

# wwPDB EM Validation Summary Report (i)

Nov 11, 2024 – 06:22 PM EST

PDB ID	:	9E71
EMDB ID	:	EMD-47628
Title	:	Cryo-EM structure of the Pyrobaculum calidifontis 70S ribosome
Authors	:	Nissley, A.J.; Cate, J.H.D.
Deposited on	:	2024-10-31
Resolution	:	2.36  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 (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 2.36 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.



Matria	Whole archive	EM structures
Metric	$(\# {\rm Entries})$	$(\# { m Entries})$
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2	129	91%	9% •
2	1	3024	<b>•</b> 81% 13%	• 6%
3	4	1498	5% 75% 19%	• 5%
4	AA	244	95%	• •
5	AB	338	96%	•••
6	AC	285	9%	
7	AD	178	93%	7%
8	AE	196	96%	• •



Mol	Chain	Length	Quality of chain	
9	AF	149	93%	
10	AG	186	95%	• •
11	AH	157	<u>6%</u> 96%	
12	AI	144	94%	
13	A.I	103	36%	79/
13		103	36%	1 70 •
10		103	80% 8%	13%
14	AL	156	92%	6% •
15	AM	189	93%	• •
16	AN	178	92%	• 5%
17	AO	205	96%	••
18	AP	122	98%	••
19	AQ	147	95%	5% •
20	AR	78	88%	9% •
21	AS	99	97%	
22		18/		
		104		••
23	AU	81	96%	•
24	AV	128	88%	7% 5%
25	AW	62	89%	• 10%
26	AX	79	81%	15%
27	AY	179	8%	7% •
28	AZ	101	91%	6% •
20	12	01	9%	
29	Aa	91	95%	• •
30	Ab	153	88%	• 8%
31	Ac	84	96%	••
32	Ad	52	98%	•



Conti	nued fron	<i>i</i> previous	page	
Mol	Chain	Length	Quality of chain	
33	Ae	67	19%	·
34	Af	51	92%	6% •
35	Ag	53	<u>21%</u> 94%	6%
36	Ah	91	97%	•
37	Ai	102	94%	•••
38	Aj	184	95%	• •
39	Ak	93	89%	8% •
40	BA	222	26% 77% 6% •	16%
41	BB	208	37% 88%	7% 5%
42	BC	216	29% 6% 64%	
43	BD	159	94%	••
44	BE	237	92%	7%
45	BF	202	90%	5% •
46	BG	151	88%	5% 7%
47	BH	223	95%	• •
48	BI	130	90%	9% •
49	BJ	131	93%	6% •
50	BK	142	82%	12% • 6%
51	BL	106	28% 8% 64%	
52	BM	141	83%	7% 10%
53	BN	147	93%	5% ••
54	BO	153	88%	5% • 7%
55	BP	54	52% • 46%	
56	BQ	151	92%	7% •
57	BR	147	90%	7% •



Mol	Chain	Length	Quality of chain		
	Da		72%		
58	BS	71	87%	•	10%
59	BT	158	32%	6% •	15%
60	BU	158	93%		5%•
61	BV	128	38%	•	10%
62	BW	110	24% 55% 7%	38%	
63	BX	100	70% 78%	16%	• 5%
64	BY	67	19% 93%		
65	BZ	77	31%	14%	8%
66	Ba	54	24%	% 20	%
67	Bb	68	69% 76%	12%	12%
68	Bc	65	94%		5% •



# 2 Entry composition (i)

There are 72 unique types of molecules in this entry. The entry contains 171357 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	Atoms				AltConf	Trace	
1	2	129	Total 2769	C 1231	N 512	O 897	Р 129	0	0

• Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues			AltConf	Trace			
2	1	2849	Total 61386	C 27335	N 11453	O 19749	Р 2849	0	0

• Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues		A	AltConf	Trace			
3	4	1430	Total 30817	C 13730	N 5745	O 9912	Р 1430	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	5	4AC	С	conflict	GB 343200235
4	1318	4AC	С	conflict	GB 343200235

• Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms				AltConf	Trace	
4	АА	239	Total 1803	C 1136	N 354	O 308	${ m S}{ m 5}$	0	0

• Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues		At		AltConf	Trace		
5	AB	336	Total 2611	C 1681	N 476	0 450	${f S}$ $4$	0	0



• Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues		At	oms		AltConf	Trace	
6	AC	278	Total 2178	C 1406	N 395	0 371	S 6	0	0

• Molecule 7 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	AD	178	Total 1412	C 894	N 273	0 238	${f S}{7}$	0	0

• Molecule 8 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	AE	195	Total 1520	C 990	N 254	0 272	S 4	0	0

• Molecule 9 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues		At	oms		AltConf	Trace	
9	AF	145	Total 1095	C 705	N 187	O 202	S 1	0	0

• Molecule 10 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	AG	183	Total 1510	C 979	N 278	0 246	${f S}{7}$	0	0

• Molecule 11 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AH	155	Total 1244	C 785	N 249	O 209	S 1	0	0

• Molecule 12 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues		At	oms			AltConf	Trace
12	AI	138	Total 1068	C 682	N 202	0 181	${ m S} { m 3}$	0	0

• Molecule 13 is a protein called Large ribosomal subunit protein eL14.



Mol	Chain	Residues		At	oms			AltConf	Trace
12	ΛΤ	101	Total	С	Ν	Ο	S	0	0
10	AJ	101	788	500	143	144	1	0	0
12	ΔK	00	Total	С	Ν	Ο	S	0	0
10	АК	90	700	441	130	128	1	0	0

• Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AL	152	Total 1198	C 761	N 232	O 202	${ m S} { m 3}$	0	0

• Molecule 15 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues		At	oms		AltConf	Trace	
15	AM	184	Total 1558	C 992	N 315	0 245	S 6	0	0

• Molecule 16 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues		At	oms			AltConf	Trace
16	AN	169	Total 1336	C 847	N 254	0 227	S 8	0	0

• Molecule 17 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues		At		AltConf	Trace		
17	AO	200	Total 1615	C 1027	N 309	0 278	S 1	0	0

• Molecule 18 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues		At	oms		AltConf	Trace	
18	AP	121	Total 920	C 583	N 181	0 155	S 1	0	0

• Molecule 19 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	AQ	146	Total 1214	C 759	N 244	O 208	${ m S} { m 3}$	0	0

• Molecule 20 is a protein called Large ribosomal subunit protein eL20.



Mol	Chain	Residues		At	oms	AltConf	Trace		
20	AR	76	Total 603	C 382	N 109	O 109	${ m S} { m 3}$	0	0

• Molecule 21 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues		At	oms	AltConf	Trace		
21	AS	98	Total 788	C 503	N 150	0 134	S 1	0	0

• Molecule 22 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	AT	183	Total 1496	C 978	N 268	0 247	${ m S} { m 3}$	0	0

• Molecule 23 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues		At	oms	AltConf	Trace		
23	AU	81	Total 651	C 417	N 115	0 117	${ m S} { m 2}$	0	0

• Molecule 24 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues		At	oms			AltConf	Trace
24	AV	121	Total 976	C 619	N 194	0 161	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 25 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues		Atc	$\mathbf{ms}$		AltConf	Trace	
25	AW	56	Total	С	N	0	S	0	0
			449	287	86	70	6		

• Molecule 26 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
26	AX	67	Total 554	C 343	N 117	O 92	${f S}{2}$	0	0

• Molecule 27 is a protein called Large ribosomal subunit protein uL30.



Mol	Chain	Residues		At	oms			AltConf	Trace
27	AY	172	Total 1374	C 888	N 245	O 235	S 6	0	0

• Molecule 28 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues		At	oms	AltConf	Trace		
28	AZ	98	Total 742	C 481	N 128	0 132	S 1	0	0

• Molecule 29 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace	
29	Aa	88	Total 726	C 460	N 146	O 120	0	0

• Molecule 30 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	Ab	140	Total 1183	C 757	N 239	0 186	S 1	0	0

• Molecule 31 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues		At	oms			AltConf	Trace
31	Ac	83	Total 649	C 407	N 138	0 102	S 2	0	0

• Molecule 32 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
32	Ad	52	Total 429	C 265	N 93	O 65	S 6	0	0

• Molecule 33 is a protein called LSU ribosomal protein L38E.

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
33	Ae	66	Total 552	C 363	N 93	O 96	0	0

• Molecule 34 is a protein called Large ribosomal subunit protein eL39.



Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
34	Af	50	Total 415	C 260	N 96	O 59	0	0

• Molecule 35 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
35	Ag	50	Total 417	C 259	N 88	O 66	${f S}$ $4$	0	0

• Molecule 36 is a protein called eL42.

Mol	Chain	Residues		At	oms	AltConf	Trace		
36	Ah	91	Total 739	C 467	N 142	0 123	${f S}{7}$	0	0

• Molecule 37 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues		At	oms	AltConf	Trace		
37	Ai	99	Total 769	C 489	N 148	0 127	${ m S}{ m 5}$	0	0

• Molecule 38 is a protein called DJ-1/PfpI domain-containing protein.

Mol	Chain	Residues		At	oms		AltConf	Trace	
38	Aj	183	Total 1469	C 954	N 248	O 265	${S \atop 2}$	0	0

• Molecule 39 is a protein called PaREP1 domain containing protein.

Mol	Chain	Residues		At	oms		AltConf	Trace	
39	Ak	90	Total 743	C 478	N 127	O 136	${ m S} { m 2}$	0	0

• Molecule 40 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues		At	oms		AltConf	Trace	
40	ВА	187	Total 1487	C 965	N 263	O 256	${ m S} { m 3}$	0	0

• Molecule 41 is a protein called Small ribosomal subunit protein uS2.



Mol	Chain	Residues		At	AltConf	Trace			
41	BB	198	Total 1600	C 1037	N 277	O 279	${f S}$ 7	0	0

• Molecule 42 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
42	BC	77	Total 611	C 393	N 110	O 107	S 1	0	0

• Molecule 43 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
43	BD	157	Total 1284	C 831	N 240	O 209	S 4	0	0

• Molecule 44 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues		Ate	AltConf	Trace			
44	BE	236	Total 1883	C 1223	N 336	O 322	${ m S} { m 2}$	0	0

• Molecule 45 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
45	BF	194	Total 1498	C 951	N 272	0 271	$\frac{S}{4}$	0	0

• Molecule 46 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues		At	oms	AltConf	Trace		
46	BG	140	Total 1065	C 685	N 190	0 188	${ m S} { m 2}$	0	0

• Molecule 47 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues		Ate		AltConf	Trace		
47	BH	220	Total 1773	C 1128	N 325	0 313	${f S}{7}$	0	0

• Molecule 48 is a protein called Small ribosomal subunit protein uS8.



Mol	Chain	Residues		At	oms			AltConf	Trace
48	BI	129	Total 1036	C 676	N 177	O 180	${ m S} { m 3}$	0	0

• Molecule 49 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues		At	oms	AltConf	Trace		
49	BJ	130	Total 1007	C 636	N 198	0 172	S 1	0	0

• Molecule 50 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
50	BK	134	Total 1058	C 680	N 191	0 182	${ m S}{ m 5}$	0	0

• Molecule 51 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
51	BL	38	Total 315	C 201	N 64	O 49	S 1	0	0

• Molecule 52 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
52	BM	127	Total 941	C 592	N 182	0 164	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	128	IAS	ASP	conflict	UNP A3MX63

• Molecule 53 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues		At	oms	AltConf	Trace		
53	BN	144	Total 1133	C 730	N 211	0 189	${ m S} { m 3}$	0	0

• Molecule 54 is a protein called Small ribosomal subunit protein uS13.



Mol	Chain	Residues		At	AltConf	Trace			
54	BO	143	Total 1108	C 700	N 211	O 195	${ m S} { m 2}$	0	0

• Molecule 55 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
55	BP	29	Total 241	C 150	N 51	O 36	S 4	0	0

• Molecule 56 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
56	BQ	149	Total 1224	C 782	N 233	O 208	S 1	0	0

• Molecule 57 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues		At	AltConf	Trace			
57	BR	144	Total 1171	C 756	N 216	0 194	${ m S}{ m 5}$	0	0

• Molecule 58 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
58	BS	64	Total 517	C 332	N 94	O 91	0	0

• Molecule 59 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
59	BT	135	Total 1111	C 720	N 203	0 182	S 6	0	0

• Molecule 60 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BU	155	Total 1225	C 789	N 225	O 209	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 61 is a protein called Small ribosomal subunit protein eS24.



Mol	Chain	Residues		Ato	ms	AltConf	Trace	
61	BV	115	Total 950	C 597	N 185	O 168	0	0

• Molecule 62 is a protein called SSU ribosomal protein S25E.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
62	BW	68	Total	C 25.1	N OC	0	S	0	0
			544	351	96	96	T		

• Molecule 63 is a protein called SSU ribosomal protein S26E.

Mol	Chain	Residues		At	oms	AltConf	Trace		
63	BX	95	Total 772	C 490	N 150	0 128	S 4	0	0

• Molecule 64 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms				AltConf	Trace	
64	BY	65	Total 501	C 317	N 100	O 79	${ m S}{ m 5}$	0	0

• Molecule 65 is a protein called eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace	
65	BZ	71	Total 552	C 344	N 108	O 99	S 1	0	0

• Molecule 66 is a protein called SSU ribosomal protein S30E.

Mol	Chain	Residues	Atoms			AltConf	Trace	
66	Ba	43	Total 357	C 222	N 80	O 55	0	0

• Molecule 67 is a protein called aS35.

Mol	Chain	Residues	Atoms			AltConf	Trace	
67	Bb	60	Total 479	C 301	N 95	O 83	0	0

• Molecule 68 is a protein called Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein.



Mol	Chain	Residues	Atoms			AltConf	Trace		
68	Bc	64	Total	С	Ν	0	$\mathbf{S}$	0	0
00	08 DC	01	477	301	90	82	4	0	0



Mol	Chain	Residues	Atoms	AltConf
69	1	1	Total C N 14 10 4	0
69	1	1	Total         C         N           14         10         4	0
69	1	1	Total         C         N           14         10         4	0
69	1	1	Total         C         N           14         10         4	0
69	1	1	Total         C         N           14         10         4	0
69	1	1	Total         C         N           14         10         4	0
69	1	1	Total         C         N           14         10         4	0
69	1	1	Total         C         N           14         10         4	0
69	1	1	Total         C         N           14         10         4	0
69	1	1	Total         C         N           14         10         4	0
69	1	1	Total         C         N           14         10         4	0



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	
60	1	1	Total C N	0	
09	T	T	14  10  4	0	
69	1	1	Total C N	0	
0.5	T	I	14 10 4	0	
69	1	1	Total C N	0	
	-	-	14 10 4		
69	1	1	Total C N	0	
		_	14 10 4		
69	1	1	Total C N	0	
			$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		
69	1	1	Total C N	0	
			14 10 4		
69	1	1	10tal C N	0	
			$\begin{array}{ccc} 14 & 10 & 4 \\ \hline T_{a} t_{a} l & C & N \end{array}$		
69	1	1	14 10 A	0	
			Total C N		
69	1	1	14 10 A	0	
			Total C N		
69	1	1	14 10 4	0	
			Total C N		
69	1	1	14 10 4	0	
			Total C N		
69	1	1	14 10 4	0	
60	1	1	Total C N	0	
69	1	1	14  10  4	0	
60	1	1	Total C N	0	
09	1	L	14  10  4	0	
60	1	1	Total C N	0	
09	T	T	14  10  4	0	
69	1	1	Total C N	0	
0.5	T	I	14 10 4	0	
69	1	1	Total C N	0	
0.5	1	1	14 10 4	0	
69	1	1	Total C N	0	
	*	÷	14 10 4		
69	1	1	Total C N	0	
69	1	1	Total C N	0	
			14  10  4		
69	1	1	Total C N	0	
			14 10 4	Ľ Š	



Continued from previous page...

69       1       1       Total       C       N       0         69       1       1       14       10       4       0         69       1       1       14       10       4       0         69       1       1       Total       C       N       0         69 <t< th=""><th>Mol</th><th>Chain</th><th>Residues</th><th>Atoms</th><th>AltConf</th></t<>	Mol	Chain	Residues	Atoms	AltConf
1 $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ <td< td=""><td>60</td><td>1</td><td>1</td><td>Total C N</td><td>0</td></td<>	60	1	1	Total C N	0
69       1       1       1 tail tail to tail to tail tail tail tail tail tail tail tail	0.5	1	1	14 10 4	0
10       1       14       10       4       1         69       1       1       1       Total       C       N       0         69       1       1       1       Total       C       N       0         69       1       1       1       14       10       4       0         69       1       1       14       10       4       0         69       1       1       Total       C       N       0         69       4       1       Total       C       N       0	69	1	1	Total C N	0
69       1       1       1 total       C       N       0         69       1       1       14       10       4       0         69       1       1       1       Total       C       N       0         69       1       1       1       Total       C       N       0         69       1       1       14       10       4       0         69       1       1       14       10       4       0         69       1       1       Total       C       N       0         69       4       1       Total       C       N       0		-	-	14 10 4	
14 $10$ $4$ $69$ 1         1 $14$ $10$ $4$ $69$ 1         1 $14$ $10$ $4$ $69$ 1         1 $14$ $10$ $4$ $69$ 1         1 $14$ $10$ $4$ $69$ 1         1 $14$ $10$ $4$ $69$ 1         1 $14$ $10$ $4$ $69$ 1         1 $14$ $10$ $4$ $69$ 1         1 $14$ $10$ $4$ $69$ 1         1 $14$ $10$ $4$ $69$ 1         1 $14$ $10$ $4$ $69$ 1         1 $14$ $10$ $4$ $69$ 4         1 $14$ $10$ $4$ $69$ 4         1 $14$ $10$ $4$ $69$ 4         1 $14$ </td <td>69</td> <td>1</td> <td>1</td> <td>Total C N</td> <td>0</td>	69	1	1	Total C N	0
69       1       1       1 orail of a constraints of				$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
14 $10$ $4$ $10$ $4$ $69$ $1$ $1$ $14$ $10$ $4$ $69$ $1$ $1$ $14$ $10$ $4$ $69$ $1$ $1$ $14$ $10$ $4$ $69$ $1$ $1$ $14$ $10$ $4$ $69$ $1$ $1$ $14$ $10$ $4$ $69$ $1$ $1$ $14$ $10$ $4$ $69$ $1$ $1$ $14$ $10$ $4$ $69$ $1$ $1$ $14$ $10$ $4$ $69$ $1$ $1$ $14$ $10$ $4$ $69$ $4$ $1$ $14$ $10$ $4$ $69$ $4$ $1$ $14$ $10$ $4$ $69$ $4$ $1$ $14$ $10$ $4$ $69$ $4$ $1$ $14$ $10$ $4$	69	1	1	$\begin{array}{cccc} 1 \text{ otal } \text{C} & \text{N} \\ 14 & 10 & 4 \end{array}$	0
69       1       1       1 order       0       0         69       1       1       1       Total       C       N       0         69       1       1       1       Total       C       N       0         69       4       1       Total       C       N       0         69       4       1       Total       C       N       0         69       4       1       Total       C       N       0				$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
11 $11$ $111$ <	69	1	1	14 10 4	0
69       1       1       14       10       4       0         69       1       1       14       10       4       0         69       1       1       Total       C       N       0         69       1       1       14       10       4       0         69       1       1       Total       C       N       0         69       4       1       Total       C       N       0         69				Total C N	
69       1       1       Total       C       N       0         69       1       1       14       10       4       0         69       1       1       Total       C       N       0         69       4       1       Total       C       N       0         69	69	1	1	14 10 4	0
69       1       1       14       10       4       0         69       1       1       14       10       4       0         69       1       1       Total       C       N       0         69       1       1       14       10       4       0         69       1       1       Total       C       N       0         69       4       1       Total       C       N       0         69	<u> </u>	1	1	Total C N	0
69       1       1       Total       C       N       0 $69$ 1       1       14       10       4       0 $69$ 1       1       Total       C       N       0 $69$ 4       1       Total       C       N       0      <	69	1	1	14  10  4	0
1 $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$	60	1	1	Total C N	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	09	T	T	14  10  4	0
100 $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ <t< td=""><td>69</td><td>1</td><td>1</td><td>Total C N</td><td>0</td></t<>	69	1	1	Total C N	0
69       1       1       Total       C       N       0 $69$ 4       1       Total       C       N       0		-	-	14 10 4	
14 $10$ $4$ $10$ $4$ $10$ $4$ $10$ $4$ $10$ $4$ $10$ $4$ $0$ $69$ $1$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $1$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $Total$ $C$ $N$ $0$ <	69	1	1	Total C N	0
69       1       1       1 otal       C       N       0 $69$ 1       1       14       10       4       0 $69$ 1       1       Total       C       N       0 $69$ 4       1       14       10       4       0 $69$ 4       1       Total       C       N       0 <t< td=""><td></td><td></td><td></td><td><math display="block">\begin{array}{c ccccccccccccccccccccccccccccccccccc</math></td><td>_</td></t<>				$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	_
14 $10$ $4$ $69$ $1$ $1$ $14$ $10$ $4$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $Total$ $C$ $N$ $0$ $69$ $4$ $1$ $Total$ <td< td=""><td>69</td><td>1</td><td>1</td><td>Total C N</td><td>0</td></td<>	69	1	1	Total C N	0
69       1       1 $10tal$ $C$ N $0$ $69$ $4$ 1 $14$ $10$ $4$ $0$ $69$ $4$ 1 $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $Total$ $C$ $N$ $0$				$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
69 $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $Total$ $C$ $N$ $0$	69	1	1	14 10 A	0
69 $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ <td></td> <td></td> <td></td> <td>Total C N</td> <td></td>				Total C N	
69 $4$ $1$ $14$ $10$ $14$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ $69$ $4$ $1$ $14$ $10$ $4$ $0$ <td>69</td> <td>4</td> <td>1</td> <td>14 10 4</td> <td>0</td>	69	4	1	14 10 4	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$				Total C N	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	69	4	1	14  10  4	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	60	4	1	Total C N	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	09	4	L	14  10  4	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	69	4	1	Total C N	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	0.5	т	1	14 10 4	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	69	4	1	Total C N	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		_	_	14 10 4	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	69	4	1	Total C N	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$				$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	69	4	1	$\begin{array}{cccc} 10tal & U & N \\ 14 & 10 & 4 \end{array}$	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$				Total C N	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	69	4	1	14 10 A	0
$ \begin{vmatrix} 69 \\ 4 \end{vmatrix} = 1 \qquad \begin{vmatrix} 10001 \\ 14 \\ 10 \\ 4 \end{vmatrix} = 0 $				Total C N	
	69	4	1	14 10 4	0



Mol	Chain	Residues	Atom	5	AltConf	
60	4	1	Total C	Ν	0	
09	4	1	14 10	4	0	
69 /	1	Total C	Ν	0		
0.5	00 1	1	14 10	4	0	
69	4	1	Total C	Ν	0	
	-	1	14 10	4		
69	39 4	4	1	Total C	Ν	0
	-	-	14 10	4	0	
69	4	1	Total C	Ν	0	
		-	14 10	4		
69	4	1	Total C	Ν	0	
	_	_	14 10	4		
69	4	1	Total C	N	0	
			14 10	4		
69	4	1	Total C	N	0	
			14 10	4		
69	4	1	Total C	N	0	
			14 10	4		
69	69 AL	1	Total C	N	0	
			14 10	4		
69	Ah	Ah 1	Total C	N	0	
03	ЛП		14 10	4		

• Molecule 70 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
70	1	170	Total         Mg           170         170	0
70	4	78	TotalMg7878	0
70	АА	1	Total Mg 1 1	0
70	AL	2	Total Mg 2 2	0
70	BK	1	Total Mg 1 1	0

 $\bullet\,$  Molecule 71 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
71	AW	1	Total Zn 1 1	0



Mol	Chain	Residues	Atoms	AltConf
71	Ad	1	Total Zn 1 1	0
71	Ag	1	Total Zn 1 1	0
71	Ah	1	Total Zn 1 1	0
71	Ai	1	Total Zn 1 1	0
71	BF	1	Total Zn 1 1	0
71	BP	1	Total Zn 1 1	0
71	BR	1	Total Zn 1 1	0
71	BX	1	Total Zn 1 1	0
71	BY	1	Total Zn 1 1	0
71	Bc	1	Total Zn 1 1	0

Continued from previous page...

• Molecule 72 is water.

Mol	Chain	Residues	Atoms	AltConf
72	2	181	Total O 181 181	0
72	1	5640	Total O 5640 5640	0
72	4	1487	Total O 1487 1487	0
72	АА	12	Total O 12 12	0
72	AB	1	Total O 1 1	0
72	AC	6	Total O 6 6	0
72	AG	2	Total O 2 2	0
72	AH	3	Total O 3 3	0
72	AL	10	Total O 10 10	0



$\alpha \cdot \cdot \cdot \cdot$	c	•	
Continued	trom	nromanie	naae
Continucu	11011	preduous	puyc
		1	1 0

Mol	Chain	Residues	Atoms	AltConf
72	AM	2	Total O 2 2	0
72	AN	2	Total O 2 2	0
72	AO	2	Total O 2 2	0
72	AP	1	Total O 1 1	0
72	AQ	1	Total O 1 1	0
72	AT	2	Total O 2 2	0
72	AU	1	Total O 1 1	0
72	AX	22	TotalO2222	0
72	AY	2	Total O 2 2	0
72	Aa	1	Total O 1 1	0
72	Ab	6	Total O 6 6	0
72	Ad	3	Total O 3 3	0
72	Ah	1	Total O 1 1	0
72	ВА	18	Total         O           18         18	0
72	BB	18	Total         O           18         18	0
72	BC	9	Total O 9 9	0
72	BD	28	TotalO2828	0
72	BE	23	TotalO2323	0
72	BF	32	TotalO3232	0
72	BG	19	Total         O           19         19	0
72	BH	26	Total         O           26         26	0



Mol	Chain	Residues	Atoms	AltConf
72	BI	20	Total O 20 20	0
72	BJ	13	Total         O           13         13	0
72	BK	12	Total         O           12         12	0
72	BL	7	Total O 7 7	0
72	BM	9	Total O 9 9	0
72	BN	12	Total         O           12         12	0
72	BO	26	Total         O           26         26	0
72	BP	8	Total O 8 8	0
72	BQ	15	Total         O           15         15	0
72	BR	12	Total         O           12         12	0
72	BS	5	Total O 5 5	0
72	BT	17	Total         O           17         17	0
72	BU	13	Total         O           13         13	0
72	BV	9	Total O 9 9	0
72	BW	8	Total O 8 8	0
72	BX	12	Total O 12 12	0
72	BY	10	Total         O           10         10	0
72	BZ	12	Total         O           12         12	0
72	Ba	8	Total O 8 8	0
72	Bb	7	Total O 7 7	0
72	Bc	16	Total         O           16         16	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 5S rRNA













• Molecule 13: Large ribosomal subunit protein eL14









• Molecule 19: Large ribosomal subunit protein eL19





• Molecule 21: Large ribosomal subunit protein eL21

Chain AS:	97%	••
MET V2 K3 K4 K4 K14 G99		

• Molecule 22: Large ribosomal subunit protein uL22

Chain AT:	96%	
MET 19 10 10 10 10 10 12 12 12 12 12 12 12 12 12 12 12 12 12		
• Molecule 23: Large ribosomal s	subunit protein uL23	
Chain AU:	96%	
M1 17 R17 B37 B37 B37 B37 B37 B37 B37 B3		
• Molecule 24: Large ribosomal s	subunit protein uL24	



• Molecule 25: Large ribosomal subunit protein eL24







• Molecule 32: Large ribos	somal subunit protein eL37	
Chain Ad:	98%	•
M1 KB2 KB2		
• Molecule 33: LSU riboso	omal protein L38E	
Chain Ae:	99%	•
MET P2 E1 6 E2 7 A30 A50 E51 E51 E56 L5 7 K58 K68 A50		
• Molecule 34: Large ribos	somal subunit protein eL39	
Chain Af:	92%	6% •
MET A2 736 R37 R37 R37 A51		
• Molecule 35: Large ribos	somal subunit protein eL40	
Chain Ag:	94%	6%
MET PRO 13 74 15 P7 P7 P7 P7 P3 P3 R5 R5 R5 R5 R5	LYS LYS	
• Molecule 36: eL42		
Chain Ah:	97%	
M1 K5 R30 F41 V91		
• Molecule 37: Large ribos	somal subunit protein eL43	
Chain Ai:	94%	· ·
MET P2 P3 181 181 885 885 885 885 885 885 831 830 831 832 832 832 832 832 832 832 832 832 832	K95         K97           W96         K97           K97         E98           A100         A100           A105         A105	
• Molecule 38: DJ-1/PfpI	domain-containing protein	
Chain Aj:	95%	<del>.</del> .













V141			
• Molecule 53: Small ribo	somal subunit protein uS12		
Chain BN:	93%	5% ••	
MET P2 P2 P3 K4 K6 K5 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3	K67 V60 E61 E61 K64 N98 N98 H100 D101 S115 S115 C143 C143 C143	r144 T145 ARG	
• Molecule 54: Small ribo	somal subunit protein uS13		
Chain BO:	88%	5% • 7%	
MET A2 Q3 E4 E4 A7 A7 V9 K10 E111 C12 D15 D15 C12 D15 C12	R11 0.18 134 146 155 156 156 156 156 156 156 156 156 15	K62 L63 D64 W65 K165 E72 E86 E97 A101 A101 A101 K102 K103 K103 K103 S121	L122 G123
L124 K125 V126 R127 G128 Q128 Q128 Q128 T131 T131 T133 T133 T133 T133 T133 T13	1139 1140 1140 1144 1144 1148		
• Molecule 55: Small ribo	somal subunit protein uS14		
Chain BP:	48%		
Cham D1.	•	46%	
MET PRO SER FIAR FIAR PRO PRO PRO GLU CUT FIA FIA FIA FIA FIA FIA FIA FIA FIA FIA	C19 120 120 120 123 129 129 129 129 129 129 129 129 129 129	46%	
Molecule 56: Small ribo	52% 5 8 2 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	156 137 138 144 144 144 144 144 144 144 14	
<ul> <li>Molecule 56: Small ribc</li> <li>Chain BQ:</li> </ul>	52%	46%	
<ul> <li>Molecule 56: Small ribo</li> <li>Chain BQ:</li> <li>Image: Image: Image</li></ul>	52% 5	683 813 8112 ↔ 8112 ↔ 8142 ↔ 8142 ↔ 8144 ↔ 8144 ↔ 8144 ↔ 8144 ↔ 8144 ↔ 8144 ↔ 8144 ↔ 8144 ↔ 8147 ↔ 8147 ↔ 8146 ↔ 8147 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 8148 ↔ 814	
<ul> <li>Molecule 56: Small ribo</li> <li>Chain BQ:</li> <li>Molecule 57: Small ribo</li> </ul>	52% 5	B83       B87       B83       B87       B83       B87       B84       K100       K110       K100       K134       K144       K	
<ul> <li>Molecule 56: Small ribo</li> <li>Molecule 56: Small ribo</li> <li>Chain BQ:</li> <li>Molecule 57: Small ribo</li> <li>Molecule 57: Small ribo</li> <li>Molecule 57: Small ribo</li> </ul>	52% 5 S Z S S Z Z Z Z S S Z Z Z S S Z Z Z S S Z Z Z S S Z Z Z S S Z Z Z S S Z Z Z S Z Z Z S Z Z Z Z S Z Z Z Z S S Z Z Z S S Z Z Z S S Z Z Z S S S Z Z Z S S S S Z Z Z S S S S Z Z Z S S S S S Z Z Z S	46%	
<ul> <li>Molecule 56: Small ribo</li> <li>Molecule 56: Small ribo</li> <li>Chain BQ:</li> <li>Molecule 57: Small ribo</li> <li>Molecule 57: Small ribo</li> <li>Molecule 57: Small ribo</li> <li>Molecule 57: Small ribo</li> </ul>	52% 52% 52% 52% 52% 52% 52% 52%	46% 46% 46% 46% 46% 46% 46% 46%	

 $\bullet$  Molecule 58: Small ribosomal subunit protein eS17





• Molecule 63: SSU ribosomal protein S26E 70% Chain BX: 78% 16% • 5% E52 L53 E54 E54 q56 q56 g57 d58 r59 r59 r59 P47 D48 129 R32 L49 A50 AL A R37 N72 C73 A74 V75 R91 V92 К 89 P 93 L94 Q95 <mark>Q96</mark> VAL ILE E86 R88 K 90 • Molecule 64: Small ribosomal subunit protein eS27 19% Chain BY: 93% P23 D24 G26 G26 N27 • Molecule 65: eS28 31% Chain BZ: 78% 14% 8% MET ALA GLU GLU • Molecule 66: SSU ribosomal protein S30E 24% Chain Ba: 70% 9% 20% ALA SER GLN GLN ALA ALA ALA ALA ALA ALA • Molecule 67: aS35 69% Chain Bb: 76% 12% 12% G26 K27 T28 S29 E30 E30 K32 L35 L35 L35 K36 K36 K36 K36 V38 MET ALA GLU GLU E20 K40 L5 E6 A7 V8 E 321 122 123 6 124 325

 $\bullet$  Molecule 68: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein

	17%			
Chain Bc:		94%	5%	·







# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129829	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	1.526	Depositor
Minimum map value	-0.618	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.215	Depositor
Map size (Å)	504.2144, 504.2144, 504.2144	wwPDB
Map dimensions	608, 608, 608	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8293, 0.8293, 0.8293	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: MA6, 6MZ, IAS, PSU, A2M, 4AC, OMC, B8T, OMU, MG, UR3, M7A, SPM, 5MC, G7M, ZN, OMG

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	
WIOI	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	2	0.73	0/3096	0.90	1/4830~(0.0%)
2	1	0.60	0/67134	0.88	29/104802~(0.0%)
3	4	0.51	1/33464~(0.0%)	0.92	53/52215~(0.1%)
4	AA	0.37	0/1847	0.61	0/2489
5	AB	0.34	0/2678	0.56	0/3643
6	AC	0.32	0/2234	0.57	1/3024~(0.0%)
7	AD	0.36	0/1431	0.58	0/1913
8	AE	0.34	0/1548	0.55	0/2087
9	AF	0.32	0/1114	0.55	1/1513~(0.1%)
10	AG	0.32	0/1542	0.56	2/2076~(0.1%)
11	AH	0.30	0/1265	0.57	0/1692
12	AI	0.36	0/1093	0.66	1/1487~(0.1%)
13	AJ	0.35	0/795	0.68	1/1068~(0.1%)
13	AK	0.31	0/704	0.60	0/944
14	AL	0.34	0/1225	0.58	0/1639
15	AM	0.33	0/1594	0.58	0/2138
16	AN	0.34	0/1365	0.60	0/1841
17	AO	0.38	0/1647	0.58	0/2212
18	AP	0.30	0/933	0.57	0/1263
19	AQ	0.32	0/1233	0.68	2/1645~(0.1%)
20	AR	0.38	0/610	0.63	0/817
21	AS	0.43	0/805	0.61	0/1081
22	AT	0.32	0/1536	0.57	1/2075~(0.0%)
23	AU	0.30	0/655	0.58	1/877~(0.1%)
24	AV	0.34	0/990	0.67	1/1325~(0.1%)
25	AW	0.36	0/460	0.57	0/613
26	AX	0.36	0/557	0.66	0/738
27	AY	0.35	0/1407	0.62	1/1905~(0.1%)
28	AZ	0.33	$0/\overline{754}$	0.58	0/1021
29	Aa	0.32	0/735	0.64	1/986~(0.1%)
30	Ab	0.32	0/1209	0.63	2/1621~(0.1%)



Mol Chain		Bond lengths		Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
31	Ac	0.32	0/663	0.60	0/889	
32	Ad	0.34	0/442	0.59	0/587	
33	Ae	0.30	0/562	0.49	0/753	
34	Af	0.30	0/423	0.63	0/566	
35	Ag	0.31	0/424	0.59	0/564	
36	Ah	0.40	0/753	0.59	0/1001	
37	Ai	0.35	0/788	0.62	0/1057	
38	Aj	0.35	0/1497	0.56	0/2029	
39	Ak	0.35	0/754	0.49	0/1005	
40	BA	0.32	0/1515	0.69	2/2043~(0.1%)	
41	BB	0.37	1/1638~(0.1%)	0.62	0/2221	
42	BC	0.30	0/620	0.73	1/831~(0.1%)	
43	BD	0.30	0/1308	0.57	0/1755	
44	BE	0.35	0/1929	0.63	1/2621~(0.0%)	
45	BF	0.34	0/1522	0.60	3/2059~(0.1%)	
46	BG	0.32	0/1087	0.66	1/1465~(0.1%)	
47	BH	0.32	0/1809	0.59	1/2444~(0.0%)	
48	BI	0.36	0/1055	0.57	0/1425	
49	BJ	0.33	0/1023	0.61	1/1370~(0.1%)	
50	BK	0.32	0/1079	0.59	0/1452	
51	BL	0.29	0/324	0.66	0/437	
52	BM	0.33	0/951	0.63	0/1288	
53	BN	0.38	0/1157	0.63	1/1551~(0.1%)	
54	BO	0.30	0/1125	0.61	1/1518~(0.1%)	
55	BP	0.29	0/244	0.70	0/324	
56	BQ	0.30	0/1254	0.53	0/1692	
57	BR	0.33	0/1200	0.58	1/1629~(0.1%)	
58	BS	0.31	0/524	0.57	0/698	
59	BT	0.31	0/1139	0.60	0/1533	
60	BU	0.32	0/1253	0.56	0/1695	
61	BV	0.32	0/960	0.59	0/1280	
62	BW	0.36	0/551	0.58	0/741	
63	BX	0.32	0/787	0.69	0/1054	
64	BY	0.33	0/511	0.62	0/689	
65	ΒZ	0.37	0/555	0.71	0/745	
66	Ba	0.27	0/364	0.59	0/486	
67	Bb	0.30	0/478	0.67	0/634	
68	Bc	0.37	0/491	0.62	0/670	
All	All	0.49	2/172419~(0.0%)	0.80	$11\overline{1/254381}$ (0.0%)	

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



Mol	Chain	#Chirality outliers	#Planarity outliers
7	AD	0	2
13	AK	0	1
48	BI	0	3
50	BK	0	1
All	All	0	7

sidechain that are expected to be planar.

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
41	BB	90	CYS	CB-SG	-6.38	1.71	1.82
3	4	1345	G	P-O5'	5.56	1.65	1.59

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	4	102	А	OP1-P-OP2	14.34	141.12	119.60
3	4	812	С	OP1-P-O3'	-14.14	74.10	105.20
3	4	101	С	OP1-P-O3'	-14.12	74.14	105.20
3	4	812	С	OP2-P-O3'	-11.60	79.69	105.20
2	1	1603	G	OP1-P-O3'	-11.16	80.64	105.20

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Group
7	AD	77	ARG	Sidechain
7	AD	78	ARG	Sidechain
13	AK	38	GLY	Peptide
48	BI	28	TRP	Peptide
48	BI	76	ARG	Sidechain

### 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
4	AA	237/244~(97%)	228 (96%)	9~(4%)	0	100	100
5	AB	334/338~(99%)	326 (98%)	8 (2%)	0	100	100
6	AC	276/285~(97%)	271 (98%)	5(2%)	0	100	100
7	AD	176/178~(99%)	169 (96%)	7 (4%)	0	100	100
8	AE	193/196~(98%)	189 (98%)	4 (2%)	0	100	100
9	AF	143/149~(96%)	141 (99%)	2(1%)	0	100	100
10	AG	181/186~(97%)	177 (98%)	4 (2%)	0	100	100
11	AH	153/157~(98%)	151 (99%)	2(1%)	0	100	100
12	AI	136/144~(94%)	134 (98%)	2(2%)	0	100	100
13	AJ	99/103~(96%)	95 (96%)	4 (4%)	0	100	100
13	AK	88/103 (85%)	83 (94%)	5 (6%)	0	100	100
14	AL	150/156~(96%)	144 (96%)	6 (4%)	0	100	100
15	AM	182/189~(96%)	178 (98%)	4 (2%)	0	100	100
16	AN	167/178~(94%)	162 (97%)	5(3%)	0	100	100
17	AO	198/205~(97%)	198 (100%)	0	0	100	100
18	AP	119/122~(98%)	118 (99%)	1 (1%)	0	100	100
19	AQ	144/147~(98%)	143 (99%)	1 (1%)	0	100	100
20	AR	74/78~(95%)	74 (100%)	0	0	100	100
21	AS	96/99~(97%)	89 (93%)	7 (7%)	0	100	100
22	AT	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
23	AU	79/81~(98%)	76 (96%)	3 (4%)	0	100	100
24	AV	119/128~(93%)	117 (98%)	1 (1%)	1 (1%)	16	17
25	AW	54/62~(87%)	53 (98%)	1 (2%)	0	100	100
26	AX	65/79~(82%)	65 (100%)	0	0	100	100
27	AY	170/179~(95%)	161 (95%)	8 (5%)	1 (1%)	22	24



$\alpha$ $\cdots$ $1$	c		
Continued	trom	previous	page
0 0 1 0 0 1 0 0 0 0 0 0	J	r · · · · · · · · · · · · · · · · · · ·	r ~g ~···

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
28	AZ	96/101~(95%)	93~(97%)	3~(3%)	0	100	100
29	Aa	86/91~(94%)	85 (99%)	1 (1%)	0	100	100
30	Ab	138/153~(90%)	137~(99%)	1 (1%)	0	100	100
31	Ac	81/84~(96%)	80 (99%)	1 (1%)	0	100	100
32	Ad	50/52~(96%)	48 (96%)	2~(4%)	0	100	100
33	Ae	64/67~(96%)	63~(98%)	1 (2%)	0	100	100
34	Af	48/51~(94%)	45 (94%)	3~(6%)	0	100	100
35	Ag	48/53~(91%)	48 (100%)	0	0	100	100
36	Ah	89/91~(98%)	89 (100%)	0	0	100	100
37	Ai	97/102~(95%)	89 (92%)	8 (8%)	0	100	100
38	Aj	181/184~(98%)	172 (95%)	9~(5%)	0	100	100
39	Ak	88/93~(95%)	87~(99%)	1 (1%)	0	100	100
40	BA	185/222~(83%)	180 (97%)	4 (2%)	1 (0%)	25	28
41	BB	196/208~(94%)	187 (95%)	9~(5%)	0	100	100
42	BC	75/216~(35%)	58 (77%)	16 (21%)	1 (1%)	10	8
43	BD	155/159~(98%)	153 (99%)	2(1%)	0	100	100
44	BE	234/237~(99%)	219 (94%)	13~(6%)	2(1%)	14	14
45	BF	192/202~(95%)	180 (94%)	11 (6%)	1 (0%)	25	28
46	BG	138/151~(91%)	130 (94%)	8~(6%)	0	100	100
47	BH	218/223~(98%)	206 (94%)	12~(6%)	0	100	100
48	BI	127/130~(98%)	121~(95%)	5~(4%)	1 (1%)	16	17
49	BJ	128/131~(98%)	124 (97%)	4(3%)	0	100	100
50	BK	132/142~(93%)	119 (90%)	11 (8%)	2(2%)	8	7
51	BL	36/106~(34%)	30~(83%)	5(14%)	1 (3%)	4	2
52	BM	123/141~(87%)	116 (94%)	7~(6%)	0	100	100
53	BN	142/147~(97%)	130 (92%)	10 (7%)	2(1%)	9	7
54	BO	141/153~(92%)	129~(92%)	12 (8%)	0	100	100
55	BP	27/54~(50%)	21 (78%)	5(18%)	1 (4%)	2	1
56	BQ	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
57	BR	$142/14\overline{7}\ (97\%)$	139 (98%)	3~(2%)	0	100	100
58	BS	62/71~(87%)	57 (92%)	5 (8%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
59	BT	133/158~(84%)	128 (96%)	4 (3%)	1 (1%)	16	17
60	BU	153/158~(97%)	146 (95%)	7 (5%)	0	100	100
61	BV	113/128~(88%)	111 (98%)	2 (2%)	0	100	100
62	BW	66/110~(60%)	64 (97%)	1 (2%)	1 (2%)	8	7
63	BX	93/100~(93%)	69~(74%)	18 (19%)	6 (6%)	1	0
64	BY	63/67~(94%)	57 (90%)	6 (10%)	0	100	100
65	BZ	69/77~(90%)	63 (91%)	6 (9%)	0	100	100
66	Ba	41/54~(76%)	41 (100%)	0	0	100	100
67	Bb	58/68~(85%)	57 (98%)	1 (2%)	0	100	100
68	Bc	62/65~(95%)	59 (95%)	3(5%)	0	100	100
All	All	8331/9068 (92%)	7998 (96%)	311 (4%)	22 (0%)	38	43

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
44	BE	185	GLY
44	BE	186	GLY
50	BK	10	ASN
53	BN	5	LYS
53	BN	6	SER

### 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	AA	181/186~(97%)	174 (96%)	7 (4%)	27 36
5	AB	280/282~(99%)	269~(96%)	11 (4%)	27 36
6	AC	226/231~(98%)	218 (96%)	8 (4%)	31 40
7	AD	149/149~(100%)	138~(93%)	11 (7%)	11 11
8	AE	165/165~(100%)	159~(96%)	6 (4%)	30 39
9	AF	115/118~(98%)	110 (96%)	5 (4%)	25 31



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
10	AG	163/165~(99%)	158~(97%)	5(3%)	35	44
11	AH	133/135~(98%)	128 (96%)	5 (4%)	28	37
12	AI	115/118 (98%)	114 (99%)	1 (1%)	75	85
13	AJ	87/89~(98%)	81 (93%)	6 (7%)	13	13
13	AK	77/89~(86%)	70 (91%)	7 (9%)	7	7
14	AL	121/125~(97%)	112 (93%)	9~(7%)	11	11
15	AM	161/165~(98%)	153 (95%)	8 (5%)	20	25
16	AN	134/140~(96%)	128 (96%)	6 (4%)	23	29
17	AO	166/169~(98%)	163 (98%)	3 (2%)	54	67
18	AP	99/100~(99%)	97~(98%)	2 (2%)	50	63
19	AQ	127/128~(99%)	122 (96%)	5 (4%)	27	36
20	AR	69/71~(97%)	62 (90%)	7 (10%)	6	5
21	AS	84/85~(99%)	82 (98%)	2 (2%)	44	55
22	AT	157/158~(99%)	152 (97%)	5 (3%)	34	43
23	AU	71/71~(100%)	69 (97%)	2(3%)	38	49
24	AV	107/112~(96%)	100 (94%)	7 (6%)	14	15
25	AW	48/53~(91%)	47 (98%)	1 (2%)	48	61
26	AX	58/65~(89%)	55 (95%)	3(5%)	19	23
27	AY	147/152~(97%)	137 (93%)	10 (7%)	13	14
28	AZ	77/79~(98%)	71 (92%)	6 (8%)	10	10
29	Aa	78/81~(96%)	77 (99%)	1 (1%)	65	77
30	Ab	125/137~(91%)	122 (98%)	3 (2%)	44	55
31	Ac	67/68~(98%)	65~(97%)	2(3%)	36	46
32	Ad	44/44~(100%)	43 (98%)	1 (2%)	45	56
33	Ae	60/61~(98%)	60 (100%)	0	100	100
34	Af	42/43~(98%)	39~(93%)	3~(7%)	12	12
35	Ag	46/49~(94%)	46 (100%)	0	100	100
36	Ah	82/82~(100%)	79~(96%)	3 (4%)	29	38
37	Ai	77/80~(96%)	74 (96%)	3 (4%)	27	36
38	Aj	161/162~(99%)	153 (95%)	8 (5%)	20	25
39	Ak	$79/\overline{82}\ (96\%)$	72 (91%)	7(9%)	8	7



Mol	Chain	Analysed	Rotameric	Outliers	Percen	tiles
40	BA	157/181~(87%)	143 (91%)	14 (9%)	8	7
41	BB	174/182~(96%)	161 (92%)	13~(8%)	11	11
42	BC	63/183~(34%)	49 (78%)	14 (22%)	1	0
43	BD	136/138 (99%)	129 (95%)	7 (5%)	20	24
44	BE	203/204~(100%)	189 (93%)	14 (7%)	13	13
45	BF	161/169~(95%)	151 (94%)	10 (6%)	15	17
46	BG	114/121 (94%)	108 (95%)	6(5%)	19	23
47	BH	191/193~(99%)	183 (96%)	8 (4%)	25	32
48	BI	109/110~(99%)	100 (92%)	9 (8%)	9	9
49	BJ	105/106~(99%)	98~(93%)	7 (7%)	13	14
50	BK	110/117 (94%)	93 (84%)	17 (16%)	2	2
51	BL	34/94~(36%)	27 (79%)	7 (21%)	1	1
52	BM	93/106~(88%)	84 (90%)	9 (10%)	6	6
53	BN	117/120~(98%)	111 (95%)	6 (5%)	20	24
54	BO	113/119~(95%)	104 (92%)	9 (8%)	10	10
55	BP	25/48~(52%)	25~(100%)	0	100	100
56	BQ	135/137~(98%)	125~(93%)	10 (7%)	11	11
57	BR	131/134~(98%)	121 (92%)	10 (8%)	11	11
58	BS	55/59~(93%)	53~(96%)	2(4%)	30	39
59	BT	120/137~(88%)	110 (92%)	10 (8%)	9	9
60	BU	127/130~(98%)	119 (94%)	8 (6%)	15	16
61	BV	101/111 (91%)	96~(95%)	5(5%)	20	25
62	BW	59/94~(63%)	52 (88%)	7 (12%)	4	4
63	BX	85/89~(96%)	73~(86%)	12 (14%)	3	2
64	BY	55/57~(96%)	52 (94%)	3 (6%)	18	20
65	BZ	59/63~(94%)	48 (81%)	11 (19%)	1	1
66	Ba	39/44~(89%)	34 (87%)	5 (13%)	3	3
67	Bb	49/56~(88%)	41 (84%)	8 (16%)	2	1
68	Bc	51/52~(98%)	48 (94%)	3 (6%)	16	18
All	All	7149/7643~(94%)	6726 (94%)	423 (6%)	19	18

 $5~{\rm of}~423$  residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
44	BE	66	ILE
50	BK	33	MET
65	BZ	30	GLU
44	BE	214	GLU
47	BH	156	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
45	BF	61	GLN
48	BI	108	GLN
38	Aj	131	HIS
38	Aj	150	ASN
42	BC	178	HIS

### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers		
1	2	129/129~(100%)	10 (7%)	2(1%)		
2	1	2841/3024~(93%)	341 (12%)	28~(0%)		
3	4	1418/1498 (94%)	258 (18%)	38~(2%)		
All	All	4388/4651 (94%)	609~(13%)	68~(1%)		

5 of 609 RNA backbone outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	2	2	С
1	2	8	А
1	2	28	G
1	2	48	А
1	2	54	G

5 of 68 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	4	1162	А
3	4	1178	А
3	4	1444	G
2	1	2420	G
2	1	2361	G



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

106 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	Bond angle		les
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	M7A	4	508	3	$19,\!25,\!26$	0.29	0	$25,\!37,\!40$	0.57	0
3	OMG	4	462	3	$19,\!26,\!27$	0.93	1 (5%)	21,38,41	1.12	2 (9%)
3	OMG	4	674	3	19,26,27	0.89	1 (5%)	21,38,41	1.05	2 (9%)
3	4AC	4	1318	3	21,24,25	0.39	0	$28,\!34,\!37$	0.70	0
3	A2M	4	1060	3	$18,\!25,\!26$	0.67	0	20,36,39	0.85	1 (5%)
2	OMC	1	2018	2	19,22,23	0.79	0	25,31,34	0.75	0
2	OMC	1	2624	2	$19,\!22,\!23$	0.80	0	$25,\!31,\!34$	0.85	1 (4%)
2	OMC	1	2555	2	19,22,23	0.80	0	25,31,34	0.86	1 (4%)
2	OMG	1	2366	2	19,26,27	0.93	1 (5%)	21,38,41	1.07	2 (9%)
3	OMG	4	1289	3,70	19,26,27	0.90	1 (5%)	21,38,41	1.03	2 (9%)
2	PSU	1	1911	2	18,21,22	0.93	1 (5%)	21,30,33	0.78	0
2	OMC	1	492	2	19,22,23	0.77	0	25,31,34	0.82	0
3	A2M	4	569	3,70	$18,\!25,\!26$	0.67	0	20,36,39	0.72	1 (5%)
2	G7M	1	3023	2	20,26,27	2.36	3 (15%)	16,39,42	0.59	0
2	OMU	1	2574	2	19,22,23	1.25	3 (15%)	25,31,34	1.76	4 (16%)
2	OMG	1	1949	2	$19,\!26,\!27$	0.90	1 (5%)	21,38,41	1.05	2 (9%)
2	OMG	1	2066	2	$19,\!26,\!27$	0.91	1 (5%)	21,38,41	1.08	2 (9%)
2	OMC	1	2704	2	19,22,23	0.80	0	25,31,34	0.88	0
3	PSU	4	263	3	18,21,22	0.93	1 (5%)	21,30,33	0.63	0
2	OMU	1	2077	2	19,22,23	1.32	3 (15%)	25,31,34	1.78	5 (20%)
3	B8T	4	1469	3	19,22,23	0.43	0	$25,\!31,\!34$	0.42	0
2	OMC	1	1816	2	19,22,23	0.80	0	25,31,34	0.71	0
3	OMC	4	572	3	19,22,23	0.80	0	25,31,34	0.79	0
2	OMG	1	2362	2	$19,\!26,\!27$	0.91	1 (5%)	21,38,41	1.07	2 (9%)
2	B8T	1	2937	2	19,22,23	0.41	0	25,31,34	0.32	0
2	OMU	1	875	2	19,22,23	1.27	3 (15%)	25,31,34	1.87	5 (20%)
3	OMU	4	15	3	19,22,23	1.33	4 (21%)	25,31,34	1.82	4 (16%)
2	OMC	1	2720	2	19,22,23	0.79	0	25,31,34	0.93	1 (4%)



Mal	<b>T</b>	Chain	Dec	T : 1-	Bond lengths		Bond angles			
NIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	PSU	1	1987	2	18,21,22	0.91	1 (5%)	21,30,33	0.68	0
3	A2M	4	880	3	18,25,26	0.69	0	20,36,39	0.80	1 (5%)
2	OMG	1	1957	2	19,26,27	0.93	1 (5%)	21,38,41	1.09	2 (9%)
2	OMC	1	2538	2	19,22,23	0.78	0	25,31,34	0.79	0
3	B8T	4	1035	3	19,22,23	0.41	0	25,31,34	0.56	0
2	OMU	1	2628	2	19,22,23	1.27	3 (15%)	25,31,34	1.81	5 (20%)
3	OMC	4	1045	3	19,22,23	0.76	0	25,31,34	0.80	0
2	OMG	1	2176	2,70	19,26,27	0.92	1 (5%)	21,38,41	1.09	2 (9%)
2	5MC	1	2056	2,70	19,22,23	1.52	3 (15%)	26,32,35	1.16	3 (11%)
2	OMU	1	2851	2	19,22,23	1.28	4 (21%)	25,31,34	1.84	4 (16%)
2	OMG	1	2103	2	19,26,27	0.94	1 (5%)	21,38,41	1.06	2 (9%)
3	OMG	4	1211	3	19,26,27	0.93	1 (5%)	21,38,41	1.09	1 (4%)
3	OMG	4	908	3	19,26,27	0.90	1 (5%)	21,38,41	1.09	2 (9%)
2	PSU	1	2607	2	18,21,22	0.96	1 (5%)	21,30,33	0.81	0
2	OMC	1	872	2	19,22,23	0.78	0	25,31,34	0.83	1 (4%)
2	OMG	1	2388	2	19,26,27	0.91	1 (5%)	21,38,41	1.18	2 (9%)
3	OMG	4	7	3	19,26,27	0.93	1 (5%)	21,38,41	1.36	3 (14%)
2	A2M	1	2691	2,70	18,25,26	0.66	0	20,36,39	0.73	1 (5%)
2	A2M	1	1990	2	18,25,26	0.69	0	20,36,39	0.86	1 (5%)
3	OMG	4	1163	3	19,26,27	0.90	1 (5%)	21,38,41	1.12	2 (9%)
3	OMG	4	465	3	19,26,27	0.94	1 (5%)	21,38,41	1.05	2 (9%)
3	OMG	4	1210	3	19,26,27	0.91	1 (5%)	21,38,41	1.04	1 (4%)
2	OMC	1	2143	2	19,22,23	0.27	0	25,31,34	0.30	0
3	OMG	4	1212	3	19,26,27	0.93	1 (5%)	21,38,41	1.11	2 (9%)
2	OMU	1	2408	2	19,22,23	1.33	4 (21%)	25,31,34	1.92	4 (16%)
2	OMC	1	2116	2	19,22,23	0.81	0	25,31,34	0.72	0
2	A2M	1	2011	2	18,25,26	0.67	0	20,36,39	0.71	1 (5%)
2	B8T	1	79	2	19,22,23	0.41	0	25,31,34	0.37	0
2	OMU	1	2623	2	19,22,23	1.26	3 (15%)	25,31,34	1.85	5 (20%)
2	OMC	1	493	2	19,22,23	0.79	0	25,31,34	0.81	0
3	OMG	4	19	3	19,26,27	0.95	1 (5%)	21,38,41	1.13	2 (9%)
3	A2M	4	40	3	18,25,26	0.67	0	20,36,39	0.73	1 (5%)
3	OMC	4	1184	3	19,22,23	0.80	0	25,31,34	0.85	1 (4%)
3	OMG	4	906	3	19,26,27	0.89	1 (5%)	21,38,41	1.11	2 (9%)
2	PSU	1	2625	2	18,21,22	0.92	1 (5%)	21,30,33	0.71	0
2	OMC	1	673	2	19,22,23	0.79	0	25,31,34	0.83	0



Mal	Tune	Chain	Dec	Tink	Bo	ond leng	Bond lengths		Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
3	MA6	4	1478	3	$19,\!26,\!27$	0.92	1 (5%)	18,38,41	0.83	1 (5%)	
2	A2M	1	2059	2,70	18,25,26	0.71	0	20,36,39	0.91	0	
2	4AC	1	2016	2	21,24,25	0.39	0	28,34,37	0.60	0	
3	OMG	4	511	3	19,26,27	0.89	1(5%)	21,38,41	1.06	2(9%)	
3	MA6	4	1477	3	19,26,27	0.93	1 (5%)	18,38,41	0.82	1 (5%)	
2	OMU	1	2155	2	$19,\!22,\!23$	1.26	3 (15%)	$25,\!31,\!34$	1.86	5 (20%)	
2	OMG	1	902	2,70	$19,\!26,\!27$	0.87	1 (5%)	21,38,41	1.14	2 (9%)	
2	OMG	1	1971	2	19,26,27	0.92	1 (5%)	21,38,41	1.08	2 (9%)	
3	OMG	4	475	3	19,26,27	0.94	1 (5%)	21,38,41	1.06	2 (9%)	
3	4AC	4	5	3	21,24,25	0.43	0	$28,\!34,\!37$	0.66	0	
2	OMG	1	2667	2	19,26,27	0.91	1 (5%)	21,38,41	1.08	2 (9%)	
3	A2M	4	879	3	18,25,26	0.66	0	20,36,39	0.73	1 (5%)	
2	OMG	1	2104	2	19,26,27	0.93	1 (5%)	21,38,41	1.14	2 (9%)	
3	OMC	4	1034	3	19,22,23	0.80	0	25,31,34	0.81	0	
3	OMG	4	1202	3,70	19,26,27	0.91	1 (5%)	21,38,41	1.12	2 (9%)	
2	UR3	1	2698	2	19,22,23	0.93	0	26,32,35	1.72	2 (7%)	
3	A2M	4	496	3	18,25,26	0.67	0	20,36,39	0.82	1 (5%)	
2	OMG	1	2071	2	19,26,27	0.90	1 (5%)	21,38,41	1.05	2 (9%)	
2	OMG	1	2017	2	19,26,27	0.90	1 (5%)	21,38,41	1.04	2 (9%)	
2	OMU	1	908	2,70	19,22,23	1.32	4 (21%)	25,31,34	1.96	7 (28%)	
2	OMG	1	2601	2,70	19,26,27	0.92	1 (5%)	21,38,41	1.08	2(9%)	
3	6MZ	4	1459	3,70	17,25,26	0.82	0	15,36,39	1.96	2 (13%)	
2	OMU	1	2707	2	19,22,23	1.28	4 (21%)	25,31,34	1.88	5 (20%)	
3	OMC	4	1368	3	19,22,23	0.79	0	25,31,34	0.79	0	
3	OMC	4	489	3	19,22,23	0.81	0	25,31,34	0.88	0	
2	PSU	1	2571	2	18,21,22	0.94	1(5%)	21,30,33	0.73	0	
2	PSU	1	2044	2	18,21,22	0.90	1 (5%)	$21,\!30,\!33$	0.67	0	
2	OMG	1	2608	2	19,26,27	0.92	1 (5%)	21,38,41	1.12	2 (9%)	
2	OMC	1	1976	2	19,22,23	0.83	0	25,31,34	0.91	1 (4%)	
2	PSU	1	2610	2	18,21,22	0.90	1 (5%)	21,30,33	0.79	0	
2	OMC	1	2885	2	19,22,23	0.81	0	25,31,34	0.78	0	
52	IAS	BM	128	52	6,7,8	1.32	1 (16%)	3,8,10	1.47	1 (33%)	
2	OMC	1	2115	2	19,22,23	0.80	0	$25,\!31,\!34$	0.80	0	
2	OMG	1	2537	2	19,26,27	0.91	1 (5%)	21,38,41	1.08	2 (9%)	
3	OMU	4	877	3	19,22,23	1.26	3 (15%)	25,31,34	1.84	5 (20%)	
2	5MC	1	38	2	19,22,23	1.46	3 (15%)	26,32,35	1.21	3 (11%)	



Mal	Turne	Type Chain Bes		og Link	Bo	Bond lengths			Bond angles		
WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
3	OMG	4	467	3	$19,\!26,\!27$	0.84	1 (5%)	21,38,41	1.06	1 (4%)	
2	OMC	1	2884	2	19,22,23	0.79	0	25,31,34	0.81	0	
3	OMC	4	514	3	$19,\!22,\!23$	0.82	0	25,31,34	0.91	1 (4%)	
2	OMU	1	2666	2	$19,\!22,\!23$	1.26	3 (15%)	25,31,34	1.85	5 (20%)	
2	OMU	1	2088	2	$19,\!22,\!23$	1.28	3 (15%)	25,31,34	1.80	4 (16%)	
2	OMG	1	1947	2	19,26,27	0.90	1 (5%)	21,38,41	1.22	2 (9%)	

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	M7A	4	508	3	-	3/7/37/38	0/3/3/3
3	OMG	4	462	3	-	1/5/27/28	0/3/3/3
3	OMG	4	674	3	-	0/5/27/28	0/3/3/3
3	4AC	4	1318	3	-	0/11/29/30	0/2/2/2
3	A2M	4	1060	3	-	3/5/27/28	0/3/3/3
2	OMC	1	2018	2	-	0/9/27/28	0/2/2/2
2	OMC	1	2624	2	-	0/9/27/28	0/2/2/2
2	OMC	1	2555	2	-	2/9/27/28	0/2/2/2
2	OMG	1	2366	2	-	0/5/27/28	0/3/3/3
3	OMG	4	1289	3,70	-	0/5/27/28	0/3/3/3
2	PSU	1	1911	2	-	0/7/25/26	0/2/2/2
2	OMC	1	492	2	-	2/9/27/28	0/2/2/2
3	A2M	4	569	3,70	-	0/5/27/28	0/3/3/3
2	G7M	1	3023	2	-	1/3/25/26	0/3/3/3
2	OMU	1	2574	2	-	0/9/27/28	0/2/2/2
2	OMG	1	1949	2	-	0/5/27/28	0/3/3/3
2	OMG	1	2066	2	-	0/5/27/28	0/3/3/3
2	OMC	1	2704	2	-	0/9/27/28	0/2/2/2
3	PSU	4	263	3	-	0/7/25/26	0/2/2/2
2	OMU	1	2077	2	-	1/9/27/28	0/2/2/2
3	B8T	4	1469	3	-	0/7/27/28	0/2/2/2
2	OMC	1	1816	2	-	0/9/27/28	0/2/2/2
3	OMC	4	572	3	-	1/9/27/28	0/2/2/2
2	OMG	1	2362	2	-	1/5/27/28	0/3/3/3
2	B8T	1	2937	2	-	1/7/27/28	0/2/2/2
2	OMU	1	875	2	-	1/9/27/28	0/2/2/2
3	OMU	4	15	3	-	0/9/27/28	0/2/2/2
2	OMC	1	2720	2	-	0/9/27/28	0/2/2/2



Mol		Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	1	1987	2	-	0/7/25/26	0/2/2/2
3	A2M	4	880	3	_	0/1/20/20 0/5/27/28	0/2/2/2
2	OMG	1	1957	2	_	0/5/27/28	0/3/3/3
2	OMC	1	2538	2	_	0/9/27/28	0/2/2/2
3	B8T	4	1035	3	-	0/7/27/28	0/2/2/2
2	OMU	1	2628	2	-	0/9/27/28	0/2/2/2
3	OMC	4	1045	3	-	2/9/27/28	0/2/2/2
2	OMG	1	2176	2,70	-	0/5/27/28	0/3/3/3
2	5MC	1	2056	2,70	-	1/7/25/26	0/2/2/2
2	OMU	1	2851	2	-	2/9/27/28	0/2/2/2
2	OMG	1	2103	2	-	0/5/27/28	0/3/3/3
3	OMG	4	1211	3	-	2/5/27/28	0/3/3/3
3	OMG	4	908	3	-	4/5/27/28	0/3/3/3
2	PSU	1	2607	2	-	0/7/25/26	0/2/2/2
2	OMC	1	872	2	-	0/9/27/28	0/2/2/2
2	OMG	1	2388	2	-	2/5/27/28	0/3/3/3
3	OMG	4	7	3	-	0/5/27/28	0/3/3/3
2	A2M	1	2691	2,70	-	1/5/27/28	0/3/3/3
2	A2M	1	1990	2	-	0/5/27/28	0/3/3/3
3	OMG	4	1163	3	-	3/5/27/28	0/3/3/3
3	OMG	4	465	3	-	2/5/27/28	0/3/3/3
3	OMG	4	1210	3	-	1/5/27/28	0/3/3/3
2	OMC	1	2143	2	-	0/9/27/28	0/2/2/2
3	OMG	4	1212	3	-	0/5/27/28	0/3/3/3
2	OMU	1	2408	2	-	0/9/27/28	0/2/2/2
2	OMC	1	2116	2	-	2/9/27/28	0/2/2/2
2	A2M	1	2011	2	-	0/5/27/28	0/3/3/3
2	B8T	1	79	2	-	0/7/27/28	0/2/2/2
2	OMU	1	2623	2	-	2/9/27/28	0/2/2/2
2	OMC	1	493	2	-	1/9/27/28	0/2/2/2
3	OMG	4	19	3	-	1/5/27/28	0/3/3/3
3	A2M	4	40	3	-	1/5/27/28	0/3/3/3
3	OMC	4	1184	3	-	1/9/27/28	0/2/2/2
3	OMG	4	906	3	-	0/5/27/28	0/3/3/3
2	PSU	1	2625	2	-	2/7/25/26	0/2/2/2
2	OMC	1	673	2	-	0/9/27/28	0/2/2/2
3	MA6	4	1478	3	-	2/7/29/30	0/3/3/3
2	A2M	1	2059	2,70	-	1/5/27/28	0/3/3/3
2	4AC	1	2016	2	-	0/11/29/30	0/2/2/2



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	4	511	3	-	3/5/27/28	0/3/3/3
3	MA6	4	1477	3	-	0/7/29/30	0/3/3/3
2	OMU	1	2155	2	-	2/9/27/28	0/2/2/2
2	OMG	1	902	2,70	_	0/5/27/28	0/3/3/3
2	OMG	1	1971	2	-	0/5/27/28	0/3/3/3
3	OMG	4	475	3	-	0/5/27/28	0/3/3/3
3	4AC	4	5	3	-	2/11/29/30	0/2/2/2
2	OMG	1	2667	2	-	0/5/27/28	0/3/3/3
3	A2M	4	879	3	_	4/5/27/28	0/3/3/3
2	OMG	1	2104	2	-	0/5/27/28	0/3/3/3
3	OMC	4	1034	3	_	0/9/27/28	0/2/2/2
3	OMG	4	1202	3,70	-	3/5/27/28	0/3/3/3
2	UR3	1	2698	2	-	0/7/25/26	0/2/2/2
3	A2M	4	496	3	_	3/5/27/28	0/3/3/3
2	OMG	1	2071	2	_	0/5/27/28	0/3/3/3
2	OMG	1	2017	2	-	$\frac{3}{1/5/27/28}$	0/3/3/3
2	OMU	1	908	2,70	-	$\frac{4}{9}/27/28$	0/2/2/2
2	OMG	1	2601	2.70	_	0/5/27/28	0/3/3/3
3	6MZ	4	1459	3,70	-	$\frac{0/5/27/28}{0/5/27/28}$	0/3/3/3
2	OMU	1	2707	2	-	0/9/27/28	0/2/2/2
3	OMC	4	1368	3	-	1/9/27/28	0/2/2/2
3	OMC	4	489	3	-	1/9/27/28	0/2/2/2
2	PSU	1	2571	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2044	2	-	2/7/25/26	0/2/2/2
2	OMG	1	2608	2	-	2/5/27/28	0/3/3/3
2	OMC	1	1976	2	-	1/9/27/28	0/2/2/2
2	PSU	1	2610	2	-	0/7/25/26	0/2/2/2
2	OMC	1	2885	2	-	0/9/27/28	0/2/2/2
52	IAS	BM	128	52	-	1/7/7/8	-
2	OMC	1	2115	2	-	0/9/27/28	0/2/2/2
2	OMG	1	2537	2	-	2/5/27/28	0/3/3/3
3	OMU	4	877	3	-	0/9/27/28	0/2/2/2
2	5MC	1	38	2	-	1/7/25/26	0/2/2/2
3	OMG	4	467	3	-	0/5/27/28	0/3/3/3
2	OMC	1	2884	2	-	0/9/27/28	0/2/2/2
3	OMC	4	514	3	-	1/9/27/28	0/2/2/2
2	OMU		2666	2	-	$\frac{0/9/27/28}{0/9/27/28}$	0/2/2/2
2	OMU		2088	2	-	0/9/27/28	0/2/2/2
2	OMG	1	1947	2	-	2/5/27/28	+0/3/3/3



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	3023	G7M	C8-N9	7.19	1.46	1.33
2	1	3023	G7M	C8-N7	6.72	1.45	1.33
2	1	2056	5MC	C5-C4	5.34	1.48	1.44
2	1	38	5MC	C5-C4	5.00	1.47	1.44
2	1	2607	PSU	C6-C5	3.62	1.39	1.35

The worst 5 of 101 bond length outliers are listed below:

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	1	2698	UR3	C4-N3-C2	-6.86	119.06	124.58
3	4	1459	6MZ	C2-N1-C6	6.07	121.31	116.60
2	1	2408	OMU	C4-N3-C2	-5.28	120.06	126.61
2	1	2155	OMU	C4-N3-C2	-5.07	120.31	126.61
3	4	877	OMU	C4-N3-C2	-5.02	120.38	126.61

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
3	4	40	A2M	C1'-C2'-O2'-CM'
3	4	496	A2M	C1'-C2'-O2'-CM'
3	4	879	A2M	C3'-C4'-C5'-O5'
3	4	879	A2M	C1'-C2'-O2'-CM'
3	4	1045	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 327 ligands modelled in this entry, 263 are monoatomic - leaving 64 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



					Be	ond leng	ths	В	ond ang	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
69	SPM	1	3109	_	13,13,13	0.17	0	12,12,12	0.36	0
69	SPM	1	3115	-	13,13,13	0.18	0	12,12,12	0.45	0
69	SPM	1	3116	-	13,13,13	0.15	0	12,12,12	0.26	0
69	SPM	4	3017	-	13,13,13	0.21	0	12,12,12	1.70	1 (8%)
69	SPM	AL	201	-	13,13,13	0.16	0	12,12,12	0.40	0
69	SPM	1	3108	-	13,13,13	0.19	0	12,12,12	0.66	0
69	SPM	1	3121	-	13,13,13	0.24	0	12,12,12	0.30	0
69	SPM	1	3135	-	13,13,13	0.16	0	12,12,12	0.64	0
69	SPM	1	3138	-	13,13,13	0.17	0	12,12,12	0.82	0
69	SPM	1	3132	-	13,13,13	0.16	0	12,12,12	0.40	0
69	SPM	1	3129	-	13,13,13	0.17	0	12,12,12	0.37	0
69	SPM	1	3101	-	13,13,13	0.18	0	12,12,12	0.66	0
69	SPM	1	3133	-	13,13,13	0.17	0	12,12,12	0.37	0
69	SPM	4	3007	-	13,13,13	0.24	0	12,12,12	0.53	0
69	SPM	1	3111	-	13,13,13	0.15	0	12,12,12	0.25	0
69	SPM	1	3117	-	13,13,13	0.17	0	12,12,12	0.36	0
69	SPM	1	3105	-	13,13,13	0.15	0	12,12,12	0.16	0
69	SPM	1	3126	-	13,13,13	0.17	0	12,12,12	0.59	0
69	SPM	1	3144	-	13,13,13	0.16	0	12,12,12	0.40	0
69	SPM	4	3010	-	13,13,13	0.15	0	12,12,12	0.69	0
69	SPM	1	3127	-	13,13,13	0.17	0	12,12,12	0.30	0
69	SPM	1	3120	-	13,13,13	0.18	0	12,12,12	0.22	0
69	SPM	1	3103	-	13,13,13	0.16	0	12,12,12	0.44	0
69	SPM	1	3122	-	13,13,13	0.18	0	12,12,12	0.25	0
69	SPM	1	3102	-	13,13,13	0.16	0	12,12,12	0.43	0
69	SPM	4	3014	-	13,13,13	0.19	0	12,12,12	0.57	0
69	SPM	4	3011	-	13,13,13	0.16	0	$12,\!12,\!12$	0.43	0
69	SPM	Ah	101	-	13,13,13	0.17	0	$12,\!12,\!12$	0.19	0
69	SPM	4	3009	-	13,13,13	0.17	0	$12,\!12,\!12$	0.35	0
69	SPM	1	3130	-	$13,\!13,\!13$	0.14	0	$12,\!12,\!12$	0.18	0
69	SPM	4	3016	-	13,13,13	0.16	0	$12,\!12,\!12$	0.22	0
69	SPM	1	3113	-	13,13,13	0.18	0	$12,\!12,\!12$	0.19	0
69	SPM	1	3125	-	13,13,13	0.17	0	$12,\!12,\!12$	0.29	0
69	SPM	1	3128	-	13,13,13	0.18	0	12,12,12	0.21	0
69	SPM	1	3136	-	13,13,13	0.14	0	12,12,12	0.29	0
69	SPM	1	3106	-	13,13,13	0.17	0	12,12,12	0.19	0
69	SPM	4	3003	-	13,13,13	0.18	0	$12,\!12,\!12$	0.38	0
69	SPM	4	3013	-	13,13,13	0.16	0	12,12,12	0.28	0
69	SPM	1	3123	-	13,13,13	0.16	0	12,12,12	0.36	0

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	В	ond ang	gles
	Type	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
69	SPM	1	3110	-	13,13,13	0.16	0	12,12,12	0.29	0
69	SPM	1	3119	-	13,13,13	0.21	0	12,12,12	0.26	0
69	SPM	1	3114	-	13,13,13	0.16	0	12,12,12	0.19	0
69	SPM	1	3137	-	13,13,13	0.17	0	12,12,12	0.43	0
69	SPM	1	3104	-	13,13,13	0.16	0	12,12,12	0.31	0
69	SPM	4	3001	-	13,13,13	0.16	0	12,12,12	0.33	0
69	SPM	4	3002	-	13,13,13	0.21	0	12,12,12	0.47	0
69	SPM	4	3008	-	13,13,13	0.15	0	12,12,12	0.27	0
69	SPM	4	3005	-	13,13,13	0.14	0	12,12,12	0.16	0
69	SPM	1	3131	-	13,13,13	0.16	0	12,12,12	0.34	0
69	SPM	1	3112	-	13,13,13	0.17	0	12,12,12	0.32	0
69	SPM	1	3134	-	13,13,13	0.15	0	12,12,12	0.43	0
69	SPM	1	3118	-	13,13,13	0.15	0	12,12,12	0.17	0
69	SPM	1	3107	-	13,13,13	0.18	0	12,12,12	0.19	0
69	SPM	1	3124	-	13,13,13	0.15	0	12,12,12	0.23	0
69	SPM	4	3006	-	13,13,13	0.15	0	12,12,12	0.24	0
69	SPM	1	3140	-	13,13,13	0.15	0	12,12,12	0.39	0
69	SPM	1	3142	-	13,13,13	0.18	0	12,12,12	0.34	0
69	SPM	4	3012	-	13,13,13	0.19	0	12,12,12	0.20	0
69	SPM	1	3143	-	13,13,13	0.21	0	12,12,12	0.46	0
69	SPM	4	3004	-	13,13,13	0.16	0	12,12,12	0.26	0
69	SPM	4	3018	-	13,13,13	0.15	0	12,12,12	0.32	0
69	SPM	1	3141	-	13,13,13	0.20	0	12,12,12	0.62	0
69	SPM	1	3139	-	13,13,13	0.16	0	12,12,12	0.25	0
69	SPM	4	3015	-	13,13,13	0.15	0	12,12,12	0.35	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
69	SPM	1	3109	-	-	1/11/11/11	-
69	SPM	1	3115	-	-	1/11/11/11	-
69	SPM	1	3116	-	-	2/11/11/11	-
69	SPM	4	3017	-	-	4/11/11/11	-
69	SPM	AL	201	-	-	1/11/11/11	-
69	SPM	1	3108	-	-	3/11/11/11	-
69	SPM	1	3121	-	-	1/11/11/11	-
69	SPM	1	3135	-	-	2/11/11/11	-
69	SPM	1	3138	-	_	6/11/11/11	_



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	SPM	1	3132	_	-	3/11/11/11	-
69	SPM	1	3129	_	_	$\frac{2}{11}$	-
69	SPM	1	3101	_	-	4/11/11/11	-
69	SPM	1	3133	_	_	3/11/11/11	-
69	SPM	4	3007	_	-	5/11/11/11	-
69	SPM	1	3111	_	-	0/11/11/11	-
69	SPM	1	3117	-	_	2/11/11/11	_
69	SPM	1	3105	_	_	1/11/11/11	-
69	SPM	1	3126	-	-	3/11/11/11	-
69	SPM	1	3144	-	-	3/11/11/11	-
69	SPM	4	3010	-	-	2/11/11/11	-
69	SPM	1	3127	-	-	0/11/11/11	-
69	SPM	1	3120	-	-	1/11/11/11	-
69	SPM	1	3103	-	-	0/11/11/11	-
69	SPM	1	3122	-	-	1/11/11/11	-
69	SPM	1	3102	-	-	0/11/11/11	-
69	SPM	4	3014	-	-	2/11/11/11	-
69	SPM	4	3011	-	-	2/11/11/11	-
69	SPM	Ah	101	-	-	2/11/11/11	-
69	SPM	4	3009	-	-	2/11/11/11	-
69	SPM	1	3130	-	-	0/11/11/11	-
69	SPM	4	3016	-	-	1/11/11/11	-
69	SPM	1	3113	-	-	4/11/11/11	-
69	SPM	1	3125	-	-	1/11/11/11	-
69	SPM	1	3128	-	-	2/11/11/11	-
69	SPM	1	3136	-	-	2/11/11/11	-
69	SPM	1	3106	-	-	5/11/11/11	-
69	SPM	4	3003	-	-	5/11/11/11	-
69	SPM	4	3013	-	-	1/11/11/11	-
69	SPM	1	3123	-	-	1/11/11/11	-
69	SPM	1	3110	-	-	1/11/11/11	-
69	SPM	1	3119	-	-	4/11/11/11	-
69	SPM	1	3114	-	-	4/11/11/11	-
69	SPM	1	3137	-	-	2/11/11/11	-
69	SPM	1	3104	-	-	3/11/11/11	-
69	SPM	4	3001	-	-	0/11/11/11	-
69	SPM	4	3002	-	-	4/11/11/11	-

Continued from previous page...



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	SPM	4	3008	-	-	0/11/11/11	-
69	SPM	4	3005	-	-	1/11/11/11	-
69	SPM	1	3131	-	-	4/11/11/11	-
69	SPM	1	3112	-	-	1/11/11/11	-
69	SPM	1	3134	-	-	3/11/11/11	-
69	SPM	1	3118	-	-	0/11/11/11	-
69	SPM	1	3107	-	-	1/11/11/11	-
69	SPM	1	3124	-	-	0/11/11/11	-
69	SPM	4	3006	-	-	2/11/11/11	-
69	SPM	1	3140	-	-	1/11/11/11	-
69	SPM	1	3142	-	-	3/11/11/11	-
69	SPM	4	3012	-	-	4/11/11/11	-
69	SPM	1	3143	-	-	1/11/11/11	-
69	SPM	4	3004	-	-	3/11/11/11	-
69	SPM	4	3018	-	-	0/11/11/11	-
69	SPM	1	3141	-	-	4/11/11/11	-
69	SPM	1	3139	-	-	1/11/11/11	-
69	SPM	4	3015	-	-	2/11/11/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
69	4	3017	SPM	C7-C8-C9	5.69	139.82	113.56

There are no chirality outliers.

5 of 130 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1	3106	SPM	C12-C11-N10-C9
69	4	3017	SPM	C6-C7-C8-C9
69	1	3101	SPM	C7-C8-C9-N10
69	4	3007	SPM	C7-C8-C9-N10
69	1	3134	SPM	N5-C6-C7-C8

There are no ring outliers.

No monomer is involved in short contacts.



# 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



#### 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-47628. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

#### Orthogonal projections (i) 6.1

#### 6.1.1Primary map



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

#### Central slices (i) 6.2

#### 6.2.1Primary map



X Index: 304

Y Index: 304



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: 334

Y Index: 288

Z Index: 326

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



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

### 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 756  $\rm nm^3;$  this corresponds to an approximate mass of 683 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 0.424  $\rm \AA^{-1}$ 



# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-47628 and PDB model 9E71. Per-residue inclusion information can be found in section 3 on page 23.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.215 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 (0.215).



### 9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 82% 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 (0.215) and Q-score for the entire model and for each chain.

$\mathbf{Chain}$	Atom inclusion	$\mathbf{Q} ext{-score}$
All	0.8160	0.6140
1	0.9300	0.6510
2	0.9230	0.6430
4	0.8380	0.5700
AA	0.8830	0.6710
AB	0.8490	0.6750
AC	0.8070	0.6490
AD	0.7750	0.6090
AE	0.5900	0.5970
AF	0.5750	0.5870
AG	0.8080	0.6520
AH	0.8180	0.6540
AI	0.8270	0.6530
AJ	0.5520	0.5570
AK	0.5190	0.5690
AL	0.7420	0.6260
AM	0.8600	0.6640
AN	0.7920	0.6340
AO	0.8770	0.6530
AP	0.8330	0.6490
AQ	0.8250	0.6440
AR	0.6960	0.6010
AS	0.9430	0.6800
AT	0.8680	0.6700
AU	0.8050	0.6680
AV	0.7400	0.6280
AW	0.8320	0.6530
AX	0.6420	0.6150
AY	0.8380	0.6470
AZ	0.6670	0.5790
Aa	0.8080	0.6560
Ab	0.8120	0.6530
Ac	0.9160	0.6590
Ad	0.9830	0.7140
Ae	0.7110	0.6450



Chain	Atom inclusion	Q-score
Af	0.9470	0.6810
Ag	0.6910	0.6150
Ah	0.9020	0.6710
Ai	0.7920	0.6270
Aj	0.6470	0.6020
Ak	0.6880	0.6160
BA	0.5200	0.5220
BB	0.4950	0.5050
BC	0.1640	0.3990
BD	0.7110	0.5830
BE	0.6780	0.5840
BF	0.6980	0.5740
BG	0.3720	0.4690
BH	0.6510	0.5460
BI	0.7930	0.5960
BJ	0.7190	0.5880
BK	0.6360	0.5360
BL	0.1690	0.4480
BM	0.6630	0.5330
BN	0.7040	0.5810
BO	0.5280	0.5410
BP	0.1730	0.4250
BQ	0.6570	0.5710
BR	0.6460	0.5780
BS	0.2220	0.4030
BT	0.5290	0.5350
BU	0.6990	0.5720
BV	0.4610	0.5190
BW	0.5220	0.5330
BX	0.2220	0.4380
BY	0.6210	0.5710
BZ	0.5230	0.5050
Ba	0.5900	0.5470
Bb	0.2760	0.4360
Bc	0.6180	0.5340

