wwPDB EM Validation Summary Report (i)

Apr 17, 2024 – 10:24 am BST

PDB ID	:	7OTC
EMDB ID	:	EMD-13058
Title	:	Cryo-EM structure of an Escherichia coli 70S ribosome in complex with elongation factor G and the antibiotic Argyrin B
Authors	:	Wieland, M.; Koller, T.O.; Wilson, D.N.
Deposited on	:	2021-06-10
Resolution	:	2.90 Å(reported)
Based on initial models	:	7K00, 4V9P

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:

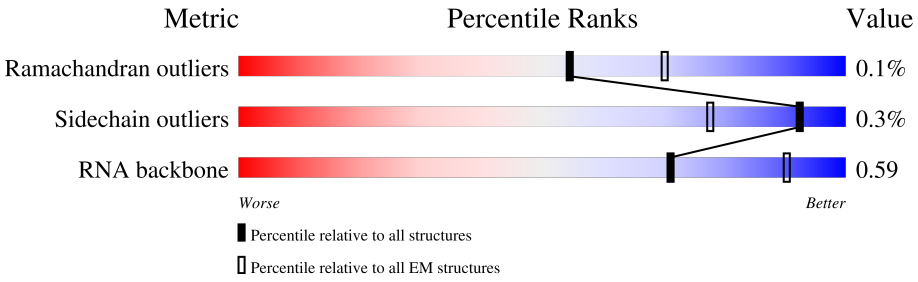
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	a	1533	82% 18%
2	b	226	12% 98%
3	c	206	100%
4	d	205	100%
5	e	157	99%
6	f	106	8% 99%
7	g	156	43% 99%
8	h	129	100%

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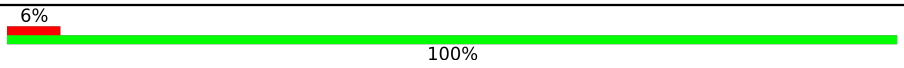
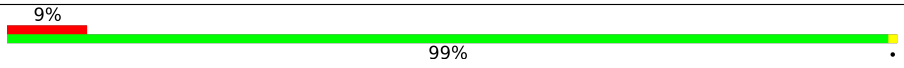
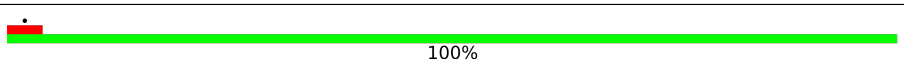
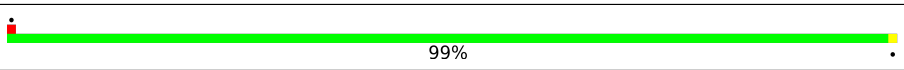
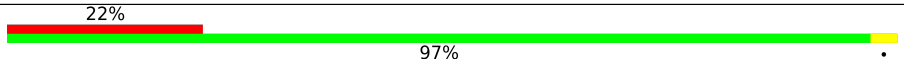
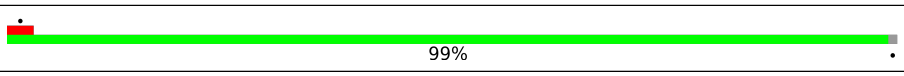
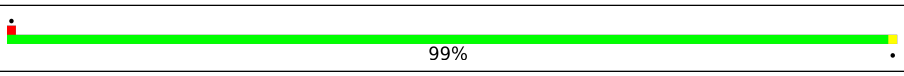
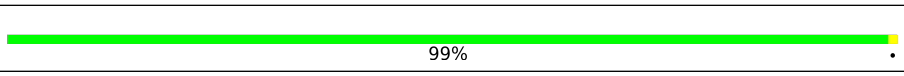
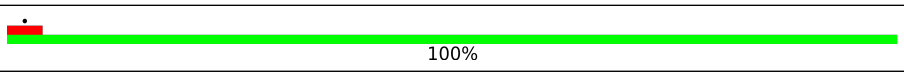
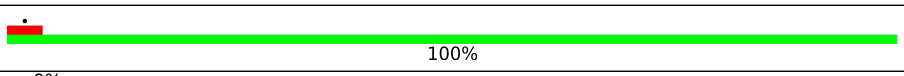
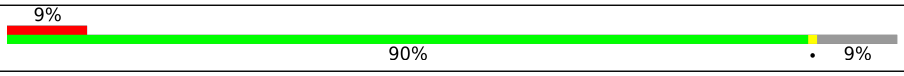
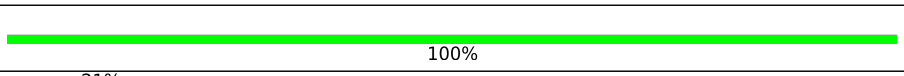
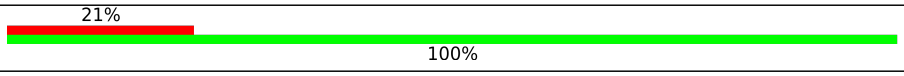
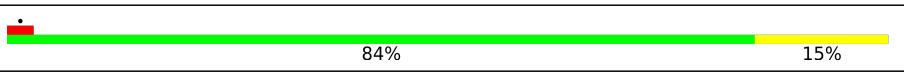
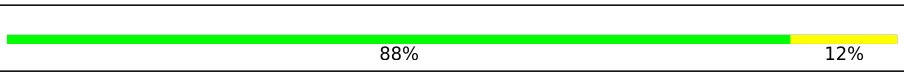
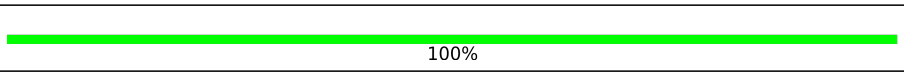
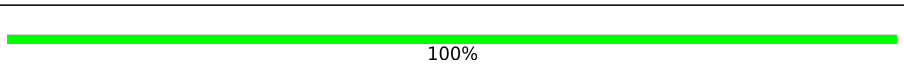
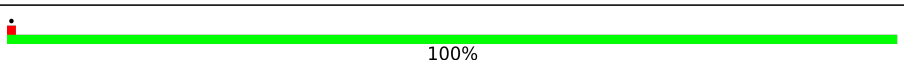
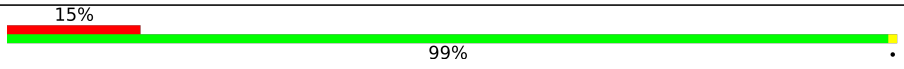
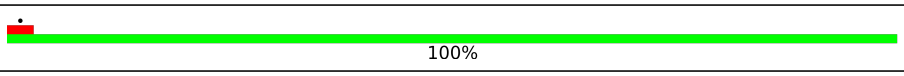
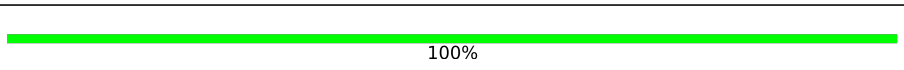
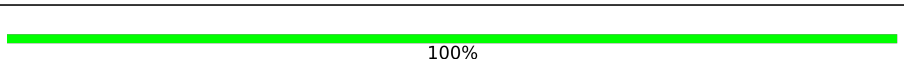
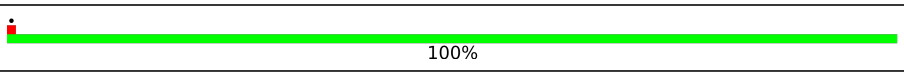
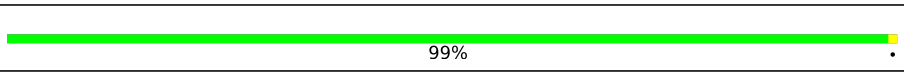
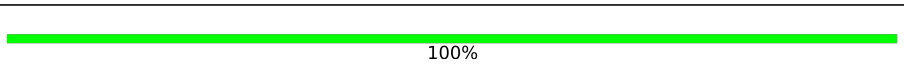
Mol	Chain	Length	Quality of chain
9	i	127	
10	j	99	
11	k	117	
12	l	123	
13	m	115	
14	n	101	
15	o	88	
16	p	82	
17	q	80	
18	r	67	
19	s	92	
20	t	86	
21	u	70	
22	A	2903	
23	B	120	
24	C	271	
25	D	209	
26	E	201	
27	F	177	
28	G	176	
29	J	142	
30	K	123	
31	L	144	
32	M	136	
33	N	120	

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Mol	Chain	Length	Quality of chain
34	O	116	100%
35	P	114	99%
36	Q	117	100%
37	R	103	98%
38	S	110	100%
39	T	93	100%
40	U	102	92% 8%
41	V	94	100%
42	W	84	10% 100%
43	X	77	100%
44	Y	63	6% 98%
45	Z	58	5% 100%
46	5	67	48% 99%
47	0	56	100%
48	1	50	100%
49	2	46	100%
50	3	64	100%
51	4	38	100%
52	w	704	14% 95%

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 147132 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1533	32907	14683	6036	10655	1533	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	226	1769	1119	317	325	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	206	1624	1028	305	288	3	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	205	1642	1026	315	297	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	155	1144	711	216	211	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	151	GLU	ALA	conflict	UNP A0A140N6Z9

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	106	Total 862	C 545	N 156	O 154	S 7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	156	Total 1236	C 773	N 238	O 221	S 4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	157	LEU	-	expression tag	UNP A0A140N6W8

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total 978	C 616	N 173	O 183	S 6	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total 1021	C 634	N 206	O 178	S 3	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	99	Total 806	C 504	N 156	O 145	S 1	1	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	117	Total 876	C 540	N 174	O 159	S 3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			804	499	164	138	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP A0A140N7K8

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			713	439	144	129	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	67	Total	C	N	O	S	0	0
			555	351	106	97	1		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	2903	Total	C	N	O	P	0	0
			62334	27815	11467	20149	2903		

- Molecule 23 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	271	Total	C	N	O	S	1	0
			2090	1292	425	366	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	J	142	Total	C	N	O	S	1	0
			1139	720	215	200	4		

- Molecule 30 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 31 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	144	Total	C	N	O	S	1	0
			1064	660	211	191	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	77	ILE	VAL	conflict	UNP A0A140N711

- Molecule 32 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 33 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 34 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 35 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	P	114	Total	C	N	O	S	0	0
			916	574	179	162	1		

- Molecule 36 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 37 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 38 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 40 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	U	94	Total	C	N	O	0	0
			721	454	136	131		

- Molecule 41 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	V	94	Total	C	N	O	S	0	0
			752	479	137	133	3		

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	W	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	X	77	Total	C	N	O	S	0	0
			624	388	129	105	2		

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 46 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	5	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 50 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	64	Total	C	N	O	S	1	0
			512	329	107	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	675	Total	C	N	O	S	0	0
			5196	3277	899	997	23		

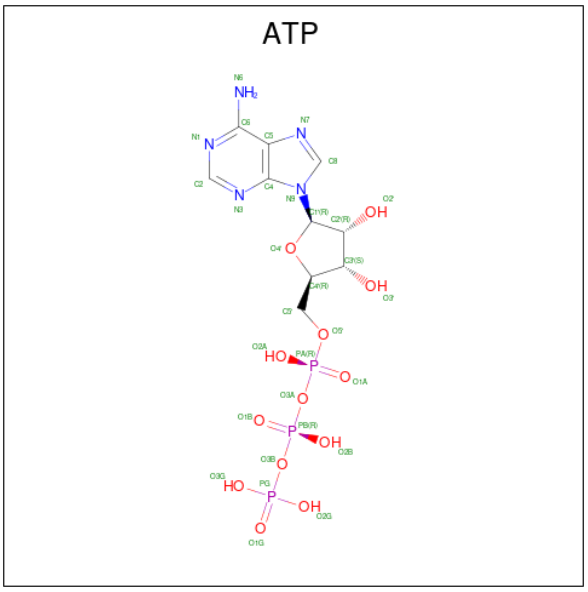
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	1	SER	-	expression tag	UNP A0A140N7C7
w	237	THR	TYR	variant	UNP A0A140N7C7
w	258	ASP	ASN	variant	UNP A0A140N7C7

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

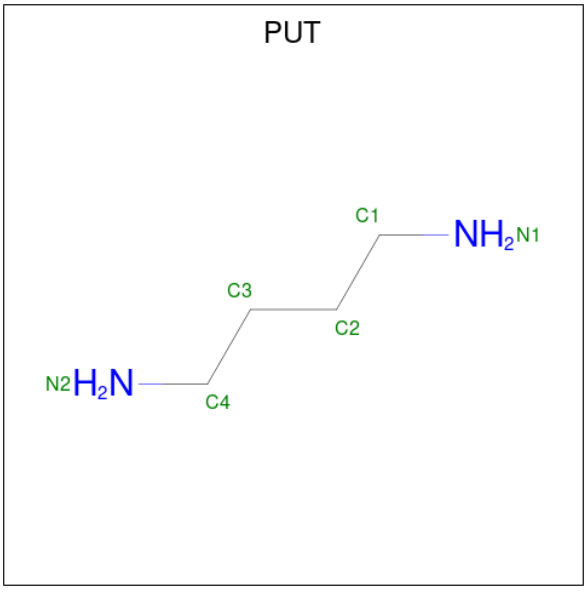
Mol	Chain	Residues	Atoms		AltConf
53	a	61	Total	Mg	0
			61	61	
53	n	1	Total	Mg	0
			1	1	
53	A	219	Total	Mg	0
			219	219	
53	B	4	Total	Mg	0
			4	4	
53	C	2	Total	Mg	0
			2	2	
53	D	1	Total	Mg	0
			1	1	
53	N	1	Total	Mg	0
			1	1	
53	Q	1	Total	Mg	0
			1	1	
53	0	1	Total	Mg	0
			1	1	
53	w	1	Total	Mg	0
			1	1	

- Molecule 54 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
54	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 55 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
55	A	1	Total	C	N	0
			6	4	2	
55	A	1	Total	C	N	0
			6	4	2	
55	A	1	Total	C	N	0
			6	4	2	

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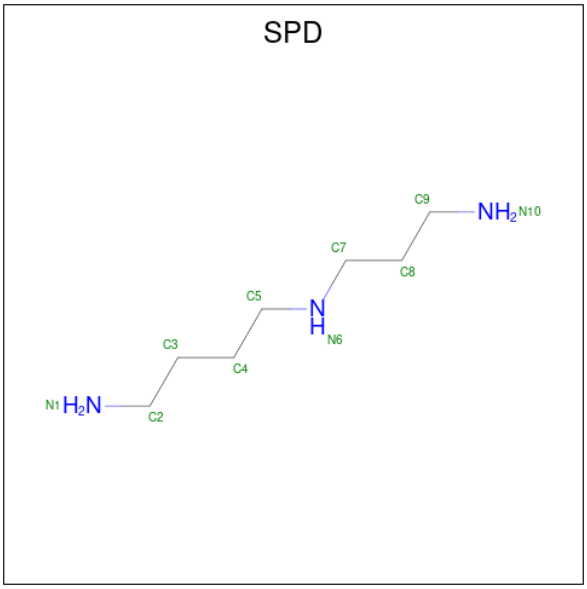
Mol	Chain	Residues	Atoms	AltConf
55	A	1	Total C N 6 4 2	0
55	A	1	Total C N 6 4 2	0
55	A	1	Total C N 6 4 2	0
55	A	1	Total C N 6 4 2	0
55	A	1	Total C N 6 4 2	0

- Molecule 56 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).

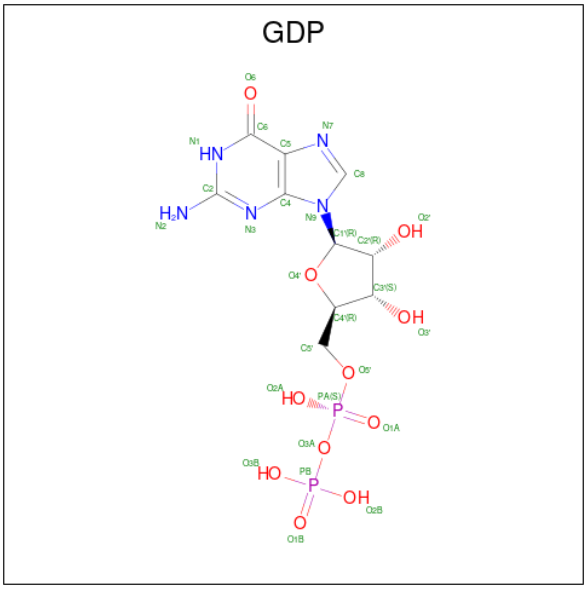


Mol	Chain	Residues	Atoms	AltConf
56	A	1	Total C N 10 7 3	0
56	A	1	Total C N 10 7 3	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

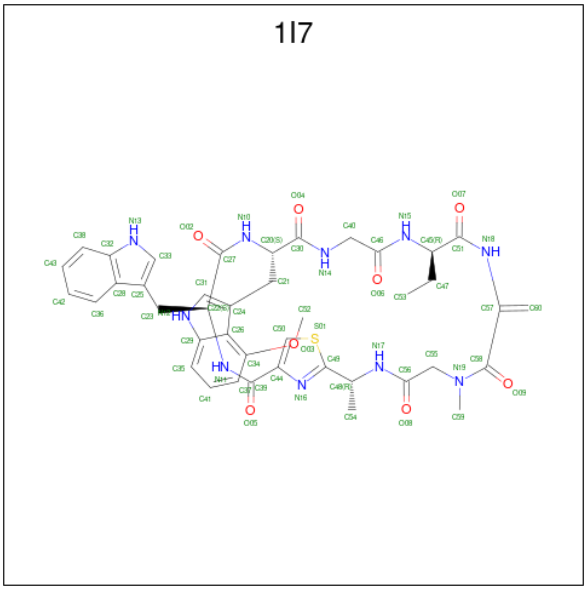
Mol	Chain	Residues	Atoms	AltConf
57	5	1	Total Zn 1 1	0
57	4	1	Total Zn 1 1	0

- Molecule 58 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
58	w	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 59 is Argyrin B (three-letter code: 1I7) (formula: $C_{41}H_{46}N_{10}O_8S$) (labeled as "Ligand of Interest" by depositor).



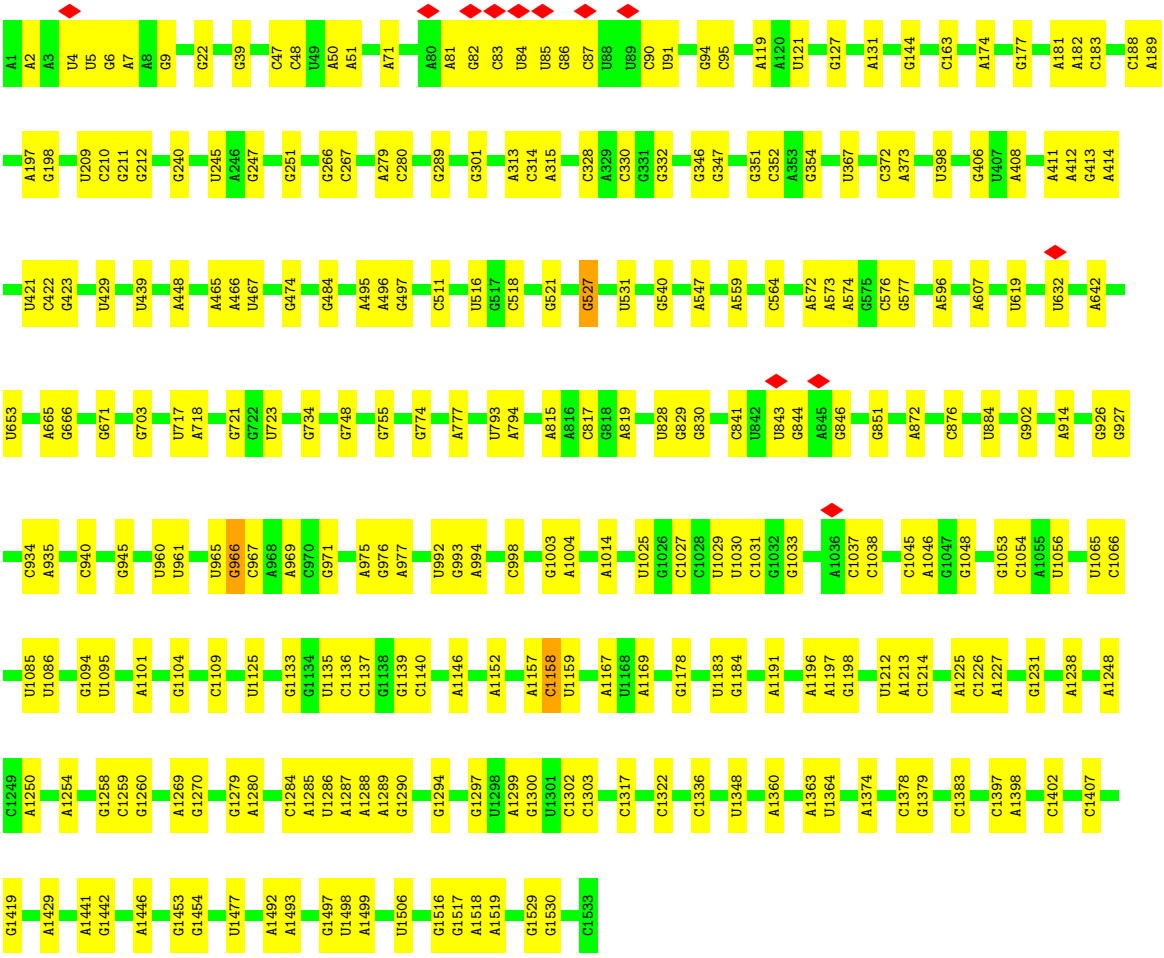
Mol	Chain	Residues	Atoms					AltConf
59	w	1	Total	C	N	O	S	0
			60	41	10	8	1	

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.

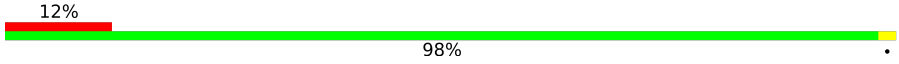
• Molecule 1: 16S ribosomal RNA

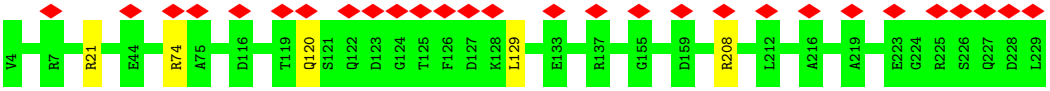
Chain a:



• Molecule 2: 30S ribosomal protein S2

Chain b:



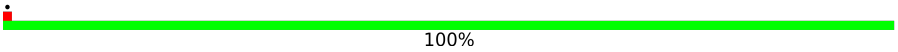


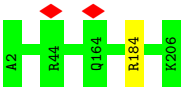
• Molecule 3: 30S ribosomal protein S3

Chain c: 

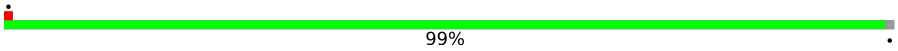
There are no outlier residues recorded for this chain.

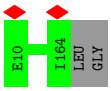
• Molecule 4: 30S ribosomal protein S4

Chain d: 

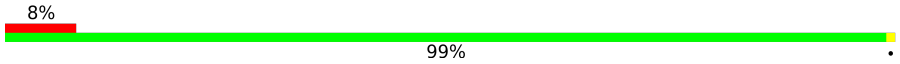


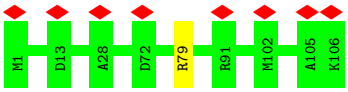
• Molecule 5: 30S ribosomal protein S5

Chain e: 

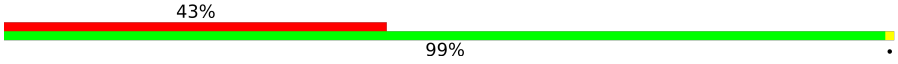


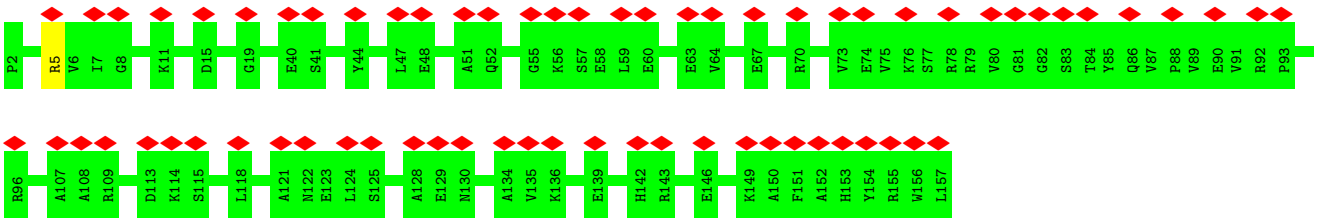
• Molecule 6: 30S ribosomal protein S6

Chain f: 

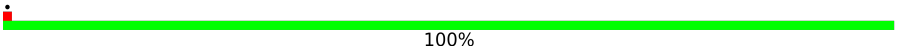


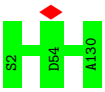
• Molecule 7: 30S ribosomal protein S7

Chain g: 



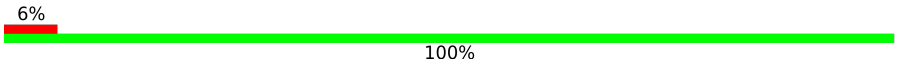
• Molecule 8: 30S ribosomal protein S8

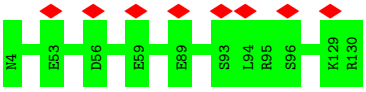
Chain h: 



• Molecule 9: 30S ribosomal protein S9

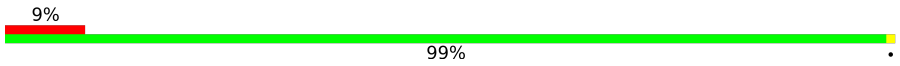
Chain i:

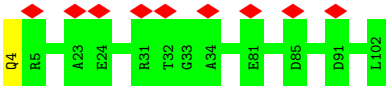




• Molecule 10: 30S ribosomal protein S10

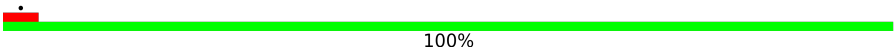
Chain j:

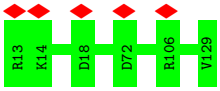




• Molecule 11: 30S ribosomal protein S11

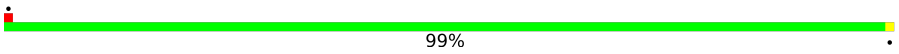
Chain k:

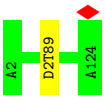




• Molecule 12: 30S ribosomal protein S12

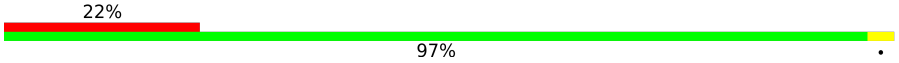
Chain l:

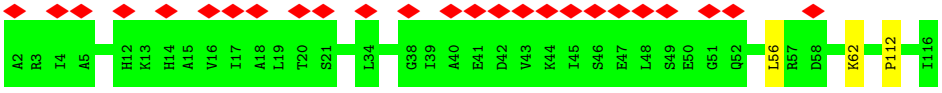




• Molecule 13: 30S ribosomal protein S13

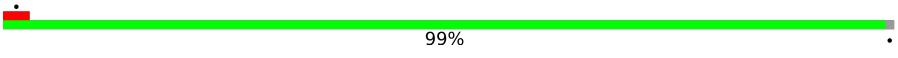
Chain m:

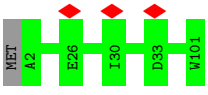




• Molecule 14: 30S ribosomal protein S14

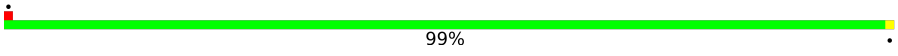
Chain n:





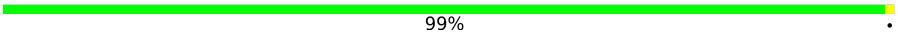
• Molecule 15: 30S ribosomal protein S15

Chain o:



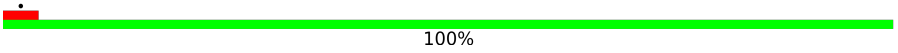
• Molecule 16: 30S ribosomal protein S16

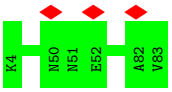
Chain p:



• Molecule 17: 30S ribosomal protein S17

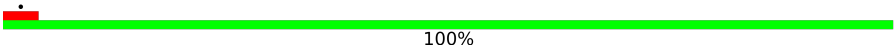
Chain q:

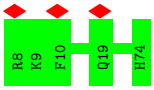




• Molecule 18: 30S ribosomal protein S18

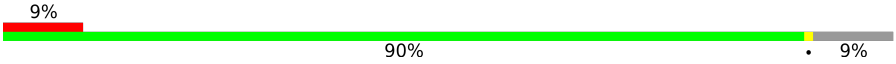
Chain r:

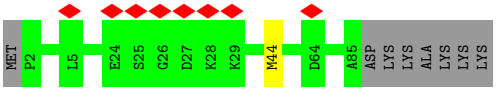




• Molecule 19: 30S ribosomal protein S19

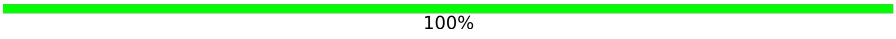
Chain s:





• Molecule 20: 30S ribosomal protein S20

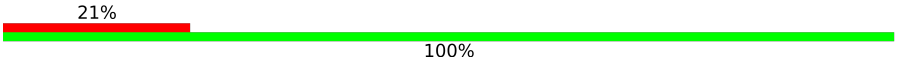
Chain t:

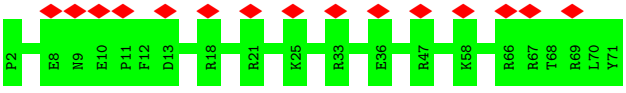


There are no outlier residues recorded for this chain.

• Molecule 21: 30S ribosomal protein S21

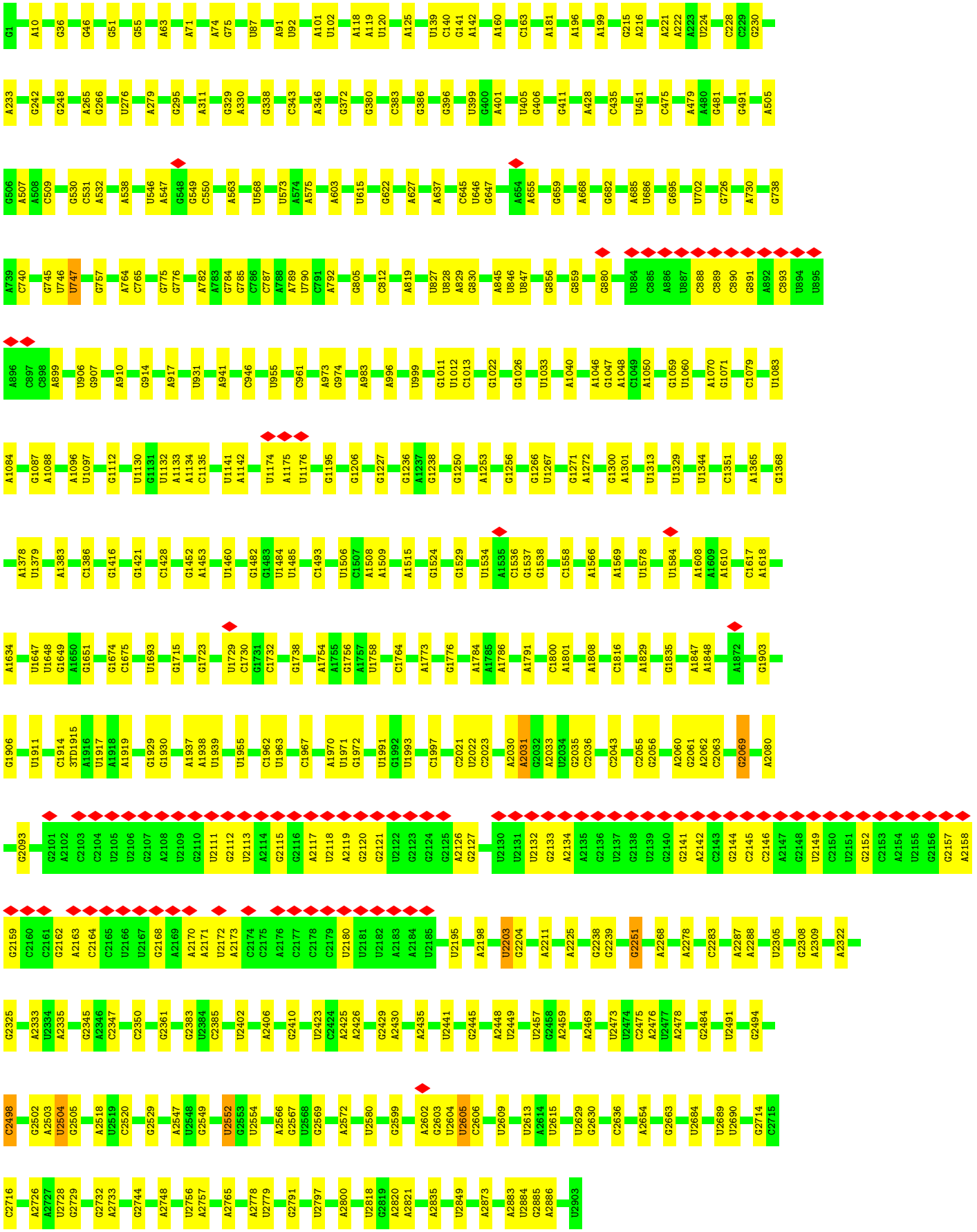
Chain u:





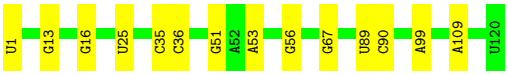
• Molecule 22: 23S ribosomal RNA

Chain A:


G1 A10 G36 G46 G51 G55 A63 A71 A74 G75 U87 A91 U92 A101 U102 A118 A119 U120 A125 U139 C140 G141 A142 A160 C163 A181 A196 A199 G215 A216 A221 A222 A223 U224 C228 C229 G230
A233 G242 G248 A265 G266 U276 A279 G295 A311 G329 A330 G338 C343 A346 G372 G380 C383 G386 G396 U399 G400 A401 U405 G406 G411 A428 C435 U451 C475 A479 A480 G481 G491 A505
G506 A507 A508 C509 G530 C531 A532 A538 U546 A547 G548 G549 C550 A563 U568 U573 A574 A575 A603 U615 G622 A627 A637 C645 U646 G647 A654 A655 G659 A668 G682 A685 U686 G695 U702 G726 A730 G738
A739 C740 G745 U746 U747 G757 A764 C765 G775 G776 A782 A783 G784 G785 C786 C787 A788 A789 U790 C791 A792 G805 C812 A819 U827 U828 A829 G830 A845 U846 U847 G856 G859 G880 U884 C885 A886 U887 C888 C889 C890 G891 A892 C893 U894 U895
A896 C897 C898 A899 U906 G907 A910 G914 A917 U931 A941 C946 U955 C961 A973 G974 A983 A996 U999 G1011 U1012 C1013 G1022 G1026 U1033 A1040 A1046 G1047 A1048 C1049 A1050 G1059 U1060 A1070 G1071 C1079 U1083
A1084 G1087 A1088 A1096 U1097 G1112 U1130 G1131 U1132 A1133 A1134 C1135 U1141 A1142 U1174 A1175 U1176 G1195 G1206 G1227 G1236 A1237 G1238 G1250 A1253 G1256 G1266 U1267 G1271 A1272 G1300 A1301 U1313 U1329 U1344 C1351 A1365 G1368
A1378 U1379 A1383 C1386 G1416 G1421 C1428 G1452 A1453 U1460 G1482 G1483 U1484 U1485 C1493 U1506 C1507 A1508 A1509 A1515 G1524 G1529 U1534 A1535 C1536 G1537 G1538 C1558 A1566 A1569 U1578 U1684 A1608 A1609 A1610 C1617 A1618
A1634 U1647 U1648 G1649 A1650 G1651 G1674 C1675 U1693 G1715 G1723 U1729 C1730 G1731 C1732 G1738 A1754 A1755 G1756 A1757 U1758 C1764 A1773 G1776 A1784 A1785 A1786 A1791 C1800 A1801 A1808 C1816 A1829 G1835 A1847 A1848 A1872 G1903
G1906 U1911 C1914 3TD1915 A1916 U1917 A1918 A1919 G1929 G1930 A1937 A1938 U1939 U1955 C1962 U1963 C1967 A1970 U1971 G1972 U1991 G1992 U1993 C1997 C2021 U2022 C2023 A2030 A2031 G2032 A2033 U2034 G2035 C2036 C2043 C2055 G2056 A2060 G2061 A2062 C2063 G2069 A2080
G2093 G2101 A2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140 G2141 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G2157 A2158
G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2185 U2195 A2198 U2203 G2204 A2211 A2225 G2238 G2239 G2251 A2268 A2278 C2283 A2287 A2288 U2305 G2308 A2309 A2322
G2325 A2333 U2334 A2335 G2345 A2346 C2347 C2350 G2361 G2383 U2384 C2385 U2402 A2406 G2410 U2423 C2424 A2425 A2426 G2429 A2430 A2435 U2441 G2445 A2448 U2449 U2457 G2458 A2459 A2469 U2473 U2474 C2475 A2476 U2477 A2478 C2484 U2491 G2494
C2498 G2502 A2503 U2504 G2505 A2518 U2519 C2520 G2529 A2547 U2548 G2549 U2552 G2553 U2554 A2566 G2567 U2568 G2569 A2572 U2580 G2599 A2602 G2603 U2604 U2605 C2606 U2609 U2613 A2614 U2615 U2629 G2630 C2636 A2654 G2663 U2684 U2689 U2690 G2714 C2715
C2716 A2726 A2727 U2728 G2729 G2732 A2733 G2744 A2748 U2756 A2757 A2765 A2778 U2779 G2791 U2797 A2800 U2818 G2819 A2820 A2821 A2835 U2849 A2873 A2883 U2884 G2885 A2886 U2903

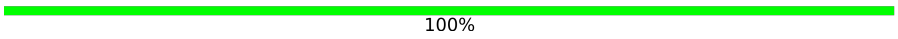
• Molecule 23: 5S ribosomal RNA

Chain B:



• Molecule 24: 50S ribosomal protein L2

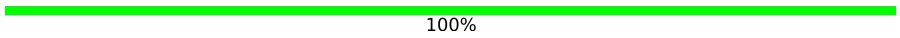
Chain C:



There are no outlier residues recorded for this chain.

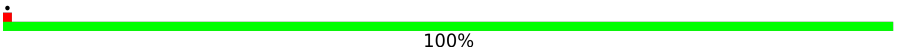
• Molecule 25: 50S ribosomal protein L3

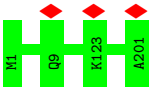
Chain D:



• Molecule 26: 50S ribosomal protein L4

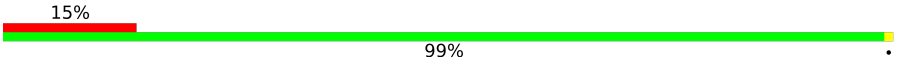
Chain E:

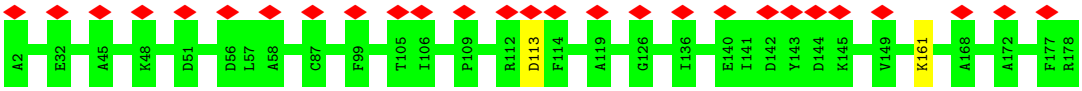




• Molecule 27: 50S ribosomal protein L5

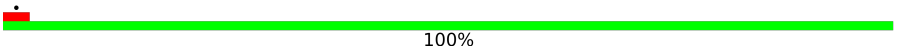
Chain F:

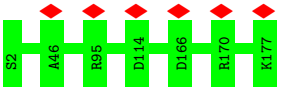




• Molecule 28: 50S ribosomal protein L6

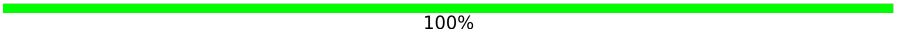
Chain G:





• Molecule 29: 50S ribosomal protein L13

Chain J:



There are no outlier residues recorded for this chain.

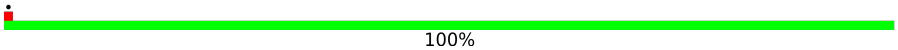
• Molecule 30: 50S ribosomal protein L14

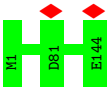
Chain K:

There are no outlier residues recorded for this chain.

• Molecule 31: 50S ribosomal protein L15

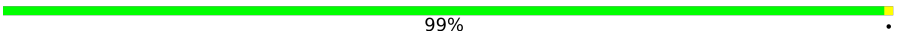
Chain L:





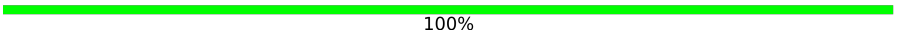
• Molecule 32: 50S ribosomal protein L16

Chain M:



• Molecule 33: 50S ribosomal protein L17

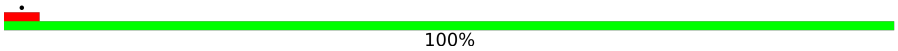
Chain N:

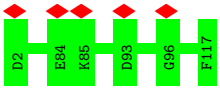


There are no outlier residues recorded for this chain.

• Molecule 34: 50S ribosomal protein L18

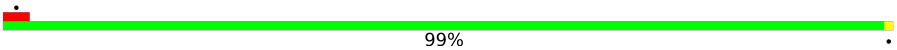
Chain O:

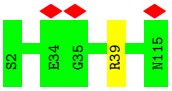




• Molecule 35: 50S ribosomal protein L19

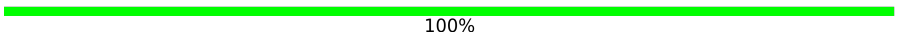
Chain P:





• Molecule 36: 50S ribosomal protein L20

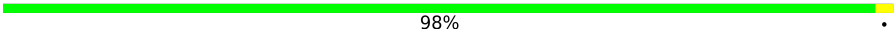
Chain Q:

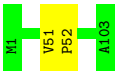


There are no outlier residues recorded for this chain.

• Molecule 37: 50S ribosomal protein L21

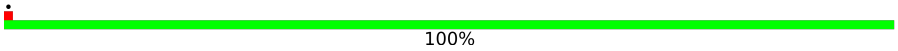
Chain R:

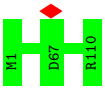




• Molecule 38: 50S ribosomal protein L22

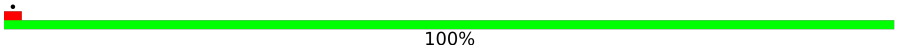
Chain S:

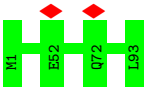




• Molecule 39: 50S ribosomal protein L23

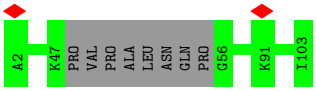
Chain T:





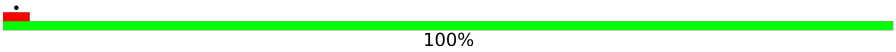
• Molecule 40: 50S ribosomal protein L24

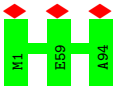
Chain U:



• Molecule 41: 50S ribosomal protein L25

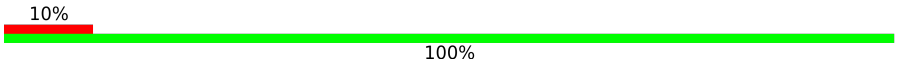
Chain V:

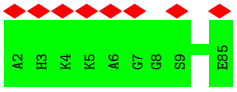




• Molecule 42: 50S ribosomal protein L27

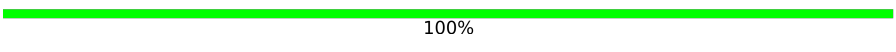
Chain W:





• Molecule 43: 50S ribosomal protein L28

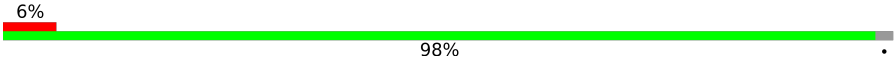
Chain X:

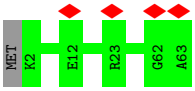


There are no outlier residues recorded for this chain.

• Molecule 44: 50S ribosomal protein L29

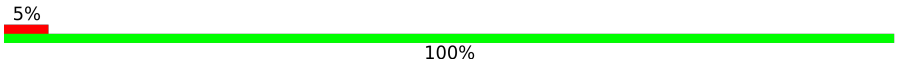
Chain Y:





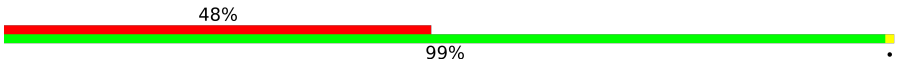
• Molecule 45: 50S ribosomal protein L30

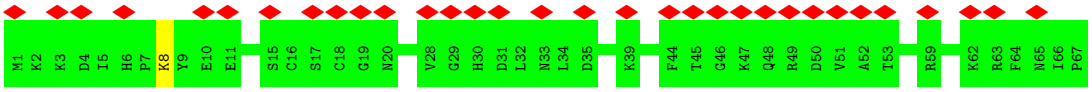
Chain Z:



• Molecule 46: 50S ribosomal protein L31

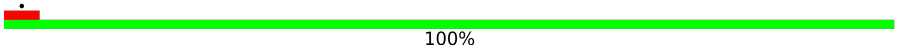
Chain 5:





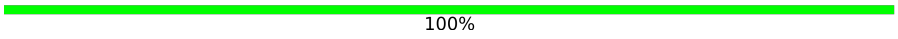
• Molecule 47: 50S ribosomal protein L32

Chain 0:



• Molecule 48: 50S ribosomal protein L33

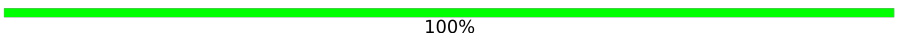
Chain 1:



There are no outlier residues recorded for this chain.

• Molecule 49: 50S ribosomal protein L34

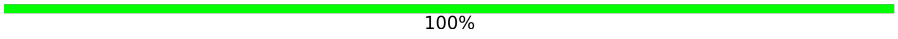
Chain 2:



There are no outlier residues recorded for this chain.

• Molecule 50: 50S ribosomal protein L35

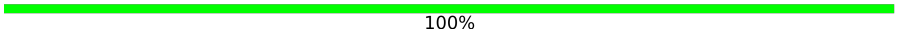
Chain 3:



There are no outlier residues recorded for this chain.

• Molecule 51: 50S ribosomal protein L36

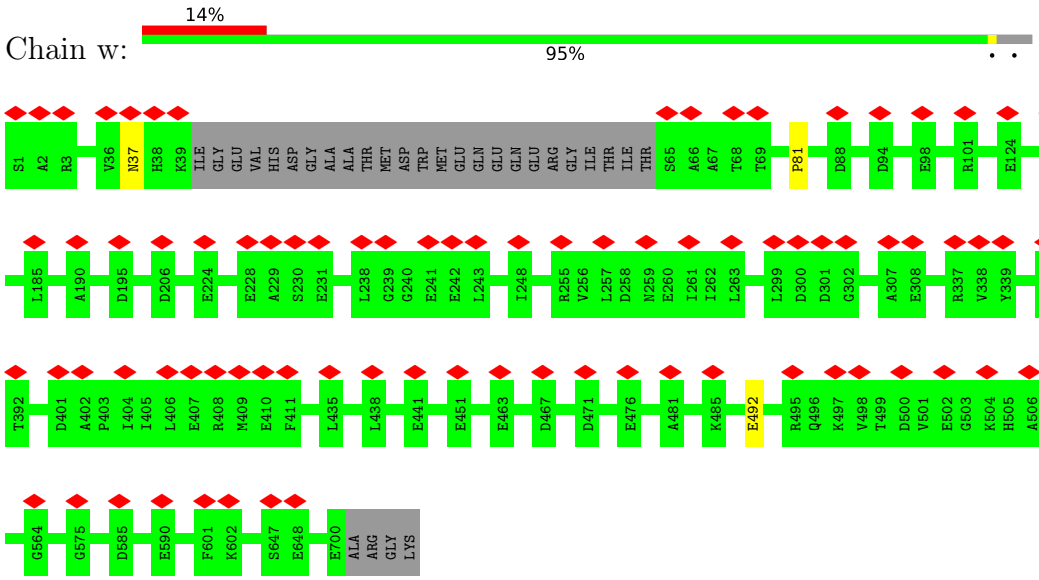
Chain 4:



There are no outlier residues recorded for this chain.

• Molecule 52: Elongation factor G

Chain w:


14%
95%
S1 A2 R3 V36 N37 H38 K39 ILE GLY GLU VAL HIS ASP GLY ALA ALA THR MET ASP TRP MET GLU GLN GLU GLN GLU ARG GLY ILE THR ILE THR S65 A66 A67 T68 T69 P81 D88 D94 E98 R101 E124 R161 L162 P166 L169 Q170 E177
L185 A190 D195 D206 E224 E228 A229 S230 E231 L238 G239 G240 E241 E242 L243 I248 R255 V256 L257 D258 N259 E260 I261 I262 L263 L299 D300 D301 G302 A307 E308 R337 V338 Y339 K354 A355 A356 K370 R378 A379 G380 D381 D390 V391
T392 D401 A402 P403 I404 I405 L406 E407 R408 M409 E410 F411 L435 L438 E441 E451 E463 D467 D471 E476 A481 K485 E492 R495 Q496 K497 V498 T499 D500 V501 E502 G503 K504 H505 A506 G511 D521 N530 I540 E548 E559
G564 G575 D585 E590 F601 K602 S647 E648 E700 ALA ARG GLY LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153360	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.614	Depositor
Minimum map value	-0.390	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	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: G7M, H2U, OMG, D2T, UR3, 3TD, OMU, SPD, 2MA, 6MZ, MG, GDP, PUT, MA6, 2MG, 1I7, OMC, ATP, PSU, ZN, 1MG, 4OC, 4D4, 5MU, 5MC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	a	0.36	0/36594	0.75	4/57083 (0.0%)
2	b	0.29	0/1800	0.65	3/2425 (0.1%)
3	c	0.27	0/1651	0.59	0/2225
4	d	0.28	0/1664	0.61	0/2227
5	e	0.28	0/1157	0.58	0/1557
6	f	0.32	0/881	0.68	0/1189
7	g	0.26	0/1254	0.62	0/1683
8	h	0.29	0/988	0.59	0/1326
9	i	0.31	0/1033	0.68	0/1375
10	j	0.30	0/816	0.72	0/1103
11	k	0.29	0/892	0.66	0/1205
12	l	0.31	0/960	0.64	0/1286
13	m	0.32	0/900	0.81	3/1204 (0.2%)
14	n	0.29	0/816	0.68	0/1088
15	o	0.26	0/721	0.57	0/964
16	p	0.30	0/659	0.64	0/884
17	q	0.31	0/657	0.65	0/881
18	r	0.29	0/564	0.57	0/756
19	s	0.32	0/685	0.66	0/922
20	t	0.27	0/675	0.51	0/895
21	u	0.28	0/597	0.64	0/792
22	A	0.37	0/69239	0.74	7/108014 (0.0%)
23	B	0.32	1/2873 (0.0%)	0.74	0/4478
24	C	0.32	0/2129	0.60	0/2863
25	D	0.30	0/1586	0.56	0/2134
26	E	0.27	0/1571	0.55	0/2113
27	F	0.34	0/1434	0.78	1/1926 (0.1%)
28	G	0.29	0/1343	0.57	0/1816
29	J	0.29	0/1163	0.52	0/1566
30	K	0.30	0/955	0.59	0/1279
31	L	0.29	0/1073	0.63	0/1427

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	M	0.28	0/1081	0.58	0/1443
33	N	0.27	0/973	0.58	0/1301
34	O	0.30	0/902	0.65	0/1209
35	P	0.31	0/928	0.65	1/1242 (0.1%)
36	Q	0.30	0/960	0.56	0/1278
37	R	0.29	0/829	0.59	0/1107
38	S	0.27	0/864	0.56	0/1156
39	T	0.27	0/744	0.60	0/994
40	U	0.29	0/725	0.61	0/961
41	V	0.28	0/765	0.56	0/1025
42	W	0.29	0/642	0.57	0/848
43	X	0.29	0/634	0.65	0/848
44	Y	0.25	0/502	0.64	0/667
45	Z	0.27	0/452	0.57	0/605
46	5	0.27	0/539	0.65	0/721
47	0	0.27	0/450	0.60	0/599
48	1	0.27	0/416	0.55	0/554
49	2	0.27	0/380	0.67	0/498
50	3	0.26	0/521	0.57	0/687
51	4	0.28	0/303	0.58	0/397
52	w	0.30	0/5293	0.63	0/7166
All	All	0.34	1/158233 (0.0%)	0.71	19/235992 (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 sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
37	R	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1	U	OP3-P	-10.64	1.48	1.61

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	129	LEU	CA-CB-CG	8.95	135.88	115.30
2	b	21	ARG	CB-CG-CD	-8.77	88.79	111.60
13	m	112	PRO	CA-N-CD	-7.81	100.56	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	21	ARG	CG-CD-NE	-7.32	96.42	111.80
22	A	790	U	C2-N1-C1'	6.73	125.78	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	R	51	VAL	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	224/226 (99%)	210 (94%)	14 (6%)	0	100	100
3	c	204/206 (99%)	199 (98%)	5 (2%)	0	100	100
4	d	203/205 (99%)	201 (99%)	2 (1%)	0	100	100
5	e	153/157 (98%)	144 (94%)	9 (6%)	0	100	100
6	f	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
7	g	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
8	h	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
9	i	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
10	j	98/99 (99%)	92 (94%)	6 (6%)	0	100	100
11	k	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
12	l	120/123 (98%)	116 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	113/115 (98%)	103 (91%)	10 (9%)	0	100	100
14	n	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
15	o	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
16	p	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	q	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
18	r	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
19	s	82/92 (89%)	82 (100%)	0	0	100	100
20	t	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
21	u	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
24	C	270/271 (100%)	260 (96%)	10 (4%)	0	100	100
25	D	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
26	E	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
27	F	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
28	G	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
29	J	141/142 (99%)	140 (99%)	1 (1%)	0	100	100
30	K	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
31	L	143/144 (99%)	140 (98%)	3 (2%)	0	100	100
32	M	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
33	N	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
34	O	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
35	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
36	Q	115/117 (98%)	115 (100%)	0	0	100	100
37	R	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	15	45
38	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
39	T	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
40	U	90/102 (88%)	86 (96%)	4 (4%)	0	100	100
41	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
42	W	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
43	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
44	Y	60/63 (95%)	60 (100%)	0	0	100	100
45	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
46	5	65/67 (97%)	61 (94%)	4 (6%)	0	100 100
47	0	54/56 (96%)	52 (96%)	2 (4%)	0	100 100
48	1	48/50 (96%)	48 (100%)	0	0	100 100
49	2	44/46 (96%)	44 (100%)	0	0	100 100
50	3	63/64 (98%)	58 (92%)	5 (8%)	0	100 100
51	4	36/38 (95%)	36 (100%)	0	0	100 100
52	w	671/704 (95%)	634 (94%)	33 (5%)	4 (1%)	25 58
All	All	6139/6287 (98%)	5914 (96%)	220 (4%)	5 (0%)	54 82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	w	540	ILE
52	w	166	PRO
52	w	81	PRO
52	w	492	GLU
37	R	52	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain 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
2	b	188/188 (100%)	185 (98%)	3 (2%)	62 86
3	c	170/170 (100%)	170 (100%)	0	100 100
4	d	172/172 (100%)	171 (99%)	1 (1%)	86 96
5	e	118/119 (99%)	118 (100%)	0	100 100
6	f	92/92 (100%)	91 (99%)	1 (1%)	73 92
7	g	129/129 (100%)	128 (99%)	1 (1%)	81 94
8	h	104/104 (100%)	104 (100%)	0	100 100
9	i	105/105 (100%)	105 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	j	88/87 (101%)	87 (99%)	1 (1%)	73 92
11	k	90/90 (100%)	90 (100%)	0	100 100
12	l	102/102 (100%)	102 (100%)	0	100 100
13	m	93/93 (100%)	92 (99%)	1 (1%)	73 92
14	n	83/84 (99%)	83 (100%)	0	100 100
15	o	76/76 (100%)	75 (99%)	1 (1%)	69 90
16	p	65/65 (100%)	64 (98%)	1 (2%)	65 87
17	q	74/74 (100%)	74 (100%)	0	100 100
18	r	58/58 (100%)	58 (100%)	0	100 100
19	s	72/79 (91%)	71 (99%)	1 (1%)	67 89
20	t	65/65 (100%)	65 (100%)	0	100 100
21	u	60/60 (100%)	60 (100%)	0	100 100
24	C	217/216 (100%)	217 (100%)	0	100 100
25	D	164/164 (100%)	164 (100%)	0	100 100
26	E	165/165 (100%)	165 (100%)	0	100 100
27	F	148/148 (100%)	147 (99%)	1 (1%)	84 95
28	G	137/137 (100%)	137 (100%)	0	100 100
29	J	117/116 (101%)	117 (100%)	0	100 100
30	K	104/104 (100%)	104 (100%)	0	100 100
31	L	104/103 (101%)	104 (100%)	0	100 100
32	M	108/108 (100%)	108 (100%)	0	100 100
33	N	100/100 (100%)	100 (100%)	0	100 100
34	O	86/86 (100%)	86 (100%)	0	100 100
35	P	99/99 (100%)	99 (100%)	0	100 100
36	Q	89/89 (100%)	89 (100%)	0	100 100
37	R	84/84 (100%)	84 (100%)	0	100 100
38	S	93/93 (100%)	93 (100%)	0	100 100
39	T	80/80 (100%)	80 (100%)	0	100 100
40	U	76/83 (92%)	76 (100%)	0	100 100
41	V	78/78 (100%)	78 (100%)	0	100 100
42	W	62/62 (100%)	62 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	X	67/67 (100%)	67 (100%)	0	100 100
44	Y	54/55 (98%)	54 (100%)	0	100 100
45	Z	48/48 (100%)	48 (100%)	0	100 100
46	5	60/60 (100%)	59 (98%)	1 (2%)	60 86
47	0	47/47 (100%)	47 (100%)	0	100 100
48	1	45/45 (100%)	45 (100%)	0	100 100
49	2	38/38 (100%)	38 (100%)	0	100 100
50	3	52/51 (102%)	52 (100%)	0	100 100
51	4	34/34 (100%)	34 (100%)	0	100 100
52	w	549/578 (95%)	546 (100%)	3 (0%)	88 96
All	All	5109/5150 (99%)	5093 (100%)	16 (0%)	92 98

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	w	370	LYS
52	w	37	ASN
15	o	88	ARG
46	5	8	LYS
13	m	62	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
40	U	99	ASN
52	w	496	GLN
52	w	505	HIS
52	w	220	GLN
24	C	115	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1529/1533 (99%)	262 (17%)	0
22	A	2897/2903 (99%)	427 (14%)	6 (0%)
23	B	119/120 (99%)	13 (10%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4545/4556 (99%)	702 (15%)	6 (0%)

5 of 702 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	2	A
1	a	4	U
1	a	5	U
1	a	6	G
1	a	7	A

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	A	1847	A
22	A	2602	A
22	A	2756	U
22	A	888	C
22	A	784	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	G7M	A	2069	22	20,26,27	2.41	7 (35%)	17,39,42	1.13	1 (5%)
1	2MG	a	1516	1	18,26,27	2.46	3 (16%)	16,38,41	1.31	3 (18%)
22	PSU	A	2605	22	18,21,22	2.69	6 (33%)	22,30,33	1.84	5 (22%)
1	UR3	a	1498	1	19,22,23	2.89	7 (36%)	26,32,35	1.30	2 (7%)
1	5MC	a	1407	1	18,22,23	3.17	7 (38%)	26,32,35	2.32	7 (26%)
22	PSU	A	2457	22	18,21,22	2.68	6 (33%)	22,30,33	1.87	5 (22%)
22	2MA	A	2503	53,22	17,25,26	2.47	5 (29%)	17,37,40	1.31	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	2MG	A	2445	22	18,26,27	2.41	3 (16%)	16,38,41	1.36	3 (18%)
12	D2T	l	89	12	7,9,10	1.34	1 (14%)	6,11,13	1.48	0
1	PSU	a	516	1	18,21,22	2.72	7 (38%)	22,30,33	1.83	6 (27%)
22	3TD	A	1915	22	18,22,23	4.09	7 (38%)	22,32,35	1.86	3 (13%)
1	MA6	a	1519	1	18,26,27	1.16	2 (11%)	19,38,41	3.20	2 (10%)
22	PSU	A	746	53,22	18,21,22	2.70	6 (33%)	22,30,33	1.73	5 (22%)
22	PSU	A	1917	22	18,21,22	2.73	6 (33%)	22,30,33	1.89	5 (22%)
1	MA6	a	1518	1	18,26,27	1.16	2 (11%)	19,38,41	3.09	2 (10%)
22	6MZ	A	2030	22	18,25,26	2.48	2 (11%)	16,36,39	2.40	4 (25%)
1	5MC	a	967	1	18,22,23	3.25	7 (38%)	26,32,35	2.33	7 (26%)
22	OMC	A	2498	53,22	19,22,23	2.93	6 (31%)	26,31,34	2.00	5 (19%)
22	OMG	A	2251	53,22	18,26,27	1.16	2 (11%)	19,38,41	0.85	1 (5%)
1	G7M	a	527	1	20,26,27	2.42	7 (35%)	17,39,42	1.10	1 (5%)
22	5MC	A	1962	22	18,22,23	3.15	7 (38%)	26,32,35	2.41	6 (23%)
22	PSU	A	2580	22	18,21,22	2.66	7 (38%)	22,30,33	1.96	6 (27%)
22	H2U	A	2449	22	18,21,22	2.11	4 (22%)	21,30,33	2.11	4 (19%)
22	2MG	A	1835	22	18,26,27	2.42	3 (16%)	16,38,41	1.25	3 (18%)
1	2MG	a	966	1	18,26,27	2.53	3 (16%)	16,38,41	1.30	2 (12%)
22	PSU	A	2604	22	18,21,22	2.68	6 (33%)	22,30,33	1.90	5 (22%)
1	4OC	a	1402	1	20,23,24	3.12	8 (40%)	26,32,35	0.94	1 (3%)
22	PSU	A	2504	22	18,21,22	2.70	6 (33%)	22,30,33	1.87	5 (22%)
22	PSU	A	1911	22	18,21,22	2.76	6 (33%)	22,30,33	1.84	5 (22%)
22	5MU	A	747	22	19,22,23	2.29	6 (31%)	28,32,35	2.28	8 (28%)
22	PSU	A	955	22	18,21,22	2.68	6 (33%)	22,30,33	1.92	5 (22%)
22	OMU	A	2552	22	19,22,23	2.04	6 (31%)	26,31,34	1.73	5 (19%)
22	5MU	A	1939	22	19,22,23	2.29	6 (31%)	28,32,35	2.24	8 (28%)
22	1MG	A	745	22	18,26,27	2.78	6 (33%)	19,39,42	1.43	4 (21%)
22	6MZ	A	1618	22	18,25,26	2.51	3 (16%)	16,36,39	2.04	3 (18%)
32	4D4	M	81	32	9,11,12	2.11	2 (22%)	8,13,15	2.09	4 (50%)

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
22	G7M	A	2069	22	-	2/3/25/26	0/3/3/3
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
22	PSU	A	2605	22	-	2/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
22	PSU	A	2457	22	-	0/7/25/26	0/2/2/2
22	2MA	A	2503	53,22	-	2/3/25/26	0/3/3/3
22	2MG	A	2445	22	-	2/5/27/28	0/3/3/3
12	D2T	l	89	12	-	1/7/12/14	-
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
22	3TD	A	1915	22	-	2/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	2/7/29/30	0/3/3/3
22	PSU	A	746	53,22	-	1/7/25/26	0/2/2/2
22	PSU	A	1917	22	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
22	6MZ	A	2030	22	-	2/5/27/28	0/3/3/3
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
22	OMC	A	2498	53,22	-	2/9/27/28	0/2/2/2
22	OMG	A	2251	53,22	-	3/5/27/28	0/3/3/3
1	G7M	a	527	1	-	2/3/25/26	0/3/3/3
22	5MC	A	1962	22	-	1/7/25/26	0/2/2/2
22	PSU	A	2580	22	-	0/7/25/26	0/2/2/2
22	H2U	A	2449	22	-	0/7/38/39	0/2/2/2
22	2MG	A	1835	22	-	2/5/27/28	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
22	PSU	A	2604	22	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	1/9/29/30	0/2/2/2
22	PSU	A	2504	22	-	0/7/25/26	0/2/2/2
22	PSU	A	1911	22	-	1/7/25/26	0/2/2/2
22	5MU	A	747	22	-	2/7/25/26	0/2/2/2
22	PSU	A	955	22	-	0/7/25/26	0/2/2/2
22	OMU	A	2552	22	-	2/9/27/28	0/2/2/2
22	5MU	A	1939	22	-	0/7/25/26	0/2/2/2
22	1MG	A	745	22	-	0/3/25/26	0/3/3/3
22	6MZ	A	1618	22	-	3/5/27/28	0/3/3/3
32	4D4	M	81	32	-	5/11/12/14	-

The worst 5 of 184 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1915	3TD	C6-C5	12.20	1.49	1.35
22	A	1618	6MZ	C6-N6	9.58	1.50	1.35
22	A	2030	6MZ	C6-N6	9.34	1.50	1.35
1	a	967	5MC	O2-C2	9.02	1.40	1.23
22	A	2498	OMC	O2-C2	8.92	1.40	1.23

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1519	MA6	N1-C6-N6	-12.29	104.12	117.06
1	a	1518	MA6	N1-C6-N6	-12.01	104.41	117.06
22	A	1962	5MC	C6-N1-C2	-7.99	109.81	120.87
1	a	967	5MC	C6-N1-C2	-7.84	110.02	120.87
1	a	1407	5MC	C6-N1-C2	-7.78	110.09	120.87

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	527	G7M	C3'-C4'-C5'-O5'
32	M	81	4D4	NE-CD-CG-CB
22	A	747	5MU	C3'-C4'-C5'-O5'
22	A	747	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 307 ligands modelled in this entry, 294 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	PUT	A	3008	-	5,5,5	0.17	0	4,4,4	0.17	0
56	SPD	A	3010	-	9,9,9	0.31	0	8,8,8	0.88	0
55	PUT	A	3002	-	5,5,5	0.15	0	4,4,4	0.15	0
55	PUT	A	3005	-	5,5,5	0.12	0	4,4,4	0.16	0
55	PUT	A	3144	-	5,5,5	0.13	0	4,4,4	0.15	0
55	PUT	A	3003	-	5,5,5	0.10	0	4,4,4	0.17	0
55	PUT	A	3007	-	5,5,5	0.11	0	4,4,4	0.16	0
55	PUT	A	3004	-	5,5,5	0.09	0	4,4,4	0.18	0
56	SPD	A	3009	-	9,9,9	0.33	0	8,8,8	0.91	0
58	GDP	w	802	-	24,30,30	2.48	7 (29%)	30,47,47	1.71	9 (30%)
59	1I7	w	803	-	58,65,65	2.63	22 (37%)	69,92,92	1.42	9 (13%)
55	PUT	A	3006	-	5,5,5	0.14	0	4,4,4	0.16	0
54	ATP	A	3001	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PUT	A	3008	-	-	1/3/3/3	-
56	SPD	A	3010	-	-	2/7/7/7	-
55	PUT	A	3002	-	-	0/3/3/3	-
55	PUT	A	3005	-	-	0/3/3/3	-
55	PUT	A	3144	-	-	0/3/3/3	-
55	PUT	A	3003	-	-	0/3/3/3	-
55	PUT	A	3007	-	-	1/3/3/3	-
55	PUT	A	3004	-	-	1/3/3/3	-
56	SPD	A	3009	-	-	0/7/7/7	-
58	GDP	w	802	-	-	1/12/32/32	0/3/3/3
59	1I7	w	803	-	-	12/58/69/69	0/5/6/6
55	PUT	A	3006	-	-	1/3/3/3	-
54	ATP	A	3001	-	-	2/18/38/38	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	w	802	GDP	O6-C6	8.28	1.40	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	w	803	1I7	C51-N18	7.19	1.49	1.36
59	w	803	1I7	C27-N10	6.72	1.48	1.34
59	w	803	1I7	C46-N15	6.64	1.48	1.34
59	w	803	1I7	C56-N17	6.61	1.48	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	w	803	1I7	C60-C57-N18	-3.89	117.10	126.07
59	w	803	1I7	C44-C50-S01	3.77	116.42	111.79
58	w	802	GDP	C5-C6-N1	3.45	120.04	113.95
58	w	802	GDP	C3'-C2'-C1'	3.45	106.17	100.98
59	w	803	1I7	C52-O03-C34	-3.27	113.18	117.75

There are no chirality outliers.

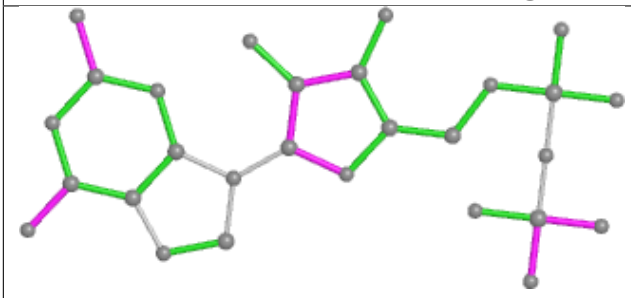
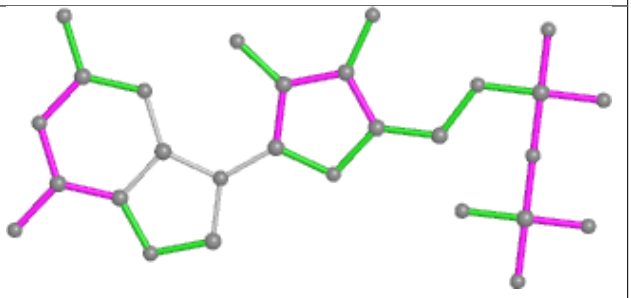
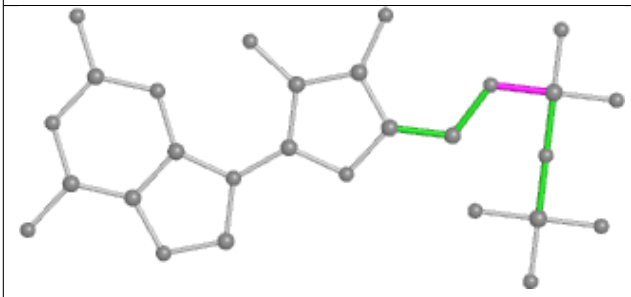
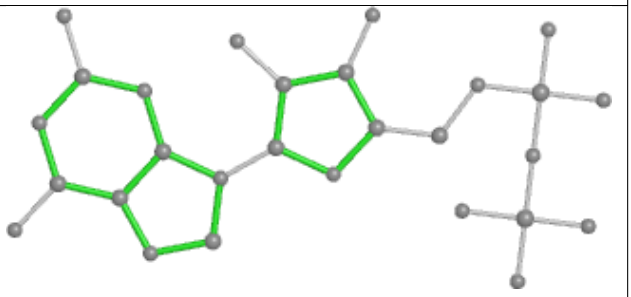
5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	w	803	1I7	C26-C34-O03-C52
59	w	803	1I7	C49-C48-N17-C56
59	w	803	1I7	C56-C55-N19-C58
59	w	803	1I7	C56-C55-N19-C59
59	w	803	1I7	N18-C57-C58-N19

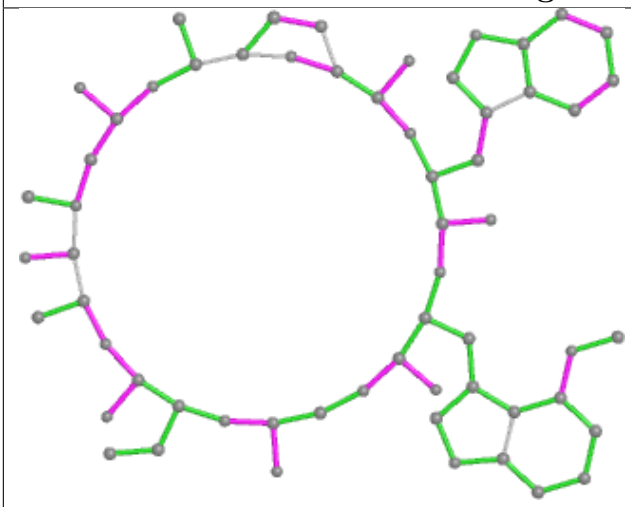
There are no ring outliers.

No monomer is involved in short contacts.

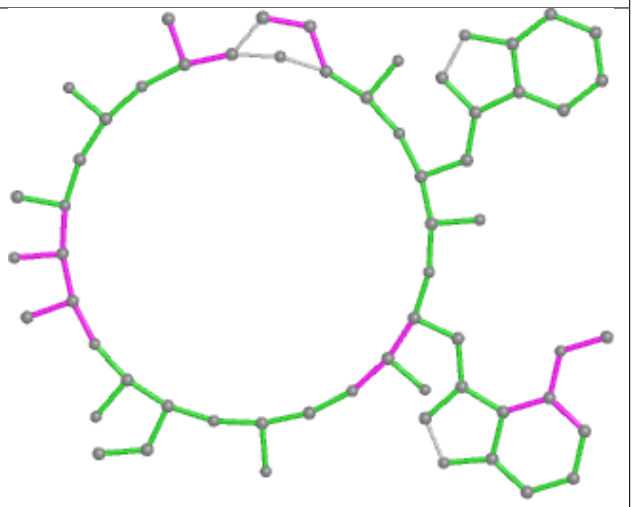
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP w 802	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

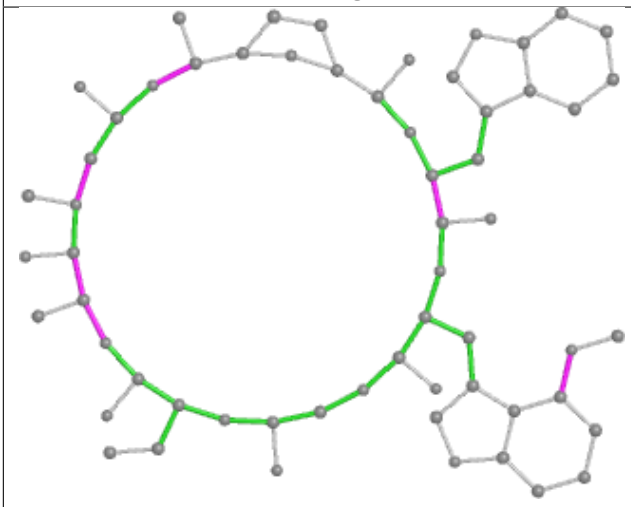
Ligand 1I7 w 803



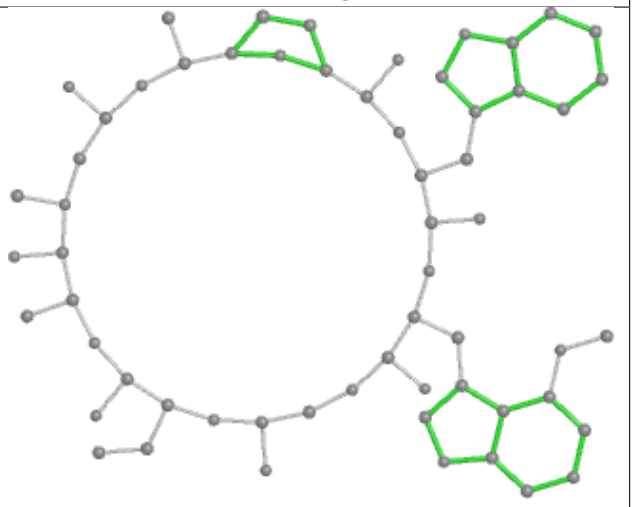
Bond lengths



Bond angles

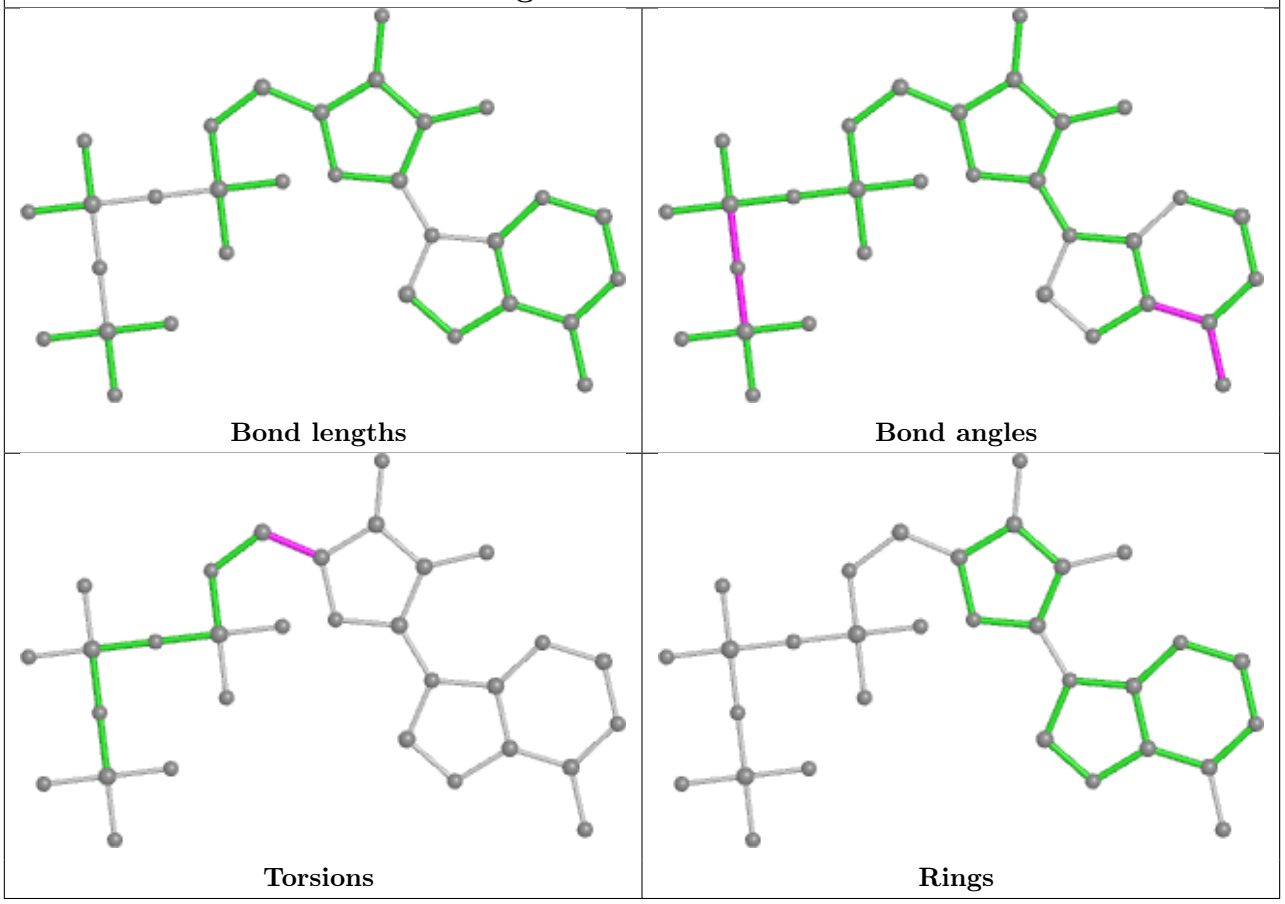


Torsions



Rings

Ligand ATP A 3001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1618:6MZ	O3'	1619:G	P	4.10

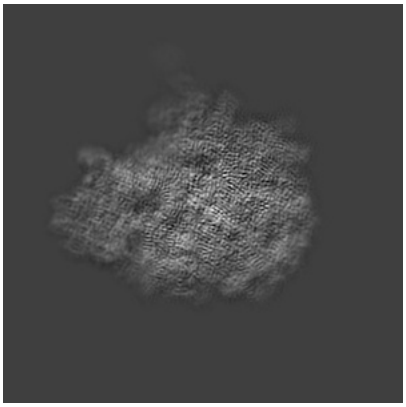
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13058. These allow visual inspection of the internal detail of the map and identification of artifacts.

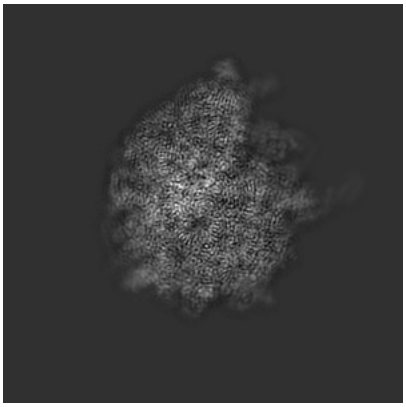
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

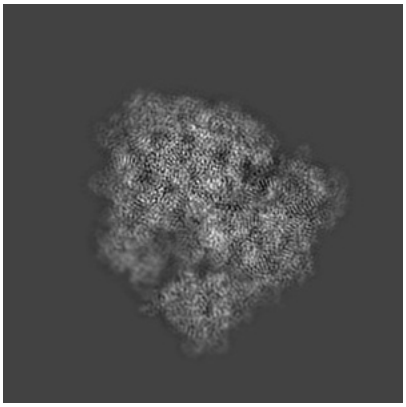
6.1.1 Primary map



X



Y



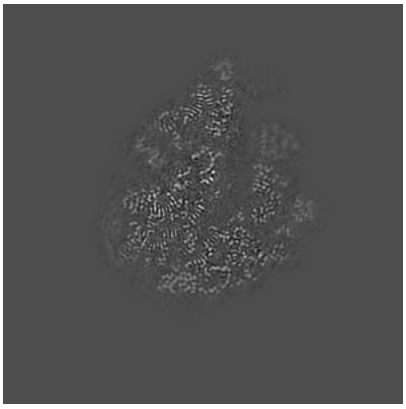
Z

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

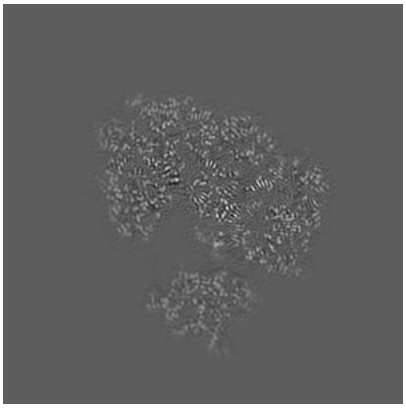
6.2 Central slices

6.2.1 Primary map

X Index: 180



Y Index: 180

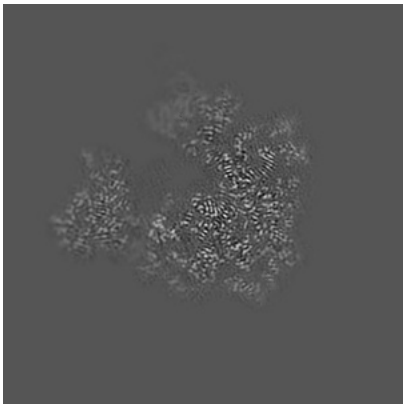


Z Index: 180

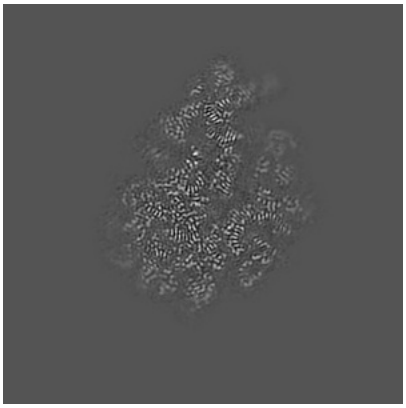
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

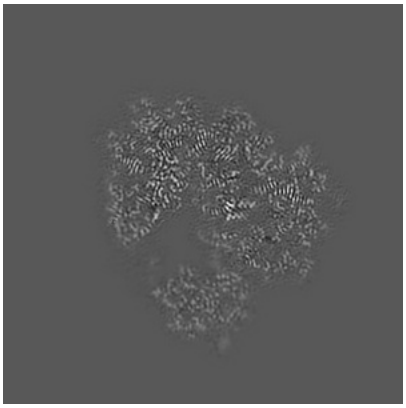
6.3.1 Primary map



X Index: 179



Y Index: 187

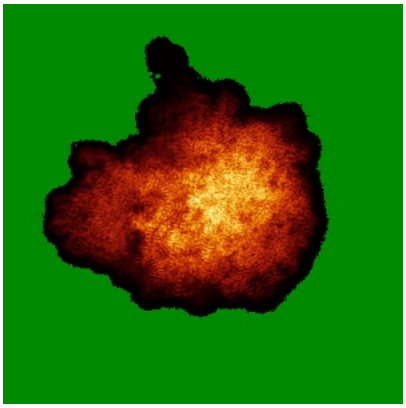


Z Index: 187

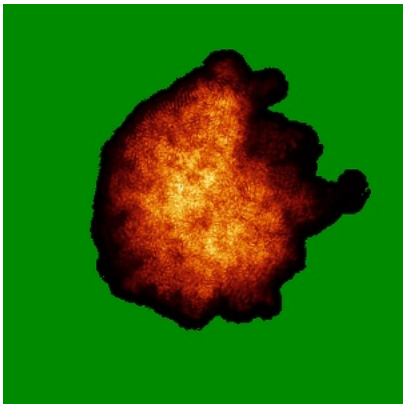
The images above show the largest variance slices of the map in three orthogonal directions.

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

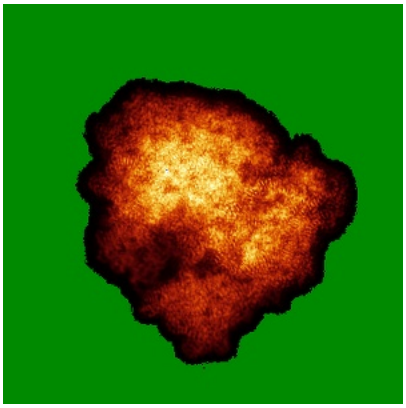
6.4.1 Primary map



X



Y

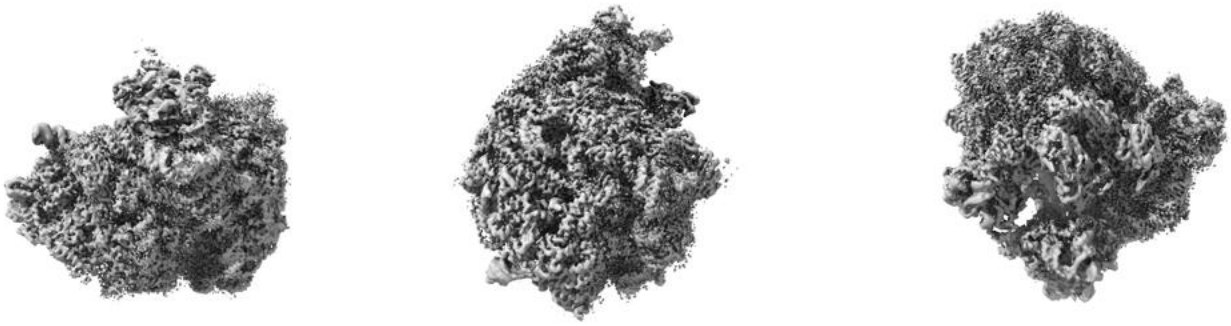


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

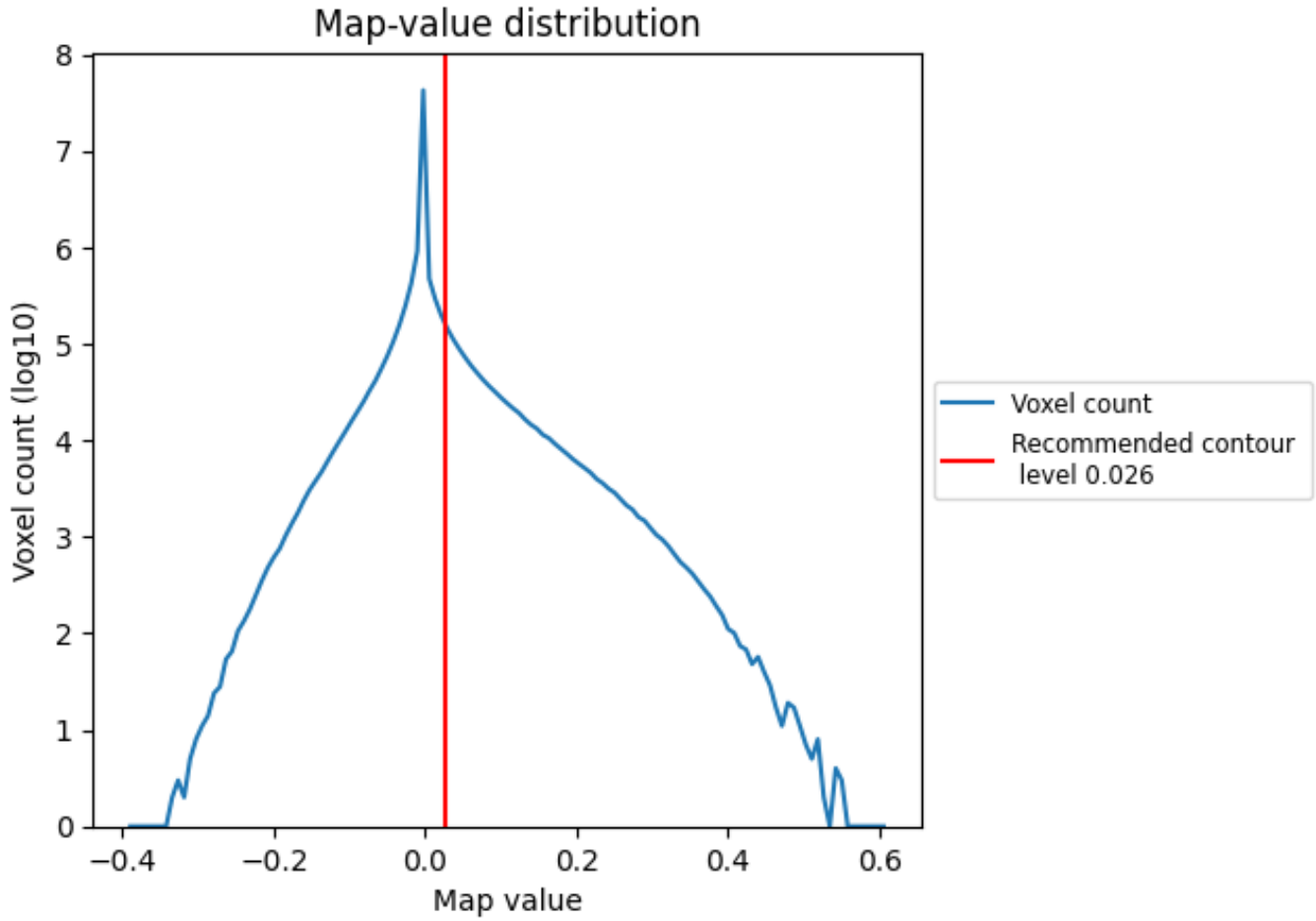
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

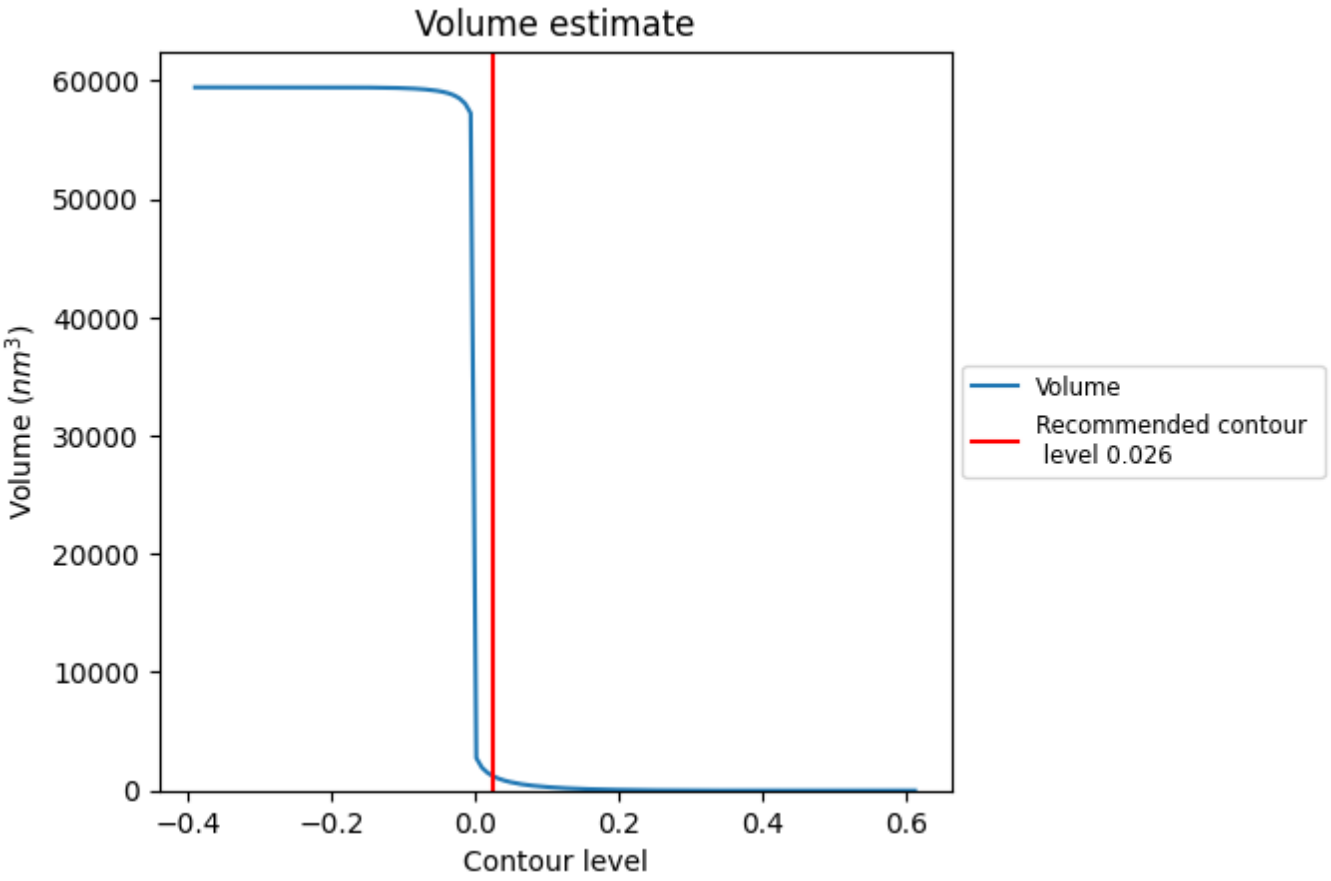
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

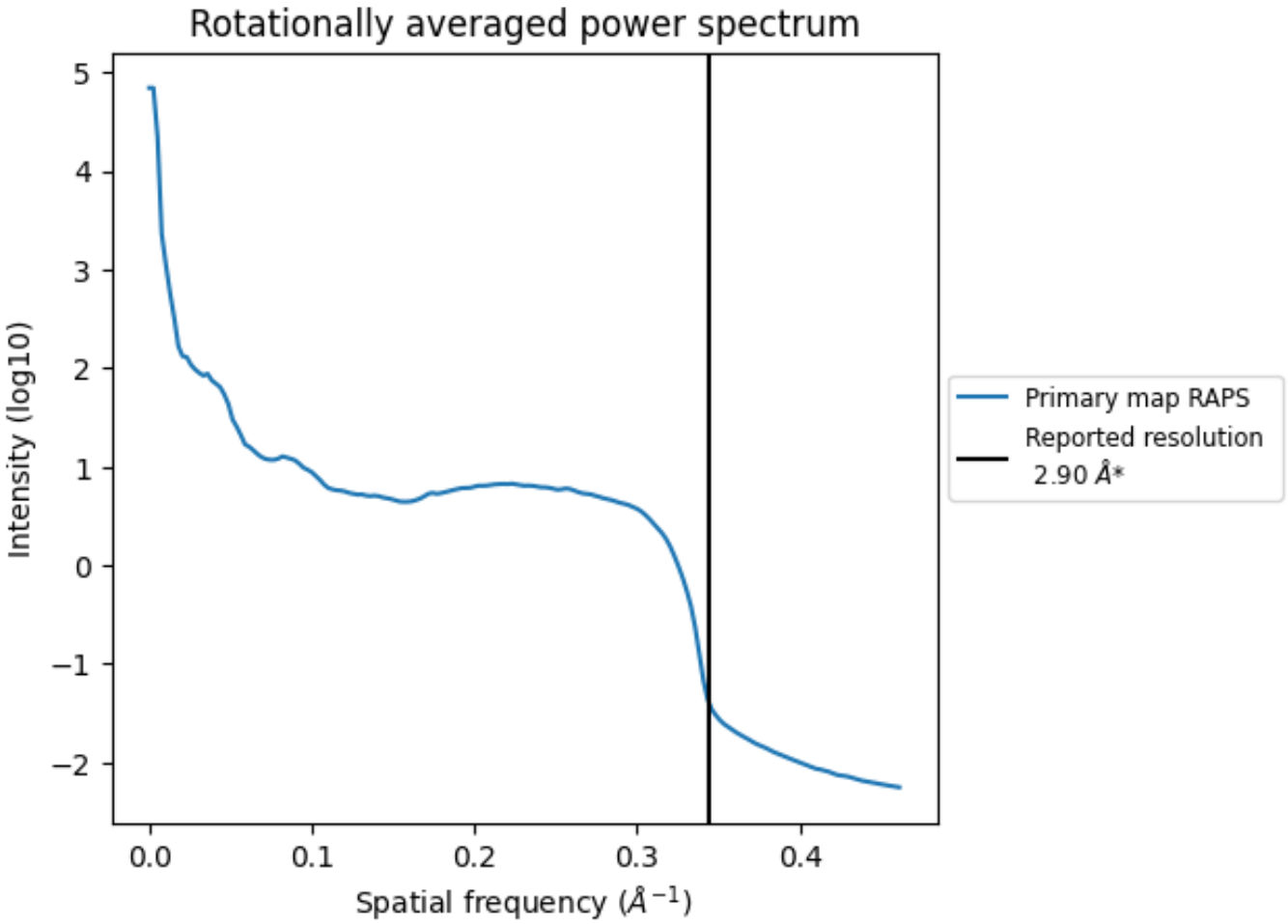
7.2 Volume estimate (i)



The volume at the recommended contour level is 1206 nm^3; this corresponds to an approximate mass of 1089 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 0.345 $Å^{-1}$

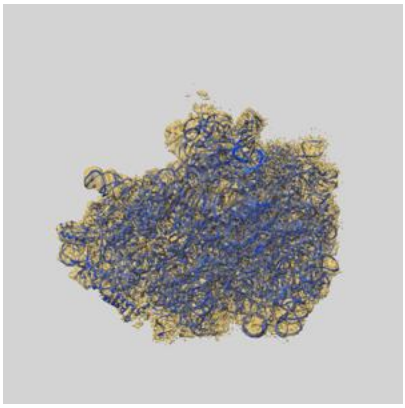
8 Fourier-Shell correlation (i)

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

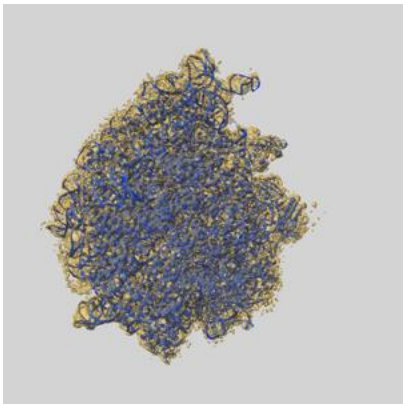
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13058 and PDB model 7OTC. Per-residue inclusion information can be found in section 3 on page 17.

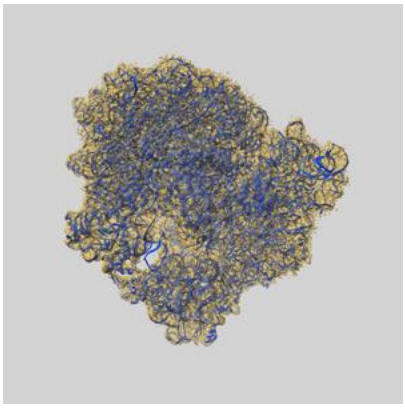
9.1 Map-model overlay



X



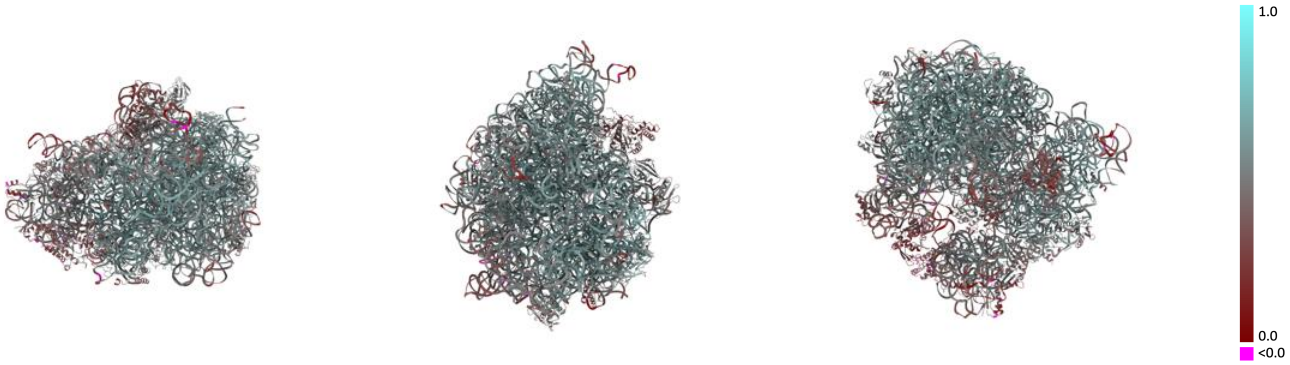
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 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.

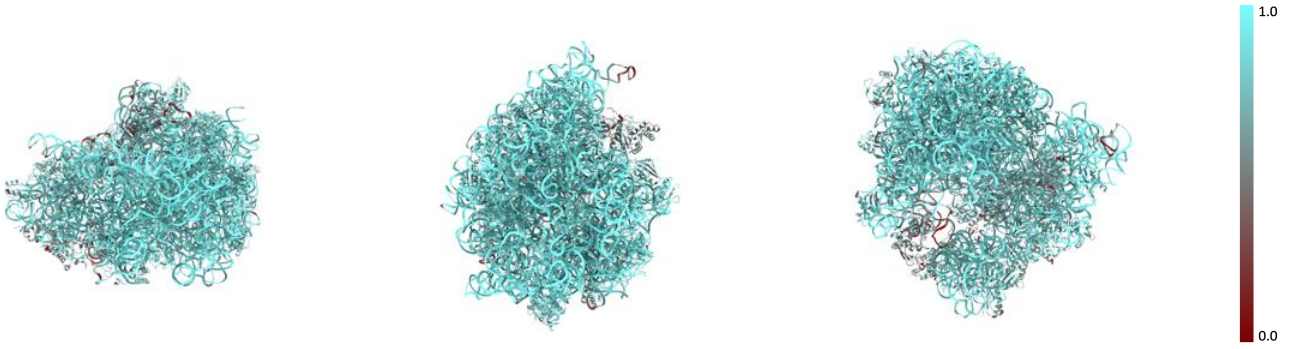
9.2 Q-score mapped to coordinate model



X Y Z

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.

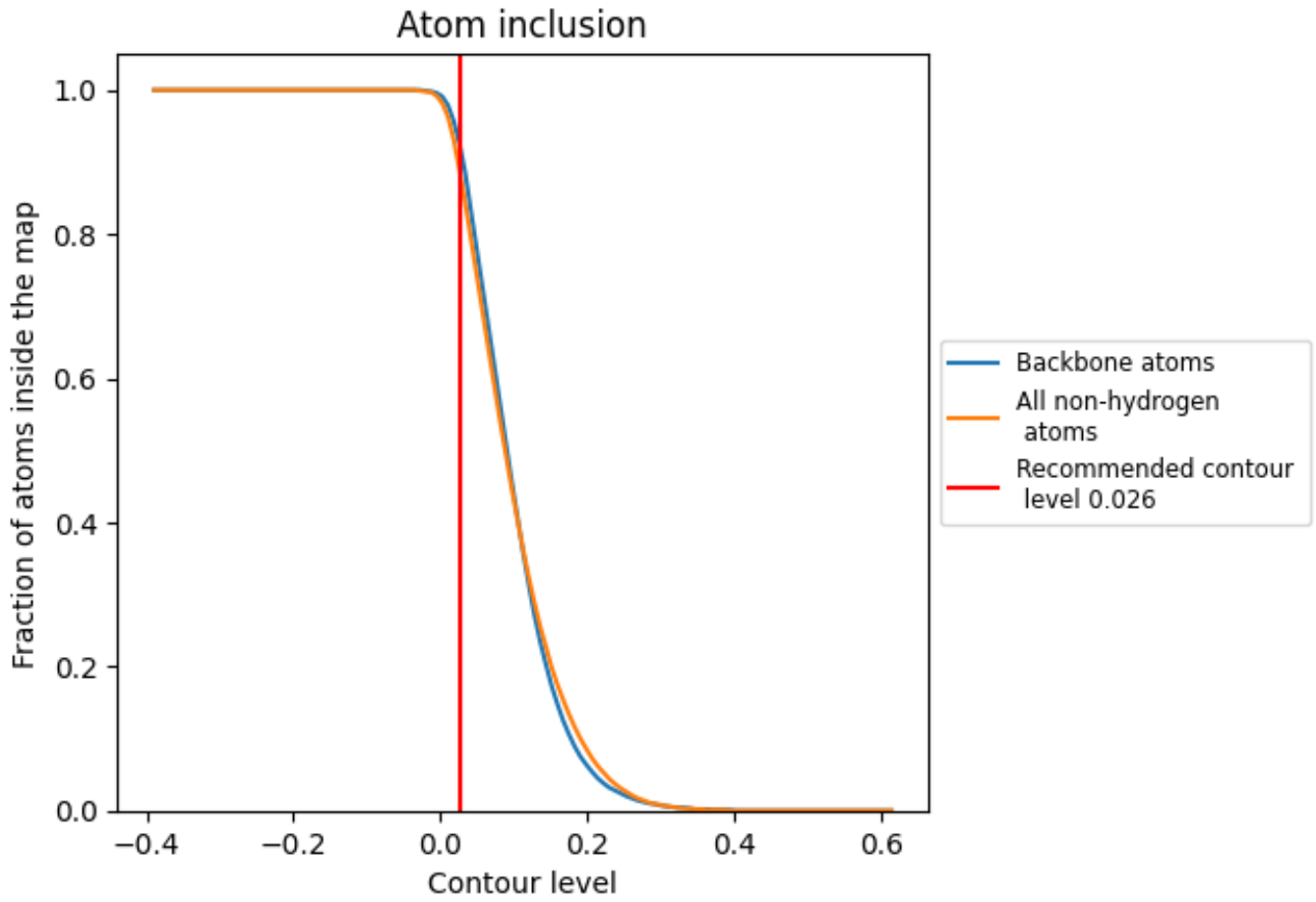
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8880	0.5040
0	0.8790	0.5420
1	0.8050	0.4840
2	0.9350	0.5890
3	0.9180	0.5670
4	0.8870	0.5380
5	0.4260	0.2120
A	0.9300	0.5330
B	0.9260	0.4250
C	0.9450	0.5780
D	0.9040	0.5610
E	0.8320	0.5020
F	0.5880	0.2800
G	0.8090	0.4730
J	0.9320	0.5780
K	0.8940	0.5630
L	0.8640	0.5080
M	0.8730	0.5210
N	0.8940	0.5420
O	0.7490	0.3620
P	0.8480	0.5100
Q	0.9480	0.5930
R	0.9170	0.5610
S	0.9010	0.5600
T	0.7840	0.4580
U	0.8170	0.4600
V	0.8140	0.4830
W	0.7880	0.5020
X	0.8650	0.5310
Y	0.7300	0.4010
Z	0.8490	0.5380
a	0.9460	0.5250
b	0.6710	0.3800
c	0.8140	0.4470
d	0.8280	0.4670

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Chain	Atom inclusion	Q-score
e	0.8590	0.4970
f	0.7420	0.3890
g	0.4920	0.2280
h	0.8580	0.5250
i	0.7850	0.4000
j	0.7350	0.3630
k	0.8150	0.4140
l	0.9090	0.5340
m	0.6270	0.2860
n	0.8220	0.4360
o	0.8810	0.5020
p	0.8820	0.5060
q	0.8560	0.4920
r	0.8200	0.4580
s	0.7670	0.3880
t	0.8930	0.5310
u	0.6010	0.3710
w	0.6170	0.3470