

# wwPDB EM Validation Summary Report (i)

Nov 6, 2023 – 11:17 AM JST

PDB ID	:	8IDY
EMDB ID	:	EMD-35371
Title	:	human nuclear pre-60S ribosomal particle - State F
Authors	:	Zhang, Y.; Gao, N.
Deposited on	:	2023-02-14
Resolution	:	3.00  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 70
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)	:	2.36

# 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 3.00 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	5	120	74%	25% •
2	6	245	99%	·
3	7	163	83%	17%
4	8	156	65% 31°	% •
5	9	134	69% ·	28%
6	В	403	99%	·
7	С	159	<b>6%</b> <b>58%</b> • 429	%
8	D	427	83%	• 16%

Continued on next page...



Mol	Chain	Length	Quality of chain	
0	F	115	12%	
9	E	110	84% • 15%	
10	F	117	92%	7%
11	G	266	15%	
11	u	200	90% 9%	0
12	Н	123	99%	•
13	Ι	192	96%	•••
14	Κ	105	97%	·
15	L	148	99%	-
16	М	07	000/	
10	101	51	42%	/0
17	Ν	178	90%	7%
18	0	70	97%	••
19	Р	51	98%	•
20	Q	211	<mark>6%</mark> 99%	_
	, and the second	0.1 ×		
21	S	215	61% · 37%	
22	U	204	100%	
23	V	203	99%	
24	W	106	8%	6%
25	x	02	7%	
20	<u> </u>	52	99%	•
26	Z	188	99%	•
27	a	196	• 74% • 24%	
28	b	176	100%	_
29	с	160	<b>•</b> 96%	•••
30	е	140	91%	5%
31	o	156	76%	
20	5 1	145	1070 Z4%	
32	n	145	92% 8	3%
33	i	136	98%	••

Continued from previous page...

Continued on next page...



Mol	Chain	Length	Quality of chain
34	1	137	91% 9%
35	m	257	95% • •
36	n	110	96%
37	О	288	10% 81% • 18%
38	р	248	91% 9%
39	r	297	97%
40	А	731	7% 42% 58%
41	R	203	
42	J	239	87% 92% • 7%
43	Т	99	44% 56%
44	2	5054	8% 46% 23% • 28%
45	У	165	95% 99%
46	4	634	94%
47	d	128	5% • 19%
48	j	125	88% • 11%
49	k	135	95% • •
50	Υ	184	6% 89% ·· 9%
51	Z	129	16% 50% • 48%
52	t	217	98% 96% · ·
53	u	687	75% 79% • 19%
54	v	260	13%

Continued from previous page...



# 2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 155910 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 5S rRNA.

Mol	Chain	Residues		A	AltConf	Trace			
1	5	120	Total 2558	C 1141	N 456	0 842	Р 119	0	0

• Molecule 2 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	244	Total 1852	C 1149	N 318	0 372	S 13	0	0

• Molecule 3 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues		A	toms	AltConf	Trace		
3	7	135	Total 1159	C 737	N 225	0 187	S 10	0	0

• Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	156	Total 3315	C 1481	N 585	O 1094	Р 155	0	0

• Molecule 5 is a protein called Zinc finger protein 593.

Mol	Chain	Residues		At	oms	AltConf	Trace		
5	9	97	Total 793	C 484	N 171	0 134	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	В	402	Total 3244	C 2065	N 609	O 556	S 14	1	0



• Molecule 7 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues		At	$\mathbf{oms}$			AltConf	Trace
7	С	93	Total 764	C 476	N 167	0 117	${S \atop 4}$	0	0

• Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	D	358	Total 2853	C 1797	N 570	0 473	S 13	0	0

• Molecule 9 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues		At	oms	AltConf	Trace		
9	Е	98	Total 764	C 485	N 135	0 138	S 6	0	0

• Molecule 10 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	F	109	Total 868	C 544	N 179	0 139	S 6	0	0

• Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues		Ate	AltConf	Trace			
11	G	241	Total 1935	C 1233	N 374	0 324	S 4	1	0

• Molecule 12 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues		At	oms	AltConf	Trace		
12	Н	122	Total 1015	C 641	N 205	0 168	S 1	0	0

• Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues		At	oms			AltConf	Trace
13	Ι	190	Total 1518	C 956	N 284	0 272	S 6	0	0

• Molecule 14 is a protein called 60S ribosomal protein L36.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	K	102	Total 832	C 521	N 177	O 129	${f S}{5}$	0	0

• Molecule 15 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues		At	oms			AltConf	Trace
15	L	147	Total 1162	C 736	N 237	0 186	${ m S} { m 3}$	0	0

• Molecule 16 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues		At	oms			AltConf	Trace
16	М	86	Total 705	С 434	N 155	0 111	${f S}{5}$	0	0

• Molecule 17 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
17	Ν	165	Total 1319	C 836	N 245	O 233	${ m S}{ m 5}$	0	0

• Molecule 18 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues		Ate	oms	Atoms					
18	О	69	Total 569	C 366	N 103	O 99	S 1	0	0		

• Molecule 19 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues		Atc	$\mathbf{ms}$			AltConf	Trace
10	р	50	Total	С	Ν	Ο	$\mathbf{S}$	0	0
15	1	50	444	281	98	64	1	0	0

• Molecule 20 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
20	Q	210	Total 1701	C 1064	N 352	0 281	${f S}{4}$	0	0

• Molecule 21 is a protein called 60S ribosomal protein L14.



Mol	Chain	Residues		At	oms			AltConf	Trace
21	S	135	Total 1111	C 713	N 213	0 178	${f S}$ 7	0	0

• Molecule 22 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues		Ate	AltConf	Trace			
22	U	203	Total 1701	C 1072	N 359	O 266	$\frac{S}{4}$	0	0

• Molecule 23 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues		At	AltConf	Trace			
23	V	201	Total 1650	C 1063	N 321	0 261	$\frac{S}{5}$	0	0

• Molecule 24 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues		Atoms					Trace
24	W	100	Total 818	C 512	N 168	0 132	S 6	0	0

• Molecule 25 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues		At	oms	AltConf	Trace		
25	Х	91	Total 708	C 445	N 136	0 120	S 7	0	0

• Molecule 26 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues		At	oms			AltConf	Trace
26	Z	187	Total 1513	C 944	N 314	O 250	${ m S}{ m 5}$	0	0

• Molecule 27 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues		At	oms			AltConf	Trace
27	a	148	Total 1239	С 772	N 266	0 192	S 9	0	0

• Molecule 28 is a protein called 60S ribosomal protein L18a.



Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
28	b	176	Total 1461	C 930	N 284	O 236	S 11	0	0

• Molecule 29 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues		Atoms					Trace
29	с	155	Total 1264	C 801	N 248	0 210	${S \atop 5}$	0	0

• Molecule 30 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues		At	oms			AltConf	Trace
30	е	131	Total 979	C 618	N 184	0 172	${ m S}{ m 5}$	0	0

• Molecule 31 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues		At	oms			AltConf	Trace
31	g	118	Total	C 619	N 101	0	S 1	0	0
	_		907	018	181	107	T		

• Molecule 32 is a protein called 60S ribosomal protein L26.

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

• Molecule 33 is a protein called 60S ribosomal protein L27.

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

• Molecule 34 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues		At	oms			AltConf	Trace
34	1	125	Total 1002	C 622	N 207	0 168	${f S}{5}$	0	0

• Molecule 35 is a protein called 60S ribosomal protein L8.



Mol	Chain	Residues		At	oms			AltConf	Trace
35	m	248	Total	С	N	0	S	0	0
			1898	1189	389	314	6		

• Molecule 36 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues		At	oms		Atoms					
36	n	109	Total 876	$\begin{array}{c} \mathrm{C} \\ 555 \end{array}$	N 174	0 144	${ m S} { m 3}$	0	0			

• Molecule 37 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
37	О	235	Total 1897	C 1217	N 360	O 316	$\frac{S}{4}$	0	0

• Molecule 38 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
38	р	225	Total 1878	C 1207	N 361	O 301	S 9	1	0

• Molecule 39 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues		At	oms			AltConf	Trace
39	r	293	Total 2382	C 1507	N 434	O 427	S 14	0	0

• Molecule 40 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues		At	oms			AltConf	Trace
40	А	307	Total 2460	C 1576	N 419	O 457	S 8	0	0

• Molecule 41 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues		At	oms	AltConf	Trace		
41	R	153	Total 1296	C 810	N 248	0 233	${S \atop 5}$	0	0

• Molecule 42 is a protein called mRNA turnover protein 4 homolog.



Mol	Chain	Residues		At	oms			AltConf	Trace
42	J	223	Total 1809	C 1140	N 309	O 349	S 11	0	0

• Molecule 43 is a protein called Leydig cell tumor 10 kDa protein homolog.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
43	Т	44	Total 343	C 215	N 71	O 56	S 1	0	0

• Molecule 44 is a RNA chain called 28S rRNA.

Mol	Chain	Residues			Atoms			AltConf	Trace
44	2	3641	Total 77442	C 34506	N 14094	O 25202	Р 3640	0	0

• Molecule 45 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues		At	oms			AltConf	Trace
45	У	165	Total 1250	C 779	N 232	0 234	${S \atop 5}$	0	0

• Molecule 46 is a protein called GTP-binding protein 4.

Mol	Chain	Residues		At	oms			AltConf	Trace
46	4	611	Total 5016	C 3151	N 918	0 920	$\frac{S}{27}$	0	0

• Molecule 47 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues		At	oms			AltConf	Trace
47	d	104	Total 850	С 542	N 149	0 157	${ m S} { m 2}$	0	0

• Molecule 48 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues		At	oms			AltConf	Trace
48	j	111	Total 918	C 578	N 178	0 160	$\frac{\mathrm{S}}{2}$	0	0

• Molecule 49 is a protein called 60S ribosomal protein L32.



Mol	Chain	Residues		At	oms			AltConf	Trace
49	k	129	Total 1064	C 673	N 220	O 166	${ m S}{ m 5}$	0	0

• Molecule 50 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues		At	oms			AltConf	Trace
50	Y	167	Total 1355	C 848	N 260	O 238	S 9	0	0

• Molecule 51 is a protein called Protein LLP homolog.

Mol	Chain	Residues		At	oms			AltConf	Trace
51	Z	67	Total 581	C 363	N 128	O 88	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 52 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues		At	oms			AltConf	Trace
52	t	212	Total 1708	C 1092	N 308	O 300	S 8	0	0

• Molecule 53 is a protein called Protein SDA1 homolog.

Mol	Chain	Residues		At	oms			AltConf	Trace
53	u	554	Total 4536	C 2890	N 810	0 804	S 32	0	0

• Molecule 54 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues		Aton	ıs		AltConf	Trace
54	v	35	Total 316	C 196	N 68	O 52	0	0

• Molecule 55 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).





Mol	Chain	Residues	Residues Atoms											
55	А	1	Total	С	Ν	0	Р	0						
- 55	Π		28	10	5	11	2	0						

• Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
56	А	1	Total Mg 1 1	0

• Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf			
57	А	1	Total K 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.

 $\bullet$  Molecule 1: 5S rRNA







• Molecule 11: 60S ribo	osomal protein L7a	
Chain G:	90%	9%
MET PRO LLYS LLYS LLYS LLYS LLYS LLYS LLYS LLY	VAL VAL LYS LYS GLN GLN GLN K26 V27 V26 V27 V27 V28 K11 A114 A114 A114 A113 K120 K120 K120 K120 K120 K120 K120	K125 K126 G126 P129 P129 K131 K131 F130 F130 F130 F130 F130 F130 F130 F130 F130 F130 F130 F130 F130 F130 F130 F130 F120
A266 K257 A258 K259 E260 E260 L261 A262 T263 K264 L265 C265 C265 C266		
• Molecule 12: 60S ribo	osomal protein L35	
Chain H:	99%	:
MET A2		
• Molecule 13: 60S ribo	osomal protein L9	
Chain I:	96%	
M1 K50 K51 K53 K53 R54 R93 R93 L111 U104 0138	K141 L176 Q189 A190 ASP GLU	
• Molecule 14: 60S ribo	osomal protein L36	
Chain K:	97%	
MET A2 L3 R4 R98 R98 A100 A100 A101 A101 A101 A102 K102 K102 K102 K102 ASP		
• Molecule 15: 60S ribo	osomal protein L27a	
Chain L:	99%	
MET P2 K94 A148		
• Molecule 16: 60S ribo	osomal protein L37	
Chain M:	89%	11%
MET 172 K87 ARG ARA ALA ALA ALA ALA ALA ALA SER SER SER SER		

 $\bullet$  Molecule 17: 60S ribosomal protein L11



	42%		
Chain N:	90%		• 7%
MET ALA ALA ASP ASP GLN GLV GLV GLV GLU ASN AND AND	RIG FIL FIL FIL FIL FIL FIL FIL FIL	A36 A37 K38 V39 E41 E41 E41 645 645 C45 C45 S51 K52 K52	I62 R63 R63 R64 N65 E66 K76 K76 K76 K78 K78 K78 E80 E80 E81 I83 L83
E84 K85 C86 L87 K88 K98 K98 K92 E91 E93	L94 R95 R110 E111 E111 L115 C116 G116 G116 C116 C116 C116 Y119 Y119 Y119	5122 1123 1125 1126 1126 1128 1128 1128 1128 1128 1128	E160 M163 M163 0167 0167 0168 K169 M171 0171 0171 1174 1174 1174 1175 6177 K178
• Molecule 18: 60	0S ribosomal protein L38		
Chain O:	97	%	
MET P2 E7 R16 K29 D30 D49	K50 E51 F61 P61 P62 C63 C63 K70		
• Molecule 19: 60	0S ribosomal protein L39		
Chain P:	98	%	·
MET 22 L51			
• Molecule 20: 60	0S ribosomal protein L13		
Chain Q:	99	9%	
MET A.2 K.1 45 V.1 54 A.202 A.203 E.204	q205 D206 V207 E208 K209 K210 K211		
• Molecule 21: 60	0S ribosomal protein L14		
Chain S:	61%	• 37%	
MET V2 D32 L130 A131 A133 A133 A133 A133 A133 A133 A	LYS LYS SER SER PRO PRO LYS CLY THR CLY CLYS CLY THR THR ALA ALA ALA ALA	ALA ALA ALA ALA ALA ALA ALA CYS ALA ALA CYS SER CYS SER ALA ALA	ALA ALA GLN CLYS ALA PRO ALA ALA ALA ALA THR THR
GLY GLN GLN LLYS ALA ALA PRO PRO CLY CLYS CLN CLYS	GLN LYS ALA ALA ALA ALA ALA PRO CLYS CLYS CLYS CLYS CLYS CLYS CLYS CLYS		
• Molecule 22: 60	0S ribosomal protein L15	-	
Chain U:	10	00%	
MET G2 R204			

• Molecule 23: 60S ribosomal protein L13a



Chain V: 99%
• Molecule 24: 60S ribosomal protein L36a
Chain W: 94% 6%
V2 N76 C77 R78 R96 K96 K98 K99 C101 C101 C101 C101 C101 C101 C101 C1
• Molecule 25: 60S ribosomal protein L37a
Chain X: 99% .
• Molecule 26: 60S ribosomal protein L18
Chain Z: 99%
• Molecule 27: 60S ribosomal protein L19
Chain a: 74% • 24%
Radia and a constraint of the
• Molecule 28: 60S ribosomal protein L18a
Chain b: 100%
There are no outlier residues recorded for this chain.
• Molecule 29: 60S ribosomal protein L21
Chain c: 96%
T2 V8 V123 C123 PHE ALA

• Molecule 30: 60S ribosomal protein L23



Chain e:	91%	• 6%
MET SER LYS LYS ARG ARG GLY SER SER SIO RH8	196 11 00 140	
• Molecule 31: 60	S ribosomal protein L23a	
Chain g:	76%	24%
MET PRO PRO LYS LYS LYS GLU GLU PRO PRO PRO	LYS ALA ALA GLU GLU CYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 32: 60	S ribosomal protein L26	
Chain h:	92%	8%
M K132 6133 K134 K134 K134 CLU CLU CLU CLU	NET RET GLU	
• Molecule 33: 60	S ribosomal protein L27	
Chain i:	98%	
MET G2 D30 B30 B88 R102 R103 E113	F136	
• Molecule 34: 60	S ribosomal protein L28	
Chain l:	91%	9%
MET 22 22 22 22 12 17 25 17 28 28 28 28 28 28 28 28 28 28 28 29 29 20 20 20 20 20 20 20 20 20 20 20 20 20	LIVE SER SER	
• Molecule 35: 60	S ribosomal protein L8	
Chain m:	95%	
MET G2 R54 L102 N132 T143 G248	1245 LYS THR GLN GLU GLU ASN ASN	
• Molecule 36: 60	S ribosomal protein L35a	
Chain n:	96%	
MET 82 15 1106 11106 1110		



$\bullet$ Molecule 37: 60S $\bullet$	ribosomal protein I	L6				
10%						
Chain o:	81%		·	18%		
MET ALA ALA GLU CLYS GLU CLYS PRO ASP THR THR THR CLU CLY CLU CLYS CLU	PRO GLU GLU LYS LYS LYS VAL ALA ALA GLY GLY CYS CVS	LYS GLY ASN ASN LEU LYS LYS LYS LYS CLY	LYS P42 R56 A75 A75 LYS CVS	JEN VAL GLU CYS LYS LYS LYS LYS	GLU LYS VAL L89	
G97 G98 G98 G103 T104 K207 K207	L222 R223 P225 P225 P225 Q228 Q228 C229 C230 C230 C231 C231 C231 C231 C231 C231 C231 C231	1232 F233 D234 D234 E236 K237 K237 K239 K239 K239				
• Molecule 38: 60S 1	ribosomal protein I	L7	•			
Chain p:	9	1%		9%		
MET GLU GLU GLU CLU CLU CLU CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV	GLU THR LEU LYS LYS LYS ARG ARG ARG ARG ARG					
• Molecule 39: 60S 1	ribosomal protein I	L5				
Chain r:		97%		••		
MET G2 F3 F3 K5 K5 V7 V7 V86 K89	L104 E124 D128 E133 S134 L135 D136 0137	L146 D147 E186 \$187 K188 A205 A205	r207 R209 Y210 L211 M212 E213 E213	D215 E216 D217 A218 Y219 K220	K221 1227 S230 D234	M235 M236 E237 E238
K241 K242 E254 K255 K255 K255 F257 K258 K258 K259 E260 V261	K263 K264 R265 R265 P269 K270 L273	K277 D278 K279 V280 A281 Q282 K283 K283 K283	5286 F287 L288 R289 A290 Q291 E292	A294 ALA GLU SER		
• Molecule 40: G Pr	otein Nucleolar 2					
Chain A:	42%		58%			
MET VAL LYS LYS PRO LYS GLY GLY GLY ARG SER THR THR THR THR THR SER SER	LYS ALA SER THR ASP ASP ASP ASP GLY GLY GLY GLY	GLY GLN ASN ASP ASP ASP ASP ALA ALA ALA ALA ARG ARG	LEU ASN MET TYR ARG GLN LYS GLU ARG	ARG ASN SER ARG GLY ILE TLE	LEU	
GLN TYR GLN GLN SER SER VAL ALA SER SER SER ALA ALA ALA ALA OLU	PRO ASN ILLE LYS TRP PHE PHE GLY ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	GLM SER SER SER SER CLU CLU GLU GLU MET ASP	THR VAL MET LYS ASP PRO TYR LYS VAL	VAL MET LYS GLN SER LYS LEU PRU	MET SER LEU	
LEU HIS AKSP AKSP ARG ARG ARG ARG ARSN HILE ULL LLL LLL LLL LLL	ASP THR THR SER SER SER HHE HHE HHE HHE CYS CYS SER	ARG ARG ARG ARG ARN ASN ASN ALA ARA ARA ARA ARA ARA ARA ARA ARA	1161 5162 1163 1164 1164 1165	ALO( E168 5170 5171 E172 E172	51/3 174 0175 176 3177 K178 K178	R180
•• •••• • •		• • •• • •	•• •• •	••		
D181 1182 1184 1184 E185 E185 D186 R197 A193	E196 K200 G201 Q202 D228 G302 K303 K303 B307	K308 K309 Q310 B371 D371 D375 L398	E399 R400 D413 S414 E419	L432 N464 A465 GLU PRO	VAL ALA PRO GLN LEU PRO SER	SER LEU
GLU VAL VAL PRO PRO GLU ALA ALA ALA ASN ASN ASN ASN ASN ASN ASN VAL VAL	THR GLU THR ALA GLU GLU SER SER SER ILE ILE	GLU THR GLU GLU GLU GLU GLU ASN ASN ASP ASN	THR GLU GLU GLN GLN ILE LEU THR ARG	VAL ARG GLN ASN PHE GLY LYS TTE	ASN VAL VAL	
PRO GLN GLN SER SER GLY ASP LEU VAL PRO GLU VAL SER SP	LEU GLU GLU GLU GLU SER SER SER GLU GLU GLU	GLU GLU GLU GLU GLU ASP ALS ALS GLU GLU GLU	SER SER SER GLU GLU GLU ASN	VAL GLY ASN ASP THR LYS ALA VAL	ILE LYS ALA	



#### LEU LYS LYS CHURNER CHURNER CHURNER LYS CHURNER LYS CHURNER LYS CHURNER CHURNE

#### LLYS ARIG GLUU GLUU GLUU GLUU GLUU HHISS ARIG GLUU LLYS ARIG GLUU LLYS ARIG GLUU LLYS ARIG GLUU LLYS ARIG GLUV VAL LLINS ARIG GLUV VAL LLINS ARIG GLUV VAL ARIG GLUV VAL LLINS ARIG GLUV VAL ARIG CUV VAL ARIG VAL A VAL A VAL VAL VAL VAL V

#### GLN LYS HIS LYS LYS LYS LYS PHE ARG GLN CLNS GLN

• Molecule 41: Translation machinery-associated protein 16



• Molecule 42: mRNA turnover protein 4 homolog

Chain J:       92%       7%         Statistics       Statistics<		87%		
	Chain J:	92%	• 7%	]
		••• ••••• ••••	• •• •••••	•
	MET PRO LYS SER LYS ARC ASP LYS VAC VAC CEU THR THR THR THR THR THR	K17 K18 G19 C21 L20 L22 K23 Q24 N26 C33 C33 C33 C33 C33 C33 C33 C33 C33 C3	T36 Y37 K38 K38 Y39 F41 F41 F42 F43 F43 S44 V45 S44 V45 N47 M48	R49 N50 L53 K54 D55 R57 R57 N58 N58 N58 N59 N60 N60 N60
<ul> <li></li></ul>	••• •• • ••••	· · · · · · · · · · · · · · · · · · ·	*** *******	******
************************************	S63 R64 M65 F66 F67 G68 K71 V72 M73 M74 V75 A76	L77 G78 R79 S80 P81 P81 P81 P81 F84 K86 B83 E84 N88 N88 N88 N88 N88 S93 S93	R95 L96 R97 G98 E99 C100 L102 L102 L103 F104 F104 T105 N106	T108 K109 E110 E111 V112 V112 F115 F115 F115 T117 T120 F112 T120 F121 M122 D123
• Molecule 43: Leydig cell tumor 10 kDa protein homolog         10%				
• Molecule 43: Leydig cell tumor 10 kDa protein homolog	Y124 A125 R126 A127 G128 G128 K130 A131 A131 A132 F133 T134 V135	<pre>\$136 \$1137 \$1137 \$1139 \$1139 \$1140 \$1141 \$1142 \$1142 \$1142 \$1144 \$1144 \$1144 \$1144 \$1144 \$1144 \$1144 \$1144 \$1144 \$1146 \$1151 \$1153 \$1155 \$1</pre>	R154 Q155 L156 G157 G157 L156 P159 P159 P159 A161 L162 K163 R164 R164 G165	V166 V167 L1168 L1169 L1170 L1170 L1170 S171 S171 S171 S171 C176 K177 K177 E178 G179 G179 D180 V181 V181 V181 V182 C176
• Molecule 43: Leydig cell tumor 10 kDa protein homolog				
Molecule 43: Leydig cell tumor 10 kDa protein homolog	P184 E185 Q186 A187 A187 R188 V189 L190 L192 F193 F193 F193 G194 G194	E196 M197 A198 E199 E199 F200 F200 T203 T203 T203 T204 V205 W205 W205 W205 W205 W206 W205 W206 W201 S213 S210 S213 S213	R214 F215 Q216 Q217 M218 G219 D220 D221 L222 P223 F223 F223 F223 S225	A.220 5227 5228 5229 5233 5233 5233 5233 5233 5233 5233
10%	• Molecule 43: Levdig	g cell tumor 10 kDa protein hor	molog	
Chain T: 56%	10%	<b>J</b>	0	
	Chain T:	44%	56%	
• • • • • • • • • • • • • • • • • • •		• • • • •	• • • • •	
MET MET ARG GLN GLN GLN GLN GLN GLN GLN GLN GLN GL	MET ALA GLN GLN GLN GLN GLN FLS PHE CLN HIS PHE CLN HIS TLS SER SER	LYS THR ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	149 153 153 153 153 153 153 854 857 153 150 150 150 150 150	ALA LEU LYS LYS ALA PRO ALA LYS
LLYS ALA ALA ALA ALA ALA THR SER SER SER SER SER	LYS LYS GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA THR THR SER SER SER SER SER SER			
- Malanda 44, 200 - DNA	- Malassila 44, 200 T			















G3839 U3840	<mark>U3851</mark>	A3852 U3853	C3858	C3866	A3867 G3868	C3869	A3871	A3876	A3877 C3878	G3879 G3880	G3881 C3882	C3887	COOCII	03893 C3893	G3897	63899 63899	G3900 A3901	A3902 A3903	G3904 A3905	A3906	C3909	C3911 C3911	63913 63913	U3914 U3915	C3919	A3923	<mark>c3926</mark>	<mark>U3932</mark>	<mark>C3935</mark>	63938 63939								
A3942	A3943 G3944	A3945		C3948 A3949	U3950	G3951	G3953	A3954	63956 (3956	U3957	G3958 U3959	A3960	G3961	A3963	U3964	A3966	G3967	0.3969 G3969	G3970	G3971 A3972	G3973	G3974 C3975	C3976	C3977	C3979	G3980 G3981	C3982	C3984	C3985	C3987	C3389	G3991	G 3992	G3994	U3995 C3996	C3997 C3998	C3999 G4000	
C4001	44003	G4004 <b>G</b> 4005	G4006	G4007 C4008	C4009	C4010	G4011 G4012	G4013	G4014 C4015	G4016	G4017 G4018	G4019	U4020	C4021 C4022	G4023	C4025	G4026	G4027 C4028	C4029	C4030	G4032	C4033	G4035	G4036	C4038	G4039 C4040	C4041	G4042 G4043	U4044	A4046	A4041 A4048	04049 A4050	C4051	C4052 A4053	C4054	A4056	U4058	U4060
G4061	U4063	C4064	U4066	U4067	VLOVJ	04074 U4075	G4076 A4077	C4078	U4083 G4084	C4088		G4094 G4095	C4096	G4097 A4098	G4099	C4100 C4101	C4102	C4103	A4105	G4106 G4107	G4108	G4109		C4112	C4114	G4115 C4116	U4117 U4118	C4119 U4120	C4123	G4129	C4133 C4134	G4135	G4136 C4137	C4138	C4140			
G4141	G4143	C4144 C4145	G4146	G4147 C4148	C4149	00155	C4162 U4163	A4170	C4171	G4183 G4184	G4185	U4189	04190 G4191	A4192 C4193	U4194 G4195	G4196 G4197	G4198	C4199	G4200 G4201	U4202 A4203	C4204 A4205	C4206	A4212 A2213	A4214	44220	C4221	64225 64226	04227 04228 64228	U4229	A4233 A4234	C4243	G4247						
A4248 G4249	G4250 A4251	C4252 A4253	G4254 A4255	A4256 A4257	C4258	04260 U4260	C4261 C4262	C4263 G4264	U4265	A4268	A4271	A4273	A4279	A4280 A4281	C4284	U4285 C4286	U4289	U4290 C4291	44292 A4292	04293 C4294	04295 U4296	G4297 A4298	U4299	C4303 A4304	G4305 U4306	A4307 C4308	C4314	C4319	G4329	64330 64331 C4332								
C4335	A4339	U4340 C4341	C4342	C4349 C4350	U4351 U4352	U4353 114254	04355 G4355	U4360	U4361	G4364 C4365	G4370	G4371 U4372	G4373	G4377	A4379	A4380 A4381	G4382	C4387	U4395 A4396	C P		500	C4402	04406	C4413 A4414	G4415	C4417 G4418	U4419	C4421	A4422 U4423	A4424 G4425							
C4426 G4427	A4428	C4423	U4435	U4436 U4437	n	G	4 D U	00	o D	С G4448	G4451	U4452 C4453	C4456		C4461	A4464	04465 C4466	U4469	G4470 U4471	G4472	G4475 C4476	A4477	U4481	C4483	A4404	64489 64489		114498	G4499	C4502 A4503	C4504							
C4505	C4508	U4512 A4513	A4518	C4519	G4522 A4523	G4524	G4529		A4535 C4536	C4537	G4545 A4546	C4547	64549 64549	G4550	U4555 U4556	U4557 U4558	A4559 C4560	C4561 C4562	04563 N4563	1001H	G4570	A4571	G4575	A4584	A4589 A4590	U4594	G4595 C4596	U4597 C4598	64600 64600									
A4607 G4608	C4612	C4613 G4614	U4620	G4623	U4627	U4628	A4635	04637 G4637	04638 G4639	A4656	U4657	C4662 G4663	A4664	C4667	04000 A4669	C4671 C4671	A4672 U4673	C4674	G4678	U4682	U4685 C4686	A4687	G4690	C4693	G4694 C4695	04697 04697	C4698 U4699	A4/00 A4701	A4708 114709	C4710 C4711 C4711								
C4712 G4713	C4714	G4719 C4720	<mark>G4721</mark> G4722	C4730	G4731	C4733	A4734 G4735	C4738	C4739	C4741	G4742	G4745 C4746	C4747	U4752	G4754	C4757	04759 C4759	G4760 G4761	A4764	G4765 C4766	C4771	C4772	C4774	C4775 G4776	ი ი	υυ	50	00	ບບ	υυυ	00							
o a	A C	ບອ	0 5	00	υυ	00	טטני	ט ט ז	U U	ප ප	5 5	A G	000	500	500	e c	ი ი	ບບ	0 5	00	) <del>(</del> )		5 5 5	500	9 9 8	A A A	C4858	U4864	G4870 C4871	G4872 G4873								
A4874	G4877 C4878	<mark>C4879</mark> C4880	U4881 U4882	C4883	C4886 C4887	U4888	000 00 00 00 00 00 00 00 00 00 00 00 00		C4900 G4901	G4910	A4911 64912	64913 64913	G4915 G4915	C4923	C4926	G4927 C4928	A4934	44938	C4939	G4941	C4942 A4943	C4944 G4945	G4949	G4960	C4969	C4970 A4971	U4972 U4973	U4976	G4981	A4962 C4983	•							









• Molecule 53: Protein SDA1 homolog







LEU LYVAL LYVAL CILY GULY GULY ALL LLYS CULYS CU

ALA THR THR PPRO CUU CLUEU CLUEU CLUEU PPRO CLUEU THR PPRO CLUEU C

TYR ALA GLN VAL THR ASN THR ASN PRO GLU PRO GLU ASN ASP ASP ASP ASP LLEU VAL LLEU VAL LLEU VAL



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41193	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 $(e^-/\text{\AA}^2)$	1.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.223	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0365	Depositor
Map size (Å)	548.0, 548.0, 548.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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: M7A, 6MZ, B9H, B8H, I4U, P7G, 7MG, A2M, B8W, 1MA, GDP, E7G, E6G, K, B8K, B9B, OMG, MHG, B8T, 2MG, B8Q, UR3, P4U, 5MU, BGH, MG, 5MC, OMC, OMU

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	Bo	ond lengths		Bond angles
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	5	0.43	0/2858	1.35	38/4455~(0.9%)
2	6	0.34	0/1877	0.75	2/2554~(0.1%)
3	7	0.37	0/1181	0.68	0/1563
4	8	0.45	0/3679	1.40	64/5732~(1.1%)
5	9	0.34	0/808	0.84	3/1076~(0.3%)
6	В	0.32	0/3315	0.70	3/4435~(0.1%)
7	С	0.29	0/777	0.77	1/1026~(0.1%)
8	D	0.31	0/2907	0.75	4/3905~(0.1%)
9	Ε	0.32	0/774	0.67	1/1038~(0.1%)
10	F	0.29	0/878	0.72	0/1170
11	G	0.34	0/1971	0.73	2/2651~(0.1%)
12	Н	0.35	0/1023	0.71	0/1351
13	Ι	0.33	0/1537	0.75	3/2066~(0.1%)
14	Κ	0.30	0/843	0.65	0/1115
15	L	0.29	0/1191	0.65	0/1591
16	М	0.31	0/720	0.70	0/952
17	Ν	0.39	0/1341	0.88	2/1793~(0.1%)
18	0	0.37	0/575	0.90	2/761~(0.3%)
19	Р	0.31	0/454	0.66	0/599
20	Q	0.33	0/1732	0.70	0/2315
21	S	0.36	0/1133	0.76	3/1516~(0.2%)
22	U	0.29	0/1746	0.66	0/2338
23	V	0.31	0/1682	0.67	1/2250~(0.0%)
24	W	0.33	0/831	0.70	0/1095
25	Х	0.30	0/718	0.61	0/953
26	Ζ	0.30	0/1537	0.68	0/2052
27	a	0.33	0/1255	0.75	2/1662~(0.1%)
28	b	0.32	0/1501	0.65	0/2013
29	с	0.33	0/1291	0.71	$2\overline{/1725}~(0.1\%)$
30	е	0.33	0/993	0.75	1/1332~(0.1%)
31	g	0.29	0/984	0.60	0/1323



Mal	Chain	Bo	ond lengths	Bond angles	
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
32	h	0.31	0/1132	0.68	0/1504
33	i	0.35	0/1130	0.70	1/1507~(0.1%)
34	1	0.30	0/1017	0.69	0/1364
35	m	0.32	0/1936	0.71	1/2596~(0.0%)
36	n	0.30	0/895	0.76	3/1198~(0.3%)
37	0	0.31	0/1935	0.69	0/2596
38	р	0.34	0/1916	0.69	0/2553
39	r	0.33	0/2428	0.70	3/3252~(0.1%)
40	А	0.31	0/2515	0.60	3/3403~(0.1%)
41	R	0.36	0/1317	0.72	2/1757~(0.1%)
42	J	0.39	0/1844	0.72	1/2476~(0.0%)
43	Т	0.29	0/345	0.77	0/455
44	2	0.44	7/84533~(0.0%)	1.36	1230/131714~(0.9%)
45	У	0.31	0/1269	0.71	1/1712~(0.1%)
46	4	0.33	0/5099	0.77	12/6840~(0.2%)
47	d	0.37	0/864	0.78	2/1160~(0.2%)
48	j	0.34	0/933	0.73	0/1256
49	k	0.31	0/1082	0.71	1/1443~(0.1%)
50	Y	0.30	0/1383	0.66	2/1856~(0.1%)
51	Z	0.33	0/587	0.84	1/767~(0.1%)
52	t	0.31	0/1736	0.62	2/2328~(0.1%)
53	u	0.39	2/4614~(0.0%)	0.65	4/6191~(0.1%)
54	V	0.31	0/321	0.55	0/418
All	All	0.39	9/164943~(0.0%)	1.14	$14\overline{03/240753}\ (0.6\%)$

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	В	0	1
11	G	0	1
17	Ν	0	1
20	Q	0	1
29	с	0	1
30	е	0	1
35	m	0	2
36	n	0	1
42	J	0	1
50	Y	0	1
53	u	0	3
All	All	0	14



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	u	668	PHE	CD2-CE2	11.13	1.61	1.39
53	u	668	PHE	CE2-CZ	9.61	1.55	1.37
44	2	4060	U	O3'-P	7.15	1.69	1.61
44	2	4062	А	O3'-P	6.91	1.69	1.61
44	2	4061	G	O3'-P	6.69	1.69	1.61

The worst 5 of 9 bond length outliers are listed below:

The worst 5 of 1403 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
44	2	485	C	C2-N1-C1'	14.89	135.18	118.80
18	0	30	ASP	CB-CG-OD1	12.50	129.55	118.30
44	2	753	C	N1-C2-O2	12.46	126.38	118.90
44	2	485	С	N1-C2-O2	12.20	126.22	118.90
4	8	128	С	N1-C2-O2	12.03	126.12	118.90

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	В	16	PHE	Peptide
11	G	162	ASP	Peptide
17	N	117	ILE	Peptide
20	Q	154	VAL	Peptide
29	с	80	VAL	Peptide

## 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
2	6	242/245~(99%)	225~(93%)	17 (7%)	0	100	100
3	7	133/163~(82%)	129~(97%)	4 (3%)	0	100	100
5	9	93/134~(69%)	81 (87%)	12 (13%)	0	100	100
6	В	401/403~(100%)	376 (94%)	25 (6%)	0	100	100
7	С	89/159~(56%)	87 (98%)	2 (2%)	0	100	100
8	D	356/427~(83%)	331 (93%)	25 (7%)	0	100	100
9	Е	96/115~(84%)	92 (96%)	4 (4%)	0	100	100
10	F	107/117~(92%)	104 (97%)	3 (3%)	0	100	100
11	G	240/266~(90%)	229 (95%)	11 (5%)	0	100	100
12	Н	120/123~(98%)	116 (97%)	4 (3%)	0	100	100
13	Ι	188/192~(98%)	178 (95%)	10 (5%)	0	100	100
14	К	100/105~(95%)	95 (95%)	5 (5%)	0	100	100
15	L	145/148~(98%)	135 (93%)	10 (7%)	0	100	100
16	М	84/97~(87%)	78 (93%)	6 (7%)	0	100	100
17	Ν	163/178~(92%)	140 (86%)	21 (13%)	2 (1%)	13	48
18	Ο	67/70~(96%)	63 (94%)	4 (6%)	0	100	100
19	Р	48/51~(94%)	47 (98%)	1 (2%)	0	100	100
20	Q	208/211~(99%)	195 (94%)	13 (6%)	0	100	100
21	S	133/215~(62%)	127 (96%)	6 (4%)	0	100	100
22	U	201/204~(98%)	192 (96%)	9 (4%)	0	100	100
23	V	199/203~(98%)	193 (97%)	6 (3%)	0	100	100
24	W	98/106~(92%)	94 (96%)	4 (4%)	0	100	100
25	Х	89/92~(97%)	85 (96%)	4 (4%)	0	100	100
26	Z	185/188~(98%)	180 (97%)	5 (3%)	0	100	100
27	a	146/196~(74%)	140 (96%)	6 (4%)	0	100	100
28	b	174/176~(99%)	168 (97%)	6 (3%)	0	100	100
29	с	153/160~(96%)	149 (97%)	4 (3%)	0	100	100
30	е	129/140~(92%)	114 (88%)	15 (12%)	0	100	100
31	g	116/156~(74%)	113 (97%)	3 (3%)	0	100	100
32	h	132/145~(91%)	130 (98%)	2 (2%)	0	100	100
33	i	133/136~(98%)	121 (91%)	12 (9%)	0	100	100
34	1	123/137~(90%)	117 (95%)	6 (5%)	0	100	100

Continued on next page...



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
35	m	246/257~(96%)	216 (88%)	30 (12%)	0	100	100
36	n	107/110~(97%)	103 (96%)	3~(3%)	1 (1%)	17	55
37	0	231/288~(80%)	215~(93%)	16 (7%)	0	100	100
38	р	224/248~(90%)	213~(95%)	11 (5%)	0	100	100
39	r	291/297~(98%)	278~(96%)	13~(4%)	0	100	100
40	А	305/731~(42%)	296 (97%)	8(3%)	1 (0%)	41	76
41	R	151/203~(74%)	143~(95%)	7 (5%)	1 (1%)	22	60
42	J	221/239~(92%)	209 (95%)	12 (5%)	0	100	100
43	Т	42/99~(42%)	42 (100%)	0	0	100	100
45	У	163/165~(99%)	159 (98%)	4 (2%)	0	100	100
46	4	607/634~(96%)	559~(92%)	45 (7%)	3~(0%)	29	68
47	d	102/128~(80%)	94 (92%)	8 (8%)	0	100	100
48	j	109/125~(87%)	103 (94%)	6 (6%)	0	100	100
49	k	127/135~(94%)	121 (95%)	6 (5%)	0	100	100
50	Y	165/184~(90%)	154 (93%)	11 (7%)	0	100	100
51	Z	63/129~(49%)	60~(95%)	2(3%)	1 (2%)	9	40
52	t	210/217~(97%)	201 (96%)	9 (4%)	0	100	100
53	u	546/687~(80%)	515 (94%)	30 (6%)	1 (0%)	47	82
54	v	33/260~(13%)	33 (100%)	0	0	100	100
All	All	8834/10594 (83%)	8338 (94%)	486 (6%)	10 (0%)	54	85

Continued from previous page...

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Ν	176	PRO
36	n	106	TYR
40	А	160	MET
53	u	326	GLY
17	N	21	CYS

#### 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.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	6	212/213~(100%)	212 (100%)	0	100	100
3	7	126/149~(85%)	126 (100%)	0	100	100
5	9	82/114~(72%)	80~(98%)	2(2%)	49	79
6	В	349/349~(100%)	348 (100%)	1 (0%)	92	97
7	С	78/126~(62%)	78 (100%)	0	100	100
8	D	298/348~(86%)	297 (100%)	1 (0%)	92	97
9	Е	83/97~(86%)	83 (100%)	0	100	100
10	F	94/100~(94%)	93~(99%)	1 (1%)	73	90
11	G	204/223~(92%)	204 (100%)	0	100	100
12	Н	109/110 (99%)	109 (100%)	0	100	100
13	Ι	169/171~(99%)	167 (99%)	2 (1%)	71	90
14	К	86/89~(97%)	86 (100%)	0	100	100
15	L	120/121 (99%)	120 (100%)	0	100	100
16	М	73/80~(91%)	73 (100%)	0	100	100
17	Ν	138/149~(93%)	138 (100%)	0	100	100
18	О	64/65~(98%)	64 (100%)	0	100	100
19	Р	47/48~(98%)	47 (100%)	0	100	100
20	Q	176/177~(99%)	176 (100%)	0	100	100
21	S	115/161 (71%)	114 (99%)	1 (1%)	78	92
22	U	171/172~(99%)	171 (100%)	0	100	100
23	V	173/174 (99%)	173 (100%)	0	100	100
24	W	88/94~(94%)	88 (100%)	0	100	100
25	Х	74/75~(99%)	74 (100%)	0	100	100
26	Z	164/165~(99%)	164 (100%)	0	100	100
27	a	133/175~(76%)	133 (100%)	0	100	100
28	b	157/157~(100%)	157 (100%)	0	100	100
29	с	136/140~(97%)	136 (100%)	0	100	100
30	е	101/107~(94%)	100 (99%)	1 (1%)	76	91
31	g	106/133~(80%)	106 (100%)	0	100	100
32	h	124/135~(92%)	124 (100%)	0	100	100

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

Continued on next page...



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles	3
33	i	117/118~(99%)	116 (99%)	1 (1%)	78	92	
34	1	109/121~(90%)	109 (100%)	0	100	100	
35	m	190/199~(96%)	190 (100%)	0	100	100	
36	n	88/89~(99%)	88 (100%)	0	100	100	
37	0	208/252~(82%)	206 (99%)	2 (1%)	76	91	
38	р	195/215~(91%)	195 (100%)	0	100	100	
39	r	246/250~(98%)	245 (100%)	1 (0%)	91	97	
40	А	272/654~(42%)	272 (100%)	0	100	100	
41	R	141/184~(77%)	140 (99%)	1 (1%)	84	94	
42	J	199/214~(93%)	199 (100%)	0	100	100	
43	Т	37/76~(49%)	37~(100%)	0	100	100	
45	У	137/137~(100%)	137 (100%)	0	100	100	
46	4	554/574~(96%)	553~(100%)	1 (0%)	93	98	
47	d	94/115~(82%)	93~(99%)	1 (1%)	73	90	
48	j	101/110~(92%)	100 (99%)	1 (1%)	76	91	
49	k	115/121~(95%)	115 (100%)	0	100	100	
50	Y	147/163~(90%)	146 (99%)	1 (1%)	84	94	
51	Z	61/115~(53%)	60~(98%)	1 (2%)	62	86	
52	t	191/196~(97%)	189 (99%)	2 (1%)	76	91	
53	u	509/629~(81%)	507 (100%)	2(0%)	91	97	
54	v	$\overline{32/228}\ (14\%)$	31 (97%)	1 (3%)	40	75	
All	All	7793/9177 (85%)	7769 (100%)	24 (0%)	92	97	

Continued from previous page...

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	4	385	ARG
50	Y	97	ASN
48	j	100	ASN
51	Z	112	ARG
13	Ι	93	ARG

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



Mol	Chain	Res	Type
48	j	100	ASN
52	t	171	HIS
54	V	10	HIS
53	u	155	ASN
35	m	215	ASN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	119/120~(99%)	14 (11%)	0
4	8	155/156~(99%)	28~(18%)	0
44	2	3543/5054~(70%)	868~(24%)	22~(0%)
All	All	3817/5330~(71%)	910~(23%)	22~(0%)

5 of 910 RNA backbone outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	5	11	А
1	5	22	А
1	5	24	С
1	5	33	U
1	5	40	U

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	2	4202	U
44	2	4382	G
44	2	4380	А
44	2	4498	U
44	2	2760	G

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

78 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.



Mol	Type	Chain	Res	Link	B	Bond lengths Counts $  BMSZ   \#  Z  > 2$			Bond angles Counts   $BMSZ   \#  Z  > 2$		
44	A2M	2	1871	53,44	18,25,26	3.58	$\frac{1}{2} = \frac{1}{2}$	18,36,39	3.47	$\frac{\pi}{2} > 2$ 3 (16%)	
44	A2M	2	2401	44	18,25,26	3.62	8 (44%)	18,36,39	3.37	3 (16%)	
44	OMG	2	1883	44	18,26,27	2.90	8 (44%)	19,38,41	1.56	4 (21%)	
44	OMG	2	1316	44	18,26,27	2.85	8 (44%)	19,38,41	1.54	5 (26%)	
44	A2M	2	1326	44	18,25,26	3.63	8 (44%)	18,36,39	<b>3.53</b>	4 (22%)	
44	B9B	2	1574	44	21,28,29	1.95	3 (14%)	23,40,43	6.43	5 (21%)	
44	OMG	2	4637	44	18,26,27	2.86	8 (44%)	19,38,41	1.54	4 (21%)	
44	A2M	2	3718	44	18,25,26	3.58	8 (44%)	18,36,39	<b>3.39</b>	4 (22%)	
44	B8W	2	4129	44	18,26,27	2.11	2 (11%)	21,38,41	2.42	7 (33%)	
44	A2M	2	398	44	18,25,26	3.61	8 (44%)	18,36,39	3.44	4 (22%)	
44	B8H	2	1860	44	20,22,23	6.60	6 (30%)	21,32,35	2.36	5 (23%)	
44	2MG	2	978	44	18,26,27	2.72	6 (33%)	16,38,41	1.38	4 (25%)	
44	5MC	2	4335	44	18,22,23	<mark>3.59</mark>	7 (38%)	26,32,35	1.11	2 (7%)	
44	OMU	2	4620	44	19,22,23	2.97	8 (42%)	26,31,34	1.69	4 (15%)	
44	5MU	2	4083	44	19,22,23	7.22	8 (42%)	28,32,35	3.42	10 (35%)	
44	OMG	2	4370	44	18,26,27	2.87	8 (44%)	19,38,41	1.50	5 (26%)	
44	OMG	2	2424	44	18,26,27	2.87	8 (44%)	19,38,41	1.50	4 (21%)	
44	OMC	2	4536	44	19,22,23	2.98	8 (42%)	26,31,34	1.13	3 (11%)	
44	E6G	2	4355	44	20,27,28	2.81	3 (15%)	22,39,42	<b>3.26</b>	7 (31%)	
44	OMC	2	3869	44	19,22,23	<mark>3.06</mark>	8 (42%)	26,31,34	1.56	4 (15%)	
44	OMG	2	4494	44	18,26,27	2.85	8 (44%)	19,38,41	1.45	4 (21%)	
44	B8W	2	2380	44	18,26,27	2.09	2 (11%)	21,38,41	2.46	7 (33%)	
44	B8W	2	4529	44	18,26,27	2.13	2 (11%)	21,38,41	2.71	7 (33%)	
44	A2M	2	3825	44	18,25,26	3.58	8 (44%)	18,36,39	<mark>3.38</mark>	3 (16%)	
44	OMC	2	2804	44	19,22,23	2.91	8 (42%)	26,31,34	1.36	3 (11%)	
44	B8W	2	4185	44	18,26,27	2.12	2 (11%)	21,38,41	2.49	6 (28%)	
44	B9B	2	2754	44	21,28,29	2.00	3 (14%)	23,40,43	<mark>6.39</mark>	5 (21%)	
44	2MG	2	1517	44	18,26,27	2.71	6 (33%)	16,38,41	1.55	4 (25%)	
44	7MG	2	2522	44	22,26,27	<mark>3.73</mark>	10 (45%)	29,39,42	1.96	9 (31%)	
44	OMG	2	373	44	18,26,27	2.88	8 (44%)	19,38,41	1.59	5 (26%)	
44	OMC	2	3701	44	19,22,23	2.99	8 (42%)	26,31,34	0.78	0	
44	OMC	2	2861	44	19,22,23	3.06	8 (42%)	26,31,34	1.18	3 (11%)	
44	B8T	2	4483	44	19,22,23	<mark>3.65</mark>	8 (42%)	26,31,34	1.31	3 (11%)	

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	Bond angles		
WIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
44	B8W	2	4472	44	$18,\!26,\!27$	2.15	2 (11%)	21,38,41	2.59	7 (33%)
44	A2M	2	1534	44	18,25,26	<mark>3.58</mark>	8 (44%)	18,36,39	3.56	4 (22%)
44	OMG	2	1522	44	18,26,27	2.81	8 (44%)	19,38,41	1.50	5 (26%)
44	OMG	2	2364	44	18,26,27	2.85	8 (44%)	19,38,41	1.50	5 (26%)
44	UR3	2	1866	53,44	19,22,23	2.95	<mark>6 (31%)</mark>	26,32,35	2.11	<mark>6 (23%)</mark>
44	M7A	2	4564	44	20,25,26	1.99	3(15%)	28,37,40	3.87	7 (25%)
44	A2M	2	3867	44	18,25,26	<mark>-3.57</mark>	8 (44%)	18,36,39	3.45	4 (22%)
44	B8K	2	3897	44	24,28,29	<b>3.43</b>	11 (45%)	30,42,45	2.51	11 (36%)
44	E7G	2	1797	44	24,27,28	4.07	11 (45%)	30,40,43	2.18	<mark>9 (30%)</mark>
44	OMG	2	4870	44	18,26,27	2.87	8 (44%)	19,38,41	1.56	4 (21%)
44	OMC	2	3887	44	19,22,23	<mark>3.03</mark>	8 (42%)	26,31,34	0.83	1 (3%)
44	2MG	2	729	44	18,26,27	2.68	<mark>6 (33%)</mark>	16,38,41	1.42	4 (25%)
44	B8Q	2	1456	44	17,22,23	2.95	<mark>5 (29%)</mark>	22,32,35	2.30	<mark>6 (27%)</mark>
44	2MG	2	4872	44	18,26,27	<mark>2.61</mark>	6 (33%)	16,38,41	1.72	4 (25%)
44	UR3	2	4597	44	19,22,23	2.78	7 (36%)	26,32,35	1.93	4 (15%)
44	OMC	2	2365	44	19,22,23	3.00	8 (42%)	26,31,34	0.76	0
44	P7G	2	3880	44	24,28,29	4.09	11 (45%)	27,41,44	1.47	4 (14%)
44	7MG	2	1605	44	22,26,27	3.82	10 (45%)	29,39,42	1.96	9 (31%)
44	MHG	2	4371	44	29,32,33	<mark>3.93</mark>	11 (37%)	34,46,49	2.37	12 (35%)
44	A2M	2	3723	44	18,25,26	3.56	8 (44%)	18,36,39	3.37	4 (22%)
44	1MA	2	4415	44	16,25,26	4.38	5 (31%)	18,37,40	1.67	3 (16%)
44	B8H	2	4296	44	20,22,23	<mark>6.62</mark>	<mark>6 (30%)</mark>	21,32,35	2.39	<mark>5 (23%)</mark>
44	UR3	2	4530	44	19,22,23	2.86	<mark>6 (31%)</mark>	26,32,35	1.28	2 (7%)
44	E7G	2	2297	44	24,27,28	4.02	11 (45%)	30,40,43	2.15	10 (33%)
44	P4U	2	1348	44	21,24,25	<mark>3.62</mark>	8 (38%)	27,33,36	1.06	1 (3%)
44	BGH	2	3899	44	25,29,30	4.62	17 (68%)	31,43,46	2.59	12 (38%)
44	B9B	2	237	44	21,28,29	2.00	3 (14%)	23,40,43	6.42	<b>5</b> (21%)
44	7MG	2	4550	44	22,26,27	<mark>3.82</mark>	10 (45%)	29,39,42	1.92	8 (27%)
44	B8T	2	4671	44	19,22,23	<mark>3.59</mark>	8 (42%)	26,31,34	0.93	1 (3%)
44	OMU	2	4306	44	19,22,23	<mark>3.04</mark>	8 (42%)	26,31,34	1.69	4 (15%)
44	OMG	2	2050	44	18,26,27	2.83	8 (44%)	19,38,41	1.49	4 (21%)
44	6MZ	2	4220	44	18,25,26	1.87	3 (16%)	16,36,39	3.75	3 (18%)
44	B8K	2	4690	44	24,28,29	3.42	11 (45%)	30,42,45	2.59	11 (36%)
44	P7G	2	1909	44	24,28,29	4.05	11 (45%)	27,41,44	1.55	3 (11%)
44	I4U	2	1659	44	21,24,25	3.59	9 (42%)	27,34,37	1.20	1 (3%)



Mal	Turne	Chain	Dec	Tinle	B	ond leng	gths	Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
44	A2M	2	2363	44	18,25,26	<mark>3.60</mark>	8 (44%)	18,36,39	3.40	4 (22%)
44	B9H	2	2786	44	20,25,26	3.28	5 (25%)	22,35,38	2.40	7 (31%)
44	A2M	2	4571	44	18,25,26	<mark>3.58</mark>	8 (44%)	18,36,39	3.42	4 (22%)
44	A2M	2	4523	44	18,25,26	<mark>-3.57</mark>	8 (44%)	18,36,39	3.45	4 (22%)
44	A2M	2	1524	44	18,25,26	3.62	8 (44%)	18,36,39	3.44	4 (22%)
44	OMC	2	3909	44	19,22,23	3.01	8 (42%)	26,31,34	1.24	5 (19%)
44	OMG	2	2773	44	18,26,27	2.91	8 (44%)	19,38,41	1.54	5 (26%)
4	OMU	8	14	4,44	19,22,23	2.99	8 (42%)	26,31,34	1.78	5 (19%)
44	OMG	2	1625	44	18,26,27	2.91	8 (44%)	19,38,41	1.50	4 (21%)
44	OMG	2	4623	44	18,26,27	2.86	8 (44%)	19,38,41	1.55	5 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
44	A2M	2	1871	53,44	-	0/5/27/28	0/3/3/3
44	A2M	2	2401	44	-	1/5/27/28	0/3/3/3
44	OMG	2	1883	44	-	2/5/27/28	0/3/3/3
44	OMG	2	1316	44	-	0/5/27/28	0/3/3/3
44	A2M	2	1326	44	-	3/5/27/28	0/3/3/3
44	B9B	2	1574	44	-	3/7/29/30	0/3/3/3
44	OMG	2	4637	44	-	3/5/27/28	0/3/3/3
44	A2M	2	3718	44	-	0/5/27/28	0/3/3/3
44	B8W	2	4129	44	-	2/5/27/28	0/3/3/3
44	A2M	2	398	44	-	2/5/27/28	0/3/3/3
44	B8H	2	1860	44	-	2/7/25/26	0/2/2/2
44	2MG	2	978	44	-	0/5/27/28	0/3/3/3
44	5MC	2	4335	44	-	0/7/25/26	0/2/2/2
44	OMU	2	4620	44	-	0/9/27/28	0/2/2/2
44	5MU	2	4083	44	-	0/7/25/26	0/2/2/2
44	OMG	2	4370	44	-	1/5/27/28	0/3/3/3
44	OMG	2	2424	44	-	2/5/27/28	0/3/3/3
44	OMC	2	4536	44	-	0/9/27/28	0/2/2/2
44	E6G	2	4355	44	-	2/6/28/29	0/3/3/3
44	OMC	2	3869	44	-	4/9/27/28	0/2/2/2
44	OMG	2	4494	44	-	0/5/27/28	0/3/3/3

Continued on next page...



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	B8W	2	2380	44	-	2/5/27/28	0/3/3/3
44	B8W	2	4529	44	-	0/5/27/28	0/3/3/3
44	A2M	2	3825	44	-	0/5/27/28	0/3/3/3
44	OMC	2	2804	44	-	0/9/27/28	0/2/2/2
44	B8W	2	4185	44	-	2/5/27/28	0/3/3/3
44	B9B	2	2754	44	-	2/7/29/30	0/3/3/3
44	2MG	2	1517	44	-	0/5/27/28	0/3/3/3
44	7MG	2	2522	44	-	0/7/37/38	0/3/3/3
44	OMG	2	373	44	-	1/5/27/28	0/3/3/3
44	OMC	2	3701	44	-	4/9/27/28	0/2/2/2
44	OMC	2	2861	44	-	0/9/27/28	0/2/2/2
44	B8T	2	4483	44	-	0/7/27/28	0/2/2/2
44	B8W	2	4472	44	-	2/5/27/28	0/3/3/3
44	A2M	2	1534	44	-	1/5/27/28	0/3/3/3
44	OMG	2	1522	44	-	0/5/27/28	0/3/3/3
44	OMG	2	2364	44	-	2/5/27/28	0/3/3/3
44	UR3	2	1866	53,44	-	3/7/25/26	0/2/2/2
44	M7A	2	4564	44	-	0/7/37/38	0/3/3/3
44	A2M	2	3867	44	-	2/5/27/28	0/3/3/3
44	B8K	2	3897	44	-	3/11/41/42	0/3/3/3
44	E7G	2	1797	44	-	2/9/39/40	0/3/3/3
44	OMG	2	4870	44	-	3/5/27/28	0/3/3/3
44	OMC	2	3887	44	-	1/9/27/28	0/2/2/2
44	2MG	2	729	44	-	2/5/27/28	0/3/3/3
44	B8Q	2	1456	44	-	0/7/42/43	0/2/2/2
44	2MG	2	4872	44	-	2/5/27/28	0/3/3/3
44	UR3	2	4597	44	-	0/7/25/26	0/2/2/2
44	OMC	2	2365	44	-	0/9/27/28	0/2/2/2
44	P7G	2	3880	44	-	4/10/40/41	0/3/3/3
44	7MG	2	1605	44	-	0/7/37/38	0/3/3/3
44	MHG	2	4371	44	-	3/16/46/47	0/3/3/3
44	A2M	2	3723	44	-	2/5/27/28	0/3/3/3
44	1MA	2	4415	44	-	3/3/25/26	0/3/3/3
44	B8H	2	4296	44	-	2/7/25/26	0/2/2/2
44	UR3	2	4530	44	-	0/7/25/26	0/2/2/2
44	E7G	2	2297	44	-	1/9/39/40	0/3/3/3
44	P4U	2	1348	44	-	1/10/29/30	0/2/2/2
44	BGH	2	3899	44	-	1/13/43/44	0/3/3/3

Continued from previous page...

Continued on next page...



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	B9B	2	237	44	-	5/7/29/30	0/3/3/3
44	7MG	2	4550	44	-	0/7/37/38	0/3/3/3
44	B8T	2	4671	44	-	0/7/27/28	0/2/2/2
44	OMU	2	4306	44	-	0/9/27/28	0/2/2/2
44	OMG	2	2050	44	-	0/5/27/28	0/3/3/3
44	6MZ	2	4220	44	-	1/5/27/28	0/3/3/3
44	B8K	2	4690	44	-	0/11/41/42	0/3/3/3
44	P7G	2	1909	44	-	3/10/40/41	0/3/3/3
44	I4U	2	1659	44	-	2/9/29/30	0/2/2/2
44	A2M	2	2363	44	-	0/5/27/28	0/3/3/3
44	B9H	2	2786	44	-	0/12/47/48	0/2/2/2
44	A2M	2	4571	44	-	0/5/27/28	0/3/3/3
44	A2M	2	4523	44	-	4/5/27/28	0/3/3/3
44	A2M	2	1524	44	-	1/5/27/28	0/3/3/3
44	OMC	2	3909	44	-	1/9/27/28	0/2/2/2
44	OMG	2	2773	44	-	0/5/27/28	0/3/3/3
4	OMU	8	14	4,44	-	1/9/27/28	0/2/2/2
44	OMG	2	1625	44	-	3/5/27/28	0/3/3/3
44	OMG	2	4623	44	-	1/5/27/28	0/3/3/3

Continued from previous page...

The worst 5 of 574 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
44	2	4083	5MU	C4-C5	20.79	1.79	1.44
44	2	4296	B8H	C6-C5	-16.51	1.11	1.34
44	2	1860	B8H	C6-C5	-16.35	1.12	1.34
44	2	4415	1MA	C2-N3	16.16	1.48	1.29
44	2	4083	5MU	C6-N1	15.93	1.65	1.38

The worst 5 of 380 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
44	2	1574	B9B	O6-C6-N1	-29.48	94.67	120.12
44	2	237	B9B	O6-C6-N1	-29.29	94.84	120.12
44	2	2754	B9B	O6-C6-N1	-29.20	94.92	120.12
44	2	4564	M7A	C5-C6-N6	13.69	147.13	123.74
44	2	4220	6MZ	C1'-N9-C4	-12.71	104.32	126.64

There are no chirality outliers.

5 of 100 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
4	8	14	OMU	C1'-C2'-O2'-CM2
44	2	237	B9B	C5-C6-O6-C61
44	2	237	B9B	N1-C6-O6-C61
44	2	237	B9B	C3'-C4'-C5'-O5'
44	2	237	B9B	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 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).

Mol	Type	Chain	Dog	Tink	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
WIOI	Moi Type Chain		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
55	GDP	А	801	57,56	24,30,30	1.20	2 (8%)	30,47,47	1.41	5 (16%)

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
55	GDP	А	801	57,56	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	А	801	GDP	C6-N1	-3.47	1.32	1.37

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(Å)	Ideal(Å)
55	А	801	GDP	C2'-C1'	-2.22	1.50	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
55	А	801	GDP	PA-O3A-PB	-3.52	120.74	132.83
55	А	801	GDP	C3'-C2'-C1'	3.26	105.89	100.98
55	А	801	GDP	C8-N7-C5	2.47	107.69	102.99
55	А	801	GDP	O3B-PB-O2B	2.35	116.63	107.64
55	А	801	GDP	C5-C6-N1	2.32	118.05	113.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	А	801	GDP	PA-O3A-PB-O2B
55	А	801	GDP	PA-O3A-PB-O1B

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 sup 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-35371. 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: 200



Y Index: 200



Z Index: 200

#### 6.2.2 Raw map



X Index: 200

Y Index: 200



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: 206



Y Index: 182



Z Index: 202

#### 6.3.2 Raw map



X Index: 205

Y Index: 189



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



## 6.4 Orthogonal standard-deviation projections (False-color) (i)

#### 6.4.1 Primary map



#### 6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



#### 6.5 Orthogonal surface views (i)

#### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0365. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.5.2 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.

#### 6.6 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  $1145 \text{ nm}^3$ ; this corresponds to an approximate mass of 1034 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 0.333  ${\rm \AA^{-1}}$ 



# 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 0.333  $\mathrm{\AA^{-1}}$ 



## 8.2 Resolution estimates (i)

<b>Bosolution ostimato</b> $(\hat{\lambda})$	Estim	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit		
Reported by author	3.00	-	-		
Author-provided FSC curve	-	-	-		
Unmasked-calculated*	3.91	7.10	4.01		

\*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 3.91 differs from the reported value 3.0 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35371 and PDB model 8IDY. Per-residue inclusion information can be found in section 3 on page 14.

# 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0365 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



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



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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0365).



## 9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.0365) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.7920	0.4860
2	0.8620	0.4910
4	0.6540	0.4620
5	0.9190	0.4800
6	0.7350	0.5080
7	0.8090	0.5400
8	0.9440	0.5440
9	0.5540	0.4670
А	0.6590	0.4950
В	0.9060	0.5680
С	0.7520	0.4750
D	0.9290	0.5640
Е	0.6830	0.5060
F	0.8820	0.5540
G	0.7040	0.4800
Н	0.8700	0.5420
Ι	0.8030	0.5240
J	0.1120	0.1850
Κ	0.8360	0.5280
L	0.9320	0.5790
Μ	0.9660	0.5810
Ν	0.4190	0.3070
Ο	0.6770	0.4920
Р	0.9760	0.5780
Q	0.8420	0.5250
R	0.4700	0.4450
S	0.8970	0.5510
Т	0.6060	0.4370
U	0.9680	0.5860
V	0.9220	0.5660
W	0.7290	0.5170
X	0.8050	0.5360
Y	0.8660	0.5560
Z	0.9480	0.5890
a	0.8740	0.5430

0.0 <0.0

1.0

Continued on next page...



Continued from previous page...

Chain	Atom inclusion	Q-score
b	0.9330	0.5780
С	0.8790	0.5320
d	0.7520	0.5180
е	0.8800	0.5480
g	0.8960	0.5580
h	0.8860	0.5570
i	0.7600	0.5220
j	0.8340	0.5350
k	0.9400	0.5790
1	0.9250	0.5640
m	0.9030	0.5600
n	0.9530	0.5870
О	0.7650	0.4980
р	0.9150	0.5590
r	0.6190	0.4250
t	0.0010	0.1380
u	0.0710	0.2110
V	0.0860	0.2300
У	0.1120	0.2100
Z	0.5670	0.4230

