44%)	19,38,41	1.53	4 (21%)
9	E6G	A2	4007	9	20,27,28	5.76	8 (40%)	22,39,42	2.06	<u>6 (27%)</u>
9	OMC	A2	3565	9	19,22,23	<mark>3.05</mark>	8 (42%)	26,31,34	0.81	0
9	B9B	A2	237	9	21,28,29	<mark>5.60</mark>	8 (38%)	23,40,43	1.97	5 (21%)
9	OMG	A2	4022	43,9	18,26,27	<mark>2.59</mark>	8 (44%)	19,38,41	1.50	4 (21%)
9	2MG	A2	4517	9,7	18,26,27	2.14	6 (33%)	16,38,41	1.40	4 (25%)
9	PSU	A2	1496	9	18,21,22	4.34	6 (33%)	22,30,33	2.79	5 (22%)
9	B9H	A2	2541	9	20,25,26	2.93	5 (25%)	22,35,38	1.63	4 (18%)
9	OMC	A2	2177	9	19,22,23	<mark>3.03</mark>	8 (42%)	26,31,34	0.96	1 (3%)
9	A2M	A2	1673	9	18,25,26	2.62	9 (50%)	18,36,39	1.92	4 (22%)
46	B8N	m2	1250	46	24,29,30	2.47	5 (20%)	29,42,45	1.84	<mark>6 (20%)</mark>
9	B9B	A2	1387	9	21,28,29	<mark>5.62</mark>	8 (38%)	23,40,43	1.91	<mark>6 (26%)</mark>
46	OMG	m2	646	46	18,26,27	2.61	8 (44%)	19,38,41	1.49	4 (21%)
9	I4U	A2	1472	9	21,24,25	4.74	16 (76%)	27,34,37	1.16	2 (7%)
9	OMG	A2	4146	9	18,26,27	2.60	8 (44%)	19,38,41	1.50	4 (21%)
11	OMU	C2	14	11	19,22,23	3.04	8 (42%)	26,31,34	1.70	4 (15%)
9	1MA	A2	4067	9	16,25,26	<mark>3.96</mark>	3 (18%)	18,37,40	1.67	3 (16%)
9	OMG	A2	1438	9	18,26,27	2.59	8 (44%)	19,38,41	1.56	4 (21%)
9	G7M	A2	1418	9	20,26,27	<mark>3.97</mark>	9 (45%)	17,39,42	1.14	1 (5%)
9	2MG	A2	1330	9	18,26,27	<mark>2.17</mark>	6 (33%)	16,38,41	1.39	4 (25%)
9	OMG	A2	4289	9,32	18,26,27	2.59	7 (38%)	19,38,41	1.49	3 (15%)
9	OMG	A2	2119	9	18,26,27	2.58	8 (44%)	19,38,41	1.53	4 (21%)
9	PSU	A2	3371	9	18,21,22	4.34	6 (33%)	22,30,33	2.69	6 (27%)
46	PSU	m2	825	46	18,21,22	4.37	7 (38%)	22,30,33	2.78	5 (22%)
9	OMG	A2	1685	9,33	18,26,27	2.60	8 (44%)	19,38,41	1.55	4 (21%)
9	OMC	A2	2120	9	19,22,23	3.02	7 (36%)	26,31,34	1.02	3 (11%)
9	5MC	A2	3438	9	18,22,23	3.61	7 (38%)	26,32,35	0.98	1 (3%)



Mol	Type	Chain	Res	Link	В	ond leng	gths	Bond angles			
	-390		1005		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
9	OMG	A2	3448	9	18,26,27	2.59	8 (44%)	19,38,41	1.50	4 (21%)	
9	A2M	A2	3374	9	18,25,26	2.64	9 (50%)	18,36,39	1.86	4 (22%)	
9	A2M	A2	3441	9	18,25,26	2.77	9 (50%)	18,36,39	1.85	3 (16%)	
9	B8Q	A2	1269	9	17,22,23	3.10	4 (23%)	22,32,35	1.98	6 (27%)	
9	E7G	A2	2052	9	24,27,28	3.72	10 (41%)	30,40,43	2.22	9 (30%)	
9	OMC	A2	3543	9,17	19,22,23	<mark>3.03</mark>	8 (42%)	26,31,34	0.84	0	
9	OMG	A2	3848	9	18,26,27	2.60	8 (44%)	19,38,41	1.50	4 (21%)	
9	G7M	A2	4202	9	20,26,27	3.97	9 (45%)	17,39,42	1.12	1 (5%)	
79	DDE	m	714	79	14,20,21	2.00	3 (21%)	14,28,30	1.53	2 (14%)	
9	A2M	A2	398	9	18,25,26	2.63	9 (50%)	18,36,39	1.89	4 (22%)	
9	PSU	A2	2263	9	18,21,22	4.38	6 (33%)	22,30,33	2.67	5 (22%)	
9	OMG	A2	1335	9	18,26,27	2.60	8 (44%)	19,38,41	1.56	4 (21%)	
9	OMG	A2	4515	9,7	18,26,27	2.58	8 (44%)	19,38,41	1.53	4 (21%)	
9	PSU	A2	4055	9	18,21,22	4.36	6 (33%)	22,30,33	2.76	6 (27%)	
9	P7G	A2	3536	9	24,28,29	4.01	10 (41%)	27,41,44	1.52	2 (7%)	
41	MLZ	g2	98	41	8,9,10	0.70	0	4,9,11	0.90	0	
9	PSU	A2	4288	9,32	18,21,22	4.36	7 (38%)	22,30,33	2.74	5 (22%)	
9	OMG	A2	373	9	18,26,27	2.59	8 (44%)	19,38,41	1.51	4 (21%)	
9	OMG	A2	2179	9	18,26,27	2.61	8 (44%)	19,38,41	1.50	4 (21%)	
46	OMG	m2	685	46	18,26,27	2.60	8 (44%)	19,38,41	1.49	4 (21%)	
9	OMC	A2	3525	9	19,22,23	3.01	8 (42%)	26,31,34	0.74	0	
46	OMC	m2	519	46	19,22,23	3.05	8 (42%)	26,31,34	0.90	1 (3%)	
9	OMC	A2	2559	9	19,22,23	3.01	8 (42%)	26,31,34	0.73	0	
9	5MC	A2	3987	9	18,22,23	<mark>3.59</mark>	7 (38%)	26,32,35	1.04	2 (7%)	
9	PSU	A2	1490	9	18,21,22	4.36	6 (33%)	22,30,33	2.78	6 (27%)	
46	A2M	m2	166	46	18,25,26	2.65	9 (50%)	18,36,39	1.93	4 (22%)	
9	2MG	A2	878	9	18,26,27	2.16	6 (33%)	16,38,41	1.34	3 (18%)	
9	OMC	A2	2616	9	19,22,23	3.07	8 (42%)	26,31,34	0.90	1 (3%)	
9	P7G	A2	1711	9,10	24,28,29	4.09	10 (41%)	27,41,44	1.44	2 (7%)	
9	PSU	A2	3945	9	18,21,22	4.32	6 (33%)	22,30,33	2.77	5 (22%)	
9	A2M	A2	2156	9	18,25,26	2.66	9 (50%)	18,36,39	1.85	4 (22%)	

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
46	OMU	m2	116	46	-	1/9/27/28	0/2/2/2
9	B8T	A2	4135	9	-	0/7/27/28	0/2/2/2
9	UR3	A2	1668	9	-	2/7/25/26	0/2/2/2
9	6MZ	A2	3872	9	-	5/5/27/28	0/3/3/3
9	UR3	A2	4249	9	-	0/7/25/26	0/2/2/2
46	PSU	m2	614	46	-	0/7/25/26	0/2/2/2
9	A2M	A2	3523	9	-	3/5/27/28	0/3/3/3
9	PSU	A2	3385	9	-	2/7/25/26	0/2/2/2
9	B8W	A2	3837	9	-	2/5/27/28	0/3/3/3
9	5MC	A2	4099	9	-	4/7/25/26	0/2/2/2
9	OMU	A2	4272	9	-	1/9/27/28	0/2/2/2
9	PSU	A2	4280	9	-	0/7/25/26	0/2/2/2
9	A2M	A2	3379	9	-	1/5/27/28	0/3/3/3
9	PSU	A2	3420	9	-	2/7/25/26	0/2/2/2
9	G7M	A2	2277	9	-	0/3/25/26	0/3/3/3
9	A2M	A2	4223	9	-	1/5/27/28	0/3/3/3
9	OMC	A2	3357	9	-	5/9/27/28	0/2/2/2
9	A2M	A2	3481	9	-	1/5/27/28	0/3/3/3
46	A2M	m2	1033	46	-	1/5/27/28	0/3/3/3
46	A2M	m2	27	46	-	1/5/27/28	0/3/3/3
46	UR3	m2	1832	46	-	4/7/25/26	0/2/2/2
9	PSU	A2	4183	9	-	1/7/25/26	0/2/2/2
9	OMU	A2	3958	9	-	3/9/27/28	0/2/2/2
46	PSU	m2	824	46	-	3/7/25/26	0/2/2/2
9	A2M	A2	1337	9	-	0/5/27/28	0/3/3/3
9	A2M	A2	1347	9	-	2/5/27/28	0/3/3/3
9	E7G	A2	1599	9	-	1/9/39/40	0/3/3/3
9	PSU	A2	4102	9	-	3/7/25/26	0/2/2/2
46	PSU	m2	1245	46	-	3/7/25/26	0/2/2/2
46	PSU	m2	1083	46	-	1/7/25/26	0/2/2/2
9	OMC	A2	4188	9	-	0/9/27/28	0/2/2/2
9	OMG	A2	1852	9	-	0/5/27/28	0/3/3/3
9	A2M	A2	1140	9	-	1/5/27/28	0/3/3/3
9	OMG	A2	2528	9	-	2/5/27/28	0/3/3/3
9	PSU	A2	1395	9	-	2/7/25/26	0/2/2/2
9	PSU	A2	4152	9	-	4/7/25/26	0/2/2/2
9	I4U	A2	3846	9	-	2/9/29/30	0/2/2/2
46	4AC	m2	1844	46	-	0/11/29/30	0/2/2/2
9	MHG	A2	4023	9	-	4/16/46/47	0/3/3/3



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MLZ	F2	333	14	-	1/7/8/10	-
9	PSU	A2	4094	9	-	0/7/25/26	0/2/2/2
9	A2M	A2	2118	9	-	0/5/27/28	0/3/3/3
46	A2M	m2	670	46	-	1/5/27/28	0/3/3/3
9	OMG	A2	4275	9	-	0/5/27/28	0/3/3/3
9	E6G	A2	4007	9	-	3/6/28/29	0/3/3/3
9	OMC	A2	3565	9	-	0/9/27/28	0/2/2/2
9	B9B	A2	237	9	-	6/7/29/30	0/3/3/3
9	OMG	A2	4022	43,9	-	0/5/27/28	0/3/3/3
9	2MG	A2	4517	9,7	-	0/5/27/28	0/3/3/3
9	PSU	A2	1496	9	-	0/7/25/26	0/2/2/2
9	B9H	A2	2541	9	-	0/12/47/48	0/2/2/2
9	OMC	A2	2177	9	-	5/9/27/28	0/2/2/2
9	A2M	A2	1673	9	-	0/5/27/28	0/3/3/3
46	B8N	m2	1250	46	-	4/16/34/35	0/2/2/2
9	B9B	A2	1387	9	-	3/7/29/30	0/3/3/3
46	OMG	m2	646	46	-	2/5/27/28	0/3/3/3
9	I4U	A2	1472	9	-	0/9/29/30	0/2/2/2
9	OMG	A2	4146	9	-	0/5/27/28	0/3/3/3
11	OMU	C2	14	11	-	1/9/27/28	0/2/2/2
9	1MA	A2	4067	9	-	2/3/25/26	0/3/3/3
9	OMG	A2	1438	9	-	3/5/27/28	0/3/3/3
9	G7M	A2	1418	9	-	0/3/25/26	0/3/3/3
9	2MG	A2	1330	9	-	0/5/27/28	0/3/3/3
9	OMG	A2	4289	9,32	-	2/5/27/28	0/3/3/3
9	OMG	A2	2119	9	-	2/5/27/28	0/3/3/3
9	PSU	A2	3371	9	-	0/7/25/26	0/2/2/2
46	PSU	m2	825	46	-	0/7/25/26	0/2/2/2
9	OMG	A2	1685	9,33	-	2/5/27/28	0/3/3/3
9	OMC	A2	2120	9	-	0/9/27/28	0/2/2/2
9	5MC	A2	3438	9	-	2/7/25/26	0/2/2/2
9	OMG	A2	3448	9	-	0/5/27/28	0/3/3/3
9	A2M	A2	3374	9	-	1/5/27/28	0/3/3/3
9	A2M	A2	3441	9	-	2/5/27/28	0/3/3/3
9	B8Q	A2	1269	9	-	0/7/42/43	0/2/2/2
9	E7G	A2	2052	9	-	4/9/39/40	0/3/3/3
9	OMC	A2	3543	9,17	-	3/9/27/28	0/2/2/2
9	OMG	A2	3848	9	-	0/5/27/28	0/3/3/3
9	G7M	A2	4202	9	_	0/3/25/26	0/3/3/3



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
79	DDE	m	714	79	-	7/20/21/23	0/1/1/1
9	A2M	A2	398	9	-	3/5/27/28	0/3/3/3
9	PSU	A2	2263	9	-	0/7/25/26	0/2/2/2
9	OMG	A2	1335	9	-	0/5/27/28	0/3/3/3
9	OMG	A2	4515	9,7	-	1/5/27/28	0/3/3/3
9	PSU	A2	4055	9	-	0/7/25/26	0/2/2/2
9	P7G	A2	3536	9	-	3/10/40/41	0/3/3/3
41	MLZ	g2	98	41	-	1/7/8/10	-
9	PSU	A2	4288	9,32	-	6/7/25/26	0/2/2/2
9	OMG	A2	373	9	-	1/5/27/28	0/3/3/3
9	OMG	A2	2179	9	-	3/5/27/28	0/3/3/3
46	OMG	m2	685	46	-	2/5/27/28	0/3/3/3
9	OMC	A2	3525	9	-	0/9/27/28	0/2/2/2
46	OMC	m2	519	46	-	4/9/27/28	0/2/2/2
9	OMC	A2	2559	9	-	0/9/27/28	0/2/2/2
9	5MC	A2	3987	9	-	1/7/25/26	0/2/2/2
9	PSU	A2	1490	9	-	3/7/25/26	0/2/2/2
46	A2M	m2	166	46	-	3/5/27/28	0/3/3/3
9	2MG	A2	878	9	-	2/5/27/28	0/3/3/3
9	OMC	A2	2616	9	-	0/9/27/28	0/2/2/2
9	P7G	A2	1711	9,10	-	1/10/40/41	0/3/3/3
9	PSU	A2	3945	9	-	2/7/25/26	0/2/2/2
9	A2M	A2	2156	9	-	2/5/27/28	0/3/3/3

The worst 5 of 772 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3837	B8W	O4'-C1'	19.05	1.67	1.41
9	A2	1387	B9B	C2'-C1'	-15.85	1.29	1.53
9	A2	4007	E6G	O4'-C1'	15.81	1.63	1.41
9	A2	237	B9B	O4'-C1'	15.69	1.63	1.41
9	A2	4007	E6G	C2'-C1'	-15.65	1.30	1.53

The worst 5 of 378 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
9	A2	4023	MHG	C2-N3-C4	7.95	121.90	112.04
9	A2	3837	B8W	O6-C6-N1	7.88	129.96	119.03
9	A2	4183	PSU	N1-C2-N3	7.55	123.68	115.13



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\mathbf{Mol}	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
9	A2	3837	B8W	N2-C2-N3	7.54	130.08	117.79
9	A2	4152	PSU	N1-C2-N3	7.42	123.53	115.13

There are no chirality outliers.

5 of 162 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	g2	98	MLZ	C-CA-CB-CG
79	m	714	DDE	O-C-CA-CB
79	m	714	DDE	CA-CB-CG-ND1
79	m	714	DDE	NAD-CBI-CBW-NCB
79	m	714	DDE	CAT-CAU-CBW-CBI

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)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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

Mal	Type	Chain	Dog	Link	B	ond leng	gths	Bond angles		
MOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
88	GDP	m	900	-	24,30,30	3.45	14 (58%)	30,47,47	1.46	6 (20%)

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
88	GDP	m	900	-	-	5/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	m	900	GDP	O4'-C1'	7.73	1.51	1.41
88	m	900	GDP	O4'-C4'	-6.00	1.31	1.45
88	m	900	GDP	C2-N3	5.56	1.46	1.33
88	m	900	GDP	C3'-C4'	5.44	1.66	1.53
88	m	900	GDP	C4-N3	4.88	1.49	1.37

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
88	m	900	GDP	C5-C6-N1	3.37	119.90	113.95
88	m	900	GDP	C8-N7-C5	3.23	109.14	102.99
88	m	900	GDP	PA-O3A-PB	-2.98	122.59	132.83
88	m	900	GDP	C2-N1-C6	-2.85	119.85	125.10
88	m	900	GDP	O6-C6-C5	-2.24	120.00	124.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	m	900	GDP	C5'-O5'-PA-O1A
88	m	900	GDP	C5'-O5'-PA-O2A
88	m	900	GDP	PB-O3A-PA-O2A
88	m	900	GDP	C5'-O5'-PA-O3A
88	m	900	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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-23501. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 384



Y Index: 384



Z Index: 384

6.2.2 Raw map



X Index: 384

Y Index: 384



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: 390



Y Index: 376



Z Index: 375

6.3.2 Raw map



X Index: 390

Y Index: 376



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 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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 1947 nm^3 ; this corresponds to an approximate mass of 1759 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 0.323 ${\rm \AA}^{-1}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.323 ${\rm \AA}^{-1}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.71	3.14
Unmasked-calculated*	3.70	4.85	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 3.1 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23501 and PDB model 7LS2. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 4.0 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)

This section was not generated.

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 (4.0).



9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8184
А	0.4705
A1	0.7782
A2	0.8968
A3	0.7118
B1	0.7881
B2	0.9543
B3	0.7435
C1	0.7799
C2	0.9041
C3	0.7137
D1	0.7735
D2	0.7594
D3	0.7781
E1	0.7677
E2	0.7827
E3	0.6947
F1	0.8063
F2	0.7789
F3	0.7426
G1	0.8208
G2	0.8278
G3	0.5947
H1	0.8019
H2	0.8040
H3	0.7472
I2	0.7933
I3	0.7378
J2	0.8093
J3	0.7493
K2	0.7849
K3	0.6940
L1	0.5417
L2	0.7776
L3	0.7304





Chain	Atom inclusion
M2	0.8197
M3	0.5301
N2	0.7910
N3	0.7253
O2	0.7559
O3	0.7061
P2	0.7265
P3	0.7228
Q2	0.7206
Q3	0.6742
R2	0.7830
R3	0.6792
S2	0.8006
S3	0.7297
T2	0.8155
Τ3	0.6974
U2	0.8142
U3	0.6829
V2	0.7272
W2	0.7944
X2	0.7888
Y2	0.7797
Z2	0.8147
a2	0.7791
b2	0.7756
c2	0.8063
d2	0.7875
e2	0.7230
f2	0.7612
g2	0.7890
h2	0.7033
i2	0.7772
j	0.7266
j2	0.7556
k	0.6280
k2	0.8347
m	0.7038
m2	0.8857
n2	0.8429
02	0.7725
p2	0.7020
q2	0.7122


Chain	Atom inclusion
r2	0.7156
s2	0.6481
t	0.7166
u	0.6785
v2	0.7152
w2	0.6799
x2	0.7064
y2	0.7118
z2	0.7152

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