Full wwPDB EM Validation Report ⓘ

Mar 3, 2024 – 04:06 PM EST

PDB ID	:	5WE4
EMDB ID	:	EMD-8814
Title	:	70S ribosome-EF-Tu wt complex with GppNHp
Authors	:	Fislage, M.; Brown, Z.; Frank, J.
Deposited on	:	2017-07-07
Resolution	:	3.10 Å(reported)

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

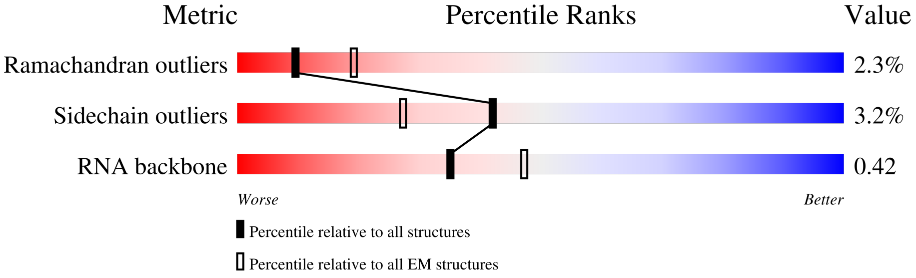
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

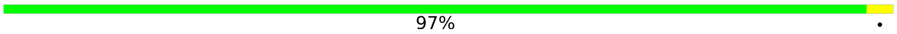
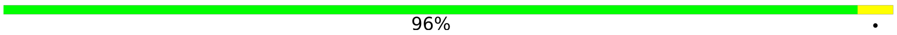
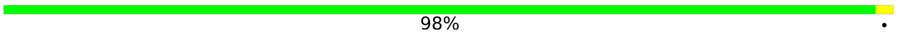
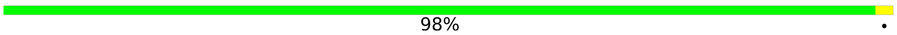
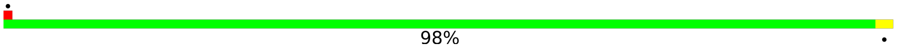
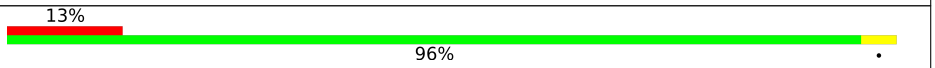
The reported resolution of this entry is 3.10 Å.

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	2903	
2	B	120	
3	C	271	
4	D	208	
5	E	200	
6	F	177	
7	G	174	
8	H	149	

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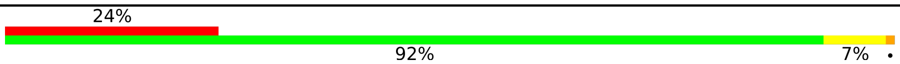
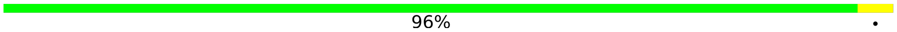
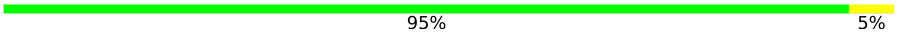
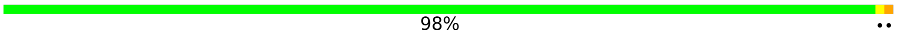
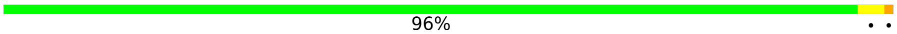
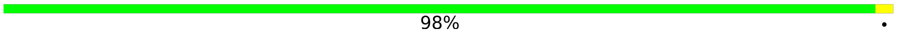
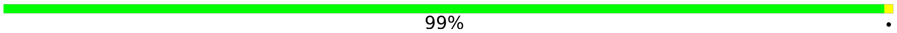
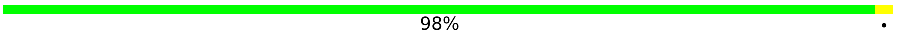
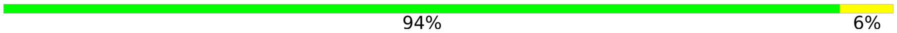
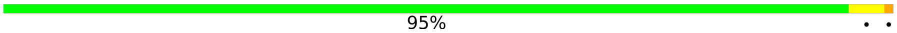
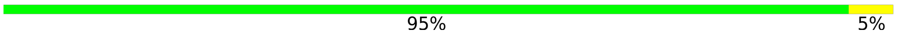
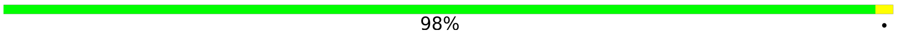
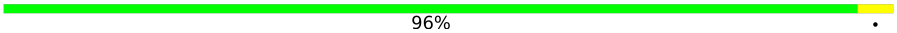
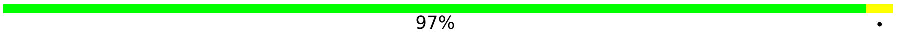
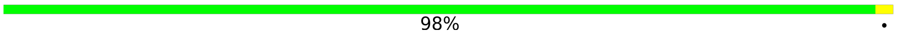
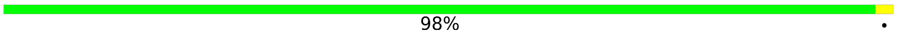
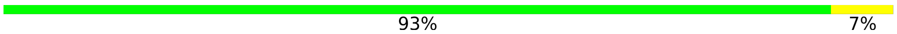
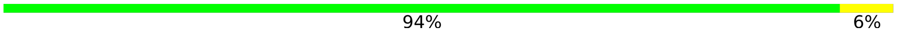
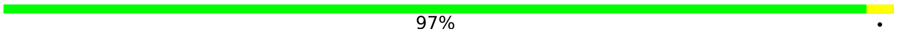
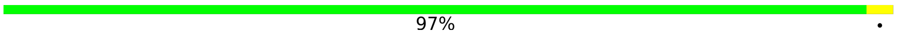
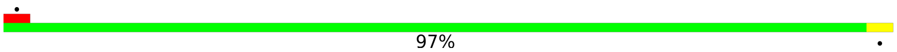
Mol	Chain	Length	Quality of chain
9	I	141	
10	J	141	
11	K	122	
12	L	143	
13	M	136	
14	N	119	
15	O	116	
16	P	114	
17	Q	115	
18	R	102	
19	S	109	
20	T	92	
21	U	102	
22	V	92	
23	W	75	
24	X	77	
25	Y	60	
26	Z	56	
27	0	55	
28	1	51	
29	2	45	
30	3	64	
31	4	38	
32	5	131	
33	6	66	

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Mol	Chain	Length	Quality of chain
34	a	1540	72% 28%
35	b	218	97% •
36	c	206	97% •
37	d	205	99% •
38	e	157	94% 6%
39	f	100	• 92% 8%
40	g	151	95% 5%
41	h	129	98% •
42	i	127	• 94% 5% •
43	j	98	93% 7%
44	k	116	94% 6%
45	l	121	• 92% 7% •
46	m	115	96% •
47	n	101	94% 6%
48	o	88	92% 7% •
49	p	82	• 95% 5%
50	q	80	94% 6%
51	r	65	• 88% 12%
52	s	79	95% 5%
53	t	85	93% 7%
54	u	65	• 82% 18%
55	v	77	• 69% 29% •
55	w	77	• 49% 45% 5%
56	x	12	92% 8%
57	y	76	• 55% 39% 5%

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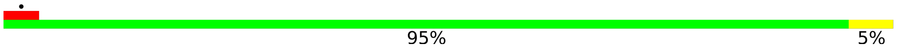
Mol	Chain	Length	Quality of chain
58	z	393	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155067 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2900	62277	27788	11459	20130	2900	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 731469900
A	1723	G	A	conflict	GB 731469900
A	1847	G	A	conflict	GB 731469900

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2572	1145	471	836	120	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1174070234

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2082	1288	423	364	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	208	1557	974	287	293	3	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	200	1544	969	282	289	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	174	1304	820	239	243	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	149	1111	699	197	214	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	141	1032	651	179	196	6	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	141	1120	708	211	197	4	0	0

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	122	938	587	180	165	6	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	115	Total	C	N	O	0	0
			933	595	190	148		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	109	Total 845	C 526	N 162	O 154	S 3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	92	Total 730	C 461	N 138	O 130	S 1	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	102	Total 779	C 492	N 146	O 141	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	92	Total 739	C 471	N 135	O 131	S 2	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total 572	C 355	N 116	O 100	S 1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	77	Total 625	C 388	N 129	O 106	S 2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	60	Total 494	C 305	N 96	O 91	S 2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	56	434	273	85	74	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	0	55	434	263	92	78	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	1	51	417	269	76	72	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	2	45	367	222	88	55	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	3	64	504	323	105	74	2	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	4	38	302	185	65	48	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	5	131	988	625	175	183	5	0	0

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total 522	C 323	N 99	O 94	S 6	0	0

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total 33050	C 14748	N 6057	O 10705	P 1540	0	0

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total 1704	C 1081	N 305	O 311	S 7	0	0

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	205	Total 1643	C 1026	N 315	O 298	S 4	0	0

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total 1164	C 724	N 221	O 213	S 6	1	0

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total 817	C 515	N 148	O 148	S 6	0	0

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total 1181	C 735	N 227	O 215	S 4	0	0

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	129	Total 979	C 616	N 173	O 184	S 6	0	0

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	127	Total 1022	C 634	N 206	O 179	S 3	0	0

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	98	Total 786	C 493	N 150	O 142	S 1	0	0

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total 869	C 535	N 173	O 158	S 3	0	0

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	121	Total 940	C 581	N 193	O 162	S 4	0	0

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	n	101	810	502	165	140	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	o	88	714	439	144	130	1	0	0

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	r	65	535	339	100	95	1	0	0

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	s	79	637	408	120	107	2	0	0

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total 665	C 411	N 137	O 114	S 3	0	0

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total 544	C 335	N 117	O 91	S 1	0	0

- Molecule 55 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0
55	w	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	12	Total 252	C 113	N 42	O 85	P 12	0	0

- Molecule 57 is a RNA chain called Phe-tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	76	Total 1632	C 731	N 290	O 533	P 76	S 2	0	0

- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total 3036	C 1918	N 524	O 581	S 13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	47	ASN	ASP	conflict	UNP P0CE48

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
59	A	1181	Total Mg 1181 1181	0
59	B	31	Total Mg 31 31	0
59	C	1	Total Mg 1 1	0
59	K	1	Total Mg 1 1	0
59	L	2	Total Mg 2 2	0
59	M	1	Total Mg 1 1	0
59	Q	1	Total Mg 1 1	0
59	R	1	Total Mg 1 1	0
59	S	1	Total Mg 1 1	0
59	T	2	Total Mg 2 2	0
59	0	2	Total Mg 2 2	0
59	1	1	Total Mg 1 1	0
59	3	1	Total Mg 1 1	0
59	4	1	Total Mg 1 1	0
59	a	373	Total Mg 373 373	0
59	d	1	Total Mg 1 1	0
59	h	1	Total Mg 1 1	0
59	i	1	Total Mg 1 1	0
59	s	1	Total Mg 1 1	0
59	u	1	Total Mg 1 1	0
59	v	7	Total Mg 7 7	0
59	w	1	Total Mg 1 1	0

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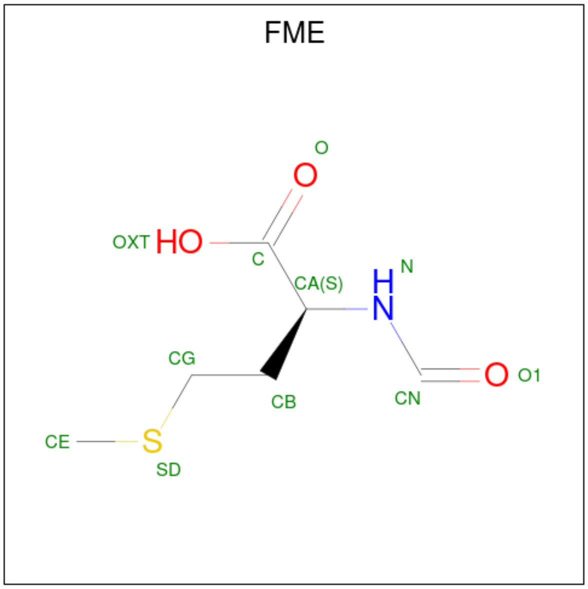
Mol	Chain	Residues	Atoms		AltConf
59	y	4	Total 4	Mg 4	0
59	z	1	Total 1	Mg 1	0

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

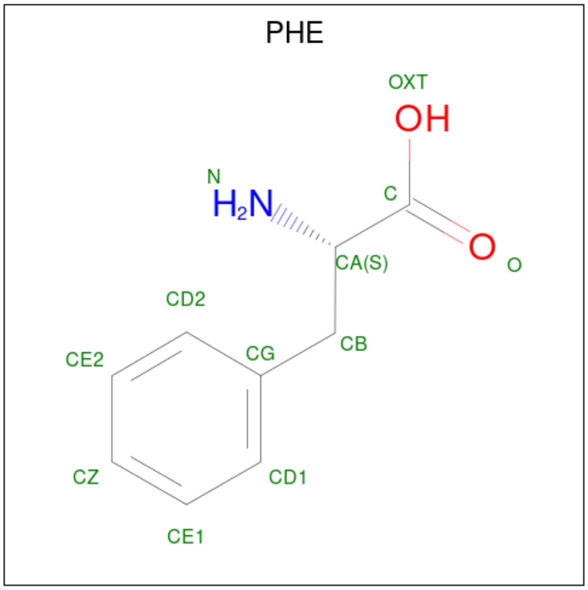
Mol	Chain	Residues	Atoms		AltConf
60	A	1	Total 1	K 1	0

- Molecule 61 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



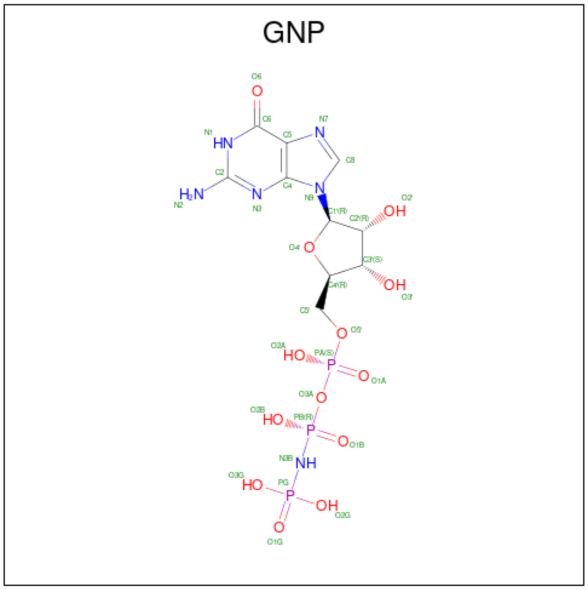
Mol	Chain	Residues	Atoms					AltConf
61	v	1	Total 10	C 6	N 1	O 2	S 1	0

- Molecule 62 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
62	z	1	Total 11	C 9	N 1	O 1	0

- Molecule 63 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
63	z	1	Total 32	C 10	N 6	O 13	P 3	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	AltConf
64	A	751	Total O 751 751	0
64	B	11	Total O 11 11	0
64	C	9	Total O 9 9	0
64	E	5	Total O 5 5	0
64	J	2	Total O 2 2	0
64	K	2	Total O 2 2	0
64	L	6	Total O 6 6	0
64	M	1	Total O 1 1	0
64	N	3	Total O 3 3	0
64	O	1	Total O 1 1	0
64	P	2	Total O 2 2	0
64	Q	3	Total O 3 3	0
64	R	1	Total O 1 1	0
64	S	2	Total O 2 2	0
64	T	3	Total O 3 3	0
64	U	2	Total O 2 2	0
64	W	1	Total O 1 1	0
64	X	1	Total O 1 1	0
64	Y	1	Total O 1 1	0
64	Z	3	Total O 3 3	0
64	2	5	Total O 5 5	0
64	3	4	Total O 4 4	0

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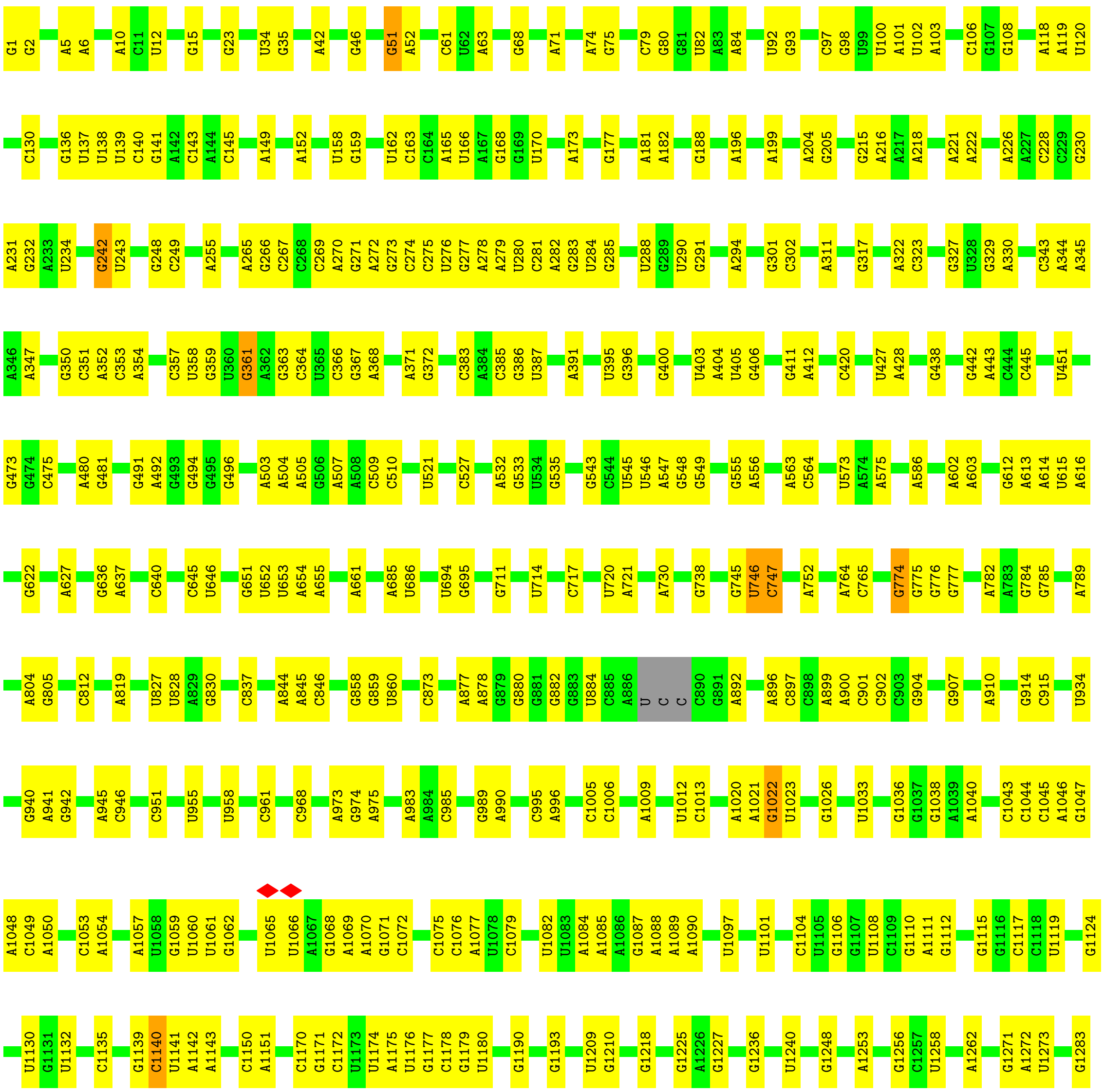
Mol	Chain	Residues	Atoms	AltConf
64	4	1	Total O 1 1	0
64	a	160	Total O 160 160	0
64	i	2	Total O 2 2	0
64	j	1	Total O 1 1	0
64	o	1	Total O 1 1	0
64	p	1	Total O 1 1	0
64	s	2	Total O 2 2	0
64	t	1	Total O 1 1	0
64	u	1	Total O 1 1	0
64	v	3	Total O 3 3	0
64	w	1	Total O 1 1	0
64	y	3	Total O 3 3	0

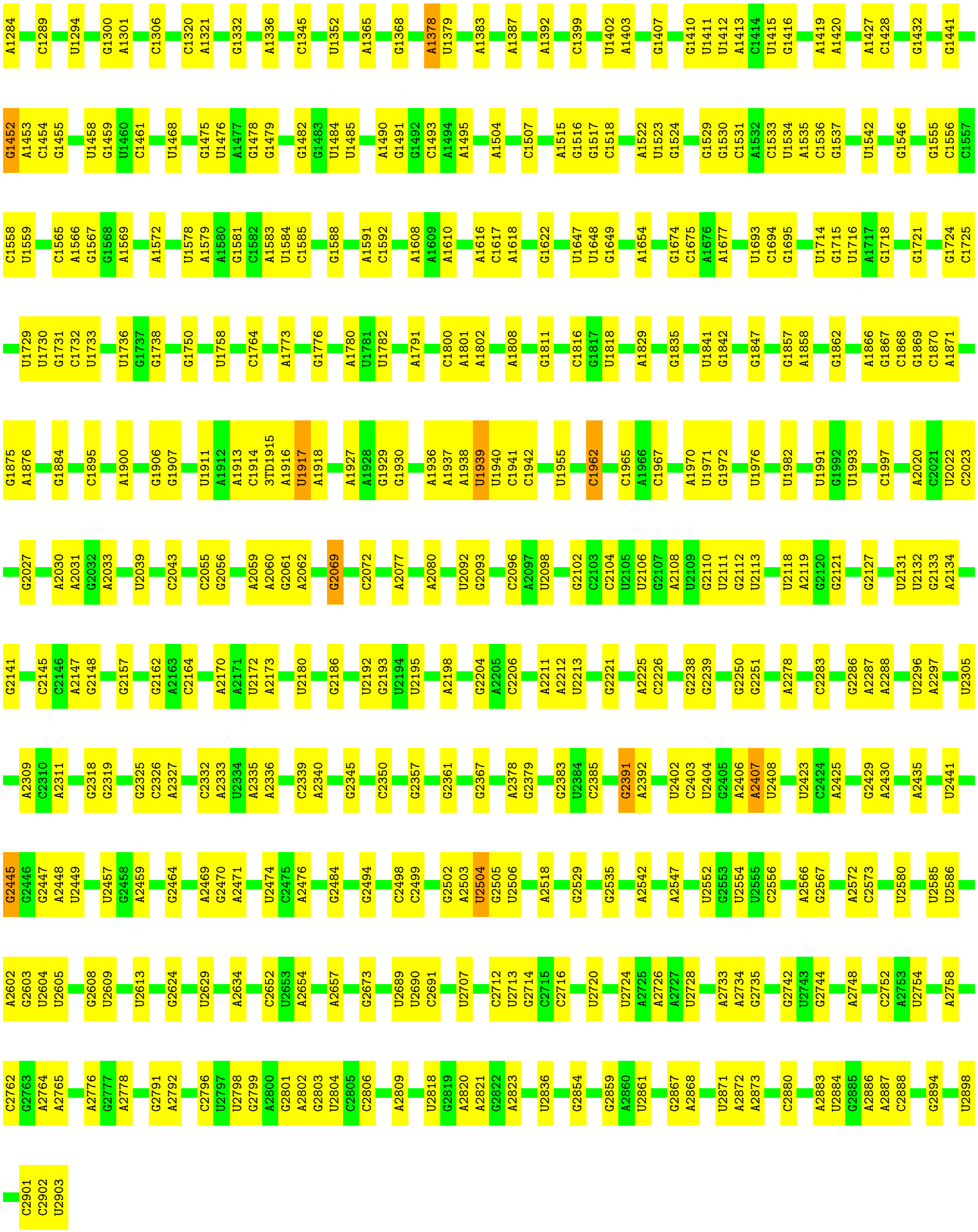
3 Residue-property plots ⓘ

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: 23S rRNA

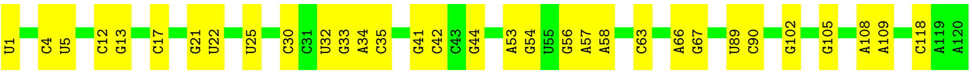
Chain A:



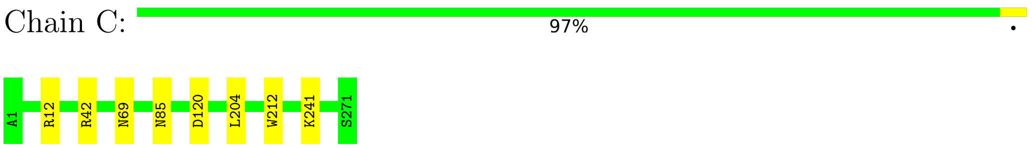


- Molecule 2: 5S rRNA

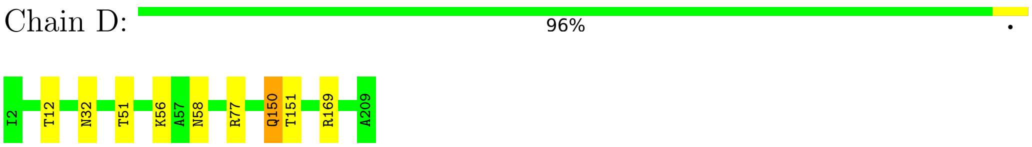
Chain B:



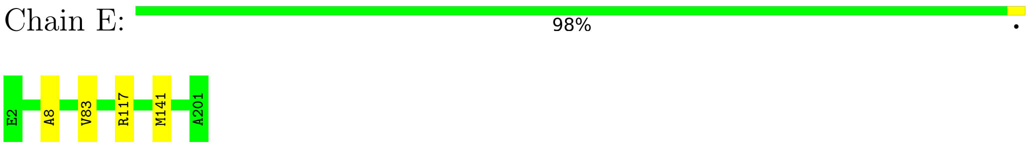
- Molecule 3: 50S ribosomal protein L2



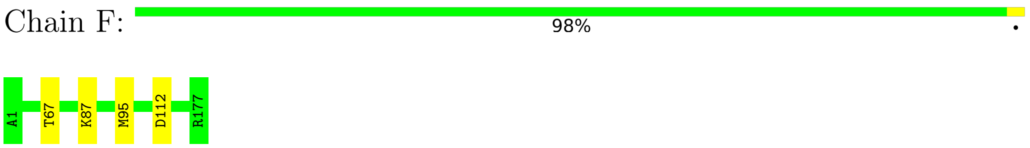
- Molecule 4: 50S ribosomal protein L3



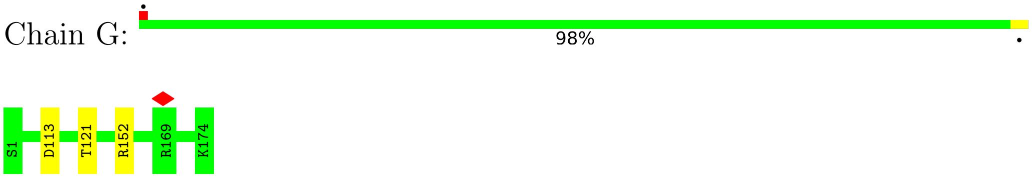
- Molecule 5: 50S ribosomal protein L4



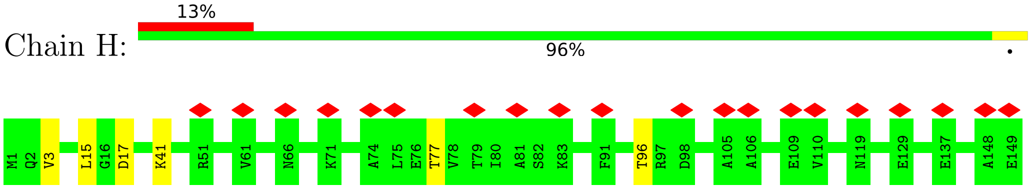
- Molecule 6: 50S ribosomal protein L5



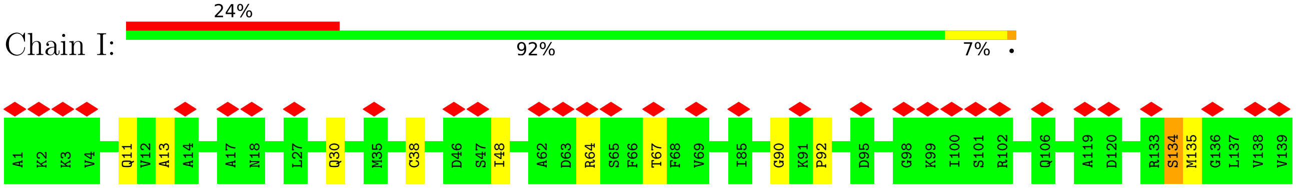
- Molecule 7: 50S ribosomal protein L6

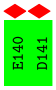


- Molecule 8: 50S ribosomal protein L9



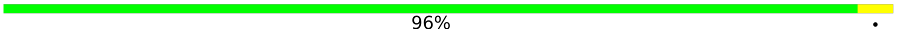
- Molecule 9: 50S ribosomal protein L11

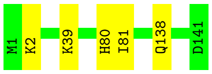




- Molecule 10: 50S ribosomal protein L13

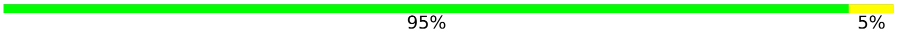
Chain J:

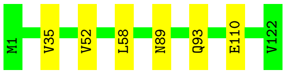




- Molecule 11: 50S ribosomal protein L14

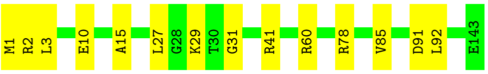
Chain K:





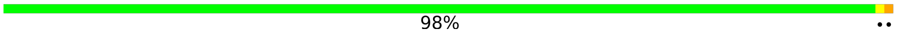
- Molecule 12: 50S ribosomal protein L15

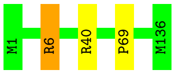
Chain L:



- Molecule 13: 50S ribosomal protein L16

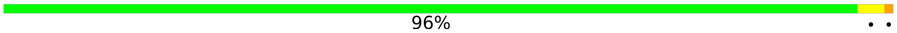
Chain M:

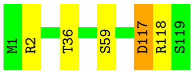




- Molecule 14: 50S ribosomal protein L17

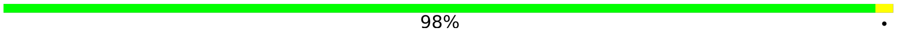
Chain N:

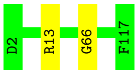




- Molecule 15: 50S ribosomal protein L18

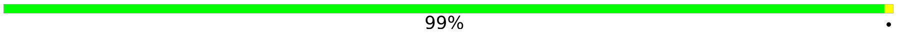
Chain O:

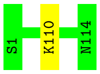




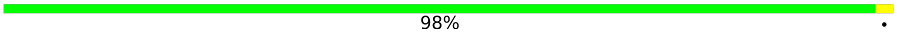
- Molecule 16: 50S ribosomal protein L19

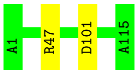
Chain P:





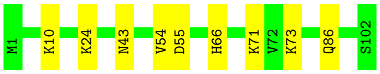
- Molecule 17: 50S ribosomal protein L20

Chain Q:


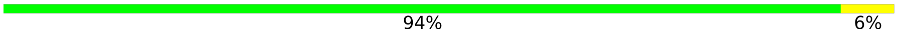


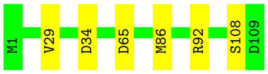
- Molecule 18: 50S ribosomal protein L21

Chain R:

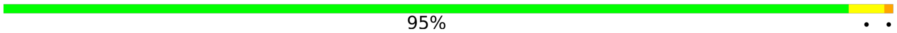



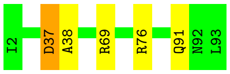
- Molecule 19: 50S ribosomal protein L22

Chain S:


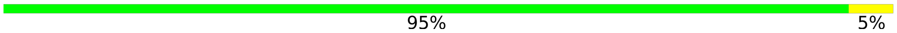


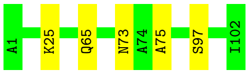
- Molecule 20: 50S ribosomal protein L23

Chain T:


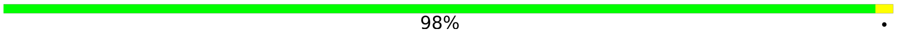


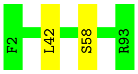
- Molecule 21: 50S ribosomal protein L24

Chain U:


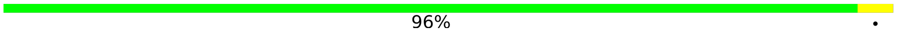


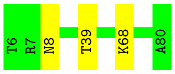
- Molecule 22: 50S ribosomal protein L25

Chain V:




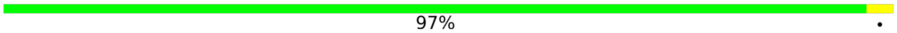
- Molecule 23: 50S ribosomal protein L27

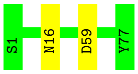
Chain W:




- Molecule 24: 50S ribosomal protein L28

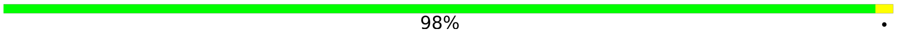
Chain X:

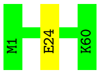




- Molecule 25: 50S ribosomal protein L29

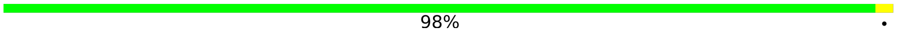
Chain Y:

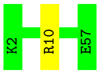




- Molecule 26: 50S ribosomal protein L30

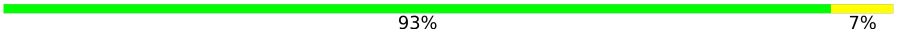
Chain Z:

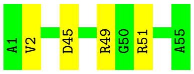




- Molecule 27: 50S ribosomal protein L32

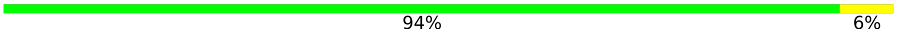
Chain 0:

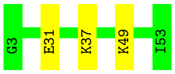




- Molecule 28: 50S ribosomal protein L33

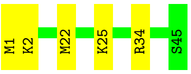
Chain 1:





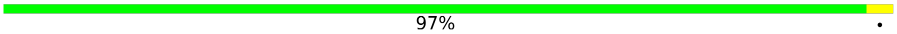
- Molecule 29: 50S ribosomal protein L34

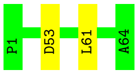
Chain 2:



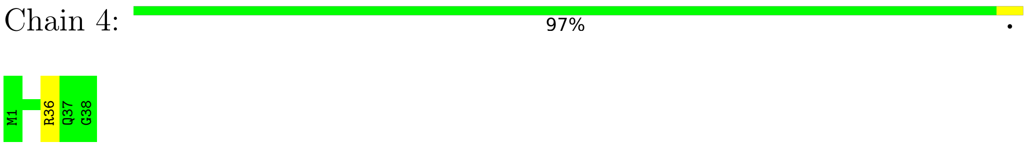
- Molecule 30: 50S ribosomal protein L35

Chain 3:

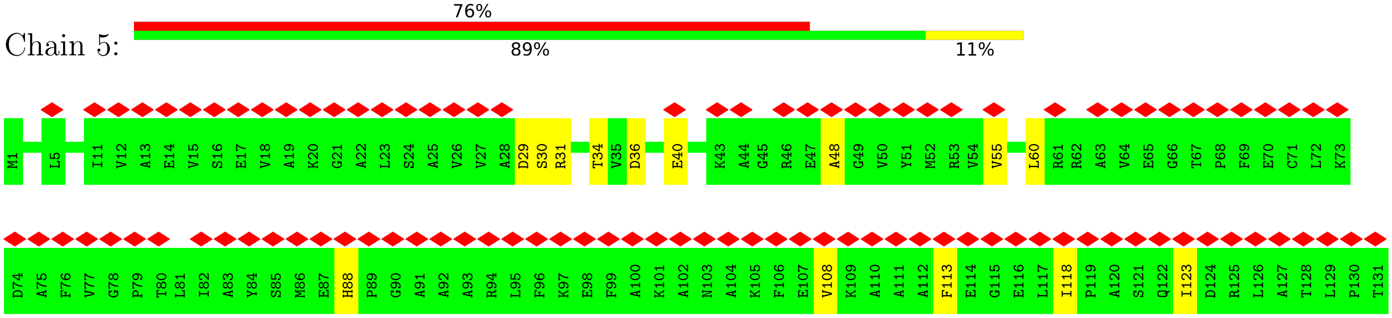




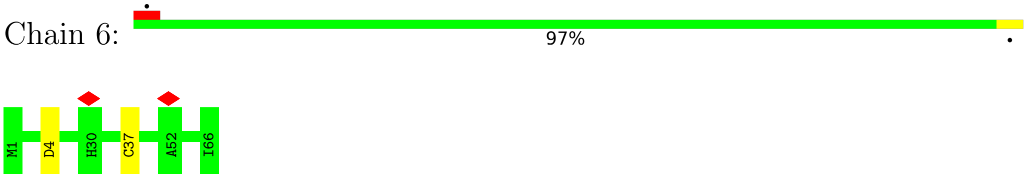
- Molecule 31: 50S ribosomal protein L36



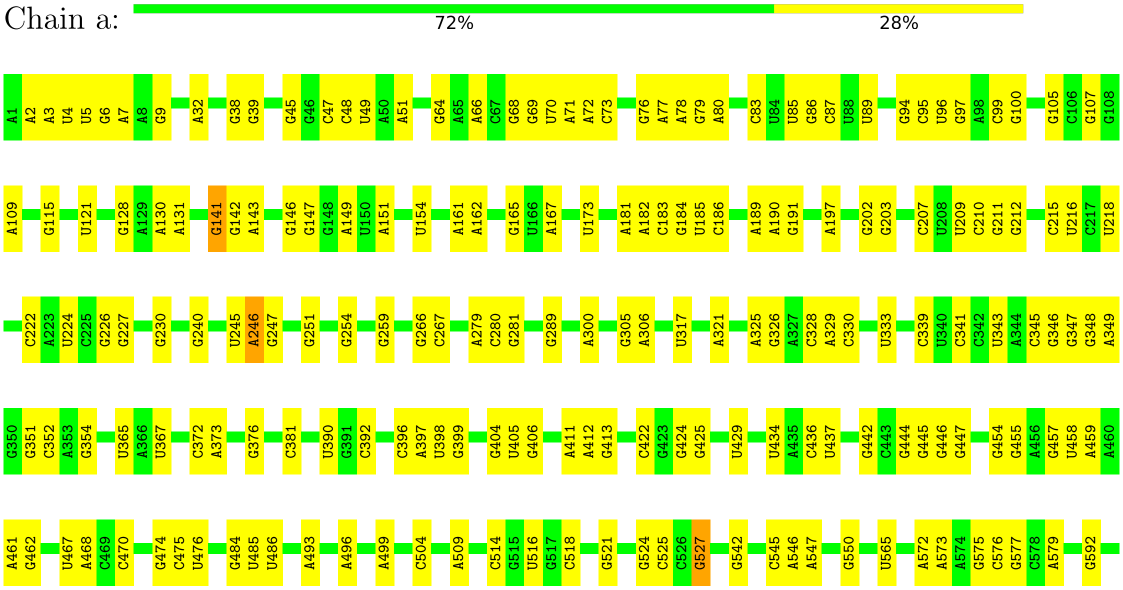
- Molecule 32: 50S ribosomal protein L10

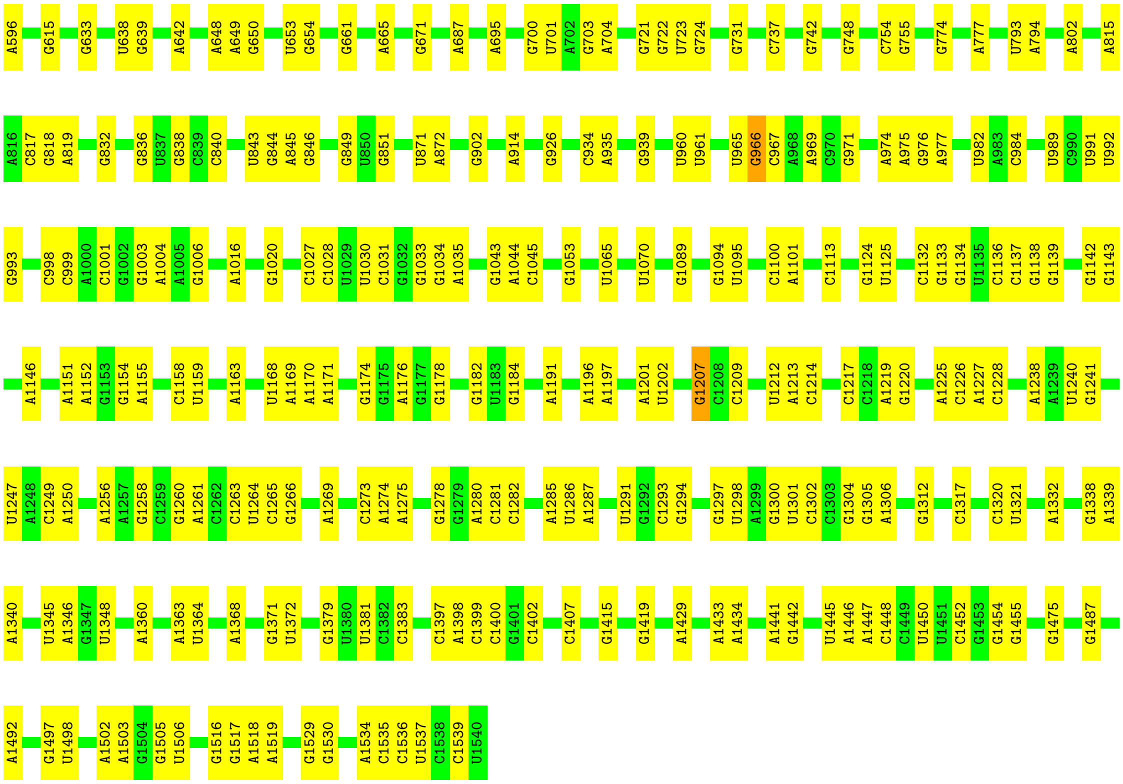


- Molecule 33: 50S ribosomal protein L31



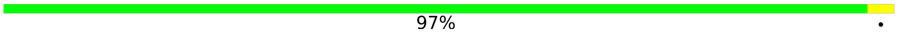
- Molecule 34: 16S rRNA

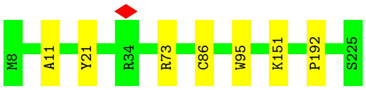




- Molecule 35: 30S ribosomal protein S2

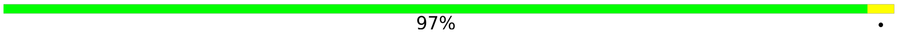
Chain b:

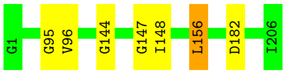




- Molecule 36: 30S ribosomal protein S3

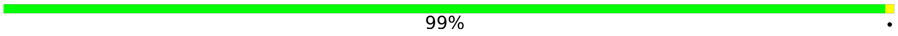
Chain c:

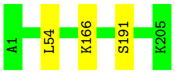




- Molecule 37: 30S ribosomal protein S4

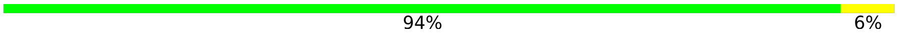
Chain d:

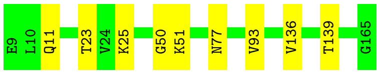




- Molecule 38: 30S ribosomal protein S5

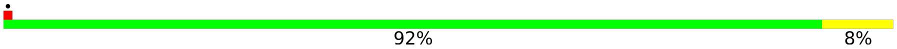
Chain e:

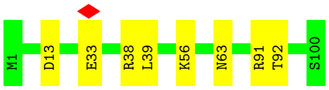




- Molecule 39: 30S ribosomal protein S6

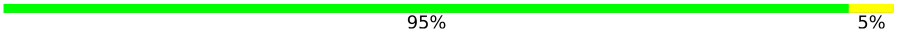
Chain f:

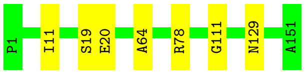




- Molecule 40: 30S ribosomal protein S7

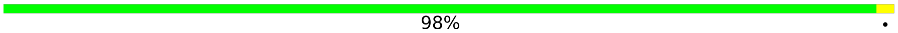
Chain g:

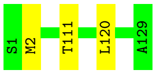




- Molecule 41: 30S ribosomal protein S8

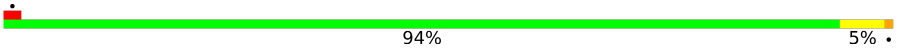
Chain h:

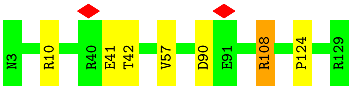




- Molecule 42: 30S ribosomal protein S9

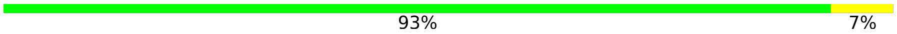
Chain i:

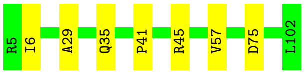




- Molecule 43: 30S ribosomal protein S10

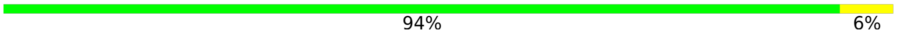
Chain j:

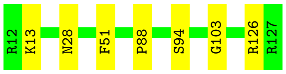




- Molecule 44: 30S ribosomal protein S11

Chain k:



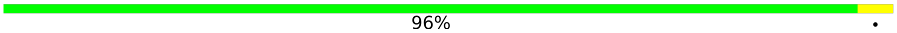


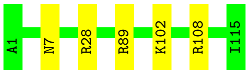
- Molecule 45: 30S ribosomal protein S12

Chain l:

- Molecule 46: 30S ribosomal protein S13

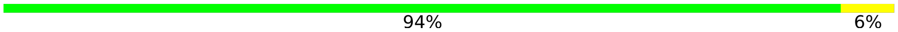
Chain m:

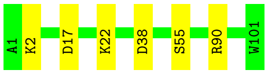




- Molecule 47: 30S ribosomal protein S14

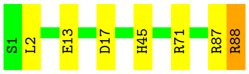
Chain n:





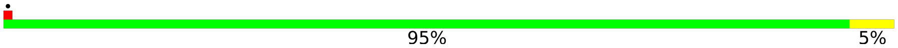
- Molecule 48: 30S ribosomal protein S15

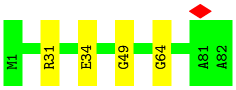
Chain o:



- Molecule 49: 30S ribosomal protein S16

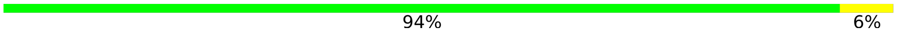
Chain p:

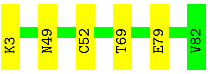




- Molecule 50: 30S ribosomal protein S17

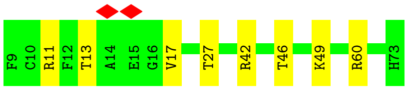
Chain q:





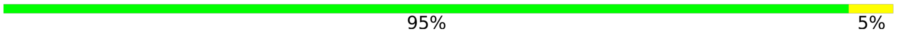
- Molecule 51: 30S ribosomal protein S18

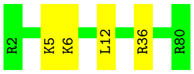
Chain r:



- Molecule 52: 30S ribosomal protein S19

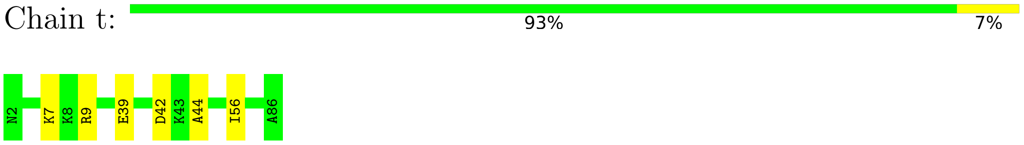
Chain s:





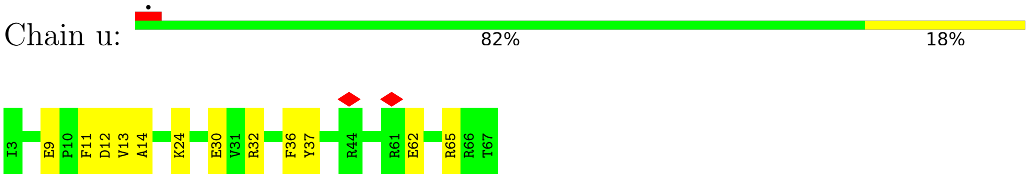
- Molecule 53: 30S ribosomal protein S20

Chain t:



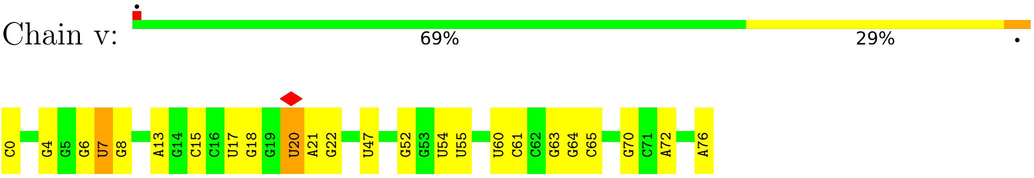
- Molecule 54: 30S ribosomal protein S21

Chain u:



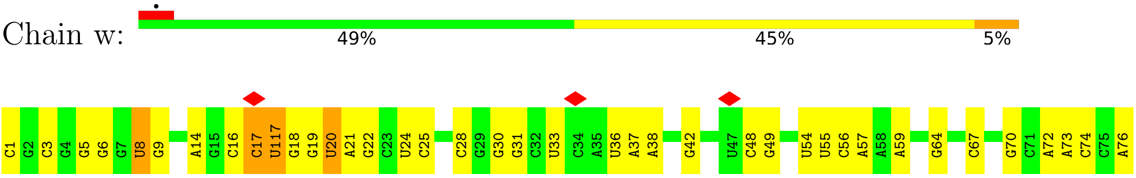
- Molecule 55: tRNA-fMet

Chain v:



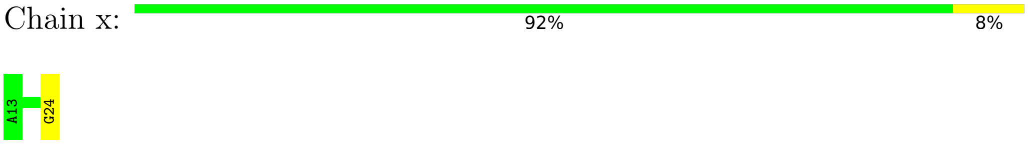
- Molecule 55: tRNA-fMet

Chain w:



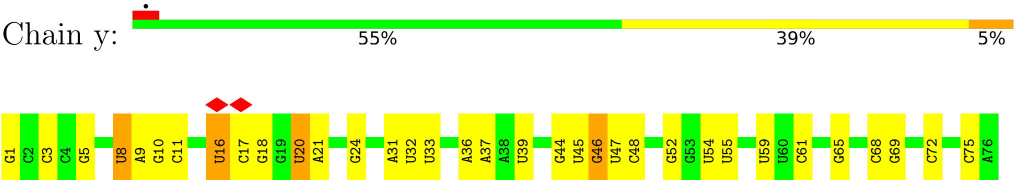
- Molecule 56: mRNA

Chain x:



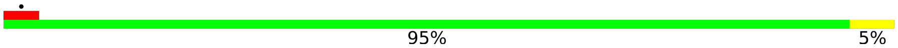
- Molecule 57: Phe-tRNA-Phe

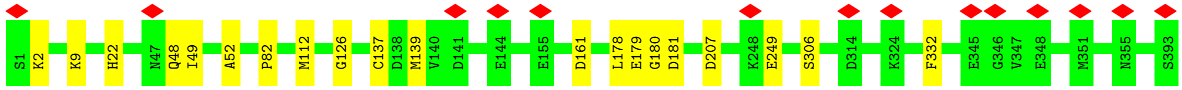
Chain y:



- Molecule 58: Elongation factor Tu 2

Chain z:




S1
K2
K9
H22
N47
Q48
I49
A52
P82
M112
G126
C137
D138
M139
V140
D141
E144
E155
D161
L178
E179
G180
D181
D207
K248
E249
S306
D314
K324
F332
E345
G346
V347
E348
M351
N355
S393

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56963	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^{-}/\text{Å}^{2})$	67	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51020	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.307	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.00677	Depositor
Map size (Å)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, 5MU, OMG, 2MG, 3TD, MA6, 7MG, H2U, OMC, PSU, 2MA, MG, 4OC, 5MC, FME, 6MZ, 1MG, K, MIA, 4SU, OMU, UR3

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	0.26	1/69174 (0.0%)	0.70	10/107907 (0.0%)
2	B	0.30	1/2876 (0.0%)	0.69	0/4483
3	C	0.34	0/2121	0.68	0/2852
4	D	0.35	0/1578	0.61	0/2124
5	E	0.36	0/1563	0.63	0/2103
6	F	0.37	0/1434	0.60	0/1926
7	G	0.35	0/1324	0.54	0/1794
8	H	0.38	0/1122	0.51	0/1515
9	I	0.42	0/1046	0.61	0/1410
10	J	0.35	0/1143	0.61	0/1540
11	K	0.36	0/947	0.69	0/1268
12	L	0.36	0/1052	0.70	0/1401
13	M	0.37	0/1093	0.62	0/1460
14	N	0.38	0/964	0.66	0/1289
15	O	0.37	0/902	0.63	0/1209
16	P	0.36	0/929	0.64	0/1242
17	Q	0.36	0/946	0.70	0/1260
18	R	0.35	0/823	0.61	0/1100
19	S	0.35	0/852	0.68	0/1142
20	T	0.35	0/736	0.63	0/984
21	U	0.35	0/787	0.60	0/1051
22	V	0.34	0/752	0.55	0/1008
23	W	0.35	0/579	0.66	0/767
24	X	0.37	0/635	0.66	0/848
25	Y	0.37	0/495	0.60	0/658
26	Z	0.36	0/438	0.60	0/586
27	0	0.35	0/440	0.75	0/588
28	1	0.35	0/424	0.55	0/565
29	2	0.38	0/370	0.81	0/487
30	3	0.34	0/513	0.64	0/676
31	4	0.32	0/303	0.66	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
32	5	0.45	0/1001	0.65	0/1350
33	6	0.40	0/531	0.54	0/709
34	a	0.24	0/36725	0.70	2/57285 (0.0%)
35	b	0.38	0/1735	0.53	0/2338
36	c	0.36	0/1651	0.59	0/2225
37	d	0.38	0/1665	0.59	0/2227
38	e	0.35	0/1180	0.62	0/1587
39	f	0.36	0/835	0.63	0/1128
40	g	0.36	0/1195	0.60	0/1602
41	h	0.33	0/989	0.60	0/1326
42	i	0.39	0/1034	0.69	0/1375
43	j	0.37	0/796	0.65	0/1077
44	k	0.35	0/885	0.62	0/1195
45	l	0.37	0/954	0.69	0/1282
46	m	0.36	0/900	0.65	0/1204
47	n	0.37	0/822	0.65	0/1095
48	o	0.37	0/722	0.67	1/964 (0.1%)
49	p	0.37	0/659	0.58	0/884
50	q	0.37	0/657	0.64	0/881
51	r	0.39	0/544	0.65	0/731
52	s	0.37	0/652	0.62	0/877
53	t	0.37	0/671	0.63	0/888
54	u	0.45	0/550	0.75	0/728
55	v	0.34	1/1747 (0.1%)	0.69	0/2721
55	w	0.61	2/1747 (0.1%)	0.80	2/2721 (0.1%)
56	x	0.21	0/280	0.65	0/433
57	y	0.33	1/1607 (0.1%)	0.67	0/2501
58	z	0.37	0/3092	0.58	0/4183
All	All	0.30	6/164187 (0.0%)	0.68	15/245157 (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
9	I	0	1
32	5	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	117	U	O3'-P	-21.55	1.35	1.61
55	v	0	C	OP3-P	-10.20	1.49	1.61
57	y	1	G	OP3-P	-10.19	1.49	1.61
2	B	1	U	OP3-P	-10.15	1.49	1.61
1	A	1	G	OP3-P	-10.14	1.49	1.61
55	w	1	C	OP3-P	-10.03	1.49	1.61

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	w	17	C	O3'-P-O5'	17.11	136.50	104.00
55	w	17	C	OP1-P-O3'	-9.94	83.33	105.20
1	A	2407	A	C2'-C3'-O3'	7.86	126.78	109.50
1	A	1140	C	C2'-C3'-O3'	7.76	126.56	109.50
1	A	242	G	C2'-C3'-O3'	7.72	126.49	109.50
1	A	1022	G	C2'-C3'-O3'	6.76	124.51	113.70
1	A	51	G	C2'-C3'-O3'	6.49	124.08	113.70
1	A	774	G	C2'-C3'-O3'	5.76	122.92	113.70
1	A	1378	A	C4'-C3'-O3'	5.73	124.46	113.00
1	A	361	G	N9-C1'-C2'	5.64	121.33	114.00
1	A	1452	G	C2'-C3'-O3'	-5.64	97.10	109.50
48	o	88	ARG	NE-CZ-NH2	5.58	123.09	120.30
34	a	141	G	O4'-C1'-N9	5.49	112.59	108.20
34	a	246	A	C4'-C3'-O3'	5.40	123.81	113.00
1	A	2391	G	C4'-C3'-O3'	5.30	123.59	113.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	5	30	SER	Peptide
9	I	134	SER	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
3	C	269/271 (99%)	240 (89%)	27 (10%)	2 (1%)	22	57
4	D	206/208 (99%)	190 (92%)	15 (7%)	1 (0%)	29	64
5	E	198/200 (99%)	181 (91%)	15 (8%)	2 (1%)	15	49
6	F	175/177 (99%)	156 (89%)	19 (11%)	0	100	100
7	G	172/174 (99%)	159 (92%)	13 (8%)	0	100	100
8	H	147/149 (99%)	125 (85%)	19 (13%)	3 (2%)	7	31
9	I	139/141 (99%)	104 (75%)	29 (21%)	6 (4%)	2	16
10	J	139/141 (99%)	130 (94%)	7 (5%)	2 (1%)	11	40
11	K	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	4	21
12	L	141/143 (99%)	117 (83%)	19 (14%)	5 (4%)	3	20
13	M	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	10	39
14	N	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	5	26
15	O	114/116 (98%)	107 (94%)	6 (5%)	1 (1%)	17	52
16	P	112/114 (98%)	98 (88%)	14 (12%)	0	100	100
17	Q	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
18	R	100/102 (98%)	84 (84%)	13 (13%)	3 (3%)	4	23
19	S	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	17	52
20	T	90/92 (98%)	79 (88%)	9 (10%)	2 (2%)	6	29
21	U	100/102 (98%)	87 (87%)	11 (11%)	2 (2%)	7	31
22	V	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	14	46
23	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	11	40
24	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
25	Y	58/60 (97%)	54 (93%)	3 (5%)	1 (2%)	9	36
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
27	0	53/55 (96%)	45 (85%)	7 (13%)	1 (2%)	8	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1	49/51 (96%)	44 (90%)	5 (10%)	0	100	100
29	2	43/45 (96%)	40 (93%)	3 (7%)	0	100	100
30	3	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	96 (74%)	24 (19%)	9 (7%)	1	7
33	6	64/66 (97%)	56 (88%)	7 (11%)	1 (2%)	9	37
35	b	216/218 (99%)	187 (87%)	24 (11%)	5 (2%)	6	28
36	c	204/206 (99%)	180 (88%)	18 (9%)	6 (3%)	4	24
37	d	203/205 (99%)	182 (90%)	19 (9%)	2 (1%)	15	49
38	e	156/157 (99%)	136 (87%)	16 (10%)	4 (3%)	5	26
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	3	16
40	g	149/151 (99%)	131 (88%)	13 (9%)	5 (3%)	3	21
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/127 (98%)	94 (75%)	27 (22%)	4 (3%)	4	22
43	j	96/98 (98%)	70 (73%)	20 (21%)	6 (6%)	1	8
44	k	114/116 (98%)	101 (89%)	8 (7%)	5 (4%)	2	15
45	l	119/121 (98%)	94 (79%)	19 (16%)	6 (5%)	2	13
46	m	113/115 (98%)	104 (92%)	7 (6%)	2 (2%)	8	34
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	2	13
48	o	86/88 (98%)	77 (90%)	6 (7%)	3 (4%)	3	20
49	p	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	5	27
50	q	78/80 (98%)	67 (86%)	8 (10%)	3 (4%)	3	19
51	r	63/65 (97%)	51 (81%)	10 (16%)	2 (3%)	4	22
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
53	t	83/85 (98%)	77 (93%)	4 (5%)	2 (2%)	6	27
54	u	63/65 (97%)	39 (62%)	14 (22%)	10 (16%)	0	0
58	z	391/393 (100%)	350 (90%)	29 (7%)	12 (3%)	4	23
All	All	6219/6322 (98%)	5469 (88%)	609 (10%)	141 (2%)	9	28

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	81	ILE

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Mol	Chain	Res	Type
11	K	89	ASN
32	5	55	VAL
32	5	123	ILE
33	6	4	ASP
36	c	96	VAL
36	c	156	LEU
40	g	64	ALA
42	i	90	ASP
43	j	57	VAL
44	k	88	PRO
44	k	94	SER
45	l	75	GLU
47	n	55	SER
53	t	39	GLU
54	u	13	VAL
54	u	14	ALA
54	u	37	TYR
5	E	8	ALA
5	E	83	VAL
15	O	66	GLY
18	R	55	ASP
20	T	37	ASP
20	T	38	ALA
22	V	58	SER
32	5	31	ARG
32	5	108	VAL
35	b	73	ARG
38	e	77	ASN
38	e	93	VAL
40	g	20	GLU
40	g	129	ASN
42	i	57	VAL
42	i	108	ARG
42	i	124	PRO
43	j	29	ALA
44	k	51	PHE
45	l	42	LYS
46	m	7	ASN
47	n	22	LYS
47	n	90	ARG
51	r	17	VAL
54	u	30	GLU

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Mol	Chain	Res	Type
3	C	120	ASP
9	I	38	CYS
9	I	64	ARG
12	L	15	ALA
12	L	92	LEU
13	M	69	PRO
14	N	59	SER
14	N	117	ASP
18	R	54	VAL
23	W	39	THR
25	Y	24	GLU
27	0	2	VAL
32	5	48	ALA
32	5	60	LEU
32	5	88	HIS
35	b	86	CYS
37	d	191	SER
39	f	33	GLU
39	f	92	THR
44	k	103	GLY
45	l	46	SER
45	l	88	ASP
46	m	102	LYS
47	n	2	LYS
47	n	38	ASP
49	p	49	GLY
51	r	46	THR
54	u	9	GLU
54	u	11	PHE
54	u	12	ASP
54	u	36	PHE
58	z	126	GLY
58	z	161	ASP
58	z	249	GLU
58	z	332	PHE
3	C	204	LEU
8	H	15	LEU
9	I	90	GLY
11	K	35	VAL
11	K	110	GLU
12	L	29	LYS
18	R	43	ASN

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Mol	Chain	Res	Type
21	U	75	ALA
21	U	97	SER
32	5	113	PHE
32	5	118	ILE
36	c	95	GLY
36	c	147	GLY
36	c	148	ILE
37	d	166	LYS
39	f	56	LYS
39	f	63	ASN
40	g	19	SER
43	j	35	GLN
43	j	41	PRO
44	k	13	LYS
48	o	13	GLU
48	o	45	HIS
49	p	64	GLY
50	q	79	GLU
58	z	137	CYS
4	D	150	GLN
8	H	3	VAL
8	H	41	LYS
9	I	13	ALA
10	J	2	LYS
13	M	6	ARG
19	S	65	ASP
35	b	11	ALA
35	b	151	LYS
38	e	23	THR
43	j	75	ASP
45	l	33	CYS
48	o	2	LEU
50	q	49	ASN
50	q	69	THR
53	t	44	ALA
54	u	24	LYS
58	z	9	LYS
58	z	82	PRO
58	z	179	GLU
58	z	180	GLY
58	z	207	ASP
9	I	92	PRO

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Mol	Chain	Res	Type
11	K	93	GLN
12	L	85	VAL
14	N	118	ARG
43	j	6	ILE
45	l	77	SER
54	u	65	ARG
58	z	2	LYS
58	z	52	ALA
35	b	192	PRO
12	L	31	GLY
36	c	144	GLY
40	g	111	GLY
38	e	50	GLY
9	I	48	ILE

5.3.2 Protein sidechains ⓘ

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	
3	C	216/216 (100%)	210 (97%)	6 (3%)	43	73
4	D	163/163 (100%)	154 (94%)	9 (6%)	21	53
5	E	164/164 (100%)	162 (99%)	2 (1%)	71	88
6	F	148/148 (100%)	144 (97%)	4 (3%)	44	74
7	G	135/135 (100%)	132 (98%)	3 (2%)	52	78
8	H	114/114 (100%)	111 (97%)	3 (3%)	46	74
9	I	109/109 (100%)	104 (95%)	5 (5%)	27	59
10	J	115/115 (100%)	112 (97%)	3 (3%)	46	74
11	K	103/103 (100%)	101 (98%)	2 (2%)	57	81
12	L	102/102 (100%)	93 (91%)	9 (9%)	10	36
13	M	109/109 (100%)	107 (98%)	2 (2%)	59	82
14	N	99/99 (100%)	96 (97%)	3 (3%)	41	71
15	O	86/86 (100%)	85 (99%)	1 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	99/99 (100%)	98 (99%)	1 (1%)	76	90
17	Q	88/88 (100%)	86 (98%)	2 (2%)	50	77
18	R	84/84 (100%)	78 (93%)	6 (7%)	14	44
19	S	92/92 (100%)	87 (95%)	5 (5%)	22	53
20	T	79/79 (100%)	75 (95%)	4 (5%)	24	56
21	U	83/83 (100%)	80 (96%)	3 (4%)	35	67
22	V	77/77 (100%)	76 (99%)	1 (1%)	69	87
23	W	57/57 (100%)	55 (96%)	2 (4%)	36	68
24	X	67/67 (100%)	65 (97%)	2 (3%)	41	71
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	47/47 (100%)	46 (98%)	1 (2%)	53	79
27	0	46/46 (100%)	43 (94%)	3 (6%)	17	47
28	1	46/46 (100%)	43 (94%)	3 (6%)	17	47
29	2	37/37 (100%)	32 (86%)	5 (14%)	4	16
30	3	51/51 (100%)	49 (96%)	2 (4%)	32	65
31	4	34/34 (100%)	33 (97%)	1 (3%)	42	72
32	5	100/100 (100%)	96 (96%)	4 (4%)	31	65
33	6	59/59 (100%)	58 (98%)	1 (2%)	60	83
35	b	180/180 (100%)	178 (99%)	2 (1%)	73	89
36	c	170/170 (100%)	168 (99%)	2 (1%)	71	88
37	d	172/172 (100%)	171 (99%)	1 (1%)	86	94
38	e	120/119 (101%)	115 (96%)	5 (4%)	30	62
39	f	87/87 (100%)	83 (95%)	4 (5%)	27	59
40	g	124/124 (100%)	122 (98%)	2 (2%)	62	84
41	h	104/104 (100%)	101 (97%)	3 (3%)	42	72
42	i	105/105 (100%)	101 (96%)	4 (4%)	33	66
43	j	86/86 (100%)	85 (99%)	1 (1%)	71	88
44	k	89/89 (100%)	87 (98%)	2 (2%)	52	78
45	l	102/102 (100%)	96 (94%)	6 (6%)	19	50
46	m	93/93 (100%)	90 (97%)	3 (3%)	39	69
47	n	83/83 (100%)	82 (99%)	1 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	o	76/76 (100%)	72 (95%)	4 (5%)	22	54
49	p	65/65 (100%)	63 (97%)	2 (3%)	40	70
50	q	74/74 (100%)	72 (97%)	2 (3%)	44	74
51	r	56/56 (100%)	50 (89%)	6 (11%)	6	26
52	s	70/70 (100%)	66 (94%)	4 (6%)	20	52
53	t	65/65 (100%)	61 (94%)	4 (6%)	18	49
54	u	55/55 (100%)	53 (96%)	2 (4%)	35	67
58	z	326/326 (100%)	318 (98%)	8 (2%)	47	75
All	All	5166/5165 (100%)	5000 (97%)	166 (3%)	42	69

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	12	ARG
3	C	42	ARG
3	C	69	ASN
3	C	85	ASN
3	C	212	TRP
3	C	241	LYS
4	D	12	THR
4	D	32	ASN
4	D	51	THR
4	D	56	LYS
4	D	58	ASN
4	D	77	ARG
4	D	150	GLN
4	D	151	THR
4	D	169	ARG
5	E	117	ARG
5	E	141	MET
6	F	67	THR
6	F	87	LYS
6	F	95	MET
6	F	112	ASP
7	G	113	ASP
7	G	121	THR
7	G	152	ARG
8	H	17	ASP
8	H	77	THR

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Mol	Chain	Res	Type
8	H	96	THR
9	I	11	GLN
9	I	30	GLN
9	I	67	THR
9	I	134	SER
9	I	135	MET
10	J	39	LYS
10	J	80	HIS
10	J	138	GLN
11	K	52	VAL
11	K	58	LEU
12	L	1	MET
12	L	2	ARG
12	L	3	LEU
12	L	10	GLU
12	L	27	LEU
12	L	41	ARG
12	L	60	ARG
12	L	78	ARG
12	L	91	ASP
13	M	6	ARG
13	M	40	ARG
14	N	2	ARG
14	N	36	THR
14	N	117	ASP
15	O	13	ARG
16	P	110	LYS
17	Q	47	ARG
17	Q	101	ASP
18	R	10	LYS
18	R	24	LYS
18	R	66	HIS
18	R	71	LYS
18	R	73	LYS
18	R	86	GLN
19	S	29	VAL
19	S	34	ASP
19	S	86	MET
19	S	92	ARG
19	S	108	SER
20	T	37	ASP
20	T	69	ARG

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Mol	Chain	Res	Type
20	T	76	ARG
20	T	91	GLN
21	U	25	LYS
21	U	65	GLN
21	U	73	ASN
22	V	42	LEU
23	W	8	ASN
23	W	68	LYS
24	X	16	ASN
24	X	59	ASP
26	Z	10	ARG
27	0	45	ASP
27	0	49	ARG
27	0	51	ARG
28	1	31	GLU
28	1	37	LYS
28	1	49	LYS
29	2	1	MET
29	2	2	LYS
29	2	22	MET
29	2	25	LYS
29	2	34	ARG
30	3	53	ASP
30	3	61	LEU
31	4	36	ARG
32	5	29	ASP
32	5	34	THR
32	5	36	ASP
32	5	40	GLU
33	6	37	CYS
35	b	21	TYR
35	b	95	TRP
36	c	156	LEU
36	c	182	ASP
37	d	54	LEU
38	e	11	GLN
38	e	25	LYS
38	e	51	LYS
38	e	136	VAL
38	e	139	THR
39	f	13	ASP
39	f	38	ARG

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Mol	Chain	Res	Type
39	f	39	LEU
39	f	91	ARG
40	g	11	ILE
40	g	78	ARG
41	h	2	MET
41	h	111	THR
41	h	120	LEU
42	i	10	ARG
42	i	41	GLU
42	i	42	THR
42	i	108	ARG
43	j	45	ARG
44	k	28	ASN
44	k	126	ARG
45	l	9	LYS
45	l	38	THR
45	l	77	SER
45	l	88	ASP
45	l	93	ARG
45	l	111	GLN
46	m	28	ARG
46	m	89	ARG
46	m	108	ARG
47	n	17	ASP
48	o	17	ASP
48	o	71	ARG
48	o	87	ARG
48	o	88	ARG
49	p	31	ARG
49	p	34	GLU
50	q	3	LYS
50	q	52	CYS
51	r	11	ARG
51	r	13	THR
51	r	27	THR
51	r	42	ARG
51	r	49	LYS
51	r	60	ARG
52	s	5	LYS
52	s	6	LYS
52	s	12	LEU
52	s	36	ARG

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Mol	Chain	Res	Type
53	t	7	LYS
53	t	9	ARG
53	t	42	ASP
53	t	56	ILE
54	u	32	ARG
54	u	62	GLU
58	z	22	HIS
58	z	48	GLN
58	z	49	ILE
58	z	112	MET
58	z	139	MET
58	z	178	LEU
58	z	181	ASP
58	z	306	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	85	ASN
7	G	37	ASN
14	N	62	ASN
16	P	114	ASN
45	l	111	GLN
53	t	69	ASN
58	z	51	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2892/2903 (99%)	744 (25%)	78 (2%)
2	B	119/120 (99%)	29 (24%)	3 (2%)
34	a	1536/1540 (99%)	426 (27%)	0
55	v	76/77 (98%)	21 (27%)	0
55	w	76/77 (98%)	36 (47%)	0
56	x	11/12 (91%)	1 (9%)	0
57	y	74/76 (97%)	28 (37%)	0
All	All	4784/4805 (99%)	1285 (26%)	81 (1%)

All (1285) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	5	A
1	A	6	A
1	A	10	A
1	A	12	U
1	A	15	G
1	A	23	G
1	A	34	U
1	A	35	G
1	A	42	A
1	A	46	G
1	A	52	A
1	A	61	C
1	A	63	A
1	A	68	G
1	A	71	A
1	A	74	A
1	A	75	G
1	A	79	C
1	A	80	G
1	A	82	U
1	A	84	A
1	A	92	U
1	A	93	G
1	A	97	C
1	A	98	G
1	A	100	U
1	A	101	A
1	A	102	U
1	A	103	A
1	A	106	C
1	A	108	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	130	C
1	A	136	G
1	A	137	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	143	C
1	A	145	C

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Mol	Chain	Res	Type
1	A	149	A
1	A	152	A
1	A	158	U
1	A	159	G
1	A	162	U
1	A	163	C
1	A	165	A
1	A	166	U
1	A	168	G
1	A	170	U
1	A	173	A
1	A	181	A
1	A	188	G
1	A	196	A
1	A	205	G
1	A	215	G
1	A	216	A
1	A	218	A
1	A	221	A
1	A	222	A
1	A	226	A
1	A	228	C
1	A	230	G
1	A	231	A
1	A	232	G
1	A	234	U
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	265	A
1	A	266	G
1	A	267	C
1	A	269	C
1	A	270	A
1	A	271	G
1	A	272	A
1	A	273	G
1	A	274	C
1	A	275	C
1	A	276	U

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Mol	Chain	Res	Type
1	A	277	G
1	A	278	A
1	A	279	A
1	A	280	U
1	A	281	C
1	A	283	G
1	A	284	U
1	A	285	G
1	A	288	U
1	A	290	U
1	A	291	G
1	A	294	A
1	A	301	G
1	A	302	C
1	A	311	A
1	A	317	G
1	A	322	A
1	A	323	C
1	A	327	G
1	A	329	G
1	A	330	A
1	A	343	C
1	A	344	A
1	A	345	A
1	A	347	A
1	A	350	G
1	A	351	C
1	A	352	A
1	A	353	C
1	A	354	A
1	A	357	C
1	A	358	U
1	A	359	G
1	A	361	G
1	A	363	G
1	A	364	C
1	A	366	C
1	A	367	G
1	A	368	A
1	A	371	A
1	A	372	G
1	A	383	C

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Mol	Chain	Res	Type
1	A	385	C
1	A	386	G
1	A	387	U
1	A	391	A
1	A	395	U
1	A	396	G
1	A	400	G
1	A	403	U
1	A	404	A
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	420	C
1	A	427	U
1	A	428	A
1	A	438	G
1	A	442	G
1	A	443	A
1	A	445	C
1	A	451	U
1	A	473	G
1	A	475	C
1	A	480	A
1	A	481	G
1	A	491	G
1	A	492	A
1	A	494	G
1	A	496	G
1	A	503	A
1	A	504	A
1	A	505	A
1	A	507	A
1	A	509	C
1	A	510	C
1	A	521	U
1	A	527	C
1	A	532	A
1	A	533	G
1	A	535	G
1	A	543	G
1	A	545	U

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Mol	Chain	Res	Type
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	555	G
1	A	556	A
1	A	563	A
1	A	564	C
1	A	573	U
1	A	575	A
1	A	586	A
1	A	602	A
1	A	603	A
1	A	612	G
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	622	G
1	A	627	A
1	A	636	G
1	A	637	A
1	A	640	C
1	A	645	C
1	A	646	U
1	A	651	G
1	A	653	U
1	A	654	A
1	A	655	A
1	A	661	A
1	A	685	A
1	A	686	U
1	A	694	U
1	A	695	G
1	A	711	G
1	A	714	U
1	A	717	C
1	A	720	U
1	A	721	A
1	A	730	A
1	A	738	G
1	A	747	5MC

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Mol	Chain	Res	Type
1	A	752	A
1	A	764	A
1	A	765	C
1	A	774	G
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	804	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	837	C
1	A	844	A
1	A	845	A
1	A	846	C
1	A	858	G
1	A	860	U
1	A	873	C
1	A	877	A
1	A	878	A
1	A	880	G
1	A	882	G
1	A	892	A
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	C
1	A	902	C
1	A	904	G
1	A	907	G
1	A	910	A
1	A	914	G
1	A	915	C
1	A	934	U

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Mol	Chain	Res	Type
1	A	940	G
1	A	941	A
1	A	942	G
1	A	945	A
1	A	946	C
1	A	951	C
1	A	958	U
1	A	961	C
1	A	968	C
1	A	973	A
1	A	974	G
1	A	975	A
1	A	983	A
1	A	985	C
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	1005	C
1	A	1006	C
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1026	G
1	A	1033	U
1	A	1036	G
1	A	1038	G
1	A	1040	A
1	A	1043	C
1	A	1044	C
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1048	A
1	A	1049	C
1	A	1050	A
1	A	1053	C
1	A	1054	A

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Mol	Chain	Res	Type
1	A	1057	A
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1075	C
1	A	1076	C
1	A	1077	A
1	A	1079	C
1	A	1082	U
1	A	1084	A
1	A	1085	A
1	A	1087	G
1	A	1088	A
1	A	1090	A
1	A	1097	U
1	A	1101	U
1	A	1104	C
1	A	1106	G
1	A	1108	U
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1115	G
1	A	1117	C
1	A	1119	U
1	A	1130	U
1	A	1132	U
1	A	1135	C
1	A	1139	G
1	A	1141	U
1	A	1142	A
1	A	1143	A
1	A	1150	C
1	A	1151	A

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Mol	Chain	Res	Type
1	A	1170	C
1	A	1171	G
1	A	1172	C
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1179	G
1	A	1180	U
1	A	1193	G
1	A	1209	U
1	A	1210	G
1	A	1218	G
1	A	1225	G
1	A	1227	G
1	A	1236	G
1	A	1248	G
1	A	1253	A
1	A	1256	G
1	A	1258	U
1	A	1262	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1283	G
1	A	1284	A
1	A	1289	C
1	A	1294	U
1	A	1300	G
1	A	1301	A
1	A	1306	C
1	A	1320	C
1	A	1321	A
1	A	1332	G
1	A	1336	A
1	A	1345	C
1	A	1352	U
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U

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Mol	Chain	Res	Type
1	A	1383	A
1	A	1387	A
1	A	1392	A
1	A	1402	U
1	A	1403	A
1	A	1407	G
1	A	1410	G
1	A	1411	U
1	A	1412	U
1	A	1413	A
1	A	1415	U
1	A	1416	G
1	A	1419	A
1	A	1420	A
1	A	1427	A
1	A	1428	C
1	A	1441	G
1	A	1452	G
1	A	1453	A
1	A	1454	C
1	A	1455	G
1	A	1458	U
1	A	1459	G
1	A	1461	C
1	A	1468	U
1	A	1475	G
1	A	1476	U
1	A	1478	G
1	A	1479	G
1	A	1482	G
1	A	1484	U
1	A	1485	U
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1495	A
1	A	1504	A
1	A	1507	C
1	A	1515	A
1	A	1516	G
1	A	1517	G
1	A	1518	C

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Mol	Chain	Res	Type
1	A	1522	A
1	A	1523	U
1	A	1524	G
1	A	1529	G
1	A	1530	G
1	A	1531	C
1	A	1533	C
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1542	U
1	A	1546	G
1	A	1555	G
1	A	1556	C
1	A	1559	U
1	A	1565	C
1	A	1566	A
1	A	1567	G
1	A	1569	A
1	A	1572	A
1	A	1578	U
1	A	1579	A
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1588	G
1	A	1591	A
1	A	1592	C
1	A	1608	A
1	A	1610	A
1	A	1616	A
1	A	1617	C
1	A	1622	G
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1654	A
1	A	1674	G
1	A	1675	C
1	A	1677	A

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Mol	Chain	Res	Type
1	A	1693	U
1	A	1694	C
1	A	1695	G
1	A	1714	U
1	A	1715	G
1	A	1716	U
1	A	1718	G
1	A	1721	G
1	A	1724	G
1	A	1725	C
1	A	1729	U
1	A	1730	U
1	A	1731	G
1	A	1732	C
1	A	1733	U
1	A	1736	U
1	A	1738	G
1	A	1750	G
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1776	G
1	A	1780	A
1	A	1782	U
1	A	1791	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1811	G
1	A	1816	C
1	A	1829	A
1	A	1841	U
1	A	1842	G
1	A	1847	G
1	A	1858	A
1	A	1862	G
1	A	1866	A
1	A	1867	G
1	A	1868	C
1	A	1869	G
1	A	1870	C

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Mol	Chain	Res	Type
1	A	1871	A
1	A	1875	G
1	A	1876	A
1	A	1884	G
1	A	1895	C
1	A	1906	G
1	A	1907	G
1	A	1913	A
1	A	1914	C
1	A	1916	A
1	A	1917	PSU
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1940	U
1	A	1941	C
1	A	1942	C
1	A	1955	U
1	A	1962	5MC
1	A	1965	C
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1982	U
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2027	G
1	A	2031	A
1	A	2033	A
1	A	2039	U
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2059	A

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Mol	Chain	Res	Type
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	7MG
1	A	2072	C
1	A	2077	A
1	A	2080	A
1	A	2092	U
1	A	2093	G
1	A	2096	C
1	A	2098	U
1	A	2102	G
1	A	2104	C
1	A	2106	U
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2118	U
1	A	2119	A
1	A	2121	G
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2141	G
1	A	2145	C
1	A	2147	A
1	A	2148	G
1	A	2157	G
1	A	2162	G
1	A	2164	C
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2180	U
1	A	2186	G
1	A	2192	U
1	A	2193	G
1	A	2195	U

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Mol	Chain	Res	Type
1	A	2198	A
1	A	2204	G
1	A	2206	C
1	A	2211	A
1	A	2212	A
1	A	2213	U
1	A	2221	G
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2250	G
1	A	2278	A
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2288	A
1	A	2297	A
1	A	2305	U
1	A	2309	A
1	A	2311	A
1	A	2318	G
1	A	2319	G
1	A	2325	G
1	A	2326	C
1	A	2327	A
1	A	2332	C
1	A	2333	A
1	A	2335	A
1	A	2336	A
1	A	2339	C
1	A	2340	A
1	A	2345	G
1	A	2350	C
1	A	2357	G
1	A	2361	G
1	A	2367	G
1	A	2378	A
1	A	2379	G
1	A	2383	G
1	A	2385	C
1	A	2392	A

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Mol	Chain	Res	Type
1	A	2402	U
1	A	2403	C
1	A	2404	U
1	A	2406	A
1	A	2408	U
1	A	2423	U
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2441	U
1	A	2445	2MG
1	A	2447	G
1	A	2448	A
1	A	2459	A
1	A	2464	G
1	A	2469	A
1	A	2470	G
1	A	2471	A
1	A	2474	U
1	A	2476	A
1	A	2484	G
1	A	2494	G
1	A	2499	C
1	A	2502	G
1	A	2504	PSU
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2529	G
1	A	2535	G
1	A	2542	A
1	A	2547	A
1	A	2554	U
1	A	2556	C
1	A	2566	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2585	U
1	A	2586	U
1	A	2602	A

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Mol	Chain	Res	Type
1	A	2603	G
1	A	2608	G
1	A	2609	U
1	A	2613	U
1	A	2624	G
1	A	2629	U
1	A	2634	A
1	A	2652	C
1	A	2654	A
1	A	2657	A
1	A	2673	G
1	A	2689	U
1	A	2690	U
1	A	2691	C
1	A	2707	U
1	A	2713	U
1	A	2714	G
1	A	2716	C
1	A	2720	U
1	A	2724	U
1	A	2726	A
1	A	2728	U
1	A	2733	A
1	A	2734	A
1	A	2735	G
1	A	2742	G
1	A	2744	G
1	A	2748	A
1	A	2752	C
1	A	2754	U
1	A	2758	A
1	A	2762	C
1	A	2764	A
1	A	2765	A
1	A	2776	A
1	A	2778	A
1	A	2791	G
1	A	2792	A
1	A	2796	C
1	A	2798	U
1	A	2799	G
1	A	2801	G

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Mol	Chain	Res	Type
1	A	2802	A
1	A	2803	G
1	A	2804	U
1	A	2806	C
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2821	A
1	A	2823	A
1	A	2836	U
1	A	2854	G
1	A	2859	G
1	A	2861	U
1	A	2867	G
1	A	2868	A
1	A	2871	U
1	A	2872	A
1	A	2873	A
1	A	2880	C
1	A	2883	A
1	A	2884	U
1	A	2886	A
1	A	2887	A
1	A	2888	C
1	A	2894	G
1	A	2898	U
1	A	2901	C
1	A	2902	C
1	A	2903	U
2	B	4	C
2	B	5	U
2	B	12	C
2	B	13	G
2	B	17	C
2	B	21	G
2	B	22	U
2	B	25	U
2	B	30	C
2	B	32	U
2	B	33	G
2	B	35	C
2	B	41	G

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Mol	Chain	Res	Type
2	B	42	C
2	B	44	G
2	B	53	A
2	B	54	G
2	B	56	G
2	B	57	A
2	B	58	A
2	B	63	C
2	B	67	G
2	B	89	U
2	B	90	C
2	B	102	G
2	B	105	G
2	B	108	A
2	B	109	A
2	B	118	C
34	a	2	A
34	a	3	A
34	a	4	U
34	a	5	U
34	a	6	G
34	a	7	A
34	a	9	G
34	a	32	A
34	a	38	G
34	a	39	G
34	a	45	G
34	a	47	C
34	a	48	C
34	a	49	U
34	a	51	A
34	a	64	G
34	a	66	A
34	a	68	G
34	a	69	G
34	a	70	U
34	a	71	A
34	a	72	A
34	a	73	C
34	a	76	G
34	a	77	A
34	a	78	A

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Mol	Chain	Res	Type
34	a	79	G
34	a	80	A
34	a	83	C
34	a	85	U
34	a	86	G
34	a	87	C
34	a	89	U
34	a	94	G
34	a	95	C
34	a	96	U
34	a	97	G
34	a	99	C
34	a	100	G
34	a	105	G
34	a	107	G
34	a	109	A
34	a	115	G
34	a	121	U
34	a	128	G
34	a	130	A
34	a	131	A
34	a	141	G
34	a	142	G
34	a	143	A
34	a	146	G
34	a	147	G
34	a	149	A
34	a	151	A
34	a	154	U
34	a	161	A
34	a	162	A
34	a	165	G
34	a	167	A
34	a	173	U
34	a	181	A
34	a	182	A
34	a	183	C
34	a	184	G
34	a	185	U
34	a	186	C
34	a	189	A
34	a	190	A

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Mol	Chain	Res	Type
34	a	191	G
34	a	197	A
34	a	202	G
34	a	203	G
34	a	207	C
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	215	C
34	a	216	U
34	a	218	U
34	a	222	C
34	a	224	U
34	a	226	G
34	a	227	G
34	a	230	G
34	a	240	G
34	a	245	U
34	a	246	A
34	a	247	G
34	a	251	G
34	a	254	G
34	a	259	G
34	a	266	G
34	a	267	C
34	a	279	A
34	a	280	C
34	a	281	G
34	a	289	G
34	a	300	A
34	a	305	G
34	a	306	A
34	a	317	U
34	a	321	A
34	a	325	A
34	a	326	G
34	a	328	C
34	a	329	A
34	a	330	C
34	a	333	U
34	a	339	C

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Mol	Chain	Res	Type
34	a	341	C
34	a	343	U
34	a	345	C
34	a	346	G
34	a	347	G
34	a	348	G
34	a	349	A
34	a	351	G
34	a	352	C
34	a	354	G
34	a	365	U
34	a	367	U
34	a	372	C
34	a	373	A
34	a	376	G
34	a	381	C
34	a	390	U
34	a	392	C
34	a	396	C
34	a	397	A
34	a	398	U
34	a	399	G
34	a	404	G
34	a	405	U
34	a	406	G
34	a	411	A
34	a	412	A
34	a	413	G
34	a	422	C
34	a	424	G
34	a	425	G
34	a	429	U
34	a	434	U
34	a	436	C
34	a	437	U
34	a	442	G
34	a	444	G
34	a	445	G
34	a	446	G
34	a	447	G
34	a	454	G
34	a	455	G

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Mol	Chain	Res	Type
34	a	457	G
34	a	458	U
34	a	459	A
34	a	461	A
34	a	462	G
34	a	467	U
34	a	468	A
34	a	470	C
34	a	474	G
34	a	475	C
34	a	476	U
34	a	484	G
34	a	485	U
34	a	486	U
34	a	493	A
34	a	496	A
34	a	499	A
34	a	504	C
34	a	509	A
34	a	514	C
34	a	518	C
34	a	521	G
34	a	524	G
34	a	525	C
34	a	527	7MG
34	a	542	G
34	a	545	C
34	a	546	A
34	a	547	A
34	a	550	G
34	a	565	U
34	a	572	A
34	a	573	A
34	a	575	G
34	a	576	C
34	a	577	G
34	a	579	A
34	a	592	G
34	a	596	A
34	a	615	G
34	a	633	G
34	a	638	U

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Mol	Chain	Res	Type
34	a	639	G
34	a	642	A
34	a	648	A
34	a	649	A
34	a	650	G
34	a	653	U
34	a	654	G
34	a	661	G
34	a	665	A
34	a	671	G
34	a	687	A
34	a	695	A
34	a	700	G
34	a	701	U
34	a	703	G
34	a	704	A
34	a	721	G
34	a	722	G
34	a	723	U
34	a	724	G
34	a	731	G
34	a	737	C
34	a	742	G
34	a	748	G
34	a	754	C
34	a	755	G
34	a	774	G
34	a	777	A
34	a	793	U
34	a	794	A
34	a	802	A
34	a	815	A
34	a	817	C
34	a	818	G
34	a	819	A
34	a	832	G
34	a	836	G
34	a	838	G
34	a	840	C
34	a	843	U
34	a	844	G
34	a	845	A

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Mol	Chain	Res	Type
34	a	846	G
34	a	849	G
34	a	851	G
34	a	871	U
34	a	872	A
34	a	902	G
34	a	914	A
34	a	926	G
34	a	934	C
34	a	935	A
34	a	939	G
34	a	960	U
34	a	961	U
34	a	965	U
34	a	966	2MG
34	a	969	A
34	a	971	G
34	a	974	A
34	a	975	A
34	a	976	G
34	a	977	A
34	a	982	U
34	a	984	C
34	a	989	U
34	a	991	U
34	a	992	U
34	a	993	G
34	a	998	C
34	a	999	C
34	a	1001	C
34	a	1003	G
34	a	1004	A
34	a	1006	G
34	a	1016	A
34	a	1020	G
34	a	1027	C
34	a	1028	C
34	a	1030	U
34	a	1031	C
34	a	1033	G
34	a	1034	G
34	a	1035	A

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Mol	Chain	Res	Type
34	a	1043	G
34	a	1044	A
34	a	1045	C
34	a	1053	G
34	a	1065	U
34	a	1070	U
34	a	1089	G
34	a	1094	G
34	a	1095	U
34	a	1100	C
34	a	1101	A
34	a	1113	C
34	a	1124	G
34	a	1125	U
34	a	1132	C
34	a	1133	G
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1142	G
34	a	1143	G
34	a	1146	A
34	a	1151	A
34	a	1152	A
34	a	1154	G
34	a	1155	A
34	a	1158	C
34	a	1159	U
34	a	1163	A
34	a	1168	U
34	a	1169	A
34	a	1170	A
34	a	1171	A
34	a	1174	G
34	a	1176	A
34	a	1178	G
34	a	1182	G
34	a	1184	G
34	a	1191	A
34	a	1196	A

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Mol	Chain	Res	Type
34	a	1197	A
34	a	1201	A
34	a	1202	U
34	a	1207	2MG
34	a	1209	C
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1217	C
34	a	1219	A
34	a	1220	G
34	a	1225	A
34	a	1226	C
34	a	1227	A
34	a	1228	C
34	a	1238	A
34	a	1240	U
34	a	1241	G
34	a	1247	U
34	a	1249	C
34	a	1250	A
34	a	1256	A
34	a	1258	G
34	a	1260	G
34	a	1261	A
34	a	1263	C
34	a	1264	U
34	a	1265	C
34	a	1266	G
34	a	1269	A
34	a	1273	C
34	a	1274	A
34	a	1275	A
34	a	1278	G
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1291	U
34	a	1293	C

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Mol	Chain	Res	Type
34	a	1294	G
34	a	1297	G
34	a	1298	U
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1304	G
34	a	1305	G
34	a	1306	A
34	a	1312	G
34	a	1317	C
34	a	1320	C
34	a	1321	U
34	a	1332	A
34	a	1338	G
34	a	1339	A
34	a	1340	A
34	a	1345	U
34	a	1346	A
34	a	1348	U
34	a	1360	A
34	a	1363	A
34	a	1364	U
34	a	1368	A
34	a	1371	G
34	a	1372	U
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1400	C
34	a	1415	G
34	a	1419	G
34	a	1429	A
34	a	1433	A
34	a	1434	A
34	a	1441	A
34	a	1442	G
34	a	1445	U
34	a	1446	A

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Mol	Chain	Res	Type
34	a	1447	A
34	a	1448	C
34	a	1450	U
34	a	1452	C
34	a	1454	G
34	a	1455	G
34	a	1475	G
34	a	1487	G
34	a	1492	A
34	a	1497	G
34	a	1502	A
34	a	1503	A
34	a	1505	G
34	a	1506	U
34	a	1517	G
34	a	1529	G
34	a	1530	G
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1537	U
34	a	1539	C
55	v	4	G
55	v	6	G
55	v	7	4SU
55	v	8	G
55	v	13	A
55	v	15	C
55	v	17	U
55	v	18	G
55	v	20	H2U
55	v	21	A
55	v	22	G
55	v	47	U
55	v	52	G
55	v	60	U
55	v	61	C
55	v	63	G
55	v	64	G
55	v	65	C
55	v	70	G
55	v	72	A

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Mol	Chain	Res	Type
55	v	76	A
55	w	3	C
55	w	5	G
55	w	6	G
55	w	8	4SU
55	w	9	G
55	w	14	A
55	w	16	C
55	w	17	C
55	w	117	U
55	w	18	G
55	w	19	G
55	w	20	H2U
55	w	21	A
55	w	22	G
55	w	24	U
55	w	25	C
55	w	28	C
55	w	30	G
55	w	31	G
55	w	33	U
55	w	36	U
55	w	37	A
55	w	38	A
55	w	42	G
55	w	48	C
55	w	49	G
55	w	56	C
55	w	57	A
55	w	59	A
55	w	64	G
55	w	67	C
55	w	70	G
55	w	72	A
55	w	73	A
55	w	74	C
55	w	76	A
56	x	24	G
57	y	3	C
57	y	5	G
57	y	8	4SU
57	y	9	A

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Mol	Chain	Res	Type
57	y	10	G
57	y	11	C
57	y	16	H2U
57	y	17	C
57	y	18	G
57	y	20	H2U
57	y	21	A
57	y	24	G
57	y	31	A
57	y	33	U
57	y	36	A
57	y	44	G
57	y	45	U
57	y	46	7MG
57	y	47	U
57	y	48	C
57	y	52	G
57	y	59	U
57	y	61	C
57	y	65	G
57	y	68	C
57	y	69	G
57	y	72	C
57	y	75	C

All (81) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	97	C
1	A	141	G
1	A	162	U
1	A	163	C
1	A	177	G
1	A	182	A
1	A	199	A
1	A	204	A
1	A	231	A
1	A	242	G
1	A	265	A
1	A	278	A
1	A	282	A

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Mol	Chain	Res	Type
1	A	301	G
1	A	322	A
1	A	353	C
1	A	361	G
1	A	403	U
1	A	503	A
1	A	527	C
1	A	555	G
1	A	616	A
1	A	645	C
1	A	652	U
1	A	746	PSU
1	A	764	A
1	A	774	G
1	A	776	G
1	A	784	G
1	A	859	G
1	A	884	U
1	A	1020	A
1	A	1022	G
1	A	1046	A
1	A	1070	A
1	A	1089	A
1	A	1111	A
1	A	1124	G
1	A	1130	U
1	A	1132	U
1	A	1140	C
1	A	1141	U
1	A	1175	A
1	A	1178	C
1	A	1190	G
1	A	1240	U
1	A	1378	A
1	A	1399	C
1	A	1432	G
1	A	1452	G
1	A	1454	C
1	A	1458	U
1	A	1459	G
1	A	1475	G
1	A	1493	C

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Mol	Chain	Res	Type
1	A	1555	G
1	A	1558	C
1	A	1608	A
1	A	1647	U
1	A	1729	U
1	A	1730	U
1	A	1818	U
1	A	1857	G
1	A	1900	A
1	A	1918	A
1	A	1939	5MU
1	A	1940	U
1	A	1976	U
1	A	2296	U
1	A	2333	A
1	A	2391	G
1	A	2407	A
1	A	2566	A
1	A	2585	U
1	A	2712	C
1	A	2798	U
1	A	2873	A
2	B	34	A
2	B	56	G
2	B	66	A

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

52 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	$\#\|Z\| > 2$
55	PSU	v	55	55	18,21,22	1.30	3 (16%)	22,30,33	1.87	5 (22%)
57	H2U	y	20	57	18,21,22	0.84	1 (5%)	21,30,33	1.56	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	PSU	A	2457	1,59	18,21,22	1.51	3 (16%)	22,30,33	1.94	5 (22%)
34	MA6	a	1518	34	19,26,27	1.29	2 (10%)	18,38,41	1.81	4 (22%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	28,32,35	2.04	10 (35%)
1	2MG	A	1835	1	18,26,27	1.03	2 (11%)	16,38,41	1.22	2 (12%)
57	PSU	y	55	57	18,21,22	1.37	2 (11%)	22,30,33	1.93	5 (22%)
34	MA6	a	1519	34,59	19,26,27	1.17	2 (10%)	18,38,41	1.78	3 (16%)
34	2MG	a	1207	34	18,26,27	0.94	0	16,38,41	1.27	3 (18%)
55	H2U	v	20	55	18,21,22	0.81	1 (5%)	21,30,33	1.70	3 (14%)
1	H2U	A	2449	1	18,21,22	1.10	2 (11%)	21,30,33	1.67	5 (23%)
34	5MC	a	967	34	18,22,23	1.02	1 (5%)	26,32,35	1.38	4 (15%)
34	2MG	a	966	34	18,26,27	1.04	2 (11%)	16,38,41	1.35	3 (18%)
57	MIA	y	37	57	24,31,32	2.23	4 (16%)	26,44,47	2.55	11 (42%)
1	PSU	A	1911	1	18,21,22	1.39	2 (11%)	22,30,33	1.98	4 (18%)
57	PSU	y	39	57	18,21,22	1.42	2 (11%)	22,30,33	1.80	4 (18%)
1	2MA	A	2503	1,59	17,25,26	1.01	1 (5%)	17,37,40	1.27	3 (17%)
1	OMG	A	2251	1,55,59	18,26,27	1.05	1 (5%)	19,38,41	1.00	1 (5%)
57	PSU	y	32	57	18,21,22	1.32	2 (11%)	22,30,33	2.04	5 (22%)
1	7MG	A	2069	1,59	22,26,27	1.51	4 (18%)	29,39,42	2.42	9 (31%)
55	5MU	v	54	55	19,22,23	1.45	5 (26%)	28,32,35	1.94	8 (28%)
55	H2U	w	20	55	18,21,22	0.81	0	21,30,33	1.75	3 (14%)
1	OMU	A	2552	1,59	19,22,23	1.31	3 (15%)	26,31,34	2.07	8 (30%)
34	5MC	a	1407	34	18,22,23	0.97	1 (5%)	26,32,35	1.53	4 (15%)
1	PSU	A	746	1,59	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	A	2604	1	18,21,22	1.34	2 (11%)	22,30,33	1.73	4 (18%)
57	4SU	y	8	57	18,21,22	1.75	5 (27%)	26,30,33	2.28	7 (26%)
57	7MG	y	46	57	22,26,27	1.42	4 (18%)	29,39,42	2.39	7 (24%)
1	5MU	A	1939	1	19,22,23	1.35	4 (21%)	28,32,35	2.00	8 (28%)
1	6MZ	A	2030	1,59	18,25,26	1.02	1 (5%)	16,36,39	2.29	5 (31%)
1	PSU	A	2580	1	18,21,22	1.45	3 (16%)	22,30,33	1.88	5 (22%)
34	2MG	a	1516	34	18,26,27	0.95	0	16,38,41	1.13	2 (12%)
55	PSU	w	55	55	18,21,22	1.30	2 (11%)	22,30,33	1.90	5 (22%)
57	5MU	y	54	57	19,22,23	1.41	4 (21%)	28,32,35	2.03	8 (28%)
1	PSU	A	1917	1	18,21,22	1.42	2 (11%)	22,30,33	1.85	5 (22%)
1	OMC	A	2498	1,59	19,22,23	0.86	1 (5%)	26,31,34	1.33	4 (15%)
1	PSU	A	2504	1	18,21,22	1.41	2 (11%)	22,30,33	1.92	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	3TD	A	1915	1	18,22,23	7.23	14 (77%)	22,32,35	1.78	4 (18%)
34	PSU	a	516	34	18,21,22	1.34	2 (11%)	22,30,33	1.98	5 (22%)
1	5MC	A	747	1	18,22,23	0.99	2 (11%)	26,32,35	1.50	4 (15%)
55	4SU	v	7	55	18,21,22	1.71	5 (27%)	26,30,33	2.38	7 (26%)
34	7MG	a	527	34	22,26,27	1.46	4 (18%)	29,39,42	2.45	8 (27%)
1	PSU	A	2605	1	18,21,22	1.39	2 (11%)	22,30,33	1.88	4 (18%)
1	2MG	A	2445	1,59	18,26,27	1.05	1 (5%)	16,38,41	1.13	1 (6%)
55	4SU	w	8	55	18,21,22	1.73	5 (27%)	26,30,33	2.16	6 (23%)
57	H2U	y	16	57	18,21,22	0.81	1 (5%)	21,30,33	1.50	4 (19%)
34	4OC	a	1402	34	20,23,24	0.80	0	26,32,35	1.31	4 (15%)
34	UR3	a	1498	34	19,22,23	1.10	2 (10%)	26,32,35	1.66	4 (15%)
1	6MZ	A	1618	1	18,25,26	0.92	1 (5%)	16,36,39	2.58	6 (37%)
1	PSU	A	955	1	18,21,22	1.41	3 (16%)	22,30,33	1.93	4 (18%)
1	1MG	A	745	1	18,26,27	0.95	0	19,39,42	1.46	3 (15%)
1	5MC	A	1962	1	18,22,23	1.00	1 (5%)	26,32,35	1.45	3 (11%)

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	PSU	v	55	55	-	2/7/25/26	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
1	PSU	A	2457	1,59	-	2/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	2/7/29/30	0/3/3/3
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
34	MA6	a	1519	34,59	-	3/7/29/30	0/3/3/3
34	2MG	a	1207	34	-	1/5/27/28	0/3/3/3
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
57	MIA	y	37	57	-	3/11/33/34	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
1	2MA	A	2503	1,59	-	2/3/25/26	0/3/3/3
1	OMG	A	2251	1,55,59	-	0/5/27/28	0/3/3/3
57	PSU	y	32	57	-	0/7/25/26	0/2/2/2
1	7MG	A	2069	1,59	-	3/7/37/38	0/3/3/3
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
55	H2U	w	20	55	-	2/7/38/39	0/2/2/2
1	OMU	A	2552	1,59	-	2/9/27/28	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	PSU	A	746	1,59	-	1/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
57	4SU	y	8	57	-	2/7/25/26	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	5MU	A	1939	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1,59	-	3/5/27/28	0/3/3/3
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
55	PSU	w	55	55	-	0/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
1	OMC	A	2498	1,59	-	0/9/27/28	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	5/7/25/26	0/2/2/2
34	PSU	a	516	34	-	2/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
34	7MG	a	527	34	-	2/7/37/38	0/3/3/3
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1,59	-	2/5/27/28	0/3/3/3
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	2/5/27/28	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.83	1.66	1.43
1	A	1915	3TD	C2'-C1'	-15.02	1.34	1.53
1	A	1915	3TD	C6-C5	14.81	1.52	1.35
1	A	1915	3TD	C2-N1	8.13	1.47	1.37
57	y	37	MIA	C13-C14	7.39	1.53	1.32
1	A	1915	3TD	O4'-C4'	-5.96	1.31	1.45
1	A	1915	3TD	C2-N3	5.92	1.51	1.38
57	y	37	MIA	C2-S10	-5.61	1.70	1.75
1	A	1915	3TD	C6-N1	5.29	1.45	1.36
1	A	2069	7MG	C4-N9	-4.62	1.32	1.37
57	y	8	4SU	C4-S4	-4.50	1.59	1.68
55	w	8	4SU	C4-S4	-4.44	1.60	1.68
55	v	7	4SU	C4-S4	-4.43	1.60	1.68
57	y	39	PSU	C6-C5	4.19	1.40	1.35
57	y	55	PSU	C6-C5	4.10	1.40	1.35
1	A	2457	PSU	C6-C5	4.05	1.40	1.35
1	A	2605	PSU	C6-C5	3.99	1.40	1.35
34	a	516	PSU	C6-C5	3.96	1.39	1.35
1	A	1917	PSU	C6-C5	3.89	1.39	1.35
1	A	2580	PSU	C6-C5	3.88	1.39	1.35
1	A	1911	PSU	C6-C5	3.84	1.39	1.35
55	w	55	PSU	C6-C5	3.82	1.39	1.35
57	y	32	PSU	C6-C5	3.78	1.39	1.35
55	v	55	PSU	C6-C5	3.75	1.39	1.35
34	a	527	7MG	C4-N9	-3.74	1.33	1.37
1	A	2504	PSU	C6-C5	3.73	1.39	1.35
1	A	746	PSU	C6-C5	3.62	1.39	1.35
1	A	2604	PSU	C6-C5	3.35	1.39	1.35
57	y	46	7MG	C4-N9	-3.30	1.33	1.37
1	A	955	PSU	C6-C5	3.28	1.39	1.35
55	w	54	5MU	C6-C5	3.21	1.39	1.34
55	v	54	5MU	C6-C5	3.18	1.39	1.34
57	y	46	7MG	C5-C4	3.15	1.48	1.38
1	A	1915	3TD	O2'-C2'	3.13	1.50	1.43
1	A	2552	OMU	C2-N1	3.13	1.43	1.38
34	a	967	5MC	C6-C5	3.09	1.39	1.34
55	v	7	4SU	C2-N1	3.04	1.43	1.38
55	w	54	5MU	C2-N1	3.00	1.43	1.38
34	a	527	7MG	C5-C4	3.00	1.47	1.38
1	A	1962	5MC	C6-C5	3.00	1.39	1.34
57	y	8	4SU	C2-N1	2.96	1.43	1.38
34	a	1518	MA6	C5-C4	2.95	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	8	4SU	C2-N1	2.93	1.43	1.38
57	y	54	5MU	C2-N1	2.93	1.43	1.38
57	y	8	4SU	C4-N3	-2.90	1.34	1.37
55	w	8	4SU	C4-N3	-2.88	1.34	1.37
1	A	1939	5MU	C6-C5	2.88	1.39	1.34
34	a	1407	5MC	C6-C5	2.86	1.39	1.34
57	y	54	5MU	C6-C5	2.85	1.39	1.34
1	A	2449	H2U	C4-N3	-2.81	1.32	1.37
55	w	54	5MU	C4-C5	2.77	1.49	1.44
1	A	1915	3TD	C4-N3	2.76	1.46	1.40
1	A	955	PSU	C4-N3	-2.73	1.33	1.38
1	A	2457	PSU	C4-N3	-2.69	1.33	1.38
1	A	2069	7MG	C5-N7	-2.69	1.32	1.35
1	A	2449	H2U	C2-N3	-2.68	1.33	1.38
1	A	1915	3TD	C10-N3	-2.67	1.42	1.47
1	A	2580	PSU	C4-N3	-2.66	1.33	1.38
1	A	955	PSU	C2-N3	-2.64	1.33	1.37
55	v	54	5MU	C4-N3	-2.64	1.33	1.38
1	A	2504	PSU	C4-N3	-2.63	1.34	1.38
1	A	1917	PSU	C4-N3	-2.62	1.34	1.38
1	A	2069	7MG	C5-C4	2.62	1.46	1.38
1	A	2445	2MG	C6-N1	-2.58	1.34	1.37
1	A	2251	OMG	C6-N1	-2.57	1.34	1.37
55	v	7	4SU	C4-N3	-2.55	1.34	1.37
1	A	747	5MC	C6-C5	2.52	1.38	1.34
34	a	1518	MA6	C6-N1	2.50	1.36	1.33
55	v	54	5MU	C4-C5	2.50	1.48	1.44
1	A	1915	3TD	O3'-C3'	-2.50	1.37	1.43
1	A	2030	6MZ	C5-C4	2.48	1.47	1.40
1	A	1915	3TD	O2-C2	-2.46	1.18	1.23
34	a	966	2MG	O4'-C1'	2.46	1.44	1.41
1	A	746	PSU	C4-N3	-2.45	1.34	1.38
1	A	2552	OMU	C4-N3	-2.45	1.34	1.38
57	y	54	5MU	C4-C5	2.44	1.48	1.44
1	A	1835	2MG	C6-N1	-2.44	1.34	1.37
34	a	1519	MA6	C5-C4	2.39	1.47	1.40
57	y	37	MIA	C5-C4	2.38	1.47	1.40
57	y	37	MIA	C6-N1	2.38	1.36	1.32
1	A	2605	PSU	C4-N3	-2.37	1.34	1.38
34	a	1498	UR3	C2-N1	2.36	1.41	1.38
1	A	1915	3TD	C3'-C4'	2.35	1.59	1.53
1	A	1911	PSU	C4-N3	-2.35	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1939	5MU	C4-N3	-2.34	1.34	1.38
55	v	54	5MU	C2-N1	2.32	1.42	1.38
57	y	8	4SU	C5-C4	-2.32	1.39	1.42
1	A	2604	PSU	C4-N3	-2.31	1.34	1.38
55	w	8	4SU	C5-C4	-2.30	1.39	1.42
34	a	516	PSU	C4-N3	-2.29	1.34	1.38
1	A	1939	5MU	C4-C5	2.29	1.48	1.44
57	y	55	PSU	C4-N3	-2.28	1.34	1.38
57	y	39	PSU	C4-N3	-2.27	1.34	1.38
55	w	54	5MU	C4-N3	-2.26	1.34	1.38
57	y	54	5MU	C4-N3	-2.26	1.34	1.38
1	A	747	5MC	C6-N1	-2.25	1.34	1.38
55	w	55	PSU	C4-N3	-2.24	1.34	1.38
55	v	55	PSU	C4-N3	-2.21	1.34	1.38
55	v	7	4SU	C5-C4	-2.18	1.39	1.42
34	a	527	7MG	C8-N9	2.16	1.47	1.46
1	A	1835	2MG	O4'-C1'	2.14	1.44	1.41
34	a	966	2MG	C6-N1	-2.12	1.34	1.37
1	A	2580	PSU	C2-N3	-2.11	1.33	1.37
1	A	2503	2MA	C2-N3	2.11	1.35	1.31
1	A	2552	OMU	C6-C5	2.11	1.39	1.35
34	a	527	7MG	C5-N7	-2.10	1.33	1.35
57	y	32	PSU	C4-N3	-2.10	1.34	1.38
1	A	2069	7MG	C6-N1	-2.09	1.35	1.38
57	y	16	H2U	C2-N3	-2.09	1.34	1.38
55	v	54	5MU	C2-N3	-2.08	1.34	1.38
57	y	46	7MG	C8-N9	2.08	1.47	1.46
34	a	1519	MA6	O4'-C1'	2.08	1.44	1.41
1	A	2498	OMC	C6-C5	2.07	1.39	1.35
57	y	8	4SU	C6-C5	2.07	1.39	1.35
57	y	20	H2U	C2-N3	-2.06	1.34	1.38
1	A	1618	6MZ	C5-C4	2.05	1.46	1.40
1	A	2457	PSU	C2-N3	-2.05	1.34	1.37
55	w	8	4SU	C6-C5	2.04	1.39	1.35
55	v	7	4SU	C6-C5	2.03	1.39	1.35
34	a	1498	UR3	C5-C4	-2.03	1.38	1.43
55	v	55	PSU	C4-C5	2.02	1.49	1.44
55	v	20	H2U	C2-N3	-2.02	1.34	1.38
1	A	1915	3TD	O4-C4	-2.02	1.18	1.23
57	y	46	7MG	C5-C6	2.01	1.48	1.43
1	A	1939	5MU	C6-N1	-2.01	1.34	1.38

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	46	7MG	N9-C4-N3	7.98	137.40	125.47
34	a	527	7MG	N9-C4-N3	7.97	137.39	125.47
1	A	2069	7MG	N9-C4-N3	7.10	136.08	125.47
55	v	7	4SU	C4-N3-C2	-6.81	120.73	127.34
57	y	37	MIA	C12-C13-C14	-6.74	114.03	127.14
1	A	1618	6MZ	C2-N1-C6	6.44	122.11	116.59
57	y	8	4SU	C4-N3-C2	-6.38	121.14	127.34
55	w	8	4SU	C4-N3-C2	-6.23	121.28	127.34
1	A	2030	6MZ	C2-N1-C6	5.97	121.71	116.59
1	A	2504	PSU	N1-C2-N3	5.86	121.77	115.13
1	A	955	PSU	N1-C2-N3	5.81	121.71	115.13
57	y	55	PSU	N1-C2-N3	5.67	121.55	115.13
1	A	746	PSU	N1-C2-N3	5.66	121.54	115.13
55	v	7	4SU	C5-C4-N3	5.65	119.93	114.69
57	y	32	PSU	N1-C2-N3	5.64	121.52	115.13
55	w	55	PSU	N1-C2-N3	5.63	121.51	115.13
1	A	1911	PSU	N1-C2-N3	5.62	121.50	115.13
1	A	2605	PSU	N1-C2-N3	5.53	121.39	115.13
34	a	516	PSU	N1-C2-N3	5.51	121.37	115.13
1	A	2457	PSU	N1-C2-N3	5.50	121.37	115.13
55	v	55	PSU	N1-C2-N3	5.49	121.35	115.13
57	y	39	PSU	N1-C2-N3	5.47	121.33	115.13
34	a	1498	UR3	C4-N3-C2	-5.47	119.41	124.56
55	v	54	5MU	N3-C2-N1	5.40	122.06	114.89
55	w	8	4SU	C5-C4-N3	5.38	119.67	114.69
55	v	20	H2U	O4'-C1'-N1	5.36	116.59	109.30
57	y	8	4SU	C5-C4-N3	5.34	119.65	114.69
1	A	1917	PSU	N1-C2-N3	5.24	121.07	115.13
1	A	2604	PSU	N1-C2-N3	5.17	120.98	115.13
1	A	2580	PSU	N1-C2-N3	5.16	120.97	115.13
57	y	46	7MG	C5-C4-N3	-5.03	118.55	128.13
1	A	1915	3TD	N1-C2-N3	5.02	120.10	116.14
34	a	527	7MG	C5-C4-N3	-5.00	118.60	128.13
1	A	1618	6MZ	C9-N6-C6	-4.90	118.65	122.87
1	A	2069	7MG	C5-C4-N3	-4.90	118.79	128.13
1	A	1915	3TD	C4-N3-C2	-4.85	119.34	124.61
57	y	8	4SU	N3-C2-N1	4.84	121.31	114.89
55	w	54	5MU	N3-C2-N1	4.83	121.31	114.89
1	A	2552	OMU	C4-N3-C2	-4.81	120.23	126.58
57	y	37	MIA	C16-C14-C13	-4.81	108.75	122.65
1	A	2069	7MG	N9-C8-N7	-4.79	96.53	103.38
55	w	20	H2U	O4'-C1'-N1	4.79	115.82	109.30
1	A	1939	5MU	N3-C2-N1	4.78	121.24	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1939	5MU	C4-N3-C2	-4.78	121.17	127.35
55	v	7	4SU	N3-C2-N1	4.69	121.11	114.89
1	A	2069	7MG	C2-N3-C4	4.64	120.57	112.30
1	A	2552	OMU	N3-C2-N1	4.64	121.05	114.89
57	y	46	7MG	C2-N3-C4	4.57	120.44	112.30
57	y	54	5MU	N3-C2-N1	4.55	120.93	114.89
34	a	1519	MA6	C4-C5-N7	-4.52	104.69	109.40
55	w	54	5MU	C4-N3-C2	-4.49	121.54	127.35
34	a	527	7MG	N9-C8-N7	-4.47	96.99	103.38
57	y	46	7MG	N9-C8-N7	-4.46	97.00	103.38
34	a	527	7MG	C2-N3-C4	4.45	120.23	112.30
1	A	747	5MC	CM5-C5-C6	-4.45	116.91	122.85
55	w	8	4SU	N3-C2-N1	4.44	120.79	114.89
57	y	54	5MU	C4-N3-C2	-4.40	121.65	127.35
1	A	2449	H2U	N3-C2-N1	4.36	121.26	116.65
55	v	54	5MU	C4-N3-C2	-4.31	121.77	127.35
57	y	37	MIA	C2-N3-C4	4.30	121.25	115.32
57	y	54	5MU	C5-C4-N3	4.28	118.97	115.31
55	v	7	4SU	C5-C4-S4	-4.20	119.06	124.47
1	A	1939	5MU	C5-C4-N3	4.19	118.89	115.31
55	w	54	5MU	C5-C4-N3	4.15	118.85	115.31
1	A	1911	PSU	O2-C2-N1	-4.12	118.25	122.79
1	A	955	PSU	C4-N3-C2	-4.05	120.50	126.34
34	a	1518	MA6	N3-C2-N1	-4.02	122.40	128.68
55	w	20	H2U	C4-N3-C2	-3.99	122.48	125.79
1	A	1917	PSU	C6-C5-C4	-3.83	115.52	118.20
57	y	54	5MU	O4-C4-C5	-3.83	120.46	124.90
1	A	1962	5MC	CM5-C5-C6	-3.82	117.75	122.85
1	A	2552	OMU	C5-C4-N3	3.82	120.55	114.84
57	y	55	PSU	C4-N3-C2	-3.79	120.89	126.34
1	A	746	PSU	C4-N3-C2	-3.77	120.90	126.34
1	A	2605	PSU	C4-N3-C2	-3.77	120.91	126.34
57	y	37	MIA	C5-C6-N1	-3.77	117.68	120.81
1	A	1911	PSU	C4-N3-C2	-3.74	120.95	126.34
55	v	55	PSU	C4-N3-C2	-3.73	120.97	126.34
34	a	1518	MA6	C3'-C2'-C1'	3.71	106.56	100.98
57	y	39	PSU	O2-C2-N1	-3.70	118.72	122.79
55	w	55	PSU	C4-N3-C2	-3.67	121.06	126.34
1	A	1618	6MZ	N3-C2-N1	-3.60	123.04	128.68
55	v	54	5MU	C5-C4-N3	3.60	118.38	115.31
34	a	516	PSU	C4-N3-C2	-3.60	121.15	126.34
1	A	2504	PSU	C4-N3-C2	-3.60	121.15	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	y	32	PSU	C6-C5-C4	-3.56	115.71	118.20
1	A	2504	PSU	O2-C2-N1	-3.54	118.89	122.79
1	A	746	PSU	O2-C2-N1	-3.53	118.90	122.79
57	y	32	PSU	C4-N3-C2	-3.52	121.27	126.34
1	A	1939	5MU	O4-C4-C5	-3.51	120.83	124.90
34	a	1407	5MC	CM5-C5-C6	-3.50	118.18	122.85
34	a	1498	UR3	C1'-N1-C2	3.49	122.88	116.99
1	A	1911	PSU	C6-C5-C4	-3.49	115.76	118.20
34	a	967	5MC	CM5-C5-C6	-3.45	118.23	122.85
57	y	32	PSU	O2-C2-N1	-3.44	119.00	122.79
57	y	37	MIA	C3'-C2'-C1'	3.44	106.16	100.98
1	A	2030	6MZ	C3'-C2'-C1'	3.43	106.14	100.98
57	y	20	H2U	C4-N3-C2	-3.43	122.95	125.79
57	y	8	4SU	C5-C4-S4	-3.42	120.06	124.47
1	A	2030	6MZ	C9-N6-C6	-3.42	119.93	122.87
1	A	955	PSU	C6-C5-C4	-3.41	115.81	118.20
34	a	1407	5MC	O2-C2-N3	-3.41	116.79	122.33
34	a	1407	5MC	C5-C4-N3	-3.40	118.00	121.67
1	A	2580	PSU	C6-C5-C4	-3.40	115.82	118.20
34	a	1519	MA6	N3-C2-N1	-3.40	123.37	128.68
1	A	2604	PSU	C4-N3-C2	-3.38	121.46	126.34
57	y	16	H2U	C4-N3-C2	-3.36	123.00	125.79
55	v	20	H2U	C4-N3-C2	-3.34	123.02	125.79
1	A	2457	PSU	C6-C5-C4	-3.34	115.86	118.20
1	A	2605	PSU	C6-C5-C4	-3.32	115.88	118.20
55	w	8	4SU	C5-C4-S4	-3.32	120.19	124.47
1	A	745	1MG	O6-C6-C5	-3.31	118.34	124.19
1	A	2457	PSU	O2-C2-N1	-3.30	119.16	122.79
1	A	2457	PSU	C4-N3-C2	-3.26	121.64	126.34
57	y	37	MIA	C15-C14-C13	-3.25	113.26	122.65
1	A	2552	OMU	O4-C4-C5	-3.24	119.47	125.16
57	y	55	PSU	O2-C2-N1	-3.24	119.23	122.79
1	A	747	5MC	C5-C4-N3	-3.23	118.19	121.67
57	y	20	H2U	O4'-C1'-N1	3.22	113.69	109.30
55	w	55	PSU	O2-C2-N1	-3.21	119.25	122.79
1	A	2580	PSU	C4-N3-C2	-3.20	121.72	126.34
57	y	54	5MU	C5M-C5-C4	3.20	122.29	118.77
57	y	32	PSU	C3'-C2'-C1'	3.18	105.34	101.64
55	w	54	5MU	C5M-C5-C4	3.18	122.27	118.77
1	A	2030	6MZ	N3-C2-N1	-3.14	123.76	128.68
1	A	1962	5MC	O2-C2-N3	-3.14	117.22	122.33
57	y	37	MIA	C2-N1-C6	3.13	122.80	117.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2498	OMC	O2-C2-N3	-3.13	117.24	122.33
34	a	516	PSU	C3'-C2'-C1'	3.12	105.27	101.64
1	A	1917	PSU	O2-C2-N1	-3.11	119.36	122.79
1	A	1962	5MC	C5-C4-N3	-3.09	118.34	121.67
1	A	2552	OMU	C1'-N1-C2	3.08	123.15	117.57
55	w	54	5MU	O4-C4-C5	-3.00	121.43	124.90
34	a	527	7MG	C5-C6-N1	3.00	116.27	110.99
1	A	745	1MG	C5-C6-N1	2.99	118.40	113.90
55	v	55	PSU	C6-C5-C4	-2.99	116.11	118.20
57	y	46	7MG	C5-C6-N1	2.98	116.24	110.99
57	y	39	PSU	C4-N3-C2	-2.97	122.06	126.34
1	A	2449	H2U	C5-C4-N3	2.96	119.98	116.65
57	y	8	4SU	C6-N1-C2	-2.96	117.21	120.99
1	A	2580	PSU	C3'-C2'-C1'	2.94	105.07	101.64
1	A	2449	H2U	O4'-C1'-N1	2.92	113.28	109.30
1	A	1917	PSU	C4-N3-C2	-2.91	122.14	126.34
1	A	2069	7MG	C5-C6-N1	2.91	116.12	110.99
55	w	55	PSU	C3'-C2'-C1'	2.91	105.02	101.64
57	y	37	MIA	N3-C2-N1	-2.91	121.63	126.98
1	A	1915	3TD	C10-N3-C4	2.89	122.12	117.69
1	A	2552	OMU	C2'-C1'-N1	-2.88	108.64	114.22
34	a	516	PSU	O2-C2-N1	-2.88	119.62	122.79
34	a	1518	MA6	C4-C5-N7	-2.87	106.41	109.40
1	A	2504	PSU	C6-C5-C4	-2.87	116.19	118.20
34	a	516	PSU	C6-C5-C4	-2.87	116.19	118.20
34	a	1207	2MG	C5-C6-N1	2.86	119.00	113.95
34	a	967	5MC	O2-C2-N3	-2.85	117.69	122.33
34	a	966	2MG	C5-C6-N1	2.84	118.97	113.95
57	y	39	PSU	C6-C5-C4	-2.84	116.21	118.20
1	A	1939	5MU	C5-C6-N1	-2.84	120.42	123.34
34	a	967	5MC	C5-C4-N3	-2.83	118.62	121.67
34	a	1402	4OC	C6-C5-C4	2.82	120.42	116.96
1	A	1618	6MZ	C4-C5-N7	-2.81	106.47	109.40
1	A	1618	6MZ	C3'-C2'-C1'	2.79	105.18	100.98
55	v	55	PSU	O2-C2-N1	-2.76	119.75	122.79
57	y	55	PSU	C6-C5-C4	-2.75	116.27	118.20
1	A	747	5MC	C5-C6-N1	-2.74	120.52	123.34
1	A	2604	PSU	C6-C5-C4	-2.74	116.28	118.20
1	A	2449	H2U	C4-N3-C2	-2.74	123.52	125.79
1	A	2030	6MZ	C4-C5-N7	-2.73	106.55	109.40
1	A	2605	PSU	O2-C2-N1	-2.68	119.83	122.79
55	v	54	5MU	O4-C4-C5	-2.67	121.81	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	20	H2U	C5-C6-N1	-2.64	102.92	111.61
1	A	2445	2MG	C5-C6-N1	2.63	118.60	113.95
55	v	54	5MU	C6-N1-C2	-2.62	118.65	121.30
34	a	1402	4OC	O4'-C1'-N1	2.61	114.32	108.36
1	A	1939	5MU	O2-C2-N1	-2.60	119.33	122.79
57	y	20	H2U	C5-C4-N3	2.60	119.57	116.65
1	A	1835	2MG	C5-C6-N1	2.59	118.53	113.95
57	y	16	H2U	O4'-C1'-N1	2.58	112.82	109.30
1	A	955	PSU	O2-C2-N1	-2.58	119.95	122.79
1	A	2503	2MA	C3'-C2'-C1'	2.58	104.86	100.98
34	a	1519	MA6	C10-N6-C6	-2.57	111.73	119.51
1	A	2604	PSU	O2-C2-N1	-2.56	119.97	122.79
34	a	966	2MG	C8-N7-C5	2.55	107.85	102.99
34	a	1518	MA6	C9-N6-C6	-2.53	111.85	119.51
57	y	55	PSU	C3'-C2'-C1'	2.53	104.58	101.64
1	A	2457	PSU	C3'-C2'-C1'	2.52	104.58	101.64
1	A	2552	OMU	O4'-C1'-N1	2.51	114.09	108.36
34	a	1207	2MG	C8-N7-C5	2.50	107.76	102.99
55	v	20	H2U	C5-C4-N3	2.50	119.46	116.65
1	A	747	5MC	O2-C2-N3	-2.50	118.27	122.33
57	y	16	H2U	C5-C4-N3	2.49	119.45	116.65
55	v	54	5MU	C5M-C5-C4	2.44	121.46	118.77
57	y	37	MIA	C4-C5-N7	-2.44	106.85	109.40
1	A	1939	5MU	C5M-C5-C4	2.44	121.45	118.77
1	A	1917	PSU	C3'-C2'-C1'	2.43	104.47	101.64
55	w	55	PSU	C6-C5-C4	-2.43	116.50	118.20
1	A	1915	3TD	C3'-C2'-C1'	2.43	104.47	101.64
34	a	1402	4OC	C5-C4-N3	-2.43	118.69	122.59
34	a	1516	2MG	C5-C6-N1	2.42	118.22	113.95
55	w	8	4SU	C6-N1-C2	-2.41	117.91	120.99
1	A	2580	PSU	O2-C2-N1	-2.39	120.16	122.79
55	v	7	4SU	C6-N1-C2	-2.38	117.95	120.99
55	w	54	5MU	C3'-C2'-C1'	2.37	105.93	101.43
1	A	2498	OMC	O4'-C1'-N1	2.37	113.78	108.36
57	y	8	4SU	O2-C2-N3	-2.37	117.09	121.50
34	a	527	7MG	O4'-C1'-N9	2.35	112.50	109.30
1	A	2552	OMU	O2-C2-N3	-2.35	117.12	121.50
34	a	527	7MG	O6-C6-C5	-2.34	121.80	127.54
1	A	2503	2MA	C5-C6-N1	2.34	118.05	114.02
34	a	1516	2MG	C8-N7-C5	2.34	107.44	102.99
34	a	527	7MG	CM7-N7-C5	2.33	132.43	126.40
34	a	1402	4OC	O2-C2-N3	-2.33	118.54	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1498	UR3	C3U-N3-C2	2.33	121.40	117.31
1	A	2069	7MG	N2-C2-N3	-2.33	115.20	119.73
55	v	55	PSU	C3'-C2'-C1'	2.32	104.34	101.64
57	y	46	7MG	CM7-N7-C5	2.32	132.38	126.40
1	A	745	1MG	C8-N7-C5	2.32	107.40	102.99
55	w	54	5MU	C5-C6-N1	-2.31	120.96	123.34
55	w	54	5MU	C5M-C5-C6	-2.31	119.76	122.85
55	w	54	5MU	O4'-C1'-N1	2.31	113.65	108.36
1	A	2503	2MA	C8-N7-C5	2.30	107.37	102.99
57	y	16	H2U	C3'-C2'-C1'	2.29	105.78	101.43
57	y	20	H2U	C3'-C2'-C1'	2.26	105.71	101.43
34	a	1207	2MG	O6-C6-C5	-2.24	119.99	124.37
1	A	1939	5MU	O4'-C1'-N1	2.24	113.48	108.36
57	y	37	MIA	C16-C14-C15	-2.23	109.67	114.60
1	A	2069	7MG	N2-C2-N1	2.23	121.45	116.71
1	A	2251	OMG	C5-C6-N1	2.22	117.87	113.95
1	A	2069	7MG	O6-C6-C5	-2.22	122.11	127.54
55	v	54	5MU	C5-C6-N1	-2.20	121.08	123.34
1	A	2498	OMC	C2'-C1'-N1	-2.18	109.98	114.22
1	A	1618	6MZ	C1'-N9-C4	-2.16	122.84	126.64
34	a	1498	UR3	C6-N1-C2	-2.13	119.88	121.79
55	v	7	4SU	O2-C2-N3	-2.13	117.54	121.50
57	y	37	MIA	C11-S10-C2	2.12	103.85	102.27
57	y	54	5MU	C5M-C5-C6	-2.10	120.04	122.85
55	w	54	5MU	O2-C2-N3	-2.10	117.60	121.50
57	y	46	7MG	O6-C6-C5	-2.10	122.40	127.54
1	A	2449	H2U	O2-C2-N1	-2.09	120.49	123.11
1	A	1835	2MG	C8-N7-C5	2.07	106.94	102.99
1	A	2069	7MG	O4'-C1'-N9	2.07	112.12	109.30
55	v	7	4SU	O4'-C1'-N1	2.06	113.07	108.36
57	y	54	5MU	C1'-N1-C2	2.06	121.29	117.57
57	y	8	4SU	C1'-N1-C2	2.06	121.29	117.57
34	a	1407	5MC	O4'-C1'-N1	2.05	113.05	108.36
57	y	54	5MU	C6-N1-C2	-2.05	119.22	121.30
34	a	966	2MG	C3'-C2'-C1'	2.01	104.01	100.98
55	w	8	4SU	O2-C2-N3	-2.01	117.75	121.50
34	a	967	5MC	C5-C6-N1	-2.01	121.27	123.34
1	A	2498	OMC	C6-C5-C4	2.01	120.74	117.50
55	v	54	5MU	O2-C2-N3	-2.01	117.76	121.50

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1618	6MZ	O4'-C4'-C5'-O5'
1	A	1618	6MZ	C3'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	C2'-C1'-C5-C6
1	A	1915	3TD	O4'-C1'-C5-C6
1	A	1915	3TD	C3'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C4'-C5'-O5'
1	A	1917	PSU	O4'-C4'-C5'-O5'
1	A	1962	5MC	O4'-C4'-C5'-O5'
1	A	1962	5MC	C3'-C4'-C5'-O5'
1	A	2030	6MZ	C4'-C5'-O5'-P
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2069	7MG	C3'-C4'-C5'-O5'
1	A	2445	2MG	O4'-C4'-C5'-O5'
1	A	2445	2MG	C3'-C4'-C5'-O5'
1	A	2552	OMU	O4'-C1'-N1-C2
1	A	2552	OMU	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C2
34	a	1518	MA6	C5-C6-N6-C9
34	a	1519	MA6	C5-C6-N6-C10
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
55	w	8	4SU	C3'-C4'-C5'-O5'
55	w	8	4SU	O4'-C4'-C5'-O5'
57	y	20	H2U	O4'-C1'-N1-C2
57	y	20	H2U	O4'-C1'-N1-C6
57	y	37	MIA	O4'-C4'-C5'-O5'
57	y	37	MIA	C3'-C4'-C5'-O5'
57	y	37	MIA	C12-C13-C14-C15
57	y	46	7MG	O4'-C4'-C5'-O5'
1	A	1917	PSU	C3'-C4'-C5'-O5'
34	a	966	2MG	C3'-C4'-C5'-O5'
55	v	7	4SU	O4'-C4'-C5'-O5'
57	y	46	7MG	C3'-C4'-C5'-O5'
1	A	2030	6MZ	O4'-C4'-C5'-O5'
34	a	966	2MG	O4'-C4'-C5'-O5'
34	a	1402	4OC	O4'-C4'-C5'-O5'
55	v	7	4SU	C3'-C4'-C5'-O5'
34	a	1518	MA6	N1-C6-N6-C9
34	a	1519	MA6	N1-C6-N6-C10
55	w	8	4SU	C2'-C1'-N1-C6
34	a	1402	4OC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	2069	7MG	O4'-C4'-C5'-O5'
1	A	2503	2MA	O4'-C4'-C5'-O5'
57	y	16	H2U	O4'-C4'-C5'-O5'
57	y	16	H2U	C3'-C4'-C5'-O5'
34	a	966	2MG	C4'-C5'-O5'-P
1	A	2457	PSU	O4'-C4'-C5'-O5'
34	a	527	7MG	C3'-C4'-C5'-O5'
55	w	8	4SU	C2'-C1'-N1-C2
57	y	46	7MG	C2'-C1'-N9-C8
1	A	2504	PSU	O4'-C4'-C5'-O5'
55	w	8	4SU	O4'-C1'-N1-C6
1	A	2503	2MA	C3'-C4'-C5'-O5'
34	a	527	7MG	C4'-C5'-O5'-P
55	w	8	4SU	O4'-C1'-N1-C2
34	a	1207	2MG	C3'-C4'-C5'-O5'
1	A	2457	PSU	C3'-C4'-C5'-O5'
34	a	1519	MA6	C4'-C5'-O5'-P
34	a	516	PSU	O4'-C1'-C5-C4
57	y	46	7MG	O4'-C1'-N9-C8
1	A	2504	PSU	C3'-C4'-C5'-O5'
57	y	8	4SU	C2'-C1'-N1-C2
55	w	20	H2U	C2'-C1'-N1-C6
1	A	746	PSU	O4'-C1'-C5-C6
34	a	516	PSU	O4'-C1'-C5-C6
57	y	8	4SU	O4'-C4'-C5'-O5'
55	w	20	H2U	C2'-C1'-N1-C2
1	A	2069	7MG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1622 ligands modelled in this entry, 1619 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	**Type**	**Chain**	**Res**	**Link**	**Bond lengths**			**Bond angles**		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
62	PHE	z	401	-	10,11,12	0.43	0	10,13,15	0.31	0
61	FME	v	101	-	8,9,10	0.62	0	7,9,11	1.92	2 (28%)
63	GNP	z	402	59	29,34,34	2.57	7 (24%)	33,54,54	2.05	9 (27%)

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**
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1
61	FME	v	101	-	-	2/7/9/11	-
63	GNP	z	402	59	-	6/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(Å)**	**Ideal(Å)**
63	z	402	GNP	PG-O1G	9.60	1.61	1.46
63	z	402	GNP	C5-C6	4.49	1.49	1.41
63	z	402	GNP	PG-N3B	4.48	1.75	1.63
63	z	402	GNP	PB-N3B	4.47	1.75	1.63
63	z	402	GNP	PG-O3G	-3.12	1.48	1.56
63	z	402	GNP	C5-C4	2.54	1.47	1.40
63	z	402	GNP	PB-O3A	2.22	1.61	1.59

All (11) bond angle outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(^{o})**	**Ideal(^{o})**
63	z	402	GNP	C2-N3-C4	5.22	121.32	115.36
63	z	402	GNP	C4-C5-C6	-4.20	116.78	120.80
63	z	402	GNP	C2-N1-C6	3.81	121.98	115.93
61	v	101	FME	C-CA-N	3.77	116.53	109.73
63	z	402	GNP	N3-C2-N1	-3.58	122.44	127.22
63	z	402	GNP	PB-O3A-PA	-3.57	120.04	132.62
63	z	402	GNP	C5-C6-N1	-3.44	118.72	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	z	402	GNP	C4-C5-N7	-2.59	106.70	109.40
63	z	402	GNP	O1B-PB-N3B	-2.50	108.10	111.77
63	z	402	GNP	O3A-PB-N3B	2.25	112.83	106.59
61	v	101	FME	O1-CN-N	-2.12	119.69	125.27

There are no chirality outliers.

All (9) torsion outliers are listed below:

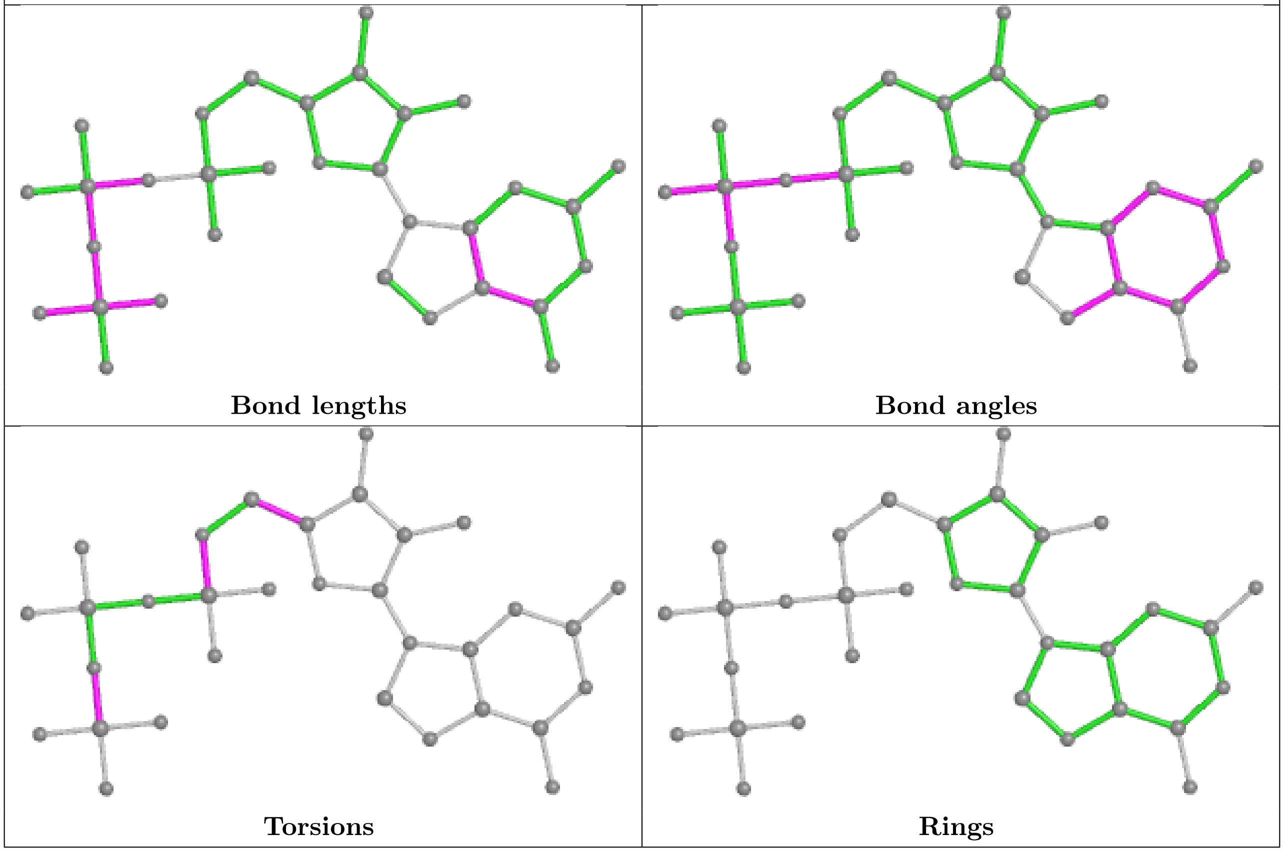
Mol	Chain	Res	Type	Atoms
61	v	101	FME	O1-CN-N-CA
62	z	401	PHE	O-C-CA-CB
63	z	402	GNP	PB-N3B-PG-O1G
63	z	402	GNP	C5'-O5'-PA-O3A
63	z	402	GNP	O4'-C4'-C5'-O5'
63	z	402	GNP	C3'-C4'-C5'-O5'
63	z	402	GNP	C5'-O5'-PA-O1A
63	z	402	GNP	C5'-O5'-PA-O2A
61	v	101	FME	CA-CB-CG-SD

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 GNP z 402



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
55	w	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	2.24
1	A	2030:6MZ	O3'	2031:A	P	1.77
1	w	117:U	O3'	18:G	P	1.35

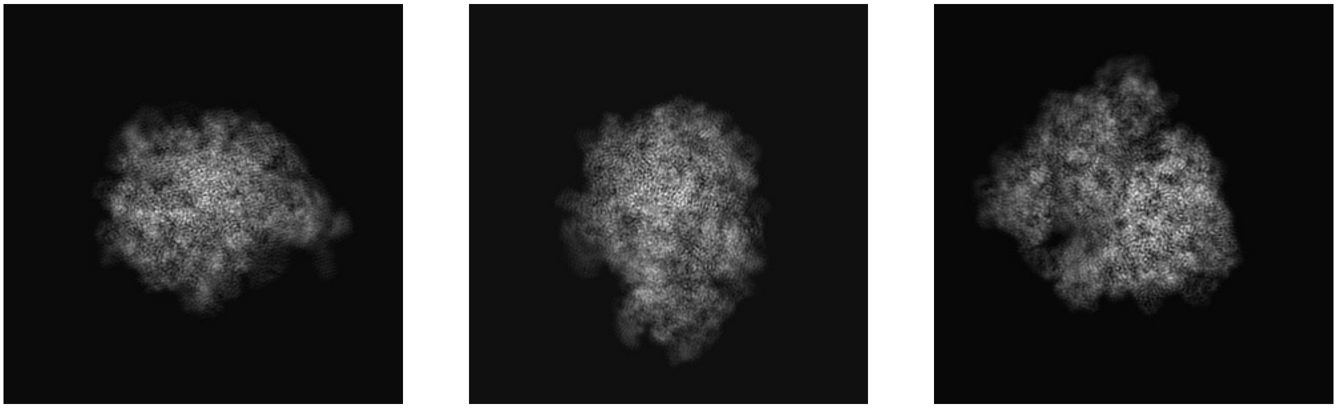
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-8814. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

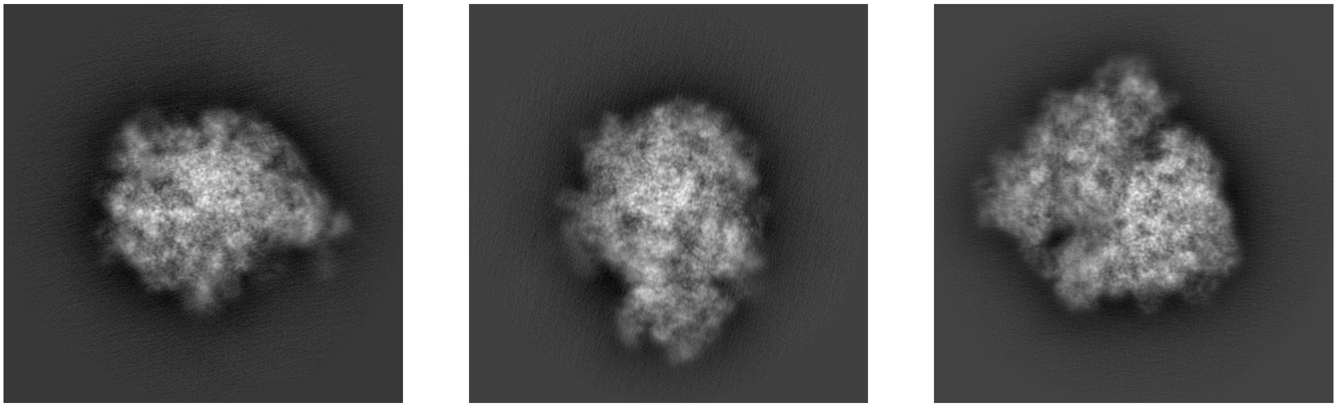
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

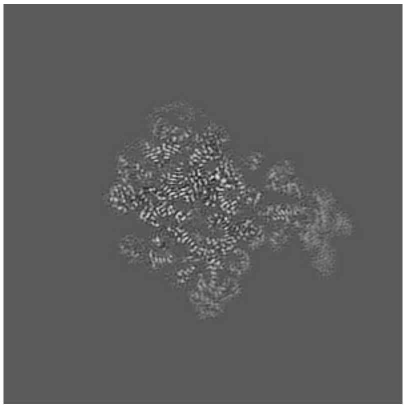


X Y Z

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

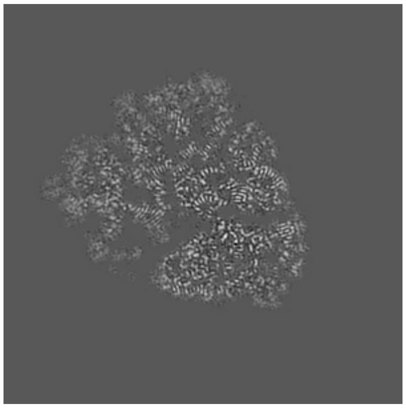
6.2 Central slices

6.2.1 Primary map



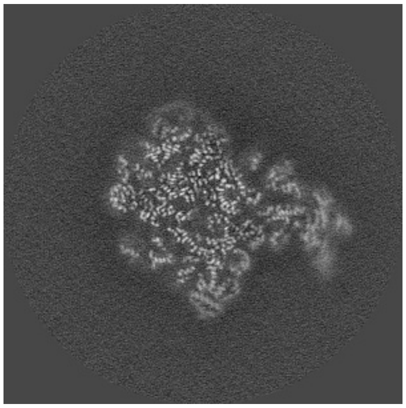
X Index: 199

Y Index: 199

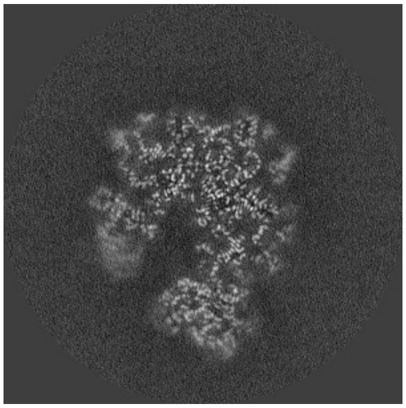


Z Index: 199

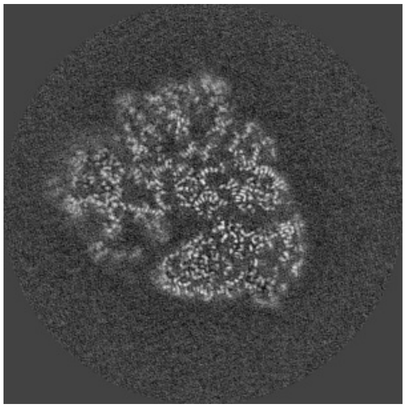
6.2.2 Raw map



X Index: 199



Y Index: 199

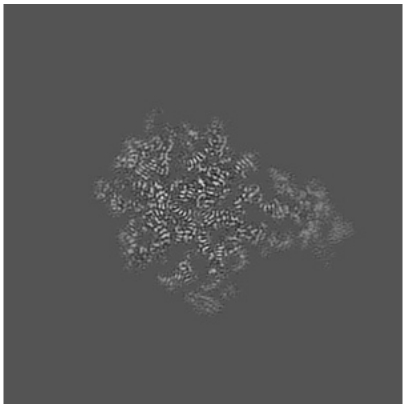


Z Index: 199

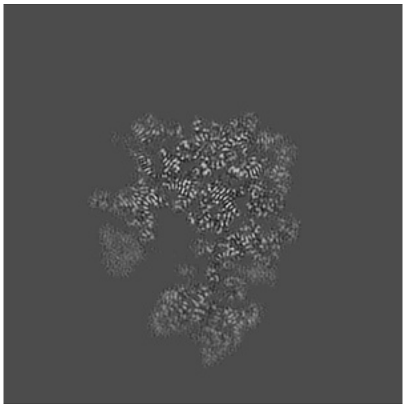
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

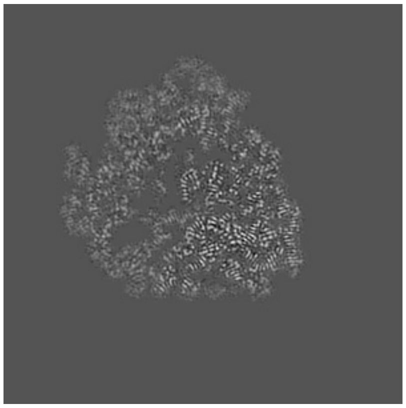
6.3.1 Primary map



X Index: 208

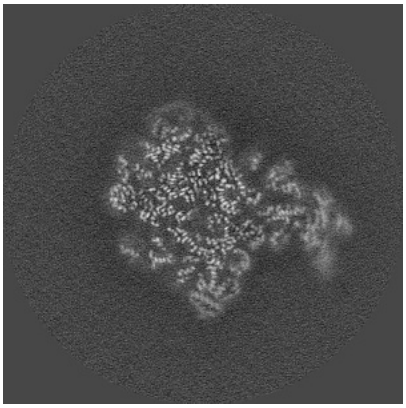


Y Index: 208

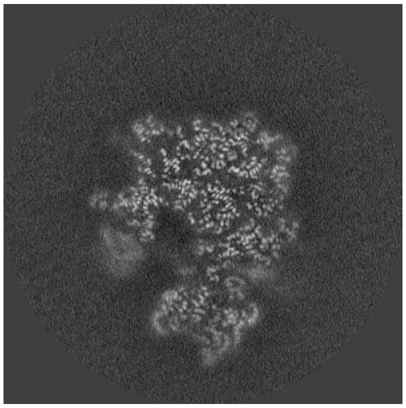


Z Index: 189

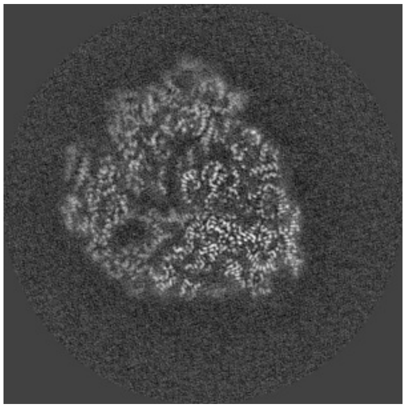
6.3.2 Raw map



X Index: 199



Y Index: 208

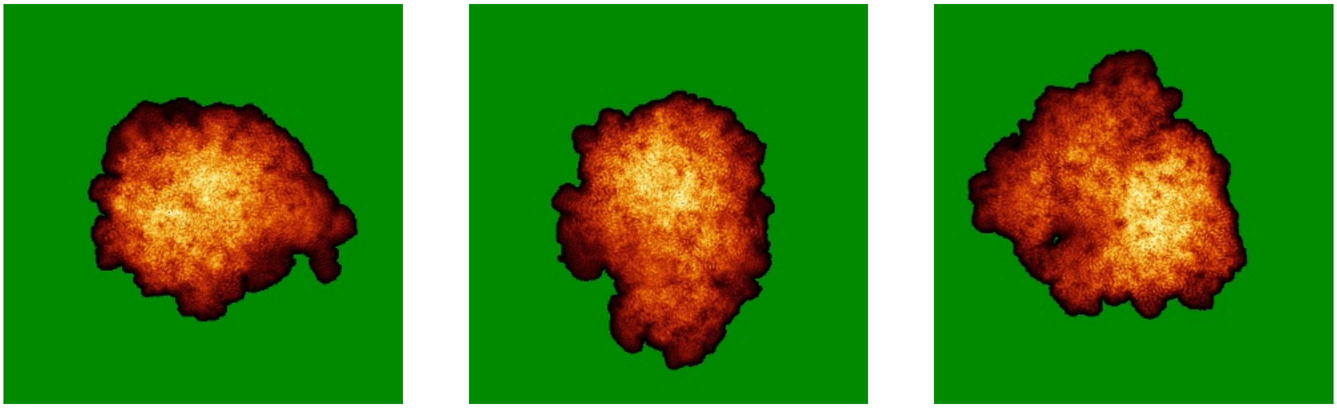


Z Index: 190

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

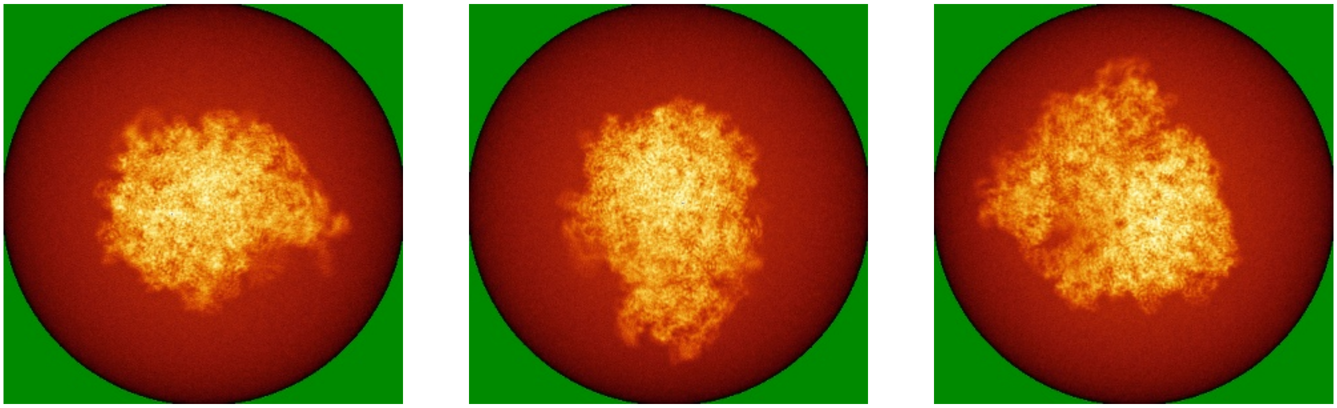
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map

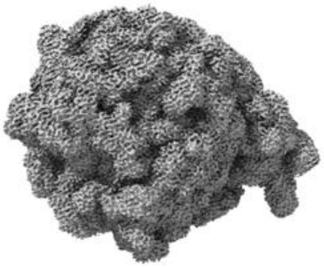


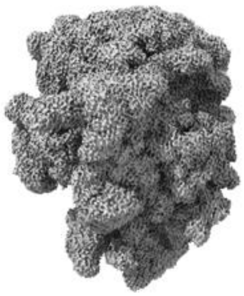
X Y Z

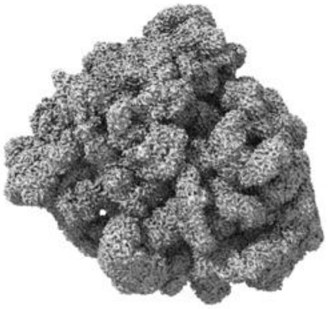
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

6.5.1 Primary map

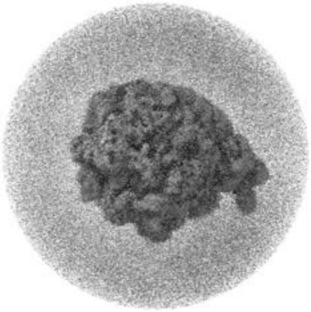

X

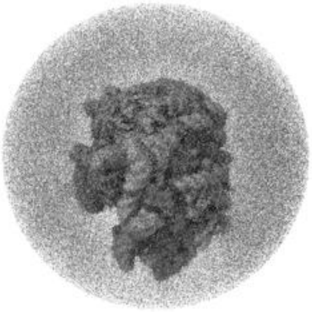

Y

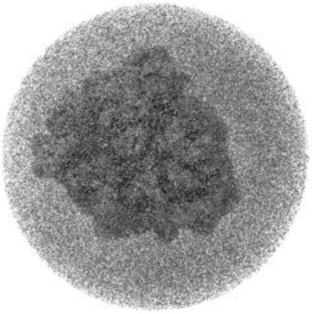

Z

The images above show the 3D surface view of the map at the recommended contour level 0.00677. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map


X


Y


Z

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

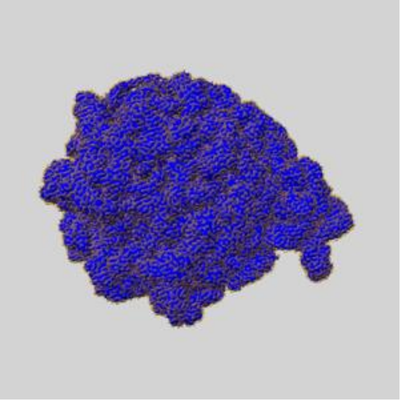
6.6 Mask visualisation

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

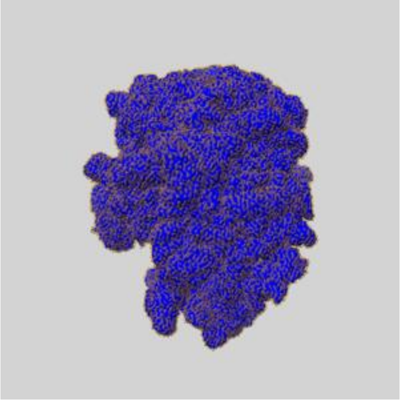
A mask typically either:

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

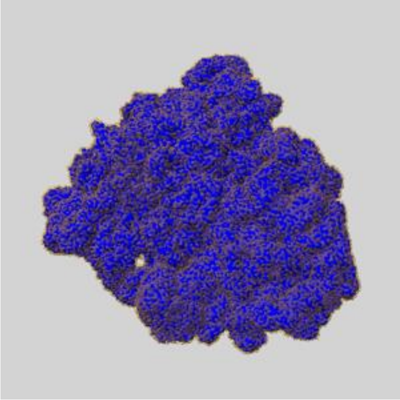
6.6.1 emd_8814_msk_1.map



X



Y

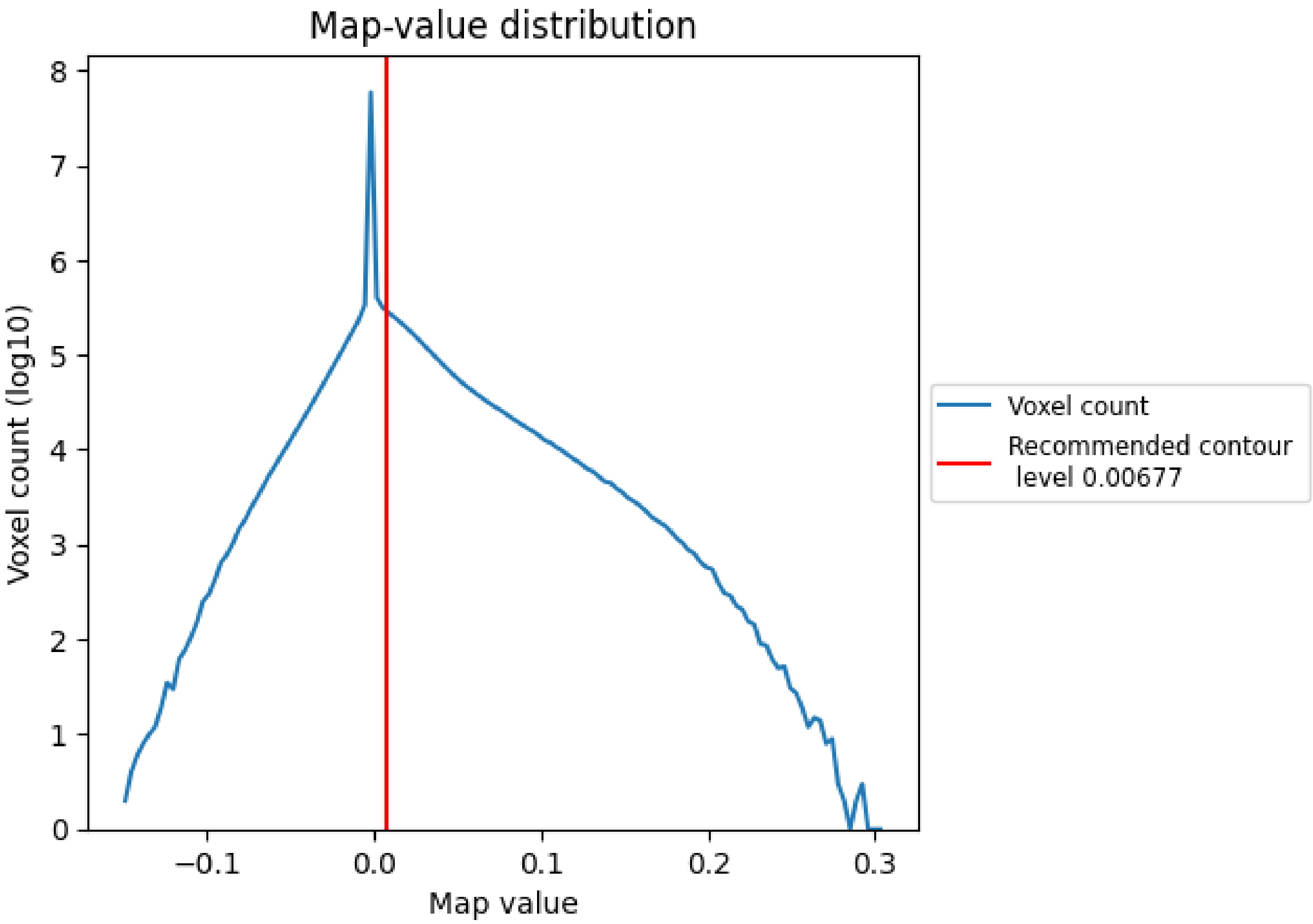


Z

7 Map analysis ⓘ

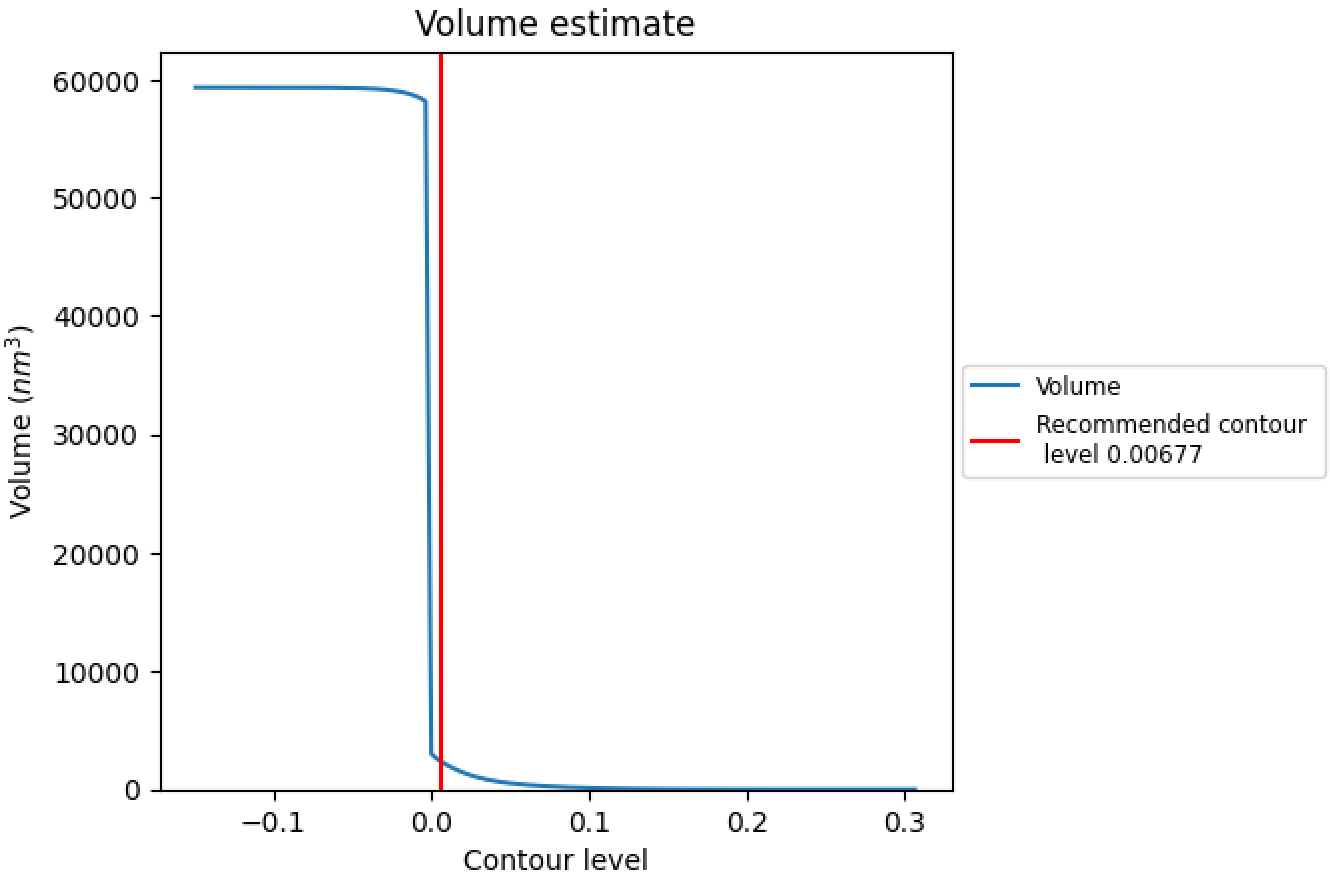
This section contains the results of statistical analysis of the map.

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.

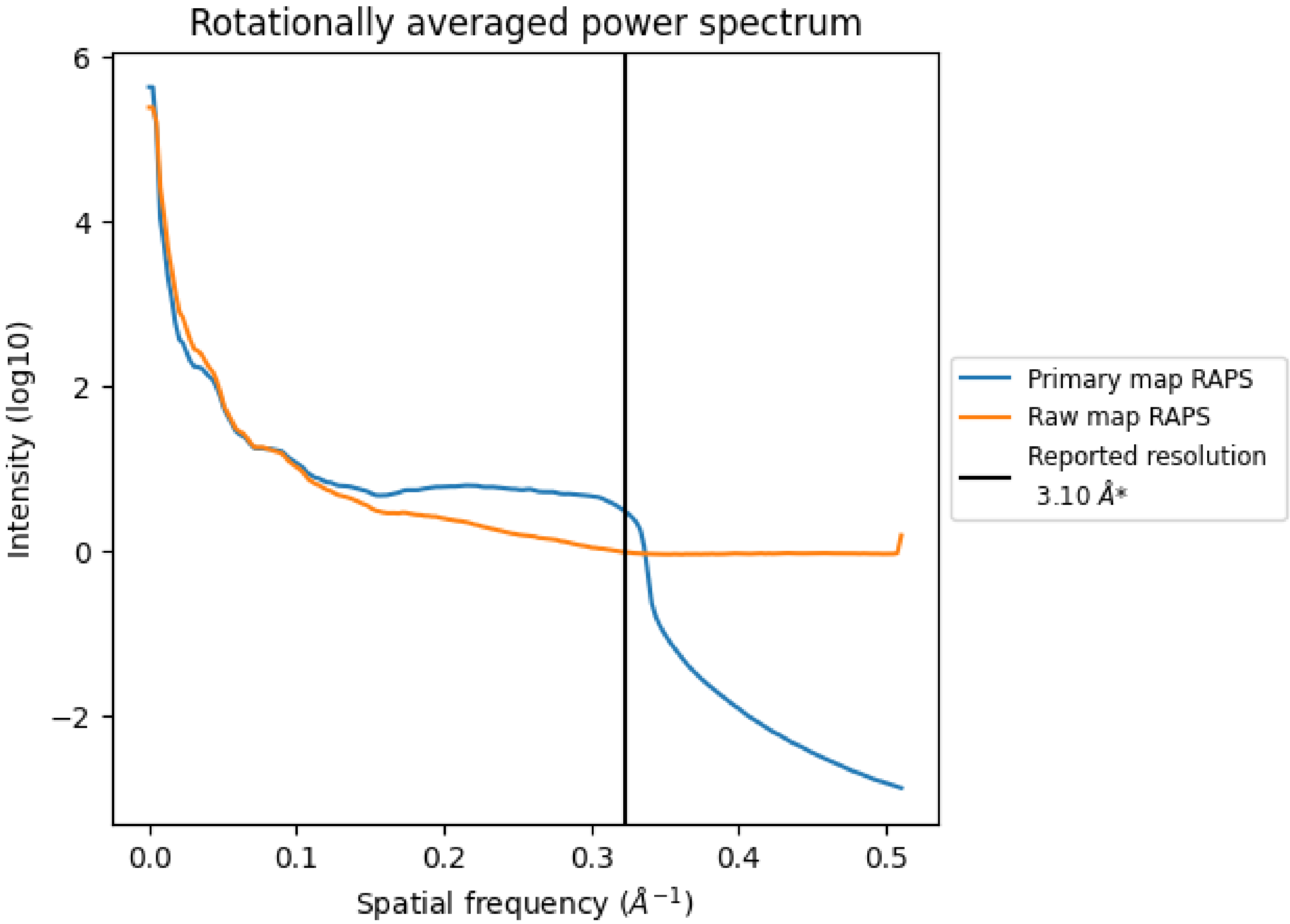
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2337 nm^3; this corresponds to an approximate mass of 2111 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)

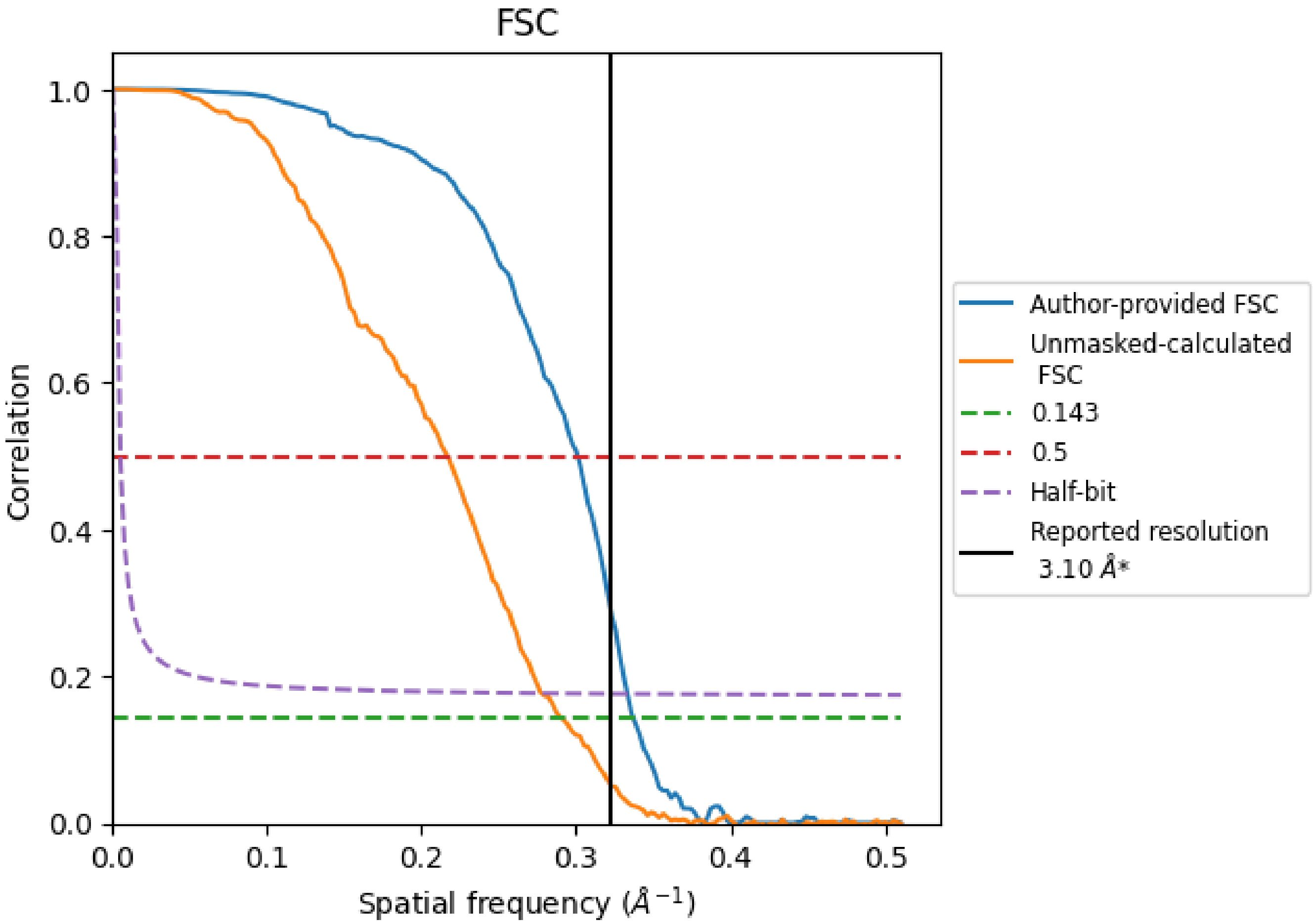


*Reported resolution corresponds to spatial frequency of 0.323 $\AA^{-1}$

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8.2 Resolution estimates

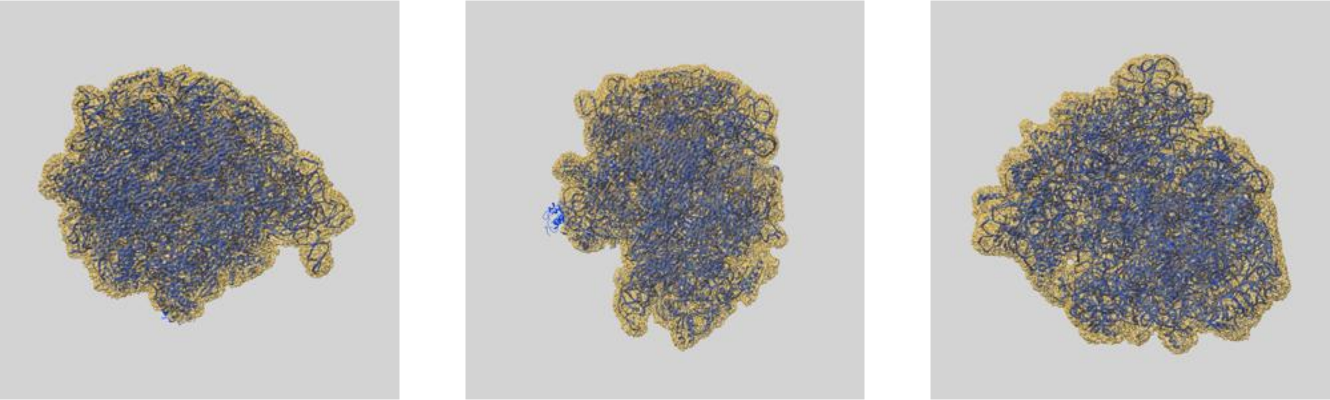
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	2.97	3.32	3.00
Unmasked-calculated*	3.44	4.61	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 3.1 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-8814 and PDB model 5WE4. Per-residue inclusion information can be found in section 3 on page 20.

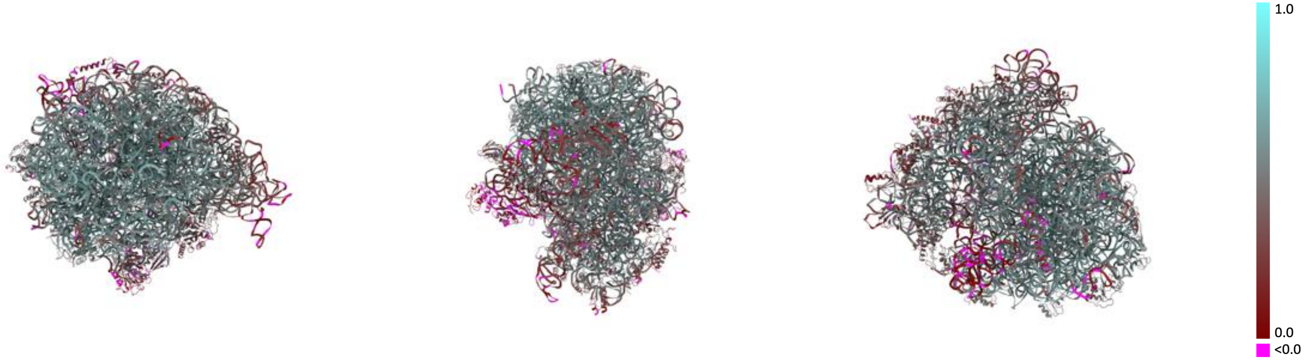
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00677 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.

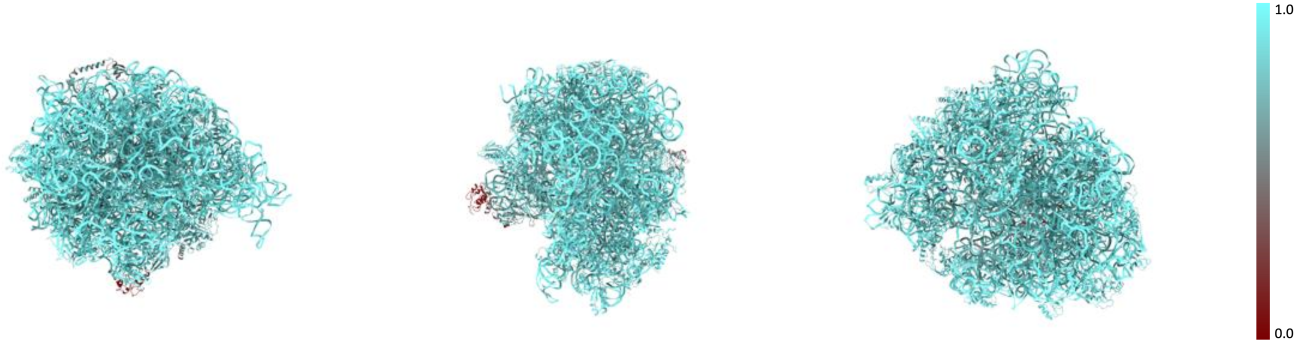
9.2 Q-score mapped to coordinate model (i)



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.

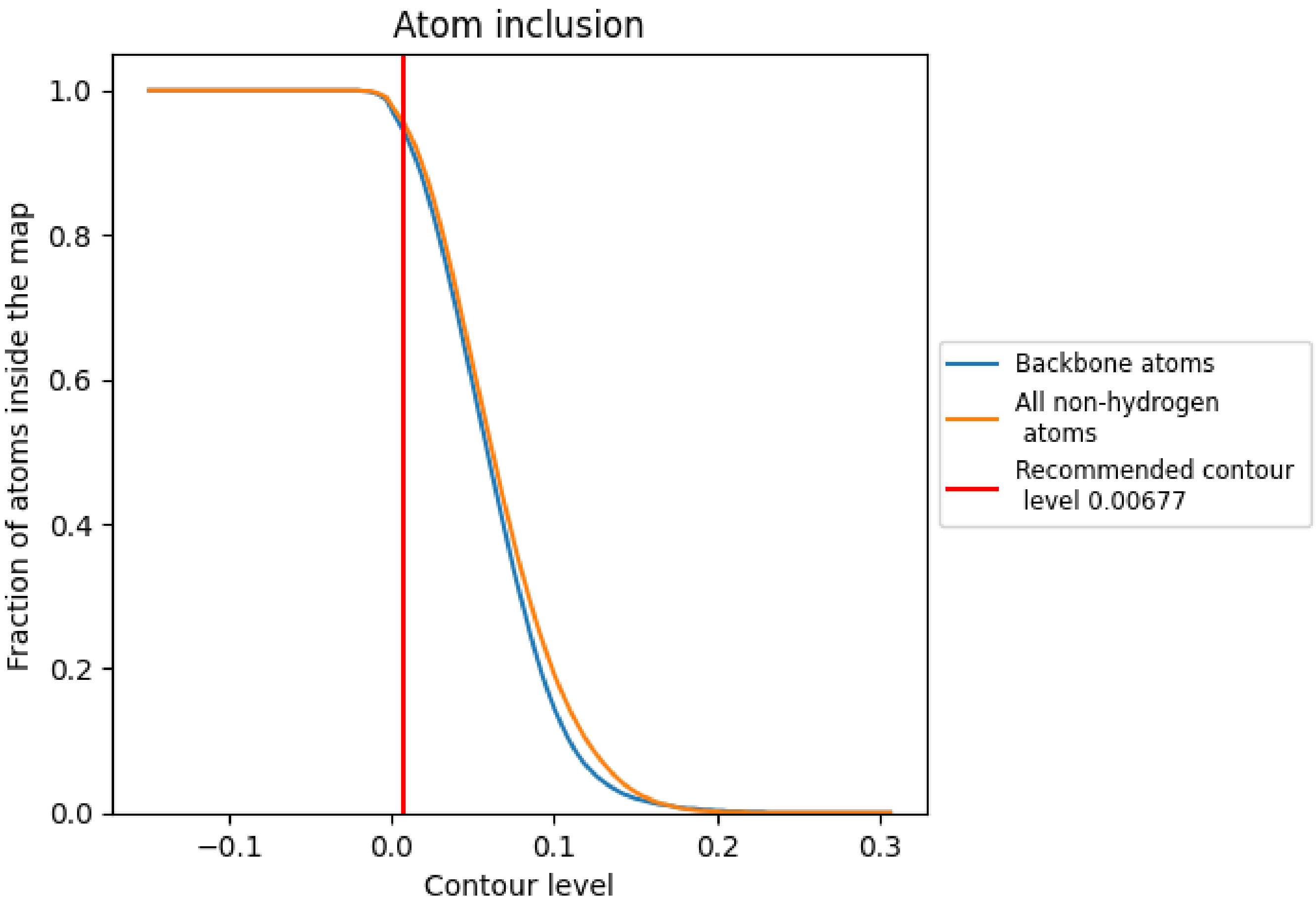
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00677).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.00677) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9570	0.4810
0	0.9620	0.5180
1	0.9510	0.4830
2	0.9800	0.5960
3	0.9780	0.5800
4	0.9660	0.5270
5	0.1930	-0.0150
6	0.8590	0.2790
A	0.9860	0.5370
B	0.9930	0.5010
C	0.9690	0.5610
D	0.9670	0.5420
E	0.9580	0.5050
F	0.9480	0.4040
G	0.9240	0.3720
H	0.6810	0.1800
I	0.5860	0.0360
J	0.9620	0.5340
K	0.9510	0.5220
L	0.9690	0.5240
M	0.9580	0.5320
N	0.9830	0.5580
O	0.9640	0.4620
P	0.9570	0.5190
Q	0.9720	0.5670
R	0.9610	0.5120
S	0.9770	0.5500
T	0.9320	0.4640
U	0.9510	0.4710
V	0.9420	0.4660
W	0.9680	0.5420
X	0.9570	0.5450
Y	0.9230	0.4250
Z	0.9550	0.5250
a	0.9870	0.4870

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Chain	Atom inclusion	Q-score
b	0.9050	0.3400
c	0.9360	0.4370
d	0.9130	0.3180
e	0.9460	0.4860
f	0.9110	0.4000
g	0.9110	0.3590
h	0.9490	0.4850
i	0.9280	0.3820
j	0.9160	0.3340
k	0.9570	0.4700
l	0.9340	0.4540
m	0.9460	0.4210
n	0.9400	0.4220
o	0.9420	0.4460
p	0.9120	0.3620
q	0.9420	0.4140
r	0.9360	0.4610
s	0.9570	0.4380
t	0.9290	0.3770
u	0.8150	0.2750
v	0.9760	0.4880
w	0.7620	0.0970
x	0.9680	0.4610
y	0.8980	0.2860
z	0.8150	0.2680