

# wwPDB EM Validation Summary Report (i)

Mar 18, 2023 - 09:47 am GMT

PDB ID	:	8A3D
EMDB ID	:	EMD-15113
Title	:	Human mature large subunit of the ribosome with eIF6 and homoharringtonine
		bound
Authors	:	Faille, A.; Warren, A.J.; Dent, K.C.
Deposited on	:	2022-06-08
Resolution	:	1.67 Å(reported)
Based on initial model	:	6EK0

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

# 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 1.67 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{f Entries})$		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
Sidechain outliers	154315	3826		
RNA backbone	4643	859		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq=3, 2, 1$  and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq=5\%$  The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	А	5069	16%	35%
			11%	
2	В	121	84%	13% ••
0	C	1 5 5	16%	
3	C	157	65%	22% 6% • 6%
4	D	257	92%	• •
5	Е	403	20%	
6	F	427	10%	• 16%
_	a	207	45%	
7	G	297	93%	• •



Mol	Chain	Length	Quality of chain	
8	Н	288	37% 74%	24%
9	m	248	85%	15%
10	n	266	45%	• 16%
11	0	102	34%	
	0	192	25%	
12	р	214	94%	• 5%
13	q	178	95%	• •
14	r	211	96%	• •
15	S	220	63% 33	7%
16	1	204	99%	
17	Ι	203	97%	••
18	J	184	78% 59	<mark>% 17%</mark>
19	K	188	97%	
20	L	196	79%	20%
21	М	176	<mark>6%</mark> 96%	
22	Ν	160	25%	
23	0	128	73%	23%
24	Р	140	18%	• 6%
25	Q	157	10% 39% • 61%	
26	R	156	72%	24%
27	S	145	91%	• 8%
28	Т	136	59% 96%	
29	U	148	97%	
30	V	159	<u>31%</u> 56% • 41%	<u> </u>
31	W	115	50% 81%	6% 13%
32	Х	125	82%	• 15%



Mol	Chain	Length	Quality of chain	
33	Y	135	8%	7% 5%
34	Z	110	5% 95%	•••
35	a	117	90%	• 9%
36	b	196	61% · 38%	
37	с	105	41% 92%	5% •
38	d	97	88%	• 11%
39	е	70	76% 99%	·
40	f	51	96%	••
41	g	99	13% 53% 47%	
42	i	106	96%	••
43	j	92	98%	••
44	k	137	91%	9%
45	h	245	92%	• 8%



# 2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 142233 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 28S ribosomal RNA.

Mol	Chain	Residues			Atoms			AltConf	Trace
1	А	3303	Total 70928	C 31625	N 12983	O 23017	Р 3303	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	4910	А	G	conflict	GB 86475748

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

Mol	Chain	Residues		A	toms			AltConf	Trace
2	В	120	Total 2558	C 1141	N 456	0 842	Р 119	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
3	С	148	Total 3153	C 1408	N 563	O 1035	Р 147	0	0

• Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms				AltConf	Trace	
4	D	246	Total 1887	C 1183	N 387	0 311	S 6	0	0

• Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Е	395	Total 3194	C 2034	N 600	O 545	${ m S}$ 15	1	0

• Molecule 6 is a protein called 60S ribosomal protein L4.



Mol	Chain	Residues		At	oms			AltConf	Trace
6	F	359	Total 2855	C 1797	N 571	O 474	S 13	0	0

• Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues		At	AltConf	Trace			
7	G	285	Total 2308	C 1460	N 419	O 415	S 14	0	0

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

Mol	Chain	Residues		Ate	AltConf	Trace			
8	Н	219	Total 1757	C 1132	N 333	O 288	$\frac{S}{4}$	0	0

• Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	m	212	Total 1755	C 1127	N 334	O 285	S 9	0	0

• Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	n	223	Total 1809	C 1153	N 349	O 303	S 4	0	0

• Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues		At	AltConf	Trace			
11	О	190	Total 1518	C 956	N 284	0 272	S 6	0	0

• Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues		At	AltConf	Trace			
12	р	204	Total 1654	C 1051	N 318	0 272	S 13	0	0

• Molecule 13 is a protein called 60S ribosomal protein L11.



Mol	Chain	Residues		At	oms			AltConf	Trace
13	q	170	Total 1358	C 858	N 253	0 241	S 6	0	0

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

Mol	Chain	Residues		Ate	AltConf	Trace			
14	r	206	Total 1664	C 1041	N 345	0 274	${f S}$ $4$	0	0

• Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	s	139	Total 1138	C 730	N 218	0 183	${f S}{7}$	0	0

• Molecule 16 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues		Ate	oms		AltConf	Trace	
16	1	203	Total 1708	C 1077	N 360	O 267	${S \atop 4}$	1	0

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

Mol	Chain	Residues		At	AltConf	Trace			
17	Ι	199	Total 1634	C 1053	N 319	O 257	$\frac{S}{5}$	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
18	J	152	Total 1233	С 771	N 240	0 213	${ m S} 9$	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
19	K	187	Total 1513	C 944	N 314	O 250	${S \atop 5}$	0	0

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



Mol	Chain	Residues		At	oms			AltConf	Trace
20	L	157	Total 1304	C 813	N 280	O 202	S 9	0	0

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

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

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	Ν	159	Total 1298	C 823	N 252	0 217	S 6	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
23	Ο	99	Total 804	C 516	N 140	0 146	${ m S} { m 2}$	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
24	Р	132	Total 985	C 621	N 185	0 174	${ m S}{ m 5}$	0	0

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

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
25	Q	62	Total	С	N	0	S	0	0
-	-0	-	519	332	101	83	3	-	-

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
26	R	119	Total 976	C 624	N 183	0 168	S 1	0	0

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



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

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

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

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

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

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	V	94	Total 773	C 480	N 171	0 119	${ m S} { m 3}$	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
31	W	100	Total 772	C 490	N 136	0 139	S 7	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
32	X	106	Total 868	C 551	N 170	0 145	${ m S} { m 2}$	0	0

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

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

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



Mol	Chain	Residues		At	oms			AltConf	Trace
34	Z	109	Total 879	$\begin{array}{c} \mathrm{C} \\ 557 \end{array}$	N 174	0 144	$\frac{S}{4}$	1	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
35	a	106	Total 845	C 530	N 174	0 135	S 6	0	0

• Molecule 36 is a protein called Ribosomal protein uL29.

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

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

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
37	С	102	Total 832	C 521	N 177	0 129	${ m S}{ m 5}$	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
38	d	86	Total 713	C 442	N 155	0 111	${ m S}{ m 5}$	1	0

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

Mol	Chain	Residues		Ate	oms			AltConf	Trace
39	е	69	Total 569	C 366	N 103	O 99	S 1	0	0

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

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
40	f	50	Total 444	C 281	N 98	0 64	S 1	0	0

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



Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
41	g	52	Total 429	C 266	N 90	O 67	S 6	0	0

 $\bullet\,$  Molecule 42 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms				AltConf	Trace	
42	i	103	Total 842	C 528	N 172	O 136	S 6	0	0

• Molecule 43 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	91	Total 708	C 445	N 136	O 120	${f S}{7}$	0	0

• Molecule 44 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	124	Total 992	C 615	N 206	0 167	${f S}$ $4$	0	0

• Molecule 45 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	h	225	Total 1712	C 1065	N 295	O 340	S 12	0	0

• Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
46	А	214	Total         Mg           214         214	0
46	В	3	Total Mg 3 3	0
46	С	6	Total Mg 6 6	0
46	J	1	Total Mg 1 1	0
46	L	2	Total Mg 2 2	0
46	Р	1	Total Mg 1 1	0



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Mol	Chain	Residues	Atoms	AltConf
46	U	1	Total Mg 1 1	0
46	d	1	Total Mg 1 1	0

• Molecule 47 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
47	А	139	Total K 139 139	0
47	В	1	Total K 1 1	0
47	D	3	Total K 3 3	0
47	0	1	Total K 1 1	0
47	р	1	Total K 1 1	0
47	1	2	Total K 2 2	0
47	J	1	Total K 1 1	0
47	Ν	1	Total K 1 1	0
47	V	1	Total K 1 1	0
47	Y	1	Total K 1 1	0
47	Ζ	1	Total K 1 1	0
47	a	1	Total K 1 1	0
47	f	1	Total K 1 1	0
47	i	1	Total K 1 1	0

• Molecule 48 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
48	А	2	Total Na 2 2	0



• Molecule 49 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano yl]cephalotaxine (three-letter code: HMT) (formula:  $C_{29}H_{39}NO_9$ ).



Mol	Chain	Residues	Atoms				AltConf
40	Λ	1	Total	С	Ν	Ο	0
49	A	1	39	29	1	9	0

• Molecule 50 is SPERMINE (three-letter code: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms	AltConf
50	А	1	Total         C         N           14         10         4	0



• Molecule 51 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms				AltConf	
51	Δ	1	Total	С	Ν	0	$\mathbf{S}$	0
01	11	1	15	8	2	4	1	0

• Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
52	a	1	Total Zn 1 1	0
52	d	1	Total Zn 1 1	0
52	g	1	Total Zn 1 1	0
52	i	1	Total Zn 1 1	0
52	j	1	Total Zn 1 1	0

• Molecule 53 is water.

Mol	Chain	Residues	Atoms	AltConf
53	А	8641	Total O 8641 8641	0
53	В	261	Total         O           261         261	0



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Mol	Chain	Residues	Atoms	AltConf
52	C	262	Total O	0
- 55	U	202	363  363	0
52	р	191	Total O	0
- 55	D	101	131 131	0
53	F	177	Total O	0
- 55	Ľ	111	177 177	0
53	F	202	Total O	0
00	T,	202	202 202	0
53	G	67	Total O	0
		01	67 67	0
53	Н	49	Total O	0
	**	10	49 49	0
53	m	131	Total O	0
		101	131 131	Ŭ
53	n	46	Total O	0
			46 46	Ŭ
53	0	43	Total O	0
	-		43 43	
53	р	81	Total O	0
	r		81 81	
53	a	13	Total O	0
	1		13 13	
53	r	101	Total O	0
53	s	38	Total O	0
			38 38	
53	1	155	Total O	0
53	Ι	117	Total O	0
53	J	63	Iotal O	0
			03 03 Total 0	
53	Κ	139	10tal U 120 120	0
			159 159 Total O	
53	L	57	57 57	0
			Total O	
53	М	100	100 100	0
			Total O	
53	Ν	87	87 87	0
			Total O	
53	Ο	5	5 5	0
			0 0	



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Mol	Chain	Residues	Atoms	AltConf
53	Р	40	Total O 40 40	0
53	Q	21	$\begin{array}{c c} \hline Total & O \\ \hline 21 & 21 \\ \end{array}$	0
53	R	35	$\begin{array}{c c} \hline & & -1 \\ \hline & & \\ \hline \\ \hline$	0
53	S	49	Total         O           49         49	0
53	Т	13	Total O 13 13	0
53	U	92	Total O 92 92	0
53	V	39	Total O 39 39	0
53	W	9	Total O 9 9	0
53	Х	37	Total O 37 37	0
53	Y	112	Total O 112 112	0
53	Z	72	Total O 72 72	0
53	a	58	$\begin{array}{cc} \text{Total} & \text{O} \\ 58 & 58 \end{array}$	0
53	b	29	Total O 29 29	0
53	с	32	Total O 32 32	0
53	d	62	Total O 62 62	0
53	е	3	Total O 3 3	0
53	f	19	Total O 19 19	0
53	g	14	Total O 14 14	0
53	i	52	$\begin{array}{cc} \text{Total} & \text{O} \\ 52 & 52 \end{array}$	0
53	j	40	Total O 40 40	0
53	k	78	Total         O           78         78	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: 28S ribosomal RNA















PROTEIN DATA BANK













• Molecule 13: 60S ribosomal protein L11





• Molecule 17: 60S ribosomal protein L13a





• Molecule 23: 60S ribosomal protein L22





• Molecule 28: 60S ribosomal protein L27





Chain Y:	87%	7% 5%	
MET A2 A3 A3 P5 P6 P5 V8 P10	M. 1 W35 R39 R48 R48 V82 V82 V82 V82 K48 C83 K83 K83 K83 K83 K83 K83 K14 K114 K114 K128 K128 K128 K84 K128 K83 K83 K83 K83 K83 K83 K83 K83 K83 K8	SER GLU GLU GLU	
• Molecule 34: 6	0S ribosomal protein L35a		
Chain Z:	95%		
MET 82 82 960 960 661 662 663 K63			
• Molecule 35: 6	0S ribosomal protein L34		
Chain a:	90%	• 9%	
MET V2 N28 R29 C47 C49 P60	H73 H73 G1002 K1013 V103 V103 V103 V103 K105 C107 ALA GLN GLN GLN GLN GLN GLN GLN GLN C1VS C1VS C1VS C1VS C1VS C1VS C1VS C1VS		
• Molecule 36: R	tibosomal protein uL29		
Chain b:	% 61% •	38%	
MET ARG ARG ALA LEU GLY GLY ALA ALA ALA ALA LEU	PRIO GLY GLY ALA ALA ALA THR THR THR ALA ALD CLU ALA ALA ALA ALA ALA ALA ALA ALA ALA A	ARG ARG ARG ARG ARG ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
	**** ** ****** ** ***	···· · · · · · · · · ·	•• •
PRO SER GLU ALA ALA ALA ALA ALA ALA ALA	ALA MET MET 14 X5 X5 X6 X6 X12 C11 K12 K13 K13 K13 K13 K13 K13 K13 K13 K13 K13	639 A40 A41 842 842 842 847 843 877 877 877 875 875 875 875 875 875 875	R89 K97 H98 E99 E100
NIO1 + 100 K110 E111 K113 L113 L115 K122 + 100			
• Molecule 37: 6	0S ribosomal protein L36		
Chain c:	41% 92%	5% •	
MET A2 L3 R4 K4 K16 V17 V17 T18	K19 N20 V21 S22 F24 F24 R25 E46 E46 E46 E46 E59 F55 F55 F55 F55 F55 F55 F55 F55 F55 F	D66 K67 R68 K71 K71 E88 E89 C93 C93 C93 C93 C93 C93 C93 C93 C93 C9	A100 A101 A102 K103 LYS ASP
• Molecule 38: 6	0S ribosomal protein L37		
Chain d:	88%	• 11%	
MET 12 K36 F38 F38 F38 F38 F38 F38 F38 F38 F38 F38	ARG ALA ALA ALA ALA ALA SER SER SER SER		

 $\bullet$  Molecule 39: 60S ribosomal protein L38





 $\bullet$  Molecule 45: Eukaryotic translation initiation factor 6







# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1088709	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 $(e^-/\text{\AA}^2)$	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.602	Depositor
Minimum map value	-0.207	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	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: HMT, NA, UR3, MG, 5MC, PSU, A2M, OMC, OMG, 1MA, EPE, 6MZ, OMU, SPM, K, ZN

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		
	Ullaill	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.81	10/76619~(0.0%)	1.32	313/119498~(0.3%)	
2	В	0.75	0/2858	1.27	7/4455~(0.2%)	
3	С	0.78	0/3450	1.33	15/5372~(0.3%)	
4	D	0.57	0/1925	0.85	0/2581	
5	Е	0.58	0/3265	0.79	0/4369	
6	F	0.58	0/2909	0.82	0/3908	
7	G	0.60	0/2352	0.76	0/3152	
8	Н	0.60	0/1791	0.75	0/2403	
9	m	0.56	0/1789	0.80	1/2388~(0.0%)	
10	n	0.60	0/1840	0.79	1/2476~(0.0%)	
11	0	0.59	0/1537	0.78	0/2066	
12	р	0.58	0/1692	0.77	0/2258	
13	q	0.62	0/1381	0.78	0/1848	
14	r	0.59	0/1695	0.82	1/2270~(0.0%)	
15	s	0.57	0/1161	0.76	0/1554	
16	l	0.57	0/1753	0.89	0/2348	
17	Ι	0.56	0/1666	0.83	1/2228~(0.0%)	
18	J	0.58	0/1259	0.81	0/1689	
19	Κ	0.58	0/1537	0.90	1/2052~(0.0%)	
20	L	0.59	0/1320	0.79	1/1749~(0.1%)	
21	М	0.55	0/1501	0.80	0/2013	
22	Ν	0.58	0/1326	0.80	0/1770	
23	0	0.64	0/818	0.81	0/1098	
24	Р	0.59	0/999	0.81	0/1340	
25	Q	0.58	0/532	0.76	0/708	
26	R	0.57	0/993	0.73	0/1334	
27	S	0.59	0/1132	0.81	0/1504	
28	Т	0.60	0/1130	0.80	0/1507	
29	U	0.57	0/1191	0.83	0/1591	
30	V	0.62	0/786	0.88	2/1038~(0.2%)	
31	W	0.62	0/783	0.75	0/1052	
32	Х	0.57	0/883	0.81	0/1190	



Mol Chain		В	ond lengths	Bond angles		
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
33	Y	0.59	0/1071	0.86	2/1429~(0.1%)	
34	Ζ	0.55	0/901	0.81	0/1206	
35	a	0.61	0/855	0.85	0/1140	
36	b	0.59	0/1023	0.80	1/1351~(0.1%)	
37	с	0.59	0/843	0.86	0/1115	
38	d	0.61	0/732	0.92	0/968	
39	е	0.62	0/575	0.79	0/761	
40	f	0.58	0/454	0.83	0/599	
41	g	0.63	0/435	0.81	0/575	
42	i	0.60	0/855	0.86	0/1128	
43	j	0.65	0/718	0.80	0/953	
44	k	0.58	0/1007	0.82	0/1351	
45	h	0.70	0/1736	0.79	0/2362	
All	All	0.73	10/137078~(0.0%)	1.17	346/201747~(0.2%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	16
3	С	0	1
All	All	0	17

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	4291	G	P-O5'	6.95	1.66	1.59
1	А	4633	G	P-O5'	-6.86	1.52	1.59
1	А	2090	U	P-O5'	6.08	1.65	1.59
1	А	1723	А	P-O5'	5.84	1.65	1.59
1	А	347	А	P-O5'	5.45	1.65	1.59

The worst 5 of 346 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	417	G	O4'-C1'-N9	12.12	117.89	108.20
1	А	1925	G	O5'-P-OP2	-11.77	95.11	105.70
1	А	1947	U	P-O3'-C3'	-10.87	106.66	119.70
1	А	73	А	O5'-P-OP1	-10.40	96.34	105.70
1	А	3776	G	O4'-C1'-N9	9.95	116.16	108.20



There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Group
1	А	292	G	Sidechain
1	А	307	А	Sidechain
1	А	369	G	Sidechain
1	А	417	G	Sidechain
1	А	93	G	Sidechain

### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	70928	0	35879	138	0
2	В	2558	0	1295	3	0
3	С	3153	0	1603	15	0
4	D	1887	0	1983	6	0
5	Е	3194	0	3336	14	0
6	F	2855	0	3021	13	0
7	G	2308	0	2318	3	0
8	Н	1757	0	1910	2	0
9	m	1755	0	1859	0	0
10	n	1809	0	1941	0	0
11	0	1518	0	1600	0	0
12	р	1654	0	1705	0	0
13	q	1358	0	1388	0	0
14	r	1664	0	1773	0	0
15	s	1138	0	1204	0	0
16	l	1708	0	1756	0	0
17	Ι	1634	0	1779	1	0
18	J	1233	0	1263	5	0
19	Κ	1513	0	1628	3	0
20	L	1304	0	1433	0	0
21	М	1461	0	1502	6	0
22	Ν	1298	0	1366	4	0
23	0	804	0	825	1	0
24	Р	985	0	1044	2	0
25	Q	519	0	533	1	0
26	R	976	0	1053	3	0



		N	$\frac{puyc}{\mathbf{TT}(\dots,\dots,1,1)}$	$\mathbf{TT}(-1,1,-1)$		C
IVI01	Chain	INON-H	H(model)	H(added)	Clasnes	Symm-Clasnes
27	S	1115	0	1205	1	0
28	Т	1107	0	1182	1	0
29	U	1162	0	1213	2	0
30	V	773	0	828	2	0
31	W	772	0	808	4	0
32	X	868	0	913	2	0
33	Y	1053	0	1147	5	0
34	Z	879	0	917	3	0
35	a	845	0	933	0	0
36	b	1015	0	1148	0	0
37	с	832	0	917	0	0
38	d	713	0	746	0	0
39	е	569	0	637	0	0
40	f	444	0	482	0	0
41	g	429	0	465	0	0
42	i	842	0	912	0	0
43	j	708	0	756	0	0
44	k	992	0	1052	0	0
45	h	1712	0	1689	0	0
46	А	214	0	0	0	0
46	В	3	0	0	0	0
46	С	6	0	0	0	0
46	J	1	0	0	0	0
46	L	2	0	0	0	0
46	Р	1	0	0	0	0
46	U	1	0	0	0	0
46	d	1	0	0	0	0
47	А	139	0	0	0	0
47	В	1	0	0	0	0
47	D	3	0	0	0	0
47	J	1	0	0	0	0
47	N	1	0	0	0	0
47	V	1	0	0	0	0
47	Y	1	0	0	0	0
47	Ζ	1	0	0	0	0
47	a	1	0	0	0	0
47	f	1	0	0	0	0
47	i	1	0	0	0	0
47	1	2	0	0	0	0
47	0	1	0	0	0	0
47	р	1	0	0	0	0
48	A	2	0	0	0	0



Moi         Chain         Non-H         H(model)         H(added)         Clashes         Symm-Clashes           49         A         39         0         39         1         0           50         A         14         0         26         0         0           51         A         15         0         17         0         0           52         a         1         0         0         0         0           52         g         1         0         0         0         0           52         j         1         0         0         0         0           53         B         261         0         0         0         0           53         B         261         0         0         0         0           53         B         261         0         0         0         0           53         F         202         0         0         3         0           53         F         202         0         0         0         0           53         J         63         0         0         0         0 <th colspan="8">Continuea from previous page</th>	Continuea from previous page							
49         A         39         0         39         1         0           50         A         14         0         26         0         0           51         A         15         0         17         0         0           52         a         1         0         0         0         0           52         d         1         0         0         0         0           52         g         1         0         0         0         0           52         j         1         0         0         0         0           53         B         261         0         0         0         0           53         D         131         0         0         1         0           53         E         177         0         0         0         0           53         G         67         0         0         0         0           53         G         67         0         0         0         0           53         J         63         0         0         0         0           53 <t< th=""><th>Mol</th><th>Chain</th><th>Non-H</th><th>H(model)</th><th>H(added)</th><th>Clashes</th><th>Symm-Clashes</th></t<>	Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
50         A         14         0         26         0         0           51         A         15         0         17         0         0           52         a         1         0         0         0         0           52         d         1         0         0         0         0           52         g         1         0         0         0         0           52         g         1         0         0         0         0           52         j         1         0         0         0         0           53         A         8641         0         0         9         0           53         B         261         0         0         1         0           53         D         131         0         0         1         0           53         F         202         0         0         3         0           53         J         63         0         0         0         0           53         J         177         0         0         0         0           53         <	49	A	39	0	39	1	0	
51         A         15         0         17         0         0           52         a         1         0         0         0         0           52         d         1         0         0         0         0           52         g         1         0         0         0         0           52         j         1         0         0         0         0           52         j         1         0         0         0         0           53         B         261         0         0         0         0           53         D         131         0         0         1         0           53         E         177         0         0         0         0           53         G         67         0         0         0         0           53         G         67         0         0         0         0           53         G         67         0         0         0         0           53         J         63         0         0         0         0           53         J	50	A	14	0	26	0	0	
52         a         1         0         0         0         0           52         d         1         0         0         0         0           52         g         1         0         0         0         0           52         i         1         0         0         0         0           52         j         1         0         0         0         0           53         A         8641         0         0         9         0           53         C         363         0         0         1         0           53         E         177         0         0         0         0           53         G         67         0         0         0         0           53         G         67         0         0         0         0           53         I         117         0         0         0         0           53         J         63         0         0         0         0           53         J         63         0         0         0         0           54	51	A	15	0	17	0	0	
52         d         1         0         0         0         0           52         i         1         0         0         0         0           52         i         1         0         0         0         0           52         j         1         0         0         0         0           53         A         8641         0         0         9         0           53         B         261         0         0         0         0           53         C         363         0         0         1         0           53         E         177         0         0         0         0           53         F         202         0         0         3         0           53         H         49         0         0         0         0           53         J         63         0         0         0         0           53         J         63         0         0         0         0           53         K         139         0         0         0         0           53         <	52	a	1	0	0	0	0	
52         g         1         0         0         0         0           52         i         1         0         0         0         0           52         j         1         0         0         0         0           53         A         8641         0         0         9         0           53         B         261         0         0         1         0           53         C         363         0         0         1         0           53         E         177         0         0         0         0           53         F         202         0         0         3         0           53         G         67         0         0         0         0           53         H         49         0         0         0         0           53         I         17         0         0         0         0           53         I         57         0         0         0         0           53         M         100         0         0         0         0           53	52	d	1	0	0	0	0	
52         i         1         0         0         0         0           52         j         1         0         0         0         0           53         B         261         0         0         0         0           53         C         363         0         0         1         0           53         D         131         0         0         1         0           53         E         177         0         0         0         0           53         F         202         0         0         3         0           53         G         67         0         0         0         0           53         H         49         0         0         0         0           53         J         63         0         0         0         0           53         J         53         0         0         0         0         0           53         J         63         0         0         0         0         0           53         N         87         0         0         1         0 </td <td>52</td> <td>g</td> <td>1</td> <td>0</td> <td>0</td> <td>0</td> <td>0</td>	52	g	1	0	0	0	0	
52         j         1         0         0         0         0           53         A         8641         0         0         9         0           53         B         261         0         0         0         0           53         C         363         0         0         1         0           53         D         131         0         0         1         0           53         E         177         0         0         0         0           53         F         202         0         0         3         0           53         H         49         0         0         0         0           53         H         49         0         0         0         0           53         J         63         0         0         0         0           53         J         63         0         0         0         0           53         L         57         0         0         0         0           53         N         87         0         0         1         0           53	52	i	1	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	52	j	1	0	0	0	0	
53         B $261$ 0         0         0         0 $53$ C $363$ 0         0         1         0 $53$ D $131$ 0         0         1         0 $53$ E $177$ 0         0         0         0 $53$ F $202$ 0         0         3         0 $53$ G $67$ 0         0         0         0 $53$ H $49$ 0         0         0         0 $53$ I $117$ 0         0         0         0 $53$ H $49$ 0         0         0         0 $53$ J $63$ 0         0         0         0 $53$ M $100$ 0         0         0         0 $53$ M $100$ 0         0         0         0 $53$ N $87$ 0         0         0 <td>53</td> <td>А</td> <td>8641</td> <td>0</td> <td>0</td> <td>9</td> <td>0</td>	53	А	8641	0	0	9	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	В	261	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	С	363	0	0	1	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	D	131	0	0	1	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	Е	177	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	F	202	0	0	3	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	G	67	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	Н	49	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	Ι	117	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	J	63	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	K	139	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	L	57	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	М	100	0	0	2	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	N	87	0	0	1	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	0	5	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	Р	40	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	Q	21	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	R	35	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	S	49	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	Т	13	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	U	92	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	V	39	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	W	9	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	Х	37	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	Y	112	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	Z	72	0	0	2	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	a	58	0	0	0	0	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	53	b	29	0	0	0	0	
	53	с	32	0	0	0	0	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	53	d	62	0	0	0	0	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	53	е	3	0	0	0	0	
53         g         14         0         0         0         0           53         i         52         0         0         0         0	53	f	19	0	0	0	0	
53 i $52$ 0 0 0 0	53	g	14	0	0	0	0	
	53	i	52	0	0	0	0	



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	j	40	0	0	0	0
53	k	78	0	0	0	0
53	l	155	0	0	0	0
53	m	131	0	0	0	0
53	n	46	0	0	0	0
53	0	43	0	0	0	0
53	р	81	0	0	0	0
53	q	13	0	0	0	0
53	r	101	0	0	0	0
53	s	38	0	0	0	0
All	All	142233	0	95029	215	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 215 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1721:G:N2	1:A:1841:C:O2	1.87	1.08
34:Z:95:LYS:NZ	53:Z:301:HOH:O	1.81	1.08
1:A:1721:G:N2	1:A:1841:C:C2	2.26	1.03
21:M:70:LYS:NZ	53:M:201:HOH:O	1.94	1.01
1:A:5028:G:O2'	1:A:5029:C:O5'	1.91	0.86

There are no symmetry-related clashes.

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
4	D	244/257~(95%)	240 (98%)	4 (2%)	0	100	100
5	Е	394/403~(98%)	389~(99%)	5 (1%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
6	F	357/427~(84%)	350~(98%)	7~(2%)	0	100	100
7	G	281/297~(95%)	279 (99%)	2(1%)	0	100	100
8	Н	213/288~(74%)	209~(98%)	4(2%)	0	100	100
9	m	210/248~(85%)	206 (98%)	4 (2%)	0	100	100
10	n	219/266~(82%)	214 (98%)	5(2%)	0	100	100
11	О	188/192~(98%)	183 (97%)	5(3%)	0	100	100
12	р	200/214~(94%)	198 (99%)	2(1%)	0	100	100
13	q	168/178~(94%)	166 (99%)	2(1%)	0	100	100
14	r	204/211~(97%)	202 (99%)	2(1%)	0	100	100
15	s	137/220~(62%)	136 (99%)	1 (1%)	0	100	100
16	1	202/204~(99%)	198 (98%)	4 (2%)	0	100	100
17	Ι	197/203~(97%)	194 (98%)	3 (2%)	0	100	100
18	J	150/184~(82%)	148 (99%)	2 (1%)	0	100	100
19	K	185/188~(98%)	181 (98%)	4 (2%)	0	100	100
20	L	155/196~(79%)	155 (100%)	0	0	100	100
21	М	174/176~(99%)	172 (99%)	2 (1%)	0	100	100
22	Ν	157/160~(98%)	153 (98%)	4 (2%)	0	100	100
23	О	97/128~(76%)	93 (96%)	3(3%)	1 (1%)	15	3
24	Р	130/140~(93%)	128 (98%)	2(2%)	0	100	100
25	Q	60/157~(38%)	59 (98%)	1 (2%)	0	100	100
26	R	117/156~(75%)	116 (99%)	1 (1%)	0	100	100
27	S	132/145~(91%)	130 (98%)	2(2%)	0	100	100
28	Т	133/136~(98%)	130 (98%)	3 (2%)	0	100	100
29	U	145/148~(98%)	140 (97%)	4 (3%)	1 (1%)	22	8
30	V	90/159~(57%)	86 (96%)	4 (4%)	0	100	100
31	W	98/115~(85%)	98 (100%)	0	0	100	100
32	Х	104/125~(83%)	103 (99%)	1 (1%)	0	100	100
33	Y	126/135~(93%)	125 (99%)	1 (1%)	0	100	100
34	Z	108/110 (98%)	108 (100%)	0	0	100	100
35	a	104/117~(89%)	102 (98%)	2 (2%)	0	100	100
36	b	120/196~(61%)	119 (99%)	1 (1%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
37	с	100/105~(95%)	97~(97%)	3~(3%)	0	100	100
38	d	85/97~(88%)	84 (99%)	1 (1%)	0	100	100
39	е	67/70~(96%)	66~(98%)	1 (2%)	0	100	100
40	f	48/51~(94%)	48 (100%)	0	0	100	100
41	g	50/99~(50%)	50 (100%)	0	0	100	100
42	i	101/106~(95%)	100 (99%)	1 (1%)	0	100	100
43	j	89/92~(97%)	84 (94%)	5~(6%)	0	100	100
44	k	122/137~(89%)	121 (99%)	1 (1%)	0	100	100
45	h	223/245~(91%)	215 (96%)	7(3%)	1 (0%)	34	17
All	All	6484/7481 (87%)	6375 (98%)	106 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	0	67	LYS
29	U	15	VAL
45	h	58	ILE

#### 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	Percentiles
4	D	189/199~(95%)	187~(99%)	2(1%)	73 61
5	Ε	345/349~(99%)	343~(99%)	2(1%)	86 79
6	F	297/348~(85%)	295~(99%)	2(1%)	84 76
7	G	237/250~(95%)	234~(99%)	3~(1%)	69 54
8	Η	193/252~(77%)	192 (100%)	1 (0%)	88 83
9	m	182/215~(85%)	182 (100%)	0	100 100
10	n	193/223~(86%)	190 (98%)	3~(2%)	62 46
11	0	169/171 (99%)	168(99%)	1 (1%)	86 79



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
12	р	174/181~(96%)	172~(99%)	2(1%)	73	61
13	q	142/149~(95%)	141 (99%)	1 (1%)	84	76
14	r	172/177~(97%)	170~(99%)	2(1%)	71	57
15	s	118/161~(73%)	118 (100%)	0	100	100
16	1	172/172~(100%)	171 (99%)	1 (1%)	86	79
17	Ι	171/174~(98%)	171 (100%)	0	100	100
18	J	133/163~(82%)	131 (98%)	2(2%)	65	48
19	К	164/165~(99%)	164 (100%)	0	100	100
20	L	138/175~(79%)	137~(99%)	1 (1%)	84	76
21	М	157/157~(100%)	156 (99%)	1 (1%)	86	79
22	Ν	139/140~(99%)	137 (99%)	2(1%)	67	51
23	О	88/115~(76%)	86 (98%)	2(2%)	50	30
24	Р	102/107~(95%)	101 (99%)	1 (1%)	76	65
25	Q	54/126~(43%)	54 (100%)	0	100	100
26	R	107/133~(80%)	106~(99%)	1 (1%)	78	69
27	S	124/135~(92%)	123 (99%)	1 (1%)	81	72
28	Т	117/118~(99%)	115~(98%)	2(2%)	60	43
29	U	120/121~(99%)	120 (100%)	0	100	100
30	V	79/126~(63%)	78~(99%)	1 (1%)	69	54
31	W	84/97~(87%)	84 (100%)	0	100	100
32	Х	93/110~(84%)	93 (100%)	0	100	100
33	Y	114/121~(94%)	114 (100%)	0	100	100
34	Ζ	89/89~(100%)	89 (100%)	0	100	100
35	a	92/100~(92%)	91~(99%)	1 (1%)	73	61
36	b	109/153~(71%)	108~(99%)	1 (1%)	78	69
37	с	86/89~(97%)	81 (94%)	5~(6%)	20	5
38	d	74/80~(92%)	73~(99%)	1 (1%)	67	51
39	е	$64/\overline{65}~(98\%)$	64 (100%)	0	100	100
40	f	47/48~(98%)	46 (98%)	1 (2%)	53	33
41	g	48/91~(53%)	48 (100%)	0	100	100
42	i	$91/\overline{94}\ (97\%)$	90 (99%)	1 (1%)	73	61



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	j	74/75~(99%)	73~(99%)	1 (1%)	67 51
44	k	107/121~(88%)	107 (100%)	0	100 100
45	h	195/213~(92%)	192~(98%)	3~(2%)	65 48
All	All	5643/6348~(89%)	5595~(99%)	48 (1%)	79 69

Continued from previous page...

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
24	Р	48	ARG
36	b	113	LEU
26	R	156	ILE
28	Т	102	ARG
37	с	18	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
43	j	56	HIS
29	U	60	HIS
19	Κ	45	GLN
16	l	29	GLN
24	Р	135	ASN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	А	3278/5069~(64%)	510 (15%)	71 (2%)
2	В	119/121~(98%)	8~(6%)	0
3	С	146/157~(92%)	20 (13%)	2(1%)
All	All	3543/5347~(66%)	538 (15%)	73~(2%)

5 of 538 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	А	2	G
1	А	39	А
1	А	42	А
1	А	43	U
1	А	48	G



5 of 73 RNA pucker outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	4116	С
3	С	51	U
1	А	4266	G
1	А	4870	G
1	А	1501	С

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

117 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	Type	Chain	Dog	Link	Bo	ond leng	ths	Bond angles		
MOI	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	OMG	А	1316	47,1	18,26,27	1.01	1 (5%)	19,38,41	1.24	2 (10%)
1	A2M	А	2401	46,1	18,25,26	0.83	0	18,36,39	1.81	4 (22%)
1	OMC	А	2422	46,1	19,22,23	1.12	2 (10%)	26,31,34	0.84	1 (3%)
1	5MC	А	3782	46,1	18,22,23	1.11	1 (5%)	26,32,35	1.29	4 (15%)
1	PSU	А	4299	1	18,21,22	1.40	4 (22%)	22,30,33	2.36	5 (22%)
1	PSU	А	3853	46,1	18,21,22	1.28	3 (16%)	22,30,33	2.33	5 (22%)
1	PSU	А	1792	47,1	18,21,22	1.44	3 (16%)	22,30,33	2.29	7 (31%)
1	OMU	А	4306	1	19,22,23	1.28	3 (15%)	26,31,34	1.78	<mark>6 (23%)</mark>
1	PSU	А	4493	47,1	18,21,22	1.31	2 (11%)	22,30,33	2.34	<mark>6 (27%)</mark>
1	OMC	А	2824	1	19,22,23	0.89	0	26,31,34	0.97	1 (3%)
1	PSU	А	3844	1	18,21,22	1.39	3 (16%)	22,30,33	2.32	5 (22%)
1	PSU	А	4353	47,1	18,21,22	1.53	3 (16%)	22,30,33	2.37	5 (22%)
1	PSU	А	4361	47,1	18,21,22	1.77	4 (22%)	22,30,33	2.12	5 (22%)
1	OMC	А	3841	1	19,22,23	0.75	0	26,31,34	1.13	2 (7%)
1	A2M	А	4590	1	18,25,26	0.76	0	18,36,39	1.74	3 (16%)
1	PSU	А	3884	47,1	18,21,22	1.23	3 (16%)	22,30,33	2.05	4 (18%)
1	PSU	А	1781	1	18,21,22	1.43	2 (11%)	22,30,33	2.13	5 (22%)
1	PSU	А	3851	1	18,21,22	1.31	3 (16%)	22,30,33	2.35	6 (27%)



Mal	Type	Chain	Dog	Link	Bo	ond leng	ths	Bond angles		
10101	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	A2M	А	2363	46,1	18,25,26	0.76	0	18,36,39	1.95	<mark>5 (27%)</mark>
1	OMU	А	4620	1	19,22,23	1.15	2 (10%)	$26,\!31,\!34$	2.18	6 (23%)
1	PSU	А	1860	1	18,21,22	1.37	3 (16%)	22,30,33	2.15	6 (27%)
1	PSU	А	2508	1	18,21,22	1.32	3 (16%)	22,30,33	1.99	6 (27%)
1	OMG	А	2424	1	18,26,27	1.23	1 (5%)	19,38,41	1.22	2 (10%)
1	PSU	А	4312	1	18,21,22	1.44	2 (11%)	22,30,33	2.16	4 (18%)
1	PSU	А	3920	46,1	18,21,22	1.28	1 (5%)	22,30,33	2.05	5 (22%)
1	PSU	А	3639	1	18,21,22	1.39	2 (11%)	22,30,33	2.14	3 (13%)
1	OMC	А	4456	1	19,22,23	0.85	0	26,31,34	0.85	1 (3%)
1	PSU	А	4293	1	18,21,22	1.47	3 (16%)	22,30,33	2.08	6 (27%)
1	PSU	А	4576	47,1	18,21,22	1.35	3 (16%)	22,30,33	2.18	5 (22%)
3	PSU	С	55	3	18,21,22	1.23	3 (16%)	22,30,33	1.93	5 (22%)
1	OMC	А	2365	46,1	19,22,23	1.01	1 (5%)	26,31,34	1.06	2 (7%)
1	PSU	А	5010	1	18,21,22	1.28	2 (11%)	22,30,33	1.94	5 (22%)
1	PSU	А	1677	47,1	18,21,22	1.66	3 (16%)	22,30,33	2.41	6 (27%)
1	A2M	А	2787	46,1	18,25,26	1.04	1 (5%)	18,36,39	2.03	9 (50%)
1	A2M	А	3724	1	18,25,26	1.02	2 (11%)	18,36,39	1.39	2 (11%)
1	PSU	А	3637	47,1	18,21,22	1.31	3 (16%)	22,30,33	2.29	4 (18%)
1	OMG	А	3899	1	18,26,27	0.98	0	19,38,41	1.39	3 (15%)
1	A2M	А	398	1	18,25,26	1.23	3 (16%)	18,36,39	1.62	3 (16%)
1	PSU	А	4532	47,1	18,21,22	1.50	3 (16%)	22,30,33	2.33	6 (27%)
1	A2M	А	1871	46,1	18,25,26	0.65	0	18,36,39	1.79	4 (22%)
1	OMC	А	3701	47,1	19,22,23	0.93	0	26,31,34	1.45	4 (15%)
1	OMC	А	3869	1	19,22,23	0.84	1 (5%)	26,31,34	1.21	4 (15%)
1	PSU	А	4628	1	18,21,22	1.40	4 (22%)	22,30,33	2.35	5 (22%)
1	A2M	А	3718	1	18,25,26	0.97	1 (5%)	18,36,39	1.37	2 (11%)
1	OMC	А	4536	46,1	19,22,23	0.85	0	26,31,34	0.89	1 (3%)
1	PSU	А	4420	1	18,21,22	1.35	2 (11%)	22,30,33	1.99	5 (22%)
1	PSU	А	4471	47,1	18,21,22	1.53	3 (16%)	22,30,33	1.92	4 (18%)
1	OMG	А	1522	1	18,26,27	0.97	0	19,38,41	1.09	0
1	A2M	A	1534	46, 1	18,25,26	1.08	3 (16%)	18,36,39	1.70	5 (27%)
1	OMU	A	3925	1	19,22,23	1.16	2(10%)	26,31,34	1.92	5 (19%)
1	6MZ	A	4220	1	18,25,26	1.12	0	16,36,39	2.35	4 (25%)
1	A2M	A	1524	1	18,25,26	1.02	0	18,36,39	1.61	3 (16%)
1	A2M	А	3830	1	18,25,26	0.97	1 (5%)	18,36,39	1.65	6 (33%)



Mol	Type	Chain	Bos	Link	Bo	ond leng	ths	Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
1	OMG	А	2364	1	18,26,27	1.14	2 (11%)	19,38,41	1.29	2 (10%)
1	A2M	А	2815	47,1	18,25,26	0.92	0	18,36,39	1.31	2 (11%)
1	A2M	А	1326	1	$18,\!25,\!26$	1.00	0	$18,\!36,\!39$	1.90	4 (22%)
1	PSU	А	4423	1	18,21,22	1.29	3 (16%)	22,30,33	1.88	3 (13%)
1	OMG	А	4637	47,1	18,26,27	1.05	1 (5%)	19,38,41	1.21	2 (10%)
1	PSU	А	4552	1	18,21,22	1.53	3 (16%)	22,30,33	2.25	6 (27%)
1	PSU	А	4689	1	18,21,22	1.26	3 (16%)	22,30,33	2.19	4 (18%)
1	PSU	А	1582	47,1	18,21,22	1.85	5 (27%)	22,30,33	2.12	5 (22%)
1	UR3	А	4530	1	19,22,23	0.92	1 (5%)	26,32,35	1.64	4 (15%)
1	5MC	А	4447	47,1	18,22,23	1.00	1 (5%)	26,32,35	1.51	5 (19%)
1	OMG	А	4499	1	18,26,27	1.03	1 (5%)	19,38,41	1.46	3 (15%)
1	PSU	А	4579	1	18,21,22	1.45	3 (16%)	22,30,33	2.09	4 (18%)
1	A2M	А	3785	1	18,25,26	1.01	1 (5%)	18,36,39	1.67	5 (27%)
1	A2M	А	3867	1	18,25,26	1.01	1 (5%)	18,36,39	1.49	2 (11%)
1	PSU	А	1862	1	18,21,22	1.49	3 (16%)	22,30,33	2.51	4 (18%)
1	A2M	А	4523	46,1	18,25,26	0.83	0	18,36,39	1.63	4 (22%)
1	PSU	А	1536	1	18,21,22	1.44	2 (11%)	22,30,33	2.31	4 (18%)
3	PSU	С	69	3	18,21,22	1.53	3 (16%)	22,30,33	2.20	5 (22%)
1	PSU	А	4521	47,46,1	18,21,22	1.49	3 (16%)	22,30,33	2.40	7 (31%)
1	PSU	А	1782	1	18,21,22	1.60	3 (16%)	22,30,33	2.06	5 (22%)
1	PSU	А	4296	1	18,21,22	1.41	3 (16%)	22,30,33	2.07	5 (22%)
1	PSU	А	4673	47,1	18,21,22	1.15	3 (16%)	22,30,33	1.81	3 (13%)
1	OMG	А	3627	1	18,26,27	1.09	1 (5%)	19,38,41	1.24	2 (10%)
1	PSU	А	1683	47,1	18,21,22	1.39	3 (16%)	22,30,33	2.34	6 (27%)
1	OMG	А	4392	1	18,26,27	1.02	1 (5%)	19,38,41	1.25	3 (15%)
1	OMU	А	2837	1	19,22,23	1.31	2 (10%)	26,31,34	2.02	7 (26%)
1	OMC	А	3887	1	19,22,23	0.85	1 (5%)	26,31,34	1.24	2 (7%)
1	OMG	А	4370	1	18,26,27	0.87	1 (5%)	19,38,41	1.14	2 (10%)
1	OMU	А	4498	47,1	19,22,23	1.27	3 (15%)	26,31,34	2.31	7 (26%)
3	OMG	С	75	3	18,26,27	0.91	1 (5%)	19,38,41	1.31	4 (21%)
1	PSU	А	3729	1	18,21,22	1.45	4 (22%)	22,30,33	1.95	4 (18%)
1	OMC	А	2804	1	19,22,23	0.86	1 (5%)	26,31,34	0.99	1 (3%)
1	1MA	А	1322	46,1	16,25,26	1.15	2 (12%)	18,37,40	1.37	2 (11%)
1	OMG	А	4623	1	18,26,27	0.98	1 (5%)	19,38,41	1.23	2 (10%)
1	PSU	А	5001	47,1	18,21,22	1.46	3 (16%)	22,30,33	2.37	4 (18%)



Mal	Type	Chain	Bos	Link	Bo	ond leng	ths	Bond angles		
	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	PSU	А	4500	1	18,21,22	1.44	4 (22%)	22,30,33	2.21	5 (22%)
1	A2M	А	400	1	18,25,26	1.12	2 (11%)	$18,\!36,\!39$	1.66	3 (16%)
1	OMG	А	4618	47,1	18,26,27	0.88	0	19,38,41	1.30	4 (21%)
1	PSU	А	4972	47,1	18,21,22	1.31	2 (11%)	22,30,33	2.42	6 (27%)
1	OMU	А	3818	47,1	19,22,23	1.35	3 (15%)	26,31,34	1.98	6 (23%)
1	OMG	А	4494	1	18,26,27	1.14	1 (5%)	19,38,41	1.25	1 (5%)
1	PSU	А	2839	1	18,21,22	1.41	3 (16%)	22,30,33	1.95	7 (31%)
1	PSU	А	3695	47,1	18,21,22	1.34	2 (11%)	22,30,33	2.08	6 (27%)
1	OMC	А	1340	1	19,22,23	0.92	1 (5%)	26,31,34	1.05	0
1	PSU	А	4442	1	18,21,22	1.44	2 (11%)	22,30,33	2.18	6 (27%)
1	OMC	А	3808	1	19,22,23	0.80	1 (5%)	26,31,34	0.97	1 (3%)
1	PSU	А	2632	1	18,21,22	1.46	3 (16%)	22,30,33	2.12	5 (22%)
1	OMG	А	3792	1	18,26,27	0.90	0	19,38,41	1.12	2 (10%)
1	OMC	А	2351	46,1	19,22,23	0.77	0	26,31,34	1.45	2 (7%)
1	OMU	А	2415	1	19,22,23	1.33	2 (10%)	26,31,34	1.85	8 (30%)
1	PSU	А	4431	47,1	18,21,22	1.44	3 (16%)	22,30,33	2.41	7 (31%)
1	PSU	А	3715	1	18,21,22	1.29	2 (11%)	22,30,33	2.05	4 (18%)
1	A2M	А	3825	1	18,25,26	0.84	0	18,36,39	1.46	4 (22%)
1	PSU	А	4403	47,1	18,21,22	1.64	2 (11%)	22,30,33	2.18	5 (22%)
1	A2M	А	4571	1	18,25,26	1.04	0	18,36,39	1.50	3 (16%)
1	PSU	А	4457	1	18,21,22	1.37	3 (16%)	22,30,33	2.31	5 (22%)
1	OMU	А	4227	1	19,22,23	1.24	3 (15%)	26,31,34	1.84	5 (19%)
1	OMG	А	3744	1	18,26,27	0.80	0	19,38,41	1.15	2 (10%)
1	OMG	А	4228	1	18,26,27	1.02	1 (5%)	19,38,41	1.54	4 (21%)
1	PSU	А	1744	47,1	18,21,22	1.38	2 (11%)	22,30,33	2.10	4 (18%)
1	OMG	А	1625	47,1	18,26,27	1.22	1 (5%)	19,38,41	1.59	4 (21%)
1	OMC	А	2861	1	19,22,23	0.93	2 (10%)	26,31,34	0.86	0
1	OMG	А	2876	1	18,26,27	1.05	1 (5%)	19,38,41	1.43	4 (21%)
1	OMG	А	4196	46,1	18,26,27	1.07	1 (5%)	19,38,41	1.34	4 (21%)

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
1	OMG	А	1316	47,1	-	0/5/27/28	0/3/3/3
1	A2M	А	2401	46,1	-	1/5/27/28	0/3/3/3
1	OMC	А	2422	46,1	-	2/9/27/28	0/2/2/2
1	5MC	А	3782	46,1	_	0/7/25/26	0/2/2/2
1	PSU	А	4299	1	-	0/7/25/26	0/2/2/2
1	PSU	А	3853	46,1	-	0/7/25/26	0/2/2/2
1	PSU	А	1792	47,1	-	0/7/25/26	0/2/2/2
1	OMU	А	4306	1	-	0/9/27/28	0/2/2/2
1	PSU	А	4493	47,1	-	0/7/25/26	0/2/2/2
1	OMC	А	2824	1	-	0/9/27/28	0/2/2/2
1	PSU	А	3844	1	-	1/7/25/26	0/2/2/2
1	PSU	А	4353	47,1	-	0/7/25/26	0/2/2/2
1	PSU	А	4361	47,1	-	0/7/25/26	0/2/2/2
1	OMC	А	3841	1	-	0/9/27/28	0/2/2/2
1	A2M	А	4590	1	-	1/5/27/28	0/3/3/3
1	PSU	А	3884	47,1	-	0/7/25/26	0/2/2/2
1	PSU	А	1781	1	-	0/7/25/26	0/2/2/2
1	PSU	А	3851	1	-	0/7/25/26	0/2/2/2
1	A2M	А	2363	46,1	-	1/5/27/28	0/3/3/3
1	OMU	А	4620	1	-	0/9/27/28	0/2/2/2
1	PSU	A	1860	1	-	0/7/25/26	0/2/2/2
1	PSU	А	2508	1	-	0/7/25/26	0/2/2/2
1	OMG	A	2424	1	-	0/5/27/28	0/3/3/3
1	PSU	A	4312	1	-	0/7/25/26	0/2/2/2
1	PSU	A	3920	46,1	-	0/7/25/26	0/2/2/2
1	PSU	A	3639	1	-	0/7/25/26	0/2/2/2
1	OMC	A	4456	1	-	0/9/27/28	0/2/2/2
1	PSU	A	4293	1	-	0/7/25/26	0/2/2/2
1	PSU	A	4576	47,1	-	0/7/25/26	0/2/2/2
3	PSU	С	55	3	-	0/7/25/26	0/2/2/2
1	OMC	A	2365	46,1	-	0/9/27/28	0/2/2/2
1	PSU	A	5010	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1677	47,1	-	1/7/25/26	0/2/2/2
1	A2M	A	2787	46,1	-	0/5/27/28	0/3/3/3
1	A2M	A	3724	1	-	0/5/27/28	0/3/3/3
1	PSU	A	3637	47,1	-	0/7/25/26	0/2/2/2
1	OMG	A	3899	1	-	0/5/27/28	0/3/3/3
	A2M	A	398	1	-	0/5/27/28	0/3/3/3
1	PSU	A	4532	47,1	-	0/7/25/26	0/2/2/2
1	A2M	A	1871	46,1	-	0/5/27/28	0/3/3/3
1	OMC	A	3701	47,1	-	4/9/27/28	0/2/2/2
1	OMC	A	3869	1	-	0/9/27/28	0/2/2/2
1	PSU	A	4628	1	-	0/7/25/26	0/2/2/2



Mol	Type	Chain	$\operatorname{Res}$	$\operatorname{Link}$	Chirals	Torsions	Rings
1	A2M	А	3718	1	-	0/5/27/28	0/3/3/3
1	OMC	А	4536	46,1	-	0/9/27/28	0/2/2/2
1	PSU	А	4420	1	-	0/7/25/26	0/2/2/2
1	PSU	А	4471	47,1	-	0/7/25/26	0/2/2/2
1	OMG	А	1522	1	-	0/5/27/28	0/3/3/3
1	A2M	А	1534	46,1	-	2/5/27/28	0/3/3/3
1	OMU	А	3925	1	-	0/9/27/28	0/2/2/2
1	6MZ	А	4220	1	-	0/5/27/28	0/3/3/3
1	A2M	А	1524	1	-	0/5/27/28	0/3/3/3
1	A2M	А	3830	1	-	0/5/27/28	0/3/3/3
1	OMG	А	2364	1	-	2/5/27/28	0/3/3/3
1	A2M	А	2815	47,1	-	0/5/27/28	0/3/3/3
1	A2M	А	1326	1	-	1/5/27/28	0/3/3/3
1	PSU	А	4423	1	-	0/7/25/26	0/2/2/2
1	OMG	А	4637	47,1	-	0/5/27/28	0/3/3/3
1	PSU	А	4552	1	-	0/7/25/26	0/2/2/2
1	PSU	А	4689	1	-	0/7/25/26	0/2/2/2
1	PSU	А	1582	47,1	-	0/7/25/26	0/2/2/2
1	UR3	А	4530	1	-	0/7/25/26	0/2/2/2
1	5MC	А	4447	47,1	-	4/7/25/26	0/2/2/2
1	OMG	А	4499	1	-	0/5/27/28	0/3/3/3
1	PSU	А	4579	1	-	0/7/25/26	0/2/2/2
1	A2M	А	3785	1	-	2/5/27/28	0/3/3/3
1	A2M	А	3867	1	-	0/5/27/28	0/3/3/3
1	PSU	А	1862	1	-	0/7/25/26	0/2/2/2
1	A2M	А	4523	46,1	-	0/5/27/28	0/3/3/3
1	PSU	А	1536	1	-	0/7/25/26	0/2/2/2
3	PSU	С	69	3	-	0/7/25/26	0/2/2/2
1	PSU	А	4521	47,46,1	-	0/7/25/26	0/2/2/2
1	PSU	А	1782	1	-	0/7/25/26	0/2/2/2
1	PSU	А	4296	1	-	0/7/25/26	0/2/2/2
1	PSU	А	4673	47,1	-	0/7/25/26	0/2/2/2
1	OMG	А	3627	1	-	0/5/27/28	0/3/3/3
1	PSU	А	1683	47,1	-	0/7/25/26	0/2/2/2
1	OMG	А	4392	1	-	0/5/27/28	0/3/3/3
1	OMU	A	2837	1	-	0/9/27/28	0/2/2/2
1	OMC	A	3887	1	-	$0/9/27\overline{/28}$	0/2/2/2
1	OMG	А	4370	1	_	0/5/27/28	0/3/3/3
1	OMU	A	4498	47, 1	-	$0/9/27\overline{/28}$	$0/2/\overline{2/2}$
3	OMG	С	75	3	-	0/5/27/28	0/3/3/3
1	PSU	А	3729	1	-	0/7/25/26	0/2/2/2



Contre	naca jio		is paye.	••			
Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	А	2804	1	-	0/9/27/28	0/2/2/2
1	1MA	А	1322	46,1	-	0/3/25/26	0/3/3/3
1	OMG	А	4623	1	-	0/5/27/28	0/3/3/3
1	PSU	А	5001	47,1	-	0/7/25/26	0/2/2/2
1	PSU	А	4500	1	-	1/7/25/26	0/2/2/2
1	A2M	А	400	1	-	0/5/27/28	0/3/3/3
1	OMG	А	4618	47,1	-	0/5/27/28	0/3/3/3
1	PSU	А	4972	47,1	-	0/7/25/26	0/2/2/2
1	OMU	А	3818	47,1	-	1/9/27/28	0/2/2/2
1	OMG	А	4494	1	-	1/5/27/28	0/3/3/3
1	PSU	А	2839	1	-	0/7/25/26	0/2/2/2
1	PSU	А	3695	47,1	-	0/7/25/26	0/2/2/2
1	OMC	А	1340	1	-	0/9/27/28	0/2/2/2
1	PSU	А	4442	1	-	0/7/25/26	0/2/2/2
1	OMC	А	3808	1	-	0/9/27/28	0/2/2/2
1	PSU	А	2632	1	-	0/7/25/26	0/2/2/2
1	OMG	А	3792	1	-	0/5/27/28	0/3/3/3
1	OMC	А	2351	46,1	-	1/9/27/28	0/2/2/2
1	OMU	А	2415	1	-	1/9/27/28	0/2/2/2
1	PSU	А	4431	47,1	-	0/7/25/26	0/2/2/2
1	PSU	А	3715	1	-	0/7/25/26	0/2/2/2
1	A2M	А	3825	1	-	0/5/27/28	0/3/3/3
1	PSU	А	4403	47,1	-	0/7/25/26	0/2/2/2
1	A2M	А	4571	1	-	0/5/27/28	0/3/3/3
1	PSU	А	4457	1	-	0/7/25/26	0/2/2/2
1	OMU	А	4227	1	-	0/9/27/28	0/2/2/2
1	OMG	А	3744	1	-	0/5/27/28	0/3/3/3
1	OMG	А	4228	1	-	0/5/27/28	0/3/3/3
1	PSU	A	$17\overline{44}$	47,1	-	$0/7/\overline{25/26}$	$0/2\overline{/2/2}$
1	OMG	А	1625	47,1	-	0/5/27/28	0/3/3/3
1	OMC	A	2861	1	-	0/9/27/28	0/2/2/2
1	OMG	A	2876	1	-	$0/5/\overline{27/28}$	0/3/3/3
1	OMG	A	4196	46,1	-	$0/5/\overline{27/28}$	0/3/3/3

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The worst 5 of 211 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	4403	PSU	C6-C5	4.87	1.41	1.35
1	А	4361	PSU	C6-C5	4.66	1.40	1.35
1	А	1782	PSU	C6-C5	4.21	1.40	1.35
1	А	4532	PSU	C6-C5	4.19	1.40	1.35
1	А	2632	PSU	C6-C5	4.15	1.40	1.35



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	4353	PSU	N1-C2-N3	7.77	123.94	115.13
1	А	1862	PSU	N1-C2-N3	7.45	123.57	115.13
1	А	5001	PSU	N1-C2-N3	7.41	123.53	115.13
1	А	4628	PSU	N1-C2-N3	7.17	123.26	115.13
1	А	4521	PSU	N1-C2-N3	7.15	123.23	115.13

The worst 5 of 473 bond angle outliers are listed below:

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	2415	OMU	C1'-C2'-O2'-CM2
1	А	3701	OMC	C2'-C1'-N1-C2
1	А	3701	OMC	C2'-C1'-N1-C6
1	А	4590	A2M	C4'-C5'-O5'-P
1	А	3785	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	4456	OMC	1	0
1	А	4293	PSU	1	0
1	А	2787	A2M	1	0
1	А	4220	6MZ	1	0
1	А	2364	OMG	1	0
1	А	1326	A2M	1	0
1	А	3867	A2M	2	0
1	А	4498	OMU	1	0
1	А	4500	PSU	1	0
1	А	3818	OMU	1	0
1	А	1340	OMC	1	0
1	А	2351	OMC	3	0
1	А	2415	OMU	1	0
1	А	4457	PSU	1	0
1	А	2876	OMG	1	0

# 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



# 5.6 Ligand geometry (i)

Of 394 ligands modelled in this entry, 391 are monoatomic - leaving 3 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	Bond angles			
WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
49	HMT	А	5455	-	$40,\!43,\!43$	0.62	0	$41,\!66,\!66$	0.67	0
51	EPE	А	5457	-	$15,\!15,\!15$	0.91	1 (6%)	18,20,20	1.89	2 (11%)
50	SPM	А	5456	-	13,13,13	0.22	0	12,12,12	0.24	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
49	HMT	А	5455	-	-	0/27/74/74	0/5/5/5
51	EPE	А	5457	-	-	1/9/19/19	0/1/1/1
50	SPM	А	5456	-	-	3/11/11/11	_

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	А	5457	EPE	O2S-S	3.20	1.54	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
51	А	5457	EPE	O2S-S-C10	-7.35	98.06	106.92
51	А	5457	EPE	O3S-S-O1S	2.76	118.01	111.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	А	5456	SPM	C2-C3-C4-N5



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Mol	Chain	Res	Type	Atoms
50	А	5456	SPM	C6-C7-C8-C9
51	А	5457	EPE	C9-C10-S-O3S
50	А	5456	SPM	C7-C6-N5-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	А	5455	HMT	1	0

## 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-15113. 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







Y Index: 256



Z Index: 256

#### 6.2.2 Raw map



X Index: 256

Y Index: 256

Z Index: 256

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: 253



Y Index: 239



Z Index: 258

#### 6.3.2 Raw map



X Index: 253

Y Index: 239



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

#### 6.4.2 Raw map



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



#### Mask visualisation (i) 6.5

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

#### $emd_{15113}_{msk}_{1.map}$ (i) 6.5.1



 $\mathbf{Z}$ 



# 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 222  $\rm nm^3;$  this corresponds to an approximate mass of 200 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 0.599  ${\rm \AA^{-1}}$ 



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



## 8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estim	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit		
Reported by author	1.67	-	-		
Author-provided FSC curve	1.67	1.87	1.69		
Unmasked-calculated*	1.91	2.28	1.94		

\*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 1.91 differs from the reported value 1.67 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15113 and PDB model 8A3D. Per-residue inclusion information can be found in section 3 on page 17.

# 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.07 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 (0.07).



### 9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

# 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

$\mathbf{Chain}$	Atom inclusion	Q-score
All	0.6785	0.7690
А	0.7075	0.7530
В	0.7763	0.8070
С	0.7534	0.7850
D	0.8599	0.8430
Е	0.7289	0.8170
F	0.8096	0.8270
G	0.4808	0.7720
Н	0.4476	0.7440
Ι	0.7905	0.8260
J	0.7948	0.8340
Κ	0.8481	0.8450
L	0.6363	0.7650
М	0.8233	0.8330
Ν	0.6772	0.7700
О	0.0763	0.6310
Р	0.7261	0.8190
Q	0.6560	0.8060
R	0.5975	0.7930
S	0.6800	0.8010
Т	0.3672	0.7540
U	0.8019	0.8270
V	0.4416	0.7200
W	0.3788	0.7370
Х	0.6272	0.7870
Y	0.8379	0.8400
Z	0.8636	0.8480
a	0.7506	0.8200
b	0.5586	0.7800
С	0.4712	0.7460
d	0.8546	0.8470
e	0.2352	0.6880
f	0.7028	0.8080
g	0.6683	0.7950
h	0.0000	0.5730

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Chain	Atom inclusion	Q-score
i	0.6773	0.8140
j	0.6981	0.7920
k	0.7692	0.8200
l	0.9168	0.8500
m	0.8756	0.8480
n	0.4023	0.7310
0	0.5348	0.7840
р	0.6679	0.8120
q	0.1648	0.6920
r	0.6018	0.7690
S	0.6621	0.7840

