Full wwPDB EM Validation Report ⓘ

Nov 4, 2023 – 03:37 PM EDT

PDB ID : 7K00
EMDB ID : EMD-22586
Title : Structure of the Bacterial Ribosome at 2 Angstrom Resolution
Authors : Watson, Z.L.; Ward, F.R.; Meheust, R.; Ad, O.; Schepartz, A.; Banfield, J.F.; Cate, J.H.D.
Deposited on : 2020-09-02
Resolution : 1.98 Å(reported)
Based on initial model : 4YBB

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

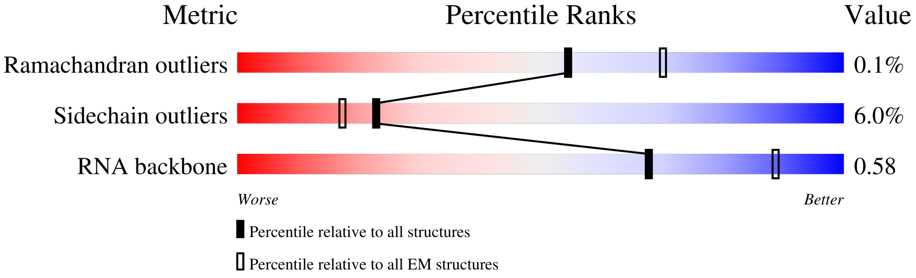
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance ⓘ

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

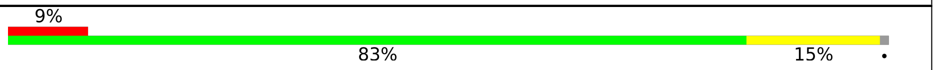
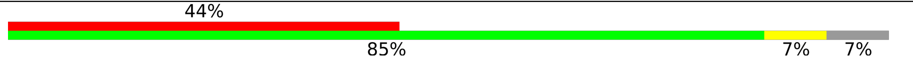
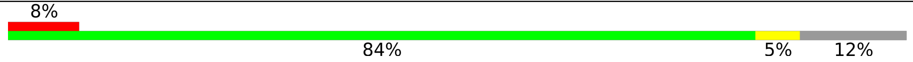
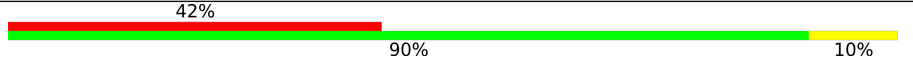
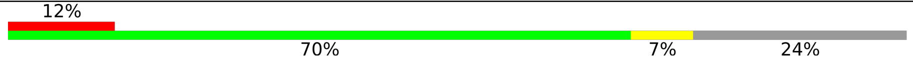
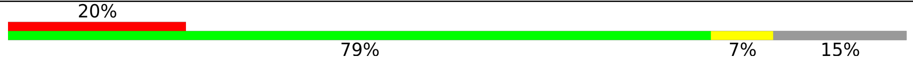
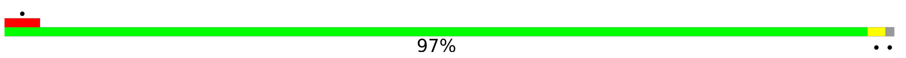
The reported resolution of this entry is 1.98 Å.

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	1542	
2	B	241	
3	C	233	
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	

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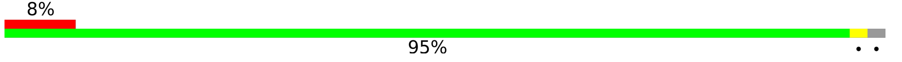
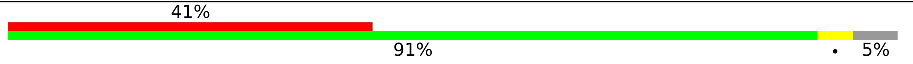
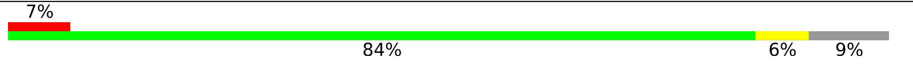
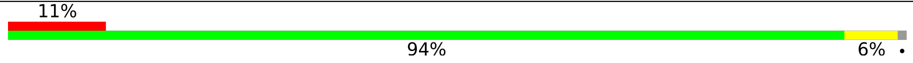
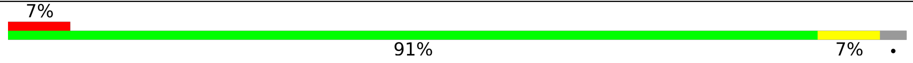
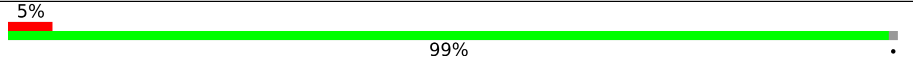
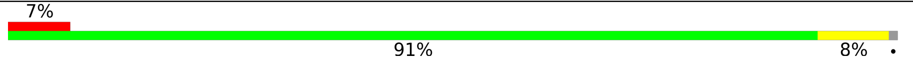
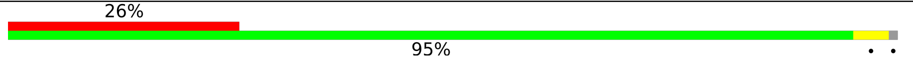
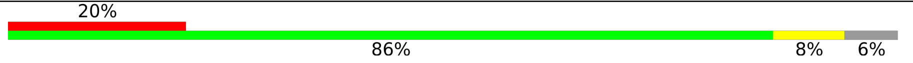
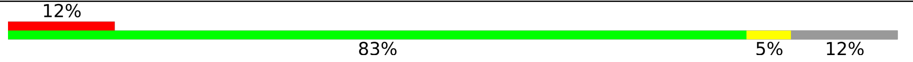
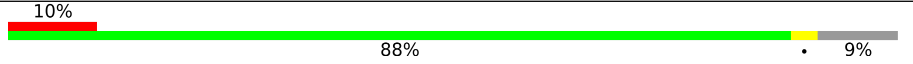
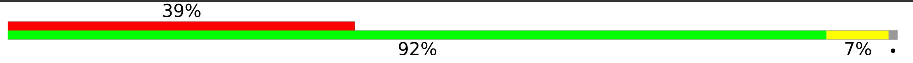
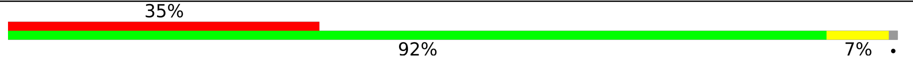
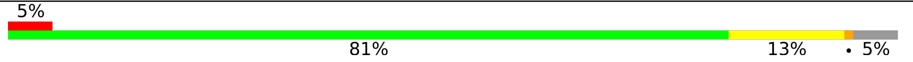
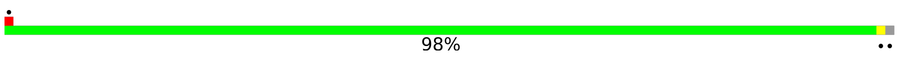
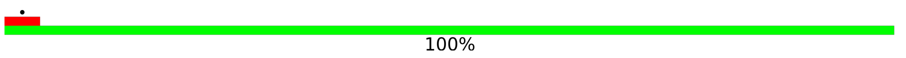
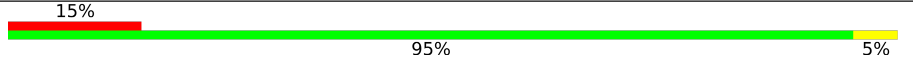
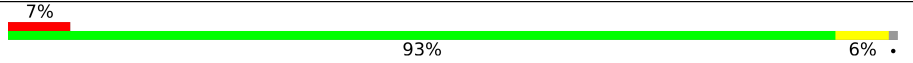
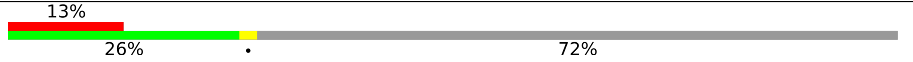
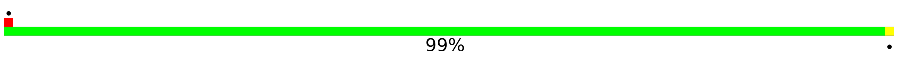
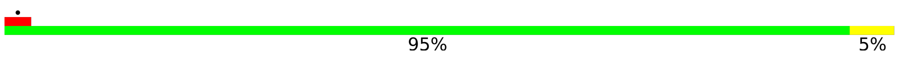
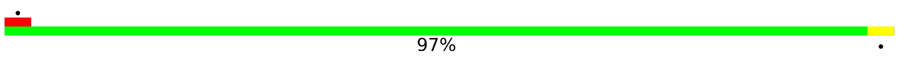
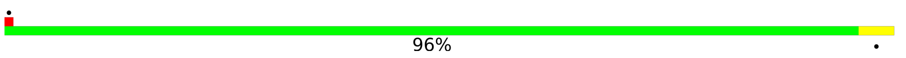
Mol	Chain	Length	Quality of chain
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	120	
24	c	273	
25	d	209	
26	e	201	
27	f	179	
28	g	177	
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	

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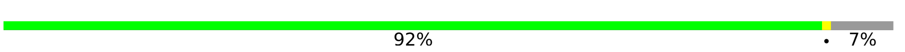
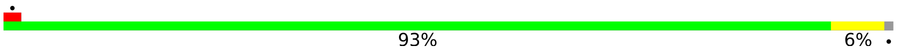
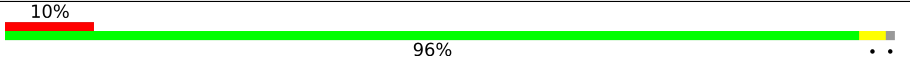
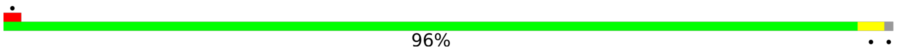
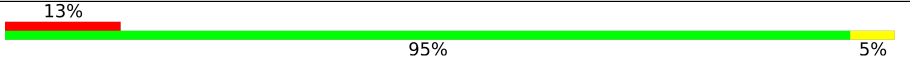
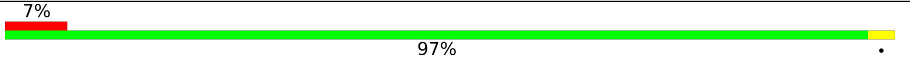
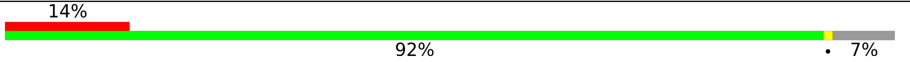
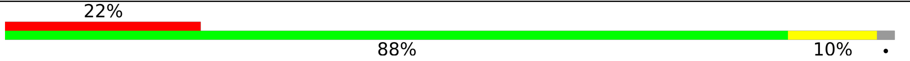
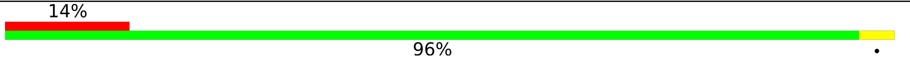
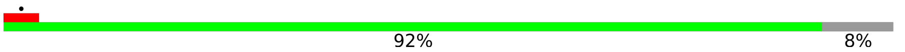
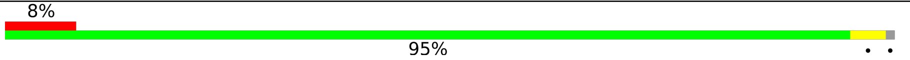
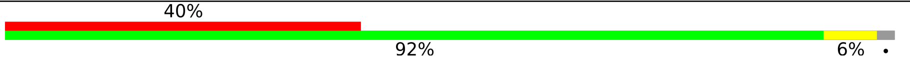
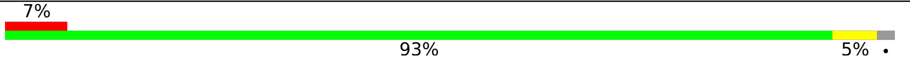
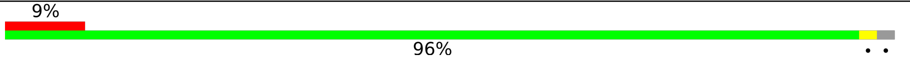
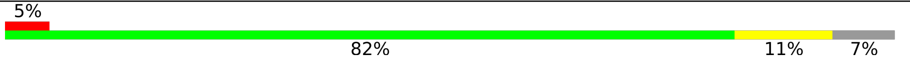
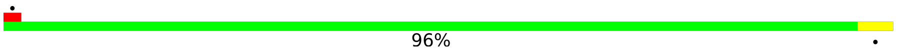
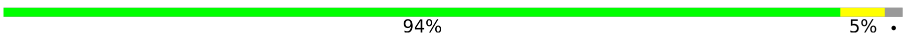
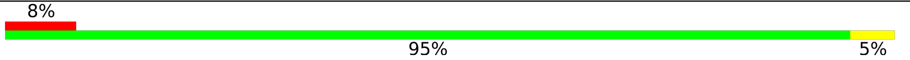
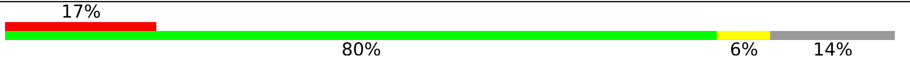
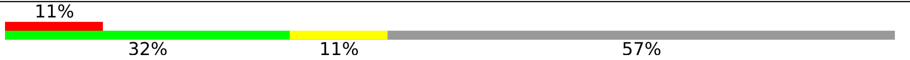
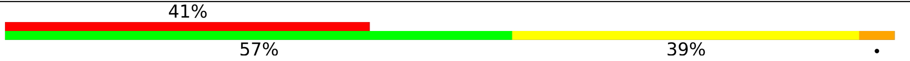
Mol	Chain	Length	Quality of chain
34	m	127	
35	n	117	
36	o	115	
37	p	118	
38	q	103	
39	r	110	
40	s	100	
41	t	104	
42	u	94	
43	v	85	
44	w	78	
45	x	63	
46	y	59	
47	z	57	
48	0	55	
49	1	46	
50	2	65	
51	3	38	
52	4	70	
53	X	28	
54	Y	76	
55	Z	76	
56	5	2	

2 Entry composition ⓘ

There are 62 unique types of molecules in this entry. The entry contains 149338 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1519	32612	14552	5986	10555	1519	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	224	1753	1109	315	321	8	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	156	1152	717	217	212	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	103	839	530	151	151	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP S1ELC2

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

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

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

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

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

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

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	h	41	303	194	54	54	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	i	142	1129	714	212	199	4	0	0

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	k	144	1053	654	207	190	2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	l	136	1075	686	205	177	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP L4V2J8

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	118	Total 945	C 585	N 194	O 161	S 5	0	0

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	u	94	753	479	137	134	3	0	0

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	78	586	362	116	107	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	y	58	449	281	87	79	2	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
48	0	51	Total 417	C 269	N 76	O 72	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total 377	C 228	N 90	O 57	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total 504	C 323	N 105	O 74	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total 302	C 185	N 65	O 48	S 4	0	0

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total 480	C 299	N 90	O 85	S 6	0	0

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	12	Total 260	C 117	N 51	O 80	P 12	0	0

- Molecule 54 is a RNA chain called A-site tRNA-val.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	Y	74	1579	705	287	514	73	0	0

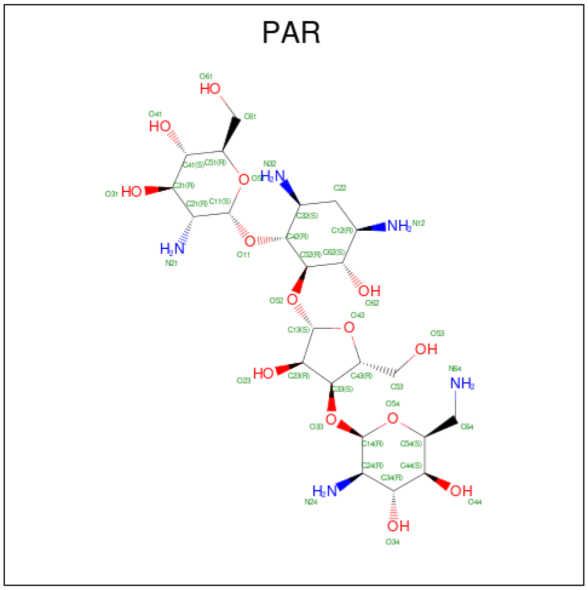
- Molecule 55 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	Z	76	1623	723	294	530	76	0	0

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	5	2	42	19	8	13	2	0	0

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
57	A	1	42	23	5	14	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	A	93	93	93	0

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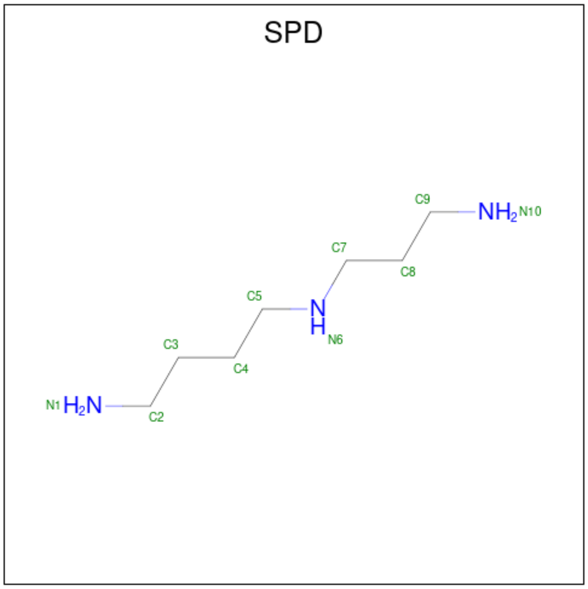
Mol	Chain	Residues	Atoms	AltConf
58	a	208	Total Mg 208 208	0
58	b	5	Total Mg 5 5	0
58	c	1	Total Mg 1 1	0
58	d	1	Total Mg 1 1	0
58	z	1	Total Mg 1 1	0

- Molecule 59 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



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

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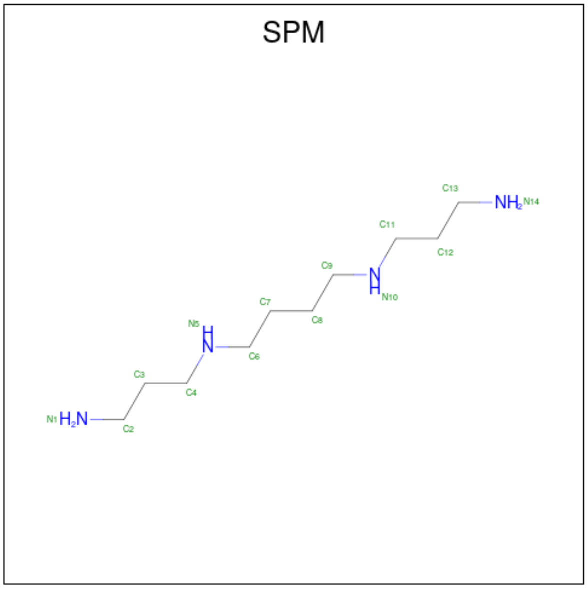
Mol	Chain	Residues	Atoms	AltConf
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0
59	a	1	Total C N 10 7 3	0

- Molecule 60 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



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

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
61	3	1	Total Zn 1 1	0
61	4	1	Total Zn 1 1	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	AltConf
62	A	2063	Total O 2063 2063	0
62	B	1	Total O 1 1	0
62	C	46	Total O 46 46	0
62	D	11	Total O 11 11	0
62	E	15	Total O 15 15	0
62	G	5	Total O 5 5	0
62	H	28	Total O 28 28	0
62	I	21	Total O 21 21	0
62	J	15	Total O 15 15	0
62	K	12	Total O 12 12	0
62	L	23	Total O 23 23	0
62	M	18	Total O 18 18	0
62	N	31	Total O 31 31	0
62	O	11	Total O 11 11	0
62	P	10	Total O 10 10	0
62	Q	4	Total O 4 4	0
62	R	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
62	S	24	Total O 24 24	0
62	T	3	Total O 3 3	0
62	U	5	Total O 5 5	0
62	a	4028	Total O 4028 4028	0
62	b	171	Total O 171 171	0
62	c	100	Total O 100 100	0
62	d	38	Total O 38 38	0
62	e	48	Total O 48 48	0
62	f	30	Total O 30 30	0
62	h	6	Total O 6 6	0
62	i	14	Total O 14 14	0
62	j	17	Total O 17 17	0
62	k	50	Total O 50 50	0
62	l	27	Total O 27 27	0
62	m	33	Total O 33 33	0
62	n	42	Total O 42 42	0
62	o	12	Total O 12 12	0
62	p	33	Total O 33 33	0
62	q	20	Total O 20 20	0
62	r	20	Total O 20 20	0
62	s	11	Total O 11 11	0

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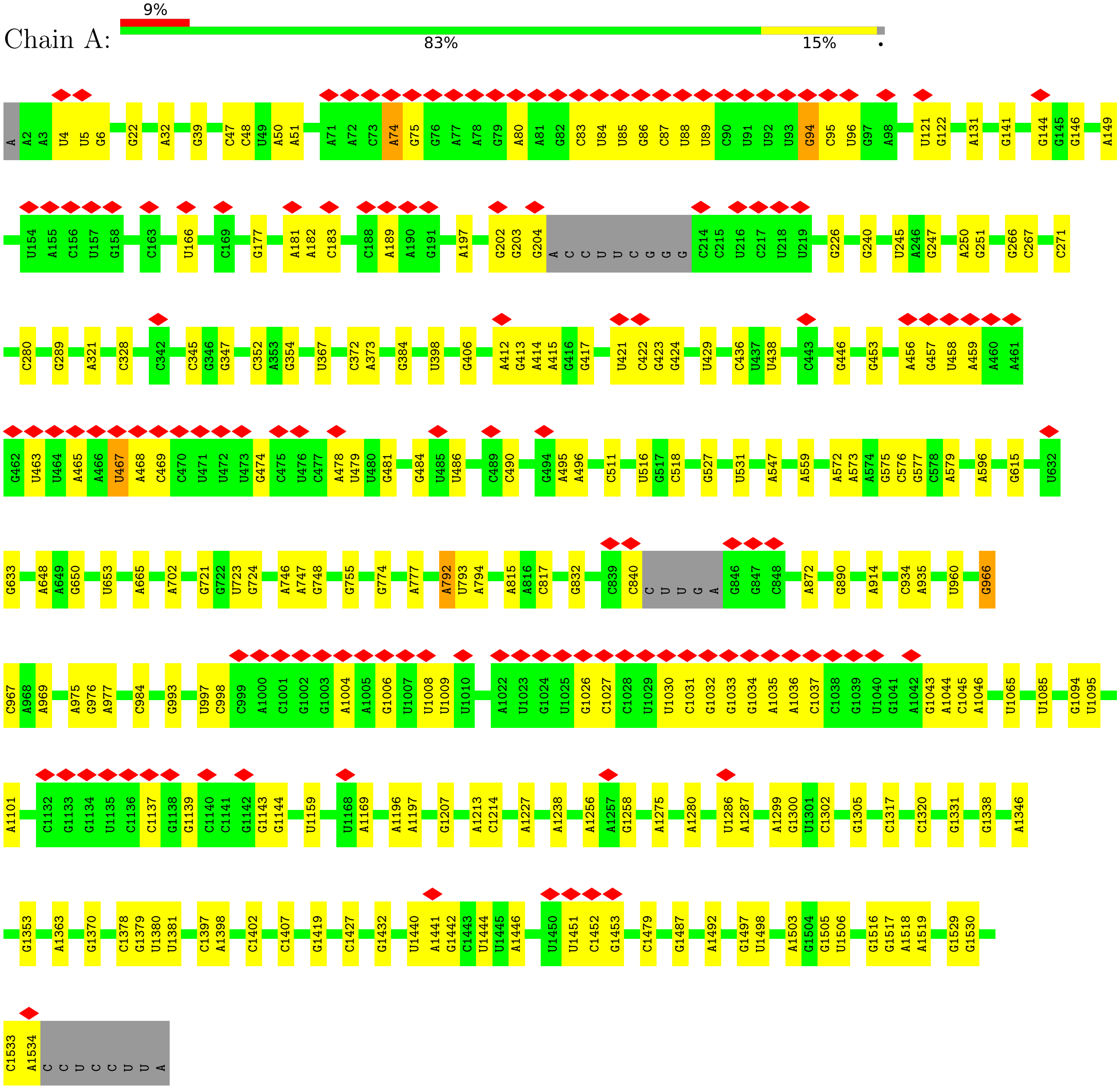
Mol	Chain	Residues	Atoms	AltConf
62	t	3	Total O 3 3	0
62	u	4	Total O 4 4	0
62	v	18	Total O 18 18	0
62	w	23	Total O 23 23	0
62	x	2	Total O 2 2	0
62	y	6	Total O 6 6	0
62	z	25	Total O 25 25	0
62	0	7	Total O 7 7	0
62	1	33	Total O 33 33	0
62	2	24	Total O 24 24	0
62	3	3	Total O 3 3	0
62	4	6	Total O 6 6	0
62	X	15	Total O 15 15	0
62	Y	13	Total O 13 13	0
62	Z	19	Total O 19 19	0

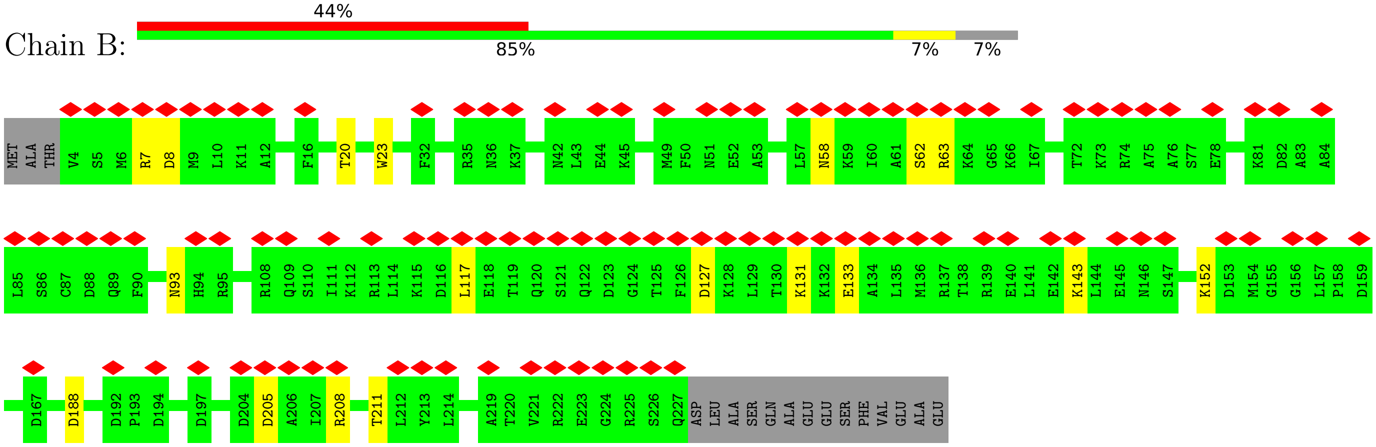
3 Residue-property plots ⓘ

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.

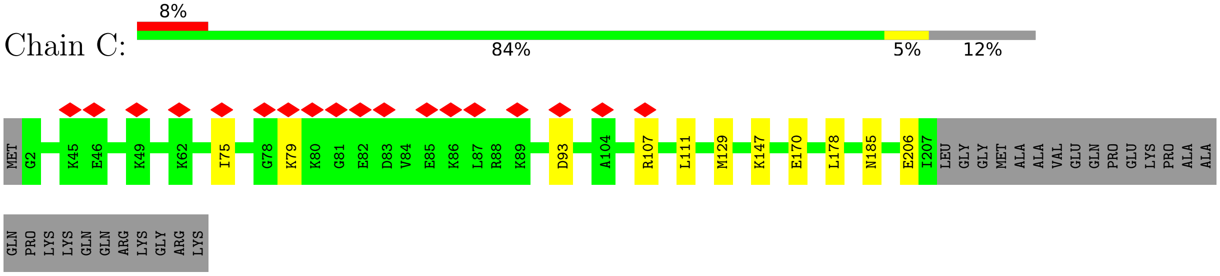
- Molecule 1: 16S rRNA



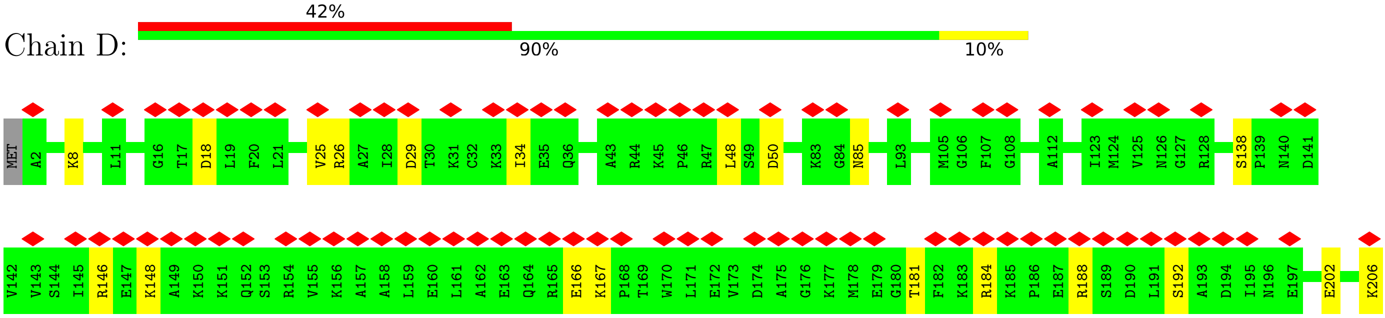
- Molecule 2: 30S ribosomal protein S2



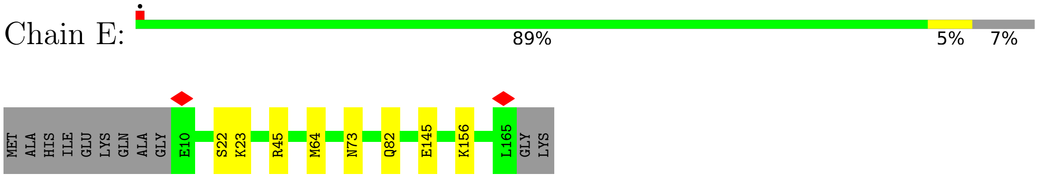
- Molecule 3: 30S ribosomal protein S3



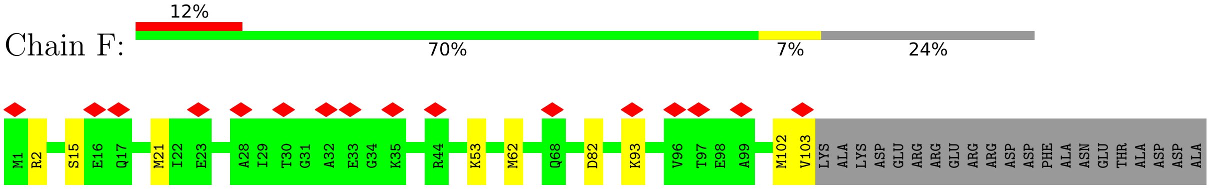
- Molecule 4: 30S ribosomal protein S4



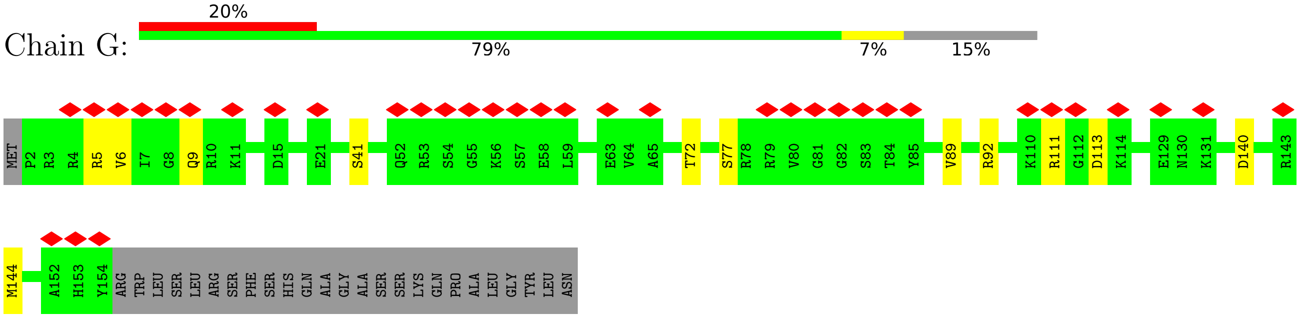
- Molecule 5: 30S ribosomal protein S5



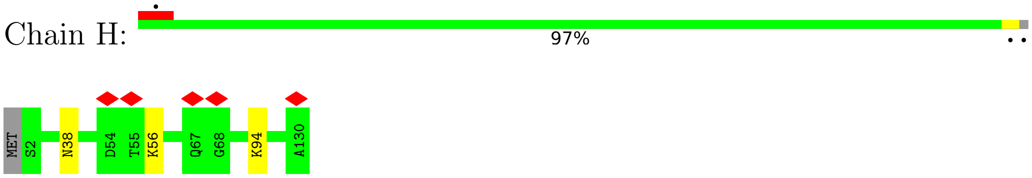
- Molecule 6: 30S ribosomal protein S6



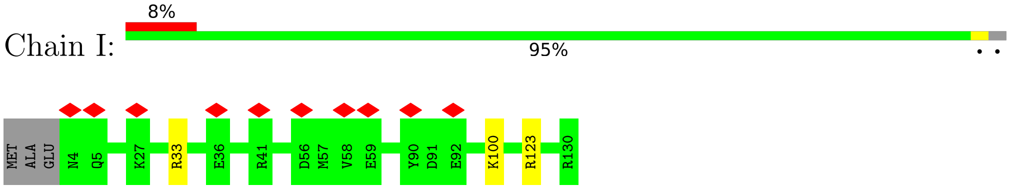
- Molecule 7: 30S ribosomal protein S7



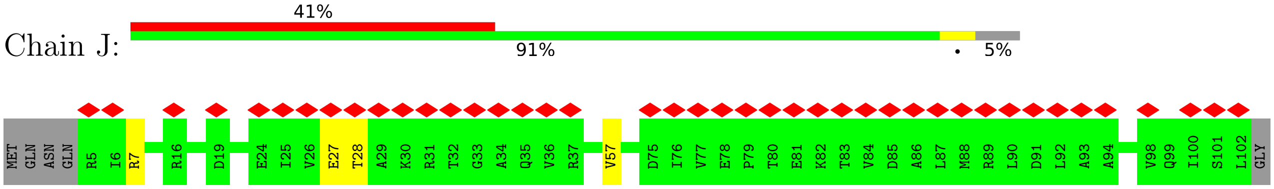
- Molecule 8: 30S ribosomal protein S8



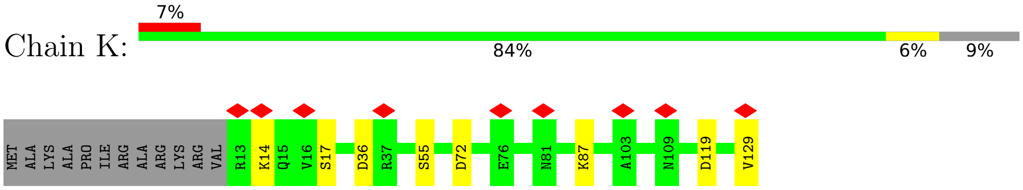
- Molecule 9: 30S ribosomal protein S9



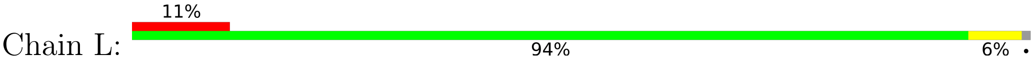
- Molecule 10: 30S ribosomal protein S10

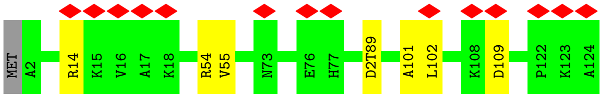


- Molecule 11: 30S ribosomal protein S11



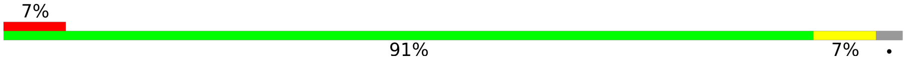
- Molecule 12: 30S ribosomal protein S12

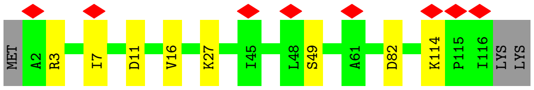




- Molecule 13: 30S ribosomal protein S13

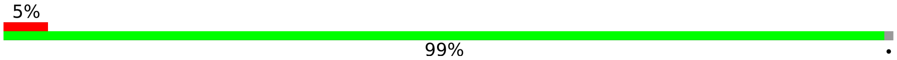
Chain M:

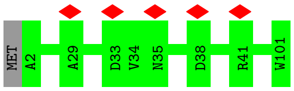




- Molecule 14: 30S ribosomal protein S14

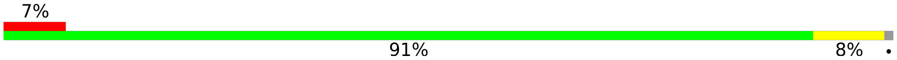
Chain N:

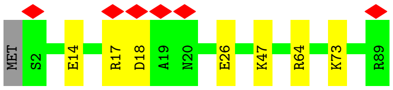




- Molecule 15: 30S ribosomal protein S15

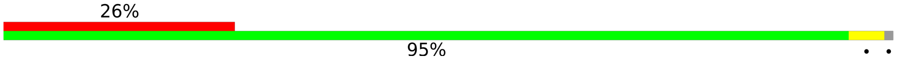
Chain O:

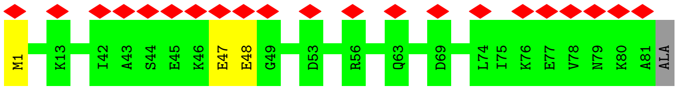




- Molecule 16: 30S ribosomal protein S16

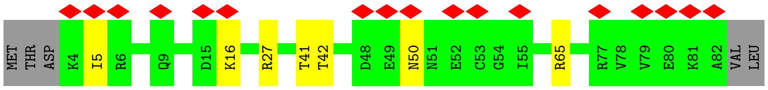
Chain P:





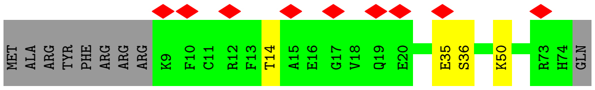
- Molecule 17: 30S ribosomal protein S17

Chain Q:

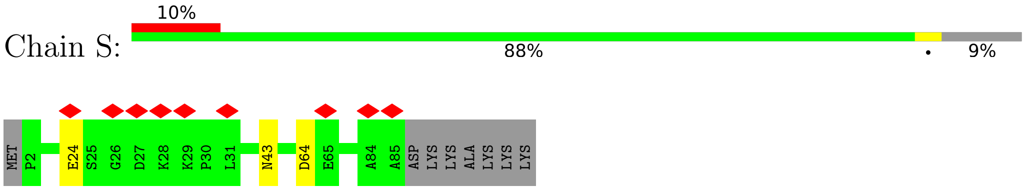


- Molecule 18: 30S ribosomal protein S18

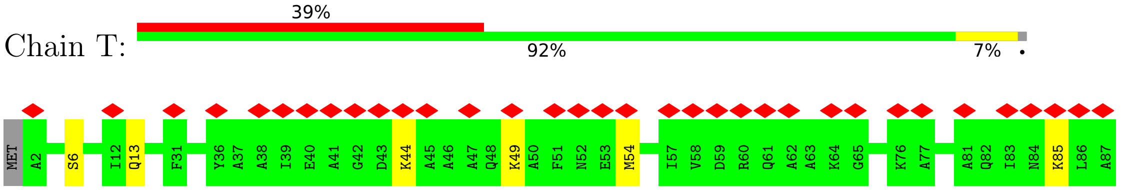
Chain R:



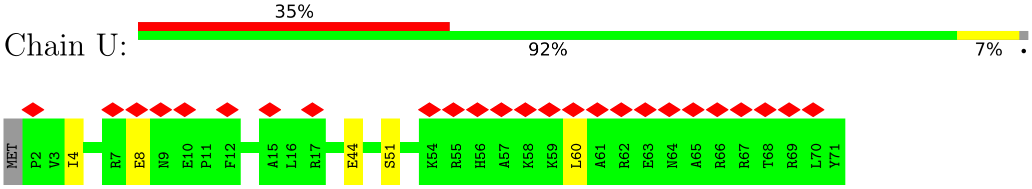
- Molecule 19: 30S ribosomal protein S19



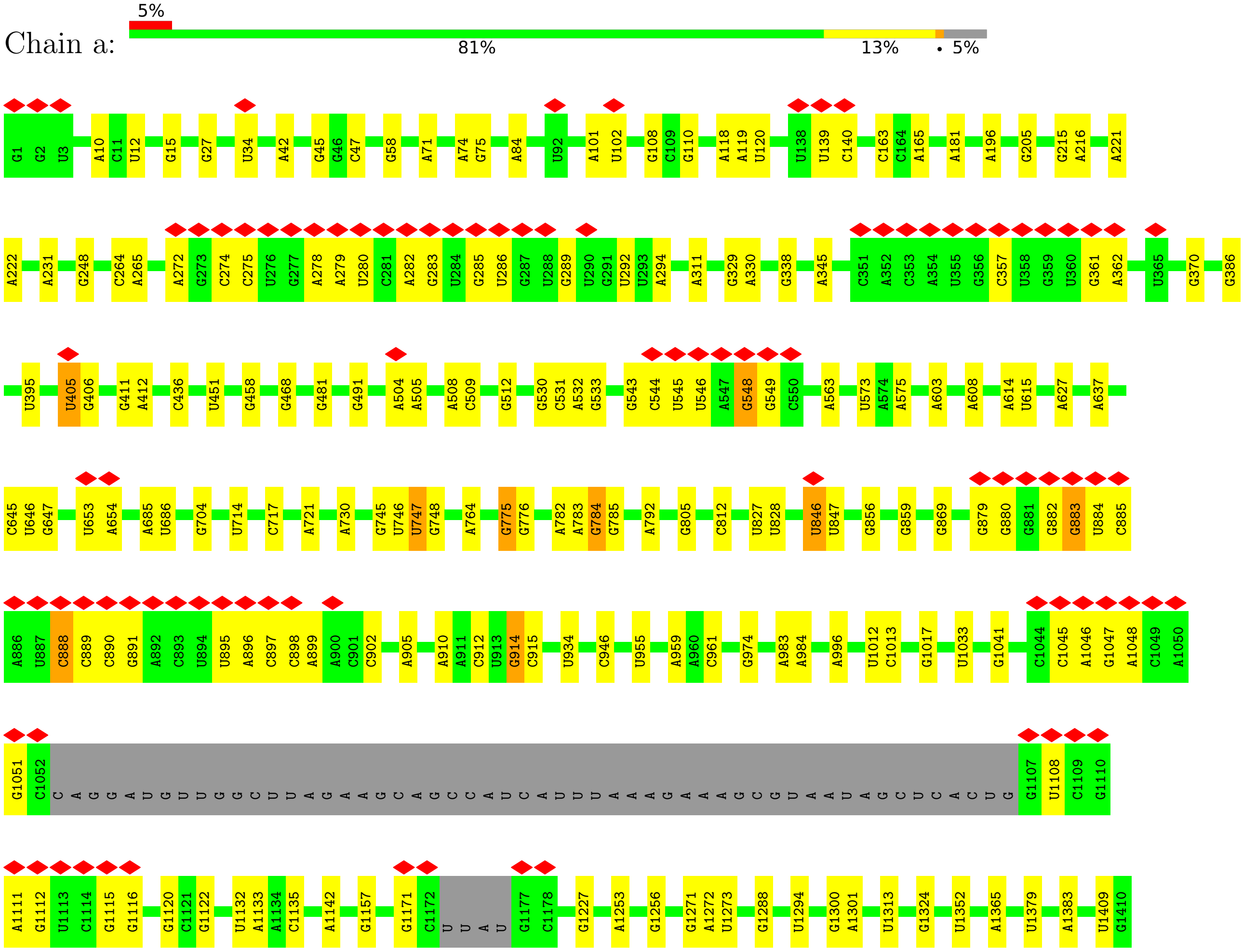
- Molecule 20: 30S ribosomal protein S20

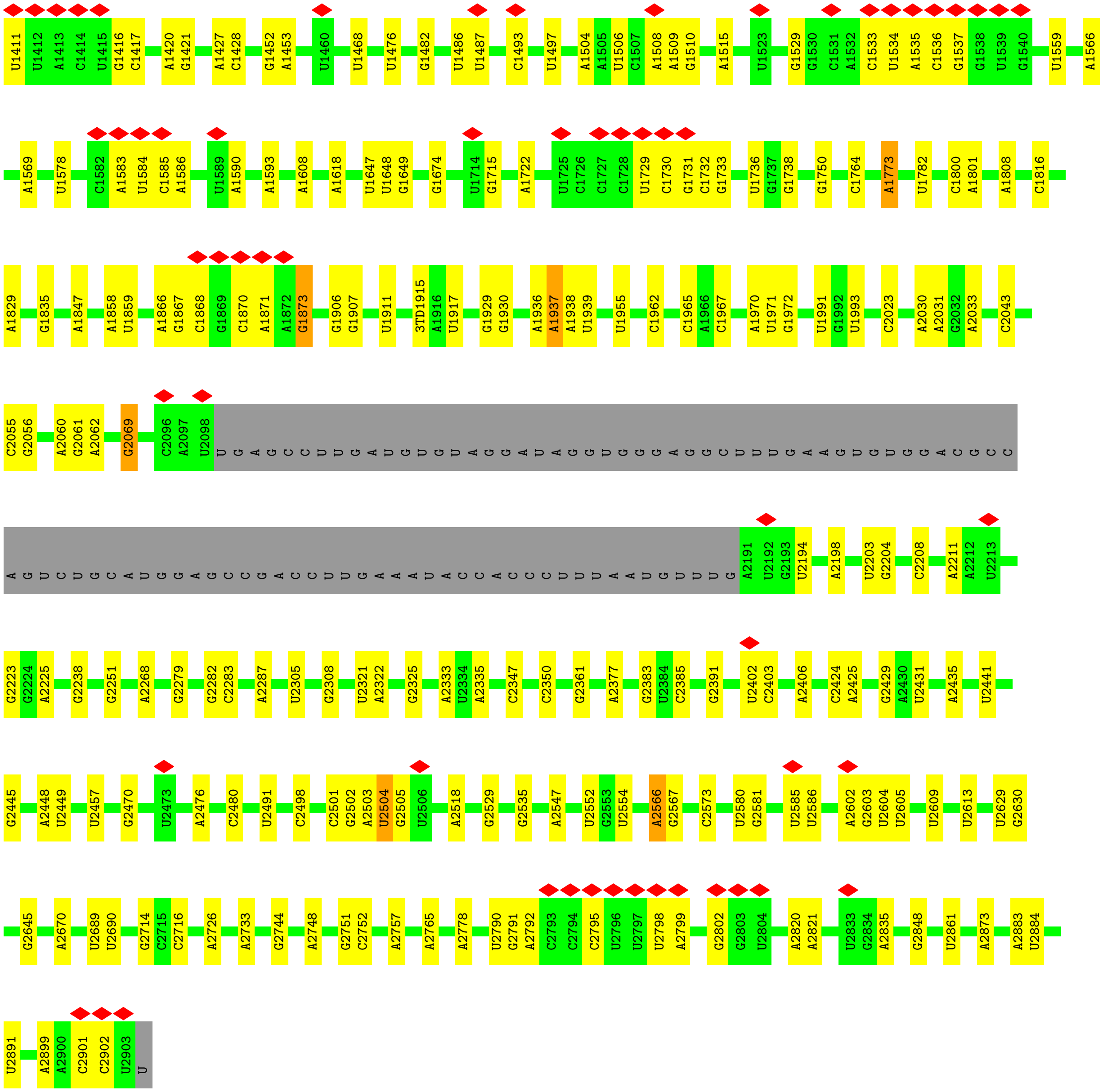


- Molecule 21: 30S ribosomal protein S21



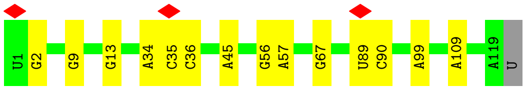
- Molecule 22: 23S rRNA





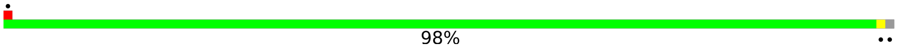
- Molecule 23: 5S rRNA

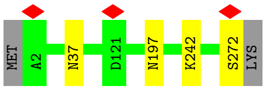
Chain b:



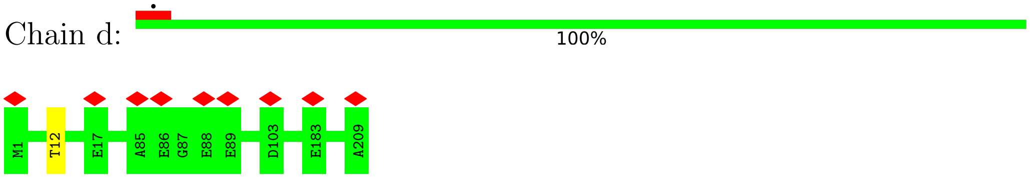
- Molecule 24: 50S ribosomal protein L2

Chain c:

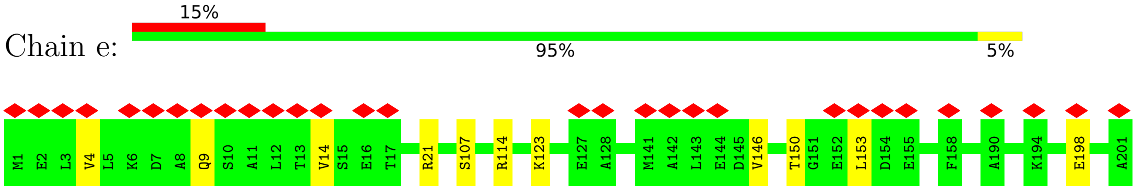




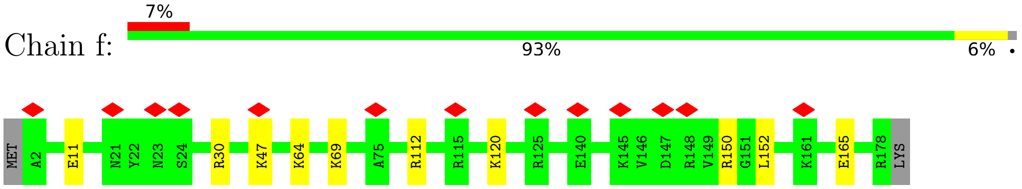
- Molecule 25: 50S ribosomal protein L3



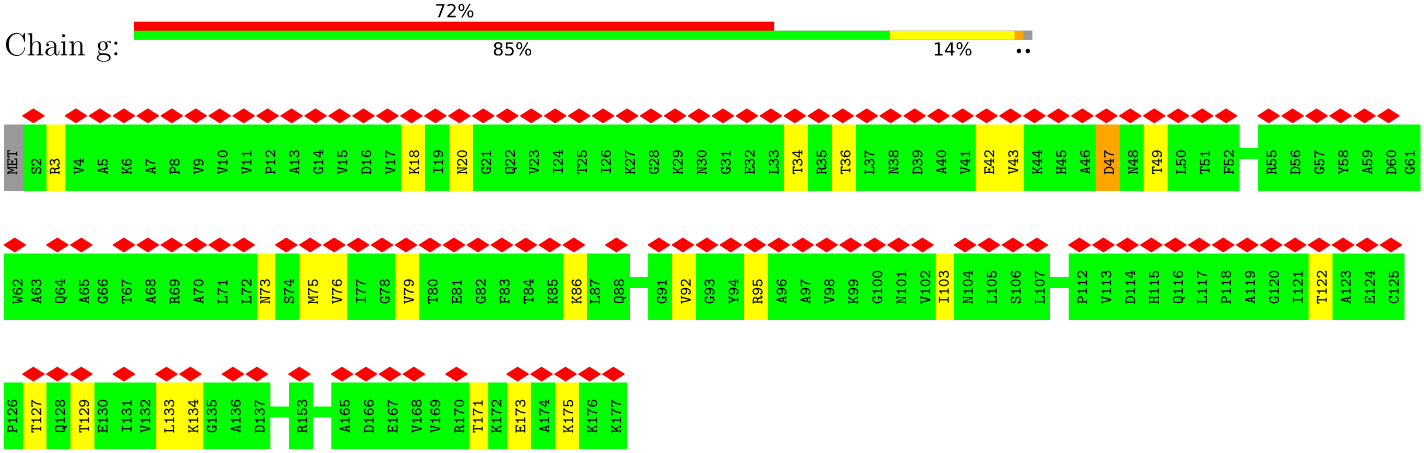
- Molecule 26: 50S ribosomal protein L4



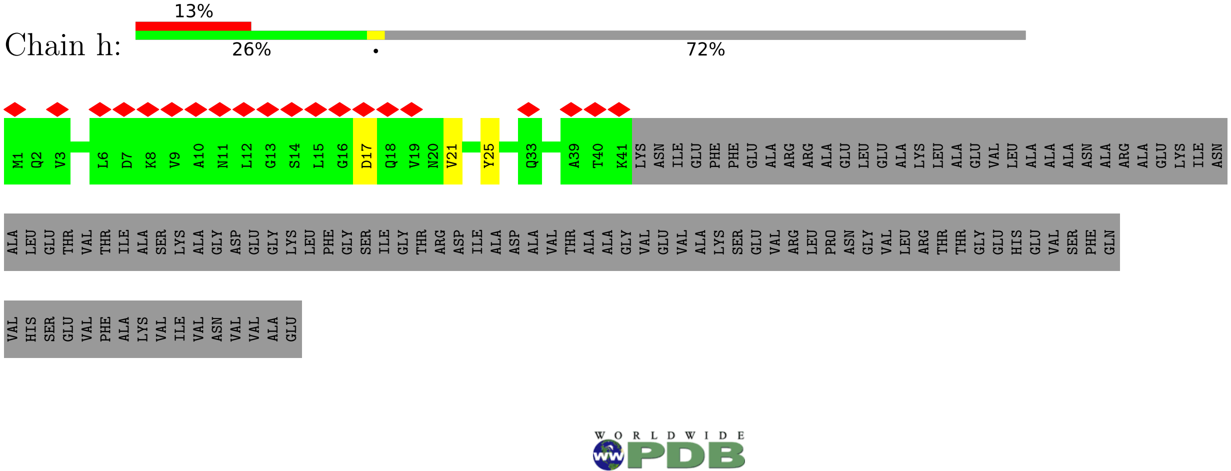
- Molecule 27: 50S ribosomal protein L5



- Molecule 28: 50S ribosomal protein L6

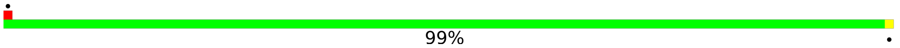


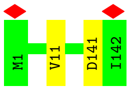
- Molecule 29: 50S ribosomal protein L9



- Molecule 30: 50S ribosomal protein L13

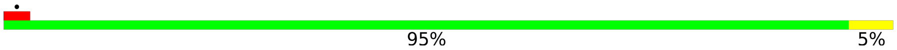
Chain i:

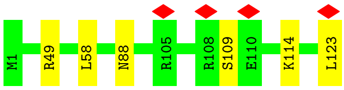




- Molecule 31: 50S ribosomal protein L14

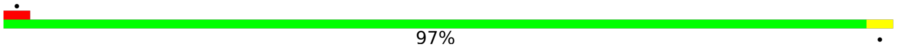
Chain j:

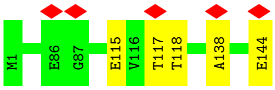




- Molecule 32: 50S ribosomal protein L15

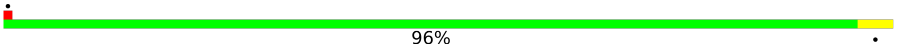
Chain k:

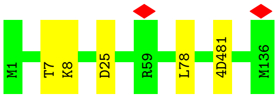




- Molecule 33: 50S ribosomal protein L16

Chain l:



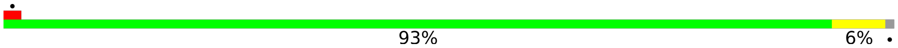


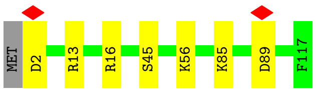
- Molecule 34: 50S ribosomal protein L17

Chain m:

- Molecule 35: 50S ribosomal protein L18

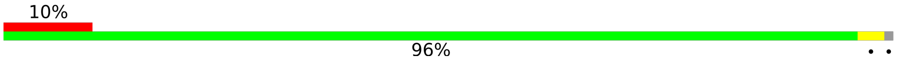
Chain n:

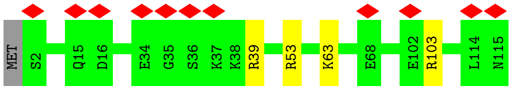




- Molecule 36: 50S ribosomal protein L19

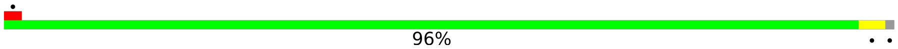
Chain o:

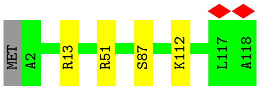




- Molecule 37: 50S ribosomal protein L20

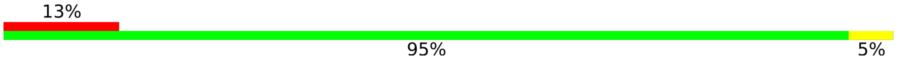
Chain p:

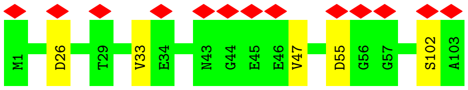




- Molecule 38: 50S ribosomal protein L21

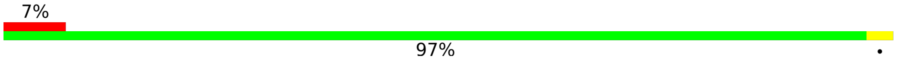
Chain q:

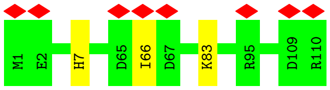




- Molecule 39: 50S ribosomal protein L22

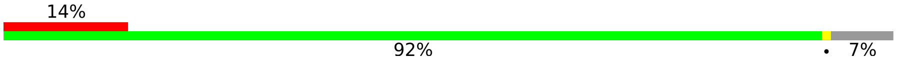
Chain r:

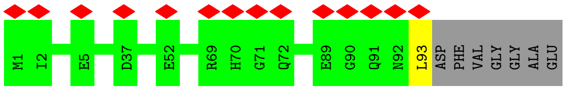




- Molecule 40: 50S ribosomal protein L23

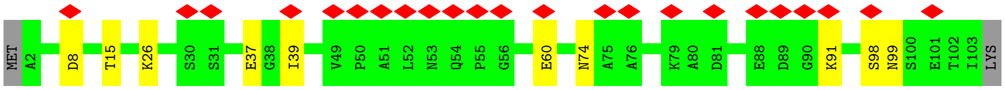
Chain s:





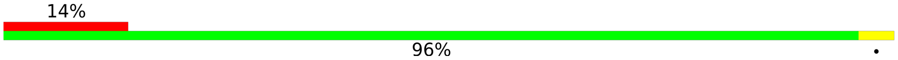
- Molecule 41: 50S ribosomal protein L24

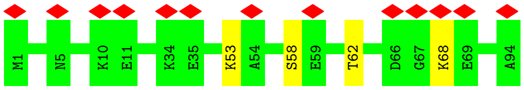
Chain t:



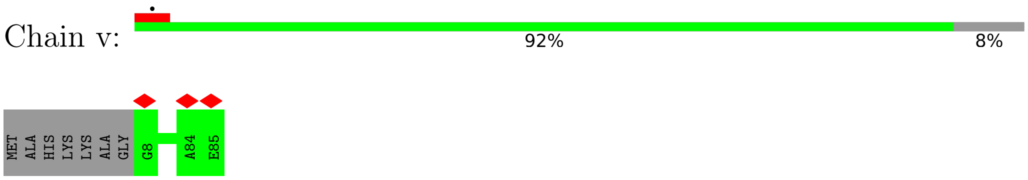
- Molecule 42: 50S ribosomal protein L25

Chain u:

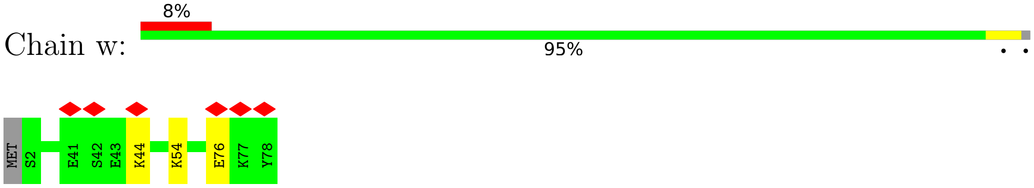




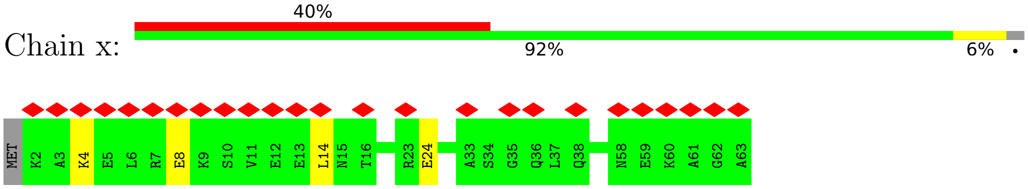
- Molecule 43: 50S ribosomal protein L27



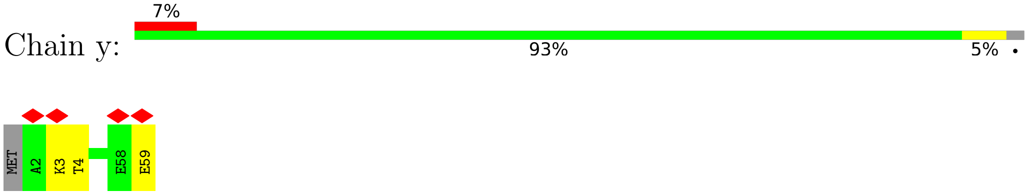
- Molecule 44: 50S ribosomal protein L28



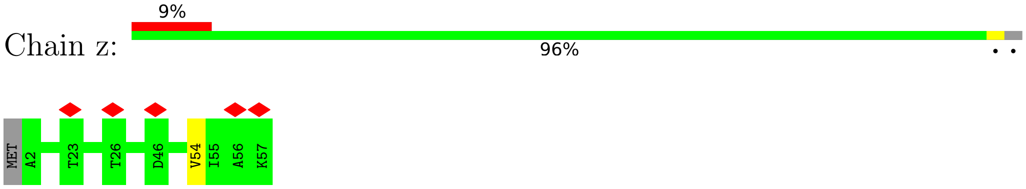
- Molecule 45: 50S ribosomal protein L29



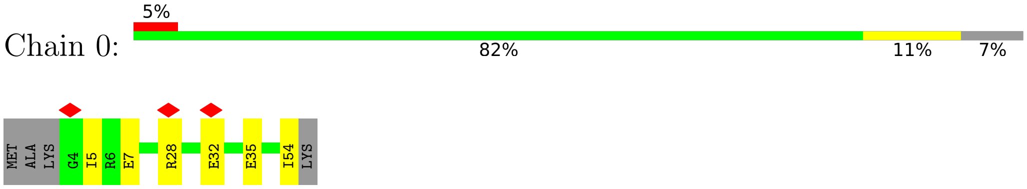
- Molecule 46: 50S ribosomal protein L30



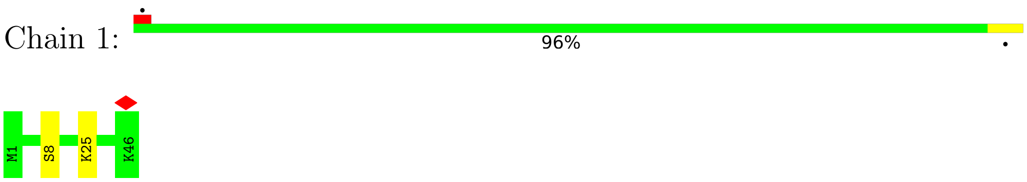
- Molecule 47: 50S ribosomal protein L32



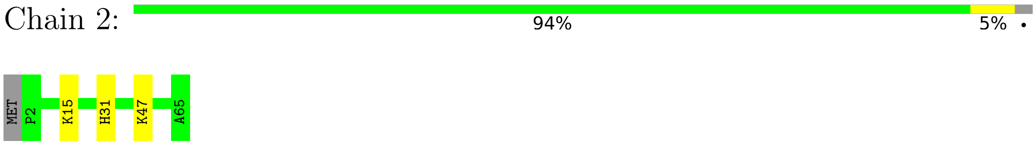
- Molecule 48: 50S ribosomal protein L33



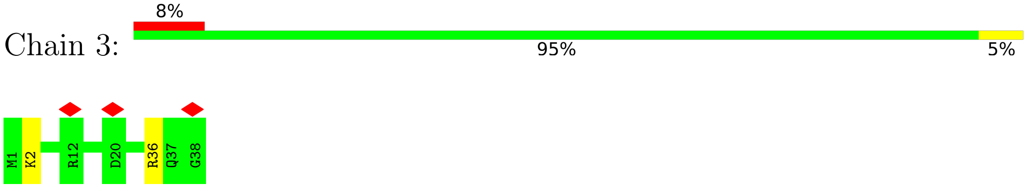
- Molecule 49: 50S ribosomal protein L34



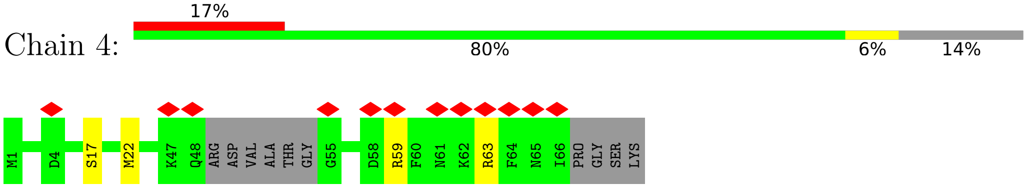
- Molecule 50: 50S ribosomal protein L35



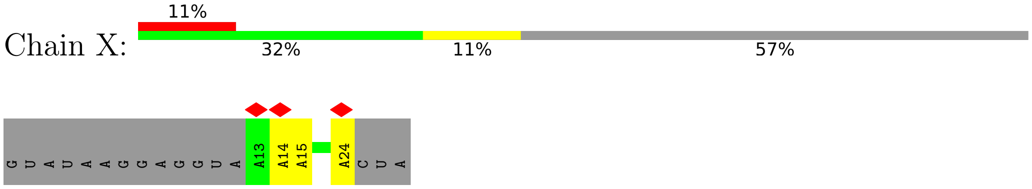
- Molecule 51: 50S ribosomal protein L36



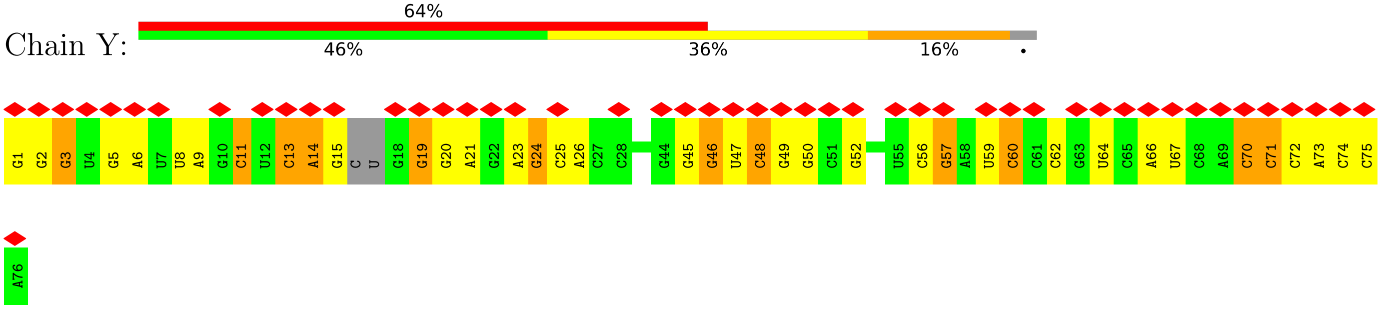
- Molecule 52: 50S ribosomal protein L31



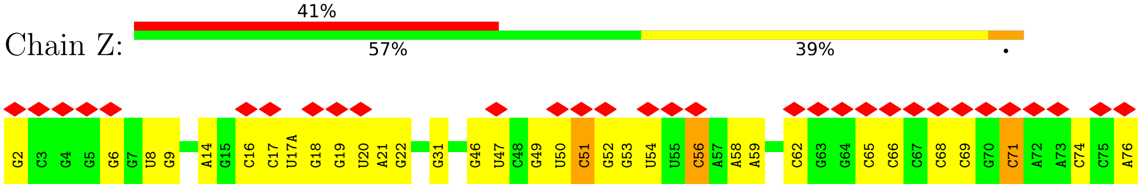
- Molecule 53: mRNA



- Molecule 54: A-site tRNA-val



- Molecule 55: P-site tRNA-fMet



- Molecule 56: E-site tRNA

Chain 5:

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	307495	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.341	Depositor
Minimum map value	-0.098	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	353.0528, 353.0528, 353.0528	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7118, 0.7118, 0.7118	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, H2U, MEQ, OMC, 2MG, PAR, SPD, OMU, D2T, 5MC, 4OC, OMG, IAS, 5MU, 1MG, SPM, G7M, ZN, 2MA, UR3, MG, PSU, 4D4, 6MZ, MS6, 3TD

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	0.46	0/36236	0.90	9/56520 (0.0%)
2	B	0.33	0/1784	0.50	0/2403
3	C	0.30	0/1651	0.47	0/2225
4	D	0.34	0/1665	0.50	0/2227
5	E	0.34	0/1165	0.55	0/1568
6	F	0.35	0/858	0.53	0/1160
7	G	0.33	0/1219	0.50	0/1635
8	H	0.32	0/989	0.51	0/1326
9	I	0.32	0/1034	0.48	0/1375
10	J	0.34	0/796	0.57	0/1077
11	K	0.34	0/884	0.51	0/1191
12	L	0.36	0/960	0.57	0/1286
13	M	0.40	0/900	0.57	0/1204
14	N	0.31	0/817	0.47	0/1088
15	O	0.38	0/722	0.53	0/964
16	P	0.32	0/653	0.52	0/877
17	Q	0.35	0/650	0.54	0/871
18	R	0.37	0/553	0.52	0/742
19	S	0.36	0/685	0.56	0/922
20	T	0.31	0/676	0.44	0/895
21	U	0.34	0/597	0.46	0/792
22	a	0.63	1/65651 (0.0%)	1.04	71/102413 (0.1%)
23	b	0.59	0/2850	0.91	1/4444 (0.0%)
24	c	0.38	0/2121	0.59	0/2852
25	d	0.33	0/1576	0.53	0/2119
26	e	0.37	0/1571	0.56	0/2113
27	f	0.37	0/1434	0.51	0/1926
28	g	0.34	0/1343	0.58	0/1816
29	h	0.37	0/306	0.61	0/413
30	i	0.35	0/1152	0.49	0/1551
31	j	0.36	0/955	0.58	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	k	0.39	0/1062	0.60	0/1413
33	l	0.39	0/1073	0.61	0/1433
34	m	0.34	0/958	0.54	0/1281
35	n	0.35	0/902	0.56	0/1209
36	o	0.35	0/929	0.56	0/1242
37	p	0.37	0/960	0.53	0/1278
38	q	0.38	0/829	0.60	0/1107
39	r	0.33	0/864	0.53	0/1156
40	s	0.37	0/744	0.56	0/994
41	t	0.36	0/787	0.58	0/1051
42	u	0.38	0/766	0.58	0/1025
43	v	0.39	0/593	0.60	0/785
44	w	0.39	0/635	0.61	0/848
45	x	0.36	0/502	0.53	0/667
46	y	0.34	0/453	0.58	0/605
47	z	0.34	0/450	0.52	0/599
48	0	0.42	0/424	0.62	0/565
49	1	0.33	0/380	0.57	0/498
50	2	0.41	0/513	0.59	0/676
51	3	0.36	0/303	0.56	0/397
52	4	0.30	0/488	0.48	0/649
53	X	0.49	0/292	0.88	0/453
54	Y	0.81	1/1764 (0.1%)	1.52	37/2747 (1.3%)
55	Z	0.67	0/1813	1.25	10/2825 (0.4%)
56	5	0.37	0/46	0.58	0/69
All	All	0.53	2/152983 (0.0%)	0.91	128/228846 (0.1%)

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
12	L	0	1
28	g	0	1
41	t	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	888	C	C2-N3	-5.22	1.31	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Y	24	G	C8-N7	-5.18	1.27	1.30

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	512	G	O4'-C1'-N9	11.53	117.42	108.20
22	a	880	G	N3-C2-N2	-10.92	112.26	119.90
54	Y	46	G	O4'-C1'-N9	9.16	115.53	108.20
22	a	846	U	N1-C2-O2	8.29	128.60	122.80
23	b	2	G	OP2-P-O3'	8.11	123.05	105.20
54	Y	24	G	C6-C5-N7	-7.72	125.77	130.40
55	Z	2	G	N3-C4-N9	-7.62	121.43	126.00
22	a	889	C	N1-C2-O2	-7.38	114.47	118.90
55	Z	51	C	C2-N1-C1'	7.33	126.86	118.80
1	A	1331	G	O4'-C1'-N9	7.27	114.02	108.20
54	Y	52	G	N3-C4-N9	-7.27	121.64	126.00
54	Y	72	C	C2-N1-C1'	7.26	126.79	118.80
54	Y	57	G	N3-C4-N9	-7.18	121.69	126.00
22	a	2501	C	C2-N1-C1'	-7.02	111.08	118.80
54	Y	52	G	N3-C4-C5	6.93	132.06	128.60
54	Y	71	C	N1-C2-O2	6.89	123.03	118.90
22	a	2321	U	N3-C2-O2	-6.79	117.44	122.20
54	Y	70	C	C2-N1-C1'	6.79	126.27	118.80
22	a	783	A	C2-N3-C4	6.75	113.98	110.60
22	a	1313	U	C2-N1-C1'	6.72	125.76	117.70
22	a	2321	U	N1-C2-O2	6.71	127.50	122.80
22	a	846	U	C2-N1-C1'	6.69	125.73	117.70
22	a	880	G	N1-C2-N2	6.67	122.20	116.20
22	a	984	A	O4'-C1'-N9	6.56	113.45	108.20
54	Y	3	G	N1-C6-O6	-6.55	115.97	119.90
22	a	2581	G	O4'-C1'-N9	6.54	113.44	108.20
22	a	2791	G	N3-C4-N9	-6.51	122.10	126.00
22	a	370	G	O4'-C1'-N9	-6.50	103.00	108.20
54	Y	3	G	C5-C6-O6	6.49	132.49	128.60
22	a	748	G	O4'-C1'-N9	6.46	113.37	108.20
55	Z	51	C	C6-N1-C1'	-6.46	113.05	120.80
22	a	1965	C	O5'-P-OP2	-6.44	99.90	105.70
55	Z	2	G	N9-C4-C5	6.37	107.95	105.40
54	Y	48	C	O5'-P-OP2	-6.37	99.97	105.70
22	a	1313	U	N1-C2-O2	6.35	127.25	122.80
55	Z	71	C	N1-C2-O2	-6.35	115.09	118.90
1	A	872	A	O4'-C1'-N9	6.31	113.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	Z	56	C	C2-N1-C1'	6.31	125.74	118.80
55	Z	2	G	N3-C2-N2	-6.30	115.49	119.90
22	a	2848	G	O4'-C1'-N9	6.21	113.17	108.20
22	a	880	G	C6-N1-C2	-6.18	121.39	125.10
54	Y	56	C	C6-N1-C2	6.17	122.77	120.30
54	Y	71	C	N3-C2-O2	-6.13	117.61	121.90
54	Y	13	C	N1-C2-O2	-6.09	115.25	118.90
55	Z	51	C	N1-C2-O2	6.07	122.54	118.90
54	Y	72	C	C6-N1-C1'	-6.05	113.54	120.80
22	a	846	U	N3-C2-O2	-6.04	117.97	122.20
54	Y	24	G	N9-C4-C5	-6.03	102.99	105.40
22	a	2501	C	C6-N1-C1'	6.00	128.00	120.80
22	a	1936	A	O4'-C1'-N9	5.97	112.97	108.20
22	a	704	G	O4'-C1'-N9	5.96	112.97	108.20
54	Y	60	C	C6-N1-C2	-5.96	117.92	120.30
54	Y	3	G	N3-C4-N9	-5.95	122.43	126.00
54	Y	72	C	N1-C2-O2	5.90	122.44	118.90
22	a	436	C	N3-C2-O2	-5.88	117.78	121.90
22	a	1533	C	C2-N1-C1'	5.87	125.26	118.80
22	a	880	G	N3-C4-N9	-5.86	122.48	126.00
22	a	205	G	O4'-C1'-N9	5.86	112.89	108.20
54	Y	46	G	N3-C4-N9	5.85	129.51	126.00
54	Y	3	G	C8-N9-C1'	5.81	134.56	127.00
22	a	395	U	O4'-C1'-N1	5.80	112.84	108.20
22	a	1313	U	N3-C2-O2	-5.74	118.18	122.20
22	a	1937	A	O4'-C1'-N9	5.71	112.77	108.20
22	a	2391	G	O4'-C1'-N9	5.68	112.75	108.20
54	Y	52	G	C4-N9-C1'	-5.67	119.12	126.50
54	Y	3	G	O4'-C1'-N9	5.66	112.73	108.20
22	a	1873	G	C6-C5-N7	-5.64	127.02	130.40
22	a	2566	A	O4'-C1'-N9	5.64	112.71	108.20
54	Y	14	A	C6-N1-C2	-5.62	115.23	118.60
1	A	74	A	O4'-C1'-N9	5.61	112.69	108.20
22	a	784	G	P-O3'-C3'	5.55	126.36	119.70
1	A	496	A	O4'-C1'-N9	5.54	112.63	108.20
22	a	912	C	N3-C4-C5	-5.54	119.69	121.90
22	a	283	G	N3-C2-N2	-5.52	116.04	119.90
22	a	436	C	N1-C2-O2	5.49	122.20	118.90
22	a	2791	G	N3-C4-C5	5.48	131.34	128.60
22	a	846	U	OP1-P-O3'	5.47	117.24	105.20
22	a	2645	G	O4'-C1'-N9	5.47	112.58	108.20
22	a	405	U	N1-C2-O2	5.46	126.62	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	Y	19	G	N1-C6-O6	-5.45	116.63	119.90
54	Y	70	C	C6-N1-C1’	-5.45	114.27	120.80
22	a	889	C	C2-N3-C4	-5.39	117.21	119.90
54	Y	24	G	C2-N3-C4	-5.38	109.21	111.90
54	Y	19	G	C5-C6-O6	5.38	131.82	128.60
54	Y	56	C	C5-C6-N1	-5.37	118.31	121.00
54	Y	74	C	N3-C4-N4	-5.36	114.25	118.00
22	a	775	G	O4’-C1’-N9	5.36	112.48	108.20
22	a	902	C	N3-C4-C5	5.35	124.04	121.90
22	a	883	G	N3-C4-N9	5.34	129.21	126.00
22	a	959	A	N1-C6-N6	-5.30	115.42	118.60
54	Y	62	C	C6-N1-C2	5.30	122.42	120.30
55	Z	56	C	C5-C6-N1	5.30	123.65	121.00
54	Y	52	G	C2-N3-C4	-5.29	109.25	111.90
54	Y	1	G	N3-C4-N9	5.29	129.17	126.00
54	Y	71	C	C2-N1-C1’	5.26	124.59	118.80
1	A	792	A	O4’-C1’-N9	5.26	112.41	108.20
22	a	275	C	C6-N1-C2	-5.25	118.20	120.30
22	a	1288	G	O4’-C1’-N9	5.23	112.39	108.20
54	Y	3	G	N9-C4-C5	5.23	107.49	105.40
1	A	438	U	O4’-C1’-N1	5.22	112.38	108.20
22	a	47	C	C2-N1-C1’	-5.22	113.06	118.80
22	a	283	G	N9-C4-C5	5.20	107.48	105.40
22	a	468	G	C2-N3-C4	5.20	114.50	111.90
22	a	889	C	C4-C5-C6	5.17	119.99	117.40
22	a	338	G	N1-C6-O6	5.16	123.00	119.90
22	a	883	G	C6-C5-N7	-5.16	127.30	130.40
22	a	1533	C	C5-C6-N1	5.16	123.58	121.00
22	a	12	U	C2-N1-C1’	5.14	123.87	117.70
22	a	880	G	C6-C5-N7	5.13	133.48	130.40
1	A	94	G	O4’-C1’-N9	-5.12	104.10	108.20
1	A	467	U	C2-N1-C1’	5.11	123.83	117.70
54	Y	71	C	C6-N1-C2	-5.11	118.25	120.30
55	Z	74	C	N1-C2-O2	-5.10	115.84	118.90
22	a	1324	G	O4’-C1’-N9	5.10	112.28	108.20
1	A	1305	G	O4’-C1’-N9	5.10	112.28	108.20
22	a	548	G	C8-N9-C4	-5.10	104.36	106.40
22	a	914	G	N3-C4-N9	5.10	129.06	126.00
22	a	27	G	O4’-C1’-N9	5.08	112.26	108.20
22	a	608	A	N1-C6-N6	5.07	121.64	118.60
22	a	1157	G	N3-C4-N9	5.06	129.04	126.00
22	a	1773	A	N9-C1’-C2’	-5.05	106.44	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	1873	G	N1-C6-O6	5.05	122.93	119.90
22	a	846	U	P-O3'-C3'	5.04	125.75	119.70
54	Y	11	C	N3-C4-C5	5.04	123.92	121.90
22	a	458	G	C8-N9-C4	5.03	108.41	106.40
22	a	108	G	C8-N9-C4	5.02	108.41	106.40
22	a	846	U	C6-N1-C1'	-5.01	114.19	121.20
22	a	2282	G	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	101	ALA	Peptide
28	g	47	ASP	Peptide
41	t	99	ASN	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	
2	B	222/241 (92%)	207 (93%)	15 (7%)	0	100	100
3	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
4	D	203/206 (98%)	194 (96%)	9 (4%)	0	100	100
5	E	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
6	F	101/135 (75%)	94 (93%)	7 (7%)	0	100	100
7	G	151/179 (84%)	137 (91%)	12 (8%)	2 (1%)	12	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	I	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
10	J	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	15	6
11	K	113/129 (88%)	107 (95%)	6 (5%)	0	100	100
12	L	120/124 (97%)	115 (96%)	4 (3%)	1 (1%)	19	9
13	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
14	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
15	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
17	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
18	R	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
19	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
20	T	84/87 (97%)	84 (100%)	0	0	100	100
21	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
24	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
25	d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
26	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
27	f	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
28	g	174/177 (98%)	151 (87%)	21 (12%)	2 (1%)	14	5
29	h	39/149 (26%)	32 (82%)	7 (18%)	0	100	100
30	i	140/142 (99%)	140 (100%)	0	0	100	100
31	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
32	k	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	22	11
33	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
34	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
35	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
36	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
37	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
38	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
39	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
40	s	91/100 (91%)	85 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
42	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
43	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
44	w	75/78 (96%)	75 (100%)	0	0	100	100
45	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
48	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
51	3	36/38 (95%)	36 (100%)	0	0	100	100
52	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
All	All	5481/5913 (93%)	5262 (96%)	212 (4%)	7 (0%)	54	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	6	VAL
28	g	47	ASP
10	J	57	VAL
7	G	5	ARG
12	L	102	LEU
32	k	138	ALA
28	g	92	VAL

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	
2	B	186/199 (94%)	168 (90%)	18 (10%)	8	1
3	C	170/190 (90%)	159 (94%)	11 (6%)	17	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	172/173 (99%)	152 (88%)	20 (12%)	5	1
5	E	119/126 (94%)	111 (93%)	8 (7%)	16	6
6	F	90/116 (78%)	81 (90%)	9 (10%)	7	1
7	G	126/147 (86%)	116 (92%)	10 (8%)	12	3
8	H	104/105 (99%)	101 (97%)	3 (3%)	42	31
9	I	105/107 (98%)	102 (97%)	3 (3%)	42	31
10	J	86/90 (96%)	83 (96%)	3 (4%)	36	24
11	K	89/98 (91%)	82 (92%)	7 (8%)	12	3
12	L	102/103 (99%)	98 (96%)	4 (4%)	32	19
13	M	93/96 (97%)	85 (91%)	8 (9%)	10	2
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	69 (91%)	7 (9%)	9	2
16	P	65/65 (100%)	62 (95%)	3 (5%)	27	14
17	Q	73/78 (94%)	66 (90%)	7 (10%)	8	1
18	R	57/65 (88%)	53 (93%)	4 (7%)	15	6
19	S	72/79 (91%)	69 (96%)	3 (4%)	30	17
20	T	65/66 (98%)	59 (91%)	6 (9%)	9	2
21	U	60/61 (98%)	55 (92%)	5 (8%)	11	3
24	c	216/218 (99%)	212 (98%)	4 (2%)	57	50
25	d	163/163 (100%)	162 (99%)	1 (1%)	86	85
26	e	165/165 (100%)	154 (93%)	11 (7%)	16	6
27	f	148/150 (99%)	138 (93%)	10 (7%)	16	6
28	g	137/138 (99%)	114 (83%)	23 (17%)	2	0
29	h	32/114 (28%)	29 (91%)	3 (9%)	8	2
30	i	116/116 (100%)	114 (98%)	2 (2%)	60	53
31	j	104/104 (100%)	98 (94%)	6 (6%)	20	9
32	k	103/103 (100%)	99 (96%)	4 (4%)	32	19
33	l	107/107 (100%)	103 (96%)	4 (4%)	34	22
34	m	98/103 (95%)	97 (99%)	1 (1%)	76	73
35	n	86/87 (99%)	79 (92%)	7 (8%)	11	3
36	o	99/100 (99%)	95 (96%)	4 (4%)	31	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	p	89/90 (99%)	85 (96%)	4 (4%)	27	15
38	q	84/84 (100%)	79 (94%)	5 (6%)	19	8
39	r	93/93 (100%)	90 (97%)	3 (3%)	39	28
40	s	80/84 (95%)	79 (99%)	1 (1%)	69	64
41	t	83/85 (98%)	74 (89%)	9 (11%)	6	1
42	u	78/78 (100%)	74 (95%)	4 (5%)	24	12
43	v	58/63 (92%)	58 (100%)	0	100	100
44	w	67/68 (98%)	64 (96%)	3 (4%)	27	15
45	x	54/55 (98%)	50 (93%)	4 (7%)	13	5
46	y	48/49 (98%)	45 (94%)	3 (6%)	18	7
47	z	47/48 (98%)	46 (98%)	1 (2%)	53	47
48	0	46/49 (94%)	40 (87%)	6 (13%)	4	1
49	1	38/38 (100%)	36 (95%)	2 (5%)	22	10
50	2	51/52 (98%)	48 (94%)	3 (6%)	19	8
51	3	34/34 (100%)	32 (94%)	2 (6%)	19	8
52	4	55/62 (89%)	51 (93%)	4 (7%)	14	5
All	All	4572/4825 (95%)	4299 (94%)	273 (6%)	23	8

All (273) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	ARG
2	B	8	ASP
2	B	20	THR
2	B	23	TRP
2	B	58	ASN
2	B	62	SER
2	B	63	ARG
2	B	93	ASN
2	B	117	LEU
2	B	127	ASP
2	B	131	LYS
2	B	133	GLU
2	B	143	LYS
2	B	152	LYS
2	B	188	ASP

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Mol	Chain	Res	Type
2	B	205	ASP
2	B	208	ARG
2	B	211	THR
3	C	75	ILE
3	C	79	LYS
3	C	93	ASP
3	C	107	ARG
3	C	111	LEU
3	C	129	MET
3	C	147	LYS
3	C	170	GLU
3	C	178	LEU
3	C	185	ASN
3	C	206	GLU
4	D	8	LYS
4	D	18	ASP
4	D	25	VAL
4	D	26	ARG
4	D	29	ASP
4	D	34	ILE
4	D	48	LEU
4	D	50	ASP
4	D	85	ASN
4	D	138	SER
4	D	146	ARG
4	D	148	LYS
4	D	166	GLU
4	D	167	LYS
4	D	181	THR
4	D	184	ARG
4	D	188	ARG
4	D	192	SER
4	D	202	GLU
4	D	206	LYS
5	E	22	SER
5	E	23	LYS
5	E	45	ARG
5	E	64	MET
5	E	73	ASN
5	E	82	GLN
5	E	145	GLU
5	E	156	LYS

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Mol	Chain	Res	Type
6	F	2	ARG
6	F	15	SER
6	F	21	MET
6	F	53	LYS
6	F	62	MET
6	F	82	ASP
6	F	93	LYS
6	F	102	MET
6	F	103	VAL
7	G	9	GLN
7	G	41	SER
7	G	72	THR
7	G	77	SER
7	G	89	VAL
7	G	92	ARG
7	G	111	ARG
7	G	113	ASP
7	G	140	ASP
7	G	144	MET
8	H	38	ASN
8	H	56	LYS
8	H	94	LYS
9	I	33	ARG
9	I	100	LYS
9	I	123	ARG
10	J	7	ARG
10	J	27	GLU
10	J	28	THR
11	K	14	LYS
11	K	17	SER
11	K	36	ASP
11	K	55	SER
11	K	72	ASP
11	K	87	LYS
11	K	129	VAL
12	L	14	ARG
12	L	54	ARG
12	L	55	VAL
12	L	109	ASP
13	M	3	ARG
13	M	7	ILE
13	M	11	ASP

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Mol	Chain	Res	Type
13	M	16	VAL
13	M	27	LYS
13	M	49	SER
13	M	82	ASP
13	M	114	LYS
15	O	14	GLU
15	O	17	ARG
15	O	18	ASP
15	O	26	GLU
15	O	47	LYS
15	O	64	ARG
15	O	73	LYS
16	P	1	MET
16	P	47	GLU
16	P	48	GLU
17	Q	5	ILE
17	Q	16	LYS
17	Q	27	ARG
17	Q	41	THR
17	Q	42	THR
17	Q	50	ASN
17	Q	65	ARG
18	R	14	THR
18	R	35	GLU
18	R	36	SER
18	R	50	LYS
19	S	24	GLU
19	S	43	ASN
19	S	64	ASP
20	T	6	SER
20	T	13	GLN
20	T	44	LYS
20	T	49	LYS
20	T	54	MET
20	T	85	LYS
21	U	4	ILE
21	U	8	GLU
21	U	44	GLU
21	U	51	SER
21	U	60	LEU
24	c	37	ASN
24	c	197	ASN

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Mol	Chain	Res	Type
24	c	242	LYS
24	c	272	SER
25	d	12	THR
26	e	4	VAL
26	e	9	GLN
26	e	14	VAL
26	e	21	ARG
26	e	107	SER
26	e	114	ARG
26	e	123	LYS
26	e	146	VAL
26	e	150	THR
26	e	153	LEU
26	e	198	GLU
27	f	11	GLU
27	f	30	ARG
27	f	47	LYS
27	f	64	LYS
27	f	69	LYS
27	f	112	ARG
27	f	120	LYS
27	f	150	ARG
27	f	152	LEU
27	f	165	GLU
28	g	3	ARG
28	g	18	LYS
28	g	20	ASN
28	g	34	THR
28	g	36	THR
28	g	42	GLU
28	g	43	VAL
28	g	49	THR
28	g	73	ASN
28	g	75	MET
28	g	76	VAL
28	g	79	VAL
28	g	86	LYS
28	g	95	ARG
28	g	103	ILE
28	g	122	THR
28	g	127	THR
28	g	129	THR

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Mol	Chain	Res	Type
28	g	133	LEU
28	g	134	LYS
28	g	171	THR
28	g	173	GLU
28	g	175	LYS
29	h	17	ASP
29	h	21	VAL
29	h	25	TYR
30	i	11	VAL
30	i	141	ASP
31	j	49	ARG
31	j	58	LEU
31	j	88	ASN
31	j	109	SER
31	j	114	LYS
31	j	123	LEU
32	k	115	GLU
32	k	117	THR
32	k	118	THR
32	k	144	GLU
33	l	7	THR
33	l	8	LYS
33	l	25	ASP
33	l	78	LEU
34	m	6	SER
35	n	2	ASP
35	n	13	ARG
35	n	16	ARG
35	n	45	SER
35	n	56	LYS
35	n	85	LYS
35	n	89	ASP
36	o	39	ARG
36	o	53	ARG
36	o	63	LYS
36	o	103	ARG
37	p	13	ARG
37	p	51	ARG
37	p	87	SER
37	p	112	LYS
38	q	26	ASP
38	q	33	VAL

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Mol	Chain	Res	Type
38	q	47	VAL
38	q	55	ASP
38	q	102	SER
39	r	7	HIS
39	r	66	ILE
39	r	83	LYS
40	s	93	LEU
41	t	8	ASP
41	t	15	THR
41	t	26	LYS
41	t	37	GLU
41	t	39	ILE
41	t	60	GLU
41	t	74	ASN
41	t	91	LYS
41	t	98	SER
42	u	53	LYS
42	u	58	SER
42	u	62	THR
42	u	68	LYS
44	w	44	LYS
44	w	54	LYS
44	w	76	GLU
45	x	4	LYS
45	x	8	GLU
45	x	14	LEU
45	x	24	GLU
46	y	3	LYS
46	y	4	THR
46	y	59	GLU
47	z	54	VAL
48	0	5	ILE
48	0	7	GLU
48	0	28	ARG
48	0	32	GLU
48	0	35	GLU
48	0	54	ILE
49	1	8	SER
49	1	25	LYS
50	2	15	LYS
50	2	31	HIS
50	2	47	LYS

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Mol	Chain	Res	Type
51	3	2	LYS
51	3	36	ARG
52	4	17	SER
52	4	22	MET
52	4	59	ARG
52	4	63	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	39	HIS
2	B	58	ASN
2	B	89	GLN
2	B	103	ASN
2	B	109	GLN
3	C	100	GLN
3	C	123	GLN
3	C	140	ASN
4	D	40	GLN
4	D	71	GLN
4	D	100	ASN
4	D	131	ASN
4	D	136	GLN
4	D	140	ASN
4	D	152	GLN
4	D	196	ASN
5	E	73	ASN
5	E	82	GLN
5	E	146	ASN
6	F	46	GLN
7	G	68	ASN
9	I	31	ASN
10	J	56	HIS
11	K	24	HIS
12	L	112	GLN
13	M	8	ASN
13	M	12	HIS
14	N	35	ASN
14	N	43	ASN
14	N	66	GLN
15	O	35	GLN
15	O	40	GLN

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Mol	Chain	Res	Type
16	P	63	GLN
19	S	52	HIS
19	S	56	GLN
19	S	83	HIS
20	T	48	GLN
20	T	68	HIS
20	T	84	ASN
24	c	115	GLN
24	c	117	GLN
24	c	197	ASN
24	c	243	HIS
26	e	136	GLN
28	g	38	ASN
28	g	48	ASN
28	g	115	HIS
28	g	139	GLN
29	h	20	ASN
30	i	47	HIS
30	i	128	ASN
31	j	93	GLN
33	l	13	HIS
33	l	60	GLN
34	m	18	GLN
34	m	31	HIS
36	o	10	GLN
36	o	12	GLN
37	p	37	GLN
37	p	52	GLN
38	q	6	GLN
38	q	43	ASN
39	r	7	HIS
39	r	31	GLN
40	s	48	GLN
40	s	92	ASN
41	t	40	ASN
41	t	53	ASN
41	t	74	ASN
42	u	5	ASN
43	v	57	HIS
44	w	6	GLN
44	w	20	HIS
44	w	36	HIS

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Mol	Chain	Res	Type
45	x	15	ASN
45	x	31	GLN
46	y	20	HIS
47	z	42	HIS
50	2	31	HIS
52	4	20	ASN
52	4	30	HIS
52	4	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1542 (98%)	218 (14%)	6 (0%)
22	a	2745/2904 (94%)	346 (12%)	0
23	b	118/120 (98%)	13 (11%)	0
53	X	11/28 (39%)	3 (27%)	0
54	Y	72/76 (94%)	32 (44%)	3 (4%)
55	Z	75/76 (98%)	31 (41%)	1 (1%)
56	5	1/2 (50%)	1 (100%)	0
All	All	4535/4748 (95%)	644 (14%)	10 (0%)

All (644) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	74	A
1	A	75	G
1	A	80	A
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G

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Mol	Chain	Res	Type
1	A	87	C
1	A	88	U
1	A	89	U
1	A	94	G
1	A	95	C
1	A	96	U
1	A	121	U
1	A	122	G
1	A	131	A
1	A	141	G
1	A	144	G
1	A	146	G
1	A	149	A
1	A	166	U
1	A	177	G
1	A	181	A
1	A	182	A
1	A	183	C
1	A	189	A
1	A	197	A
1	A	202	G
1	A	203	G
1	A	204	G
1	A	226	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	271	C
1	A	280	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	345	C
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A

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Mol	Chain	Res	Type
1	A	384	G
1	A	398	U
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	415	A
1	A	417	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	436	C
1	A	446	G
1	A	453	G
1	A	456	A
1	A	457	G
1	A	458	U
1	A	459	A
1	A	463	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	474	G
1	A	478	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	490	C
1	A	495	A
1	A	511	C
1	A	518	C
1	A	531	U
1	A	547	A
1	A	559	A
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G

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Mol	Chain	Res	Type
1	A	579	A
1	A	596	A
1	A	615	G
1	A	633	G
1	A	648	A
1	A	650	G
1	A	653	U
1	A	665	A
1	A	702	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	746	A
1	A	747	A
1	A	748	G
1	A	755	G
1	A	774	G
1	A	777	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	832	G
1	A	840	C
1	A	890	G
1	A	914	A
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	984	C
1	A	993	G
1	A	997	U
1	A	998	C
1	A	1004	A
1	A	1006	G
1	A	1008	U

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Mol	Chain	Res	Type
1	A	1009	U
1	A	1027	C
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1036	A
1	A	1037	C
1	A	1043	G
1	A	1044	A
1	A	1045	C
1	A	1046	A
1	A	1065	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1137	C
1	A	1139	G
1	A	1143	G
1	A	1144	G
1	A	1159	U
1	A	1169	A
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1256	A
1	A	1258	G
1	A	1275	A
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1302	C
1	A	1317	C
1	A	1320	C
1	A	1338	G

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Mol	Chain	Res	Type
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1380	U
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1419	G
1	A	1427	C
1	A	1432	G
1	A	1440	U
1	A	1441	A
1	A	1442	G
1	A	1444	U
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1479	C
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1503	A
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A
22	a	10	A
22	a	15	G
22	a	34	U
22	a	42	A
22	a	45	G
22	a	58	G
22	a	71	A
22	a	74	A
22	a	75	G

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Mol	Chain	Res	Type
22	a	84	A
22	a	101	A
22	a	102	U
22	a	110	G
22	a	118	A
22	a	119	A
22	a	120	U
22	a	139	U
22	a	140	C
22	a	163	C
22	a	165	A
22	a	181	A
22	a	196	A
22	a	215	G
22	a	216	A
22	a	221	A
22	a	222	A
22	a	231	A
22	a	248	G
22	a	264	C
22	a	265	A
22	a	272	A
22	a	274	C
22	a	278	A
22	a	279	A
22	a	280	U
22	a	282	A
22	a	285	G
22	a	286	U
22	a	289	G
22	a	292	U
22	a	294	A
22	a	311	A
22	a	329	G
22	a	330	A
22	a	345	A
22	a	357	C
22	a	361	G
22	a	362	A
22	a	386	G
22	a	405	U
22	a	406	G

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Mol	Chain	Res	Type
22	a	411	G
22	a	412	A
22	a	451	U
22	a	481	G
22	a	491	G
22	a	504	A
22	a	505	A
22	a	508	A
22	a	509	C
22	a	530	G
22	a	531	C
22	a	532	A
22	a	533	G
22	a	543	G
22	a	544	C
22	a	545	U
22	a	546	U
22	a	548	G
22	a	549	G
22	a	563	A
22	a	573	U
22	a	575	A
22	a	603	A
22	a	614	A
22	a	615	U
22	a	627	A
22	a	637	A
22	a	645	C
22	a	646	U
22	a	647	G
22	a	653	U
22	a	654	A
22	a	685	A
22	a	686	U
22	a	714	U
22	a	717	C
22	a	721	A
22	a	730	A
22	a	747	5MU
22	a	764	A
22	a	775	G
22	a	776	G

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Mol	Chain	Res	Type
22	a	782	A
22	a	784	G
22	a	785	G
22	a	792	A
22	a	805	G
22	a	812	C
22	a	827	U
22	a	828	U
22	a	846	U
22	a	847	U
22	a	856	G
22	a	859	G
22	a	869	G
22	a	879	G
22	a	882	G
22	a	883	G
22	a	884	U
22	a	885	C
22	a	888	C
22	a	890	C
22	a	891	G
22	a	895	U
22	a	896	A
22	a	897	C
22	a	898	C
22	a	899	A
22	a	905	A
22	a	910	A
22	a	914	G
22	a	915	C
22	a	934	U
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	996	A
22	a	1012	U
22	a	1013	C
22	a	1017	G
22	a	1033	U
22	a	1041	G
22	a	1045	C

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Mol	Chain	Res	Type
22	a	1046	A
22	a	1047	G
22	a	1048	A
22	a	1051	G
22	a	1108	U
22	a	1111	A
22	a	1112	G
22	a	1115	G
22	a	1116	G
22	a	1120	G
22	a	1122	G
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1142	A
22	a	1171	G
22	a	1227	G
22	a	1253	A
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1273	U
22	a	1294	U
22	a	1300	G
22	a	1301	A
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1409	U
22	a	1411	U
22	a	1416	G
22	a	1417	C
22	a	1420	A
22	a	1421	G
22	a	1427	A
22	a	1428	C
22	a	1452	G
22	a	1453	A
22	a	1468	U
22	a	1476	U
22	a	1482	G

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Mol	Chain	Res	Type
22	a	1486	U
22	a	1487	U
22	a	1493	C
22	a	1497	U
22	a	1504	A
22	a	1506	U
22	a	1508	A
22	a	1509	A
22	a	1510	G
22	a	1515	A
22	a	1529	G
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1559	U
22	a	1566	A
22	a	1569	A
22	a	1578	U
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1586	A
22	a	1590	A
22	a	1593	A
22	a	1608	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1674	G
22	a	1715	G
22	a	1722	A
22	a	1729	U
22	a	1730	C
22	a	1731	G
22	a	1732	C
22	a	1733	G
22	a	1736	U
22	a	1738	G
22	a	1750	G
22	a	1764	C
22	a	1773	A

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Mol	Chain	Res	Type
22	a	1782	U
22	a	1800	C
22	a	1801	A
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1847	A
22	a	1858	A
22	a	1859	U
22	a	1866	A
22	a	1867	G
22	a	1868	C
22	a	1870	C
22	a	1871	A
22	a	1873	G
22	a	1906	G
22	a	1907	G
22	a	1929	G
22	a	1930	G
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1993	U
22	a	2023	C
22	a	2031	A
22	a	2033	A
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2194	U
22	a	2198	A
22	a	2203	U
22	a	2204	G

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Mol	Chain	Res	Type
22	a	2208	C
22	a	2211	A
22	a	2223	G
22	a	2225	A
22	a	2238	G
22	a	2268	A
22	a	2279	G
22	a	2283	C
22	a	2287	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2335	A
22	a	2347	C
22	a	2350	C
22	a	2361	G
22	a	2377	A
22	a	2383	G
22	a	2385	C
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2424	C
22	a	2425	A
22	a	2429	G
22	a	2431	U
22	a	2435	A
22	a	2441	U
22	a	2448	A
22	a	2470	G
22	a	2476	A
22	a	2480	C
22	a	2491	U
22	a	2502	G
22	a	2504	PSU
22	a	2505	G
22	a	2518	A
22	a	2529	G
22	a	2535	G
22	a	2547	A

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Mol	Chain	Res	Type
22	a	2554	U
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2585	U
22	a	2586	U
22	a	2602	A
22	a	2603	G
22	a	2609	U
22	a	2613	U
22	a	2629	U
22	a	2630	G
22	a	2670	A
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2716	C
22	a	2726	A
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2751	G
22	a	2752	C
22	a	2757	A
22	a	2765	A
22	a	2778	A
22	a	2790	U
22	a	2792	A
22	a	2795	C
22	a	2798	U
22	a	2799	A
22	a	2802	G
22	a	2820	A
22	a	2821	A
22	a	2835	A
22	a	2861	U
22	a	2873	A
22	a	2883	A
22	a	2884	U
22	a	2891	U
22	a	2899	A
22	a	2901	C

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Mol	Chain	Res	Type
22	a	2902	C
23	b	9	G
23	b	13	G
23	b	34	A
23	b	35	C
23	b	36	C
23	b	45	A
23	b	56	G
23	b	57	A
23	b	67	G
23	b	89	U
23	b	90	C
23	b	99	A
23	b	109	A
53	X	14	A
53	X	15	A
53	X	24	A
54	Y	2	G
54	Y	3	G
54	Y	5	G
54	Y	6	A
54	Y	8	U
54	Y	9	A
54	Y	11	C
54	Y	13	C
54	Y	14	A
54	Y	15	G
54	Y	19	G
54	Y	20	G
54	Y	21	A
54	Y	23	A
54	Y	24	G
54	Y	25	C
54	Y	26	A
54	Y	45	G
54	Y	46	G
54	Y	47	U
54	Y	48	C
54	Y	49	G
54	Y	50	G
54	Y	57	G
54	Y	59	U

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Mol	Chain	Res	Type
54	Y	64	U
54	Y	66	A
54	Y	67	U
54	Y	70	C
54	Y	71	C
54	Y	73	A
54	Y	75	C
55	Z	6	G
55	Z	8	U
55	Z	9	G
55	Z	14	A
55	Z	16	C
55	Z	17	C
55	Z	17(A)	U
55	Z	18	G
55	Z	19	G
55	Z	20	U
55	Z	21	A
55	Z	22	G
55	Z	31	G
55	Z	46	G
55	Z	47	U
55	Z	49	G
55	Z	50	U
55	Z	51	C
55	Z	52	G
55	Z	53	G
55	Z	54	U
55	Z	56	C
55	Z	58	A
55	Z	59	A
55	Z	62	C
55	Z	65	C
55	Z	66	C
55	Z	68	C
55	Z	69	C
55	Z	71	C
55	Z	76	A
56	5	76	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	250	A
1	A	467	U
1	A	575	G
1	A	1026	G
1	A	1035	A
54	Y	13	C
54	Y	45	G
54	Y	60	C
55	Z	58	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	G7M	a	2069	22	20,26,27	1.13	2 (10%)	17,39,42	0.79	0
22	OMU	a	2552	22	19,22,23	1.20	2 (10%)	26,31,34	1.73	5 (19%)
25	MEQ	d	150	25	8,9,10	0.44	0	5,10,12	0.25	0
1	5MC	A	1407	1	18,22,23	0.98	2 (11%)	26,32,35	1.17	2 (7%)
1	G7M	A	527	1	20,26,27	1.22	2 (10%)	17,39,42	0.75	0
12	D2T	L	89	12	7,9,10	1.96	2 (28%)	6,11,13	1.48	1 (16%)
11	IAS	K	119	11	6,7,8	1.37	1 (16%)	6,8,10	0.87	0
22	PSU	a	955	22	18,21,22	1.39	3 (16%)	22,30,33	1.93	4 (18%)
1	4OC	A	1402	1	20,23,24	0.67	0	26,32,35	0.98	1 (3%)
22	PSU	a	2504	22	18,21,22	1.45	3 (16%)	22,30,33	1.74	5 (22%)
22	6MZ	a	1618	22	18,25,26	0.82	0	16,36,39	2.18	4 (25%)
22	PSU	a	1911	22	18,21,22	1.33	2 (11%)	22,30,33	1.77	3 (13%)
22	OMG	a	2251	22,55	18,26,27	0.96	1 (5%)	19,38,41	1.04	2 (10%)
22	6MZ	a	2030	22	18,25,26	0.87	1 (5%)	16,36,39	2.64	5 (31%)
1	2MG	A	1516	1	18,26,27	0.89	1 (5%)	16,38,41	1.17	3 (18%)
1	MA6	A	1518	1	19,26,27	0.93	1 (5%)	18,38,41	1.48	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
22	2MG	a	1835	22	18,26,27	0.92	1 (5%)	16,38,41	1.18	3 (18%)
22	OMC	a	2498	22,58	19,22,23	0.81	1 (5%)	26,31,34	0.85	0
22	PSU	a	1917	22	18,21,22	1.44	3 (16%)	22,30,33	1.91	5 (22%)
22	2MG	a	2445	22	18,26,27	0.94	1 (5%)	16,38,41	1.03	2 (12%)
22	2MA	a	2503	22,58	17,25,26	0.95	1 (5%)	17,37,40	1.13	2 (11%)
22	PSU	a	2604	22	18,21,22	1.46	1 (5%)	22,30,33	1.38	3 (13%)
22	1MG	a	745	22	18,26,27	0.66	0	19,39,42	1.00	2 (10%)
22	5MC	a	1962	22	18,22,23	0.91	2 (11%)	26,32,35	1.19	3 (11%)
22	PSU	a	2457	22	18,21,22	1.43	2 (11%)	22,30,33	1.92	3 (13%)
22	PSU	a	746	22,58	18,21,22	1.35	3 (16%)	22,30,33	1.95	5 (22%)
1	2MG	A	1207	1	18,26,27	0.85	1 (5%)	16,38,41	1.13	2 (12%)
33	4D4	l	81	33	9,11,12	1.87	2 (22%)	8,13,15	1.30	0
22	3TD	a	1915	22	18,22,23	1.60	4 (22%)	22,32,35	2.16	5 (22%)
1	UR3	A	1498	1	19,22,23	0.86	1 (5%)	26,32,35	1.39	3 (11%)
1	2MG	A	966	1	18,26,27	0.85	1 (5%)	16,38,41	1.22	3 (18%)
1	5MC	A	967	1	18,22,23	0.90	2 (11%)	26,32,35	1.10	3 (11%)
22	5MU	a	1939	22	19,22,23	1.49	5 (26%)	28,32,35	2.32	6 (21%)
1	MA6	A	1519	1	19,26,27	0.98	1 (5%)	18,38,41	1.53	4 (22%)
22	PSU	a	2580	22	18,21,22	1.40	3 (16%)	22,30,33	1.87	4 (18%)
1	PSU	A	516	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	4 (18%)
22	PSU	a	2605	22	18,21,22	1.30	2 (11%)	22,30,33	2.10	4 (18%)
22	5MU	a	747	22	19,22,23	1.47	6 (31%)	28,32,35	2.09	6 (21%)
22	H2U	a	2449	22	18,21,22	1.18	2 (11%)	21,30,33	1.39	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	G7M	a	2069	22	-	1/3/25/26	0/3/3/3
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
25	MEQ	d	150	25	-	2/8/9/11	-
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1	-	1/3/25/26	0/3/3/3
12	D2T	L	89	12	-	5/7/12/14	-
11	IAS	K	119	11	-	0/7/7/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
22	PSU	a	2504	22	-	2/7/25/26	0/2/2/2
22	6MZ	a	1618	22	-	0/5/27/28	0/3/3/3
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
22	OMG	a	2251	22,55	-	0/5/27/28	0/3/3/3
22	6MZ	a	2030	22	-	2/5/27/28	0/3/3/3
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
22	2MG	a	1835	22	-	0/5/27/28	0/3/3/3
22	OMC	a	2498	22,58	-	0/9/27/28	0/2/2/2
22	PSU	a	1917	22	-	1/7/25/26	0/2/2/2
22	2MG	a	2445	22	-	1/5/27/28	0/3/3/3
22	2MA	a	2503	22,58	-	2/3/25/26	0/3/3/3
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
22	1MG	a	745	22	-	0/3/25/26	0/3/3/3
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	a	746	22,58	-	3/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
33	4D4	l	81	33	-	1/11/12/14	-
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	1/5/27/28	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	2/7/29/30	0/3/3/3
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
22	5MU	a	747	22	-	1/7/25/26	0/2/2/2
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2604	PSU	C2-N1	5.04	1.43	1.36
12	L	89	D2T	CB-CG	4.08	1.59	1.52
33	l	81	4D4	CZ-NE	4.01	1.41	1.33
22	a	2457	PSU	C6-C5	3.71	1.39	1.35
22	a	2504	PSU	C6-C5	3.69	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1911	PSU	C6-C5	3.57	1.39	1.35
1	A	516	PSU	C6-C5	3.57	1.39	1.35
22	a	1915	3TD	C4-N3	-3.50	1.32	1.40
22	a	1915	3TD	C10-N3	3.27	1.53	1.47
22	a	1917	PSU	C4-N3	-3.25	1.32	1.38
22	a	746	PSU	C6-C5	3.25	1.39	1.35
22	a	2605	PSU	C4-N3	-3.21	1.32	1.38
1	A	527	G7M	C5-C4	3.20	1.45	1.39
22	a	1915	3TD	C6-C5	3.11	1.38	1.35
22	a	2580	PSU	C6-C5	3.11	1.38	1.35
22	a	1917	PSU	C6-C5	3.07	1.38	1.35
22	a	955	PSU	C4-N3	-3.06	1.33	1.38
22	a	2069	G7M	C5-C4	2.98	1.45	1.39
22	a	2605	PSU	C6-C5	2.97	1.38	1.35
22	a	2504	PSU	C4-N3	-2.94	1.33	1.38
22	a	747	5MU	C6-C5	2.89	1.39	1.34
22	a	2457	PSU	C4-N3	-2.88	1.33	1.38
22	a	1939	5MU	C6-N1	-2.86	1.33	1.38
33	l	81	4D4	CZ-NH2	2.85	1.43	1.32
1	A	1407	5MC	C6-C5	2.85	1.39	1.34
22	a	2449	H2U	C2-N3	-2.84	1.32	1.38
22	a	1911	PSU	C4-N3	-2.82	1.33	1.38
22	a	2580	PSU	C4-N3	-2.82	1.33	1.38
22	a	1835	2MG	C6-N1	-2.81	1.33	1.37
22	a	1939	5MU	C6-C5	2.81	1.39	1.34
22	a	747	5MU	C4-N3	-2.76	1.33	1.38
22	a	955	PSU	C6-C5	2.76	1.38	1.35
22	a	1939	5MU	C4-N3	-2.75	1.33	1.38
22	a	2449	H2U	C4-N3	-2.75	1.32	1.37
11	K	119	IAS	CB-CG	2.74	1.56	1.49
22	a	1939	5MU	C2-N3	-2.70	1.33	1.38
22	a	747	5MU	C4-C5	2.66	1.49	1.44
22	a	2552	OMU	C4-N3	-2.65	1.33	1.38
22	a	1962	5MC	C6-N1	-2.64	1.33	1.38
22	a	2445	2MG	C6-N1	-2.64	1.33	1.37
22	a	1917	PSU	C2-N3	-2.63	1.33	1.37
1	A	1516	2MG	C6-N1	-2.62	1.34	1.37
22	a	2251	OMG	C6-N1	-2.61	1.34	1.37
1	A	1519	MA6	C5-C4	2.60	1.47	1.40
1	A	516	PSU	C4-N3	-2.60	1.34	1.38
22	a	2552	OMU	C2-N3	-2.50	1.33	1.38
22	a	1939	5MU	C4-C5	2.48	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	89	D2T	CB-SB	2.46	1.84	1.82
1	A	967	5MC	C6-C5	2.44	1.38	1.34
22	a	746	PSU	C4-N3	-2.43	1.34	1.38
1	A	527	G7M	C6-N1	-2.36	1.34	1.37
22	a	2580	PSU	C2-N3	-2.36	1.33	1.37
1	A	967	5MC	C6-N1	-2.36	1.34	1.38
22	a	2069	G7M	C6-N1	-2.33	1.34	1.37
22	a	747	5MU	C6-N1	-2.31	1.34	1.38
22	a	747	5MU	C2-N3	-2.31	1.33	1.38
1	A	966	2MG	C6-N1	-2.30	1.34	1.37
22	a	2504	PSU	C2-N3	-2.23	1.33	1.37
22	a	1962	5MC	C6-C5	2.22	1.38	1.34
22	a	746	PSU	C2-N3	-2.20	1.33	1.37
1	A	1407	5MC	C6-N1	-2.20	1.34	1.38
1	A	1207	2MG	C6-N1	-2.18	1.34	1.37
22	a	1915	3TD	C2-N3	-2.18	1.33	1.38
22	a	2503	2MA	C2-N3	2.17	1.35	1.31
22	a	955	PSU	C2-N3	-2.13	1.33	1.37
1	A	1518	MA6	C5-C4	2.11	1.46	1.40
22	a	747	5MU	C2-N1	2.11	1.41	1.38
22	a	2498	OMC	C6-C5	2.06	1.39	1.35
1	A	1498	UR3	C6-C5	2.05	1.39	1.35
22	a	2030	6MZ	C5-C4	2.02	1.46	1.40

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	1915	3TD	N1-C2-N3	7.73	122.24	116.14
22	a	2030	6MZ	C2-N1-C6	7.59	123.10	116.59
22	a	955	PSU	N1-C2-N3	6.40	122.38	115.13
22	a	2605	PSU	N1-C2-N3	6.32	122.29	115.13
22	a	746	PSU	N1-C2-N3	6.29	122.26	115.13
22	a	1917	PSU	N1-C2-N3	6.23	122.19	115.13
22	a	1618	6MZ	C2-N1-C6	6.06	121.78	116.59
22	a	2457	PSU	N1-C2-N3	6.01	121.94	115.13
1	A	516	PSU	N1-C2-N3	5.78	121.68	115.13
22	a	2504	PSU	N1-C2-N3	5.77	121.66	115.13
22	a	1939	5MU	C4-N3-C2	-5.70	119.98	127.35
22	a	2580	PSU	N1-C2-N3	5.63	121.51	115.13
1	A	1498	UR3	C4-N3-C2	-5.56	119.33	124.56
22	a	1911	PSU	N1-C2-N3	5.45	121.31	115.13
22	a	747	5MU	N3-C2-N1	5.41	122.07	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	1939	5MU	C5-C6-N1	-5.39	117.80	123.34
22	a	747	5MU	C4-N3-C2	-5.13	120.71	127.35
22	a	1939	5MU	N3-C2-N1	4.98	121.50	114.89
22	a	2605	PSU	C4-N3-C2	-4.83	119.38	126.34
22	a	1939	5MU	C5-C4-N3	4.75	119.37	115.31
22	a	2030	6MZ	C9-N6-C6	-4.58	118.93	122.87
22	a	2552	OMU	C4-N3-C2	-4.52	120.62	126.58
22	a	2449	H2U	C4-N3-C2	-4.51	122.05	125.79
22	a	746	PSU	C4-N3-C2	-4.44	119.94	126.34
22	a	1915	3TD	C4-N3-C2	-4.28	119.97	124.61
22	a	2552	OMU	N3-C2-N1	4.27	120.56	114.89
22	a	1618	6MZ	C9-N6-C6	-4.20	119.25	122.87
22	a	1939	5MU	O4-C4-C5	-4.01	120.25	124.90
22	a	1917	PSU	C4-N3-C2	-3.96	120.63	126.34
22	a	747	5MU	C5-C4-N3	3.95	118.68	115.31
22	a	955	PSU	C4-N3-C2	-3.92	120.70	126.34
1	A	1407	5MC	C5-C6-N1	-3.91	119.31	123.34
22	a	2457	PSU	C4-N3-C2	-3.87	120.77	126.34
1	A	1518	MA6	N3-C2-N1	-3.85	122.66	128.68
22	a	2580	PSU	C4-N3-C2	-3.79	120.88	126.34
22	a	747	5MU	C5-C6-N1	-3.78	119.45	123.34
22	a	1939	5MU	O2-C2-N1	-3.71	117.85	122.79
22	a	1911	PSU	C4-N3-C2	-3.67	121.05	126.34
1	A	516	PSU	C4-N3-C2	-3.60	121.16	126.34
22	a	747	5MU	O4-C4-C5	-3.59	120.75	124.90
22	a	2552	OMU	C5-C4-N3	3.58	120.20	114.84
1	A	1519	MA6	N3-C2-N1	-3.50	123.21	128.68
22	a	2504	PSU	C4-N3-C2	-3.43	121.40	126.34
22	a	1962	5MC	C5-C6-N1	-3.42	119.82	123.34
22	a	2604	PSU	C6-C5-C4	3.40	120.57	118.20
22	a	1618	6MZ	N3-C2-N1	-3.39	123.37	128.68
22	a	747	5MU	O2-C2-N1	-3.36	118.32	122.79
22	a	2030	6MZ	C1'-N9-C4	-3.35	120.75	126.64
1	A	1518	MA6	C4-C5-N7	-3.34	105.92	109.40
22	a	2580	PSU	O2-C2-N1	-3.24	119.23	122.79
22	a	2030	6MZ	N3-C2-N1	-3.23	123.63	128.68
1	A	967	5MC	C5-C6-N1	-3.18	120.07	123.34
1	A	1519	MA6	C4-C5-N7	-3.17	106.09	109.40
1	A	1519	MA6	C1'-N9-C4	-3.17	121.07	126.64
22	a	2457	PSU	O2-C2-N1	-3.10	119.38	122.79
1	A	516	PSU	O2-C2-N1	-3.09	119.39	122.79
22	a	2552	OMU	O2-C2-N1	-3.07	118.71	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2604	PSU	O2-C2-N1	3.04	126.14	122.79
22	a	2503	2MA	C5-C6-N1	3.03	119.25	114.02
22	a	2605	PSU	O2-C2-N1	-3.00	119.49	122.79
22	a	2251	OMG	C8-N7-C5	2.79	108.31	102.99
22	a	955	PSU	O2-C2-N1	-2.79	119.72	122.79
22	a	1962	5MC	C5-C4-N3	-2.75	118.70	121.67
22	a	2604	PSU	C6-N1-C2	-2.73	119.89	122.68
1	A	1516	2MG	C5-C6-N1	2.70	118.71	113.95
22	a	1915	3TD	C5-C6-N1	-2.66	118.12	122.11
22	a	745	1MG	C5-C6-N1	2.66	117.90	113.90
22	a	2552	OMU	O4-C4-C5	-2.62	120.55	125.16
1	A	1407	5MC	C5-C4-N3	-2.60	118.87	121.67
1	A	966	2MG	C5-C6-N1	2.57	118.50	113.95
22	a	2030	6MZ	C4-C5-N7	-2.57	106.72	109.40
22	a	745	1MG	C8-N7-C5	2.53	107.81	102.99
22	a	1835	2MG	C5-C6-N1	2.51	118.38	113.95
1	A	1402	4OC	C6-C5-C4	2.50	120.03	116.96
22	a	1835	2MG	C8-N7-C5	2.47	107.70	102.99
22	a	1962	5MC	CM5-C5-C6	-2.47	119.55	122.85
22	a	2445	2MG	C5-C6-N1	2.46	118.30	113.95
1	A	1207	2MG	C8-N7-C5	2.45	107.66	102.99
12	L	89	D2T	OD1-CG-CB	-2.43	117.36	122.44
22	a	2449	H2U	N3-C2-N1	2.43	119.22	116.65
22	a	746	PSU	O2-C2-N1	-2.42	120.13	122.79
22	a	2503	2MA	C8-N7-C5	2.41	107.57	102.99
22	a	2605	PSU	C5-C6-N1	-2.35	118.58	122.11
22	a	1917	PSU	O2-C2-N3	-2.34	117.40	121.82
22	a	2580	PSU	O4'-C1'-C2'	2.33	108.43	105.14
22	a	1911	PSU	O2-C2-N1	-2.33	120.23	122.79
1	A	1207	2MG	C5-C6-N1	2.31	118.03	113.95
22	a	2251	OMG	C5-C6-N1	2.30	118.01	113.95
22	a	1618	6MZ	C4-C5-N7	-2.29	107.01	109.40
1	A	966	2MG	C8-N7-C5	2.29	107.35	102.99
1	A	967	5MC	C5-C4-N3	-2.27	119.23	121.67
22	a	1917	PSU	C5-C6-N1	-2.24	118.75	122.11
22	a	746	PSU	O2-C2-N3	-2.23	117.61	121.82
1	A	1498	UR3	C6-N1-C2	-2.23	119.79	121.79
1	A	1516	2MG	O6-C6-C5	-2.22	120.04	124.37
1	A	1518	MA6	C1'-N9-C4	-2.19	122.80	126.64
22	a	1917	PSU	O2-C2-N1	-2.16	120.41	122.79
22	a	1915	3TD	O4'-C1'-C2'	2.15	108.17	105.14
1	A	1516	2MG	C8-N7-C5	2.15	107.08	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	967	5MC	CM5-C5-C6	-2.13	120.00	122.85
1	A	966	2MG	O6-C6-C5	-2.11	120.25	124.37
22	a	2504	PSU	O2-C2-N3	-2.11	117.84	121.82
22	a	2504	PSU	O2-C2-N1	-2.09	120.49	122.79
22	a	955	PSU	O2-C2-N3	-2.08	117.89	121.82
22	a	746	PSU	C5-C6-N1	-2.06	119.02	122.11
22	a	1915	3TD	O2-C2-N3	-2.06	118.80	121.83
22	a	2445	2MG	C8-N7-C5	2.06	106.91	102.99
1	A	516	PSU	O4'-C1'-C2'	2.04	108.02	105.14
22	a	2504	PSU	C5-C6-N1	-2.03	119.06	122.11
1	A	1519	MA6	N1-C6-N6	2.03	119.19	117.06
1	A	1498	UR3	C3U-N3-C4	2.02	120.77	117.89
22	a	1835	2MG	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	89	D2T	CG-CB-SB-CB1
12	L	89	D2T	CA-CB-CG-OD1
12	L	89	D2T	CA-CB-CG-OD2
22	a	746	PSU	C2'-C1'-C5-C4
22	a	746	PSU	O4'-C1'-C5-C6
22	a	2030	6MZ	O4'-C4'-C5'-O5'
25	d	150	MEQ	NE2-CD-CG-CB
25	d	150	MEQ	OE1-CD-CG-CB
22	a	2030	6MZ	C3'-C4'-C5'-O5'
22	a	2504	PSU	O4'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
22	a	2445	2MG	C3'-C4'-C5'-O5'
22	a	747	5MU	C3'-C4'-C5'-O5'
22	a	2504	PSU	C3'-C4'-C5'-O5'
22	a	746	PSU	O4'-C1'-C5-C4
1	A	527	G7M	C4'-C5'-O5'-P
22	a	2503	2MA	C4'-C5'-O5'-P
12	L	89	D2T	CA-CB-SB-CB1
12	L	89	D2T	SB-CB-CG-OD2
22	a	1917	PSU	O4'-C4'-C5'-O5'
1	A	966	2MG	C3'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
22	a	2069	G7M	O4'-C4'-C5'-O5'
22	a	2503	2MA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
33	l	81	4D4	O-C-CA-CB

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 329 ligands modelled in this entry, 311 are monoatomic - leaving 18 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	$\#|Z| > 2$
59	SPD	a	6213	-	9,9,9	0.19	0	8,8,8	0.21	0
59	SPD	A	1695	-	9,9,9	0.18	0	8,8,8	0.35	0
59	SPD	a	6216	-	9,9,9	0.18	0	8,8,8	0.22	0
59	SPD	a	6215	-	9,9,9	0.19	0	8,8,8	0.19	0
59	SPD	a	6212	-	9,9,9	0.18	0	8,8,8	0.18	0
59	SPD	a	6217	-	9,9,9	0.18	0	8,8,8	0.18	0
59	SPD	a	6210	-	9,9,9	0.20	0	8,8,8	0.19	0
59	SPD	a	6219	-	9,9,9	0.18	0	8,8,8	0.19	0
59	SPD	a	6214	-	9,9,9	0.20	0	8,8,8	0.18	0
60	SPM	a	6223	-	13,13,13	0.17	0	12,12,12	0.19	0
59	SPD	A	1696	-	9,9,9	0.18	0	8,8,8	0.25	0
59	SPD	a	6218	-	9,9,9	0.19	0	8,8,8	0.20	0
59	SPD	a	6220	-	9,9,9	0.22	0	8,8,8	0.25	0
59	SPD	a	6222	-	9,9,9	0.18	0	8,8,8	0.17	0
59	SPD	a	6221	-	9,9,9	0.21	0	8,8,8	0.17	0
59	SPD	a	6209	-	9,9,9	0.22	0	8,8,8	0.26	0
57	PAR	A	1601	-	45,45,45	0.51	0	64,67,67	0.89	1 (1%)
59	SPD	a	6211	-	9,9,9	0.19	0	8,8,8	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SPD	a	6213	-	-	4/7/7/7	-
59	SPD	A	1695	-	-	2/7/7/7	-
59	SPD	a	6216	-	-	3/7/7/7	-
59	SPD	a	6215	-	-	4/7/7/7	-
59	SPD	a	6212	-	-	5/7/7/7	-
59	SPD	a	6217	-	-	4/7/7/7	-
59	SPD	a	6210	-	-	4/7/7/7	-
59	SPD	a	6219	-	-	7/7/7/7	-
59	SPD	a	6214	-	-	5/7/7/7	-
60	SPM	a	6223	-	-	9/11/11/11	-
59	SPD	A	1696	-	-	4/7/7/7	-
59	SPD	a	6218	-	-	3/7/7/7	-
59	SPD	a	6220	-	-	1/7/7/7	-
59	SPD	a	6222	-	-	2/7/7/7	-
59	SPD	a	6221	-	-	1/7/7/7	-
59	SPD	a	6209	-	-	0/7/7/7	-
57	PAR	A	1601	-	-	4/18/94/94	0/4/4/4
59	SPD	a	6211	-	-	3/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A	1601	PAR	C13-O52-C52	-2.33	112.20	117.96

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	1601	PAR	C44-C54-C64-N64
57	A	1601	PAR	O54-C54-C64-N64
59	a	6212	SPD	C3-C4-C5-N6
59	a	6211	SPD	N6-C7-C8-C9
59	a	6219	SPD	C3-C4-C5-N6

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Mol	Chain	Res	Type	Atoms
59	A	1695	SPD	C3-C4-C5-N6
59	a	6211	SPD	C3-C4-C5-N6
59	a	6219	SPD	N6-C7-C8-C9
59	a	6219	SPD	C8-C7-N6-C5
59	a	6216	SPD	N6-C7-C8-C9
59	a	6210	SPD	C3-C4-C5-N6
59	a	6222	SPD	C4-C5-N6-C7
60	a	6223	SPM	C3-C4-N5-C6
60	a	6223	SPM	C8-C9-N10-C11
59	a	6214	SPD	N6-C7-C8-C9
60	a	6223	SPM	C7-C8-C9-N10
59	A	1696	SPD	N6-C7-C8-C9
60	a	6223	SPM	C2-C3-C4-N5
59	a	6215	SPD	C3-C4-C5-N6
59	a	6215	SPD	C7-C8-C9-N10
59	a	6217	SPD	C7-C8-C9-N10
60	a	6223	SPM	N1-C2-C3-C4
60	a	6223	SPM	C11-C12-C13-N14
59	a	6213	SPD	N6-C7-C8-C9
59	a	6210	SPD	C8-C7-N6-C5
59	a	6219	SPD	C2-C3-C4-C5
59	a	6213	SPD	C3-C4-C5-N6
59	a	6216	SPD	C2-C3-C4-C5
59	a	6212	SPD	C2-C3-C4-C5
59	a	6212	SPD	C4-C5-N6-C7
59	a	6216	SPD	C4-C5-N6-C7
59	A	1695	SPD	C4-C5-N6-C7
59	a	6222	SPD	C8-C7-N6-C5
59	a	6217	SPD	C3-C4-C5-N6
59	a	6215	SPD	N6-C7-C8-C9
59	a	6210	SPD	C7-C8-C9-N10
59	a	6219	SPD	C7-C8-C9-N10
59	a	6221	SPD	C7-C8-C9-N10
59	a	6213	SPD	C8-C7-N6-C5
59	a	6218	SPD	N1-C2-C3-C4
59	a	6214	SPD	C3-C4-C5-N6
59	a	6212	SPD	N6-C7-C8-C9
59	A	1696	SPD	C2-C3-C4-C5
59	a	6215	SPD	N1-C2-C3-C4
60	a	6223	SPM	C12-C11-N10-C9
57	A	1601	PAR	C52-C42-O11-C11
57	A	1601	PAR	C23-C33-O33-C14

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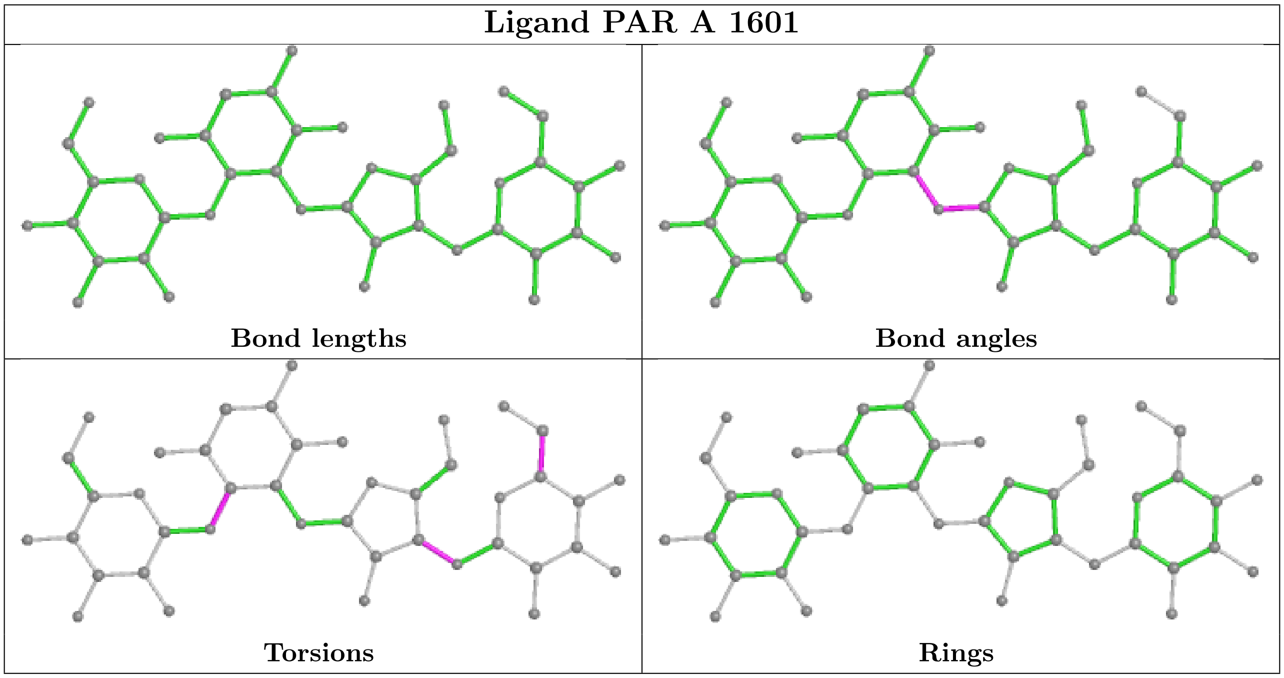
Mol	Chain	Res	Type	Atoms
60	a	6223	SPM	C6-C7-C8-C9
59	a	6217	SPD	N6-C7-C8-C9
59	a	6211	SPD	C4-C5-N6-C7
59	A	1696	SPD	C3-C4-C5-N6
59	a	6220	SPD	C3-C4-C5-N6
59	a	6214	SPD	C4-C5-N6-C7
59	a	6218	SPD	C2-C3-C4-C5
59	a	6210	SPD	C2-C3-C4-C5
59	a	6214	SPD	C2-C3-C4-C5
59	a	6212	SPD	N1-C2-C3-C4
59	a	6217	SPD	C2-C3-C4-C5
59	a	6214	SPD	C8-C7-N6-C5
59	A	1696	SPD	C7-C8-C9-N10
59	a	6218	SPD	C7-C8-C9-N10
59	a	6219	SPD	C4-C5-N6-C7
60	a	6223	SPM	C7-C6-N5-C4
59	a	6219	SPD	N1-C2-C3-C4
59	a	6213	SPD	C4-C5-N6-C7

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 PAR A 1601

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

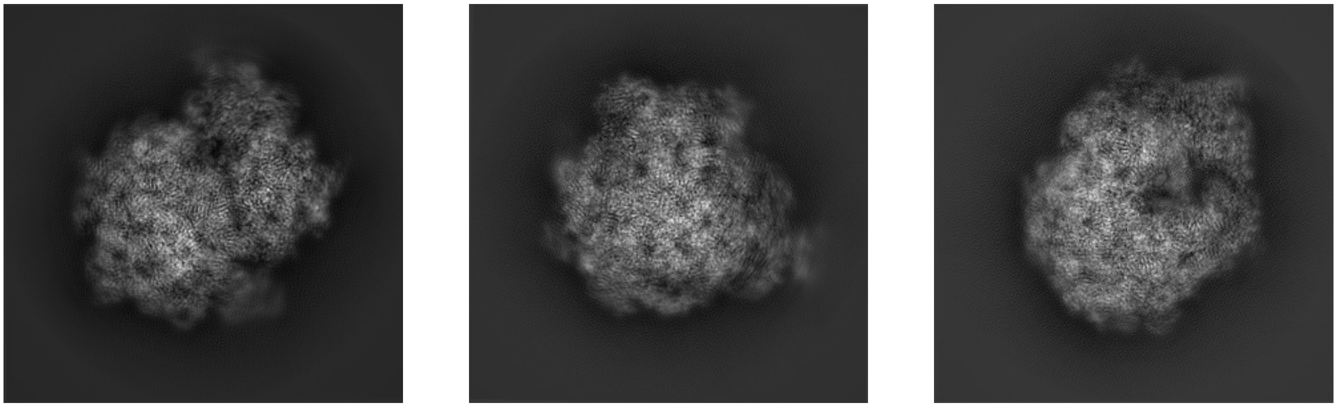
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22586. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

6.1.1 Primary map

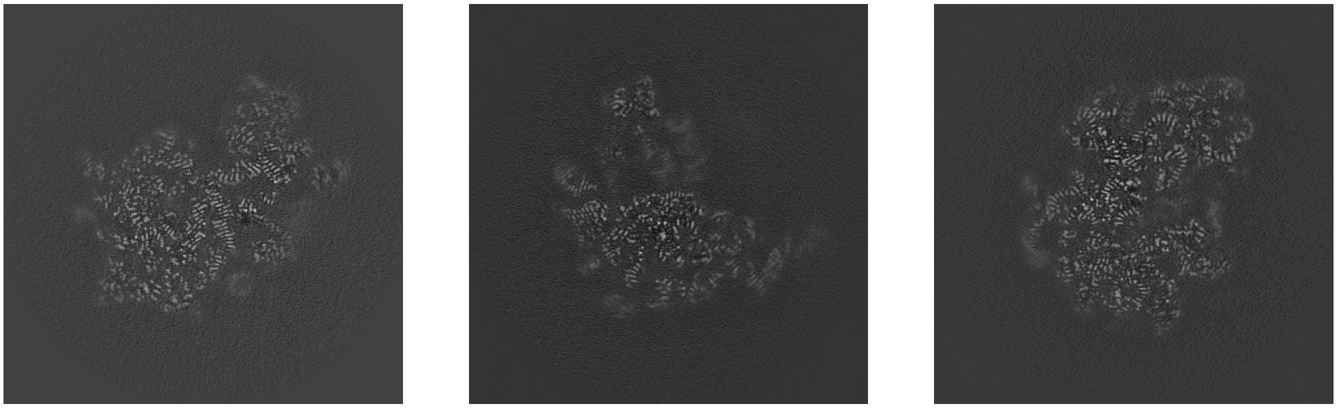


X Y Z

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

6.2 Central slices

6.2.1 Primary map

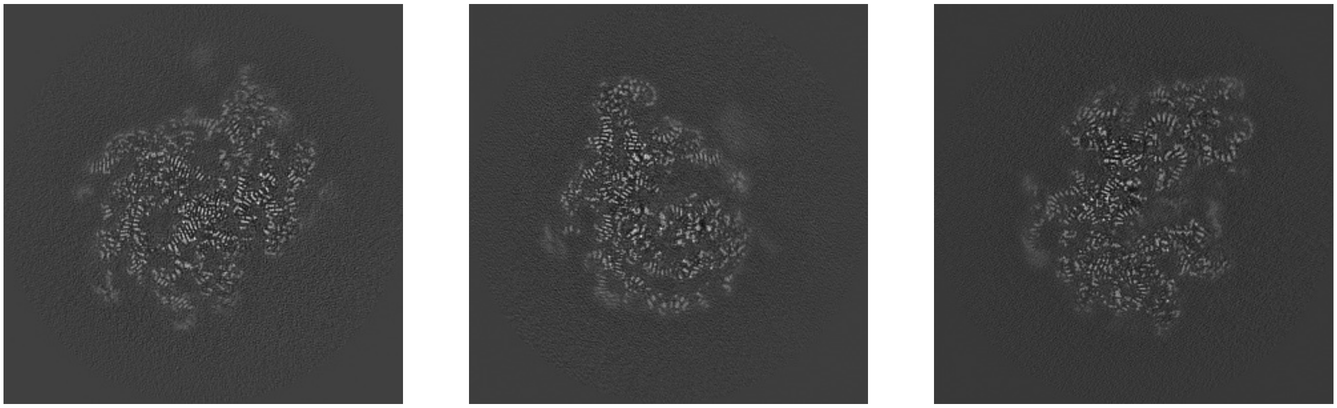


X Index: 248 Y Index: 248 Z Index: 248

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

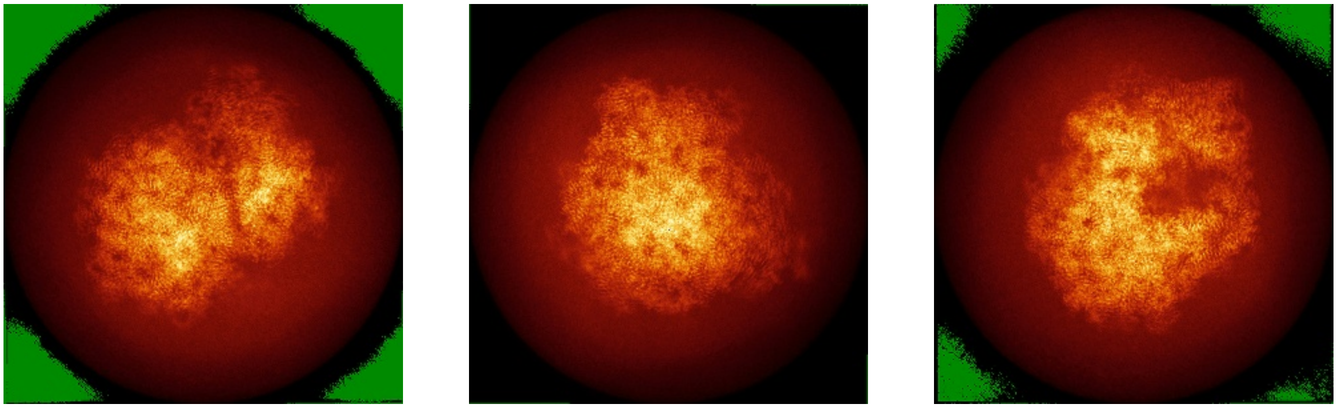


X Index: 216 Y Index: 218 Z Index: 248

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



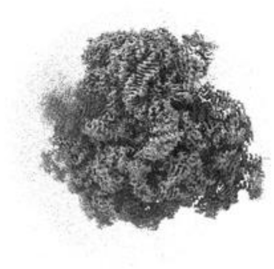
X Y Z

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.

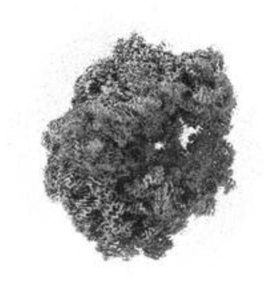
6.5 Orthogonal surface views

6.5.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

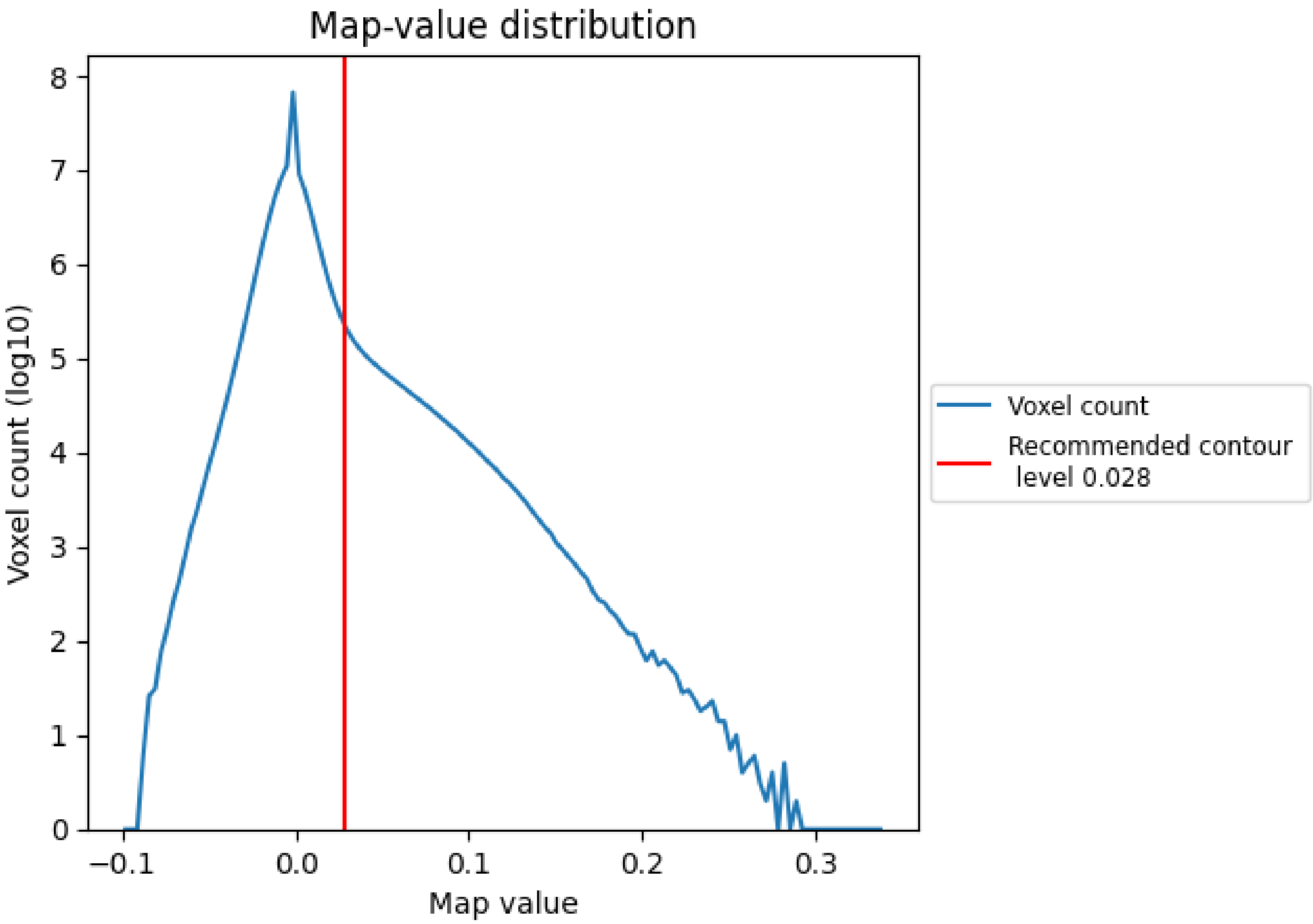
6.6 Mask visualisation

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

7 Map analysis (i)

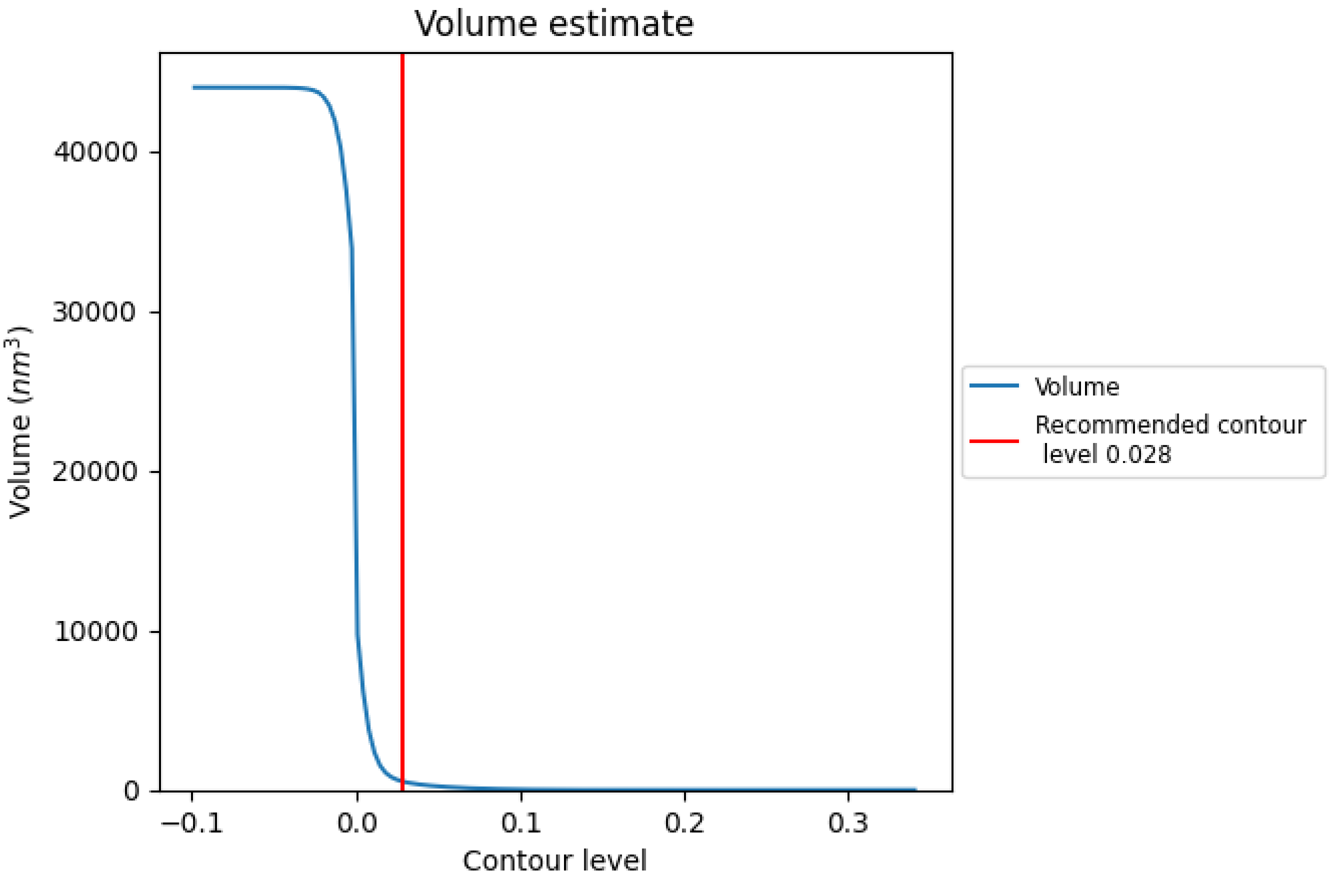
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

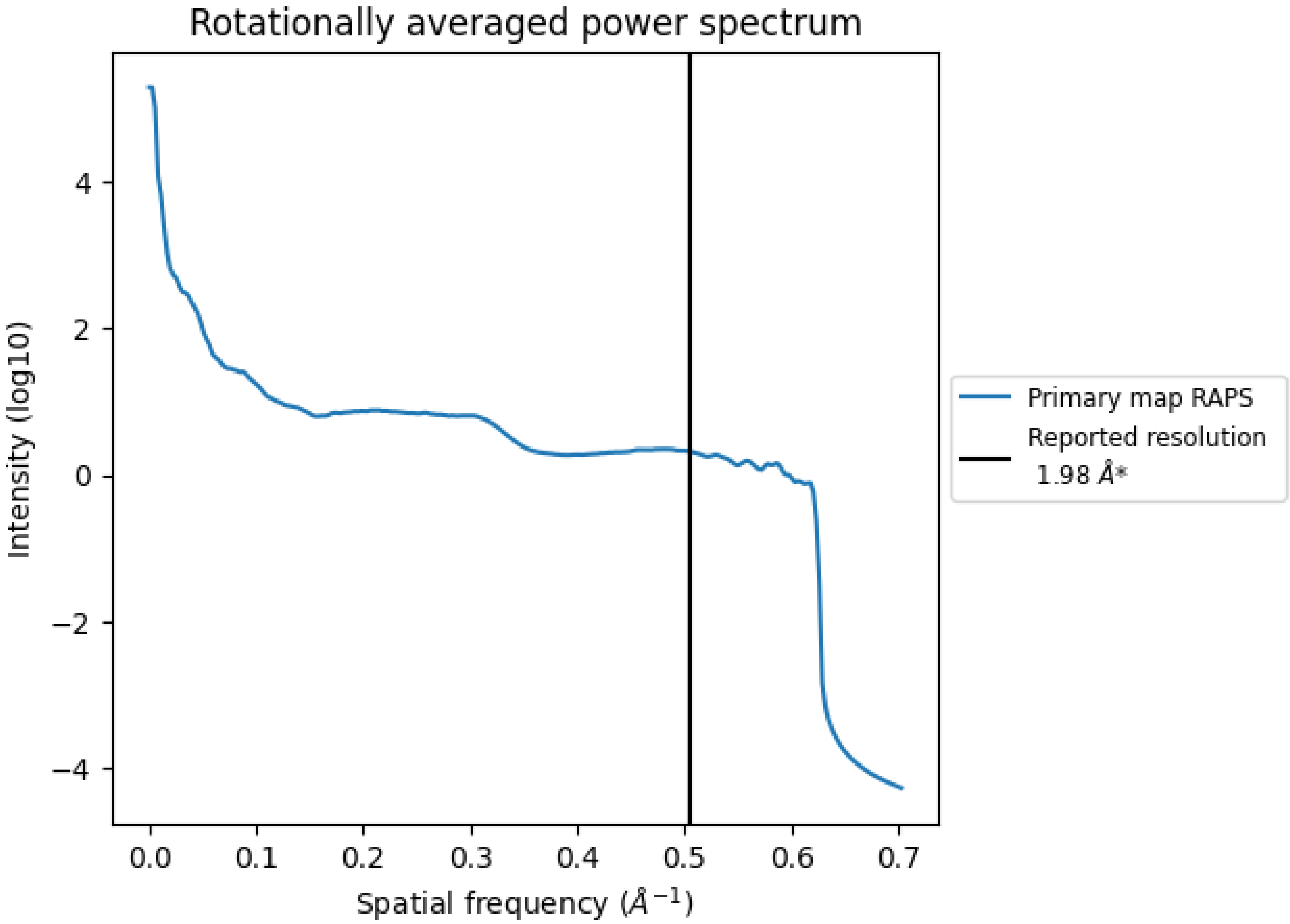
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 549 nm^3; this corresponds to an approximate mass of 496 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.505 $\AA^{-1}$

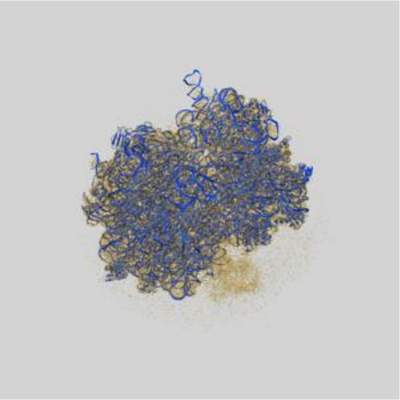
8 Fourier-Shell correlation

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

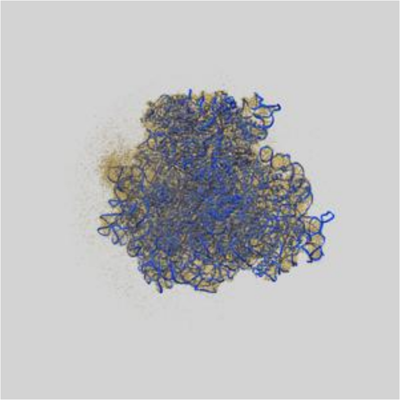
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22586 and PDB model 7K00. Per-residue inclusion information can be found in section 3 on page 19.

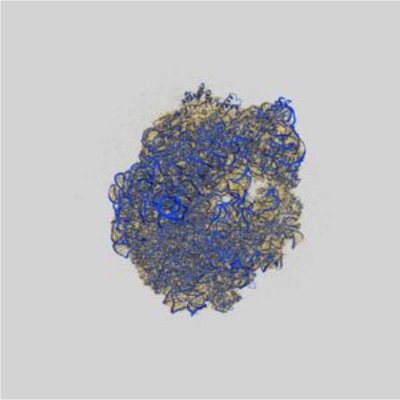
9.1 Map-model overlay



X



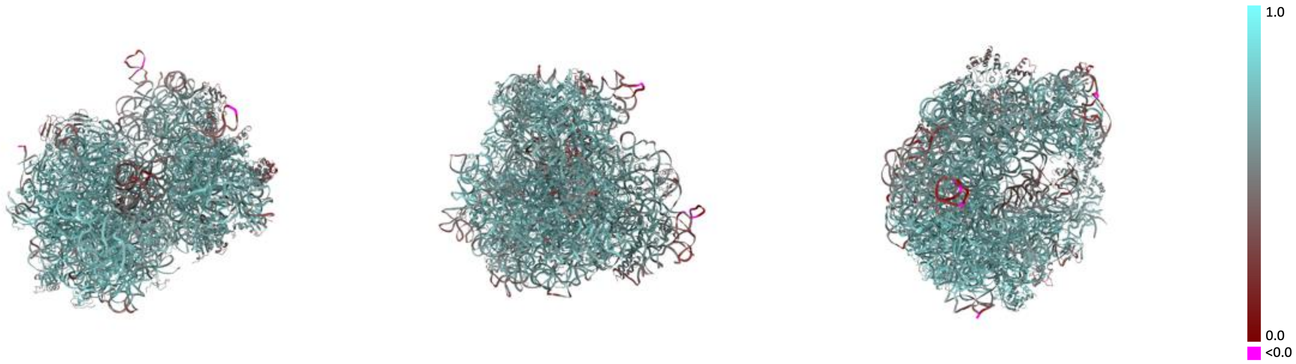
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

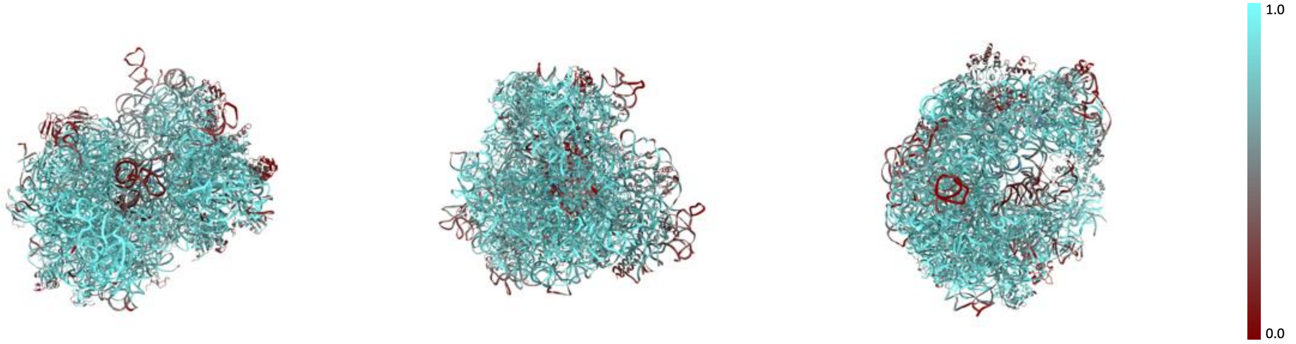
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

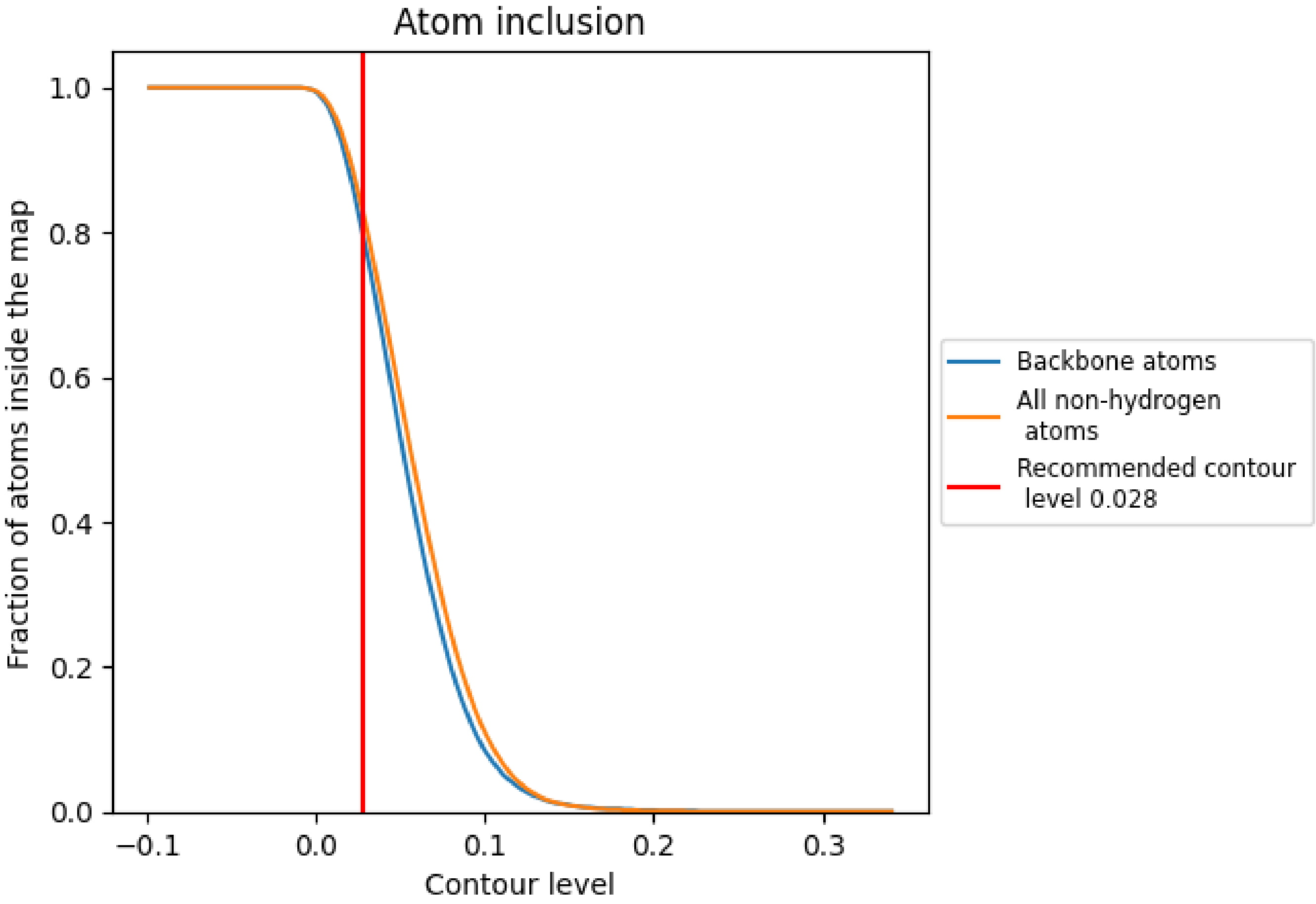
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.028).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8270	0.6770
0	0.8290	0.7010
1	0.9550	0.7930
2	0.9610	0.7840
3	0.7880	0.7110
4	0.6020	0.5410
5	0.7620	0.6530
A	0.8420	0.6520
B	0.4410	0.5030
C	0.7620	0.6510
D	0.4470	0.5260
E	0.8270	0.6710
F	0.6760	0.5710
G	0.6010	0.5560
H	0.8580	0.6910
I	0.7380	0.6370
J	0.5280	0.5540
K	0.7990	0.6430
L	0.7870	0.6700
M	0.7380	0.6290
N	0.8090	0.6810
O	0.8120	0.6390
P	0.6070	0.5960
Q	0.6180	0.5790
R	0.7840	0.6430
S	0.7510	0.6460
T	0.4900	0.5400
U	0.5040	0.5160
X	0.7390	0.6520
Y	0.3480	0.4370
Z	0.5390	0.5090
a	0.9070	0.7200
b	0.9240	0.6830
c	0.9210	0.7550
d	0.8530	0.7460

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Chain	Atom inclusion	Q-score
e	0.7350	0.6750
f	0.7560	0.6070
g	0.2810	0.4700
h	0.4430	0.5260
i	0.8750	0.7410
j	0.8130	0.7220
k	0.8570	0.7240
l	0.8670	0.7410
m	0.9260	0.7730
n	0.8620	0.6810
o	0.7930	0.7110
p	0.8980	0.7730
q	0.7490	0.6820
r	0.8330	0.7400
s	0.7040	0.6700
t	0.5950	0.5900
u	0.7140	0.6440
v	0.9110	0.7500
w	0.8500	0.7170
x	0.4990	0.5590
y	0.8400	0.7190
z	0.8350	0.7340