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PDB ID	:	7Q08
EMDB ID	:	EMD-13741
Title	:	Structure of Candida albicans 80S ribosome in complex with cycloheximide
Authors	:	Zgadzay, Y.; Kolosova, O.; Stetsenko, A.; Jenner, L.; Guskov, A.; Yusupova,
		G.; Yusupov, M.
Deposited on	:	2021-10-14
Resolution	:	2.56 Å(reported)
This is	a I	Full wwPDB EM Validation 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 following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev 8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 2.56 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	1	3359	78%	17% • •
2	3	121	94%	6%
3	4	158	84%	16%
4	j	254	98%	•
5	k	389	99%	·
6	1	363	99%	
7	m	298	98%	·
8	n	176	88%	12%

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Mol	Chain	Length	Quality of chain	
9	0	241	97%	•
10	р	262	91%	9%
11	q	191	99%	
12	r	220	95%	5%
13	s	174	98%	
14	t	202	98%	•••
15	u	131	98%	•••
16	V	204	100%	
17	W	200	100%	
18	х	185	93%	7%
19	У	186	99%	·
20	Z	190	94%	6%
21	0	172	99%	·
22	2	160	99%	••
23	5	124	81% •	17%
24	6	137	96%	•
25	7	155	40% • 59%	
26	8	142	85%	15%
27	9	127	98%	
28	AA	136	99%	·
29	AB	149	99%	·
30	AC	63	100%	
31	AD	106	91%	9%
32	AE	112	97%	·
33	AF	131	95%	5%

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Mol	Chain	Length	Quality of chain	
34	AG	107	99%	·
35	AH	122	92%	8%
36	AI	120	99%	•
37	AJ	99	98%	••
38	AK	90	94%	••
39	AL	78	99%	•
40	AM	51	98%	٠
41	AN	52	100%	
42	AO	25	92%	• •
43	AP	106	96%	••
44	AQ	92	99%	·
45	i	267	42% 58%	
46	А	1787	6 9% 26%	5%
46 47	A B	1787 261	69% 26% 80%	5%
46 47 48	A B C	1787 261 256	69% 26% 80% 82% ·	5% 20% 16%
46 47 48 49	A B C D	1787 261 256 249	69% 26% 80% 82% • 86%	5% 20% 16% 13%
46 47 48 49 50	A B C D E	1787 261 256 249 251	69% 26% 80% 80% 69% 82% 14% 88%	5% 20% 16% 13% 11%
$ \begin{array}{r} 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 51 \\ \end{array} $	A B C D E F	1787 261 256 249 251 262	69% 26% 80% 80% 82% 86% 14% 88% 99%	5% 20% 16% 13% 11%
$ \begin{array}{r} 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 51 \\ 52 \\ \end{array} $	A B C D E F G	1787 261 256 249 251 262 225	69% 26% 80% 80% 82% 86% 14% 88% 99% 13% 92%	5% 20% 16% 13% 11%
$ \begin{array}{r} 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 51 \\ 52 \\ 53 \\ \end{array} $	A B C D E F G H	1787 261 256 249 251 262 225 236	69% 26% 80% 80% 82% 86% 14% 99% 13% 92% 5% 96% 110/	5% 20% 16% 13% 11%
$ \begin{array}{r} 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 51 \\ 52 \\ 53 \\ 54 \\ \end{array} $	A B C D E F G H I	1787 261 256 249 251 262 225 236 186	69% 26% 80% 80% 82% • 86% 14% 99% 13% 92% 5% 96% 11% 97% 11%	5% 20% 16% 13% 11%
$ \begin{array}{r} 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 51 \\ 52 \\ 53 \\ 54 \\ 55 \\ \end{array} $	A B C D E F G H I J	1787 261 256 249 251 262 225 236 186 206	69% 26% 80% 80% 82% . 86% . 14% 88% 99% . 13% 92% 5% 96% 11% 97% 11% 98%	5% 20% 16% 13% 11%
$ \begin{array}{r} 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 51 \\ 52 \\ 53 \\ 54 \\ 55 \\ 56 \\ \end{array} $	A B C D E F G H I J K	1787 261 256 249 251 262 225 236 186 206 189	69% 26% 80% 80% 82% 14% 88% 99% 14% 99% 13% 99% 5% 96% 11% 97% 11% 98% 5% 98%	5% 20% 16% 13% 11%
$ \begin{array}{r} 46 \\ 47 \\ 48 \\ 49 \\ 50 \\ 51 \\ 52 \\ 53 \\ 54 \\ 55 \\ 56 \\ 57 \\ \end{array} $	A B C D E F G H I J K L	1787 261 256 249 251 262 225 236 186 206 189 118	69% 26% 80% 80% 82% 82% 88% 14% 99% 13% 99% 13% 92% 5% 92% 5% 96% 11% 98% 5% 96% 11% 98% 5%	5% 20% 16% 13% 11%

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Mol	Chain	Length	Quality of chain	
59	Ν	143	62%	19%
60	0	151	99%	••
61	Р	132	95%	• •
62	Q	142	83%	17%
63	R	142	99%	
64	S	137	91%	• 9%
65	Т	145	98%	·
66	U	145	9%	·
67	V	119	9% 82% •	16%
68	W	87	• 100%	
69	Х	130	98%	••
70	Y	145	99%	•
71	Z	135	98%	·
72	a	105	29% 69% 31%	
73	b	119	84%	16%
74	с	82	5% 99%	
75	d	67	93%	7%
76	е	56	98%	·
77	f	63	11% 89%	11%
78	g	193	26% 36% • 64%	
79	h	317	25% 97%	•••



2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 199280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues			AltConf	Trace			
1	1	3209	Total 68595	C 30642	N 12317	O 22427	Р 3209	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	3	121	Total 2579	C 1153	N 463	0 842	Р 121	0	0

• Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	158	Total 3353	C 1500	N 585	O 1110	Р 158	0	0

• Molecule 4 is a protein called Ribosomal 60S subunit protein L2A.

Mol	Chain	Residues	Atoms				AltConf	Trace	
4	j	249	Total 1894	C 1185	N 377	O 330	${S \over 2}$	1	0

• Molecule 5 is a protein called Ribosomal 60S subunit protein L3.

Mol	Chain	Residues	Atoms				AltConf	Trace	
5	k	386	Total 3084	$\begin{array}{c} \mathrm{C} \\ 1955 \end{array}$	N 584	O 538	S 7	1	0

• Molecule 6 is a protein called Ribosomal 60S subunit protein L4B.

Mol	Chain	Residues		At	oms			AltConf	Trace
6	1	361	Total 2751	C 1729	N 529	0 490	${ m S} { m 3}$	0	0



• Molecule 7 is a protein called Ribosomal 60S subunit protein L5.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	m	292	Total 2394	C 1526	N 416	0 450	${S \over 2}$	0	0

• Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
8	n	155	Total 1237	C 794	N 226	O 217	1	0

• Molecule 9 is a protein called Ribosomal 60S subunit protein L7A.

Mol	Chain	Residues		Ate		AltConf	Trace		
9	О	234	Total 1893	C 1213	N 348	0 331	S 1	1	0

• Molecule 10 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
10	р	238	Total 1839	C 1175	N 327	0 334	${ m S} { m 3}$	0	0

• Molecule 11 is a protein called Ribosomal 60S subunit protein L9B.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	q	190	Total 1519	C 958	N 276	0 281	${S \atop 4}$	0	0

• Molecule 12 is a protein called Ribosomal 60S subunit protein L10.

Mol	Chain	Residues		At	AltConf	Trace			
12	r	208	Total 1689	C 1069	N 322	0 291	$\frac{S}{7}$	0	0

• Molecule 13 is a protein called Ribosomal 60S subunit protein L11B.

Mol	Chain	Residues		At	oms			AltConf	Trace
13	S	172	Total 1385	C 864	N 262	O 255	${S \atop 4}$	1	0

• Molecule 14 is a protein called 60S ribosomal protein L13.



Mol	Chain	Residues		Ator	AltConf	Trace		
14	t	200	Total 1610	C 1009	N 318	O 283	0	0

• Molecule 15 is a protein called Ribosomal 60S subunit protein L14B.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	u	130	Total 1029	C 660	N 193	0 175	S 1	0	0

• Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues		Ate	AltConf	Trace			
16	v	203	Total 1713	C 1075	N 356	0 280	$\frac{S}{2}$	0	0

• Molecule 17 is a protein called Ribosomal 60S subunit protein L16A.

Mol	Chain	Residues		Ate		AltConf	Trace		
17	W	199	Total 1590	C 1025	N 294	O 269	${ m S} { m 2}$	0	0

• Molecule 18 is a protein called Ribosomal 60S subunit protein L17B.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
18	x	172	Total 1375	C 850	N 279	O 246	0	0

• Molecule 19 is a protein called Ribosomal 60S subunit protein L18A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
19	У	185	Total	C 030	N 302	0 246	3	0
19	У	185	1478	930	302	246	3	

• Molecule 20 is a protein called Ribosomal protein L19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
20	Z	179	Total 1462	C 904	N 311	0 244	${ m S} { m 3}$	1	0

• Molecule 21 is a protein called 60S ribosomal protein L20.



Mol	Chain	Residues		At	oms	AltConf	Trace		
21	0	171	Total 1442	C 933	N 262	0 244	${ m S} { m 3}$	2	0

• Molecule 22 is a protein called Ribosomal 60S subunit protein L21A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	2	159	Total 1276	C 807	N 244	0 223	${S \over 2}$	2	0

• Molecule 23 is a protein called Ribosomal 60S subunit protein L22B.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
23	5	103	Total 848	C 553	N 139	O 156	2	0

• Molecule 24 is a protein called Ribosomal 60S subunit protein L23B.

Mol	Chain	Residues		At	AltConf	Trace			
24	6	131	Total 986	C 621	N 186	0 171	S 8	1	0

• Molecule 25 is a protein called Ribosomal 60S subunit protein L24A.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
25	7	63	Total 524	C 334	N 103	O 86	S 1	0	0

• Molecule 26 is a protein called Ribosomal 60S subunit protein L25.

Mol	Chain	Residues		At	oms	AltConf	Trace		
26	8	121	Total 974	C 622	N 175	0 176	S 1	0	0

• Molecule 27 is a protein called Ribosomal 60S subunit protein L26B.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
27	9	126	Total 989	C 618	N 190	O 181	0	0

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



Mol	Chain	Residues		At	oms			AltConf	Trace
28	AA	135	Total 1087	C 705	N 197	O 183	${ m S} { m 2}$	0	0

• Molecule 29 is a protein called Ribosomal 60S subunit protein L28.

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	AB	148	Total 1170	С 741	N 231	O 197	S 1	0	0

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

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
30	AC	63	Total 509	C 317	N 109	O 82	S 1	1	0

• Molecule 31 is a protein called Ribosomal 60S subunit protein L30.

Mol	Chain	Residues		At	oms	AltConf	Trace		
31	AD	96	Total 729	C 469	N 121	0 137	${S \over 2}$	0	0

• Molecule 32 is a protein called Ribosomal 60S subunit protein L31B.

Mol	Chain	Residues		At	oms			AltConf	Trace
32	AE	109	Total 889	C 562	N 167	0 158	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 33 is a protein called Ribosomal 60S subunit protein L32.

Mol	Chain	Residues		At	oms	AltConf	Trace		
33	AF	125	Total 1015	C 649	N 197	0 168	S 1	1	0

• Molecule 34 is a protein called Ribosomal 60S subunit protein L33A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
34	AG	106	Total 867	C 558	N 166	0 142	S 1	3	0

• Molecule 35 is a protein called Ribosomal 60S subunit protein L34B.



Mol	Chain	Residues		At	oms	AltConf	Trace		
35	AH	112	Total 913	$\begin{array}{c} \mathrm{C} \\ 567 \end{array}$	N 188	O 154	$\frac{S}{4}$	4	0

• Molecule 36 is a protein called Ribosomal 60S subunit protein L35A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
36	AI	119	Total 990	C 629	N 195	O 166	1	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
37	AJ	98	Total 772	C 481	N 158	0 131	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	1	0

• Molecule 38 is a protein called Ribosomal protein L37.

Mol	Chain	Residues		At	oms	AltConf	Trace		
38	AK	86	Total 677	C 413	N 148	0 110	S 6	0	0

• Molecule 39 is a protein called Ribosomal 60S subunit protein L38.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
39	AL	77	Total 623	C 398	N 116	O 109	1	0

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

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
40	AM	50	Total 446	C 280	N 100	O 66	1	0

• Molecule 41 is a protein called Rpl40bp.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
41	AN	52	Total 427	C 265	N 89	O 67	S 6	1	0

• Molecule 42 is a protein called 60S ribosomal protein eL41.



Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
42	AO	24	Total 227	C 138	N 61	O 27	S 1	0	0

• Molecule 43 is a protein called Ribosomal 60S subunit protein L42A.

Mol	Chain	Residues		At	oms			AltConf	Trace
43	AP	103	Total 843	C 533	N 168	0 137	${ m S}{ m 5}$	2	0

• Molecule 44 is a protein called Ribosomal 60S subunit protein L43A.

Mol	Chain	Residues		At	oms			AltConf	Trace
44	AQ	91	Total 698	$\begin{array}{c} \mathrm{C} \\ 430 \end{array}$	N 140	0 124	${s \over 4}$	0	0

• Molecule 45 is a protein called HABP4_PAI-RBP1 domain-containing protein.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
45	i	113	Total 853	C 512	N 155	0 186	0	0

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

Mol	Chain	Residues		1	Atoms			AltConf	Trace
46	А	1692	Total 36083	C 16130	N 6412	O 11849	Р 1692	0	0

• Molecule 47 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues		At	oms			AltConf	Trace
47	В	208	Total 1627	C 1041	N 284	O 297	${f S}{5}$	0	0

• Molecule 48 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues		At	oms			AltConf	Trace
48	С	214	Total 1724	C 1094	N 313	0 313	$\frac{S}{4}$	0	0

• Molecule 49 is a protein called Ribosomal 40S subunit protein S2.



Mol	Chain	Residues		At	oms			AltConf	Trace
49	D	216	Total 1620	C 1033	N 287	O 295	${ m S}{ m 5}$	0	0

• Molecule 50 is a protein called Ribosomal 40S subunit protein S3.

Mol	Chain	Residues		Ate	AltConf	Trace			
50	Е	223	Total 1707	C 1087	N 311	O 305	$\frac{S}{4}$	0	0

• Molecule 51 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues		Ate	AltConf	Trace			
51	F	260	Total 2055	C 1306	N 386	O 358	${ m S}{ m 5}$	0	0

• Molecule 52 is a protein called Ribosomal 40S subunit protein S5.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
52	G	206	Total 1614	C 1008	N 301	O 301	${S \atop 4}$	0	0

• Molecule 53 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues		At	oms			AltConf	Trace
53	Н	226	Total 1820	C 1133	N 351	O 330	S 6	0	0

• Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
54	Ι	182	Total 1466	C 939	N 264	O 263	0	0

• Molecule 55 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues		At	AltConf	Trace			
55	J	203	Total 1579	C 973	N 322	0 283	S 1	0	0

• Molecule 56 is a protein called Ribosomal 40S subunit protein S9B.



Mol	Chain	Residues		At	oms			AltConf	Trace
56	K	178	Total 1453	C 918	N 286	0 248	S 1	0	0

• Molecule 57 is a protein called Ribosomal 40S subunit protein S10A.

Mol	Chain	Residues		At	oms			AltConf	Trace
57	L	93	Total 783	C 511	N 129	0 142	S 1	0	0

• Molecule 58 is a protein called Ribosomal 40S subunit protein S11A.

Mol	Chain	Residues		At	oms			AltConf	Trace
58	М	141	Total 1129	С 722	N 212	0 192	${ m S} { m 3}$	0	0

• Molecule 59 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues		At	oms			AltConf	Trace
59	Ν	116	Total 885	C 550	N 158	O 172	${S \over 5}$	0	0

• Molecule 60 is a protein called Ribosomal 40S subunit protein S13.

Mol	Chain	Residues		At	oms			AltConf	Trace
60	О	150	Total 1187	C 757	N 219	0 210	S 1	0	0

• Molecule 61 is a protein called Ribosomal 40S subunit protein S14B.

Mol	Chain	Residues		At	oms			AltConf	Trace
61	Р	127	Total 942	$\begin{array}{c} \mathrm{C} \\ 579 \end{array}$	N 186	0 174	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Р	119	IAS	ASP	modified residue	UNP A0A1D8PDT3

• Molecule 62 is a protein called Ribosomal 40S subunit protein S15.



Mol	Chain	Residues		At	oms			AltConf	Trace
62	Q	118	Total 935	C 598	N 169	O 162	S 6	0	0

• Molecule 63 is a protein called Ribosomal 40S subunit protein S16A.

Mol	Chain	Residues		At	oms			AltConf	Trace
63	R	140	Total 1091	C 700	N 198	0 192	S 1	0	0

• Molecule 64 is a protein called Ribosomal 40S subunit protein S17B.

Mol	Chain	Residues		At	oms			AltConf	Trace
64	S	125	Total 1002	C 631	N 184	0 186	S 1	0	0

• Molecule 65 is a protein called Ribosomal 40S subunit protein S18B.

Mol	Chain	Residues		At	oms	AltConf	Trace		
65	Т	142	Total	C 722	N 228	0 205	S 2	0	0
			1109	199	220	200	5		

• Molecule 66 is a protein called Ribosomal 40S subunit protein S19A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
66	U	141	Total 1100	C 689	N 210	O 200	S 1	0	0

• Molecule 67 is a protein called Ribosomal 40S subunit protein S20.

Mol	Chain	Residues		At	oms	AltConf	Trace		
67	V	100	Total 790	C 499	N 146	0 143	${ m S} { m 2}$	0	0

• Molecule 68 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues		At	AltConf	Trace			
68	W	87	Total 676	C 415	N 126	0 133	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 69 is a protein called 40S ribosomal protein S22-A.



Mol	Chain	Residues		At	AltConf	Trace			
69	X	129	Total 1032	$\begin{array}{c} \mathrm{C} \\ 655 \end{array}$	N 191	O 183	${ m S} { m 3}$	0	0

• Molecule 70 is a protein called Ribosomal 40S subunit protein S23B.

Mol	Chain	Residues		At	AltConf	Trace			
70	Y	143	Total	C 701	N 210	0	S	0	0
			1110	701	219	199	Ζ		

• Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
71	Z	132	Total 1072	C 670	N 216	O 186	0	0

• Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
72	a	72	Total 578	C 369	N 103	O 106	0	0

• Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues		At	AltConf	Trace			
73	b	100	Total 799	C 494	N 169	O 130	S 6	0	0

• Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues		At	AltConf	Trace			
74	С	81	Total 614	C 383	N 110	0 114	${f S}7$	0	0

• Molecule 75 is a protein called Ribosomal 40S subunit protein S28B.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
75	d	62	Total 487	C 299	N 98	O 88	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 76 is a protein called Ribosomal 40S subunit protein S29A.



Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
76	е	55	Total 454	C 281	N 94	O 75	${f S}$ 4	0	0

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

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
77	f	56	Total 444	C 278	N 89	0 75	$\frac{S}{2}$	0	0

• Molecule 78 is a protein called Ubiquitin-ribosomal 40S subunit protein S31 fusion protein.

Mol	Chain	Residues		Ate	\mathbf{oms}			AltConf	Trace
78	g	70	Total 574	C 362	N 113	O 93	S 6	0	0

• Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms		AltConf	Trace			
79	h	311	Total 2398	C 1519	N 412	0 462	${ m S}{ m 5}$	0	0

• Molecule 80 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
80	1	1	Total C N 10 7 3	0



• Molecule 81 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidi ne-2,6-dione (three-letter code: 3HE) (formula: C₁₅H₂₃NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	A	Aton	ns		AltConf
81	1	1	Total 20	C 15	N 1	0 4	0

• Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
82	AK	1	Total Zn 1 1	0
82	AN	1	Total Zn 1 1	0
82	AP	1	Total Zn 1 1	0
82	AQ	1	Total Zn 1 1	0
82	b	1	Total Zn 1 1	0
82	с	1	Total Zn 1 1	0
82	е	1	Total Zn 1 1	0
82	g	1	Total Zn 1 1	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: 25S ribosomal RNA







- Full wwPDB EM Validation Report • Molecule 4: Ribosomal 60S subunit protein L2A Chain j: 98% LYS THR ALA GLII • Molecule 5: Ribosomal 60S subunit protein L3 Chain k: 99% • Molecule 6: Ribosomal 60S subunit protein L4B Chain l: 99% • Molecule 7: Ribosomal 60S subunit protein L5 Chain m: 98% ALA GLN GLN GLU PRC PRC • Molecule 8: 60S ribosomal protein L6 Chain n: 88% 12% SER SER SER SER SER SER SER SER ALA ALA ALA ALA SER CLU CLU SER CLU CLU SER CLU CLU SER CLU MET • Molecule 9: Ribosomal 60S subunit protein L7A Chain o: 97% MET ALA THR THR LEU LYS PRO E8 E8 E8 C10 C10 C110
- Molecule 10: 60S ribosomal protein L8

Chain p:	91%	9%



MET PRO CLYS CLYS CLYS CLYS CLYS CLYS PRO PRO PRO ALA ALA ALA ALA ALA ALA ALA SER SER SER SER SER SER SER SER SER SER	V258 2261 3261
• Molecule 11: Ribosomal 60S subun	it protein L9B
Chain q:	99% .
E190	
• Molecule 12: Ribosomal 60S subuni	it protein L10
Chain r:	95% 5%
MET A2 A2 A10 EEU ALA ALA ALA GLN GLN GLN GLN GLN ALA ALA	
• Molecule 13: Ribosomal 60S subuni	it protein L11B
Chain s:	98%
MET 22 22 22 22 22 22 22 22 22 22 22 22 22	
• Molecule 14: 60S ribosomal protein	L13
Chain t:	98%
MET 13 84 85 85 85 85 85 81 86 81 178 178 178 178 178 178 178 178 178	
• Molecule 15: Ribosomal 60S subuni	it protein L14B
Chain u:	98% •••
NET S 2 2 2 4 1 3 4 1 3 1 4 1 3	
• Molecule 16: Ribosomal protein L1	5
Chain v:	100%
MET 22 8204	

• Molecule 17: Ribosomal 60S subunit protein L16A



Chain w:	100%	
MET 22 4200		
• Molecule 18: Ribosomal	60S subunit protein L17B	
Chain x:	93%	7%
MET V2 E153 ASP ASP ASP ASP ASP ASP CIU CIU CIU CIU CIU CIU CIU CIU CIU CIA AI84 AI84		
• Molecule 19: Ribosomal	60S subunit protein L18A	
Chain y:	99%	
MET 62 V186		
• Molecule 20: Ribosomal	protein L19	
Chain z:	94%	6%
MET A2 E152 Q175 Q175 Q175 C129 C178 C178 C178 C178 C178 C178 C178 C178	ALA ASN	
• Molecule 21: 60S ribosor	nal protein L20	
Chain 0:	99%	
MET 22 172 172		
• Molecule 22: Ribosomal	60S subunit protein L21A	
Chain 2:	99%	
MBT 60 1160 1160		
• Molecule 23: Ribosomal	60S subunit protein L22B	
Chain 5:	81%	• 17%
MET PICA PALA PALA PALA VAL CYS CYS CYS CYS CYS A A A A A A A A A A A A A A A A A C A A C A A C A A C A A C C A C C A C C A C C A C		
• Molecule 24: Ribosomal	60S subunit protein L23B	



Chain 6:	96	%	·
MET SER SER SER GLY GLY ALA S7 V137			
• Molecule 25:	Ribosomal 60S subunit p	rotein L24A	
Chain 7:	40% ·	59%	-
M1 D25 SER GLU GLU GLU GLU LVS	ALYS ALYS THR ARG LLYS LLYS LLYS HLS ALL ALA ALA ALA ALA ALA ALA ALA CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV	LEU LYE LYE CLU CLU ARG ARG CLU ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	ASP LYS GLU ALA LYS LYS ALA
ALA LYS ALA ALA ALA ALA CLYS CLU CYS	ALA ALA ALA ALA ALA ALA ALA ALA ALA CLN CLN CLN CLN CLN CLN CLN CLN CCN CCN	LYS LYS ALA ALA SER ARG	
• Molecule 26:	Ribosomal 60S subunit pr	rotein L25	
Chain 8:	85%	15%	-
MET ALA PRO PRO LYS LYS ALA ALA ALA ALA ALA LYS	LYS ALA ALA LEU LEU CLYS GLY CLYS CLYS LYS LYS LYS 1142		
• Molecule 27:	Ribosomal 60S subunit p	rotein L26B	
Chain 9:	9	8%	
MET A2 K3 E1 27			
• Molecule 28:	60S ribosomal protein L2'	7	
Chain AA:		99%	·
MET A2 F136			
• Molecule 29:	Ribosomal 60S subunit pr	rotein L28	
Chain AB:		99%	·
NET P2 A149			
• Molecule 30:	60S ribosomal protein L2	9	
Chain AC:		100%	_
M1 S62 A63			
		WORLDWIDE PROTEIN DATA BANK	

• Molecule 3	31: Ribosomal 60S subunit protein L30	
Chain AD:	91%	9%
MET ALA PRO LYS SER ASN LYS ASN CLN	I 106	
• Molecule 3	32: Ribosomal 60S subunit protein L31B	
Chain AE:	97%	•
MET ALA L3 D110 D111 GLU		
• Molecule 3	33: Ribosomal 60S subunit protein L32	
Chain AF:	95%	5%
MET A2 K126 LEU ASN GLU ALA		
• Molecule 3	34: Ribosomal 60S subunit protein L33A	
Chain AG:	99%	•
MET A2 1107		
• Molecule 3	35: Ribosomal 60S subunit protein L34B	
Chain AH:	92%	8%
MET A2 D110 K113 LYS ALA ALA	LYS THR GLY LYS LYS	
• Molecule 3	36: Ribosomal 60S subunit protein L35A	
Chain AI:	99%	
MET A2 A120		
• Molecule 3	37: 60S ribosomal protein L36	
Chain AJ:	98%	
M1 R98 HIS		



• Molecule 38: Ribosomal protein L37
Chain AK: 94% · ·
MET 787 PR0 SER ALA
\bullet Molecule 39: Ribosomal 60S subunit protein L38
Chain AL: 99%
MET A33 L778 L778
\bullet Molecule 40: 60S ribosomal protein L39
Chain AM: 98%
• Molecule 41: Rpl40bp
Chain AN: 100%
There are no outlier residues recorded for this chain.
• Molecule 42: 60S ribosomal protein eL41
Chain AO: 92% · ·
\bullet Molecule 43: Ribosomal 60S subunit protein L42A
Chain AP: 96% ···
MET V2 L 104 GEN
\bullet Molecule 44: Ribosomal 60S subunit protein L43A
Chain AQ: 99%
MET 1 2 492 A 92
• Molecule 45: HABP4_PAI-RBP1 domain-containing protein







99%

TYR GLN GLN GLN GLU GLU GLU GLU VAL GLU VAL GLU VAL GLU VAL ALA ALA ALA ALA ALA

• Molecule 51: 40S ribosomal protein S4

Chain F:



• Molecule 52: Ribosomal 40S subunit protein S5











	•	٠	
M1	134	G48	R87
-			

• Molecule 69: 40S ribosomal protein S22-A

Chain X:	98%		•	
MET T2 L93 Y130				
• Molecule 70: 1	Ribosomal 40S subunit protein S23B			
Chain Y:	99%			
MET G2 B97 E101 P143 R144 SER				
• Molecule 71:	40S ribosomal protein S24			
Chain Z:	98%			
MET SER D3 A4 E46 K49 A50 A50	A80 E98 A39 A39 A39			
• Molecule 72:	40S ribosomal protein $S25$			
Chain a:	29%	31%		
MET ALA PRO PRO LYS CLN GLN GLN THR LYS ALA ALA	ALA ALA ALA ALA ALA ALA ALA ALA ALA CUS CUS CUS CUS CUS CUS CUS CUS CUS CUS	D43 044 E45 Y47 Y47 P48 B49 E48 B49 E150 L51 L51 L51 L51	V54 P55 T56 Y57	D67 R68 L69
R81 982 183 184 185 186 188 188 189	T90 F91 Y101 A104 Q105			
• Molecule 73:	40S ribosomal protein S26			
Chain b:	84%	16%	-	
MET P2 K101 ARG PHE THR SER ASP ASP LYS	SER PRO AGIN AIA ALA LYS LYS AIA ASN			
• Molecule 74:	40S ribosomal protein S27			
Chain c:	99%			



MET ALA ASP



• Molecule 75: Ribosomal 40S subunit protein S28B









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	3.339	Depositor
Minimum map value	-1.298	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.122	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	426.36002, 426.36002, 426.36002	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.836, 0.836, 0.836	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: SPD, IAS, OMG, ZN, OMC, 3HE, MLZ

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).

Mol	Chain	Bond lengths		Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	1	0.79	12/76718~(0.0%)	0.83	53/119600~(0.0%)	
2	3	0.67	0/2884	0.75	0/4492	
3	4	0.80	0/3746	0.78	0/5832	
4	j	0.41	0/1931	0.58	0/2592	
5	k	0.39	0/3156	0.55	0/4246	
6	1	0.36	0/2799	0.53	0/3777	
7	m	0.34	0/2447	0.50	0/3294	
8	n	0.35	0/1258	0.53	0/1696	
9	0	0.37	0/1929	0.52	0/2589	
10	р	0.34	0/1869	0.48	0/2519	
11	q	0.33	0/1537	0.53	0/2067	
12	r	0.36	0/1724	0.54	0/2314	
13	S	0.32	0/1404	0.56	0/1880	
14	t	0.37	0/1637	0.56	0/2195	
15	u	0.35	0/1044	0.53	0/1407	
16	V	0.46	0/1753	0.58	0/2347	
17	W	0.39	0/1620	0.51	0/2167	
18	Х	0.38	0/1398	0.55	0/1879	
19	У	0.37	0/1511	0.58	0/2022	
20	Z	0.34	0/1483	0.55	0/1972	
21	0	0.40	0/1483	0.54	0/1997	
22	2	0.39	0/1305	0.53	0/1749	
23	5	0.35	0/871	0.48	0/1175	
24	6	0.36	0/994	0.56	0/1339	
25	7	0.40	0/536	0.66	1/712~(0.1%)	
26	8	0.38	0/990	0.54	0/1337	
27	9	0.36	0/999	0.53	0/1334	
28	AA	0.37	0/1112	0.48	0/1488	
29	AB	0.40	0/1199	0.53	0/1607	
30	AC	0.32	0/522	0.51	$0/\overline{692}$	
31	AD	0.36	0/738	0.49	0/994	
32	AE	0.36	0/902	0.53	0/1212	


N /L = 1		B	ond lengths	E	Bond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
33	AF	0.40	0/1039	0.54	0/1390
34	AG	0.43	0/895	0.54	0/1201
35	AH	0.40	0/934	0.59	0/1242
36	AI	0.35	0/1004	0.57	0/1337
37	AJ	0.33	0/780	0.56	0/1033
38	AK	0.40	0/690	0.61	0/916
39	AL	0.33	0/632	0.52	0/842
40	AM	0.36	0/458	0.58	0/609
41	AN	0.33	0/436	0.55	0/577
42	AO	0.25	0/228	0.78	1/293~(0.3%)
43	AP	0.38	0/840	0.54	0/1108
44	AQ	0.38	0/705	0.59	0/940
45	i	0.25	0/864	0.49	0/1156
46	А	0.39	0/40362	0.84	17/62888~(0.0%)
47	В	0.28	0/1666	0.49	0/2273
48	С	0.26	0/1750	0.53	0/2354
49	D	0.30	0/1648	0.50	0/2237
50	Е	0.28	0/1731	0.55	0/2324
51	F	0.27	0/2096	0.53	0/2822
52	G	0.25	0/1631	0.51	0/2199
53	Н	0.26	0/1845	0.53	0/2464
54	Ι	0.27	0/1490	0.53	1/2004~(0.0%)
55	J	0.30	0/1606	0.58	0/2150
56	Κ	0.26	0/1478	0.54	0/1978
57	L	0.26	0/801	0.53	0/1081
58	М	0.31	0/1154	0.54	0/1553
59	Ν	0.25	0/892	0.59	0/1203
60	Ο	0.47	1/1210~(0.1%)	0.70	3/1631~(0.2%)
61	Р	0.28	0/944	0.59	0/1265
62	Q	0.28	0/954	0.57	0/1282
63	R	0.27	0/1109	0.52	0/1486
64	S	0.25	0/1014	0.54	0/1361
65	Т	0.26	0/1186	0.56	0/1590
66	U	0.26	0/1120	0.52	0/1508
67	V	0.26	0/800	0.53	0/1082
68	W	0.30	0/683	0.57	0/918
69	Х	0.29	0/1049	0.55	1/1412 (0.1%)
70	Y	0.30	0/1128	0.57	0/1505
71	Ζ	0.27	0/1086	0.57	0/1447
72	a	0.24	0/585	0.50	0/789
73	b	0.29	0/811	0.59	0/1085
74	с	0.26	0/624	0.51	0/843
75	d	0.25	0/489	0.64	0/654



Mol	Chain	B	ond lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
76	е	0.28	0/466	0.60	0/620	
77	f	0.28	0/451	0.56	0/601	
78	g	0.25	0/585	0.58	0/778	
79	h	0.25	0/2451	0.52	0/3337	
All	All	0.56	13/213899~(0.0%)	0.73	77/313891~(0.0%)	

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1737	А	O3'-P	-15.10	1.43	1.61
60	0	82	PRO	CG-CD	-12.21	1.10	1.50
1	1	209	С	O3'-P	11.48	1.75	1.61
1	1	1738	U	O3'-P	-7.21	1.52	1.61
1	1	1573	С	O3'-P	-6.63	1.53	1.61
1	1	1738	U	P-OP1	-6.39	1.38	1.49
1	1	482	U	C1'-N1	6.12	1.57	1.48
1	1	477	U	C1'-N1	6.11	1.57	1.48
1	1	1575	A	O3'-P	-5.96	1.53	1.61
1	1	483	U	C1'-N1	5.92	1.57	1.48
1	1	479	C	C1'-N1	5.46	1.56	1.48
1	1	476	С	C1'-N1	5.45	1.56	1.48
1	1	1738	U	P-OP2	-5.02	1.40	1.49

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$			
1	1	1263	U	OP2-P-O3'	-18.84	63.74	105.20			
46	А	822	G	P-O3'-C3'	15.77	138.62	119.70			
60	0	82	PRO	N-CD-CG	-15.47	79.99	103.20			
1	1	1017	G	P-O3'-C3'	13.46	135.85	119.70			
46	А	822	G	O3'-P-O5'	11.90	126.60	104.00			
1	1	1263	U	P-O3'-C3'	11.68	133.72	119.70			
1	1	1263	U	OP1-P-O3'	10.21	127.65	105.20			
1	1	1263	U	O3'-P-O5'	8.66	120.46	104.00			
1	1	1276	С	N3-C2-O2	-8.64	115.86	121.90			
60	0	82	PRO	CA-CB-CG	-8.56	87.74	104.00			
46	А	1375	С	C2-N1-C1'	8.05	127.66	118.80			
1	1	2215	С	N3-C2-O2	-8.00	116.30	121.90			
1	1	3182	С	C2-N1-C1'	7.50	127.05	118.80			
1	1	3126	U	C2-N1-C1'	7.36	126.53	117.70			
1	1	918	U	C2-N1-C1'	7.10	126.22	117.70			
60	0	82	PRO	CA-N-CD	-7.05	101.63	111.50			
	Continued on next page									

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Continucu	jiom	previous	puye

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	1	3182	С	N1-C2-O2	6.73	122.94	118.90
1	1	1273	С	N1-C2-O2	6.58	122.85	118.90
1	1	620	А	N1-C6-N6	6.55	122.53	118.60
1	1	1017	G	OP1-P-O3'	6.50	119.49	105.20
1	1	1273	С	N3-C2-O2	-6.49	117.36	121.90
1	1	437	G	N3-C4-N9	-6.35	122.19	126.00
1	1	2215	С	N1-C2-O2	6.33	122.70	118.90
54	Ι	30	LEU	CA-CB-CG	6.13	129.40	115.30
1	1	437	G	N3-C4-C5	6.10	131.65	128.60
1	1	1099	А	OP2-P-O3'	6.06	118.53	105.20
1	1	2814	U	N1-C2-O2	6.05	127.04	122.80
46	А	1462	С	C2-N1-C1'	5.93	125.32	118.80
46	А	1067	С	C2-N1-C1'	5.92	125.31	118.80
1	1	2814	U	C2-N1-C1'	5.80	124.66	117.70
25	7	25	ASP	CB-CG-OD1	5.77	123.49	118.30
1	1	620	А	C6-C5-N7	-5.76	128.27	132.30
1	1	1276	С	N1-C2-O2	5.74	122.34	118.90
1	1	3029	U	N3-C2-O2	-5.74	118.18	122.20
1	1	1575	А	O4'-C4'-C3'	-5.73	98.27	104.00
1	1	3182	С	N3-C2-O2	-5.72	117.90	121.90
1	1	1738	U	O5'-P-OP1	-5.62	100.64	105.70
1	1	620	A	C5-C6-N6	-5.61	119.21	123.70
1	1	1552	С	N1-C2-O2	5.61	122.27	118.90
46	А	1375	С	C6-N1-C1'	-5.59	114.09	120.80
46	А	561	U	N3-C2-O2	-5.51	118.34	122.20
1	1	406	G	O4'-C1'-N9	5.48	112.59	108.20
1	1	2235	С	N1-C2-O2	5.48	122.19	118.90
1	1	3243	С	N1-C2-O2	5.47	122.18	118.90
46	А	1375	С	N1-C2-O2	5.41	122.15	118.90
1	1	3182	С	C6-N1-C1'	-5.39	114.33	120.80
1	1	1720	U	O4'-C1'-N1	5.34	112.48	108.20
1	1	1737	A	OP1-P-O3'	5.33	116.94	105.20
1	1	3030	U	C2-N1-C1'	5.33	124.09	117.70
1	1	3245	A	O4'-C1'-N9	5.33	112.46	108.20
1	1	3134	C	C2-N1-C1'	5.30	124.63	118.80
1	1	2814	U	N3-C2-O2	-5.25	$118.5\overline{2}$	$122.\overline{20}$
1	1	1229	G	C4-N9-C1'	5.22	133.29	126.50
46	A	1345	A	N1-C2-N3	5.22	131.91	129.30
42	AO	3	ASP	CB-CG-OD2	5.20	122.98	118.30
1	1	2235	C	C2-N1-C1'	5.18	124.50	118.80
1	1	620	A	C4-C5-N7	5.17	113.29	110.70
46	А	985	C	C2-N1-C1'	5.16	124.47	118.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
46	А	1375	С	C6-N1-C2	-5.16	118.24	120.30
1	1	1099	A	P-O3'-C3'	5.15	125.88	119.70
69	Х	93	LEU	C-N-CA	-5.15	108.83	121.70
46	А	1523	G	N3-C4-C5	-5.13	126.04	128.60
1	1	918	U	N1-C2-O2	5.12	126.38	122.80
46	А	802	С	C2-N1-C1'	5.11	124.42	118.80
1	1	831	G	O4'-C1'-N9	5.11	112.28	108.20
1	1	3029	U	N1-C2-O2	5.10	126.37	122.80
1	1	1033	С	C2-N1-C1'	5.09	124.40	118.80
1	1	1492	С	C2-N1-C1'	5.09	124.40	118.80
1	1	1197	С	N1-C2-O2	5.09	121.95	118.90
1	1	2842	С	C6-N1-C1'	5.08	126.90	120.80
1	1	620	А	N9-C4-C5	-5.06	103.78	105.80
46	А	1369	G	P-O3'-C3'	5.05	125.76	119.70
46	А	822	G	OP2-P-O3'	-5.03	94.13	105.20
1	1	1276	С	C6-N1-C2	-5.02	118.29	120.30
46	А	451	С	N1-C2-O2	5.01	121.91	118.90
1	1	956	U	C2-N1-C1'	5.01	123.71	117.70
46	А	1231	С	C2-N1-C1'	5.00	124.30	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	Percentiles
4	j	248/254~(98%)	240~(97%)	8 (3%)	0	100 100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
5	k	385/389~(99%)	374 (97%)	11 (3%)	0	100	100
6	1	359/363~(99%)	350 (98%)	9 (2%)	0	100	100
7	m	290/298~(97%)	280 (97%)	10 (3%)	0	100	100
8	n	152/176~(86%)	149 (98%)	3 (2%)	0	100	100
9	О	233/241~(97%)	227 (97%)	6 (3%)	0	100	100
10	р	236/262~(90%)	232 (98%)	4 (2%)	0	100	100
11	q	188/191~(98%)	181 (96%)	7 (4%)	0	100	100
12	r	204/220~(93%)	198 (97%)	6 (3%)	0	100	100
13	S	171/174~(98%)	166 (97%)	5 (3%)	0	100	100
14	t	198/202~(98%)	193 (98%)	5 (2%)	0	100	100
15	u	128/131~(98%)	124 (97%)	4 (3%)	0	100	100
16	V	201/204~(98%)	196 (98%)	5 (2%)	0	100	100
17	W	197/200~(98%)	195 (99%)	2 (1%)	0	100	100
18	х	168/185~(91%)	167 (99%)	1 (1%)	0	100	100
19	У	186/186~(100%)	183 (98%)	3 (2%)	0	100	100
20	Z	178/190~(94%)	176 (99%)	2 (1%)	0	100	100
21	0	171/172~(99%)	170 (99%)	1 (1%)	0	100	100
22	2	159/160~(99%)	158 (99%)	1 (1%)	0	100	100
23	5	103/124~(83%)	89~(86%)	13 (13%)	1 (1%)	15	21
24	6	129/137~(94%)	128 (99%)	1 (1%)	0	100	100
25	7	61/155~(39%)	60 (98%)	1 (2%)	0	100	100
26	8	119/142~(84%)	118 (99%)	1 (1%)	0	100	100
27	9	124/127~(98%)	121 (98%)	3 (2%)	0	100	100
28	AA	133/136~(98%)	131 (98%)	2 (2%)	0	100	100
29	AB	146/149~(98%)	140 (96%)	6 (4%)	0	100	100
30	AC	62/63~(98%)	60 (97%)	2 (3%)	0	100	100
31	AD	94/106~(89%)	93 (99%)	1 (1%)	0	100	100
32	AE	107/112~(96%)	106 (99%)	1 (1%)	0	100	100
33	AF	124/131~(95%)	123 (99%)	1 (1%)	0	100	100
34	AG	107/107~(100%)	103 (96%)	4 (4%)	0	100	100
35	AH	$114/122$ ($\overline{93\%}$)	112 (98%)	2 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
36	AI	118/120~(98%)	113~(96%)	5 (4%)	0	100	100
37	AJ	97/99~(98%)	94~(97%)	3(3%)	0	100	100
38	AK	84/90~(93%)	81~(96%)	3~(4%)	0	100	100
39	AL	76/78~(97%)	74 (97%)	2(3%)	0	100	100
40	AM	49/51~(96%)	47~(96%)	2(4%)	0	100	100
41	AN	51/52~(98%)	51 (100%)	0	0	100	100
42	AO	22/25~(88%)	22 (100%)	0	0	100	100
43	AP	101/106~(95%)	99~(98%)	2 (2%)	0	100	100
44	AQ	89/92~(97%)	85 (96%)	4 (4%)	0	100	100
45	i	109/267~(41%)	104 (95%)	5 (5%)	0	100	100
47	В	206/261~(79%)	196~(95%)	10 (5%)	0	100	100
48	С	212/256~(83%)	203 (96%)	9 (4%)	0	100	100
49	D	214/249~(86%)	209~(98%)	5 (2%)	0	100	100
50	Е	221/251~(88%)	216 (98%)	5 (2%)	0	100	100
51	F	258/262~(98%)	251 (97%)	7 (3%)	0	100	100
52	G	204/225~(91%)	196 (96%)	8 (4%)	0	100	100
53	Н	224/236~(95%)	220 (98%)	4 (2%)	0	100	100
54	Ι	180/186~(97%)	174 (97%)	6 (3%)	0	100	100
55	J	201/206~(98%)	197~(98%)	4 (2%)	0	100	100
56	K	176/189~(93%)	169 (96%)	7 (4%)	0	100	100
57	L	91/118 (77%)	84 (92%)	6 (7%)	1 (1%)	14	19
58	М	139/155~(90%)	133~(96%)	6 (4%)	0	100	100
59	Ν	114/143~(80%)	93~(82%)	21 (18%)	0	100	100
60	О	148/151~(98%)	146 (99%)	2 (1%)	0	100	100
61	Р	123/132~(93%)	120 (98%)	3 (2%)	0	100	100
62	Q	116/142~(82%)	107~(92%)	9 (8%)	0	100	100
63	R	138/142~(97%)	134 (97%)	4 (3%)	0	100	100
64	S	123/137~(90%)	118 (96%)	5 (4%)	0	100	100
65	Т	$\overline{140/145}~(97\%)$	129 (92%)	11 (8%)	0	100	100
66	U	139/145~(96%)	135~(97%)	4 (3%)	0	100	100
67	V	98/119~(82%)	93~(95%)	5 (5%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
68	W	85/87~(98%)	80~(94%)	5~(6%)	0	100	100
69	Х	127/130~(98%)	125~(98%)	2(2%)	0	100	100
70	Y	141/145~(97%)	136 (96%)	5 (4%)	0	100	100
71	Z	130/135~(96%)	129 (99%)	1 (1%)	0	100	100
72	a	70/105~(67%)	68~(97%)	2(3%)	0	100	100
73	b	98/119~(82%)	95~(97%)	3(3%)	0	100	100
74	с	79/82~(96%)	75~(95%)	4(5%)	0	100	100
75	d	60/67~(90%)	55~(92%)	5 (8%)	0	100	100
76	е	53/56~(95%)	50 (94%)	3~(6%)	0	100	100
77	f	54/63~(86%)	53~(98%)	1 (2%)	0	100	100
78	g	68/193~(35%)	62~(91%)	6 (9%)	0	100	100
79	h	309/317~(98%)	292 (94%)	17 (6%)	0	100	100
All	All	11010/12138 (91%)	10656 (97%)	352 (3%)	2(0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	5	20	ALA
57	L	88	PRO

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
4	j	191/194~(98%)	191 (100%)	0	100	100
5	k	326/328~(99%)	326 (100%)	0	100	100
6	1	290/292~(99%)	289 (100%)	1 (0%)	92	96
7	m	247/252~(98%)	247~(100%)	0	100	100
8	n	135/154~(88%)	135~(100%)	0	100	100
9	0	199/204~(98%)	198 (100%)	1 (0%)	88	93



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
10	р	198/216~(92%)	198 (100%)	0	100	100
11	q	169/170~(99%)	169~(100%)	0	100	100
12	r	178/186~(96%)	178 (100%)	0	100	100
13	s	148/149~(99%)	147~(99%)	1 (1%)	84	90
14	t	166/168~(99%)	163~(98%)	3(2%)	59	73
15	u	108/109~(99%)	107~(99%)	1 (1%)	78	87
16	V	177/178~(99%)	177 (100%)	0	100	100
17	W	166/167~(99%)	166 (100%)	0	100	100
18	х	142/154~(92%)	142 (100%)	0	100	100
19	у	156/154~(101%)	156 (100%)	0	100	100
20	Z	147/153~(96%)	147 (100%)	0	100	100
21	0	158/157~(101%)	158 (100%)	0	100	100
22	2	135/134~(101%)	134 (99%)	1 (1%)	84	90
23	5	95/112~(85%)	94 (99%)	1 (1%)	73	83
24	6	101/103~(98%)	101 (100%)	0	100	100
25	7	57/127~(45%)	57~(100%)	0	100	100
26	8	108/121~(89%)	108 (100%)	0	100	100
27	9	111/112~(99%)	110 (99%)	1 (1%)	78	87
28	AA	117/118~(99%)	117~(100%)	0	100	100
29	AB	120/121~(99%)	120 (100%)	0	100	100
30	AC	50/49~(102%)	50 (100%)	0	100	100
31	AD	81/90~(90%)	81 (100%)	0	100	100
32	AE	98/100~(98%)	98 (100%)	0	100	100
33	AF	111/115~(96%)	111 (100%)	0	100	100
34	AG	94/92~(102%)	94 (100%)	0	100	100
35	AH	$\overline{99/102} (97\%)$	99 (100%)	0	100	100
36	AI	106/106~(100%)	106 (100%)	0	100	100
37	AJ	79/79~(100%)	78~(99%)	1 (1%)	69	80
38	AK	70/73~(96%)	69 (99%)	1 (1%)	67	78
39	AL	$\overline{69/69}~(100\%)$	69 (100%)	0	100	100
40	AM	47/47 (100%)	47 (100%)	0	100	100



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
41	AN	48/47~(102%)	48 (100%)	0	100	100
42	AO	23/24~(96%)	23~(100%)	0	100	100
43	AP	88/89~(99%)	86~(98%)	2(2%)	50	64
44	AQ	72/73~(99%)	72~(100%)	0	100	100
45	i	92/212~(43%)	92~(100%)	0	100	100
47	В	176/215~(82%)	176 (100%)	0	100	100
48	С	194/229~(85%)	191~(98%)	3 (2%)	65	77
49	D	174/198~(88%)	173~(99%)	1 (1%)	86	92
50	Е	174/196~(89%)	173~(99%)	1 (1%)	86	92
51	F	218/220~(99%)	218 (100%)	0	100	100
52	G	178/197~(90%)	178 (100%)	0	100	100
53	Н	195/204~(96%)	195 (100%)	0	100	100
54	Ι	163/167~(98%)	162 (99%)	1 (1%)	86	92
55	J	157/160~(98%)	156 (99%)	1 (1%)	86	92
56	K	153/160~(96%)	152 (99%)	1 (1%)	84	90
57	L	87/104 (84%)	87 (100%)	0	100	100
58	М	122/134~(91%)	121 (99%)	1 (1%)	81	88
59	Ν	98/123~(80%)	98 (100%)	0	100	100
60	Ο	129/130~(99%)	128 (99%)	1 (1%)	81	88
61	Р	96/101~(95%)	95~(99%)	1 (1%)	76	84
62	Q	102/121~(84%)	102 (100%)	0	100	100
63	R	114/116~(98%)	114 (100%)	0	100	100
64	S	112/122~(92%)	111 (99%)	1 (1%)	78	87
65	Т	126/129~(98%)	126 (100%)	0	100	100
66	U	113/117~(97%)	113 (100%)	0	100	100
67	V	90/105~(86%)	88~(98%)	2 (2%)	52	66
68	W	71/71 (100%)	71 (100%)	0	100	100
69	Х	112/113~(99%)	112 (100%)	0	100	100
70	Y	116/118~(98%)	116 (100%)	0	100	100
71	Ζ	109/112~(97%)	109 (100%)	0	100	100
72	a	64/85~(75%)	64 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
73	b	86/102~(84%)	86 (100%)	0	100 100
74	с	72/73~(99%)	72~(100%)	0	100 100
75	d	54/58~(93%)	54~(100%)	0	100 100
76	е	47/48~(98%)	47~(100%)	0	100 100
77	f	48/54~(89%)	48 (100%)	0	100 100
78	g	62/175~(35%)	61~(98%)	1 (2%)	62 76
79	h	259/263~(98%)	257 (99%)	2(1%)	81 88
All	All	9443/10220 (92%)	9412 (100%)	31 (0%)	92 96

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	l	99	ARG
9	0	13	LYS
13	s	13	ARG
14	t	4	SER
14	t	5	LYS
14	t	62	THR
15	u	23	ASN
22	2	83	ARG
23	5	30	GLN
27	9	3	LYS
37	AJ	98	ARG
38	AK	84	LYS
43	AP	24[A]	LYS
43	AP	24[B]	LYS
48	С	26	ARG
48	С	95	ASN
48	С	124	ASN
49	D	136	ARG
50	Е	77	ARG
54	Ι	75	ARG
55	J	125	LYS
56	К	69	ARG
58	М	67	ARG
60	0	82	PRO
61	Р	131	ARG
64	S	80	ARG
67	V	51	LYS
67	V	100	LYS



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Mol	Chain	Res	Type
78	g	122	ARG
79	h	121	ARG
79	h	226	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
7	m	94	ASN
18	Х	118	GLN
18	Х	120	ASN
21	0	8	GLN
47	В	30	GLN
47	В	33	ASN
52	G	63	GLN
52	G	116	HIS
54	Ι	19	GLN
54	Ι	48	ASN
54	Ι	167	GLN
62	Q	79	HIS
62	Q	103	ASN
68	W	74	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3205/3359~(95%)	567~(17%)	38~(1%)
2	3	120/121~(99%)	7~(5%)	0
3	4	157/158~(99%)	26 (16%)	2(1%)
46	А	1685/1787~(94%)	439 (26%)	44 (2%)
All	All	5167/5425~(95%)	1039 (20%)	84 (1%)

All (1039) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	24	U
1	1	25	А
1	1	29	G
1	1	39	А
1	1	42	А
1	1	48	А



Mol	Chain	Res	Type
1	1	56	А
1	1	58	G
1	1	59	A
1	1	64	А
1	1	65	А
1	1	76	А
1	1	91	G
1	1	98	А
1	1	109	G
1	1	110	С
1	1	115	А
1	1	121	А
1	1	134	U
1	1	135	G
1	1	147	G
1	1	154	G
1	1	155	А
1	1	156	А
1	1	164	U
1	1	169	G
1	1	171	G
1	1	172	С
1	1	173	С
1	1	175	G
1	1	186	А
1	1	189	U
1	1	190	U
1	1	199	С
1	1	205	G
1	1	209	С
1	1	210	A
1	1	212	А
1	1	217	G
1	1	218	А
1	1	219	G
1	1	230	G
1	1	236	А
1	1	239	А
1	1	240	С
1	1	243	G
1	1	245	G
1	1	249	G



Mol	Chain	Res	Type
1	1	250	U
1	1	251	G
1	1	252	U
1	1	253	А
1	1	269	G
1	1	286	U
1	1	295	А
1	1	305	U
1	1	323	А
1	1	329	U
1	1	338	А
1	1	339	С
1	1	346	С
1	1	350	С
1	1	376	G
1	1	377	А
1	1	395	А
1	1	398	А
1	1	403	С
1	1	404	G
1	1	420	G
1	1	421	G
1	1	422	A
1	1	438	А
1	1	439	С
1	1	445	А
1	1	453	U
1	1	454	G
1	1	479	С
1	1	481	G
1	1	482	U
1	1	485	A
1	1	486	С
1	1	506	A
1	1	516	U
1	1	517	A
1	1	531	G
1	1	538	G
1	1	539	G
1	1	541	U
1	1	542	U
1	1	543	С



Mol	Chain	Res	Type
1	1	544	U
1	1	545	G
1	1	546	С
1	1	555	А
1	1	557	А
1	1	564	G
1	1	577	G
1	1	590	А
1	1	598	U
1	1	600	U
1	1	602	А
1	1	609	А
1	1	618	U
1	1	619	A
1	1	620	А
1	1	647	А
1	1	658	А
1	1	665	С
1	1	675	А
1	1	679	U
1	1	682	G
1	1	703	А
1	1	710	G
1	1	713	А
1	1	717	А
1	1	723	G
1	1	730	A
1	1	732	U
1	1	760	U
1	1	763	U
1	1	772	U
1	1	773	U
1	1	776	А
1	1	777	G
1	1	781	G
1	1	782	A
1	1	802	A
1	1	813	А
1	1	826	A
1	1	845	С
1	1	857	С
1	1	870	U



Mol	Chain	Res	Type
1	1	875	U
1	1	892	А
1	1	903	G
1	1	904	G
1	1	910	А
1	1	912	G
1	1	913	А
1	1	917	А
1	1	919	C
1	1	920	G
1	1	921	А
1	1	933	G
1	1	934	С
1	1	940	С
1	1	955	С
1	1	956	U
1	1	970	G
1	1	976	А
1	1	977	U
1	1	978	С
1	1	990	G
1	1	991	U
1	1	996	С
1	1	997	G
1	1	998	А
1	1	1006	G
1	1	1011	С
1	1	1012	U
1	1	1014	G
1	1	1019	U
1	1	1020	G
1	1	1021	А
1	1	1022	A
1	1	1023	А
1	1	1024	U
1	1	1025	G
1	1	1027	C
1	1	1030	U
1	1	1033	С
1	1	1043	A
1	1	1045	С
1	1	1060	А



Mol	Chain	Res	Type
1	1	1061	А
1	1	1068	G
1	1	1077	U
1	1	1078	U
1	1	1089	А
1	1	1090	A
1	1	1091	U
1	1	1092	U
1	1	1094	А
1	1	1099	А
1	1	1100	G
1	1	1113	G
1	1	1127	G
1	1	1140	U
1	1	1149	А
1	1	1150	A
1	1	1155	А
1	1	1176	А
1	1	1177	U
1	1	1178	G
1	1	1188	C
1	1	1189	А
1	1	1192	С
1	1	1197	С
1	1	1204	U
1	1	1215	C
1	1	1218	G
1	1	1223	C
1	1	1224	С
1	1	1225	G
1	1	1228	C
1	1	1229	G
1	1	1230	G
1	1	1231	U
1	1	1232	G
1	1	1237	U
1	1	1238	G
1	1	1239	G
1	1	1240	A
1	1	1241	A
1	1	1242	G
1	1	1243	U



Mol	Chain	Res	Type
1	1	1244	С
1	1	1245	G
1	1	1249	U
1	1	1250	С
1	1	1253	С
1	1	1255	А
1	1	1259	А
1	1	1262	G
1	1	1263	U
1	1	1264	G
1	1	1265	U
1	1	1266	А
1	1	1267	А
1	1	1268	С
1	1	1269	А
1	1	1270	А
1	1	1273	С
1	1	1274	А
1	1	1277	G
1	1	1278	G
1	1	1280	С
1	1	1282	А
1	1	1283	А
1	1	1301	U
1	1	1303	G
1	1	1304	А
1	1	1305	U
1	1	1309	G
1	1	1326	А
1	1	1327	U
1	1	1345	G
1	1	1346	U
1	1	1347	U
1	1	1348	U
1	1	1349	U
1	1	1382	A
1	1	1387	С
1	1	1395	U
1	1	1414	А
1	1	1415	А
1	1	1417	G
1	1	1421	U



Mol	Chain	Res	Type
1	1	1430	G
1	1	1433	С
1	1	1442	А
1	1	1446	G
1	1	1465	С
1	1	1477	А
1	1	1484	G
1	1	1491	U
1	1	1498	С
1	1	1504	С
1	1	1520	А
1	1	1532	G
1	1	1552	С
1	1	1556	G
1	1	1558	G
1	1	1559	С
1	1	1560	U
1	1	1561	U
1	1	1562	G
1	1	1563	А
1	1	1565	U
1	1	1566	U
1	1	1567	U
1	1	1568	U
1	1	1569	С
1	1	1571	G
1	1	1572	G
1	1	1573	С
1	1	1574	С
1	1	1575	А
1	1	1576	А
1	1	1577	С
1	1	1585	А
1	1	1589	А
1	1	1601	A
1	1	1624	С
1	1	1625	U
1	1	1635	С
1	1	1638	А
1	1	1639	A
1	1	1641	U
1	1	1653	С



Mol	Chain	Res	Type
1	1	1654	G
1	1	1701	U
1	1	1720	U
1	1	1721	С
1	1	1732	G
1	1	1746	А
1	1	1747	G
1	1	1756	А
1	1	1759	U
1	1	1760	U
1	1	1761	U
1	1	1762	G
1	1	1763	С
1	1	1771	G
1	1	1774	G
1	1	1776	G
1	1	1792	G
1	1	1793	А
1	1	1809	А
1	1	1810	А
1	1	1811	U
1	1	1812	А
1	1	1814	U
1	1	1815	U
1	1	1816	U
1	1	1817	U
1	1	1835	А
1	1	1838	A
1	1	1842	С
1	1	1845	С
1	1	1846	A
1	1	1862	C
1	1	1874	G
1	1	1876	U
1	1	1877	А
1	1	1882	A
1	1	1889	A
1	1	1902	G
1	1	1944	G
1	1	1950	G
1	1	1951	U
1	1	1958	G



Mol	Chain	Res	Type
1	1	1965	U
1	1	1968	А
1	1	1970	А
1	1	2043	G
1	1	2045	С
1	1	2051	G
1	1	2054	С
1	1	2055	G
1	1	2061	G
1	1	2066	G
1	1	2067	U
1	1	2068	U
1	1	2069	U
1	1	2070	A
1	1	2078	А
1	1	2079	С
1	1	2088	G
1	1	2089	G
1	1	2090	U
1	1	2091	А
1	1	2092	C
1	1	2099	G
1	1	2100	G
1	1	2109	А
1	1	2118	U
1	1	2122	А
1	1	2124	С
1	1	2136	A
1	1	2147	G
1	1	2149	G
1	1	2182	C
1	1	2183	U
1	1	2184	G
1	1	2185	A
1	1	2186	A
1	1	2187	U
1	1	2188	G
1	1	2200	A
1	1	2201	A
1	1	2222	A
1	1	2227	G
1	1	2234	А



Mol	Chain	Res	Type
1	1	2235	С
1	1	2250	G
1	1	2251	G
1	1	2259	А
1	1	2260	U
1	1	2276	U
1	1	2283	G
1	1	2285	G
1	1	2288	U
1	1	2291	А
1	1	2292	U
1	1	2293	G
1	1	2312	U
1	1	2314	U
1	1	2341	А
1	1	2351	А
1	1	2352	С
1	1	2353	G
1	1	2363	G
1	1	2366	U
1	1	2371	G
1	1	2375	А
1	1	2380	А
1	1	2381	G
1	1	2382	A
1	1	2389	U
1	1	2390	G
1	1	2413	G
1	1	2419	А
1	1	2420	G
1	1	2489	A
1	1	2492	U
1	1	2493	А
1	1	2511	G
1	1	2513	A
1	1	2515	G
1	1	2516	U
1	1	2517	С
1	1	2518	А
1	1	2519	A
1	1	2520	А
1	1	2521	С



Mol	Chain	Res	Type
1	1	2529	U
1	1	2530	С
1	1	2536	U
1	1	2538	А
1	1	2545	С
1	1	2546	U
1	1	2547	G
1	1	2557	G
1	1	2565	А
1	1	2566	С
1	1	2578	G
1	1	2579	G
1	1	2586	G
1	1	2598	A
1	1	2624	U
1	1	2628	А
1	1	2644	G
1	1	2646	А
1	1	2649	G
1	1	2661	А
1	1	2663	А
1	1	2666	А
1	1	2676	A
1	1	2685	U
1	1	2686	G
1	1	2700	G
1	1	2701	U
1	1	2724	U
1	1	2725	G
1	1	2734	А
1	1	2745	С
1	1	2749	G
1	1	2750	G
1	1	2768	G
1	1	2771	А
1	1	2772	G
1	1	2773	А
1	1	2774	А
1	1	2782	С
1	1	2786	G
1	1	2789	A
1	1	2790	U



Mol	Chain	Res	Type
1	1	2800	G
1	1	2814	U
1	1	2815	U
1	1	2816	С
1	1	2817	А
1	1	2833	U
1	1	2843	G
1	1	2844	А
1	1	2847	U
1	1	2859	А
1	1	2861	С
1	1	2866	С
1	1	2870	G
1	1	2871	С
1	1	2883	А
1	1	2886	G
1	1	2895	U
1	1	2907	U
1	1	2908	А
1	1	2914	С
1	1	2919	G
1	1	2943	А
1	1	2955	С
1	1	2962	G
1	1	2969	G
1	1	2984	А
1	1	3021	А
1	1	3028	U
1	1	3031	G
1	1	3050	A
1	1	3051	С
1	1	3052	G
1	1	3058	A
1	1	3064	С
1	1	3066	А
1	1	3073	G
1	1	3076	U
1	1	3094	A
1	1	3102	A
1	1	3103	U
1	1	3114	А
1	1	3115	С



Mol	Chain	Res	Type
1	1	3125	U
1	1	3134	С
1	1	3141	U
1	1	3143	G
1	1	3144	А
1	1	3146	G
1	1	3149	U
1	1	3151	С
1	1	3157	А
1	1	3160	С
1	1	3162	U
1	1	3163	U
1	1	3164	U
1	1	3165	U
1	1	3171	С
1	1	3172	U
1	1	3175	А
1	1	3182	С
1	1	3183	А
1	1	3184	G
1	1	3192	А
1	1	3194	G
1	1	3208	А
1	1	3210	А
1	1	3212	G
1	1	3214	U
1	1	3224	U
1	1	3228	G
1	1	3235	А
1	1	3241	G
1	1	3246	С
1	1	3251	G
1	1	3252	С
1	1	3259	A
1	1	3260	А
1	1	3268	G
1	1	3269	C
1	1	3278	U
1	1	3281	A
1	1	3282	U
1	1	3284	U
1	1	3285	А



Mol	Chain	Res	Type
1	1	3306	U
1	1	3307	А
1	1	3309	А
1	1	3310	G
1	1	3316	U
1	1	3317	U
1	1	3318	G
1	1	3319	U
1	1	3320	U
1	1	3321	G
1	1	3334	G
1	1	3343	С
1	1	3347	U
1	1	3351	G
1	1	3361	U
2	3	22	A
2	3	54	U
2	3	65	G
2	3	73	С
2	3	76	А
2	3	102	А
2	3	112	G
3	4	23	U
3	4	34	U
3	4	35	С
3	4	59	А
3	4	62	С
3	4	63	G
3	4	70	G
3	4	81	A
3	4	84	С
3	4	85	G
3	4	86	U
3	4	87	G
3	4	92	A
3	4	95	G
3	4	102	U
3	4	104	A
3	4	106	С
3	4	107	G
3	4	111	A
3	4	112	U
	I	· _	



Mol	Chain	Res	Type
3	4	113	U
3	4	125	U
3	4	126	А
3	4	148	G
3	4	156	U
3	4	157	U
46	А	4	С
46	А	17	С
46	А	25	С
46	А	26	А
46	А	27	U
46	А	34	G
46	А	42	G
46	А	43	А
46	А	47	А
46	А	57	G
46	А	66	U
46	А	68	А
46	А	74	U
46	А	76	А
46	А	78	А
46	А	79	С
46	А	81	G
46	А	84	А
46	А	104	А
46	А	114	С
46	А	115	G
46	А	116	U
46	А	123	G
46	А	124	А
46	A	127	G
46	А	128	U
46	A	129	А
46	A	138	С
46	A	139	U
46	A	141	G
46	A	142	G
46	A	143	A
46	A	149	G
46	A	151	G
46	A	152	G
46	А	154	А



Mol	Chain	Res	Type
46	А	156	U
46	А	157	U
46	А	158	С
46	А	164	С
46	А	166	A
46	А	167	A
46	А	168	U
46	А	173	G
46	А	174	С
46	А	176	U
46	А	177	А
46	А	179	A
46	А	187	С
46	А	190	U
46	А	193	G
46	А	199	G
46	А	200	А
46	А	202	G
46	А	211	А
46	А	213	А
46	А	215	А
46	А	216	А
46	А	217	A
46	А	218	А
46	А	219	А
46	А	248	С
46	А	255	А
46	А	259	U
46	А	260	U
46	А	261	С
46	А	262	G
46	А	263	A
46	А	266	С
46	А	269	A
46	А	270	U
46	А	274	С
46	А	276	U
46	А	277	G
46	А	278	U
46	А	279	G
46	А	299	A
46	Α	307	С



Mol	Chain	\mathbf{Res}	Type
46	А	312	С
46	А	314	А
46	А	318	U
46	А	319	С
46	А	320	G
46	А	331	А
46	А	335	G
46	А	336	С
46	А	350	А
46	А	357	А
46	А	358	А
46	А	359	С
46	А	388	G
46	A	398	A
46	A	400	С
46	А	402	G
46	А	414	А
46	А	416	G
46	А	417	G
46	А	421	G
46	А	422	C
46	А	423	А
46	А	424	G
46	А	432	G
46	А	433	С
46	А	437	U
46	А	442	С
46	А	452	А
46	А	457	G
46	А	458	А
46	А	466	А
46	А	467	С
46	A	474	U
46	A	475	A
46	A	480	U
46	A	482	C
46	A	483	A
46	A	485	G
46	A	501	G
46	A	502	U
46	A	$50\overline{3}$	A
46	A	504	A



Mol	Chain	\mathbf{Res}	Type
46	А	505	U
46	А	506	U
46	А	509	А
46	А	515	U
46	А	516	А
46	А	518	А
46	А	519	А
46	А	525	А
46	А	530	U
46	А	532	А
46	А	534	С
46	А	536	А
46	А	537	G
46	А	538	G
46	А	539	А
46	А	540	А
46	А	547	G
46	А	553	А
46	А	554	А
46	А	555	G
46	А	556	U
46	А	557	С
46	А	562	G
46	А	563	С
46	А	566	G
46	А	575	G
46	А	580	U
46	А	592	А
46	А	593	G
46	А	609	U
46	А	617	А
46	А	618	А
46	А	620	A
46	А	621	A
46	А	624	U
46	А	639	G
46	А	648	U
46	А	650	G
46	А	652	С
46	А	653	G
46	А	654	G
46	А	656	С



Mol	Chain	Res	Type
46	А	675	U
46	А	676	G
46	А	682	А
46	А	686	G
46	А	687	А
46	А	688	G
46	А	692	U
46	А	694	С
46	А	695	С
46	А	696	U
46	А	701	G
46	А	721	С
46	А	722	A
46	A	723	G
46	А	727	U
46	А	729	U
46	А	730	U
46	А	739	А
46	А	740	А
46	А	741	А
46	А	750	G
46	А	751	U
46	А	756	А
46	А	759	А
46	А	760	G
46	А	764	U
46	А	765	U
46	А	766	U
46	A	767	G
46	А	768	С
46	A	770	С
46	A	771	G
46	A	773	A
46	A	778	U
46	A	779	U
46	A	787	A
46	A	796	A
46	А	797	U
46	A	798	A
46	А	803	G
46	A	804	U
46	А	805	U



Mol	Chain	Res	Type
46	А	807	U
46	А	808	G
46	А	811	U
46	А	814	А
46	А	815	U
46	А	816	U
46	А	818	U
46	А	819	G
46	А	820	U
46	А	821	U
46	А	822	G
46	А	823	G
46	А	824	U
46	А	825	U
46	А	827	С
46	A	828	U
46	А	832	А
46	А	842	U
46	А	848	А
46	А	856	G
46	А	857	G
46	А	858	U
46	А	860	G
46	А	869	А
46	А	871	U
46	А	875	С
46	А	877	G
46	А	878	U
46	А	879	U
46	А	880	G
46	A	881	U
46	A	883	A
46	A	891	A
46	А	898	G
46	A	909	А
46	A	910	G
46	А	911	A
46	А	918	А
46	А	920	U
46	А	930	U
46	А	937	А
46	А	945	U



Mol	Chain	Res	Type
46	А	951	А
46	А	973	А
46	А	975	С
46	А	977	А
46	А	988	А
46	А	989	U
46	А	997	U
46	А	998	А
46	А	1005	А
46	А	1011	А
46	А	1013	С
46	А	1017	G
46	А	1024	А
46	A	1025	G
46	A	1039	U
46	A	1042	U
46	А	1043	U
46	А	1044	U
46	А	1047	U
46	А	1048	U
46	А	1054	А
46	А	1055	А
46	А	1056	U
46	А	1057	С
46	А	1058	G
46	А	1059	G
46	А	1061	А
46	А	1067	С
46	А	1077	А
46	А	1078	А
46	А	1081	С
46	А	1085	G
46	А	1123	A
46	A	1135	G
46	A	1136	A
46	A	1143	С
46	А	1145	А
46	А	1150	G
46	А	1152	G
46	A	$1\overline{163}$	G
46	A	1168	A
46	А	1169	А



Mol	Chain	Res	Type
46	А	1170	U
46	А	1179	А
46	А	1181	А
46	А	1184	G
46	А	1185	G
46	А	1186	G
46	А	1187	А
46	А	1190	С
46	А	1191	U
46	А	1200	С
46	А	1202	А
46	А	1203	G
46	А	1206	А
46	A	1207	С
46	A	1212	А
46	A	1213	G
46	А	1214	G
46	А	1215	А
46	А	1219	А
46	А	1220	С
46	А	1229	А
46	А	1230	G
46	А	1231	С
46	А	1236	U
46	А	1237	С
46	А	1241	А
46	А	1243	U
46	А	1250	G
46	А	1254	U
46	A	1263	G
46	А	1269	С
46	A	1270	U
46	A	1291	С
46	A	1299	U
46	А	1300	U
46	A	1306	A
46	A	1325	U
46	A	1329	A
46	A	1330	А
46	A	1336	G
46	A	1339	G
46	А	1342	А



Mol	Chain	Res	Type
46	А	1343	G
46	А	1345	А
46	А	1346	U
46	А	1348	U
46	А	1349	G
46	А	1352	G
46	А	1355	А
46	А	1356	U
46	А	1357	А
46	А	1359	U
46	А	1360	С
46	А	1364	U
46	А	1365	\mathbf{C}
46	А	1369	G
46	А	1370	А
46	А	1371	G
46	А	1376	U
46	А	1380	G
46	А	1381	А
46	А	1382	U
46	А	1384	U
46	А	1385	С
46	А	1396	А
46	А	1397	А
46	А	1398	G
46	А	1399	U
46	А	1400	U
46	А	1401	U
46	А	1408	А
46	А	1410	А
46	А	1413	А
46	А	1414	G
46	А	1415	G
46	A	1416	U
46	А	1418	U
46	A	1419	G
46	A	1422	A
46	A	1424	G
46	A	1431	G
46	A	1432	A
46	A	1433	C
46	А	1434	G



Mol	Chain	Res	Type
46	А	1444	G
46	А	1445	С
46	А	1454	U
46	А	1455	А
46	А	1457	А
46	А	1458	С
46	А	1461	А
46	А	1462	С
46	А	1463	G
46	А	1465	А
46	А	1468	С
46	А	1476	А
46	А	1477	U
46	А	1480	G
46	А	1483	U
46	А	1485	G
46	А	1491	G
46	А	1503	А
46	А	1510	G
46	А	1511	А
46	А	1513	А
46	А	1523	G
46	А	1524	С
46	А	1525	U
46	А	1526	G
46	А	1529	G
46	А	1530	А
46	А	1541	U
46	А	1544	U
46	А	1546	G
46	А	1551	U
46	А	1556	А
46	A	1560	A
46	А	1561	G
46	А	1571	G
46	А	1574	А
46	А	1580	А
46	А	1582	U
46	А	1583	С
46	A	1584	А
46	А	1588	G
46	A	1606	С



Mol	Chain	Res	Type
46	А	1621	С
46	А	1622	А
46	А	1644	U
46	А	1645	G
46	А	1667	G
46	А	1670	U
46	А	1671	G
46	А	1672	G
46	А	1673	U
46	А	1674	U
46	А	1677	G
46	А	1700	G
46	А	1702	А
46	А	1704	С
46	А	1717	A
46	А	1743	A
46	А	1749	A
46	А	1753	A
46	А	1756	U
46	А	1767	G
46	А	1770	С
46	А	1779	G
46	А	1780	G
46	А	1781	А
46	А	1783	С

All (84) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	172	С
1	1	403	С
1	1	538	G
1	1	563	U
1	1	601	U
1	1	759	G
1	1	912	G
1	1	1029	U
1	1	1060	А
1	1	1099	А
1	1	1346	U
1	1	1347	U
1	1	1559	С


Mol	Chain	Res	Type
1	1	1561	U
1	1	1574	С
1	1	1576	А
1	1	1762	G
1	1	1815	U
1	1	1943	G
1	1	1957	G
1	1	2044	U
1	1	2078	А
1	1	2090	U
1	1	2182	С
1	1	2183	U
1	1	2515	G
1	1	2519	А
1	1	2520	А
1	1	2545	С
1	1	2790	U
1	1	3093	U
1	1	3163	U
1	1	3193	С
1	1	3234	U
1	1	3284	U
1	1	3309	А
1	1	3315	С
1	1	3317	U
3	4	85	G
3	4	156	U
46	А	25	С
46	А	78	А
46	А	137	А
46	A	151	G
46	А	176	U
46	A	214	U
46	A	259	U
46	А	265	U
46	A	278	U
46	A	415	A
46	A	451	С
46	A	502	U
46	A	504	A
46	А	505	U
46	А	514	G

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Mol	Chain	Res	Type
46	А	518	А
46	А	529	С
46	А	533	А
46	А	553	А
46	А	638	U
46	А	685	С
46	А	740	А
46	А	763	С
46	А	820	U
46	А	824	U
46	А	855	С
46	А	874	U
46	А	876	А
46	А	1168	А
46	А	1335	U
46	А	1355	А
46	А	1359	U
46	А	1369	G
46	А	1396	А
46	А	1398	G
46	А	1457	А
46	А	1467	С
46	А	1479	А
46	А	1484	U
46	А	1523	G
46	А	1555	С
46	А	1573	А
46	А	1579	А
46	А	1581	G

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

6 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	Turne	Chain	Dec	Tink	Bo	ond leng	ths	В	ond ang	les
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	MLZ	6	110	24	8,9,10	0.74	0	4,9,11	1.04	0
1	OMC	1	2808	1	$15,\!22,\!23$	3.16	6 (40%)	17,31,34	1.24	2 (11%)
43	MLZ	AP	40	43	8,9,10	0.70	0	4,9,11	1.00	0
43	MLZ	AP	55	43	8,9,10	0.66	0	4,9,11	0.92	0
61	IAS	Р	119	61	4,7,8	0.90	0	$2,\!8,\!10$	1.77	1 (50%)
1	OMG	1	2765	1	18,26,27	3.32	8 (44%)	20,38,41	1.84	4 (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
24	MLZ	6	110	24	-	3/7/8/10	-
1	OMC	1	2808	1	-	1/7/27/28	0/2/2/2
43	MLZ	AP	40	43	-	1/7/8/10	-
43	MLZ	AP	55	43	-	3/7/8/10	-
61	IAS	Р	119	61	-	3/3/7/8	-
1	OMG	1	2765	1	-	0/5/27/28	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2765	OMG	C4-N3	7.99	1.48	1.35
1	1	2808	OMC	C6-N1	7.44	1.45	1.35
1	1	2765	OMG	C5-C6	6.62	1.52	1.41
1	1	2765	OMG	C6-N1	5.65	1.42	1.33
1	1	2808	OMC	C2-N3	5.21	1.48	1.38
1	1	2808	OMC	C4-N3	4.89	1.43	1.35
1	1	2808	OMC	C6-C5	4.66	1.48	1.38
1	1	2765	OMG	C2-N2	4.65	1.43	1.33
1	1	2765	OMG	C2-N1	4.32	1.43	1.35
1	1	2808	OMC	C4-N4	3.36	1.45	1.35
1	1	2808	OMC	C5-C4	2.81	1.48	1.41
1	1	2765	OMG	O6-C6	-2.72	1.17	1.24
1	1	2765	OMG	C2-N3	2.37	1.45	1.34
1	1	$27\overline{65}$	OMG	C5-C4	-2.03	1.35	1.40

All (7) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	1	2765	OMG	N3-C2-N1	-5.29	120.16	127.22
1	1	2765	OMG	C2-N3-C4	3.99	119.92	115.36
1	1	2808	OMC	C4-N3-C2	3.47	119.86	116.34
1	1	2765	OMG	C5-C6-N1	-2.29	120.30	123.43
1	1	2765	OMG	C2-N1-C6	2.19	119.41	115.93
61	Р	119	IAS	OD1-CG-CB	-2.18	119.07	125.43
1	1	2808	OMC	N4-C4-N3	2.05	119.73	116.49

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
1	1	2808	OMC	C1'-C2'-O2'-CM2
24	6	110	MLZ	N-CA-CB-CG
61	Р	119	IAS	N-CA-CB-CG
61	Р	119	IAS	C-CA-CB-CG
43	AP	55	MLZ	CG-CD-CE-NZ
24	6	110	MLZ	CD-CE-NZ-CM
43	AP	55	MLZ	CE-CD-CG-CB
43	AP	55	MLZ	CA-CB-CG-CD
24	6	110	MLZ	C-CA-CB-CG
43	AP	40	MLZ	CG-CD-CE-NZ
61	Р	119	IAS	CA-CB-CG-OD1

All (11) torsion outliers are listed below:

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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
80	SPD	1	3401	-	9,9,9	0.32	0	8,8,8	0.93	0
81	3HE	1	3402	-	21,21,21	0.54	0	19,30,30	0.62	0

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
80	SPD	1	3401	-	-	2/7/7/7	-
81	3HE	1	3402	-	-	2/8/36/36	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	1	3402	3HE	C6-C5-C7-C8
80	1	3401	SPD	N6-C7-C8-C9
80	1	3401	SPD	C7-C8-C9-N10
81	1	3402	3HE	C6-C5-C7-O3

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-13741. 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: 255

Y Index: 255



Z Index: 255

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: 275

Y Index: 274

Z Index: 206

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 0.3. 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 2491 nm^3 ; this corresponds to an approximate mass of 2251 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 0.391 \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 0.391 \AA^{-1}



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estim	Estimation criterion (FSC cut-off)				
Resolution estimate (A)	0.143	0.5	Half-bit			
Reported by author	2.56	-	-			
Author-provided FSC curve	2.56	2.91	2.60			
Unmasked-calculated*	-	-	-			

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13741 and PDB model 7Q08. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.3 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 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

