



Full wwPDB EM Validation Report ⓘ

Nov 7, 2023 – 01:02 PM EST

PDB ID : 8G6W
EMDB ID : EMD-29786
Title : Structure of WT E.coli 70S ribosome complexed with mRNA, P-site fMet-NH-tRNA^{fMet} and A-site ortho-aminobenzoic acid charged NH-tRNA^{Phe}
Authors : Majumdar, C.; Cate, J.H.D.
Deposited on : 2023-02-16
Resolution : 2.02 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

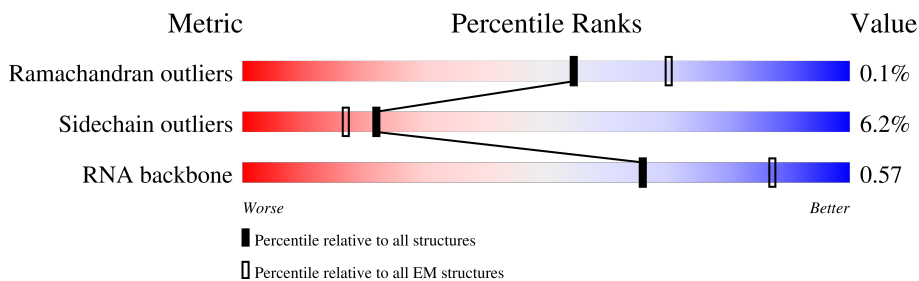
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.02 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	55	
2	1	46	
3	2	65	
4	3	38	
5	4	70	
6	A	1542	
7	B	241	
8	C	233	

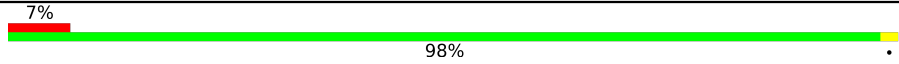
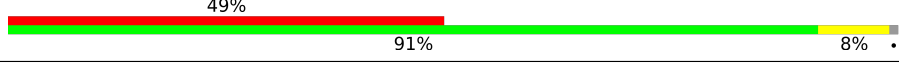
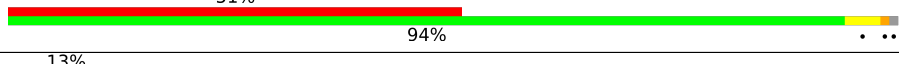

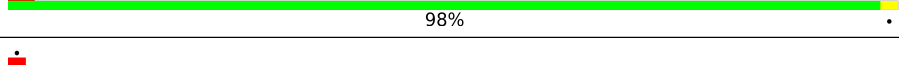
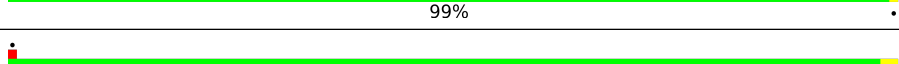
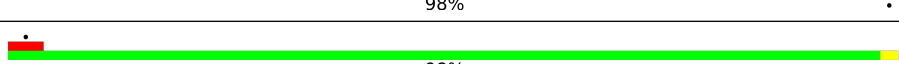
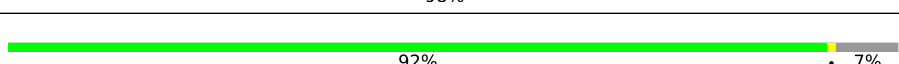
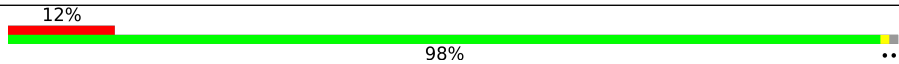
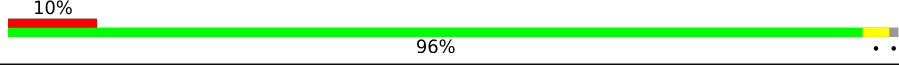
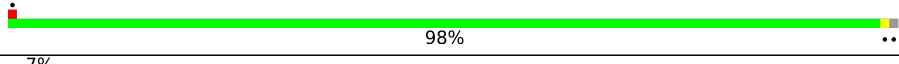
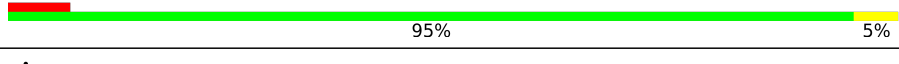
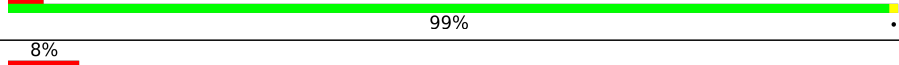
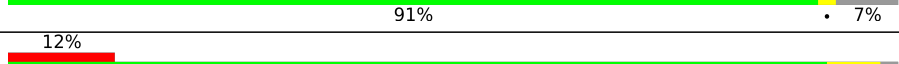
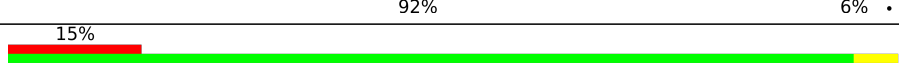
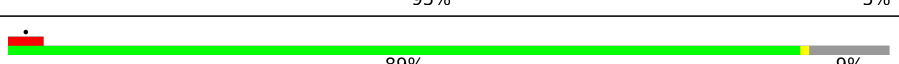
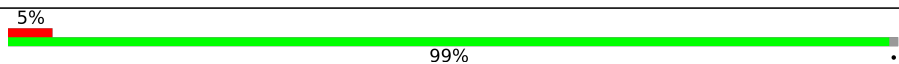
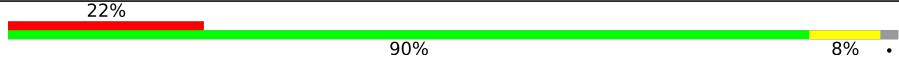
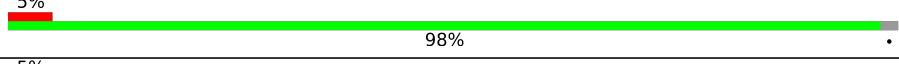
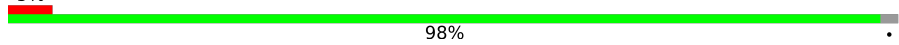


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Mol	Chain	Length	Quality of chain
9	D	206	67% 88% 12%
10	E	167	13% 90% 7%
11	F	135	39% 73% 24%
12	G	179	60% 78% 7% 15%
13	H	130	16% 94% 5%
14	I	130	75% 88% 10%
15	J	103	77% 86% 9% 5%
16	K	129	22% 83% 8% 9%
17	L	124	20% 92% 7%
18	M	118	58% 88% 8%
19	N	101	64% 92% 7%
20	O	89	27% 91% 8%
21	P	82	41% 88% 11%
22	Q	84	36% 90% 6%
23	R	75	27% 84% 12%
24	S	92	66% 82% 10% 9%
25	T	87	44% 95%
26	U	71	61% 93% 6%
27	X	28	25% 36% 14% 46%
28	Y	76	71% 58% 36%
29	Z	76	39% 68% 29%
30	a	2904	5% 82% 12% 5%
31	b	120	6% 83% 16%
32	c	273	97%
33	d	209	98%

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Mol	Chain	Length	Quality of chain
34	e	201	 7% 98%
35	f	179	 49% 91% 8%
36	g	177	 51% 94%
37	h	149	 13% 26% 72%
38	i	142	 98%
39	j	123	 99%
40	k	144	 98%
41	l	136	 98%
42	m	127	 92% 7%
43	n	117	 12% 98%
44	o	115	 10% 96%
45	p	118	 98%
46	q	103	 7% 95% 5%
47	r	110	 99%
48	s	100	 8% 91% 7%
49	t	104	 12% 92% 6%
50	u	94	 15% 95% 5%
51	v	85	 89% 9%
52	w	78	 5% 99%
53	x	63	 22% 90% 8%
54	y	59	 5% 98%
55	z	57	 5% 98%

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 145749 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 protein called 50S ribosomal protein L33.

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

- Molecule 2 is a protein called 50S ribosomal protein L34.

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

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

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

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	60	480	299	90	85	6	0	0

- Molecule 6 is a RNA chain called 16S rRNA.

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

- Molecule 7 is a protein called 30S ribosomal protein S2.

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

- Molecule 8 is a protein called 30S ribosomal protein S3.

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

- Molecule 9 is a protein called 30S ribosomal protein S4.

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

- Molecule 10 is a protein called 30S ribosomal protein S5.

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

- Molecule 11 is a protein called 30S ribosomal protein S6.

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

- Molecule 12 is a protein called 30S ribosomal protein S7.

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

- Molecule 13 is a protein called 30S ribosomal protein S8.

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

- Molecule 14 is a protein called 30S ribosomal protein S9.

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

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	J	98	785	493	149	142	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S11.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP A0A0H3PWX2

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called 30S ribosomal protein S13.

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

- Molecule 19 is a protein called 30S ribosomal protein S14.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S16.

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

- Molecule 22 is a protein called 30S ribosomal protein S17.

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

- Molecule 23 is a protein called 30S ribosomal protein S18.

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

- Molecule 24 is a protein called 30S ribosomal protein S19.

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

- Molecule 25 is a protein called 30S ribosomal protein S20.

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

- Molecule 26 is a protein called 30S ribosomal protein S21.

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

- Molecule 27 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	15	Total	C	N	O	P	0	0
			317	143	56	103	15		

- Molecule 28 is a RNA chain called A-site oABZ-tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	74	Total	C	N	O	P	0	0
			1578	705	285	515	73		

- Molecule 29 is a RNA chain called P-site fMet-tRNA^{fMet}.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	75	Total	C	N	O	P	0	0
			1601	713	289	524	75		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2753	Total	C	N	O	P	2	0
			59170	26402	10901	19112	2755		

- Molecule 31 is a RNA chain called 5S rRNA.

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

- Molecule 32 is a protein called 50S ribosomal protein L2.

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

- Molecule 33 is a protein called 50S ribosomal protein L3.

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

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

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

- Molecule 36 is a protein called 50S ribosomal protein L6.

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

- Molecule 37 is a protein called 50S ribosomal protein L9.

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

- Molecule 38 is a protein called 50S ribosomal protein L13.

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

- Molecule 39 is a protein called 50S ribosomal protein L14.

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

- Molecule 40 is a protein called 50S ribosomal protein L15.

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

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	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 E6BI61

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called Ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

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

- Molecule 48 is a protein called 50S ribosomal protein L23.

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

- Molecule 49 is a protein called 50S ribosomal protein L24.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	v	77	582	360	115	106	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L28.

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

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

- Molecule 54 is a protein called 50S ribosomal protein L30.

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

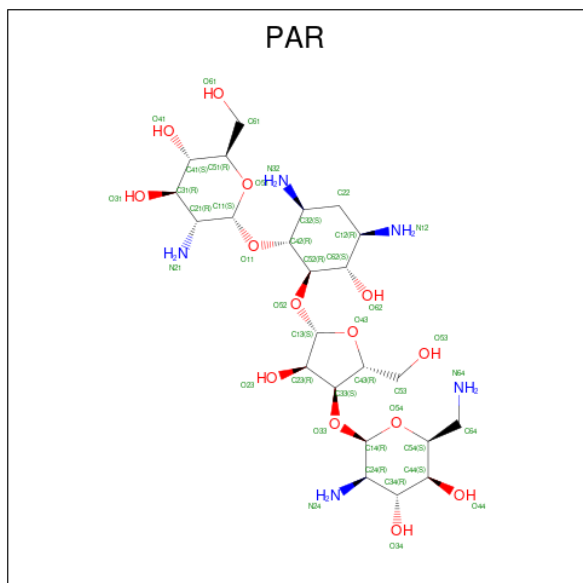
- Molecule 55 is a protein called 50S ribosomal protein L32.

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

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).

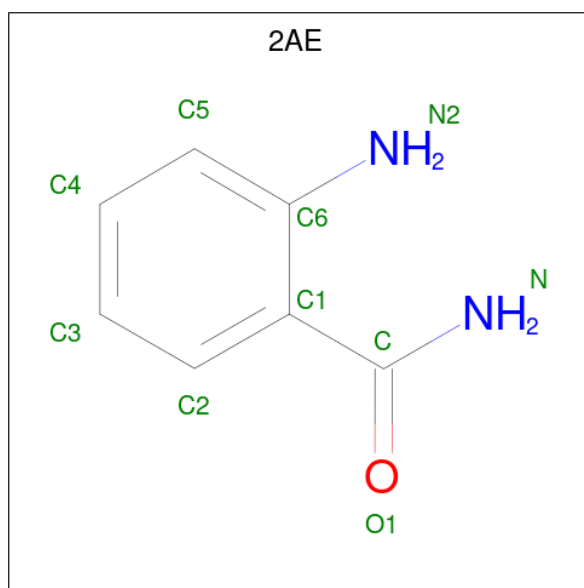


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
57	A	1	42	23	5	14	0

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

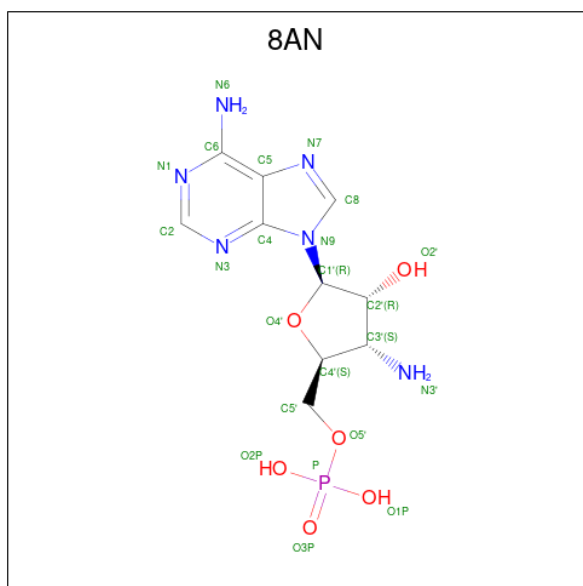
Mol	Chain	Residues	Atoms	AltConf
58	A	89	Total Mg 89 89	0
58	M	1	Total Mg 1 1	0
58	O	1	Total Mg 1 1	0
58	X	1	Total Mg 1 1	0
58	Z	1	Total Mg 1 1	0
58	a	217	Total Mg 217 217	0
58	b	5	Total Mg 5 5	0
58	c	1	Total Mg 1 1	0
58	d	1	Total Mg 1 1	0
58	m	1	Total Mg 1 1	0
58	p	1	Total Mg 1 1	0
58	z	1	Total Mg 1 1	0

- Molecule 59 is 2-AMINO-BENZAMIDE (three-letter code: 2AE) (formula: $C_7H_8N_2O$) (labeled as "Ligand of Interest" by depositor).



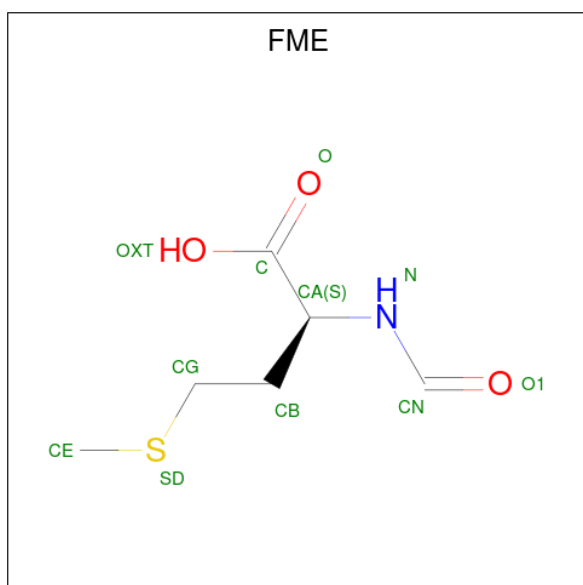
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
59	Y	1	10	7	2	1	0

- Molecule 60 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (three-letter code: 8AN) (formula: $C_{10}H_{15}N_6O_6P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	Z	1	22	10	6	5	1	0

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

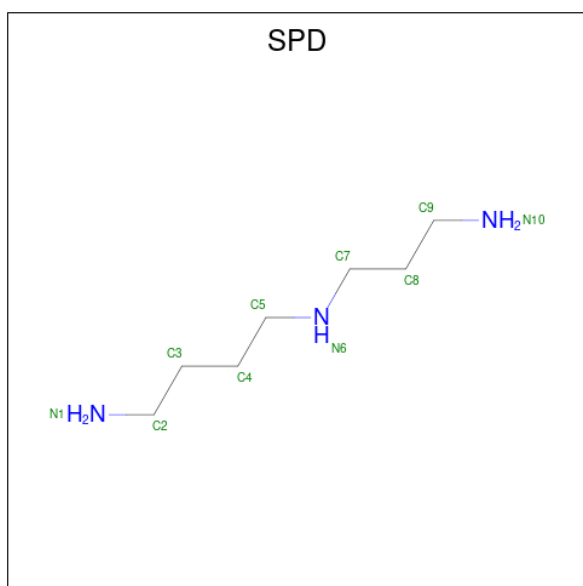


Mol	Chain	Residues	Atoms					AltConf
61	Z	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 62 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
62	a	13	Total	K	0
			13	13	
62	c	1	Total	K	0
			1	1	

- Molecule 63 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



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

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
63	d	1	10	7	3	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
64	1	16	16	16	0
64	2	19	19	19	0
64	3	2	2	2	0
64	A	10	10	10	0
64	a	3197	3197	3197	0
64	b	41	41	41	0
64	c	86	86	86	0
64	d	34	34	34	0
64	e	34	34	34	0
64	h	1	1	1	0
64	i	14	14	14	0
64	j	11	11	11	0
64	k	32	32	32	0
64	l	22	22	22	0
64	m	20	20	20	0
64	o	8	8	8	0
64	p	16	16	16	0
64	q	15	15	15	0

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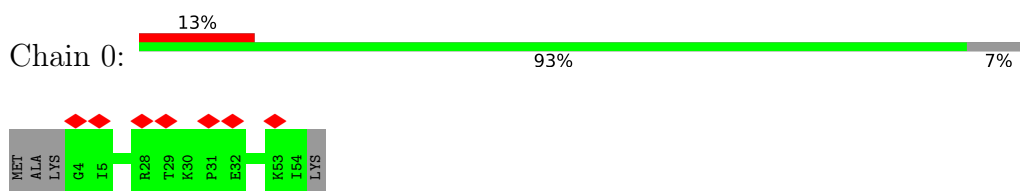
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Mol	Chain	Residues	Atoms		AltConf
64	r	25	Total 25	O 25	0
64	s	6	Total 6	O 6	0
64	t	1	Total 1	O 1	0
64	u	4	Total 4	O 4	0
64	v	11	Total 11	O 11	0
64	w	7	Total 7	O 7	0
64	x	1	Total 1	O 1	0
64	y	2	Total 2	O 2	0
64	z	24	Total 24	O 24	0

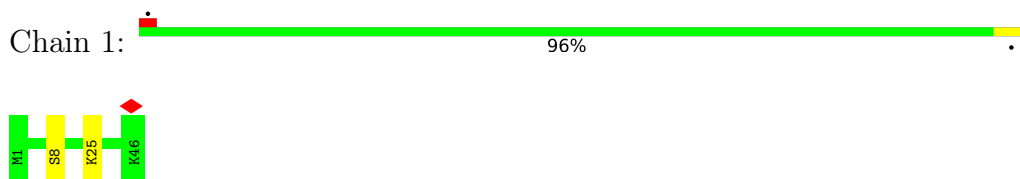
3 Residue-property plots [i](#)

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

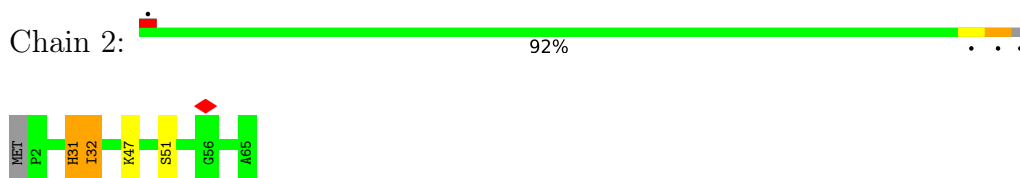
- Molecule 1: 50S ribosomal protein L33



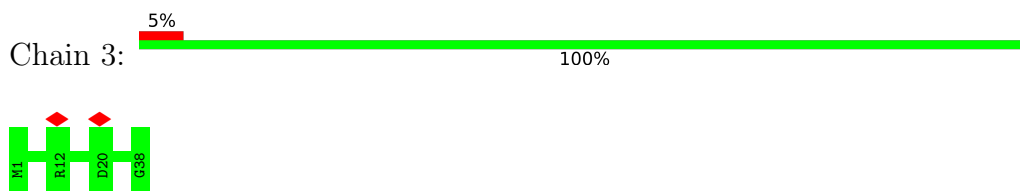
- Molecule 2: 50S ribosomal protein L34



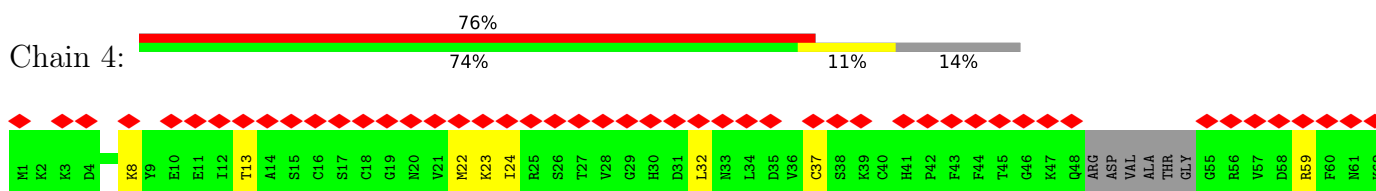
- Molecule 3: 50S ribosomal protein L35

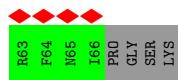


- Molecule 4: 50S ribosomal protein L36

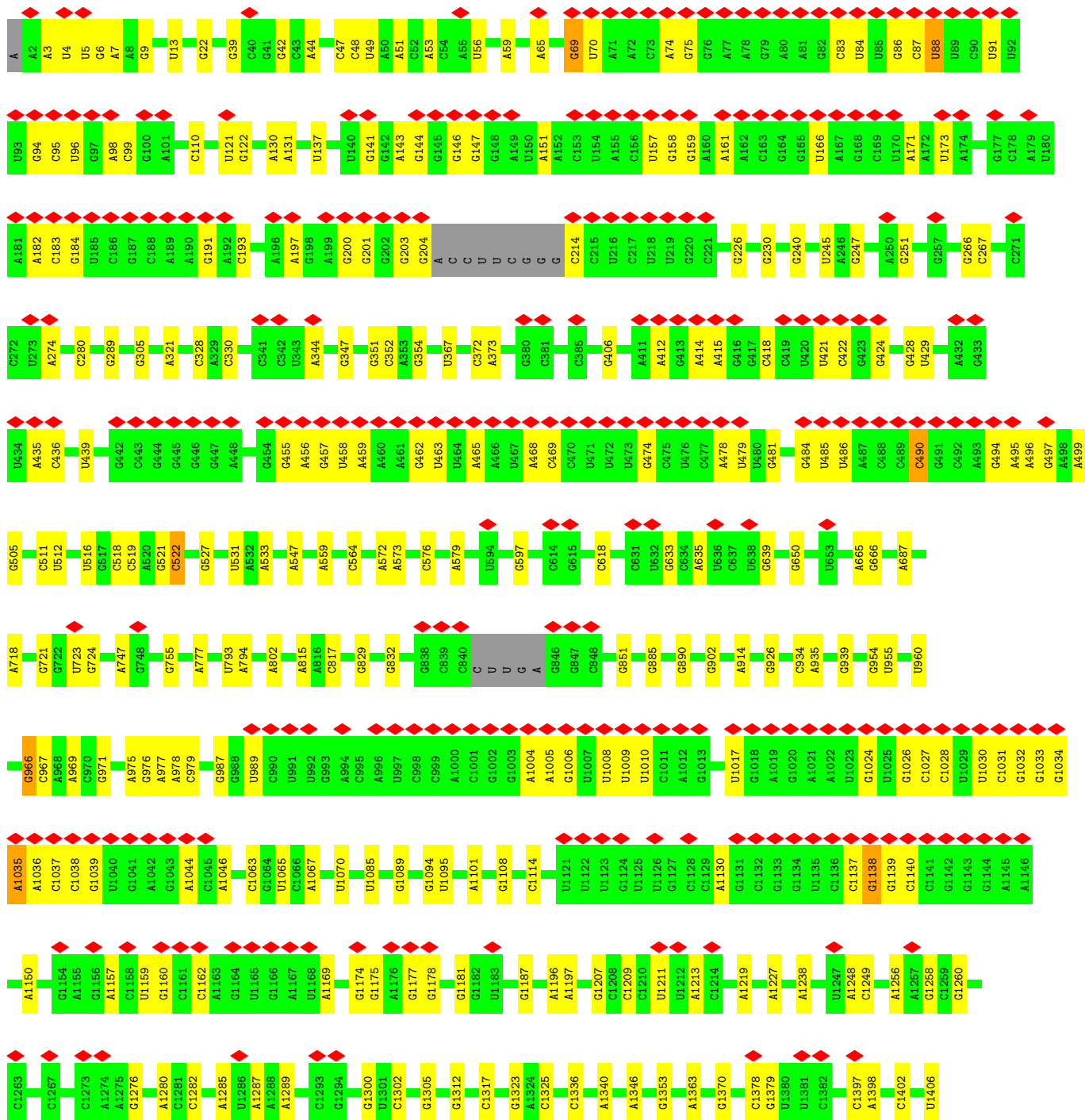
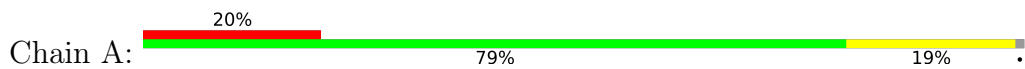


- Molecule 5: 50S ribosomal protein L31



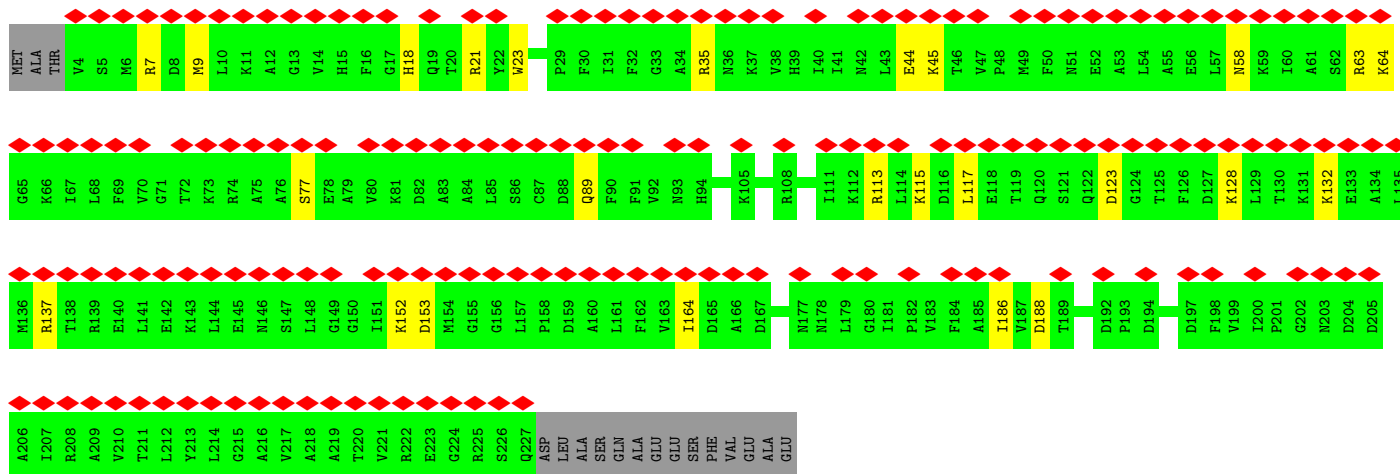
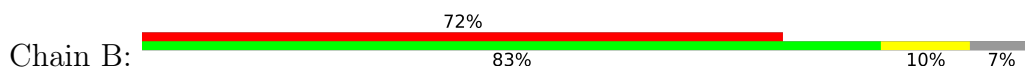


• Molecule 6: 16S rRNA

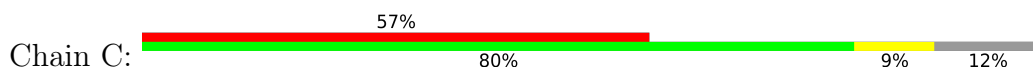




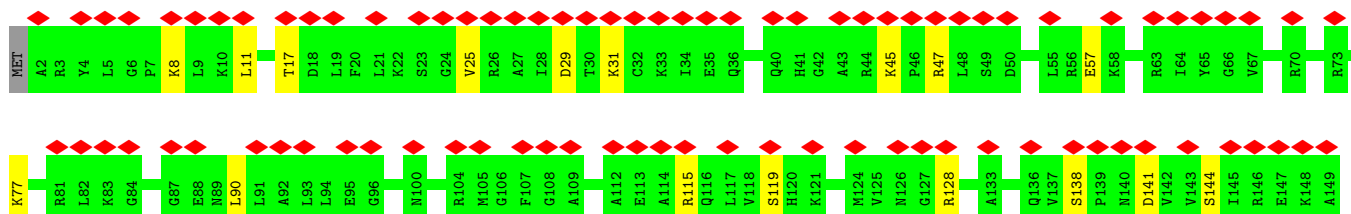
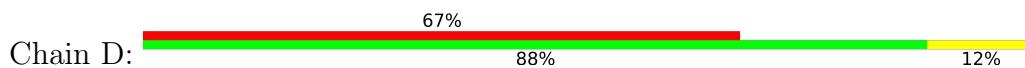
• Molecule 7: 30S ribosomal protein S2

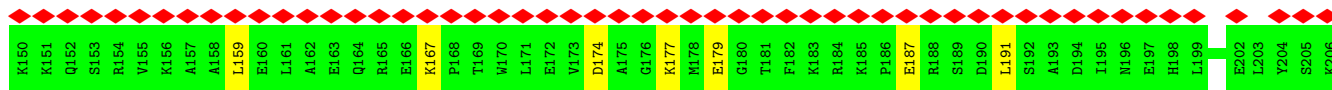


• Molecule 8: 30S ribosomal protein S3

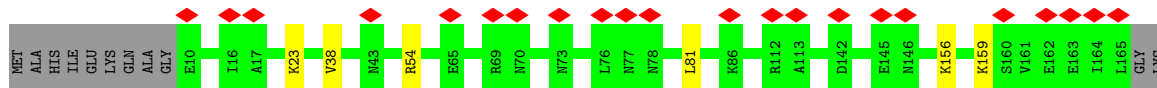
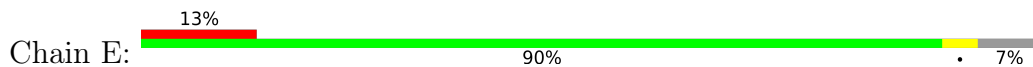


• Molecule 9: 30S ribosomal protein S4

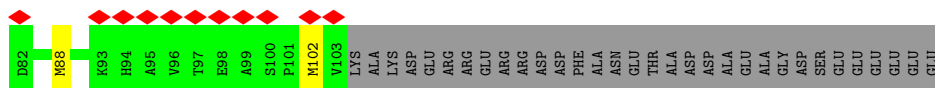
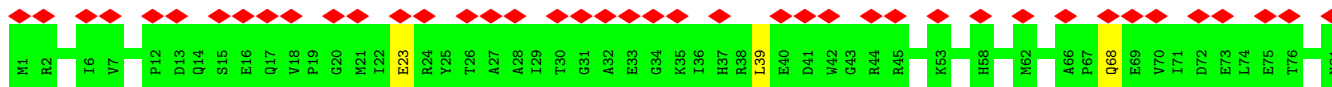
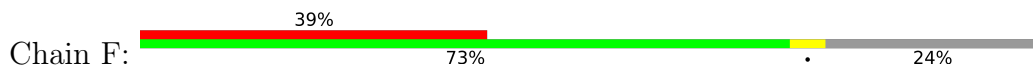




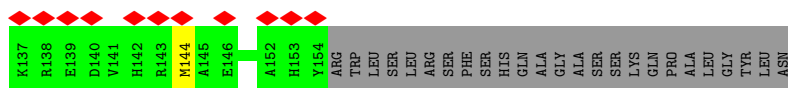
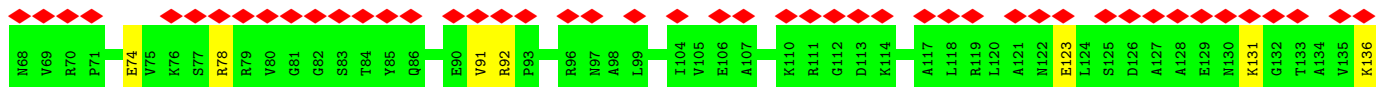
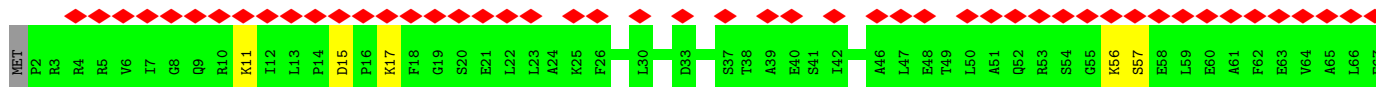
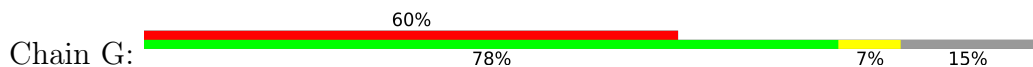
• Molecule 10: 30S ribosomal protein S5



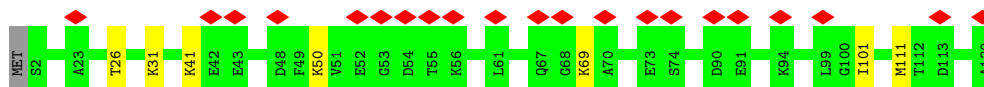
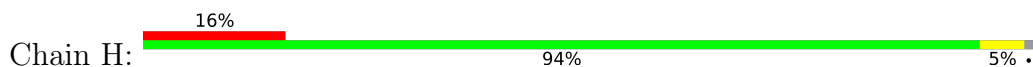
• Molecule 11: 30S ribosomal protein S6



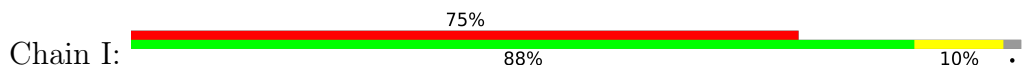
• Molecule 12: 30S ribosomal protein S7

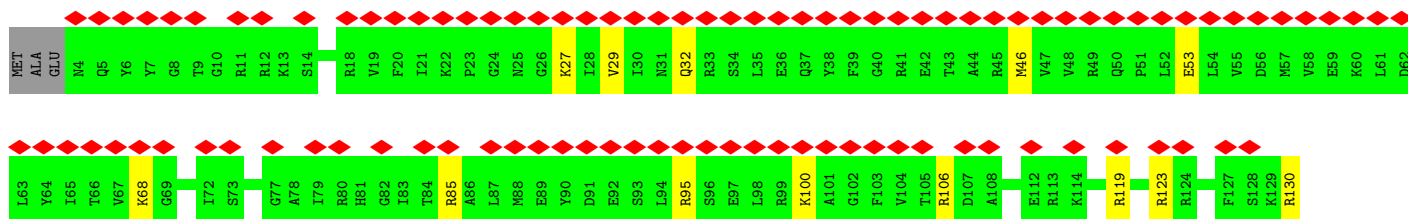


• Molecule 13: 30S ribosomal protein S8

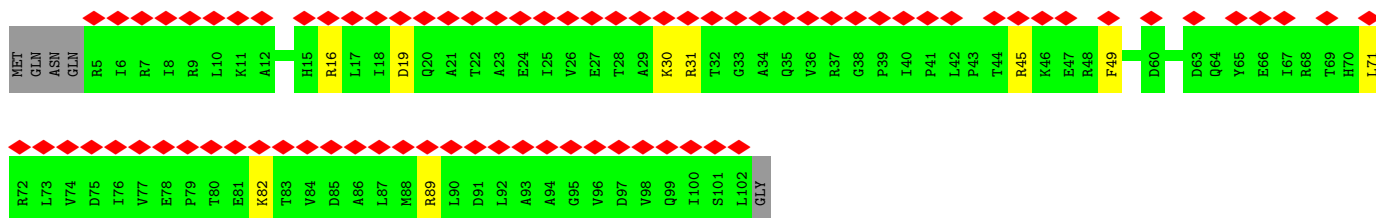
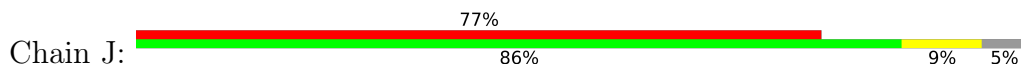


• Molecule 14: 30S ribosomal protein S9

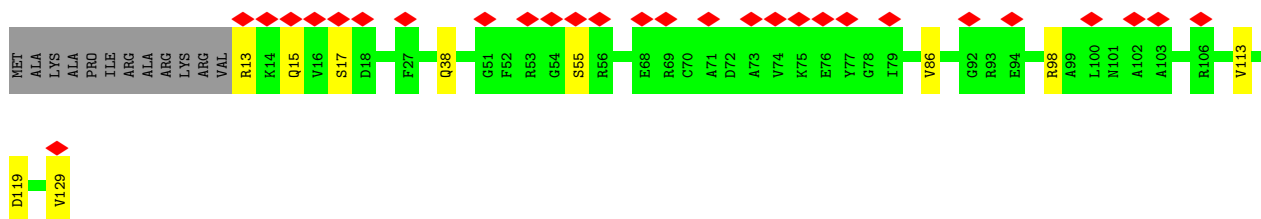
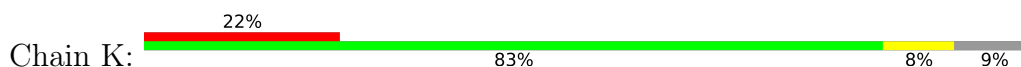




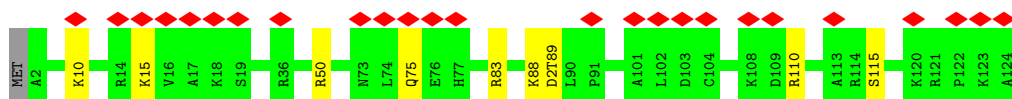
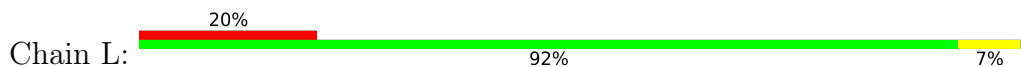
• Molecule 15: 30S ribosomal protein S10



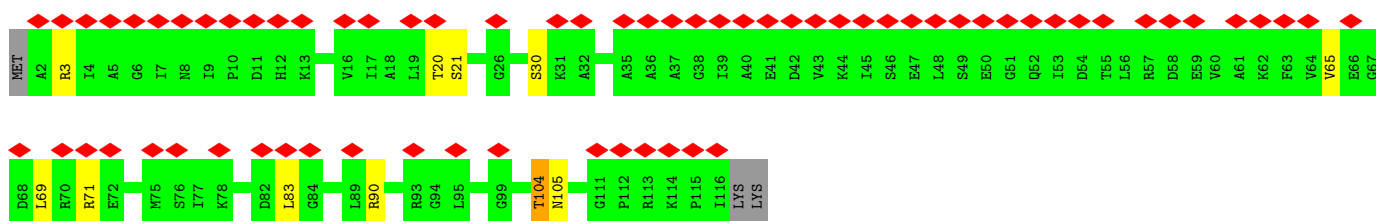
• Molecule 16: 30S ribosomal protein S11



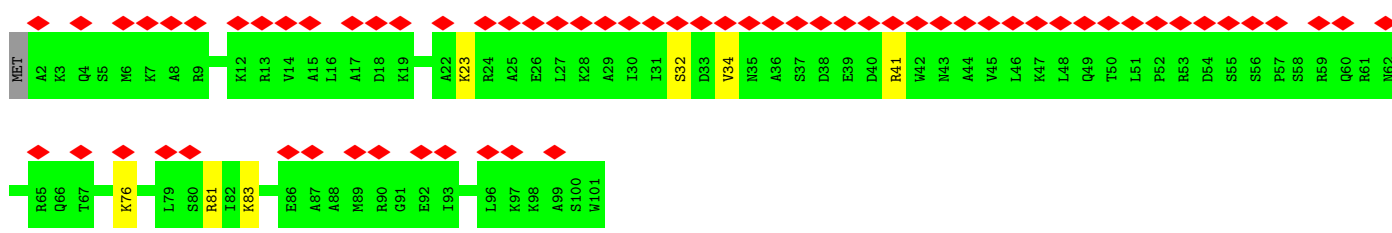
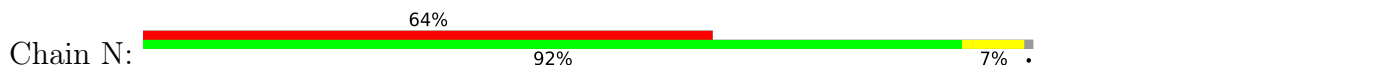
• Molecule 17: 30S ribosomal protein S12



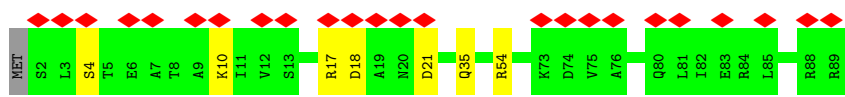
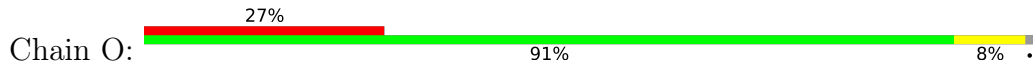
• Molecule 18: 30S ribosomal protein S13



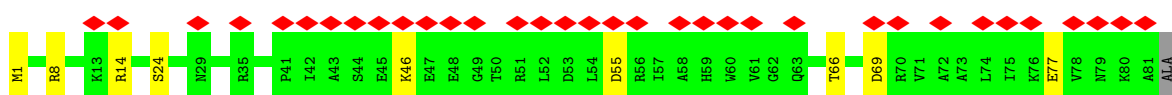
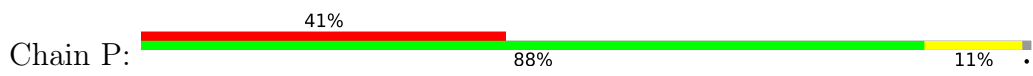
• Molecule 19: 30S ribosomal protein S14



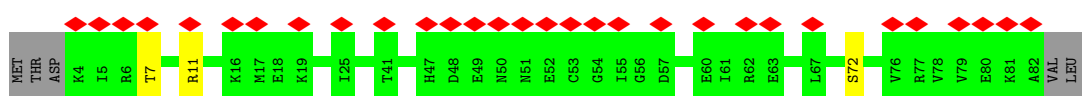
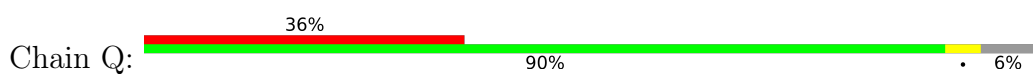
• Molecule 20: 30S ribosomal protein S15



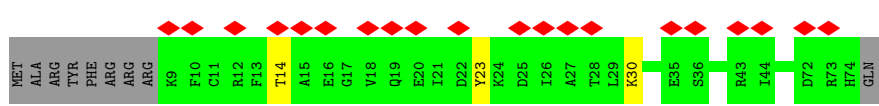
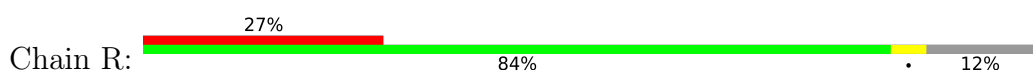
• Molecule 21: 30S ribosomal protein S16



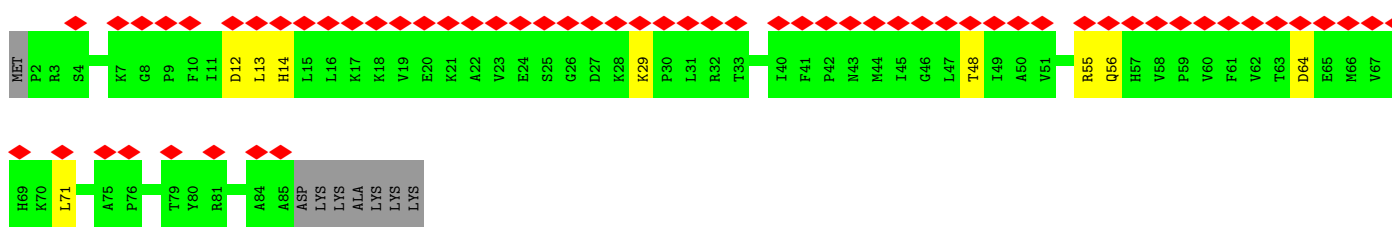
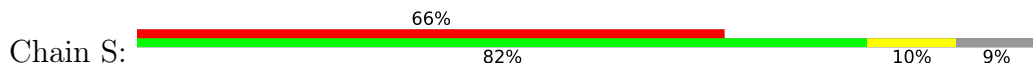
• Molecule 22: 30S ribosomal protein S17



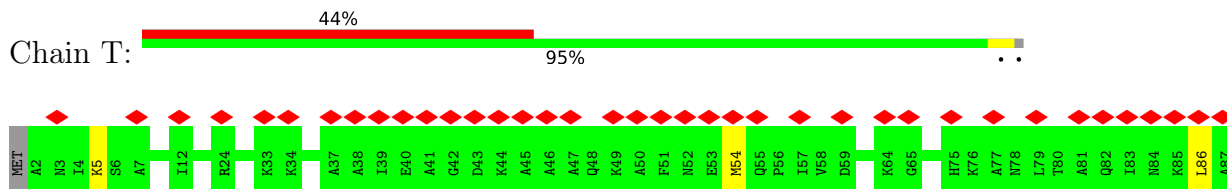
• Molecule 23: 30S ribosomal protein S18



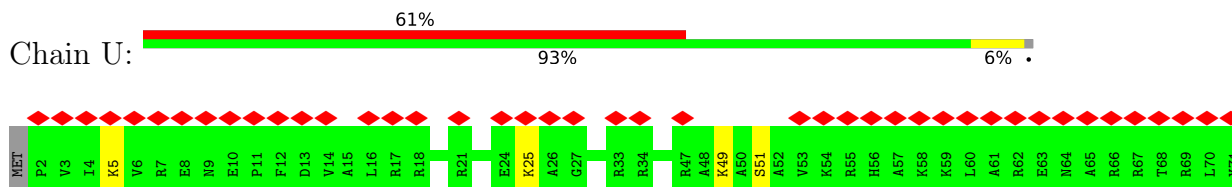
• Molecule 24: 30S ribosomal protein S19



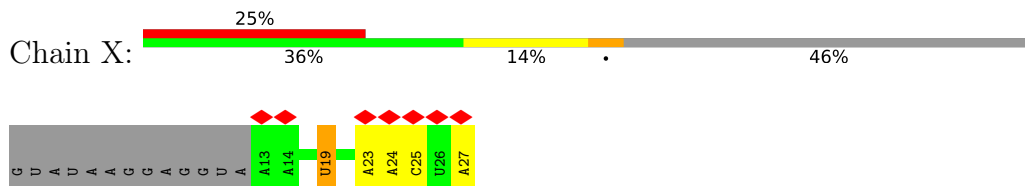
- Molecule 25: 30S ribosomal protein S20



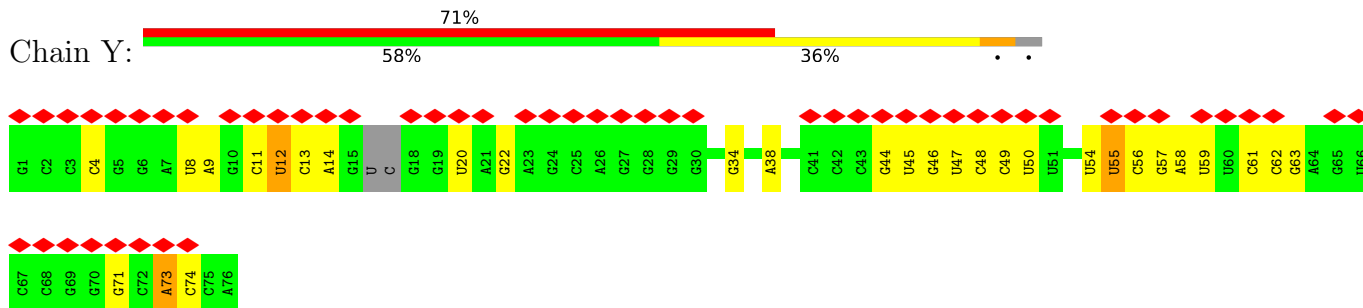
- Molecule 26: 30S ribosomal protein S21



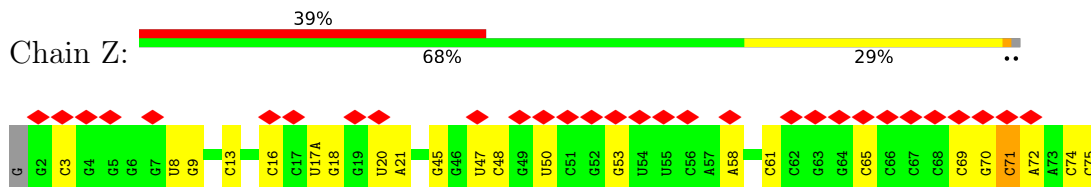
- Molecule 27: mRNA



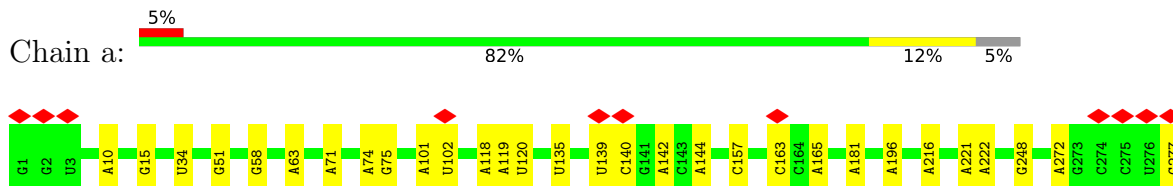
- Molecule 28: A-site oABZ-tRNA^{Phe}



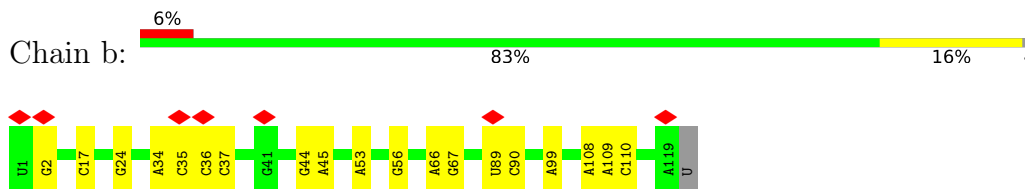
- Molecule 29: P-site fMet-tRNA^{fMet}



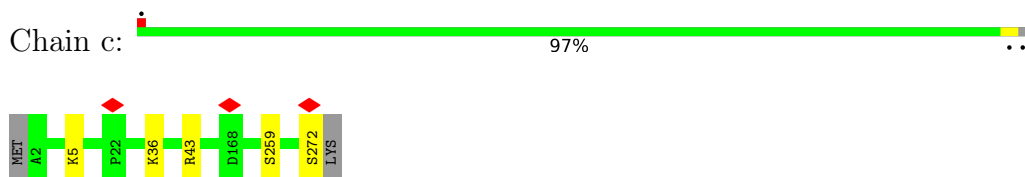
- Molecule 30: 23S rRNA



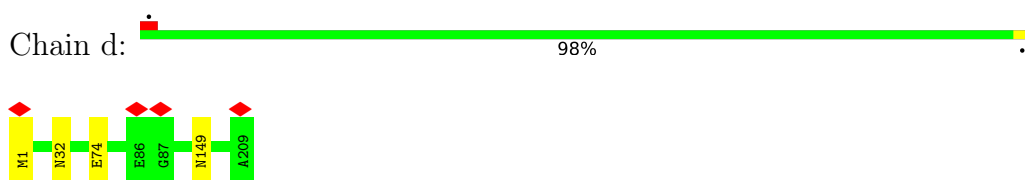
• Molecule 31: 5S rRNA



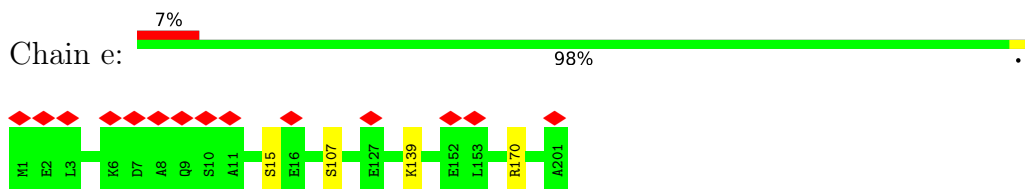
• Molecule 32: 50S ribosomal protein L2



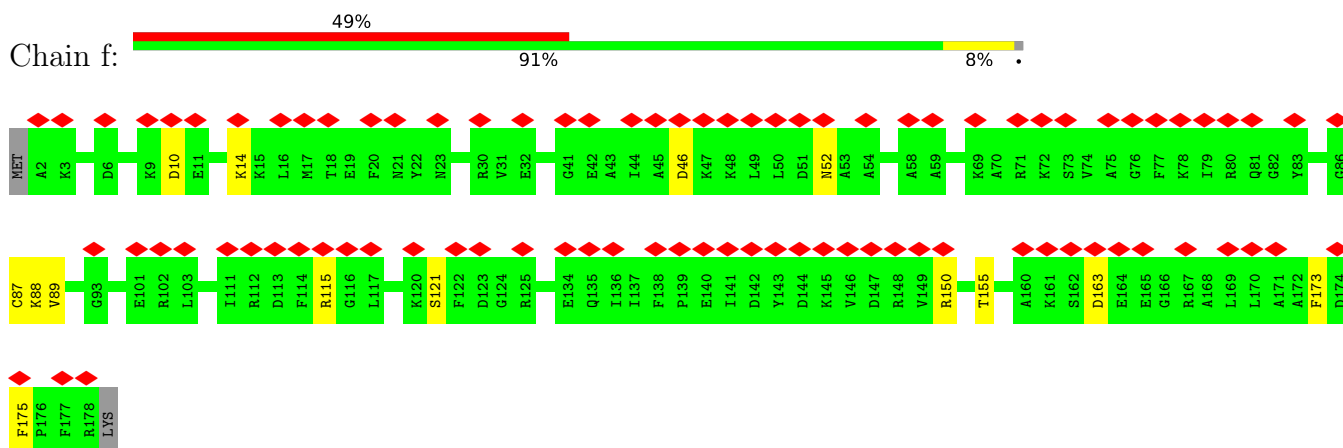
• Molecule 33: 50S ribosomal protein L3



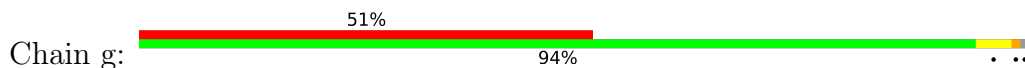
• Molecule 34: 50S ribosomal protein L4

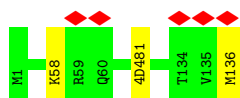


• Molecule 35: 50S ribosomal protein L5



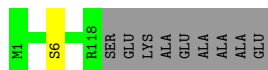
• Molecule 36: 50S ribosomal protein L6





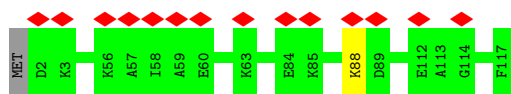
- Molecule 42: 50S ribosomal protein L17

Chain m: 92% 7%



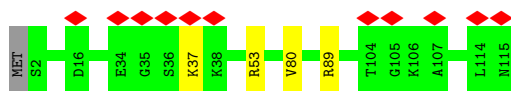
- Molecule 43: 50S ribosomal protein L18

Chain n: 12% 98%



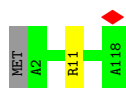
- Molecule 44: 50S ribosomal protein L19

Chain o: 10% 96%



- Molecule 45: 50S ribosomal protein L20

Chain p: 98%



- Molecule 46: Ribosomal protein L21

Chain q: 7% 95% 5%

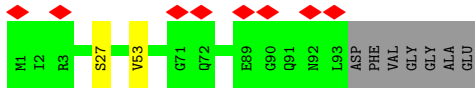
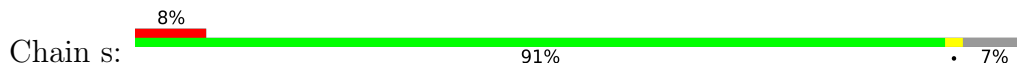


- Molecule 47: 50S ribosomal protein L22

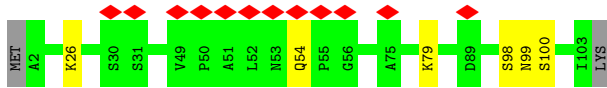
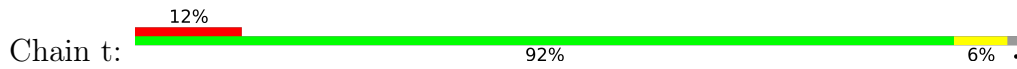
Chain r: 99%



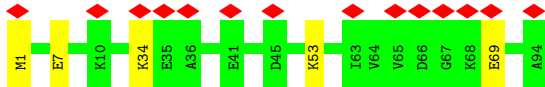
- Molecule 48: 50S ribosomal protein L23



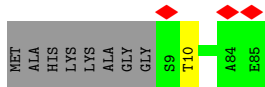
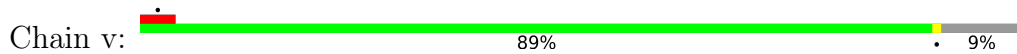
- Molecule 49: 50S ribosomal protein L24



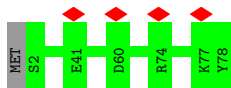
- Molecule 50: 50S ribosomal protein L25



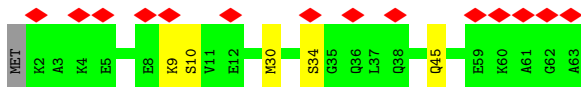
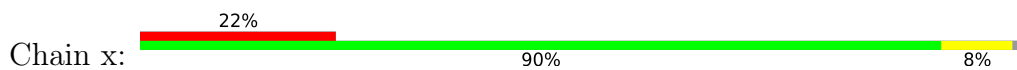
- Molecule 51: 50S ribosomal protein L27



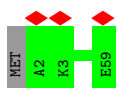
- Molecule 52: 50S ribosomal protein L28



- Molecule 53: 50S ribosomal protein L29

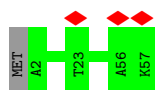


- Molecule 54: 50S ribosomal protein L30



- Molecule 55: 50S ribosomal protein L32

Chain z:  5% 98%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	339543	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0169	Depositor
Map size (Å)	381.96478, 381.96478, 381.96478	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8232, 0.8232, 0.8232	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, 8AN, MEQ, 5MU, K, 1MG, PAR, 5MC, 2AE, OMC, 4OC, OMG, 6MZ, 2MG, MG, OMU, FME, G7M, UR3, 3TD, MS6, PSU, ZN, IAS, 2MA, D2T, SPD, 4D4

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	0	0.27	0/424	0.49	0/565
2	1	0.27	0/380	0.49	0/498
3	2	0.28	0/513	0.48	0/676
4	3	0.29	0/303	0.47	0/397
5	4	0.28	0/488	0.52	0/649
6	A	0.34	0/36236	0.89	16/56520 (0.0%)
7	B	0.27	0/1784	0.47	0/2403
8	C	0.27	0/1651	0.49	0/2225
9	D	0.27	0/1665	0.48	0/2227
10	E	0.31	0/1165	0.49	0/1568
11	F	0.27	0/858	0.50	0/1160
12	G	0.28	0/1219	0.48	0/1635
13	H	0.27	0/989	0.49	0/1326
14	I	0.27	0/1034	0.50	0/1375
15	J	0.40	1/795 (0.1%)	0.64	1/1075 (0.1%)
16	K	0.28	0/884	0.49	0/1191
17	L	0.28	0/960	0.51	0/1286
18	M	0.27	0/900	0.52	0/1204
19	N	0.26	0/817	0.47	0/1088
20	O	0.26	0/722	0.45	0/964
21	P	0.27	0/653	0.51	0/877
22	Q	0.27	0/650	0.51	0/871
23	R	0.28	0/553	0.51	0/742
24	S	0.27	0/685	0.47	0/922
25	T	0.29	0/676	0.45	0/895
26	U	0.30	0/597	0.47	0/792
27	X	0.43	0/354	1.00	1/548 (0.2%)
28	Y	0.45	0/1763	1.05	8/2745 (0.3%)
29	Z	0.40	0/1788	1.01	5/2786 (0.2%)
30	a	0.46	1/65717 (0.0%)	0.91	38/102515 (0.0%)
31	b	0.37	0/2850	0.87	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.29	0/2121	0.52	0/2852
33	d	0.28	0/1576	0.51	0/2119
34	e	0.29	0/1571	0.49	0/2113
35	f	0.28	0/1434	0.50	0/1926
36	g	0.28	0/1343	0.54	0/1816
37	h	0.28	0/306	0.60	0/413
38	i	0.30	0/1152	0.47	0/1551
39	j	0.30	0/955	0.53	0/1279
40	k	0.30	0/1062	0.54	0/1413
41	l	0.29	0/1073	0.50	0/1433
42	m	0.28	0/958	0.49	0/1281
43	n	0.27	0/902	0.49	0/1209
44	o	0.30	0/929	0.50	0/1242
45	p	0.31	0/960	0.45	0/1278
46	q	0.31	0/829	0.54	0/1107
47	r	0.29	0/864	0.49	0/1156
48	s	0.28	0/744	0.47	0/994
49	t	0.29	0/787	0.52	0/1051
50	u	0.28	0/766	0.46	0/1025
51	v	0.37	0/589	0.48	0/780
52	w	0.29	0/635	0.51	0/848
53	x	0.24	0/502	0.46	0/667
54	y	0.26	0/453	0.49	0/605
55	z	0.28	0/450	0.53	0/599
All	All	0.38	2/153034 (0.0%)	0.82	69/228926 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	2	0	1
18	M	0	1
36	g	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	31	ARG	N-CA	-8.26	1.29	1.46
30	a	2605	PSU	O3'-P	-5.32	1.54	1.61

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Z	72	A	P-O3'-C3'	-9.64	108.13	119.70
30	a	2491[A]	U	P-O3'-C3'	-8.57	109.41	119.70
30	a	2491[B]	U	P-O3'-C3'	-8.57	109.41	119.70
30	a	2064	C	P-O3'-C3'	-8.48	109.52	119.70
30	a	2549	G	P-O3'-C3'	-8.19	109.87	119.70
28	Y	13	C	P-O3'-C3'	-8.07	110.01	119.70
29	Z	74	C	C6-N1-C2	-7.21	117.42	120.30
28	Y	55	U	P-O3'-C3'	-6.97	111.34	119.70
28	Y	54	U	P-O3'-C3'	-6.91	111.41	119.70
15	J	30	LYS	O-C-N	-6.55	112.22	122.70
27	X	19	U	P-O3'-C3'	-6.37	112.06	119.70
28	Y	73	A	P-O3'-C3'	-6.35	112.08	119.70
29	Z	75	C	C6-N1-C2	-6.28	117.79	120.30
6	A	214	C	C2-N1-C1'	5.93	125.33	118.80
6	A	505	G	N3-C4-N9	5.90	129.54	126.00
28	Y	12	U	P-O3'-C3'	-5.87	112.65	119.70
28	Y	71	G	P-O3'-C3'	-5.84	112.69	119.70
29	Z	74	C	C2-N1-C1'	5.79	125.16	118.80
29	Z	71	C	P-O3'-C3'	-5.74	112.81	119.70
30	a	2510	C	P-O3'-C3'	-5.73	112.83	119.70
6	A	436	C	C2-N1-C1'	5.66	125.02	118.80
30	a	703	U	P-O3'-C3'	-5.57	113.02	119.70
30	a	1937	A	O4'-C1'-N9	5.56	112.65	108.20
30	a	2321	U	C2-N1-C1'	5.54	124.35	117.70
6	A	191	G	N3-C4-N9	5.54	129.32	126.00
6	A	490	C	C5-C6-N1	5.52	123.76	121.00
30	a	1313	U	C2-N1-C1'	5.51	124.31	117.70
28	Y	38	A	P-O3'-C3'	-5.49	113.11	119.70
30	a	1774	C	N3-C2-O2	-5.47	118.07	121.90
30	a	281	C	N1-C2-O2	5.46	122.18	118.90
30	a	883	G	N3-C4-N9	5.46	129.28	126.00
30	a	2583	G	C8-N9-C4	-5.44	104.22	106.40
30	a	704	G	P-O3'-C3'	-5.44	113.18	119.70
30	a	2588	G	N9-C4-C5	5.42	107.57	105.40
30	a	2430	A	O4'-C1'-N9	5.42	112.53	108.20
30	a	2645	G	O4'-C1'-N9	5.41	112.53	108.20
30	a	775	G	O4'-C1'-N9	5.36	112.49	108.20
30	a	748	G	O4'-C1'-N9	5.36	112.49	108.20
6	A	1035	A	P-O3'-C3'	5.35	126.12	119.70
6	A	1138	G	C4-N9-C1'	5.31	133.40	126.50
30	a	281	C	C2-N1-C1'	5.31	124.64	118.80
30	a	885	C	C2-N1-C1'	5.29	124.62	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Y	74	C	P-O3'-C3'	-5.29	113.35	119.70
6	A	191	G	C4-N9-C1'	5.25	133.33	126.50
30	a	883	G	C4-N9-C1'	5.25	133.33	126.50
30	a	2247	A	N1-C6-N6	5.25	121.75	118.60
30	a	2498	OMC	OP2-P-O3'	5.25	116.75	105.20
30	a	2448	A	N1-C6-N6	5.23	121.74	118.60
6	A	191	G	C8-N9-C1'	-5.22	120.22	127.00
30	a	2250	G	C5-C6-N1	5.21	114.11	111.50
30	a	1857	G	O4'-C1'-N9	5.20	112.36	108.20
30	a	2473	U	C2-N1-C1'	5.17	123.90	117.70
30	a	2588	G	N1-C6-O6	-5.16	116.81	119.90
30	a	2588	G	C2-N3-C4	5.14	114.47	111.90
6	A	1032	G	N3-C4-C5	-5.14	126.03	128.60
30	a	2558	C	P-O3'-C3'	-5.13	113.54	119.70
30	a	1409	U	C2-N1-C1'	5.13	123.86	117.70
30	a	2557	G	C8-N9-C4	-5.13	104.35	106.40
30	a	2093	G	C6-C5-N7	5.12	133.47	130.40
6	A	88	U	C2-N1-C1'	5.12	123.84	117.70
6	A	522	C	N1-C2-O2	5.11	121.96	118.90
30	a	893	C	N1-C2-O2	5.11	121.96	118.90
6	A	69	G	N3-C4-N9	5.10	129.06	126.00
30	a	2606	C	C6-N1-C2	-5.07	118.27	120.30
6	A	462	G	C4-N9-C1'	5.06	133.08	126.50
30	a	893	C	N3-C2-O2	-5.06	118.36	121.90
30	a	2566	A	O4'-C1'-N9	5.03	112.23	108.20
6	A	979	C	N3-C2-O2	-5.03	118.38	121.90
6	A	979	C	C2-N1-C1'	5.02	124.32	118.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	31	HIS	Peptide
18	M	104	THR	Peptide
36	g	47	ASP	Peptide
36	g	48	ASN	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles

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	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	9	4
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
7	B	222/241 (92%)	207 (93%)	15 (7%)	0	100	100
8	C	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
9	D	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
10	E	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
11	F	101/135 (75%)	95 (94%)	6 (6%)	0	100	100
12	G	151/179 (84%)	143 (95%)	8 (5%)	0	100	100
13	H	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
14	I	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
15	J	96/103 (93%)	91 (95%)	5 (5%)	0	100	100
16	K	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
17	L	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
18	M	113/118 (96%)	101 (89%)	12 (11%)	0	100	100
19	N	98/101 (97%)	90 (92%)	8 (8%)	0	100	100
20	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
21	P	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
22	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
23	R	64/75 (85%)	59 (92%)	4 (6%)	1 (2%)	9	4
24	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
25	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
26	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	c	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
33	d	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	22
34	e	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
35	f	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
36	g	174/177 (98%)	156 (90%)	17 (10%)	1 (1%)	25	18
37	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
38	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
39	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
40	k	142/144 (99%)	138 (97%)	3 (2%)	1 (1%)	22	15
41	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
42	m	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
43	n	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
44	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
45	p	115/118 (98%)	115 (100%)	0	0	100	100
46	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
47	r	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
48	s	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
49	t	100/104 (96%)	94 (94%)	5 (5%)	1 (1%)	15	9
50	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
51	v	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
52	w	75/78 (96%)	75 (100%)	0	0	100	100
53	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
54	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
55	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5480/5913 (93%)	5245 (96%)	229 (4%)	6 (0%)	54	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	32	ILE
23	R	23	TYR
36	g	47	ASP
40	k	36	LYS
33	d	149	ASN

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Mol	Chain	Res	Type
49	t	99	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	36 (95%)	2 (5%)	22	17
3	2	51/52 (98%)	47 (92%)	4 (8%)	12	7
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	47 (86%)	8 (14%)	3	1
7	B	186/199 (94%)	161 (87%)	25 (13%)	4	2
8	C	170/190 (90%)	150 (88%)	20 (12%)	5	2
9	D	172/173 (99%)	148 (86%)	24 (14%)	3	1
10	E	119/126 (94%)	113 (95%)	6 (5%)	24	19
11	F	90/116 (78%)	85 (94%)	5 (6%)	21	16
12	G	126/147 (86%)	113 (90%)	13 (10%)	7	3
13	H	104/105 (99%)	97 (93%)	7 (7%)	16	11
14	I	105/107 (98%)	92 (88%)	13 (12%)	4	2
15	J	86/90 (96%)	79 (92%)	7 (8%)	11	7
16	K	89/98 (91%)	80 (90%)	9 (10%)	7	4
17	L	102/103 (99%)	94 (92%)	8 (8%)	12	7
18	M	93/96 (97%)	82 (88%)	11 (12%)	5	2
19	N	83/84 (99%)	76 (92%)	7 (8%)	11	6
20	O	76/77 (99%)	69 (91%)	7 (9%)	9	5
21	P	65/65 (100%)	56 (86%)	9 (14%)	3	1
22	Q	73/78 (94%)	70 (96%)	3 (4%)	30	27
23	R	57/65 (88%)	55 (96%)	2 (4%)	36	34
24	S	72/79 (91%)	63 (88%)	9 (12%)	4	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	T	65/66 (98%)	62 (95%)	3 (5%)	27	22
26	U	60/61 (98%)	56 (93%)	4 (7%)	16	11
32	c	216/218 (99%)	211 (98%)	5 (2%)	50	51
33	d	163/163 (100%)	160 (98%)	3 (2%)	59	61
34	e	165/165 (100%)	161 (98%)	4 (2%)	49	49
35	f	148/150 (99%)	134 (90%)	14 (10%)	8	4
36	g	137/138 (99%)	129 (94%)	8 (6%)	20	15
37	h	32/114 (28%)	29 (91%)	3 (9%)	8	4
38	i	116/116 (100%)	113 (97%)	3 (3%)	46	46
39	j	104/104 (100%)	103 (99%)	1 (1%)	76	80
40	k	103/103 (100%)	101 (98%)	2 (2%)	57	59
41	l	107/107 (100%)	105 (98%)	2 (2%)	57	59
42	m	98/103 (95%)	97 (99%)	1 (1%)	76	80
43	n	86/87 (99%)	85 (99%)	1 (1%)	71	75
44	o	99/100 (99%)	95 (96%)	4 (4%)	31	28
45	p	89/90 (99%)	88 (99%)	1 (1%)	73	77
46	q	84/84 (100%)	79 (94%)	5 (6%)	19	14
47	r	93/93 (100%)	92 (99%)	1 (1%)	73	77
48	s	80/84 (95%)	78 (98%)	2 (2%)	47	48
49	t	83/85 (98%)	78 (94%)	5 (6%)	19	14
50	u	78/78 (100%)	73 (94%)	5 (6%)	17	12
51	v	58/63 (92%)	57 (98%)	1 (2%)	60	63
52	w	67/68 (98%)	67 (100%)	0	100	100
53	x	54/55 (98%)	49 (91%)	5 (9%)	9	5
54	y	48/49 (98%)	48 (100%)	0	100	100
55	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4572/4825 (95%)	4290 (94%)	282 (6%)	22	13

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	8	SER
2	1	25	LYS

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Mol	Chain	Res	Type
3	2	31	HIS
3	2	32	ILE
3	2	47	LYS
3	2	51	SER
5	4	8	LYS
5	4	13	THR
5	4	22	MET
5	4	23	LYS
5	4	24	ILE
5	4	32	LEU
5	4	37	CYS
5	4	59	ARG
7	B	7	ARG
7	B	9	MET
7	B	18	HIS
7	B	21	ARG
7	B	23	TRP
7	B	35	ARG
7	B	44	GLU
7	B	45	LYS
7	B	58	ASN
7	B	63	ARG
7	B	64	LYS
7	B	77	SER
7	B	89	GLN
7	B	113	ARG
7	B	115	LYS
7	B	117	LEU
7	B	123	ASP
7	B	128	LYS
7	B	132	LYS
7	B	137	ARG
7	B	152	LYS
7	B	153	ASP
7	B	164	ILE
7	B	186	ILE
7	B	188	ASP
8	C	5	VAL
8	C	18	TRP
8	C	21	THR
8	C	25	ASN
8	C	52	VAL

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Mol	Chain	Res	Type
8	C	53	SER
8	C	82	GLU
8	C	88	ARG
8	C	102	ASN
8	C	107	ARG
8	C	108	LYS
8	C	119	SER
8	C	125	GLU
8	C	132	ARG
8	C	136	ARG
8	C	139	GLN
8	C	169	ARG
8	C	170	GLU
8	C	181	ASP
8	C	207	ILE
9	D	8	LYS
9	D	11	LEU
9	D	17	THR
9	D	25	VAL
9	D	29	ASP
9	D	31	LYS
9	D	45	LYS
9	D	47	ARG
9	D	57	GLU
9	D	77	LYS
9	D	90	LEU
9	D	115	ARG
9	D	119	SER
9	D	128	ARG
9	D	138	SER
9	D	141	ASP
9	D	144	SER
9	D	159	LEU
9	D	167	LYS
9	D	174	ASP
9	D	177	LYS
9	D	179	GLU
9	D	187	GLU
9	D	191	LEU
10	E	23	LYS
10	E	38	VAL
10	E	54	ARG

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Mol	Chain	Res	Type
10	E	81	LEU
10	E	156	LYS
10	E	159	LYS
11	F	23	GLU
11	F	39	LEU
11	F	68	GLN
11	F	88	MET
11	F	102	MET
12	G	11	LYS
12	G	15	ASP
12	G	17	LYS
12	G	56	LYS
12	G	57	SER
12	G	74	GLU
12	G	78	ARG
12	G	91	VAL
12	G	92	ARG
12	G	123	GLU
12	G	131	LYS
12	G	136	LYS
12	G	144	MET
13	H	26	THR
13	H	31	LYS
13	H	41	LYS
13	H	50	LYS
13	H	69	LYS
13	H	101	ILE
13	H	111	MET
14	I	27	LYS
14	I	29	VAL
14	I	32	GLN
14	I	46	MET
14	I	53	GLU
14	I	68	LYS
14	I	85	ARG
14	I	95	ARG
14	I	100	LYS
14	I	106	ARG
14	I	119	ARG
14	I	123	ARG
14	I	130	ARG
15	J	16	ARG

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Mol	Chain	Res	Type
15	J	19	ASP
15	J	45	ARG
15	J	49	PHE
15	J	71	LEU
15	J	82	LYS
15	J	89	ARG
16	K	13	ARG
16	K	15	GLN
16	K	17	SER
16	K	38	GLN
16	K	55	SER
16	K	86	VAL
16	K	98	ARG
16	K	113	VAL
16	K	129	VAL
17	L	10	LYS
17	L	15	LYS
17	L	50	ARG
17	L	75	GLN
17	L	83	ARG
17	L	88	LYS
17	L	110	ARG
17	L	115	SER
18	M	3	ARG
18	M	20	THR
18	M	21	SER
18	M	30	SER
18	M	65	VAL
18	M	69	LEU
18	M	71	ARG
18	M	83	LEU
18	M	90	ARG
18	M	104	THR
18	M	105	ASN
19	N	23	LYS
19	N	32	SER
19	N	34	VAL
19	N	41	ARG
19	N	76	LYS
19	N	81	ARG
19	N	83	LYS
20	O	4	SER

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Mol	Chain	Res	Type
20	O	10	LYS
20	O	17	ARG
20	O	18	ASP
20	O	21	ASP
20	O	35	GLN
20	O	54	ARG
21	P	1	MET
21	P	8	ARG
21	P	14	ARG
21	P	24	SER
21	P	46	LYS
21	P	55	ASP
21	P	66	THR
21	P	69	ASP
21	P	77	GLU
22	Q	7	THR
22	Q	11	ARG
22	Q	72	SER
23	R	14	THR
23	R	30	LYS
24	S	12	ASP
24	S	13	LEU
24	S	14	HIS
24	S	29	LYS
24	S	48	THR
24	S	55	ARG
24	S	56	GLN
24	S	64	ASP
24	S	71	LEU
25	T	5	LYS
25	T	54	MET
25	T	86	LEU
26	U	5	LYS
26	U	25	LYS
26	U	49	LYS
26	U	51	SER
32	c	5	LYS
32	c	36	LYS
32	c	43	ARG
32	c	259	SER
32	c	272	SER
33	d	1	MET

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Mol	Chain	Res	Type
33	d	32	ASN
33	d	74	GLU
34	e	15	SER
34	e	107	SER
34	e	139	LYS
34	e	170	ARG
35	f	10	ASP
35	f	14	LYS
35	f	46	ASP
35	f	52	ASN
35	f	87	CYS
35	f	88	LYS
35	f	89	VAL
35	f	115	ARG
35	f	121	SER
35	f	150	ARG
35	f	155	THR
35	f	163	ASP
35	f	173	PHE
35	f	175	PHE
36	g	29	LYS
36	g	48	ASN
36	g	51	THR
36	g	74	SER
36	g	99	LYS
36	g	133	LEU
36	g	137	ASP
36	g	155	GLU
37	h	8	LYS
37	h	12	LEU
37	h	14	SER
38	i	1	MET
38	i	12	LYS
38	i	96	ARG
39	j	93	GLN
40	k	112	LEU
40	k	120	VAL
41	l	58	LYS
41	l	136	MET
42	m	6	SER
43	n	88	LYS
44	o	37	LYS

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Mol	Chain	Res	Type
44	o	53	ARG
44	o	80	VAL
44	o	89	ARG
45	p	11	ARG
46	q	10	LYS
46	q	29	THR
46	q	45	GLU
46	q	46	GLU
46	q	55	ASP
47	r	27	LYS
48	s	27	SER
48	s	53	VAL
49	t	26	LYS
49	t	54	GLN
49	t	79	LYS
49	t	98	SER
49	t	100	SER
50	u	1	MET
50	u	7	GLU
50	u	34	LYS
50	u	53	LYS
50	u	69	GLU
51	v	10	THR
53	x	9	LYS
53	x	10	SER
53	x	30	MET
53	x	34	SER
53	x	45	GLN

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

Mol	Chain	Res	Type
8	C	185	ASN
11	F	63	ASN
17	L	112	GLN
24	S	57	HIS
25	T	13	GLN
39	j	93	GLN
49	t	54	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	14/28 (50%)	5 (35%)	1 (7%)
28	Y	71/76 (93%)	25 (35%)	1 (1%)
29	Z	74/76 (97%)	20 (27%)	0
30	a	2743/2904 (94%)	317 (11%)	0
31	b	118/120 (98%)	19 (16%)	0
6	A	1513/1542 (98%)	278 (18%)	5 (0%)
All	All	4533/4746 (95%)	664 (14%)	7 (0%)

All (664) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	3	A
6	A	4	U
6	A	5	U
6	A	6	G
6	A	7	A
6	A	9	G
6	A	13	U
6	A	22	G
6	A	39	G
6	A	42	G
6	A	44	A
6	A	47	C
6	A	48	C
6	A	49	U
6	A	51	A
6	A	53	A
6	A	56	U
6	A	59	A
6	A	65	A
6	A	69	G
6	A	70	U
6	A	74	A
6	A	75	G
6	A	84	U
6	A	86	G
6	A	87	C
6	A	88	U
6	A	91	U
6	A	94	G
6	A	95	C
6	A	96	U
6	A	98	A

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Mol	Chain	Res	Type
6	A	99	C
6	A	110	C
6	A	121	U
6	A	122	G
6	A	130	A
6	A	131	A
6	A	137	U
6	A	141	G
6	A	143	A
6	A	144	G
6	A	146	G
6	A	147	G
6	A	151	A
6	A	157	U
6	A	158	G
6	A	159	G
6	A	161	A
6	A	166	U
6	A	171	A
6	A	173	U
6	A	182	A
6	A	183	C
6	A	184	G
6	A	193	C
6	A	197	A
6	A	200	G
6	A	201	G
6	A	203	G
6	A	204	G
6	A	226	G
6	A	230	G
6	A	240	G
6	A	245	U
6	A	247	G
6	A	251	G
6	A	266	G
6	A	267	C
6	A	274	A
6	A	280	C
6	A	289	G
6	A	305	G
6	A	321	A

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Mol	Chain	Res	Type
6	A	328	C
6	A	330	C
6	A	344	A
6	A	347	G
6	A	351	G
6	A	352	C
6	A	354	G
6	A	367	U
6	A	372	C
6	A	373	A
6	A	406	G
6	A	412	A
6	A	414	A
6	A	415	A
6	A	418	C
6	A	421	U
6	A	422	C
6	A	424	G
6	A	428	G
6	A	429	U
6	A	435	A
6	A	439	U
6	A	455	G
6	A	456	A
6	A	457	G
6	A	458	U
6	A	459	A
6	A	463	U
6	A	465	A
6	A	468	A
6	A	469	C
6	A	474	G
6	A	478	A
6	A	479	U
6	A	481	G
6	A	484	G
6	A	485	U
6	A	486	U
6	A	490	C
6	A	494	G
6	A	495	A
6	A	496	A

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Mol	Chain	Res	Type
6	A	497	G
6	A	499	A
6	A	511	C
6	A	512	U
6	A	518	C
6	A	519	C
6	A	521	G
6	A	522	C
6	A	531	U
6	A	533	A
6	A	547	A
6	A	559	A
6	A	564	C
6	A	572	A
6	A	573	A
6	A	576	C
6	A	579	A
6	A	597	G
6	A	618	C
6	A	633	G
6	A	635	A
6	A	639	G
6	A	650	G
6	A	665	A
6	A	666	G
6	A	687	A
6	A	718	A
6	A	721	G
6	A	723	U
6	A	724	G
6	A	747	A
6	A	755	G
6	A	777	A
6	A	793	U
6	A	794	A
6	A	802	A
6	A	815	A
6	A	817	C
6	A	829	G
6	A	832	G
6	A	851	G
6	A	885	G

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Mol	Chain	Res	Type
6	A	890	G
6	A	902	G
6	A	914	A
6	A	926	G
6	A	934	C
6	A	935	A
6	A	939	G
6	A	954	G
6	A	955	U
6	A	960	U
6	A	966	2MG
6	A	969	A
6	A	971	G
6	A	975	A
6	A	976	G
6	A	977	A
6	A	978	A
6	A	987	G
6	A	989	U
6	A	1004	A
6	A	1005	A
6	A	1006	G
6	A	1008	U
6	A	1009	U
6	A	1010	U
6	A	1017	U
6	A	1024	G
6	A	1027	C
6	A	1028	C
6	A	1030	U
6	A	1031	C
6	A	1033	G
6	A	1034	G
6	A	1036	A
6	A	1037	C
6	A	1038	C
6	A	1039	G
6	A	1044	A
6	A	1046	A
6	A	1063	C
6	A	1065	U
6	A	1067	A

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Mol	Chain	Res	Type
6	A	1070	U
6	A	1085	U
6	A	1089	G
6	A	1094	G
6	A	1095	U
6	A	1101	A
6	A	1108	G
6	A	1130	A
6	A	1137	C
6	A	1138	G
6	A	1139	G
6	A	1140	C
6	A	1150	A
6	A	1157	A
6	A	1159	U
6	A	1160	G
6	A	1162	C
6	A	1169	A
6	A	1174	G
6	A	1175	G
6	A	1177	G
6	A	1178	G
6	A	1181	G
6	A	1187	G
6	A	1196	A
6	A	1197	A
6	A	1209	C
6	A	1211	U
6	A	1213	A
6	A	1219	A
6	A	1227	A
6	A	1238	A
6	A	1248	A
6	A	1249	C
6	A	1256	A
6	A	1258	G
6	A	1260	G
6	A	1276	G
6	A	1280	A
6	A	1282	C
6	A	1285	A
6	A	1287	A

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Mol	Chain	Res	Type
6	A	1289	A
6	A	1300	G
6	A	1302	C
6	A	1305	G
6	A	1312	G
6	A	1317	C
6	A	1323	G
6	A	1325	C
6	A	1336	C
6	A	1340	A
6	A	1346	A
6	A	1353	G
6	A	1363	A
6	A	1370	G
6	A	1378	C
6	A	1379	G
6	A	1397	C
6	A	1398	A
6	A	1406	U
6	A	1419	G
6	A	1432	G
6	A	1441	A
6	A	1445	U
6	A	1446	A
6	A	1451	U
6	A	1452	C
6	A	1487	G
6	A	1490	U
6	A	1492	A
6	A	1497	G
6	A	1503	A
6	A	1506	U
6	A	1517	G
6	A	1529	G
6	A	1530	G
6	A	1534	A
27	X	19	U
27	X	23	A
27	X	24	A
27	X	25	C
27	X	27	A
28	Y	4	C

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Mol	Chain	Res	Type
28	Y	8	U
28	Y	9	A
28	Y	11	C
28	Y	12	U
28	Y	14	A
28	Y	20	U
28	Y	22	G
28	Y	34	G
28	Y	44	G
28	Y	45	U
28	Y	46	G
28	Y	47	U
28	Y	48	C
28	Y	49	C
28	Y	50	U
28	Y	55	U
28	Y	56	C
28	Y	57	G
28	Y	58	A
28	Y	59	U
28	Y	61	C
28	Y	62	C
28	Y	63	G
28	Y	73	A
29	Z	3	C
29	Z	8	U
29	Z	9	G
29	Z	13	C
29	Z	16	C
29	Z	17(A)	U
29	Z	18	G
29	Z	20	U
29	Z	21	A
29	Z	45	G
29	Z	47	U
29	Z	48	C
29	Z	50	U
29	Z	53	G
29	Z	58	A
29	Z	61	C
29	Z	65	C
29	Z	69	C

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Mol	Chain	Res	Type
29	Z	70	G
29	Z	71	C
30	a	10	A
30	a	15	G
30	a	34	U
30	a	51	G
30	a	58	G
30	a	63	A
30	a	71	A
30	a	74	A
30	a	75	G
30	a	101	A
30	a	102	U
30	a	118	A
30	a	119	A
30	a	120	U
30	a	135	U
30	a	139	U
30	a	140	C
30	a	142	A
30	a	144	A
30	a	157	C
30	a	163	C
30	a	165	A
30	a	181	A
30	a	196	A
30	a	216	A
30	a	221	A
30	a	222	A
30	a	248	G
30	a	272	A
30	a	277	G
30	a	278	A
30	a	282	A
30	a	283	G
30	a	287	G
30	a	289	G
30	a	290	U
30	a	291	G
30	a	311	A
30	a	330	A
30	a	353	C

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Mol	Chain	Res	Type
30	a	362	A
30	a	386	G
30	a	405	U
30	a	411	G
30	a	481	G
30	a	491	G
30	a	504	A
30	a	505	A
30	a	509	C
30	a	530	G
30	a	532	A
30	a	544	C
30	a	545	U
30	a	546	U
30	a	547	A
30	a	548	G
30	a	549	G
30	a	563	A
30	a	573	U
30	a	575	A
30	a	603	A
30	a	613	A
30	a	615	U
30	a	627	A
30	a	637	A
30	a	645	C
30	a	646	U
30	a	647	G
30	a	653	U
30	a	654	A
30	a	655	A
30	a	686	U
30	a	711	G
30	a	715	A
30	a	719	C
30	a	730	A
30	a	747	5MU
30	a	764	A
30	a	775	G
30	a	776	G
30	a	782	A
30	a	784	G

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Mol	Chain	Res	Type
30	a	785	G
30	a	789	A
30	a	805	G
30	a	812	C
30	a	827	U
30	a	828	U
30	a	845	A
30	a	846	U
30	a	847	U
30	a	859	G
30	a	868	U
30	a	877	A
30	a	881	G
30	a	883	G
30	a	885	C
30	a	886	A
30	a	890	C
30	a	891	G
30	a	893	C
30	a	895	U
30	a	896	A
30	a	897	C
30	a	910	A
30	a	914	G
30	a	915	C
30	a	946	C
30	a	961	C
30	a	974	G
30	a	983	A
30	a	996	A
30	a	1012	U
30	a	1013	C
30	a	1017	G
30	a	1022	G
30	a	1026	G
30	a	1033	U
30	a	1042	G
30	a	1045	C
30	a	1046	A
30	a	1047	G
30	a	1048	A
30	a	1051	G

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Mol	Chain	Res	Type
30	a	1108	U
30	a	1111	A
30	a	1112	G
30	a	1113	U
30	a	1115	G
30	a	1116	G
30	a	1117	C
30	a	1122	G
30	a	1132	U
30	a	1135	C
30	a	1142	A
30	a	1171	G
30	a	1180	U
30	a	1250	G
30	a	1253	A
30	a	1256	G
30	a	1271	G
30	a	1272	A
30	a	1300	G
30	a	1301	A
30	a	1329	U
30	a	1352	U
30	a	1365	A
30	a	1379	U
30	a	1383	A
30	a	1409	U
30	a	1412	U
30	a	1416	G
30	a	1420	A
30	a	1421	G
30	a	1424	G
30	a	1427	A
30	a	1428	C
30	a	1452	G
30	a	1453	A
30	a	1460	U
30	a	1468	U
30	a	1482	G
30	a	1493	C
30	a	1494	A
30	a	1497	U
30	a	1509	A

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Mol	Chain	Res	Type
30	a	1510	G
30	a	1515	A
30	a	1524	G
30	a	1535	A
30	a	1536	C
30	a	1566	A
30	a	1569	A
30	a	1578	U
30	a	1581	G
30	a	1584	U
30	a	1585	C
30	a	1586	A
30	a	1591	A
30	a	1608	A
30	a	1647	U
30	a	1648	U
30	a	1649	G
30	a	1674	G
30	a	1715	G
30	a	1726	C
30	a	1729	U
30	a	1730	C
30	a	1733	G
30	a	1738	G
30	a	1744	A
30	a	1764	C
30	a	1773	A
30	a	1782	U
30	a	1791	A
30	a	1800	C
30	a	1801	A
30	a	1808	A
30	a	1816	C
30	a	1829	A
30	a	1847	A
30	a	1848	A
30	a	1858	A
30	a	1869	G
30	a	1871	A
30	a	1872	A
30	a	1873	G
30	a	1876	A

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Mol	Chain	Res	Type
30	a	1906	G
30	a	1907	G
30	a	1929	G
30	a	1930	G
30	a	1937	A
30	a	1938	A
30	a	1955	U
30	a	1967	C
30	a	1970	A
30	a	1971	U
30	a	1972	G
30	a	1991	U
30	a	1993	U
30	a	2023	C
30	a	2031	A
30	a	2033	A
30	a	2043	C
30	a	2055	C
30	a	2056	G
30	a	2059	A
30	a	2060	A
30	a	2061	G
30	a	2062	A
30	a	2069	G7M
30	a	2198	A
30	a	2204	G
30	a	2211	A
30	a	2223	G
30	a	2225	A
30	a	2238	G
30	a	2239	G
30	a	2268	A
30	a	2283	C
30	a	2287	A
30	a	2305	U
30	a	2307	G
30	a	2308	G
30	a	2309	A
30	a	2310	C
30	a	2322	A
30	a	2325	G
30	a	2333	A

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Mol	Chain	Res	Type
30	a	2335	A
30	a	2347	C
30	a	2350	C
30	a	2361	G
30	a	2379	G
30	a	2383	G
30	a	2385	C
30	a	2402	U
30	a	2403	C
30	a	2406	A
30	a	2425	A
30	a	2429	G
30	a	2434	A
30	a	2435	A
30	a	2441	U
30	a	2448	A
30	a	2475	C
30	a	2476	A
30	a	2478	A
30	a	2502	G
30	a	2504	PSU
30	a	2505	G
30	a	2506	U
30	a	2518	A
30	a	2520	C
30	a	2529	G
30	a	2535	G
30	a	2547	A
30	a	2566	A
30	a	2567	G
30	a	2573	C
30	a	2585	U
30	a	2602	A
30	a	2609	U
30	a	2613	U
30	a	2629	U
30	a	2653	U
30	a	2656	U
30	a	2661	G
30	a	2663	G
30	a	2667	C
30	a	2689	U

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Mol	Chain	Res	Type
30	a	2690	U
30	a	2714	G
30	a	2726	A
30	a	2733	A
30	a	2744	G
30	a	2748	A
30	a	2757	A
30	a	2765	A
30	a	2778	A
30	a	2792	A
30	a	2795	C
30	a	2797	U
30	a	2798	U
30	a	2799	A
30	a	2800	A
30	a	2820	A
30	a	2821	A
30	a	2835	A
30	a	2861	U
30	a	2873	A
30	a	2883	A
30	a	2884	U
30	a	2891	U
30	a	2902	C
30	a	2903	U
31	b	2	G
31	b	17	C
31	b	24	G
31	b	34	A
31	b	35	C
31	b	36	C
31	b	37	C
31	b	44	G
31	b	45	A
31	b	53	A
31	b	56	G
31	b	66	A
31	b	67	G
31	b	89	U
31	b	90	C
31	b	99	A
31	b	108	A

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Mol	Chain	Res	Type
31	b	109	A
31	b	110	C

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	5	U
6	A	83	C
6	A	1026	G
6	A	1035	A
6	A	1114	C
27	X	24	A
28	Y	56	C

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

38 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
6	UR3	A	1498	6	19,22,23	0.94	0	26,32,35	1.43	2 (7%)
6	5MC	A	1407	6	18,22,23	0.95	2 (11%)	26,32,35	1.27	4 (15%)
30	6MZ	a	2030	30	18,25,26	0.86	1 (5%)	16,36,39	2.27	4 (25%)
30	G7M	a	2069	30	20,26,27	1.19	2 (10%)	17,39,42	0.75	0
6	2MG	A	1516	6	18,26,27	0.89	1 (5%)	16,38,41	1.11	2 (12%)
6	5MC	A	967	6	18,22,23	0.97	2 (11%)	26,32,35	1.16	2 (7%)
30	2MG	a	1835	30	18,26,27	0.88	1 (5%)	16,38,41	1.14	2 (12%)
30	PSU	a	746	30,58	18,21,22	1.45	4 (22%)	22,30,33	1.72	4 (18%)
30	PSU	a	1911	30	18,21,22	1.34	2 (11%)	22,30,33	1.96	5 (22%)
30	2MA	a	2503	62,30,58	17,25,26	1.01	1 (5%)	17,37,40	1.26	3 (17%)
6	4OC	A	1402	6	20,23,24	0.72	0	26,32,35	0.98	1 (3%)
30	PSU	a	2457	30	18,21,22	1.27	2 (11%)	22,30,33	1.92	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	IAS	K	119	16	6,7,8	0.97	0	6,8,10	1.30	1 (16%)
30	5MU	a	747	30	19,22,23	1.38	5 (26%)	28,32,35	1.97	6 (21%)
6	MA6	A	1518	6	19,26,27	0.96	1 (5%)	18,38,41	1.28	3 (16%)
30	PSU	a	955	30	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
17	D2T	L	89	17	7,9,10	1.78	2 (28%)	6,11,13	1.28	0
6	2MG	A	966	6	18,26,27	0.93	1 (5%)	16,38,41	1.17	2 (12%)
30	PSU	a	2604	30	18,21,22	1.31	2 (11%)	22,30,33	1.97	3 (13%)
6	2MG	A	1207	6	18,26,27	0.91	1 (5%)	16,38,41	1.15	2 (12%)
30	PSU	a	2605	30	18,21,22	1.26	3 (16%)	22,30,33	2.01	4 (18%)
30	PSU	a	2580	30	18,21,22	1.38	3 (16%)	22,30,33	1.93	4 (18%)
30	1MG	a	745	30	18,26,27	0.72	0	19,39,42	0.99	2 (10%)
30	OMG	a	2251	62,30,29	18,26,27	1.00	1 (5%)	19,38,41	1.00	2 (10%)
30	5MC	a	1962	30	18,22,23	0.91	2 (11%)	26,32,35	1.16	2 (7%)
30	2MG	a	2445	30	18,26,27	1.03	1 (5%)	16,38,41	1.03	2 (12%)
30	6MZ	a	1618	30	18,25,26	0.92	1 (5%)	16,36,39	2.06	3 (18%)
33	MEQ	d	150	33	8,9,10	0.47	0	5,10,12	0.20	0
30	PSU	a	2504	62,30	18,21,22	1.50	3 (16%)	22,30,33	1.89	4 (18%)
6	G7M	A	527	6	20,26,27	1.20	2 (10%)	17,39,42	0.65	0
6	MA6	A	1519	6	19,26,27	0.98	1 (5%)	18,38,41	1.44	2 (11%)
30	5MU	a	1939	30	19,22,23	1.41	5 (26%)	28,32,35	2.10	6 (21%)
30	OMC	a	2498	30,58	19,22,23	0.88	1 (5%)	26,31,34	0.95	1 (3%)
30	OMU	a	2552	30,58	19,22,23	1.31	3 (15%)	26,31,34	1.75	5 (19%)
6	PSU	A	516	6	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
30	PSU	a	1917	30	18,21,22	1.42	2 (11%)	22,30,33	1.86	3 (13%)
30	3TD	a	1915	30	19,22,23	1.52	4 (21%)	21,32,35	1.96	2 (9%)
41	4D4	l	81	41	9,11,12	1.86	2 (22%)	8,13,15	0.75	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
30	6MZ	a	2030	30	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	G7M	a	2069	30	-	2/3/25/26	0/3/3/3
6	2MG	A	1516	6	-	0/5/27/28	0/3/3/3
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
30	2MG	a	1835	30	-	0/5/27/28	0/3/3/3
30	PSU	a	746	30,58	-	2/7/25/26	0/2/2/2
30	PSU	a	1911	30	-	0/7/25/26	0/2/2/2
30	2MA	a	2503	62,30,58	-	2/3/25/26	0/3/3/3
6	4OC	A	1402	6	-	2/9/29/30	0/2/2/2
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2
16	IAS	K	119	16	-	0/7/7/8	-
30	5MU	a	747	30	-	1/7/25/26	0/2/2/2
6	MA6	A	1518	6	-	0/7/29/30	0/3/3/3
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
17	D2T	L	89	17	-	1/7/12/14	-
6	2MG	A	966	6	-	0/5/27/28	0/3/3/3
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2
6	2MG	A	1207	6	-	2/5/27/28	0/3/3/3
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2580	30	-	0/7/25/26	0/2/2/2
30	1MG	a	745	30	-	0/3/25/26	0/3/3/3
30	OMG	a	2251	62,30,29	-	1/5/27/28	0/3/3/3
30	5MC	a	1962	30	-	2/7/25/26	0/2/2/2
30	2MG	a	2445	30	-	0/5/27/28	0/3/3/3
30	6MZ	a	1618	30	-	0/5/27/28	0/3/3/3
33	MEQ	d	150	33	-	2/8/9/11	-
30	PSU	a	2504	62,30	-	0/7/25/26	0/2/2/2
6	G7M	A	527	6	-	1/3/25/26	0/3/3/3
6	MA6	A	1519	6	-	2/7/29/30	0/3/3/3
30	5MU	a	1939	30	-	0/7/25/26	0/2/2/2
30	OMC	a	2498	30,58	-	0/9/27/28	0/2/2/2
30	OMU	a	2552	30,58	-	1/9/27/28	0/2/2/2
6	PSU	A	516	6	-	0/7/25/26	0/2/2/2
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2
30	3TD	a	1915	30	-	0/7/25/26	0/2/2/2
41	4D4	l	81	41	-	1/11/12/14	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	l	81	4D4	CZ-NE	3.95	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	527	G7M	C5-C4	3.52	1.46	1.39
30	a	2069	G7M	C5-C4	3.45	1.46	1.39
30	a	1917	PSU	C6-C5	3.33	1.39	1.35
30	a	746	PSU	C6-C5	3.31	1.39	1.35
30	a	2504	PSU	C6-C5	3.23	1.39	1.35
30	a	2552	OMU	C5-C4	-3.22	1.36	1.43
17	L	89	D2T	CB-CG	3.22	1.57	1.52
30	a	2580	PSU	C6-C5	3.20	1.39	1.35
30	a	1915	3TD	C6-C5	3.17	1.39	1.35
30	a	955	PSU	C6-C5	3.15	1.39	1.35
30	a	2457	PSU	C6-C5	3.10	1.38	1.35
30	a	1915	3TD	C4-N3	-3.06	1.33	1.40
6	A	516	PSU	C6-C5	3.01	1.38	1.35
30	a	2251	OMG	C6-N1	-2.95	1.33	1.37
6	A	967	5MC	C6-C5	2.92	1.39	1.34
30	a	1915	3TD	C10-N3	2.90	1.52	1.47
30	a	1939	5MU	C6-N1	-2.87	1.33	1.38
30	a	746	PSU	C4-N3	-2.86	1.33	1.38
30	a	955	PSU	C4-N3	-2.86	1.33	1.38
30	a	1911	PSU	C6-C5	2.84	1.38	1.35
30	a	2552	OMU	C4-N3	-2.83	1.33	1.38
30	a	1911	PSU	C4-N3	-2.81	1.33	1.38
30	a	2605	PSU	C4-N3	-2.81	1.33	1.38
30	a	2604	PSU	C6-C5	2.81	1.38	1.35
30	a	2445	2MG	C6-N1	-2.79	1.33	1.37
30	a	1939	5MU	C4-N3	-2.78	1.33	1.38
30	a	2504	PSU	C2-N1	-2.73	1.33	1.36
6	A	966	2MG	C6-N1	-2.71	1.33	1.37
30	a	2504	PSU	C4-N3	-2.69	1.33	1.38
30	a	2604	PSU	C4-N3	-2.69	1.33	1.38
30	a	1917	PSU	C4-N3	-2.68	1.33	1.38
30	a	747	5MU	C4-N3	-2.65	1.33	1.38
30	a	2457	PSU	C4-N3	-2.60	1.34	1.38
30	a	747	5MU	C6-C5	2.58	1.38	1.34
17	L	89	D2T	CB-SB	2.58	1.84	1.82
6	A	516	PSU	C4-N3	-2.57	1.34	1.38
30	a	1835	2MG	C6-N1	-2.54	1.34	1.37
6	A	1407	5MC	C6-C5	2.54	1.38	1.34
6	A	1207	2MG	C6-N1	-2.52	1.34	1.37
30	a	1962	5MC	C6-C5	2.51	1.38	1.34
6	A	1518	MA6	C5-C4	2.51	1.47	1.40
30	a	2605	PSU	C6-C5	2.50	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2580	PSU	C4-N3	-2.49	1.34	1.38
30	a	1618	6MZ	C5-C4	2.47	1.47	1.40
6	A	1519	MA6	C5-C4	2.45	1.47	1.40
6	A	1407	5MC	C6-N1	-2.41	1.33	1.38
6	A	1516	2MG	C6-N1	-2.41	1.34	1.37
30	a	2069	G7M	C6-N1	-2.40	1.34	1.37
30	a	1939	5MU	C2-N3	-2.39	1.33	1.38
30	a	1962	5MC	C6-N1	-2.37	1.34	1.38
41	l	81	4D4	CZ-NH2	2.35	1.41	1.32
30	a	747	5MU	C4-C5	2.33	1.48	1.44
30	a	1939	5MU	C6-C5	2.32	1.38	1.34
30	a	2552	OMU	C2-N3	-2.27	1.33	1.38
30	a	2580	PSU	O4'-C1'	-2.26	1.40	1.43
30	a	746	PSU	C2-N3	-2.26	1.33	1.37
30	a	747	5MU	C6-N1	-2.25	1.34	1.38
6	A	967	5MC	C6-N1	-2.21	1.34	1.38
6	A	527	G7M	C6-N1	-2.21	1.34	1.37
30	a	1939	5MU	C4-C5	2.19	1.48	1.44
30	a	747	5MU	C2-N3	-2.17	1.34	1.38
30	a	2030	6MZ	C5-C4	2.12	1.46	1.40
30	a	746	PSU	O4'-C1'	-2.11	1.40	1.43
30	a	1915	3TD	C2-N1	-2.06	1.34	1.37
30	a	2498	OMC	C6-C5	2.04	1.39	1.35
30	a	2503	2MA	C6-N1	-2.04	1.33	1.38
30	a	2605	PSU	C2-N3	-2.00	1.34	1.37

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1915	3TD	N1-C2-N3	7.16	121.79	116.14
30	a	1618	6MZ	C2-N1-C6	6.47	122.14	116.59
30	a	2030	6MZ	C2-N1-C6	6.29	121.99	116.59
30	a	1911	PSU	N1-C2-N3	6.02	121.95	115.13
30	a	2605	PSU	N1-C2-N3	5.98	121.91	115.13
30	a	2604	PSU	N1-C2-N3	5.94	121.86	115.13
30	a	2457	PSU	N1-C2-N3	5.92	121.83	115.13
30	a	955	PSU	N1-C2-N3	5.87	121.78	115.13
30	a	746	PSU	N1-C2-N3	5.86	121.77	115.13
6	A	516	PSU	N1-C2-N3	5.81	121.71	115.13
30	a	1917	PSU	N1-C2-N3	5.75	121.65	115.13
6	A	1498	UR3	C4-N3-C2	-5.66	119.24	124.56
30	a	2580	PSU	N1-C2-N3	5.58	121.45	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2552	OMU	O4-C4-C5	-5.34	115.77	125.16
30	a	1939	5MU	C4-N3-C2	-5.16	120.67	127.35
30	a	2504	PSU	N1-C2-N3	5.00	120.80	115.13
30	a	2504	PSU	C6-C5-C4	-4.66	114.94	118.20
30	a	747	5MU	C4-N3-C2	-4.64	121.34	127.35
30	a	1939	5MU	N3-C2-N1	4.63	121.04	114.89
30	a	747	5MU	N3-C2-N1	4.46	120.82	114.89
30	a	2605	PSU	C4-N3-C2	-4.42	119.97	126.34
30	a	1939	5MU	C5-C6-N1	-4.31	118.90	123.34
30	a	1911	PSU	C4-N3-C2	-4.26	120.21	126.34
6	A	967	5MC	C5-C6-N1	-4.25	118.97	123.34
30	a	1939	5MU	C5-C4-N3	4.22	118.91	115.31
30	a	2604	PSU	C4-N3-C2	-4.18	120.32	126.34
30	a	2457	PSU	C4-N3-C2	-4.16	120.34	126.34
30	a	747	5MU	O4-C4-C5	-4.13	120.11	124.90
30	a	1939	5MU	O4-C4-C5	-4.03	120.23	124.90
30	a	747	5MU	C5-C4-N3	4.01	118.73	115.31
30	a	955	PSU	C4-N3-C2	-3.95	120.65	126.34
30	a	2552	OMU	C5-C4-N3	3.86	120.62	114.84
30	a	1917	PSU	C4-N3-C2	-3.85	120.79	126.34
30	a	2604	PSU	O2-C2-N1	-3.76	118.65	122.79
30	a	2580	PSU	C4-N3-C2	-3.75	120.93	126.34
30	a	747	5MU	C5-C6-N1	-3.73	119.50	123.34
6	A	1519	MA6	C4-C5-N7	-3.72	105.53	109.40
30	a	2580	PSU	O2-C2-N1	-3.66	118.76	122.79
30	a	2030	6MZ	C9-N6-C6	-3.66	119.72	122.87
30	a	2030	6MZ	N3-C2-N1	-3.63	123.01	128.68
6	A	516	PSU	C4-N3-C2	-3.58	121.19	126.34
6	A	1407	5MC	C5-C6-N1	-3.56	119.67	123.34
30	a	1915	3TD	C4-N3-C2	-3.56	120.75	124.61
30	a	1911	PSU	O2-C2-N1	-3.55	118.88	122.79
30	a	2552	OMU	C4-N3-C2	-3.50	121.97	126.58
6	A	1519	MA6	N3-C2-N1	-3.44	123.30	128.68
30	a	2605	PSU	O2-C2-N1	-3.40	119.05	122.79
30	a	1917	PSU	O2-C2-N1	-3.38	119.07	122.79
30	a	746	PSU	C4-N3-C2	-3.36	121.50	126.34
6	A	516	PSU	O2-C2-N1	-3.33	119.13	122.79
30	a	1618	6MZ	N3-C2-N1	-3.31	123.50	128.68
30	a	1962	5MC	C5-C6-N1	-3.28	119.97	123.34
30	a	2504	PSU	C4-N3-C2	-3.27	121.63	126.34
30	a	2504	PSU	O2-C2-N1	-3.18	119.29	122.79
6	A	1518	MA6	C4-C5-N7	-3.13	106.14	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2030	6MZ	C4-C5-N7	-3.09	106.18	109.40
30	a	2457	PSU	O2-C2-N1	-3.07	119.41	122.79
6	A	1518	MA6	N3-C2-N1	-3.06	123.89	128.68
30	a	2552	OMU	O4-C4-N3	2.93	123.61	119.31
30	a	2503	2MA	C5-C6-N1	2.91	119.05	114.02
30	a	1939	5MU	O2-C2-N1	-2.86	118.99	122.79
30	a	1618	6MZ	C4-C5-N7	-2.85	106.43	109.40
30	a	747	5MU	O2-C2-N1	-2.81	119.05	122.79
30	a	955	PSU	O2-C2-N1	-2.80	119.71	122.79
30	a	1962	5MC	C5-C4-N3	-2.62	118.85	121.67
30	a	2552	OMU	N3-C2-N1	2.60	118.35	114.89
30	a	2503	2MA	C8-N7-C5	2.60	107.93	102.99
6	A	967	5MC	C5-C4-N3	-2.55	118.93	121.67
6	A	1402	4OC	C6-C5-C4	2.54	120.07	116.96
6	A	1407	5MC	C5-C4-N3	-2.54	118.93	121.67
16	K	119	IAS	OD1-CG-CB	-2.49	118.19	125.43
6	A	1407	5MC	O2-C2-N3	-2.45	118.34	122.33
30	a	1835	2MG	C8-N7-C5	2.44	107.64	102.99
30	a	2498	OMC	O2-C2-N3	-2.44	118.37	122.33
30	a	2580	PSU	O4'-C1'-C2'	2.42	108.56	105.14
30	a	745	1MG	C5-C6-N1	2.41	117.53	113.90
30	a	2251	OMG	C8-N7-C5	2.39	107.55	102.99
30	a	2605	PSU	C5-C6-N1	-2.37	118.55	122.11
6	A	1516	2MG	C5-C6-N1	2.37	118.13	113.95
30	a	1835	2MG	C5-C6-N1	2.36	118.13	113.95
6	A	1207	2MG	C8-N7-C5	2.36	107.49	102.99
6	A	516	PSU	O4'-C1'-C2'	2.34	108.44	105.14
30	a	745	1MG	C8-N7-C5	2.30	107.37	102.99
6	A	1207	2MG	C5-C6-N1	2.29	117.99	113.95
6	A	1518	MA6	N1-C6-N6	2.29	119.46	117.06
6	A	1498	UR3	C1'-N1-C2	2.27	120.82	116.99
30	a	2503	2MA	CM2-C2-N1	2.25	121.24	116.23
30	a	2445	2MG	C5-C6-N1	2.23	117.89	113.95
6	A	1516	2MG	C8-N7-C5	2.23	107.23	102.99
6	A	966	2MG	C5-C6-N1	2.22	117.88	113.95
30	a	1911	PSU	C5-C6-N1	-2.21	118.79	122.11
30	a	2251	OMG	C5-C6-N1	2.21	117.86	113.95
30	a	746	PSU	O2-C2-N1	-2.20	120.37	122.79
30	a	2445	2MG	C8-N7-C5	2.14	107.06	102.99
30	a	746	PSU	O2-C2-N3	-2.10	117.86	121.82
6	A	1407	5MC	CM5-C5-C6	-2.10	120.05	122.85
30	a	1911	PSU	O4'-C1'-C2'	2.05	108.03	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	966	2MG	C8-N7-C5	2.04	106.88	102.99
30	a	2457	PSU	O4'-C1'-C2'	2.01	107.97	105.14

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1207	2MG	N1-C2-N2-CM2
6	A	1207	2MG	N3-C2-N2-CM2
30	a	746	PSU	C2'-C1'-C5-C4
30	a	2030	6MZ	O4'-C4'-C5'-O5'
30	a	2251	OMG	C1'-C2'-O2'-CM2
33	d	150	MEQ	NE2-CD-CG-CB
6	A	1519	MA6	O4'-C4'-C5'-O5'
30	a	2030	6MZ	C3'-C4'-C5'-O5'
33	d	150	MEQ	OE1-CD-CG-CB
6	A	1402	4OC	O4'-C4'-C5'-O5'
6	A	1519	MA6	C3'-C4'-C5'-O5'
17	L	89	D2T	CG-CB-SB-CB1
30	a	747	5MU	C3'-C4'-C5'-O5'
30	a	2503	2MA	C4'-C5'-O5'-P
30	a	2552	OMU	C3'-C2'-O2'-CM2
6	A	1402	4OC	C3'-C4'-C5'-O5'
30	a	1962	5MC	C2'-C1'-N1-C6
30	a	2069	G7M	C4'-C5'-O5'-P
30	a	1962	5MC	O4'-C1'-N1-C6
30	a	2503	2MA	O4'-C4'-C5'-O5'
30	a	746	PSU	O4'-C1'-C5-C6
30	a	2069	G7M	O4'-C4'-C5'-O5'
41	l	81	4D4	O-C-CA-CB
6	A	527	G7M	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 348 ligands modelled in this entry, 336 are monoatomic - leaving 12 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
63	SPD	a	6208	-	9,9,9	0.16	0	8,8,8	0.17	0
63	SPD	a	6209	-	9,9,9	0.16	0	8,8,8	0.18	0
57	PAR	A	1601	-	45,45,45	0.35	0	64,67,67	0.60	0
63	SPD	a	6210	-	9,9,9	0.16	0	8,8,8	0.21	0
63	SPD	a	6217	-	9,9,9	0.16	0	8,8,8	0.20	0
63	SPD	d	301	-	9,9,9	0.16	0	8,8,8	0.19	0
61	FME	Z	103	60	8,9,10	0.95	0	7,9,11	0.99	1 (14%)
59	2AE	Y	101	28	10,10,10	2.40	1 (10%)	13,13,13	1.84	2 (15%)
63	SPD	a	6211	-	9,9,9	0.16	0	8,8,8	0.18	0
63	SPD	a	6213	-	9,9,9	0.15	0	8,8,8	0.21	0
63	SPD	a	6212	-	9,9,9	0.16	0	8,8,8	0.18	0
60	8AN	Z	101	61,29,58	19,24,25	1.02	2 (10%)	13,35,38	1.24	1 (7%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	SPD	a	6208	-	-	4/7/7/7	-
63	SPD	a	6209	-	-	4/7/7/7	-
57	PAR	A	1601	-	-	3/18/94/94	0/4/4/4
63	SPD	a	6210	-	-	2/7/7/7	-
63	SPD	a	6217	-	-	3/7/7/7	-
63	SPD	d	301	-	-	2/7/7/7	-
61	FME	Z	103	60	-	2/7/9/11	-
59	2AE	Y	101	28	-	0/4/4/4	0/1/1/1
63	SPD	a	6211	-	-	4/7/7/7	-
63	SPD	a	6213	-	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	SPD	a	6212	-	-	5/7/7/7	-
60	8AN	Z	101	61,29,58	-	1/3/25/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	Y	101	2AE	C1-C	-6.97	1.40	1.50
60	Z	101	8AN	C3'-N3'	-2.95	1.42	1.47
60	Z	101	8AN	C8-N7	-2.21	1.30	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	Y	101	2AE	C1-C6-N2	-4.44	116.81	122.67
59	Y	101	2AE	C5-C6-C1	4.17	122.14	118.10
60	Z	101	8AN	C1'-N9-C4	2.64	131.27	126.64
61	Z	103	FME	C-CA-N	2.15	113.61	109.73

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	Z	103	FME	N-CA-CB-CG
63	a	6209	SPD	C8-C7-N6-C5
63	a	6209	SPD	C7-C8-C9-N10
63	a	6212	SPD	C4-C5-N6-C7
63	a	6212	SPD	N6-C7-C8-C9
63	a	6217	SPD	C2-C3-C4-C5
60	Z	101	8AN	C4'-C5'-O5'-P
63	a	6209	SPD	C3-C4-C5-N6
63	a	6217	SPD	C3-C4-C5-N6
63	a	6208	SPD	N6-C7-C8-C9
63	a	6213	SPD	C2-C3-C4-C5
63	a	6208	SPD	C8-C7-N6-C5
63	a	6209	SPD	N1-C2-C3-C4
63	d	301	SPD	N6-C7-C8-C9
63	a	6211	SPD	C7-C8-C9-N10
63	a	6208	SPD	C3-C4-C5-N6
63	d	301	SPD	C2-C3-C4-C5
63	a	6211	SPD	C2-C3-C4-C5
63	a	6211	SPD	C8-C7-N6-C5

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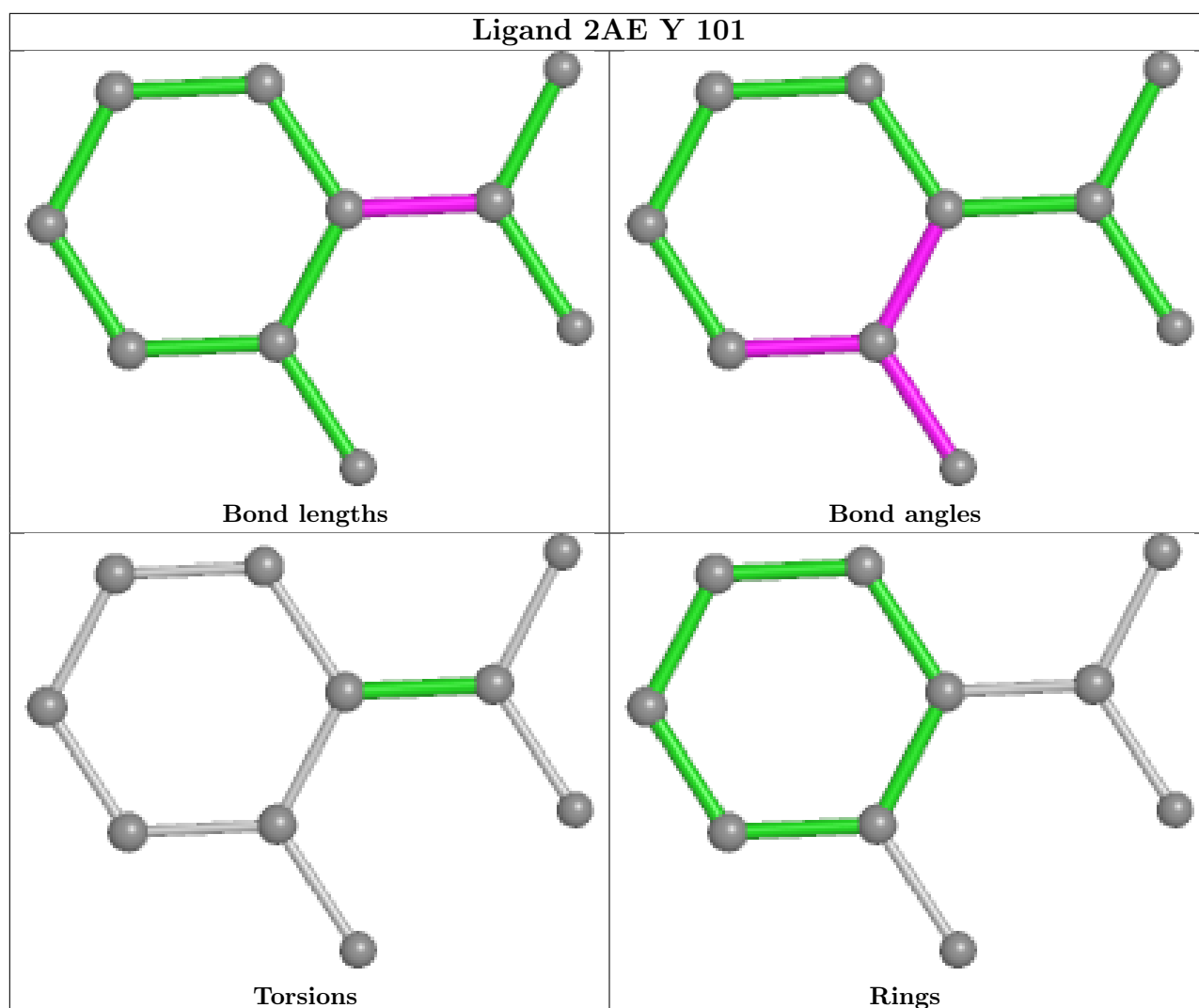
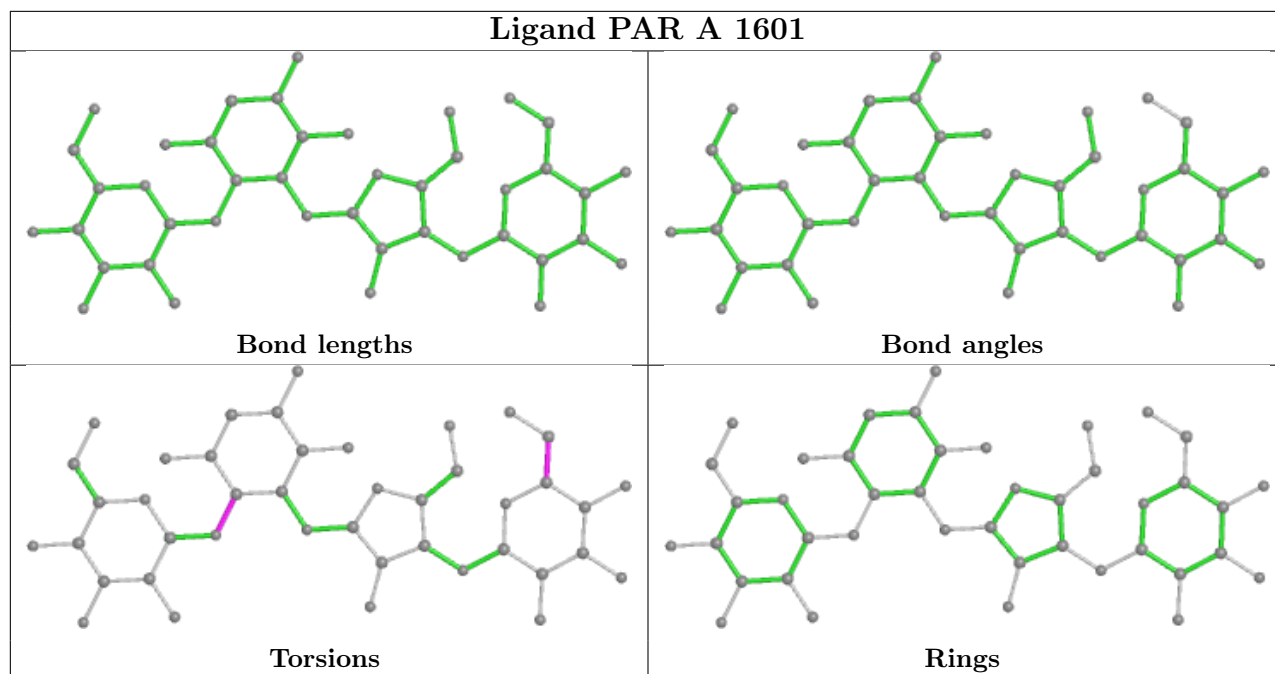
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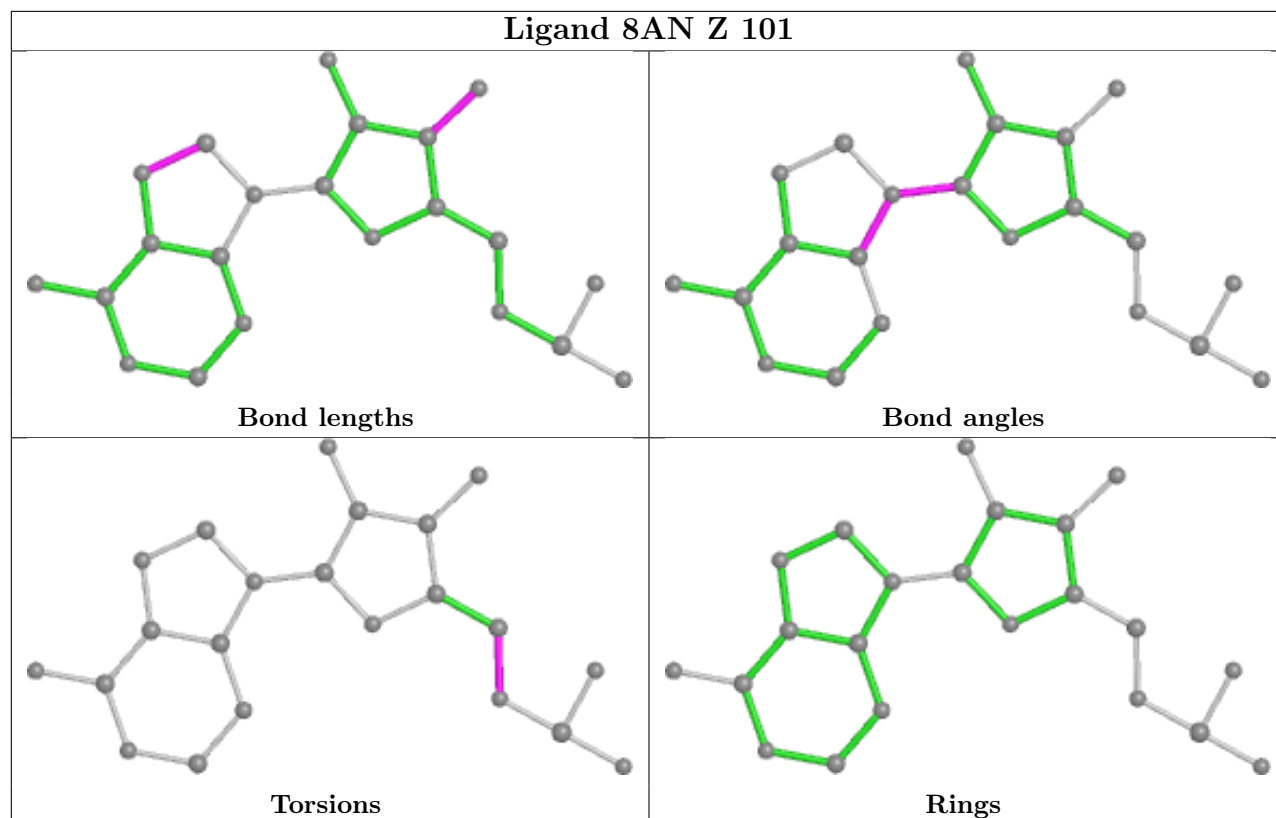
Mol	Chain	Res	Type	Atoms
63	a	6210	SPD	C8-C7-N6-C5
63	a	6211	SPD	C4-C5-N6-C7
63	a	6212	SPD	C2-C3-C4-C5
57	A	1601	PAR	O54-C54-C64-N64
57	A	1601	PAR	C52-C42-O11-C11
63	a	6212	SPD	C7-C8-C9-N10
63	a	6212	SPD	N1-C2-C3-C4
63	a	6217	SPD	C4-C5-N6-C7
61	Z	103	FME	C-CA-CB-CG
63	a	6210	SPD	C4-C5-N6-C7
57	A	1601	PAR	C44-C54-C64-N64
63	a	6208	SPD	N1-C2-C3-C4

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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

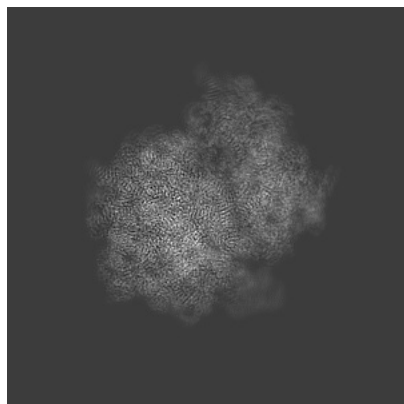
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29786. These allow visual inspection of the internal detail of the map and identification of artifacts.

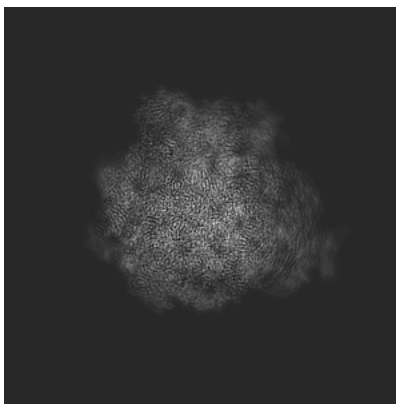
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

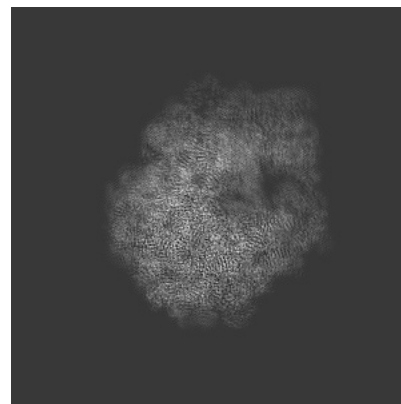
6.1.1 Primary map



X

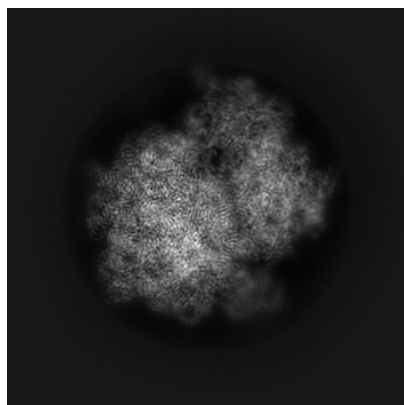


Y

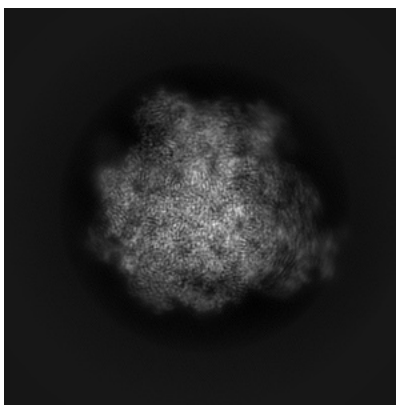


Z

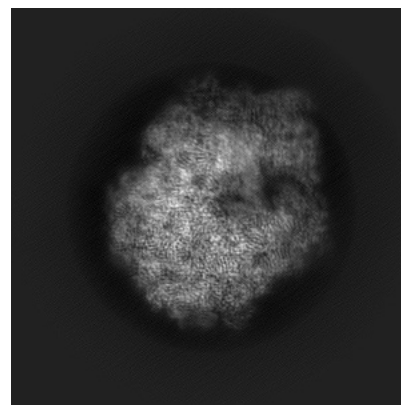
6.1.2 Raw map



X



Y

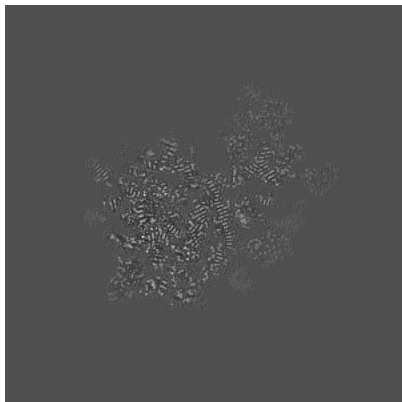


Z

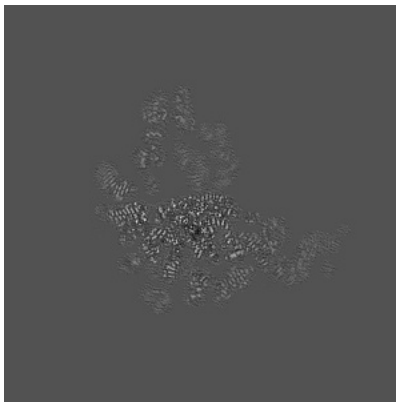
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

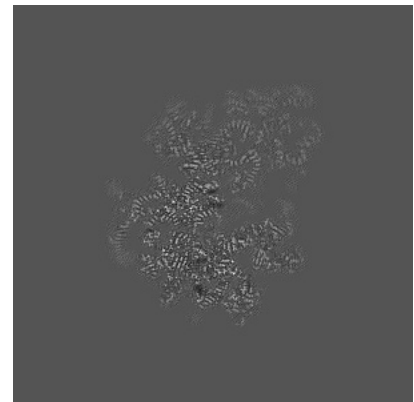
6.2.1 Primary map



X Index: 232

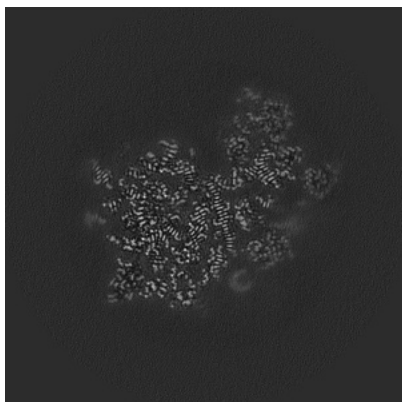


Y Index: 232

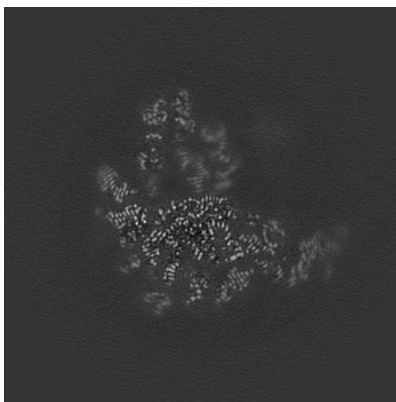


Z Index: 232

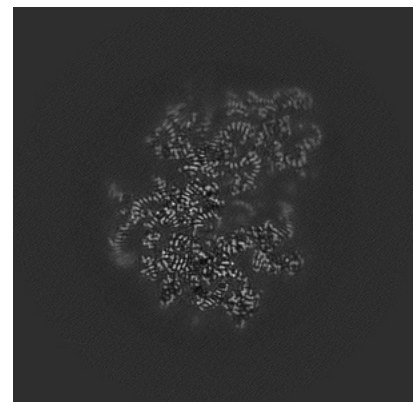
6.2.2 Raw map



X Index: 232



Y Index: 232



Z Index: 232

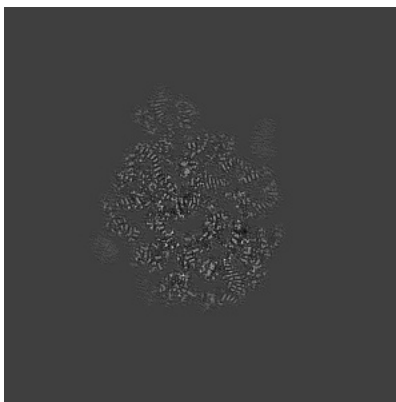
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

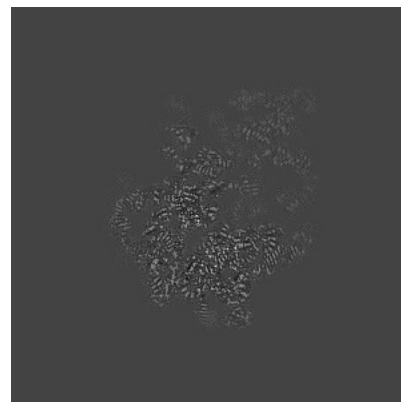
6.3.1 Primary map



X Index: 202

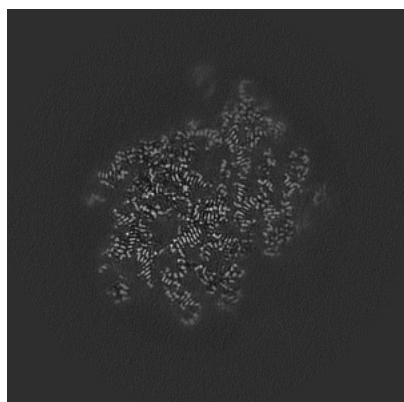


Y Index: 194

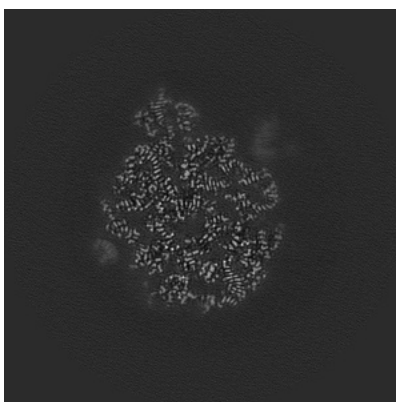


Z Index: 219

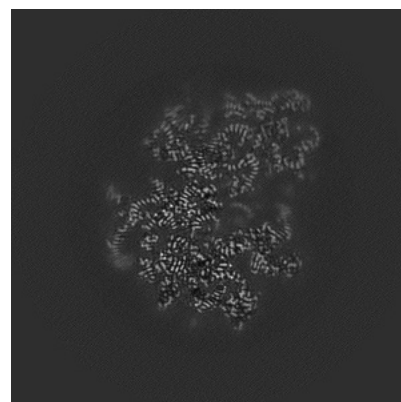
6.3.2 Raw map



X Index: 202



Y Index: 194

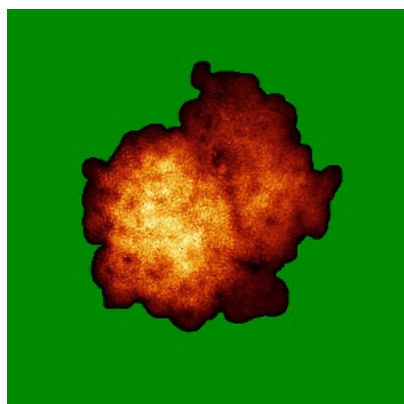


Z Index: 232

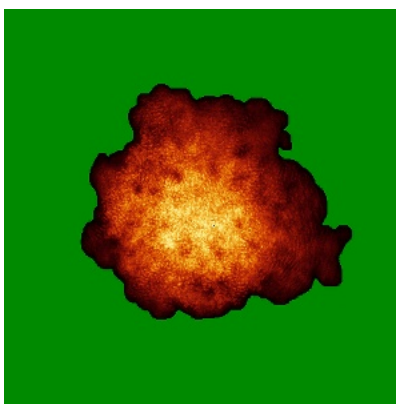
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

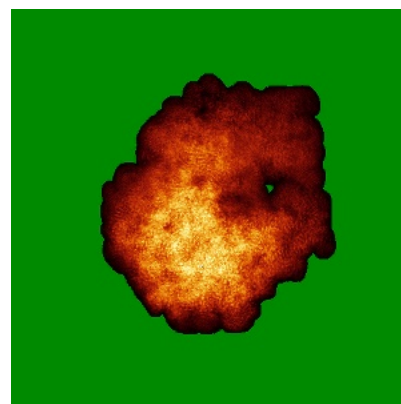
6.4.1 Primary map



X

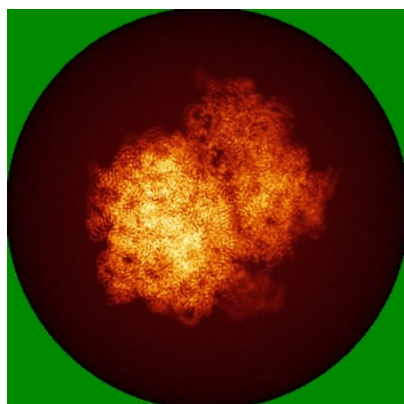


Y

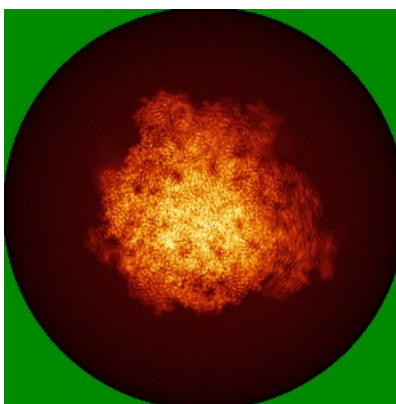


Z

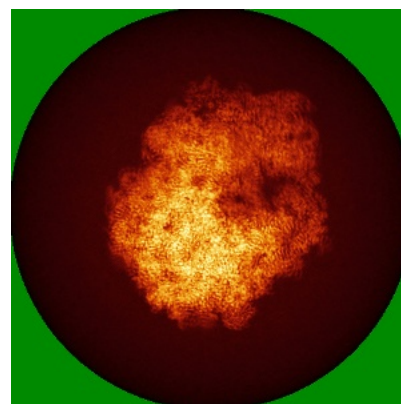
6.4.2 Raw map



X



Y

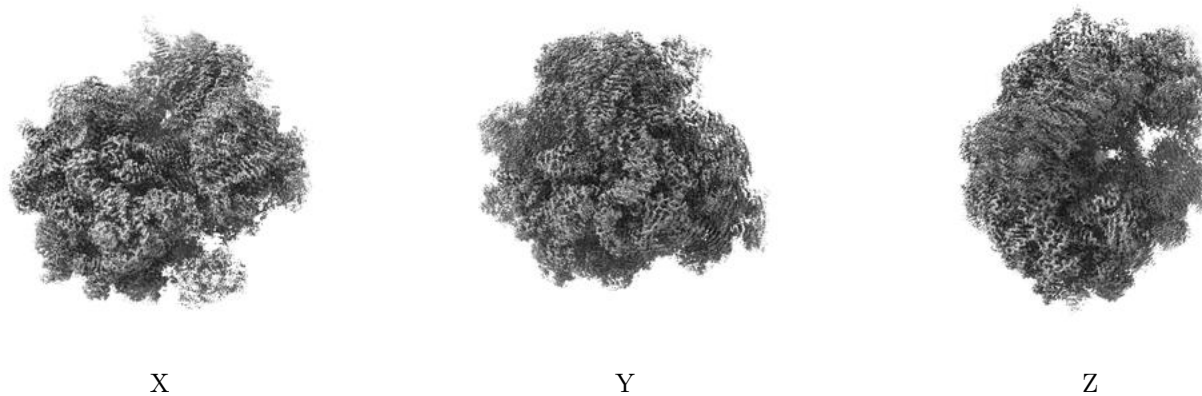


Z

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

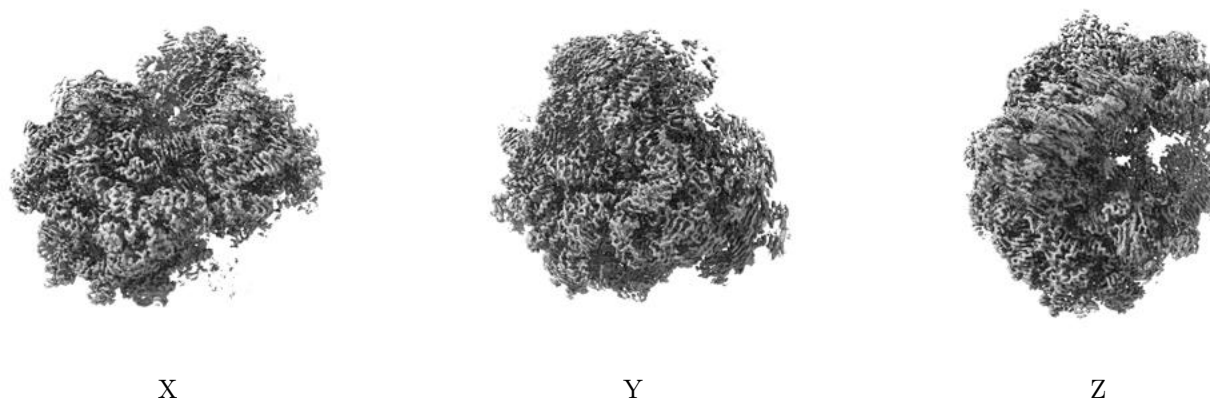
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0169. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

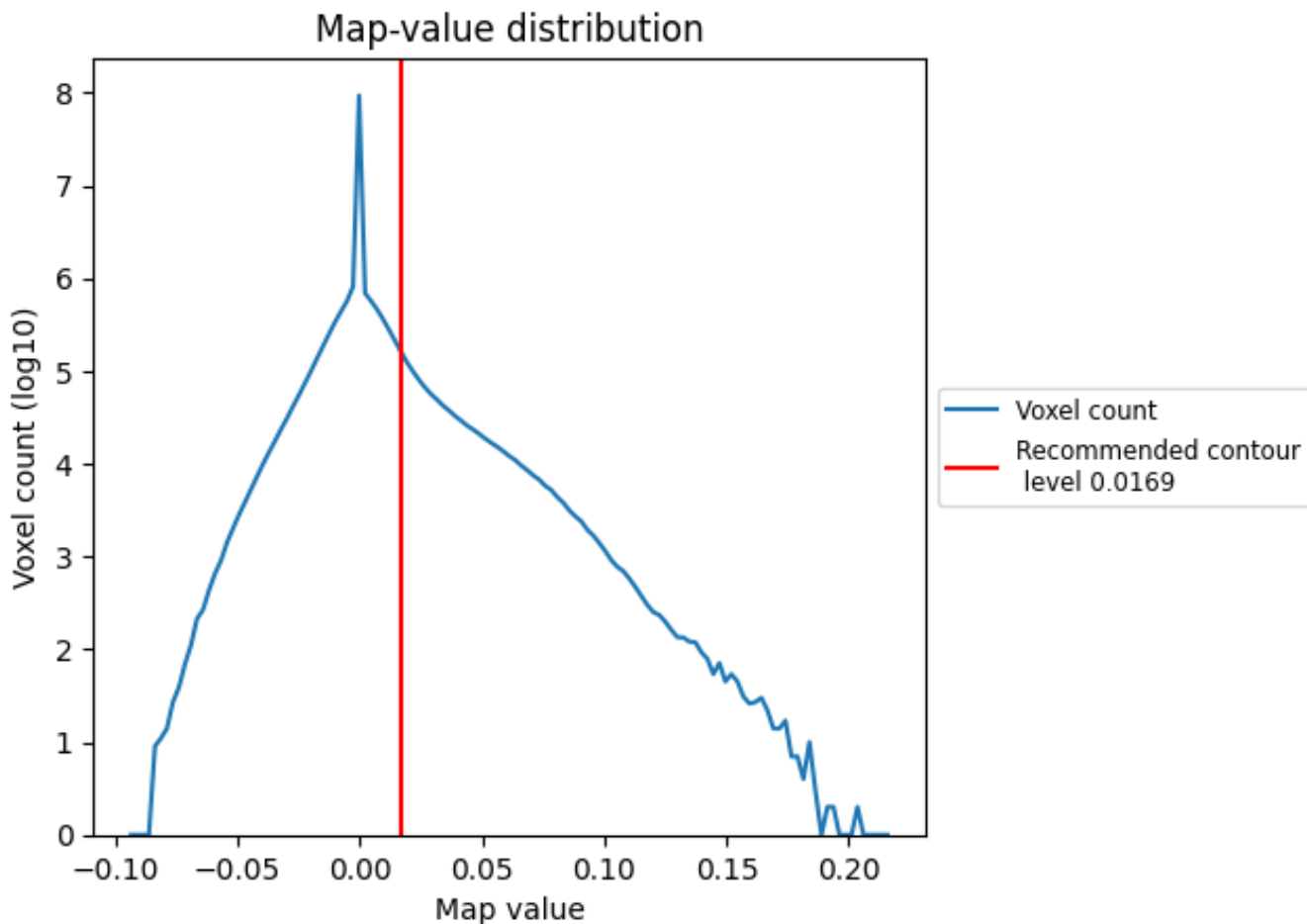
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

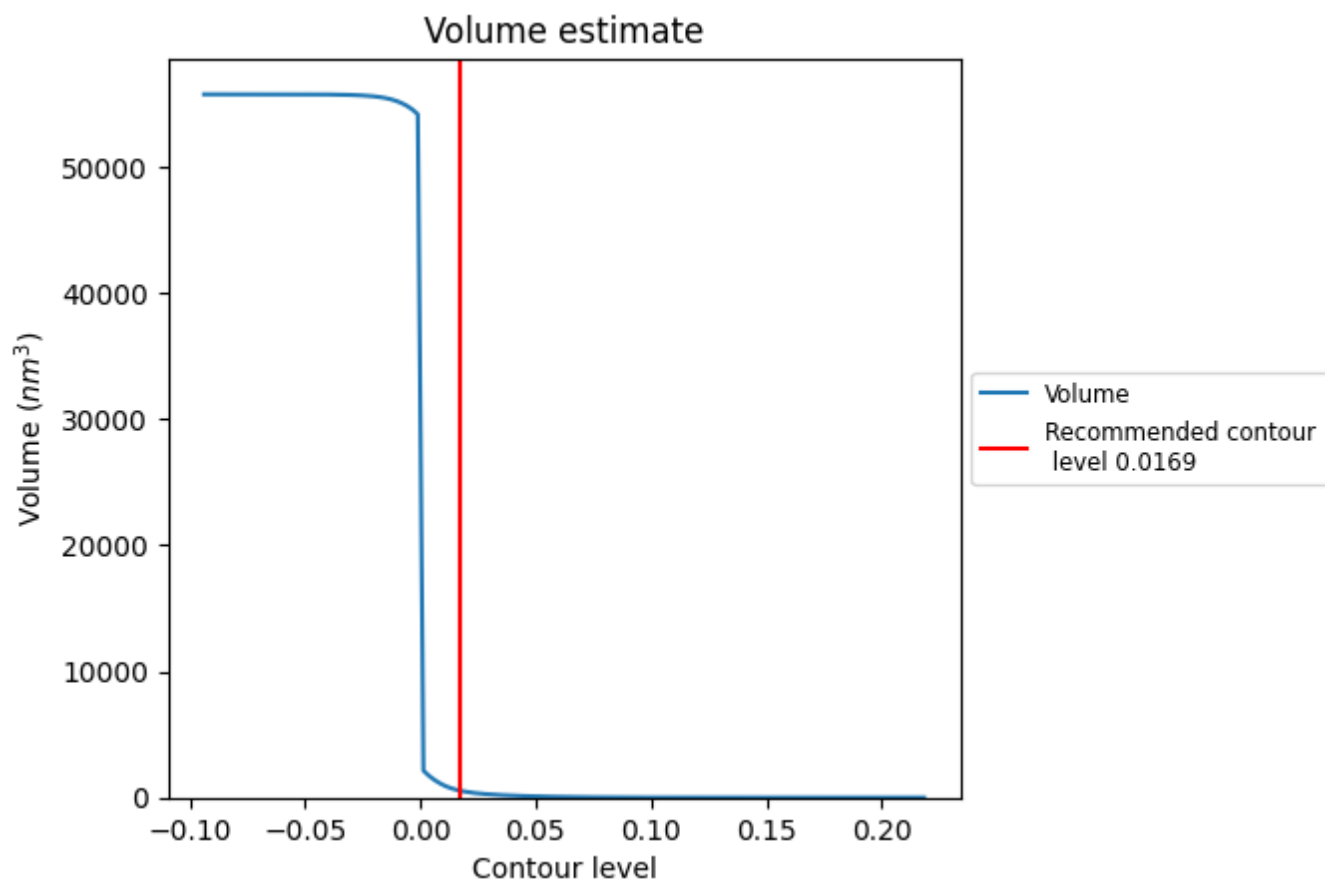
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

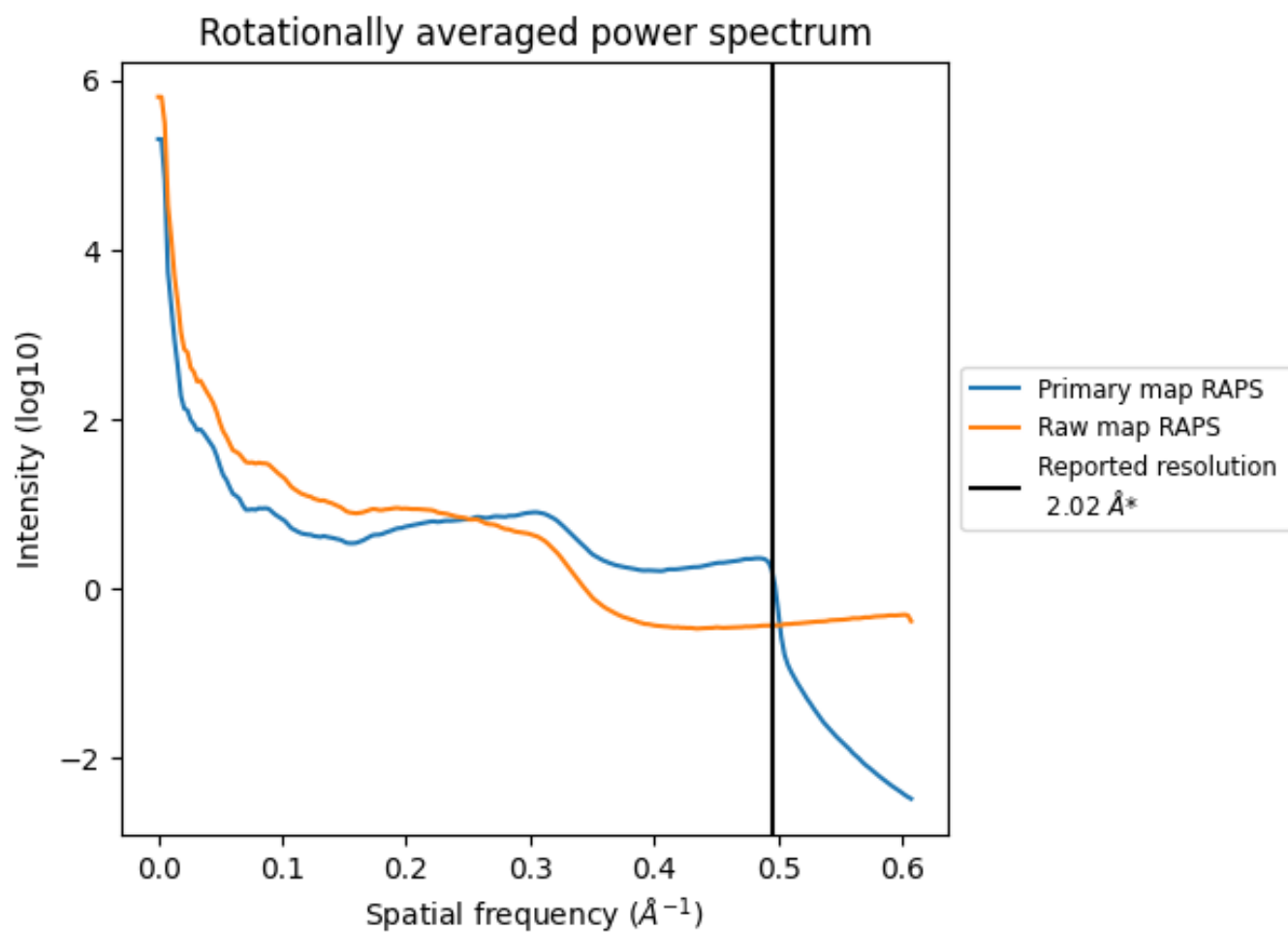
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 561 nm^3 ; this corresponds to an approximate mass of 507 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

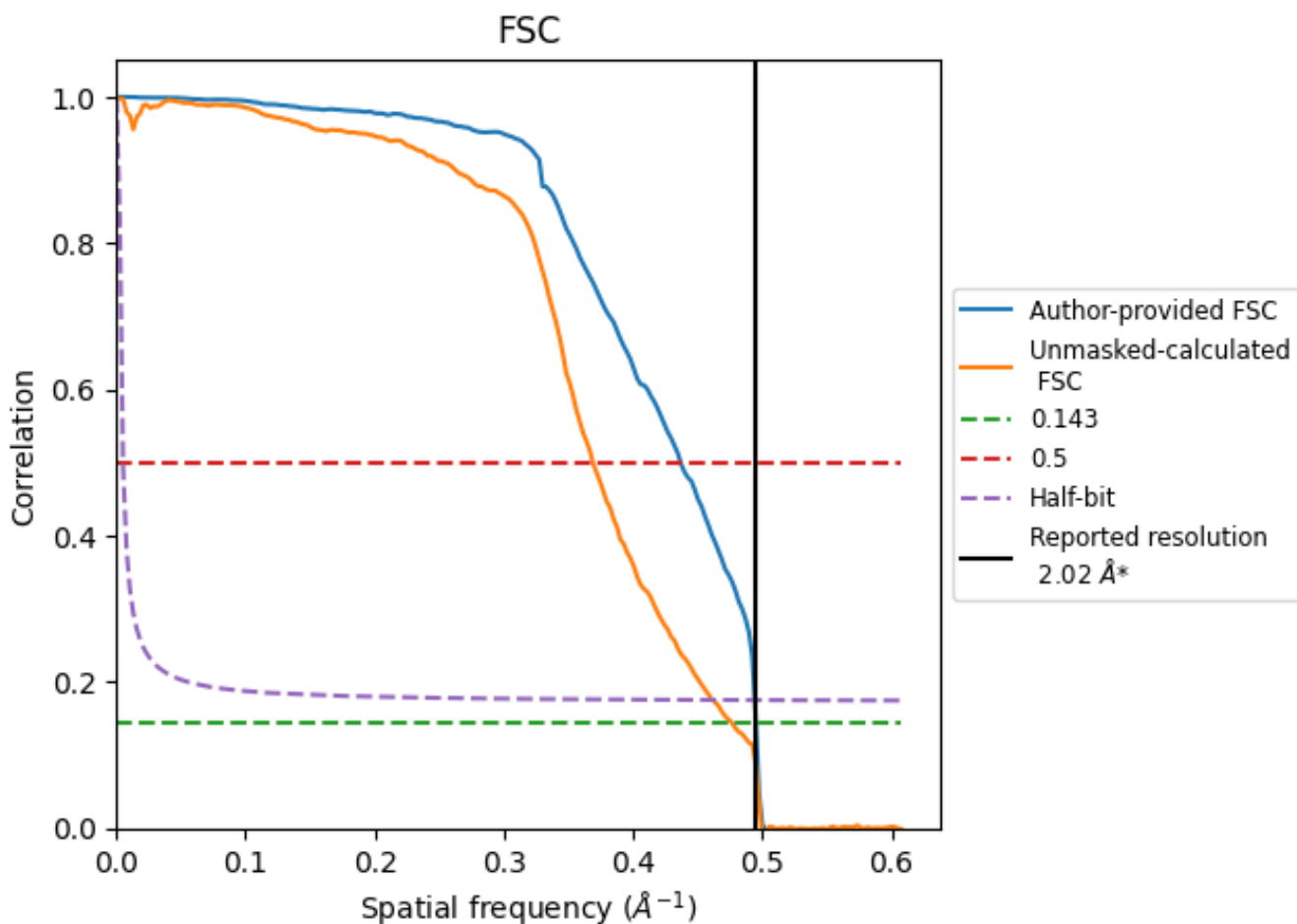


*Reported resolution corresponds to spatial frequency of 0.495 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.495 Å⁻¹

8.2 Resolution estimates [i](#)

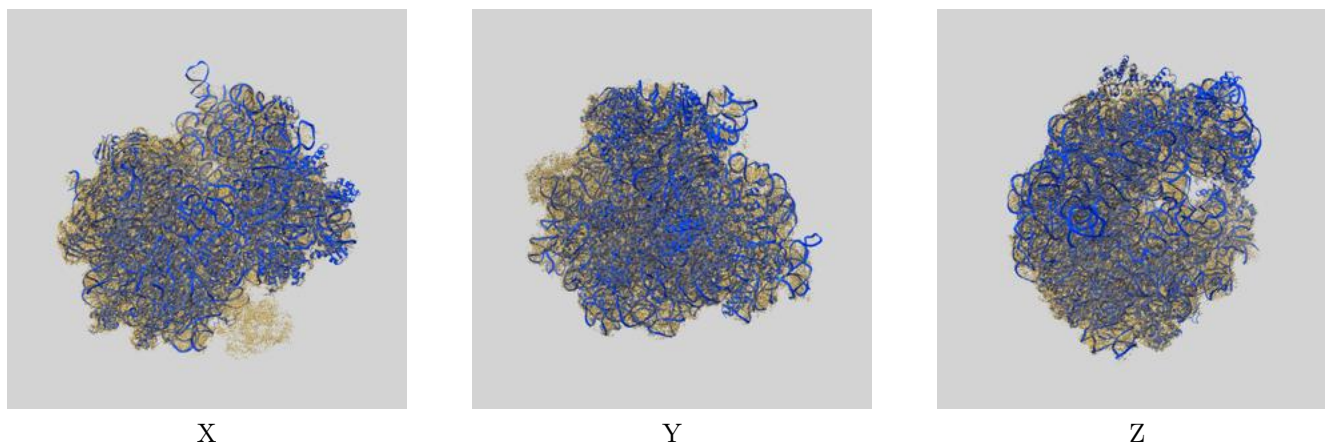
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.02	-	-
Author-provided FSC curve	2.02	2.29	2.02
Unmasked-calculated*	2.10	2.71	2.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

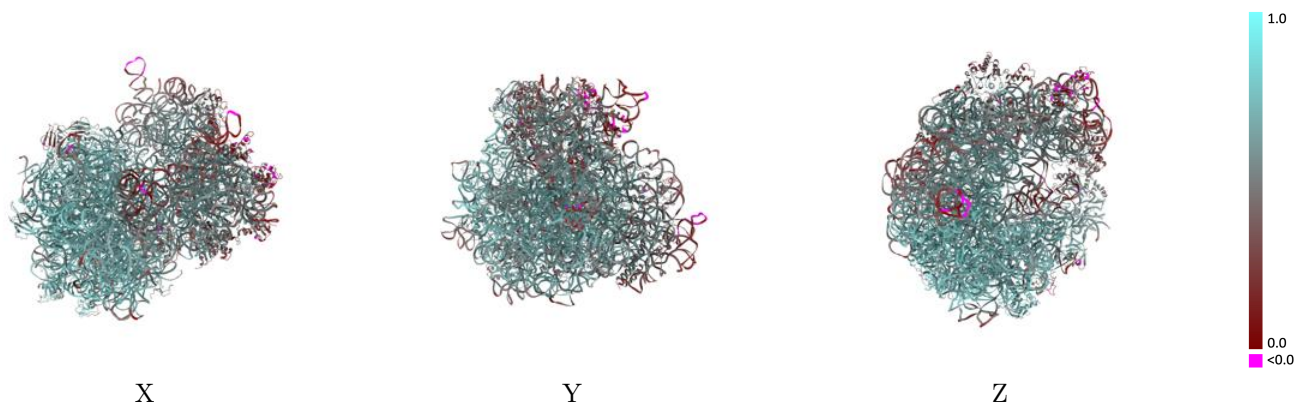
This section contains information regarding the fit between EMDB map EMD-29786 and PDB model 8G6W. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



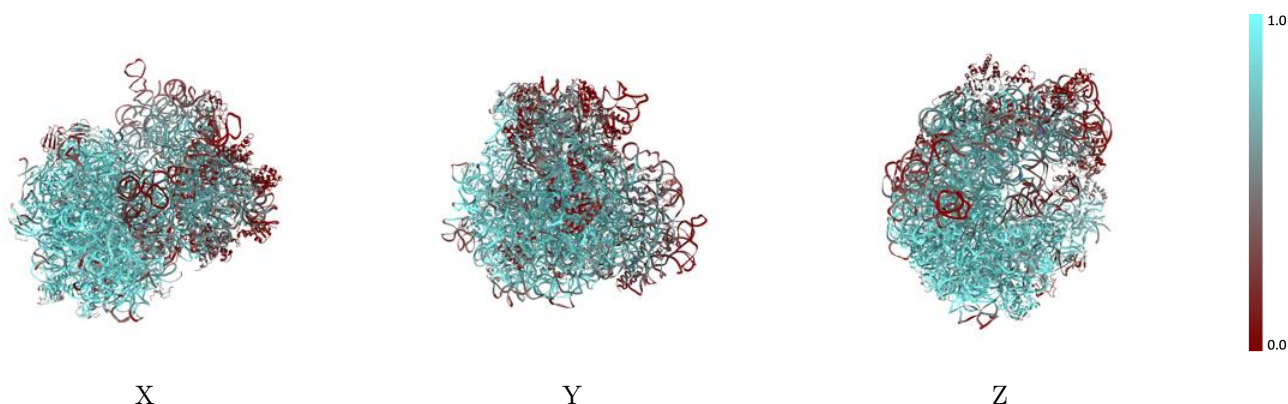
The images above show the 3D surface view of the map at the recommended contour level 0.0169 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



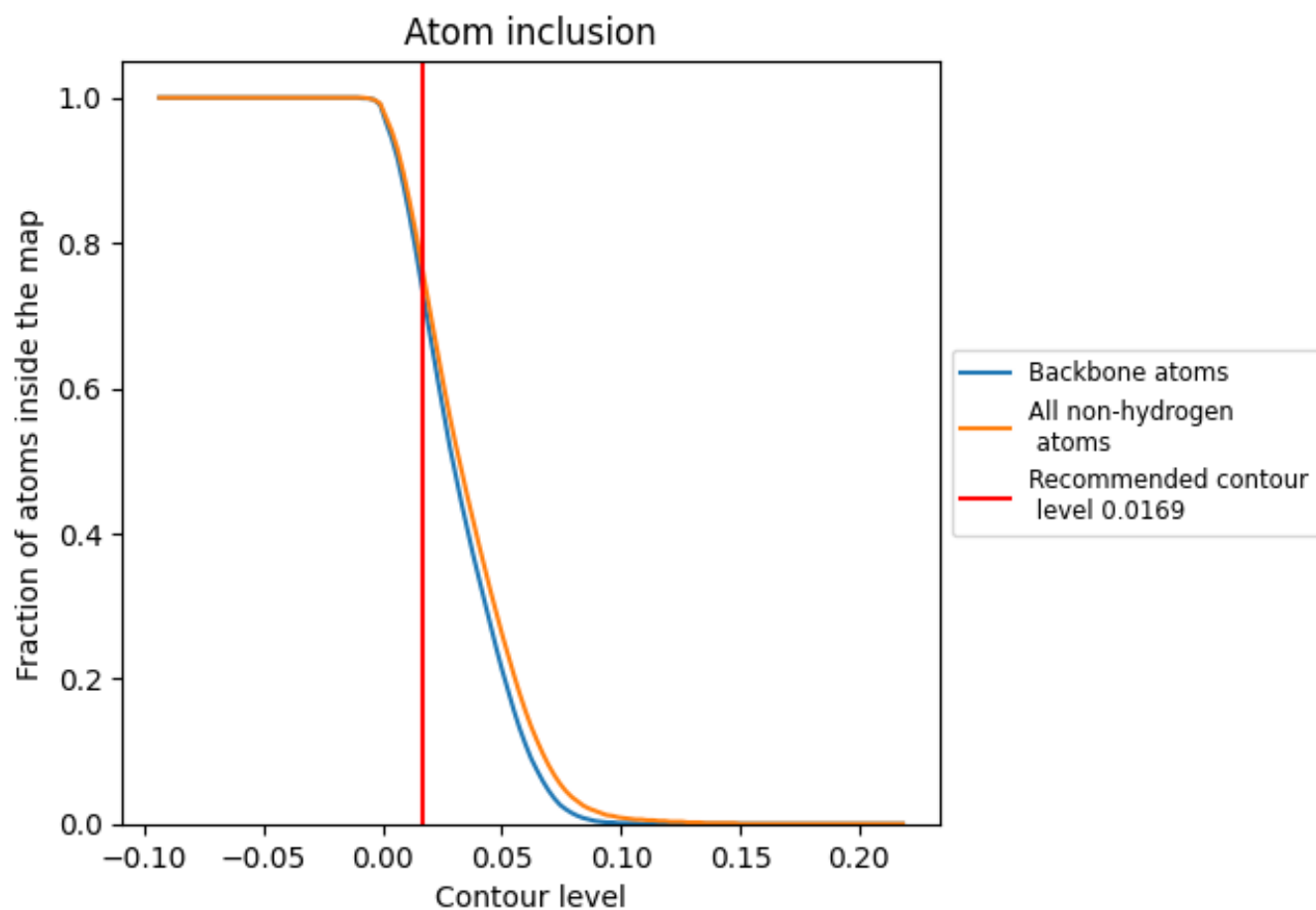
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0169).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary











































The table lists the average atom inclusion at the recommended contour level (0.0169) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.6280
0	 0.7730	 0.6740
1	 0.9410	 0.7730
2	 0.9430	 0.7650
3	 0.8460	 0.6920
4	 0.2010	 0.3590
A	 0.6870	 0.5610
B	 0.2350	 0.3930
C	 0.3070	 0.3850
D	 0.3020	 0.4210
E	 0.6860	 0.6000
F	 0.4510	 0.5200
G	 0.2760	 0.3900
H	 0.6590	 0.5790
I	 0.2750	 0.4120
J	 0.1950	 0.3030
K	 0.6250	 0.5790
L	 0.6370	 0.5920
M	 0.3780	 0.4600
N	 0.3150	 0.4430
O	 0.6220	 0.5710
P	 0.4510	 0.4920
Q	 0.4960	 0.5230
R	 0.5850	 0.5570
S	 0.2840	 0.3970
T	 0.4350	 0.4790
U	 0.3700	 0.4350
X	 0.4780	 0.4820
Y	 0.3430	 0.3620
Z	 0.5300	 0.4660
a	 0.9120	 0.7090
b	 0.8230	 0.6320
c	 0.9280	 0.7450
d	 0.9120	 0.7390
e	 0.8270	 0.7010



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Chain	Atom inclusion	Q-score
f	 0.4180	 0.4790
g	 0.4040	 0.4730
h	 0.4670	 0.5520
i	 0.9080	 0.7420
j	 0.8600	 0.7200
k	 0.8750	 0.7170
l	 0.8770	 0.7160
m	 0.9680	 0.7670
n	 0.7490	 0.6290
o	 0.8220	 0.6980
p	 0.9470	 0.7680
q	 0.8490	 0.7050
r	 0.9020	 0.7370
s	 0.8130	 0.6790
t	 0.7420	 0.6260
u	 0.7030	 0.6220
v	 0.9050	 0.7210
w	 0.8830	 0.7170
x	 0.6810	 0.6020
y	 0.8580	 0.7090
z	 0.8830	 0.7140