



## Full wwPDB EM Validation Report ⓘ

Apr 17, 2024 – 01:30 pm BST

PDB ID : 7PJV  
EMDB ID : EMD-13461  
Title : Structure of the 70S-EF-G-GDP-Pi ribosome complex with tRNAs in hybrid state 1 (H1-EF-G-GDP-Pi)  
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.  
Deposited on : 2021-08-24  
Resolution : 3.10 Å (reported)  
Based on initial models : 4AQY, 5LZD, 6YSS, 5J9Z

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

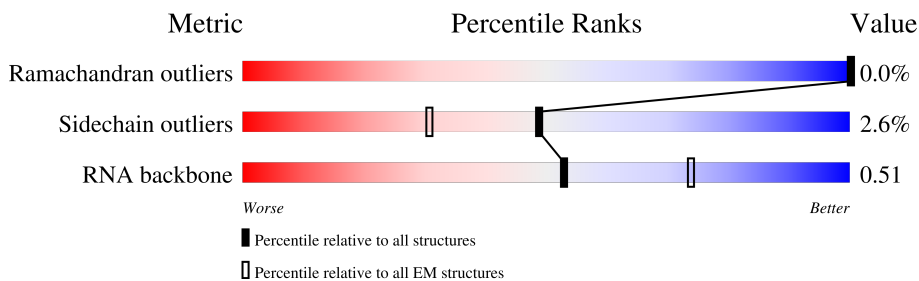
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	57	98%
2	1	55	89% 9%
3	2	46	100%
4	3	65	98%
5	4	38	97%
6	5	165	57% 79% 21%
7	6	70	90% 6%
8	A	2903	76% 23%




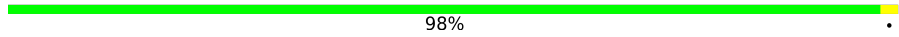
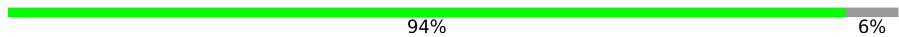


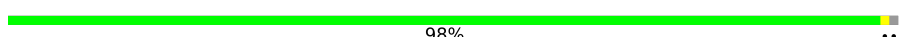
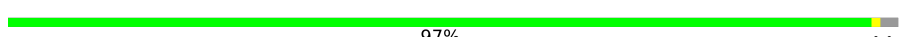




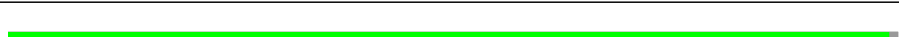


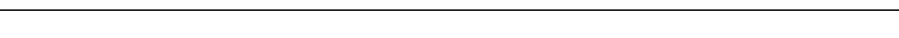
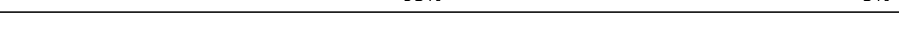


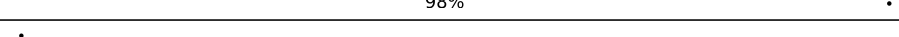
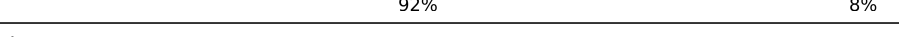



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Mol	Chain	Length	Quality of chain
9	B	120	72% 28%
10	C	273	98% ..
11	D	209	100%
12	E	201	100%
13	F	179	97% ..
14	G	177	99% ..
15	H	149	51% 100%
16	I	142	51% 99%
17	J	142	100%
18	K	123	98% ..
19	L	144	99% ..
20	M	136	99%
21	N	127	94% 6%
22	O	117	97% ..
23	P	115	97% ..
24	Q	118	98% ..
25	R	103	98%
26	S	110	100%
27	T	100	93% 7%
28	U	104	94% ..
29	V	94	100%
30	W	85	88% 12%
31	X	78	97% ..
32	Y	63	98%
33	Z	59	98%


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Mol	Chain	Length	Quality of chain
34	a	1542	 77% 22%
35	b	240	 5% 87% 9%
36	c	233	 88% 12%
37	d	206	 98%
38	e	167	 94% 6%
39	f	135	 74% 26%
40	g	179	 82% 16%
41	h	130	 98%
42	i	130	 97%
43	j	103	 93% 5%
44	k	129	 88% 10%
45	l	124	 98%
46	m	118	 96%
47	n	102	 99%
48	o	89	 99%
49	p	82	 99%
50	q	84	 93% 5%
51	r	75	 85% 13%
52	s	92	 88% 11%
53	t	87	 98%
54	u	71	 92% 8%
55	v	77	 73% 23%
56	w	76	 63% 33%
57	x	704	 6% 87% 13%
58	y	2	 50% 50%

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Mol	Chain	Length	Quality of chain
59	z	33	 21% 12% 67%

## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 153165 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 L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	50	409	263	75	71	0	0

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	5	131	647	385	131	131	0	0

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	66	522	323	99	94	6	0	0

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	A	2903	62338	27816	11471	20148	2903	0	0

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

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

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

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

- Molecule 15 is a protein called 50S ribosomal protein L9.

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

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	I	141	693	411	141	141	0	0

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

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

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	L	143	1045	649	206	189	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.



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

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

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

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 33 is a protein called 50S ribosomal protein L30.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 39 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	l	123	955	590	196	165	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	m	114	883	546	178	156	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	n	101	799	498	165	133	3	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
55	v	77	1642	733	297	534	77	1	0	0

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
56	w	76	1631	731	291	531	76	2	0	0

- Molecule 57 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	x	703	5444	3429	942	1048	25	0	0

- Molecule 58 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	y	2	21	15	2	3	1	0	0

- Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
59	z	11	230	103	35	81	11	0	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total	Mg	0
			1	1	
60	A	262	Total	Mg	0
			262	262	
60	B	7	Total	Mg	0
			7	7	
60	C	3	Total	Mg	0
			3	3	
60	D	1	Total	Mg	0
			1	1	
60	O	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
60	P	1	Total 1	Mg 1	0
60	Q	1	Total 1	Mg 1	0
60	Z	1	Total 1	Mg 1	0
60	a	85	Total 85	Mg 85	0
60	m	1	Total 1	Mg 1	0
60	n	1	Total 1	Mg 1	0
60	v	1	Total 1	Mg 1	0
60	w	1	Total 1	Mg 1	0
60	x	1	Total 1	Mg 1	0
60	z	1	Total 1	Mg 1	0

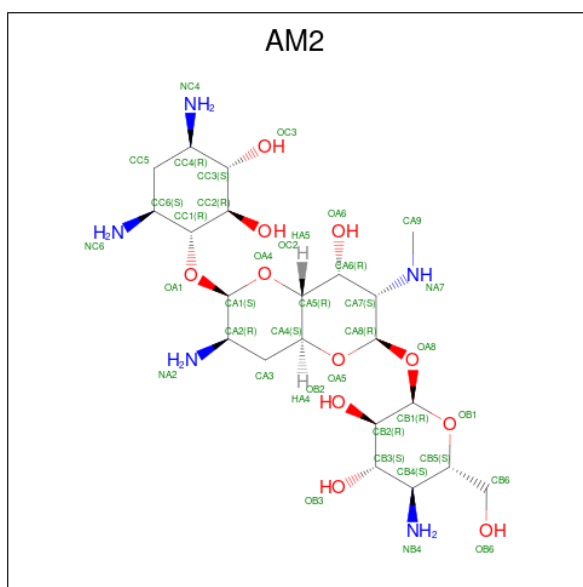
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	4	1	Total 1	Zn 1	0
61	6	1	Total 1	Zn 1	0

- Molecule 62 is SODIUM ION (three-letter code: NA) (formula: Na).

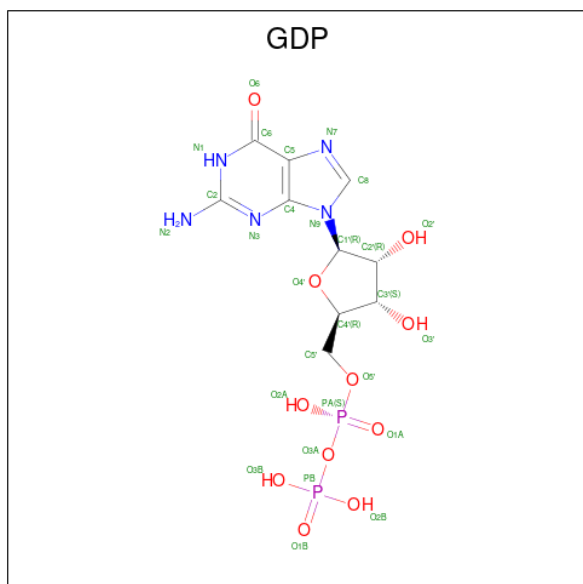
Mol	Chain	Residues	Atoms		AltConf
62	A	1	Total 1	Na 1	0
62	B	1	Total 1	Na 1	0

- Molecule 63 is APRAMYCIN (three-letter code: AM2) (formula: C<sub>21</sub>H<sub>41</sub>N<sub>5</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms				AltConf
63	a	1	Total	C	N	O	0
			37	21	5	11	
63	a	1	Total	C	N	O	0
			37	21	5	11	
63	a	1	Total	C	N	O	0
			37	21	5	11	

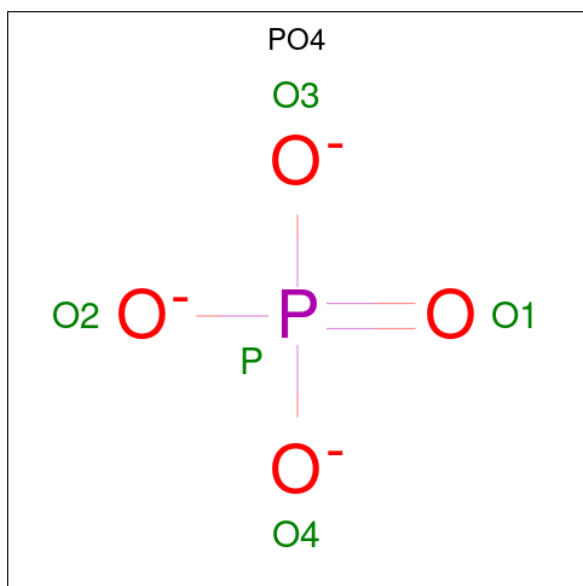
- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).





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

- Molecule 65 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
65	x	1	5	4	1	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 L32

Chain 0:  98%



- Molecule 2: 50S ribosomal protein L33

Chain 1:  89% 9%



- Molecule 3: 50S ribosomal protein L34

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: 50S ribosomal protein L35

Chain 3:  98%




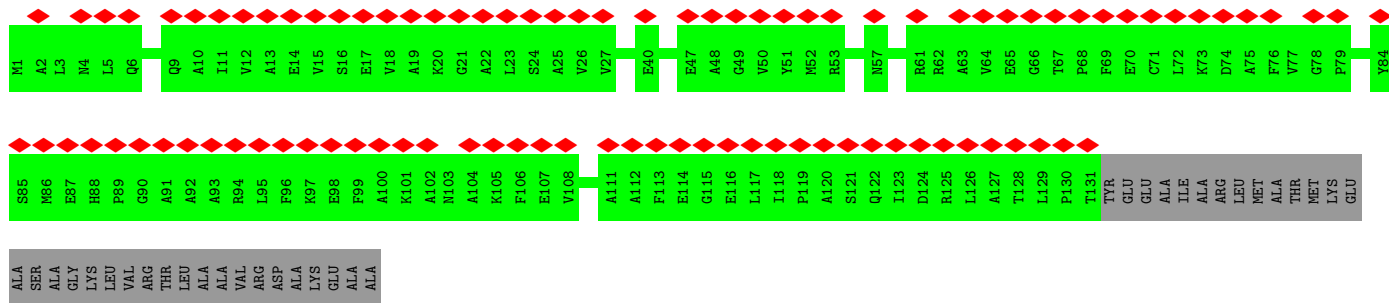
- Molecule 5: 50S ribosomal protein L36

Chain 4:  97%

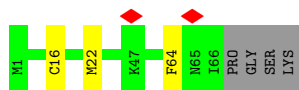
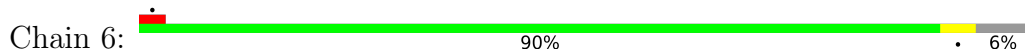


- Molecule 6: 50S ribosomal protein L10

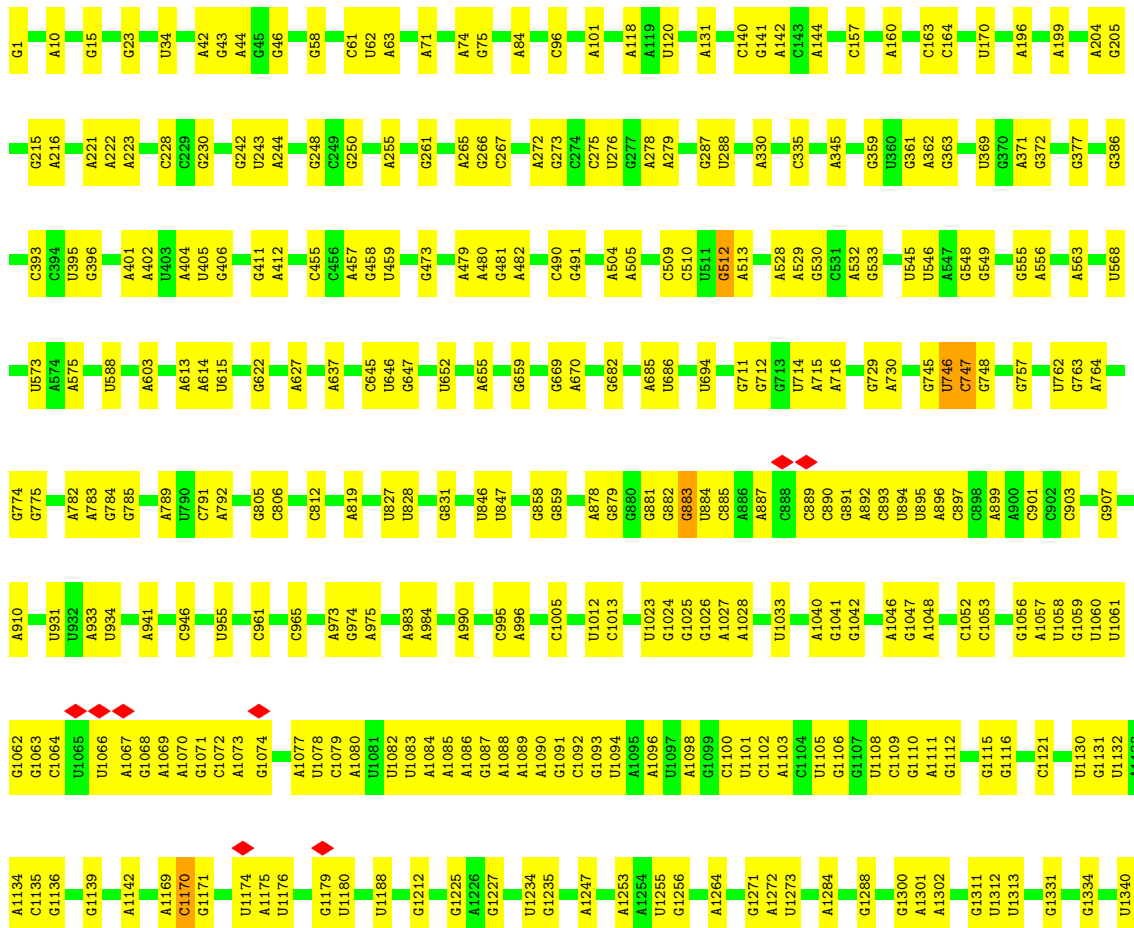
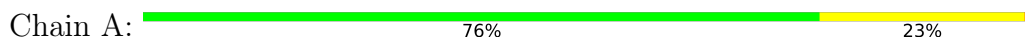
Chain 5:  57% 79% 21%

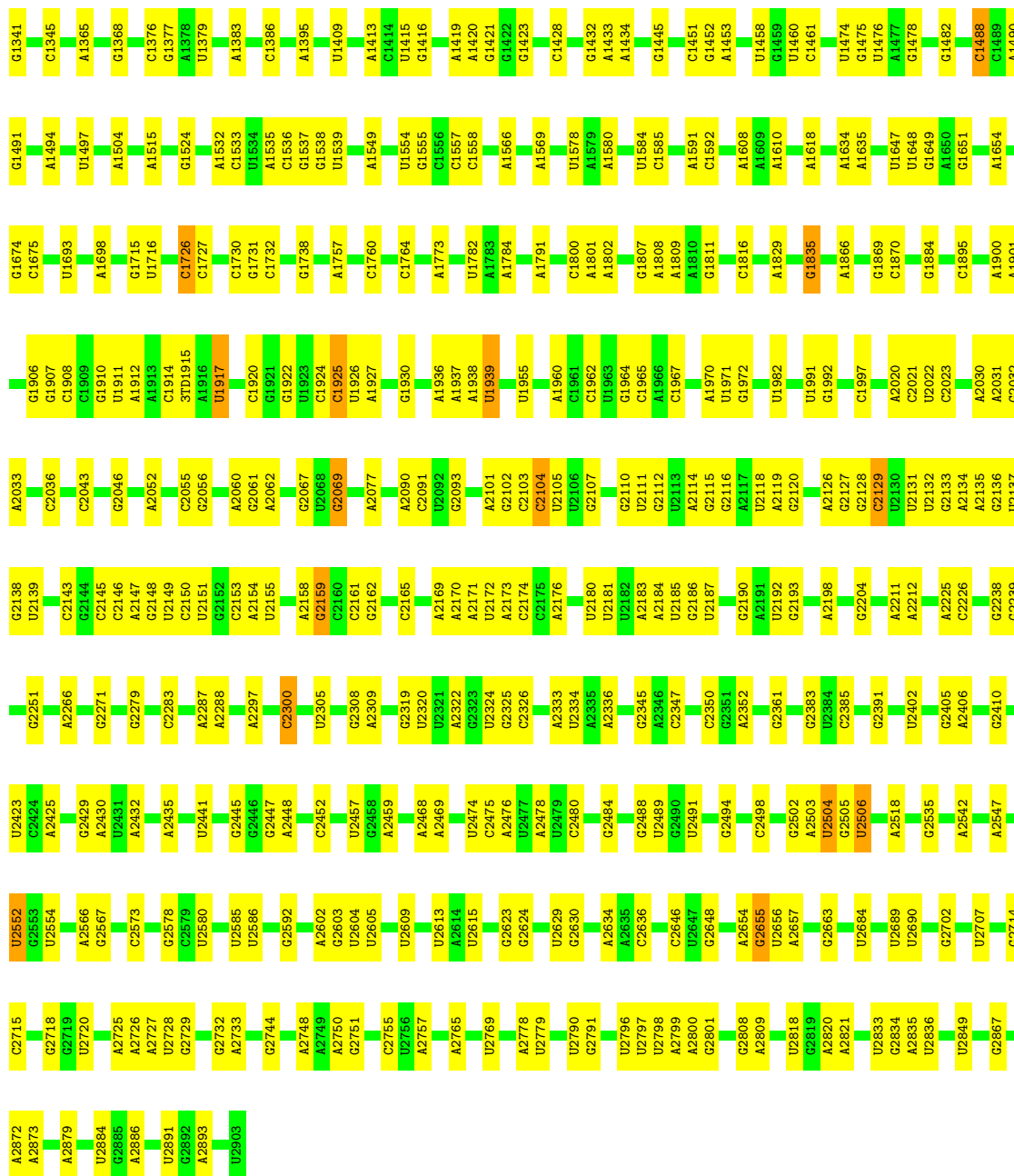


● Molecule 7: 50S ribosomal protein L31



● Molecule 8: 23S ribosomal RNA





- Molecule 9: 5S ribosomal RNA

Chain B: 72% 28%

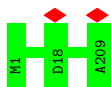


- Molecule 10: 50S ribosomal protein L2

Chain C: 98%



- Molecule 11: 50S ribosomal protein L3

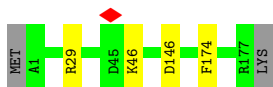


- Molecule 12: 50S ribosomal protein L4

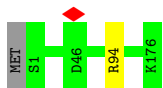


There are no outlier residues recorded for this chain.

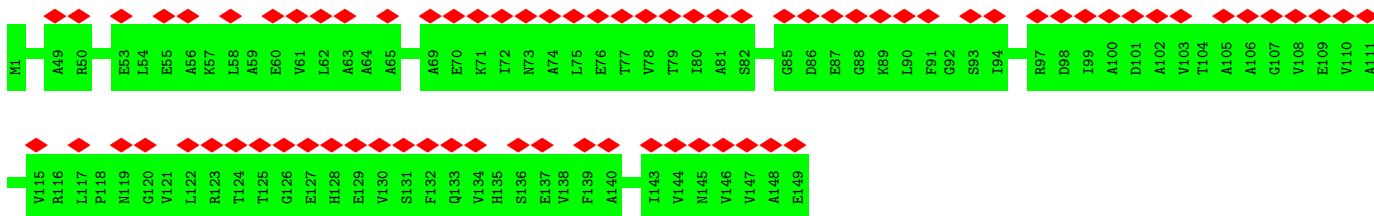
- Molecule 13: 50S ribosomal protein L5



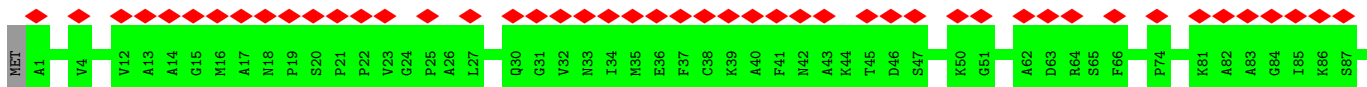
- Molecule 14: 50S ribosomal protein L6

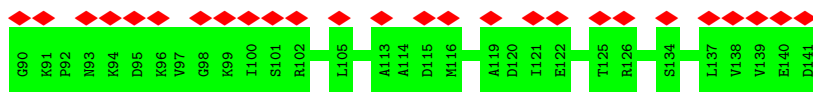


- Molecule 15: 50S ribosomal protein L9



- Molecule 16: 50S ribosomal protein L11





- Molecule 17: 50S ribosomal protein L13

Chain J: 100%

There are no outlier residues recorded for this chain.

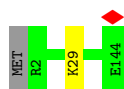
- Molecule 18: 50S ribosomal protein L14

Chain K: 98%



- Molecule 19: 50S ribosomal protein L15

Chain L: 99%



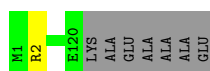
- Molecule 20: 50S ribosomal protein L16

Chain M: 99%



- Molecule 21: 50S ribosomal protein L17

Chain N: 94%



- Molecule 22: 50S ribosomal protein L18

Chain O: 97%



- Molecule 23: 50S ribosomal protein L19

Chain P: 97%



- Molecule 24: 50S ribosomal protein L20

Chain Q: 98%



- Molecule 25: 50S ribosomal protein L21

Chain R: 98%



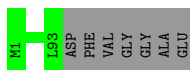
- Molecule 26: 50S ribosomal protein L22

Chain S: 100%

There are no outlier residues recorded for this chain.

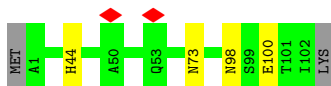
- Molecule 27: 50S ribosomal protein L23

Chain T: 93% 7%



- Molecule 28: 50S ribosomal protein L24

Chain U: 94%



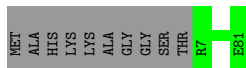
- Molecule 29: 50S ribosomal protein L25

Chain V: 100%

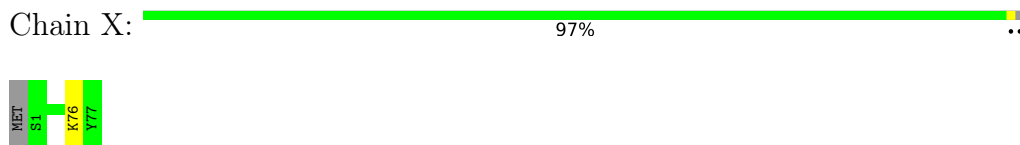
There are no outlier residues recorded for this chain.

- Molecule 30: 50S ribosomal protein L27

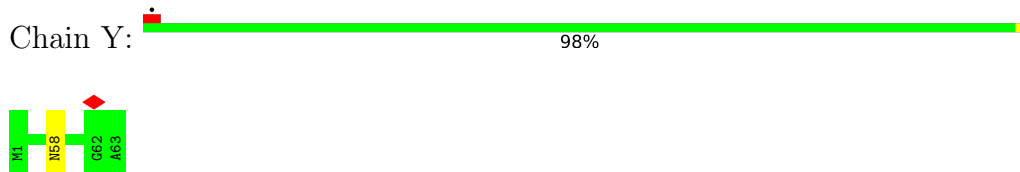
Chain W: 88% 12%



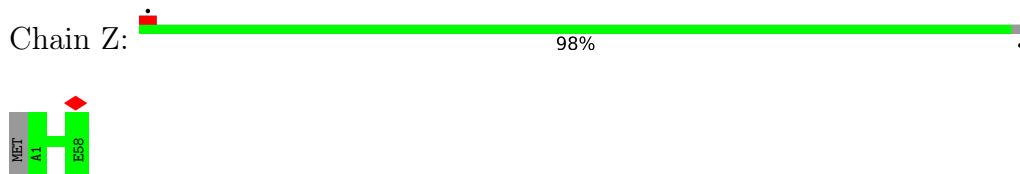
- Molecule 31: 50S ribosomal protein L28



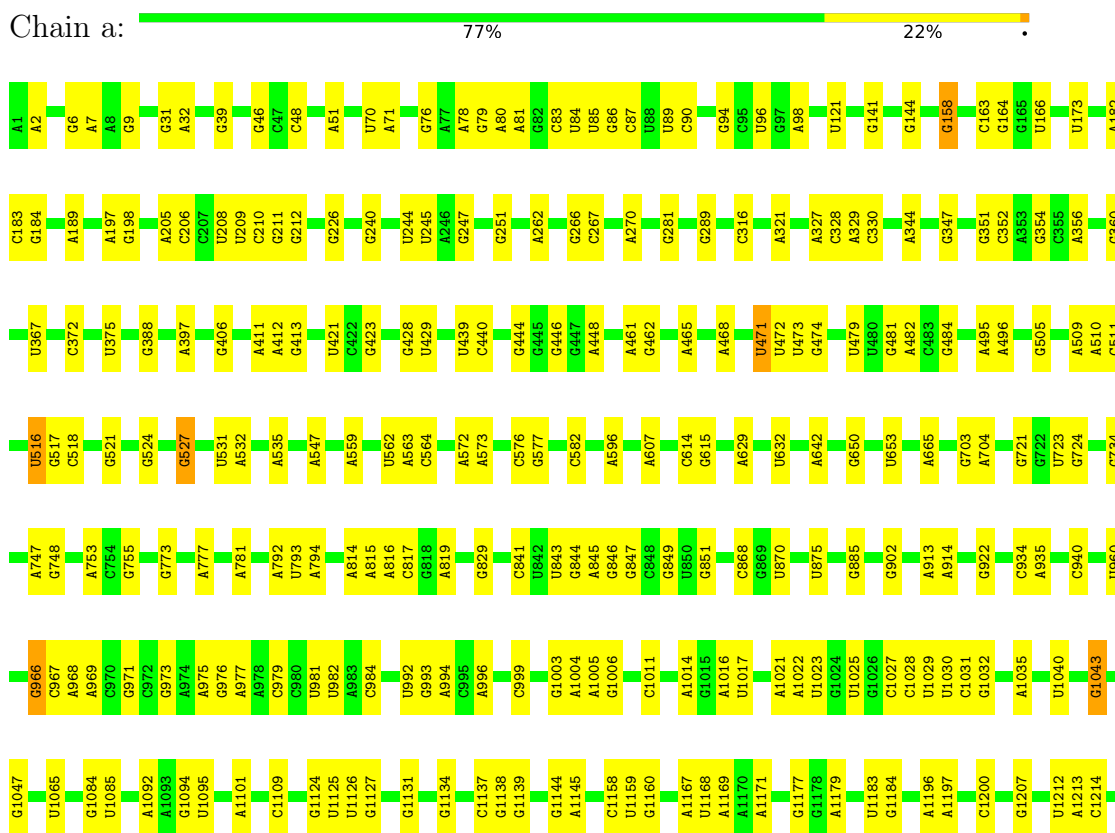
- Molecule 32: 50S ribosomal protein L29



- Molecule 33: 50S ribosomal protein L30



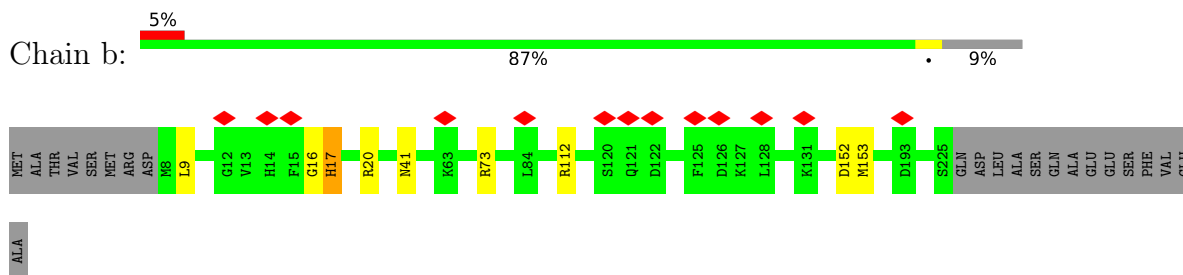
- Molecule 34: 16S ribosomal RNA



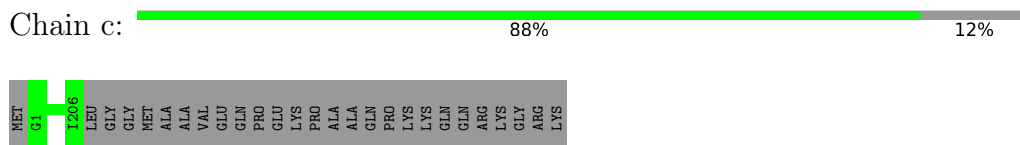




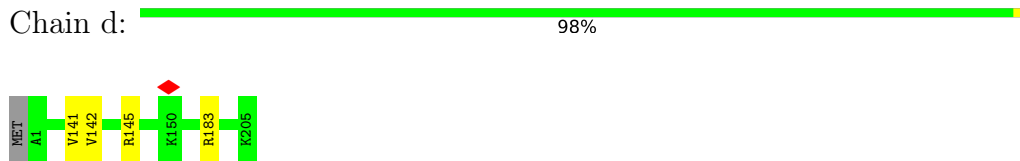
• Molecule 35: 30S ribosomal protein S2



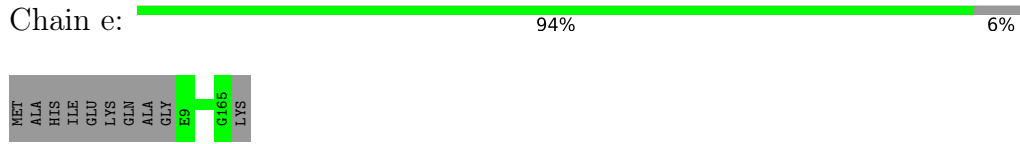
• Molecule 36: 30S ribosomal protein S3



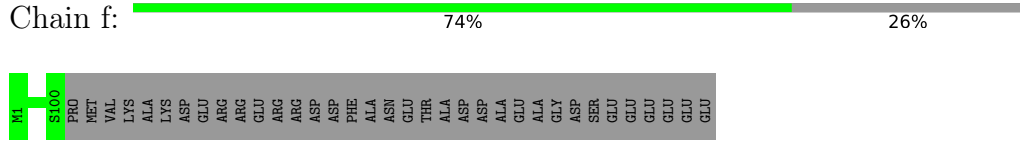
• Molecule 37: 30S ribosomal protein S4




• Molecule 38: 30S ribosomal protein S5

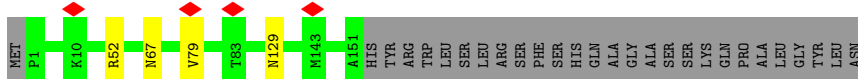


• Molecule 39: 30S ribosomal protein S6, fully modified isoform



• Molecule 40: 30S ribosomal protein S7

Chain g:  82% 16%



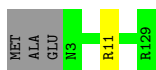
- Molecule 41: 30S ribosomal protein S8

Chain h:  98%

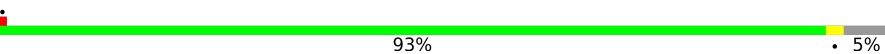


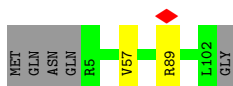
- Molecule 42: 30S ribosomal protein S9

Chain i:  97%




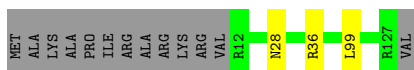
- Molecule 43: 30S ribosomal protein S10

Chain j:  93% 5%



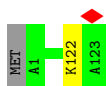
- Molecule 44: 30S ribosomal protein S11

Chain k:  88% 10%



- Molecule 45: 30S ribosomal protein S12

Chain l:  98%



- Molecule 46: 30S ribosomal protein S13

Chain m:  96%



- Molecule 47: 30S ribosomal protein S14

Chain n:  99%



- Molecule 48: 30S ribosomal protein S15

Chain o:  99%



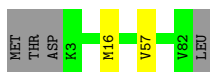
- Molecule 49: 30S ribosomal protein S16

Chain p:  99%




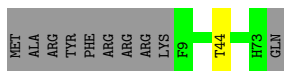
- Molecule 50: 30S ribosomal protein S17

Chain q:  93% 5%




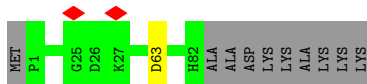
- Molecule 51: 30S ribosomal protein S18

Chain r:  85% 13%



- Molecule 52: 30S ribosomal protein S19

Chain s:  88% 11%

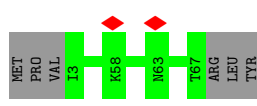
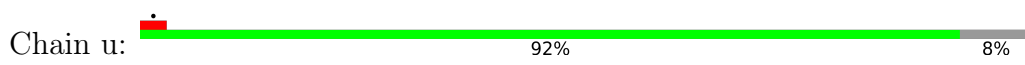


- Molecule 53: 30S ribosomal protein S20

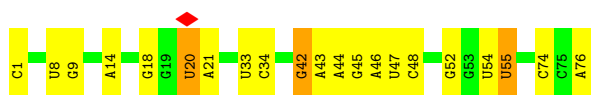
Chain t:  98%



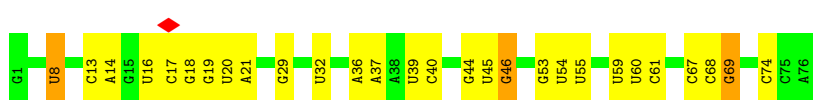
- Molecule 54: 30S ribosomal protein S21



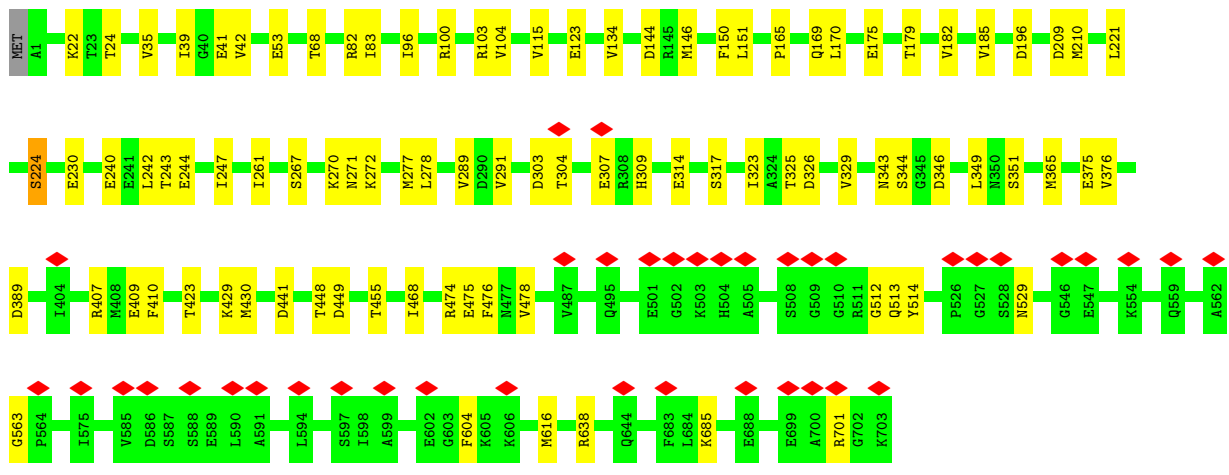
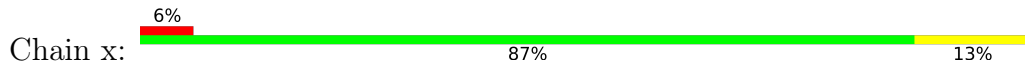
• Molecule 55: P-site tRNA(fMet)



• Molecule 56: P-site fMet-Phe-tRNA(Phe)



• Molecule 57: Elongation factor G

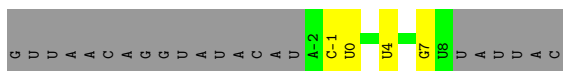


• Molecule 58: Dipeptide (FME-PHE)



• Molecule 59: mRNA





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24313	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	16.323	Depositor
Minimum map value	-7.685	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size ( $\text{\AA}$ )	334.08, 334.08, 334.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.6525, 0.6525, 0.6525	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: AM2, 2MG, G7M, 3TD, OMC, MG, 4SU, H2U, NA, FME, OMU, OMG, GDP, 6MZ, MA6, PSU, 2MA, PO4, 1MG, ZN, UR3, 5MU, 4OC, 5MC, MIA

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	0.43	0/450	0.48	0/599
2	1	0.38	0/416	0.48	0/554
3	2	0.42	0/380	0.50	0/498
4	3	0.40	0/513	0.62	0/676
5	4	0.40	0/303	0.49	0/397
6	5	0.27	0/646	0.56	0/898
7	6	0.33	0/531	0.54	0/709
8	A	0.82	2/69266 (0.0%)	0.87	46/108055 (0.0%)
9	B	0.70	1/2873 (0.0%)	0.86	0/4478
10	C	0.44	0/2121	0.55	1/2852 (0.0%)
11	D	0.43	0/1586	0.51	0/2134
12	E	0.42	0/1571	0.50	0/2113
13	F	0.34	0/1434	0.51	0/1926
14	G	0.34	0/1343	0.49	0/1816
15	H	0.30	0/1122	0.54	0/1515
16	I	0.29	0/692	0.57	0/960
17	J	0.42	0/1152	0.48	0/1551
18	K	0.40	0/947	0.58	0/1268
19	L	0.40	0/1054	0.56	0/1403
20	M	0.40	0/1093	0.51	0/1460
21	N	0.39	0/973	0.52	0/1301
22	O	0.35	0/902	0.49	0/1209
23	P	0.41	0/929	0.49	0/1242
24	Q	0.48	0/960	0.45	0/1278
25	R	0.41	0/829	0.57	0/1107
26	S	0.37	0/864	0.51	0/1156
27	T	0.36	0/744	0.52	0/994
28	U	0.39	0/787	0.57	1/1051 (0.1%)
29	V	0.38	0/766	0.45	0/1025
30	W	0.42	0/582	0.46	0/769
31	X	0.40	0/635	0.52	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Y	0.32	0/510	0.45	0/677
33	Z	0.35	0/453	0.49	0/605
34	a	0.68	0/36725	0.86	17/57285 (0.0%)
35	b	0.30	0/1735	0.56	3/2338 (0.1%)
36	c	0.35	0/1651	0.48	0/2225
37	d	0.36	0/1665	0.54	0/2227
38	e	0.37	0/1154	0.53	0/1554
39	f	0.34	0/835	0.49	0/1128
40	g	0.31	0/1195	0.49	0/1602
41	h	0.37	0/989	0.51	0/1326
42	i	0.33	0/1034	0.53	0/1375
43	j	0.34	0/796	0.60	1/1077 (0.1%)
44	k	0.36	0/885	0.51	0/1195
45	l	0.42	0/969	0.55	0/1300
46	m	0.31	0/892	0.53	0/1193
47	n	0.31	0/811	0.49	0/1081
48	o	0.34	0/722	0.46	0/964
49	p	0.37	0/659	0.52	0/884
50	q	0.40	0/657	0.56	1/881 (0.1%)
51	r	0.35	0/544	0.49	0/731
52	s	0.33	0/675	0.49	0/908
53	t	0.31	0/671	0.43	0/888
54	u	0.32	0/512	0.48	0/683
55	v	0.62	1/1745 (0.1%)	0.89	4/2716 (0.1%)
56	w	0.48	0/1650	0.89	2/2569 (0.1%)
57	x	0.56	5/5546 (0.1%)	0.90	8/7504 (0.1%)
58	y	0.63	0/11	0.37	0/13
59	z	0.71	0/255	0.87	0/394
All	All	0.67	9/164410 (0.0%)	0.80	84/245165 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1	U	OP3-P	-10.52	1.48	1.61
55	v	1	C	OP3-P	-10.23	1.48	1.61
8	A	1	G	OP3-P	-10.19	1.49	1.61
57	x	317	SER	CA-CB	-7.42	1.41	1.52
8	A	2657	A	O3'-P	-5.82	1.54	1.61
57	x	267	SER	CA-CB	-5.78	1.44	1.52
57	x	344	SER	CA-CB	-5.50	1.44	1.52
57	x	224	SER	CA-CB	-5.40	1.44	1.52
57	x	351	SER	CA-CB	-5.10	1.45	1.52



All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	x	563	GLY	N-CA-C	9.43	136.68	113.10
35	b	16	GLY	N-CA-C	9.19	136.09	113.10
8	A	2506	U	C2-N1-C1'	7.78	127.03	117.70
34	a	481	G	C4-N9-C1'	7.46	136.20	126.50
28	U	98	ASN	N-CA-C	-7.45	90.89	111.00
8	A	2104	C	N1-C2-O2	7.08	123.15	118.90
8	A	1313	U	C2-N1-C1'	7.03	126.13	117.70
8	A	2506	U	N1-C2-O2	6.97	127.68	122.80
34	a	481	G	C6-C5-N7	-6.66	126.40	130.40
8	A	2129	C	N3-C2-O2	-6.50	117.35	121.90
8	A	2159	G	N3-C4-N9	-6.43	122.14	126.00
8	A	2655	G	C1'-O4'-C4'	-6.41	104.77	109.90
34	a	1158	C	N1-C2-O2	6.35	122.71	118.90
57	x	169	GLN	CB-CA-C	-6.27	97.85	110.40
8	A	1675	C	N1-C2-O2	6.24	122.64	118.90
8	A	883	G	P-O3'-C3'	6.23	127.18	119.70
57	x	144	ASP	CB-CA-C	-6.22	97.97	110.40
8	A	2159	G	C5-C6-O6	6.20	132.32	128.60
34	a	481	G	C8-N9-C1'	-6.13	119.03	127.00
8	A	2104	C	N3-C2-O2	-6.07	117.66	121.90
8	A	2129	C	N1-C2-O2	6.03	122.52	118.90
8	A	2474	U	C2-N1-C1'	5.98	124.87	117.70
57	x	307	GLU	N-CA-C	-5.96	94.92	111.00
34	a	471	U	N3-C2-O2	-5.93	118.05	122.20
34	a	481	G	N7-C8-N9	5.93	116.06	113.10
55	v	42	G	O5'-P-OP1	-5.90	100.39	105.70
8	A	1675	C	N3-C2-O2	-5.88	117.78	121.90
8	A	512	G	O4'-C1'-N9	5.86	112.89	108.20
34	a	1158	C	C2-N1-C1'	5.84	125.22	118.80
8	A	1726	C	C2-N1-C1'	5.79	125.17	118.80
8	A	1313	U	N1-C2-O2	5.79	126.85	122.80
8	A	2104	C	C2-N1-C1'	5.78	125.16	118.80
8	A	2474	U	N1-C2-O2	5.76	126.83	122.80
8	A	2506	U	N3-C2-O2	-5.75	118.17	122.20
43	j	57	VAL	N-CA-C	5.74	126.49	111.00
35	b	9	LEU	CA-CB-CG	5.71	128.42	115.30
34	a	1356	G	C4-N9-C1'	5.66	133.85	126.50
34	a	471	U	N1-C2-O2	5.58	126.70	122.80
34	a	1158	C	N3-C2-O2	-5.57	118.00	121.90
8	A	528	A	C2-N3-C4	-5.56	107.82	110.60
8	A	1920	C	C2-N1-C1'	5.54	124.89	118.80
34	a	158	G	C4'-C3'-C2'	-5.53	97.07	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1539	U	C5-C4-O4	-5.53	122.58	125.90
57	x	512	GLY	N-CA-C	5.51	126.88	113.10
8	A	2129	C	C6-N1-C2	-5.50	118.10	120.30
8	A	883	G	N3-C4-N9	-5.48	122.71	126.00
55	v	74	C	N3-C2-O2	-5.48	118.07	121.90
34	a	1423	G	O5'-P-OP1	-5.46	100.79	105.70
57	x	271	ASN	CB-CA-C	5.45	121.30	110.40
8	A	2655	G	O4'-C1'-N9	5.42	112.53	108.20
35	b	17	HIS	N-CA-C	-5.39	96.45	111.00
8	A	2391	G	C4-N9-C1'	-5.38	119.51	126.50
8	A	2506	U	C6-N1-C1'	-5.36	113.69	121.20
8	A	2159	G	N1-C6-O6	-5.31	116.72	119.90
8	A	901	C	C2-N1-C1'	5.27	124.60	118.80
8	A	2129	C	C2-N1-C1'	5.27	124.60	118.80
50	q	57	VAL	N-CA-C	-5.27	96.78	111.00
34	a	1158	C	C6-N1-C2	-5.26	118.20	120.30
8	A	1870	C	N1-C2-O2	5.21	122.03	118.90
8	A	748	G	O4'-C1'-N9	5.18	112.34	108.20
8	A	2474	U	N3-C2-O2	-5.18	118.57	122.20
8	A	901	C	N3-C2-O2	-5.17	118.28	121.90
8	A	1925	C	C6-N1-C2	-5.17	118.23	120.30
55	v	74	C	C2-N1-C1'	5.16	124.47	118.80
8	A	2300	C	C2-N1-C1'	5.14	124.46	118.80
57	x	150	PHE	CB-CA-C	-5.14	100.11	110.40
8	A	1488	C	C2-N1-C1'	5.13	124.45	118.80
56	w	69	G	C8-N9-C1'	5.13	133.68	127.00
34	a	1397	C	N1-C2-O2	5.13	121.98	118.90
10	C	204	LEU	N-CA-C	-5.12	97.17	111.00
57	x	323	ILE	N-CA-C	-5.11	97.19	111.00
34	a	1043	G	C8-N9-C1'	5.11	133.64	127.00
8	A	1914	C	C2-N1-C1'	5.09	124.41	118.80
8	A	1920	C	N3-C2-O2	-5.08	118.34	121.90
8	A	2391	G	O4'-C1'-N9	5.08	112.27	108.20
8	A	901	C	N1-C2-O2	5.07	121.94	118.90
8	A	1533	C	C2-N1-C1'	5.07	124.37	118.80
56	w	69	G	N3-C4-N9	-5.05	122.97	126.00
8	A	2187	U	N1-C2-O2	5.04	126.33	122.80
8	A	1170	C	N1-C2-O2	5.03	121.92	118.90
34	a	979	C	C2-N1-C1'	5.03	124.33	118.80
34	a	481	G	C4-C5-N7	5.02	112.81	110.80
55	v	74	C	N1-C2-O2	5.01	121.91	118.90
8	A	61	C	N1-C2-O2	5.01	121.91	118.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
2	1	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
3	2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
4	3	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
5	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
6	5	129/165 (78%)	110 (85%)	19 (15%)	0	100	100
7	6	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
10	C	269/273 (98%)	247 (92%)	22 (8%)	0	100	100
11	D	207/209 (99%)	186 (90%)	21 (10%)	0	100	100
12	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
13	F	175/179 (98%)	153 (87%)	22 (13%)	0	100	100
14	G	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
15	H	147/149 (99%)	122 (83%)	25 (17%)	0	100	100
16	I	139/142 (98%)	114 (82%)	25 (18%)	0	100	100
17	J	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	K	120/123 (98%)	109 (91%)	11 (9%)	0	100	100
19	L	141/144 (98%)	131 (93%)	10 (7%)	0	100	100
20	M	134/136 (98%)	123 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	N	118/127 (93%)	111 (94%)	7 (6%)	0	100	100
22	O	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
23	P	112/115 (97%)	103 (92%)	9 (8%)	0	100	100
24	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
25	R	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
26	S	108/110 (98%)	98 (91%)	10 (9%)	0	100	100
27	T	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
28	U	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
29	V	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
30	W	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
31	X	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
32	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
33	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
35	b	216/240 (90%)	197 (91%)	19 (9%)	0	100	100
36	c	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
37	d	203/206 (98%)	176 (87%)	27 (13%)	0	100	100
38	e	155/167 (93%)	144 (93%)	11 (7%)	0	100	100
39	f	98/135 (73%)	88 (90%)	10 (10%)	0	100	100
40	g	149/179 (83%)	139 (93%)	10 (7%)	0	100	100
41	h	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
42	i	125/130 (96%)	109 (87%)	16 (13%)	0	100	100
43	j	96/103 (93%)	83 (86%)	13 (14%)	0	100	100
44	k	114/129 (88%)	98 (86%)	16 (14%)	0	100	100
45	l	121/124 (98%)	107 (88%)	14 (12%)	0	100	100
46	m	112/118 (95%)	100 (89%)	12 (11%)	0	100	100
47	n	99/102 (97%)	92 (93%)	7 (7%)	0	100	100
48	o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
49	p	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
50	q	78/84 (93%)	71 (91%)	7 (9%)	0	100	100
51	r	63/75 (84%)	57 (90%)	6 (10%)	0	100	100
52	s	80/92 (87%)	76 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	t	83/87 (95%)	81 (98%)	2 (2%)	0	100	100
54	u	63/71 (89%)	55 (87%)	8 (13%)	0	100	100
57	x	701/704 (100%)	652 (93%)	48 (7%)	1 (0%)	51	83
All	All	6551/6924 (95%)	5985 (91%)	565 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	x	165	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	44 (98%)	1 (2%)	52	78
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/52 (98%)	51 (100%)	0	100	100
5	4	34/34 (100%)	33 (97%)	1 (3%)	42	72
7	6	59/62 (95%)	56 (95%)	3 (5%)	24	56
10	C	216/218 (99%)	214 (99%)	2 (1%)	78	91
11	D	164/164 (100%)	164 (100%)	0	100	100
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	144 (97%)	4 (3%)	44	74
14	G	137/138 (99%)	136 (99%)	1 (1%)	84	93
15	H	114/114 (100%)	114 (100%)	0	100	100
17	J	116/116 (100%)	116 (100%)	0	100	100
18	K	103/104 (99%)	101 (98%)	2 (2%)	57	81
19	L	102/103 (99%)	101 (99%)	1 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	M	109/109 (100%)	107 (98%)	2 (2%)	59	82
21	N	100/103 (97%)	99 (99%)	1 (1%)	76	90
22	O	86/87 (99%)	84 (98%)	2 (2%)	50	77
23	P	99/100 (99%)	97 (98%)	2 (2%)	55	80
24	Q	89/90 (99%)	88 (99%)	1 (1%)	73	89
25	R	84/84 (100%)	82 (98%)	2 (2%)	49	76
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	80 (100%)	0	100	100
28	U	83/85 (98%)	80 (96%)	3 (4%)	35	67
29	V	78/78 (100%)	78 (100%)	0	100	100
30	W	57/63 (90%)	57 (100%)	0	100	100
31	X	67/68 (98%)	66 (98%)	1 (2%)	65	85
32	Y	55/55 (100%)	54 (98%)	1 (2%)	59	82
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	173 (96%)	7 (4%)	32	65
36	c	170/190 (90%)	170 (100%)	0	100	100
37	d	172/173 (99%)	168 (98%)	4 (2%)	50	77
38	e	114/126 (90%)	114 (100%)	0	100	100
39	f	87/116 (75%)	87 (100%)	0	100	100
40	g	124/147 (84%)	120 (97%)	4 (3%)	39	69
41	h	104/105 (99%)	103 (99%)	1 (1%)	76	90
42	i	105/107 (98%)	104 (99%)	1 (1%)	76	90
43	j	86/90 (96%)	85 (99%)	1 (1%)	71	88
44	k	89/99 (90%)	86 (97%)	3 (3%)	37	69
45	l	103/104 (99%)	102 (99%)	1 (1%)	76	90
46	m	92/96 (96%)	91 (99%)	1 (1%)	73	89
47	n	79/84 (94%)	79 (100%)	0	100	100
48	o	76/77 (99%)	76 (100%)	0	100	100
49	p	65/65 (100%)	64 (98%)	1 (2%)	65	85
50	q	74/78 (95%)	73 (99%)	1 (1%)	67	86
51	r	56/65 (86%)	55 (98%)	1 (2%)	59	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	s	72/79 (91%)	71 (99%)	1 (1%)	67	86
53	t	65/66 (98%)	65 (100%)	0	100	100
54	u	46/61 (75%)	46 (100%)	0	100	100
57	x	577/578 (100%)	498 (86%)	79 (14%)	3	16
58	y	1/1 (100%)	1 (100%)	0	100	100
All	All	5204/5408 (96%)	5068 (97%)	136 (3%)	49	74

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	16	THR
5	4	12	ARG
7	6	16	CYS
7	6	22	MET
7	6	64	PHE
10	C	69	ASN
10	C	239	PHE
13	F	29	ARG
13	F	46	LYS
13	F	146	ASP
13	F	174	PHE
14	G	94	ARG
18	K	49	ARG
18	K	111	LYS
19	L	29	LYS
20	M	57	VAL
20	M	58	LYS
21	N	2	ARG
22	O	31	THR
22	O	33	ARG
23	P	67	GLU
23	P	88	ARG
24	Q	36	GLN
25	R	51	VAL
25	R	72	VAL
28	U	44	HIS
28	U	73	ASN
28	U	100	GLU
31	X	76	LYS
32	Y	58	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	b	17	HIS
35	b	20	ARG
35	b	41	ASN
35	b	73	ARG
35	b	112	ARG
35	b	152	ASP
35	b	153	MET
37	d	141	VAL
37	d	142	VAL
37	d	145	ARG
37	d	183	ARG
40	g	52	ARG
40	g	67	ASN
40	g	79	VAL
40	g	129	ASN
41	h	76	ARG
42	i	11	ARG
43	j	89	ARG
44	k	28	ASN
44	k	36	ARG
44	k	99	LEU
45	l	122	LYS
46	m	13	HIS
49	p	45	GLU
50	q	16	MET
51	r	44	THR
52	s	63	ASP
57	x	22	LYS
57	x	24	THR
57	x	35	VAL
57	x	39	ILE
57	x	41	GLU
57	x	42	VAL
57	x	53	GLU
57	x	68	THR
57	x	82	ARG
57	x	83	ILE
57	x	96	ILE
57	x	100	ARG
57	x	103	ARG
57	x	104	VAL
57	x	115	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
57	x	123	GLU
57	x	134	VAL
57	x	146	MET
57	x	151	LEU
57	x	170	LEU
57	x	175	GLU
57	x	179	THR
57	x	182	VAL
57	x	185	VAL
57	x	196	ASP
57	x	209	ASP
57	x	210	MET
57	x	221	LEU
57	x	224	SER
57	x	230	GLU
57	x	240	GLU
57	x	242	LEU
57	x	243	THR
57	x	244	GLU
57	x	247	ILE
57	x	261	ILE
57	x	270	LYS
57	x	272	LYS
57	x	277	MET
57	x	278	LEU
57	x	289	VAL
57	x	291	VAL
57	x	303	ASP
57	x	304	THR
57	x	309	HIS
57	x	314	GLU
57	x	325	THR
57	x	326	ASP
57	x	329	VAL
57	x	343	ASN
57	x	346	ASP
57	x	349	LEU
57	x	365	MET
57	x	375	GLU
57	x	376	VAL
57	x	389	ASP
57	x	407	ARG

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Mol	Chain	Res	Type
57	x	409	GLU
57	x	410	PHE
57	x	423	THR
57	x	429	LYS
57	x	430	MET
57	x	441	ASP
57	x	448	THR
57	x	449	ASP
57	x	455	THR
57	x	468	ILE
57	x	474	ARG
57	x	475	GLU
57	x	476	PHE
57	x	478	VAL
57	x	513	GLN
57	x	514	TYR
57	x	529	ASN
57	x	604	PHE
57	x	616	MET
57	x	638	ARG
57	x	685	LYS
57	x	701	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
13	F	62	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	335 (21%)	0
55	v	76/77 (98%)	17 (22%)	0
56	w	74/76 (97%)	23 (31%)	0
59	z	10/33 (30%)	4 (40%)	0
8	A	2898/2903 (99%)	647 (22%)	45 (1%)
9	B	119/120 (99%)	29 (24%)	3 (2%)
All	All	4713/4751 (99%)	1055 (22%)	48 (1%)

All (1055) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	15	G
8	A	23	G
8	A	34	U
8	A	42	A
8	A	43	G
8	A	44	A
8	A	46	G
8	A	58	G
8	A	62	U
8	A	63	A
8	A	71	A
8	A	74	A
8	A	75	G
8	A	84	A
8	A	96	C
8	A	101	A
8	A	118	A
8	A	120	U
8	A	131	A
8	A	140	C
8	A	141	G
8	A	142	A
8	A	144	A
8	A	157	C
8	A	160	A
8	A	163	C
8	A	164	C
8	A	170	U
8	A	196	A
8	A	199	A
8	A	204	A
8	A	205	G
8	A	215	G
8	A	216	A
8	A	221	A
8	A	222	A
8	A	223	A
8	A	228	C
8	A	230	G
8	A	242	G
8	A	243	U
8	A	244	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	248	G
8	A	250	G
8	A	255	A
8	A	261	G
8	A	265	A
8	A	266	G
8	A	267	C
8	A	272	A
8	A	273	G
8	A	275	C
8	A	276	U
8	A	278	A
8	A	279	A
8	A	287	G
8	A	288	U
8	A	330	A
8	A	335	C
8	A	345	A
8	A	359	G
8	A	361	G
8	A	362	A
8	A	363	G
8	A	369	U
8	A	371	A
8	A	372	G
8	A	377	G
8	A	386	G
8	A	393	C
8	A	395	U
8	A	396	G
8	A	401	A
8	A	402	A
8	A	404	A
8	A	405	U
8	A	406	G
8	A	411	G
8	A	412	A
8	A	455	C
8	A	457	A
8	A	458	G
8	A	459	U
8	A	473	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	480	A
8	A	481	G
8	A	482	A
8	A	490	C
8	A	491	G
8	A	504	A
8	A	505	A
8	A	509	C
8	A	510	C
8	A	512	G
8	A	513	A
8	A	529	A
8	A	530	G
8	A	532	A
8	A	533	G
8	A	546	U
8	A	548	G
8	A	549	G
8	A	556	A
8	A	563	A
8	A	568	U
8	A	573	U
8	A	575	A
8	A	588	U
8	A	603	A
8	A	613	A
8	A	614	A
8	A	615	U
8	A	622	G
8	A	627	A
8	A	637	A
8	A	645	C
8	A	646	U
8	A	647	G
8	A	655	A
8	A	659	G
8	A	669	G
8	A	670	A
8	A	682	G
8	A	685	A
8	A	686	U
8	A	694	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	711	G
8	A	712	G
8	A	714	U
8	A	715	A
8	A	716	A
8	A	729	G
8	A	730	A
8	A	747	5MC
8	A	757	G
8	A	762	U
8	A	763	G
8	A	764	A
8	A	775	G
8	A	782	A
8	A	783	A
8	A	784	G
8	A	785	G
8	A	789	A
8	A	791	C
8	A	792	A
8	A	805	G
8	A	806	C
8	A	812	C
8	A	819	A
8	A	827	U
8	A	828	U
8	A	831	G
8	A	846	U
8	A	847	U
8	A	858	G
8	A	859	G
8	A	878	A
8	A	879	G
8	A	881	G
8	A	882	G
8	A	883	G
8	A	884	U
8	A	885	C
8	A	887	A
8	A	889	C
8	A	890	C
8	A	891	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	892	A
8	A	893	C
8	A	894	U
8	A	895	U
8	A	896	A
8	A	897	C
8	A	899	A
8	A	903	C
8	A	907	G
8	A	910	A
8	A	931	U
8	A	933	A
8	A	934	U
8	A	941	A
8	A	946	C
8	A	961	C
8	A	965	C
8	A	973	A
8	A	974	G
8	A	975	A
8	A	983	A
8	A	984	A
8	A	990	A
8	A	995	C
8	A	996	A
8	A	1005	C
8	A	1012	U
8	A	1013	C
8	A	1024	G
8	A	1025	G
8	A	1026	G
8	A	1027	A
8	A	1028	A
8	A	1033	U
8	A	1040	A
8	A	1041	G
8	A	1042	G
8	A	1046	A
8	A	1047	G
8	A	1048	A
8	A	1052	C
8	A	1053	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1056	G
8	A	1057	A
8	A	1058	U
8	A	1059	G
8	A	1060	U
8	A	1061	U
8	A	1062	G
8	A	1063	G
8	A	1064	C
8	A	1066	U
8	A	1067	A
8	A	1068	G
8	A	1069	A
8	A	1070	A
8	A	1071	G
8	A	1072	C
8	A	1073	A
8	A	1074	G
8	A	1077	A
8	A	1078	U
8	A	1079	C
8	A	1080	A
8	A	1083	U
8	A	1084	A
8	A	1085	A
8	A	1086	A
8	A	1087	G
8	A	1088	A
8	A	1089	A
8	A	1090	A
8	A	1091	G
8	A	1092	C
8	A	1094	U
8	A	1096	A
8	A	1098	A
8	A	1100	C
8	A	1101	U
8	A	1102	C
8	A	1103	A
8	A	1105	U
8	A	1106	G
8	A	1108	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1109	C
8	A	1110	G
8	A	1111	A
8	A	1112	G
8	A	1115	G
8	A	1116	G
8	A	1121	C
8	A	1130	U
8	A	1131	G
8	A	1132	U
8	A	1134	A
8	A	1135	C
8	A	1136	G
8	A	1139	G
8	A	1142	A
8	A	1169	A
8	A	1170	C
8	A	1171	G
8	A	1174	U
8	A	1175	A
8	A	1176	U
8	A	1179	G
8	A	1180	U
8	A	1188	U
8	A	1212	G
8	A	1225	G
8	A	1227	G
8	A	1234	U
8	A	1235	G
8	A	1247	A
8	A	1253	A
8	A	1255	U
8	A	1256	G
8	A	1264	A
8	A	1271	G
8	A	1272	A
8	A	1273	U
8	A	1284	A
8	A	1288	G
8	A	1300	G
8	A	1301	A
8	A	1302	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1311	G
8	A	1312	U
8	A	1334	G
8	A	1340	U
8	A	1341	G
8	A	1345	C
8	A	1365	A
8	A	1368	G
8	A	1376	C
8	A	1377	G
8	A	1379	U
8	A	1383	A
8	A	1386	C
8	A	1395	A
8	A	1409	U
8	A	1413	A
8	A	1415	U
8	A	1416	G
8	A	1419	A
8	A	1420	A
8	A	1421	G
8	A	1428	C
8	A	1432	G
8	A	1433	A
8	A	1434	A
8	A	1445	G
8	A	1452	G
8	A	1453	A
8	A	1458	U
8	A	1460	U
8	A	1461	C
8	A	1474	U
8	A	1476	U
8	A	1478	G
8	A	1482	G
8	A	1488	C
8	A	1490	A
8	A	1491	G
8	A	1494	A
8	A	1497	U
8	A	1504	A
8	A	1515	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1524	G
8	A	1532	A
8	A	1535	A
8	A	1536	C
8	A	1537	G
8	A	1538	G
8	A	1549	A
8	A	1554	U
8	A	1555	G
8	A	1557	C
8	A	1558	C
8	A	1566	A
8	A	1569	A
8	A	1578	U
8	A	1580	A
8	A	1584	U
8	A	1585	C
8	A	1591	A
8	A	1592	C
8	A	1608	A
8	A	1610	A
8	A	1634	A
8	A	1635	A
8	A	1647	U
8	A	1648	U
8	A	1649	G
8	A	1651	G
8	A	1654	A
8	A	1674	G
8	A	1693	U
8	A	1698	A
8	A	1715	G
8	A	1716	U
8	A	1726	C
8	A	1727	C
8	A	1730	C
8	A	1731	G
8	A	1732	C
8	A	1738	G
8	A	1757	A
8	A	1760	C
8	A	1764	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1773	A
8	A	1782	U
8	A	1784	A
8	A	1791	A
8	A	1800	C
8	A	1801	A
8	A	1802	A
8	A	1807	G
8	A	1808	A
8	A	1809	A
8	A	1811	G
8	A	1816	C
8	A	1829	A
8	A	1835	2MG
8	A	1866	A
8	A	1869	G
8	A	1884	G
8	A	1895	C
8	A	1900	A
8	A	1901	A
8	A	1906	G
8	A	1908	C
8	A	1910	G
8	A	1912	A
8	A	1917	PSU
8	A	1922	G
8	A	1924	C
8	A	1925	C
8	A	1926	U
8	A	1927	A
8	A	1930	G
8	A	1936	A
8	A	1937	A
8	A	1938	A
8	A	1939	5MU
8	A	1955	U
8	A	1960	A
8	A	1964	G
8	A	1965	C
8	A	1967	C
8	A	1970	A
8	A	1971	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	1972	G
8	A	1982	U
8	A	1991	U
8	A	1992	G
8	A	1997	C
8	A	2020	A
8	A	2021	C
8	A	2022	U
8	A	2023	C
8	A	2031	A
8	A	2032	G
8	A	2033	A
8	A	2036	C
8	A	2043	C
8	A	2046	G
8	A	2052	A
8	A	2055	C
8	A	2056	G
8	A	2060	A
8	A	2061	G
8	A	2062	A
8	A	2067	G
8	A	2069	G7M
8	A	2077	A
8	A	2090	A
8	A	2091	C
8	A	2093	G
8	A	2101	A
8	A	2102	G
8	A	2103	C
8	A	2104	C
8	A	2105	U
8	A	2107	G
8	A	2110	G
8	A	2111	U
8	A	2112	G
8	A	2114	A
8	A	2115	G
8	A	2116	G
8	A	2118	U
8	A	2119	A
8	A	2120	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	2126	A
8	A	2127	G
8	A	2128	G
8	A	2129	C
8	A	2131	U
8	A	2132	U
8	A	2133	G
8	A	2134	A
8	A	2135	A
8	A	2136	G
8	A	2137	U
8	A	2138	G
8	A	2139	U
8	A	2143	C
8	A	2145	C
8	A	2146	C
8	A	2147	A
8	A	2148	G
8	A	2150	C
8	A	2151	U
8	A	2153	C
8	A	2154	A
8	A	2155	U
8	A	2158	A
8	A	2159	G
8	A	2161	C
8	A	2162	G
8	A	2165	C
8	A	2169	A
8	A	2170	A
8	A	2171	A
8	A	2172	U
8	A	2173	A
8	A	2174	C
8	A	2176	A
8	A	2180	U
8	A	2181	U
8	A	2183	A
8	A	2184	A
8	A	2185	U
8	A	2186	G
8	A	2190	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	2193	G
8	A	2198	A
8	A	2204	G
8	A	2211	A
8	A	2212	A
8	A	2225	A
8	A	2226	C
8	A	2238	G
8	A	2239	G
8	A	2266	A
8	A	2271	G
8	A	2279	G
8	A	2283	C
8	A	2287	A
8	A	2288	A
8	A	2297	A
8	A	2300	C
8	A	2305	U
8	A	2309	A
8	A	2320	U
8	A	2322	A
8	A	2325	G
8	A	2326	C
8	A	2333	A
8	A	2334	U
8	A	2336	A
8	A	2345	G
8	A	2347	C
8	A	2350	C
8	A	2352	A
8	A	2361	G
8	A	2383	G
8	A	2385	C
8	A	2402	U
8	A	2406	A
8	A	2410	G
8	A	2423	U
8	A	2425	A
8	A	2429	G
8	A	2430	A
8	A	2432	A
8	A	2435	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	2441	U
8	A	2447	G
8	A	2448	A
8	A	2452	C
8	A	2459	A
8	A	2469	A
8	A	2475	C
8	A	2476	A
8	A	2478	A
8	A	2480	C
8	A	2484	G
8	A	2488	G
8	A	2489	U
8	A	2491	U
8	A	2494	G
8	A	2502	G
8	A	2504	PSU
8	A	2505	G
8	A	2506	U
8	A	2518	A
8	A	2535	G
8	A	2542	A
8	A	2547	A
8	A	2552	OMU
8	A	2554	U
8	A	2566	A
8	A	2567	G
8	A	2573	C
8	A	2578	G
8	A	2585	U
8	A	2586	U
8	A	2592	G
8	A	2602	A
8	A	2603	G
8	A	2609	U
8	A	2613	U
8	A	2615	U
8	A	2623	G
8	A	2624	G
8	A	2629	U
8	A	2630	G
8	A	2634	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	2636	C
8	A	2646	C
8	A	2648	G
8	A	2654	A
8	A	2655	G
8	A	2656	U
8	A	2663	G
8	A	2684	U
8	A	2689	U
8	A	2690	U
8	A	2702	G
8	A	2707	U
8	A	2714	G
8	A	2715	C
8	A	2718	G
8	A	2720	U
8	A	2725	A
8	A	2726	A
8	A	2727	A
8	A	2729	G
8	A	2732	G
8	A	2733	A
8	A	2744	G
8	A	2748	A
8	A	2750	A
8	A	2751	G
8	A	2755	C
8	A	2757	A
8	A	2765	A
8	A	2769	U
8	A	2778	A
8	A	2779	U
8	A	2790	U
8	A	2791	G
8	A	2796	U
8	A	2797	U
8	A	2798	U
8	A	2799	A
8	A	2800	A
8	A	2801	G
8	A	2808	G
8	A	2809	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	A	2818	U
8	A	2820	A
8	A	2821	A
8	A	2833	U
8	A	2834	G
8	A	2835	A
8	A	2836	U
8	A	2849	U
8	A	2867	G
8	A	2872	A
8	A	2873	A
8	A	2879	A
8	A	2884	U
8	A	2886	A
8	A	2891	U
8	A	2893	A
9	B	9	G
9	B	13	G
9	B	17	C
9	B	18	G
9	B	19	C
9	B	24	G
9	B	26	C
9	B	34	A
9	B	35	C
9	B	37	C
9	B	41	G
9	B	42	C
9	B	45	A
9	B	51	G
9	B	53	A
9	B	56	G
9	B	57	A
9	B	62	C
9	B	65	U
9	B	67	G
9	B	73	A
9	B	87	U
9	B	88	C
9	B	89	U
9	B	90	C
9	B	91	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	B	101	A
9	B	109	A
9	B	120	U
34	a	2	A
34	a	6	G
34	a	7	A
34	a	9	G
34	a	31	G
34	a	32	A
34	a	39	G
34	a	46	G
34	a	48	C
34	a	51	A
34	a	70	U
34	a	71	A
34	a	76	G
34	a	78	A
34	a	79	G
34	a	80	A
34	a	81	A
34	a	83	C
34	a	84	U
34	a	85	U
34	a	86	G
34	a	87	C
34	a	89	U
34	a	90	C
34	a	94	G
34	a	96	U
34	a	98	A
34	a	121	U
34	a	141	G
34	a	144	G
34	a	158	G
34	a	163	C
34	a	164	G
34	a	166	U
34	a	173	U
34	a	182	A
34	a	183	C
34	a	184	G
34	a	189	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	197	A
34	a	198	G
34	a	205	A
34	a	206	C
34	a	208	U
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	226	G
34	a	240	G
34	a	244	U
34	a	245	U
34	a	247	G
34	a	251	G
34	a	262	A
34	a	266	G
34	a	267	C
34	a	270	A
34	a	281	G
34	a	289	G
34	a	316	C
34	a	321	A
34	a	327	A
34	a	328	C
34	a	329	A
34	a	330	C
34	a	344	A
34	a	347	G
34	a	351	G
34	a	352	C
34	a	354	G
34	a	356	A
34	a	360	G
34	a	367	U
34	a	372	C
34	a	375	U
34	a	388	G
34	a	397	A
34	a	406	G
34	a	411	A
34	a	412	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	413	G
34	a	421	U
34	a	423	G
34	a	428	G
34	a	429	U
34	a	439	U
34	a	440	C
34	a	444	G
34	a	446	G
34	a	448	A
34	a	461	A
34	a	462	G
34	a	465	A
34	a	468	A
34	a	471	U
34	a	472	U
34	a	473	U
34	a	474	G
34	a	479	U
34	a	482	A
34	a	484	G
34	a	495	A
34	a	496	A
34	a	505	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	516	PSU
34	a	517	G
34	a	518	C
34	a	521	G
34	a	524	G
34	a	527	G7M
34	a	531	U
34	a	532	A
34	a	535	A
34	a	547	A
34	a	559	A
34	a	562	U
34	a	563	A
34	a	564	C
34	a	572	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	573	A
34	a	576	C
34	a	577	G
34	a	582	C
34	a	596	A
34	a	607	A
34	a	614	C
34	a	615	G
34	a	629	A
34	a	632	U
34	a	642	A
34	a	650	G
34	a	653	U
34	a	665	A
34	a	703	G
34	a	704	A
34	a	721	G
34	a	723	U
34	a	724	G
34	a	734	G
34	a	747	A
34	a	748	G
34	a	753	A
34	a	755	G
34	a	773	G
34	a	777	A
34	a	781	A
34	a	792	A
34	a	793	U
34	a	794	A
34	a	814	A
34	a	815	A
34	a	816	A
34	a	817	C
34	a	819	A
34	a	829	G
34	a	841	C
34	a	843	U
34	a	844	G
34	a	845	A
34	a	846	G
34	a	847	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	849	G
34	a	851	G
34	a	868	C
34	a	870	U
34	a	875	U
34	a	885	G
34	a	902	G
34	a	913	A
34	a	914	A
34	a	922	G
34	a	934	C
34	a	935	A
34	a	940	C
34	a	960	U
34	a	966	2MG
34	a	968	A
34	a	969	A
34	a	971	G
34	a	973	G
34	a	975	A
34	a	976	G
34	a	977	A
34	a	981	U
34	a	982	U
34	a	984	C
34	a	992	U
34	a	993	G
34	a	994	A
34	a	996	A
34	a	999	C
34	a	1003	G
34	a	1004	A
34	a	1005	A
34	a	1006	G
34	a	1011	C
34	a	1014	A
34	a	1016	A
34	a	1017	U
34	a	1021	A
34	a	1022	A
34	a	1023	U
34	a	1025	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	1027	C
34	a	1028	C
34	a	1029	U
34	a	1030	U
34	a	1031	C
34	a	1032	G
34	a	1035	A
34	a	1040	U
34	a	1043	G
34	a	1047	G
34	a	1065	U
34	a	1084	G
34	a	1085	U
34	a	1092	A
34	a	1094	G
34	a	1095	U
34	a	1101	A
34	a	1109	C
34	a	1124	G
34	a	1125	U
34	a	1126	U
34	a	1127	G
34	a	1131	G
34	a	1134	G
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1144	G
34	a	1145	A
34	a	1159	U
34	a	1160	G
34	a	1167	A
34	a	1168	U
34	a	1169	A
34	a	1171	A
34	a	1177	G
34	a	1179	A
34	a	1183	U
34	a	1184	G
34	a	1196	A
34	a	1197	A
34	a	1200	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1226	C
34	a	1227	A
34	a	1236	A
34	a	1239	A
34	a	1241	G
34	a	1251	A
34	a	1254	A
34	a	1260	G
34	a	1261	A
34	a	1267	C
34	a	1270	G
34	a	1275	A
34	a	1280	A
34	a	1286	U
34	a	1287	A
34	a	1294	G
34	a	1297	G
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1305	G
34	a	1312	G
34	a	1317	C
34	a	1320	C
34	a	1323	G
34	a	1331	G
34	a	1332	A
34	a	1346	A
34	a	1347	G
34	a	1348	U
34	a	1360	A
34	a	1361	G
34	a	1363	A
34	a	1364	U
34	a	1370	G
34	a	1378	C
34	a	1379	G
34	a	1383	C
34	a	1386	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	1397	C
34	a	1398	A
34	a	1413	A
34	a	1419	G
34	a	1422	G
34	a	1423	G
34	a	1424	U
34	a	1432	G
34	a	1433	A
34	a	1441	A
34	a	1442	G
34	a	1443	C
34	a	1444	U
34	a	1446	A
34	a	1450	U
34	a	1451	U
34	a	1452	C
34	a	1453	G
34	a	1473	G
34	a	1474	U
34	a	1475	G
34	a	1476	A
34	a	1477	U
34	a	1479	C
34	a	1482	G
34	a	1483	A
34	a	1486	G
34	a	1487	G
34	a	1488	G
34	a	1492	A
34	a	1497	G
34	a	1499	A
34	a	1503	A
34	a	1506	U
34	a	1517	G
34	a	1529	G
34	a	1530	G
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1537	U
34	a	1538	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	a	1539	C
34	a	1540	U
55	v	9	G
55	v	14	A
55	v	18	G
55	v	20	H2U
55	v	21	A
55	v	33	U
55	v	34	C
55	v	42	G
55	v	43	A
55	v	44	A
55	v	45	G
55	v	46	A
55	v	47	U
55	v	48	C
55	v	52	G
55	v	55	PSU
55	v	76	A
56	w	8	4SU
56	w	13	C
56	w	14	A
56	w	16	U
56	w	17	C
56	w	18	G
56	w	19	G
56	w	20	U
56	w	21	A
56	w	29	G
56	w	36	A
56	w	40	C
56	w	44	G
56	w	45	U
56	w	46	G7M
56	w	53	G
56	w	59	U
56	w	60	U
56	w	61	C
56	w	67	C
56	w	68	C
56	w	69	G
56	w	74	C

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Mol	Chain	Res	Type
59	z	-1	C
59	z	0	U
59	z	4	U
59	z	7	G

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	242	G
8	A	361	G
8	A	458	G
8	A	479	A
8	A	481	G
8	A	545	U
8	A	555	G
8	A	652	U
8	A	715	A
8	A	746	PSU
8	A	774	G
8	A	784	G
8	A	883	G
8	A	894	U
8	A	895	U
8	A	1023	U
8	A	1024	G
8	A	1082	U
8	A	1090	A
8	A	1093	G
8	A	1300	G
8	A	1331	G
8	A	1423	G
8	A	1432	G
8	A	1451	C
8	A	1475	G
8	A	1490	A
8	A	1715	G
8	A	1730	C
8	A	1907	G
8	A	1926	U
8	A	2149	U
8	A	2192	U
8	A	2287	A

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Mol	Chain	Res	Type
8	A	2308	G
8	A	2319	G
8	A	2324	U
8	A	2405	G
8	A	2468	A
8	A	2488	G
8	A	2505	G
8	A	2655	G
8	A	2728	U
8	A	2796	U
8	A	2808	G
9	B	36	C
9	B	52	A
9	B	66	A

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

46 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
8	PSU	A	1911	8	18,21,22	1.15	2 (11%)	22,30,33	1.95	6 (27%)
8	6MZ	A	1618	8	18,25,26	2.13	4 (22%)	16,36,39	2.03	3 (18%)
34	5MC	a	967	34	18,22,23	3.68	7 (38%)	26,32,35	1.02	1 (3%)
8	5MC	A	1962	8	18,22,23	0.95	2 (11%)	26,32,35	1.33	3 (11%)
8	PSU	A	746	8,60	18,21,22	1.03	2 (11%)	22,30,33	1.72	4 (18%)
34	UR3	a	1498	60,34	19,22,23	2.57	7 (36%)	26,32,35	1.34	3 (11%)
56	4SU	w	8	56	18,21,22	1.95	4 (22%)	26,30,33	2.31	4 (15%)
56	5MU	w	54	56	19,22,23	1.43	6 (31%)	28,32,35	2.10	9 (32%)
34	G7M	a	527	34	20,26,27	4.30	14 (70%)	17,39,42	1.45	2 (11%)
8	5MC	A	747	8	18,22,23	3.56	7 (38%)	26,32,35	1.23	2 (7%)
8	3TD	A	1915	8	18,22,23	4.24	5 (27%)	22,32,35	1.72	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	5MU	A	1939	8	19,22,23	4.64	7 (36%)	28,32,35	3.79	9 (32%)
8	OMG	A	2251	8,56	18,26,27	1.63	2 (11%)	19,38,41	1.71	6 (31%)
55	5MU	v	54	55	19,22,23	4.78	7 (36%)	28,32,35	3.60	9 (32%)
55	4SU	v	8	55	18,21,22	3.59	7 (38%)	26,30,33	2.19	4 (15%)
8	6MZ	A	2030	8	18,25,26	2.18	3 (16%)	16,36,39	2.29	3 (18%)
55	PSU	v	55	55	18,21,22	1.09	1 (5%)	22,30,33	1.72	4 (18%)
34	MA6	a	1518	34	18,26,27	0.96	1 (5%)	19,38,41	2.84	2 (10%)
8	PSU	A	2605	8	18,21,22	1.03	2 (11%)	22,30,33	1.85	3 (13%)
8	OMU	A	2552	8,60	19,22,23	2.86	8 (42%)	26,31,34	1.78	5 (19%)
56	MIA	w	37	56	24,31,32	3.23	7 (29%)	26,44,47	3.29	11 (42%)
56	PSU	w	55	56	18,21,22	1.40	2 (11%)	22,30,33	1.87	3 (13%)
8	G7M	A	2069	8,60	20,26,27	4.24	14 (70%)	17,39,42	1.57	2 (11%)
8	2MG	A	2445	8	18,26,27	1.19	1 (5%)	16,38,41	1.47	5 (31%)
34	2MG	a	966	34	18,26,27	2.62	7 (38%)	16,38,41	1.44	3 (18%)
34	2MG	a	1207	34	18,26,27	2.63	7 (38%)	16,38,41	1.42	4 (25%)
34	5MC	a	1407	34	18,22,23	3.62	7 (38%)	26,32,35	1.02	1 (3%)
34	4OC	a	1402	34	20,23,24	2.97	8 (40%)	26,32,35	0.90	2 (7%)
8	2MA	A	2503	8,60	17,25,26	2.31	5 (29%)	17,37,40	1.29	2 (11%)
58	FME	y	101	58	8,9,10	0.99	1 (12%)	7,9,11	0.86	0
34	PSU	a	516	60,34	18,21,22	0.96	1 (5%)	22,30,33	1.66	5 (22%)
8	PSU	A	1917	8	18,21,22	0.95	1 (5%)	22,30,33	1.77	4 (18%)
8	PSU	A	2580	8,60	18,21,22	1.10	3 (16%)	22,30,33	1.92	6 (27%)
8	1MG	A	745	8	18,26,27	2.57	4 (22%)	19,39,42	1.38	3 (15%)
34	MA6	a	1519	34	18,26,27	0.99	1 (5%)	19,38,41	2.69	2 (10%)
8	OMC	A	2498	8,60	19,22,23	2.84	7 (36%)	26,31,34	0.86	1 (3%)
8	PSU	A	955	8	18,21,22	1.05	2 (11%)	22,30,33	1.89	4 (18%)
8	PSU	A	2604	8	18,21,22	1.06	2 (11%)	22,30,33	2.01	4 (18%)
55	H2U	v	20	55	18,21,22	3.15	5 (27%)	21,30,33	1.96	5 (23%)
8	PSU	A	2504	8,60	18,21,22	1.03	2 (11%)	22,30,33	1.75	4 (18%)
56	PSU	w	32	56	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
56	G7M	w	46	56	20,26,27	4.29	14 (70%)	17,39,42	1.45	2 (11%)
34	2MG	a	1516	34	18,26,27	2.60	7 (38%)	16,38,41	1.47	4 (25%)
8	2MG	A	1835	8	18,26,27	2.58	7 (38%)	16,38,41	1.42	4 (25%)
8	PSU	A	2457	8	18,21,22	1.06	3 (16%)	22,30,33	1.82	5 (22%)
56	PSU	w	39	56	18,21,22	1.11	1 (5%)	22,30,33	1.84	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	0/5/27/28	0/3/3/3
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	0/7/25/26	0/2/2/2
8	PSU	A	746	8,60	-	4/7/25/26	0/2/2/2
34	UR3	a	1498	60,34	-	2/7/25/26	0/2/2/2
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
34	G7M	a	527	34	-	1/3/25/26	0/3/3/3
8	5MC	A	747	8	-	1/7/25/26	0/2/2/2
8	3TD	A	1915	8	-	2/7/25/26	0/2/2/2
8	5MU	A	1939	8	-	2/7/25/26	0/2/2/2
8	OMG	A	2251	8,56	-	2/5/27/28	0/3/3/3
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3
55	PSU	v	55	55	-	1/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	0/7/29/30	0/3/3/3
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
8	OMU	A	2552	8,60	-	3/9/27/28	0/2/2/2
56	MIA	w	37	56	-	3/11/33/34	0/3/3/3
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
8	G7M	A	2069	8,60	-	2/3/25/26	0/3/3/3
8	2MG	A	2445	8	-	0/5/27/28	0/3/3/3
34	2MG	a	966	34	-	2/5/27/28	0/3/3/3
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	1/9/29/30	0/2/2/2
8	2MA	A	2503	8,60	-	1/3/25/26	0/3/3/3
58	FME	y	101	58	-	7/7/9/11	-
34	PSU	a	516	60,34	-	0/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	3/7/25/26	0/2/2/2
8	PSU	A	2580	8,60	-	0/7/25/26	0/2/2/2
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
34	MA6	a	1519	34	-	3/7/29/30	0/3/3/3
8	OMC	A	2498	8,60	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
55	H2U	v	20	55	-	7/7/38/39	0/2/2/2
8	PSU	A	2504	8,60	-	0/7/25/26	0/2/2/2
56	PSU	w	32	56	-	3/7/25/26	0/2/2/2
56	G7M	w	46	56	-	1/3/25/26	0/3/3/3
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	3/7/25/26	0/2/2/2

All (218) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	C6-C5	12.88	1.50	1.35
56	w	37	MIA	C2-S10	-11.90	1.65	1.75
8	A	2069	G7M	C2'-C3'	-11.59	1.21	1.53
34	a	527	G7M	C2'-C3'	-11.39	1.22	1.53
55	v	54	5MU	C2-N1	10.80	1.55	1.38
56	w	46	G7M	C2'-C3'	-10.78	1.23	1.53
55	v	54	5MU	C6-N1	10.40	1.55	1.38
8	A	1939	5MU	C6-N1	10.20	1.55	1.38
8	A	1939	5MU	C2-N1	9.82	1.54	1.38
55	v	20	H2U	C2-N1	9.80	1.49	1.35
55	v	54	5MU	C4-C5	9.71	1.60	1.44
8	A	1939	5MU	C4-C5	9.53	1.60	1.44
8	A	1915	3TD	C2-N1	9.37	1.49	1.37
34	a	967	5MC	C6-C5	9.13	1.49	1.34
34	a	1407	5MC	C6-C5	9.01	1.49	1.34
8	A	747	5MC	C6-C5	8.78	1.49	1.34
55	v	8	4SU	C4-N3	8.32	1.46	1.37
8	A	1939	5MU	C4-N3	-8.14	1.23	1.38
55	v	54	5MU	C4-N3	-7.94	1.24	1.38
8	A	2030	6MZ	C6-N6	7.55	1.47	1.35
8	A	1618	6MZ	C6-N6	7.33	1.47	1.35
55	v	8	4SU	C2-N1	7.18	1.50	1.38
34	a	967	5MC	C4-N3	7.00	1.46	1.34
8	A	745	1MG	C2-N2	6.96	1.46	1.34
8	A	2503	2MA	C2-N3	6.84	1.45	1.31
8	A	2552	OMU	C2-N1	6.77	1.49	1.38
8	A	747	5MC	C4-N3	6.67	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1402	4OC	C4-N3	6.60	1.44	1.32
34	a	1407	5MC	C4-N3	6.59	1.45	1.34
55	v	20	H2U	C2-N3	6.52	1.49	1.38
34	a	966	2MG	C2-N2	6.48	1.47	1.33
34	a	527	G7M	O4'-C1'	6.35	1.49	1.41
56	w	46	G7M	O4'-C1'	6.32	1.49	1.41
8	A	2069	G7M	O4'-C1'	6.31	1.49	1.41
34	a	527	G7M	O4'-C4'	-6.17	1.31	1.45
8	A	2552	OMU	C2-N3	6.16	1.49	1.38
34	a	1207	2MG	C2-N2	6.16	1.47	1.33
8	A	1835	2MG	C2-N2	6.15	1.47	1.33
34	a	1516	2MG	C2-N2	6.15	1.47	1.33
34	a	1498	UR3	C2-N1	6.11	1.47	1.38
8	A	2498	OMC	C6-C5	6.11	1.49	1.35
8	A	747	5MC	C2-N3	6.10	1.48	1.36
34	a	967	5MC	C2-N3	6.07	1.48	1.36
34	a	1402	4OC	C6-C5	6.06	1.49	1.35
56	w	37	MIA	C13-C14	6.05	1.49	1.32
8	A	2069	G7M	O4'-C4'	-6.05	1.31	1.45
34	a	1498	UR3	C6-C5	6.00	1.49	1.35
56	w	46	G7M	O4'-C4'	-5.98	1.31	1.45
8	A	2498	OMC	C2-N3	5.93	1.48	1.36
34	a	1407	5MC	C2-N3	5.92	1.48	1.36
55	v	54	5MU	C6-C5	5.90	1.44	1.34
8	A	1939	5MU	C6-C5	5.78	1.44	1.34
55	v	8	4SU	C6-C5	5.72	1.48	1.35
8	A	1915	3TD	C6-N1	5.68	1.45	1.36
55	v	8	4SU	C2-N3	5.50	1.47	1.38
8	A	2498	OMC	C4-N3	5.45	1.45	1.34
56	w	46	G7M	C2-N3	5.45	1.46	1.33
34	a	1402	4OC	C2-N3	5.44	1.47	1.36
8	A	2552	OMU	C6-C5	5.38	1.47	1.35
34	a	527	G7M	C2-N3	5.37	1.46	1.33
34	a	966	2MG	C4-N3	5.29	1.50	1.37
8	A	745	1MG	C2-N3	5.29	1.44	1.34
56	w	46	G7M	C3'-C4'	5.15	1.66	1.53
8	A	2069	G7M	C2-N3	5.07	1.45	1.33
55	v	8	4SU	C4-S4	-5.02	1.58	1.68
8	A	1835	2MG	C4-N3	5.02	1.49	1.37
56	w	37	MIA	C2'-C1'	-5.01	1.46	1.53
55	v	20	H2U	C4-N3	5.01	1.46	1.37
56	w	8	4SU	C4-S4	-4.96	1.59	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	967	5MC	C4-N4	4.88	1.46	1.34
34	a	1207	2MG	C4-N3	4.85	1.49	1.37
34	a	527	G7M	C4-N3	4.83	1.49	1.37
34	a	1407	5MC	C4-N4	4.80	1.46	1.34
8	A	1915	3TD	C2-N3	4.80	1.49	1.38
34	a	1516	2MG	C4-N3	4.77	1.48	1.37
8	A	747	5MC	C4-N4	4.76	1.46	1.34
8	A	745	1MG	C4-N3	4.76	1.48	1.37
8	A	2069	G7M	C4-N3	4.73	1.48	1.37
56	w	46	G7M	C4-N3	4.71	1.48	1.37
8	A	2503	2MA	C4-N3	4.68	1.48	1.37
34	a	1207	2MG	C2-N1	4.64	1.44	1.36
34	a	1407	5MC	C6-N1	4.61	1.45	1.38
34	a	527	G7M	C3'-C4'	4.60	1.64	1.53
8	A	2069	G7M	C3'-C4'	4.55	1.64	1.53
34	a	1498	UR3	C2-N3	4.44	1.47	1.39
8	A	2251	OMG	C6-N1	-4.42	1.31	1.37
8	A	1835	2MG	C2-N1	4.40	1.43	1.36
34	a	1516	2MG	C2-N1	4.39	1.43	1.36
56	w	46	G7M	C2'-C1'	4.39	1.60	1.53
34	a	967	5MC	C6-N1	4.31	1.45	1.38
34	a	966	2MG	C2-N1	4.30	1.43	1.36
34	a	1407	5MC	C2-N1	4.24	1.49	1.40
34	a	527	G7M	C2-N2	4.23	1.44	1.34
8	A	747	5MC	C6-N1	4.11	1.45	1.38
34	a	1402	4OC	C4-N4	4.07	1.44	1.35
56	w	46	G7M	C2-N2	4.07	1.43	1.34
8	A	2069	G7M	C2-N2	4.05	1.43	1.34
34	a	967	5MC	C2-N1	4.03	1.48	1.40
56	w	8	4SU	C4-N3	-4.00	1.33	1.37
34	a	1402	4OC	C5-C4	3.93	1.49	1.40
34	a	527	G7M	C2'-C1'	3.82	1.59	1.53
8	A	747	5MC	C2-N1	3.81	1.48	1.40
8	A	2498	OMC	C4-N4	3.81	1.42	1.33
34	a	1207	2MG	C6-N1	3.66	1.43	1.37
55	v	55	PSU	C6-C5	3.64	1.39	1.35
56	w	46	G7M	C6-N1	3.60	1.43	1.37
8	A	2552	OMU	C4-N3	3.57	1.45	1.38
34	a	1402	4OC	C2-N1	3.52	1.47	1.40
8	A	2498	OMC	C2-N1	3.50	1.47	1.40
34	a	967	5MC	O2-C2	-3.44	1.17	1.23
8	A	2030	6MZ	C5-C4	-3.44	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	747	5MC	O2-C2	-3.42	1.17	1.23
34	a	527	G7M	C6-N1	3.41	1.43	1.37
8	A	2498	OMC	C6-N1	3.40	1.46	1.38
56	w	37	MIA	O4'-C4'	-3.38	1.37	1.45
56	w	46	G7M	C5-C6	3.37	1.54	1.45
56	w	39	PSU	C6-C5	3.34	1.39	1.35
8	A	2069	G7M	C6-N1	3.34	1.42	1.37
34	a	527	G7M	C5-C6	3.30	1.53	1.45
8	A	2069	G7M	C2'-C1'	3.29	1.58	1.53
34	a	1516	2MG	C6-N1	3.28	1.42	1.37
34	a	1407	5MC	O2-C2	-3.27	1.17	1.23
56	w	32	PSU	C6-C5	3.26	1.39	1.35
8	A	1835	2MG	C6-N1	3.24	1.42	1.37
8	A	2069	G7M	C5-C6	3.23	1.53	1.45
34	a	1402	4OC	O2-C2	-3.23	1.17	1.23
8	A	1911	PSU	C6-C5	3.22	1.39	1.35
55	v	8	4SU	C5-C4	3.22	1.46	1.42
56	w	46	G7M	O2'-C2'	3.21	1.50	1.43
8	A	1618	6MZ	C5-C4	-3.19	1.32	1.40
34	a	1516	2MG	C5-C4	-3.17	1.35	1.43
8	A	2498	OMC	O2-C2	-3.15	1.17	1.23
34	a	966	2MG	O6-C6	-3.10	1.17	1.23
8	A	1835	2MG	O6-C6	-3.09	1.17	1.23
56	w	55	PSU	C6-C5	3.06	1.38	1.35
8	A	2552	OMU	O4-C4	-3.04	1.18	1.24
34	a	1402	4OC	C6-N1	3.03	1.45	1.38
34	a	1516	2MG	C5-C6	3.00	1.53	1.47
34	a	1516	2MG	O6-C6	-3.00	1.17	1.23
8	A	1835	2MG	C5-C4	-2.96	1.35	1.43
34	a	1207	2MG	C5-C6	2.96	1.53	1.47
34	a	966	2MG	C6-N1	2.94	1.42	1.37
34	a	1207	2MG	O6-C6	-2.93	1.17	1.23
34	a	966	2MG	C5-C4	-2.92	1.35	1.43
34	a	527	G7M	O2'-C2'	2.91	1.49	1.43
34	a	1207	2MG	C5-C4	-2.90	1.35	1.43
8	A	2503	2MA	C5-C4	-2.90	1.35	1.43
34	a	1498	UR3	C6-N1	2.88	1.44	1.38
56	w	8	4SU	C5-C4	-2.87	1.38	1.42
8	A	1939	5MU	O2-C2	-2.85	1.17	1.23
8	A	2445	2MG	C6-N1	-2.84	1.33	1.37
8	A	745	1MG	C5-C4	-2.82	1.35	1.43
8	A	2069	G7M	O2'-C2'	2.80	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	46	G7M	O3'-C3'	2.79	1.49	1.43
55	v	54	5MU	O4-C4	-2.78	1.18	1.23
34	a	1498	UR3	O2-C2	-2.77	1.17	1.22
8	A	2504	PSU	C6-C5	2.76	1.38	1.35
34	a	1519	MA6	C5-C4	-2.75	1.33	1.40
56	w	55	PSU	C4-N3	-2.75	1.33	1.38
8	A	1939	5MU	O4-C4	-2.75	1.18	1.23
8	A	1962	5MC	C6-N1	-2.71	1.33	1.38
8	A	1917	PSU	C6-C5	2.69	1.38	1.35
8	A	1915	3TD	C4-N3	2.68	1.46	1.40
8	A	2604	PSU	C6-C5	2.68	1.38	1.35
55	v	8	4SU	O2-C2	-2.66	1.18	1.23
34	a	1518	MA6	C5-C4	-2.65	1.33	1.40
55	v	54	5MU	O2-C2	-2.63	1.18	1.23
34	a	516	PSU	C6-C5	2.63	1.38	1.35
8	A	746	PSU	C6-C5	2.61	1.38	1.35
56	w	54	5MU	C6-C5	2.61	1.38	1.34
8	A	2605	PSU	C6-C5	2.61	1.38	1.35
8	A	955	PSU	C6-C5	2.58	1.38	1.35
56	w	8	4SU	C2-N3	-2.56	1.33	1.38
8	A	2552	OMU	O2-C2	-2.56	1.18	1.23
8	A	2580	PSU	O4'-C1'	-2.55	1.40	1.43
34	a	966	2MG	C5-C6	2.53	1.52	1.47
56	w	54	5MU	C4-N3	-2.53	1.34	1.38
8	A	2552	OMU	C6-N1	2.52	1.44	1.38
56	w	46	G7M	O6-C6	-2.51	1.18	1.23
56	w	37	MIA	C3'-C4'	-2.50	1.46	1.53
8	A	1618	6MZ	C2-N3	2.49	1.36	1.32
34	a	527	G7M	O3'-C3'	2.48	1.48	1.43
56	w	46	G7M	C2-N1	2.46	1.43	1.37
8	A	2580	PSU	C6-C5	2.46	1.38	1.35
56	w	54	5MU	C6-N1	-2.46	1.33	1.38
8	A	2251	OMG	C2-N1	-2.45	1.31	1.37
56	w	54	5MU	C4-C5	2.42	1.48	1.44
8	A	1618	6MZ	C6-N1	-2.42	1.30	1.34
8	A	2457	PSU	C6-C5	2.41	1.38	1.35
8	A	1835	2MG	C5-C6	2.40	1.52	1.47
34	a	1498	UR3	O4-C4	-2.38	1.18	1.23
8	A	2069	G7M	O6-C6	-2.33	1.18	1.23
55	v	20	H2U	O4-C4	-2.32	1.18	1.23
55	v	20	H2U	O2-C2	-2.31	1.18	1.23
34	a	527	G7M	O6-C6	-2.29	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2503	2MA	C2-N1	2.28	1.43	1.36
8	A	2069	G7M	C2-N1	2.27	1.43	1.37
34	a	527	G7M	C2-N1	2.25	1.43	1.37
8	A	1911	PSU	C4-C5	-2.22	1.37	1.44
8	A	2580	PSU	C4-C5	-2.21	1.37	1.44
8	A	746	PSU	C4-C5	-2.18	1.38	1.44
8	A	2030	6MZ	C2-N3	2.17	1.35	1.32
8	A	2069	G7M	O3'-C3'	2.15	1.48	1.43
56	w	54	5MU	C2-N1	2.13	1.41	1.38
8	A	2457	PSU	O4'-C1'	-2.13	1.40	1.43
8	A	1962	5MC	C6-C5	2.12	1.38	1.34
8	A	2604	PSU	C4-C5	-2.09	1.38	1.44
8	A	2605	PSU	C4-C5	-2.09	1.38	1.44
8	A	955	PSU	C4-C5	-2.08	1.38	1.44
8	A	2457	PSU	C4-C5	-2.07	1.38	1.44
34	a	1498	UR3	C5-C4	2.04	1.49	1.43
56	w	54	5MU	C2-N3	-2.03	1.34	1.38
8	A	2552	OMU	C5-C4	2.03	1.48	1.43
56	w	37	MIA	O5'-C5'	-2.02	1.39	1.44
8	A	2504	PSU	C4-C5	-2.02	1.38	1.44
58	y	101	FME	CA-N	-2.01	1.43	1.46
56	w	37	MIA	C2'-C3'	-2.01	1.47	1.53
8	A	2503	2MA	C6-N1	2.01	1.42	1.38

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1939	5MU	C5-C4-N3	12.35	125.85	115.31
55	v	54	5MU	C5-C4-N3	11.91	125.48	115.31
56	w	37	MIA	C12-C13-C14	-11.05	105.63	127.14
8	A	1939	5MU	C5-C6-N1	-10.74	112.29	123.34
34	a	1518	MA6	N1-C6-N6	-10.56	105.94	117.06
55	v	54	5MU	C5-C6-N1	-9.98	113.07	123.34
34	a	1519	MA6	N1-C6-N6	-9.95	106.58	117.06
55	v	8	4SU	C4-N3-C2	-7.49	120.06	127.34
55	v	20	H2U	C4-N3-C2	-6.80	120.16	125.79
56	w	8	4SU	C4-N3-C2	-6.74	120.79	127.34
56	w	8	4SU	C5-C4-N3	6.30	120.53	114.69
56	w	55	PSU	N1-C2-N3	6.02	121.95	115.13
34	a	1519	MA6	N3-C2-N1	-5.76	119.67	128.68
34	a	1518	MA6	N3-C2-N1	-5.72	119.74	128.68
56	w	37	MIA	C16-C14-C13	-5.60	106.46	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2030	6MZ	N3-C2-N1	-5.56	119.99	128.68
8	A	1939	5MU	O4-C4-C5	-5.54	118.48	124.90
55	v	8	4SU	C5-C4-N3	5.45	119.74	114.69
8	A	1618	6MZ	N3-C2-N1	-5.39	120.25	128.68
8	A	2552	OMU	C4-N3-C2	-5.35	119.53	126.58
8	A	1939	5MU	C4-N3-C2	-5.33	120.44	127.35
8	A	1915	3TD	N1-C2-N3	5.26	120.29	116.14
8	A	1911	PSU	C4-N3-C2	-5.12	118.97	126.34
56	w	54	5MU	C4-N3-C2	-5.11	120.73	127.35
8	A	2604	PSU	C4-N3-C2	-5.08	119.02	126.34
8	A	2605	PSU	C4-N3-C2	-4.97	119.18	126.34
8	A	1618	6MZ	C9-N6-C6	-4.92	118.63	122.87
8	A	2604	PSU	N1-C2-N3	4.92	120.70	115.13
8	A	2030	6MZ	C9-N6-C6	-4.91	118.64	122.87
56	w	39	PSU	N1-C2-N3	4.91	120.69	115.13
55	v	54	5MU	C4-N3-C2	-4.89	121.02	127.35
8	A	1939	5MU	N3-C2-N1	4.87	121.35	114.89
55	v	54	5MU	O4-C4-C5	-4.85	119.28	124.90
56	w	54	5MU	N3-C2-N1	4.80	121.26	114.89
8	A	955	PSU	N1-C2-N3	4.78	120.55	115.13
8	A	1911	PSU	N1-C2-N3	4.78	120.55	115.13
56	w	37	MIA	C15-C14-C13	-4.77	108.86	122.65
8	A	2030	6MZ	C1'-N9-C4	-4.72	118.34	126.64
8	A	746	PSU	C4-N3-C2	-4.72	119.54	126.34
8	A	955	PSU	C4-N3-C2	-4.72	119.54	126.34
8	A	2457	PSU	C4-N3-C2	-4.72	119.54	126.34
55	v	54	5MU	N3-C2-N1	4.71	121.15	114.89
8	A	2580	PSU	N1-C2-N3	4.59	120.33	115.13
56	w	39	PSU	C4-N3-C2	-4.59	119.73	126.34
8	A	2457	PSU	N1-C2-N3	4.55	120.28	115.13
8	A	1917	PSU	C4-N3-C2	-4.51	119.84	126.34
55	v	55	PSU	C4-N3-C2	-4.50	119.85	126.34
56	w	32	PSU	C4-N3-C2	-4.50	119.85	126.34
55	v	55	PSU	N1-C2-N3	4.50	120.23	115.13
8	A	2504	PSU	C4-N3-C2	-4.47	119.90	126.34
8	A	2605	PSU	N1-C2-N3	4.47	120.19	115.13
8	A	1917	PSU	N1-C2-N3	4.46	120.19	115.13
56	w	37	MIA	O4'-C4'-C3'	-4.44	96.33	105.11
34	a	1498	UR3	C4-N3-C2	-4.38	120.44	124.56
34	a	516	PSU	C4-N3-C2	-4.38	120.03	126.34
8	A	2580	PSU	C4-N3-C2	-4.37	120.04	126.34
8	A	1915	3TD	C4-N3-C2	-4.35	119.89	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	32	PSU	N1-C2-N3	4.31	120.02	115.13
56	w	54	5MU	C5-C4-N3	4.30	118.98	115.31
8	A	2504	PSU	N1-C2-N3	4.30	120.00	115.13
8	A	746	PSU	N1-C2-N3	4.17	119.86	115.13
56	w	8	4SU	N3-C2-N1	4.13	120.37	114.89
56	w	55	PSU	C4-N3-C2	-4.11	120.41	126.34
8	A	745	1MG	C5-C6-N1	4.07	120.02	113.90
55	v	8	4SU	C5-C4-S4	-4.02	119.29	124.47
34	a	516	PSU	N1-C2-N3	3.89	119.53	115.13
55	v	54	5MU	C5M-C5-C6	-3.84	117.72	122.85
56	w	37	MIA	C2-N3-C4	3.81	120.58	115.32
8	A	747	5MC	C5-C6-N1	-3.81	119.42	123.34
8	A	2552	OMU	N3-C2-N1	3.77	119.90	114.89
34	a	966	2MG	C5-C6-N1	3.76	120.59	113.95
8	A	1939	5MU	O2-C2-N1	-3.67	117.90	122.79
8	A	2552	OMU	C5-C4-N3	3.66	120.31	114.84
56	w	54	5MU	O4-C4-C5	-3.63	120.69	124.90
56	w	54	5MU	C5-C6-N1	-3.59	119.65	123.34
8	A	2503	2MA	C5-C6-N1	3.58	120.20	114.02
8	A	1939	5MU	C5M-C5-C6	-3.57	118.09	122.85
8	A	2251	OMG	O2'-C2'-C1'	-3.53	102.09	109.09
8	A	1962	5MC	C5-C6-N1	-3.52	119.71	123.34
55	v	54	5MU	C5M-C5-C4	3.51	122.63	118.77
34	a	1516	2MG	C5-C6-N1	3.49	120.12	113.95
8	A	2580	PSU	O2-C2-N1	-3.43	119.02	122.79
55	v	8	4SU	N3-C2-N1	3.41	119.42	114.89
8	A	1835	2MG	C5-C6-N1	3.39	119.94	113.95
34	a	1207	2MG	C5-C6-N1	3.38	119.92	113.95
56	w	8	4SU	C5-C4-S4	-3.34	120.17	124.47
34	a	967	5MC	C5-C6-N1	-3.33	119.91	123.34
34	a	527	G7M	O4'-C1'-C2'	-3.29	102.12	106.93
8	A	2604	PSU	C6-C5-C4	3.24	120.47	118.20
56	w	37	MIA	O2'-C2'-C3'	-3.21	101.44	111.82
56	w	37	MIA	O2'-C2'-C1'	-3.21	99.02	110.85
8	A	955	PSU	O2-C2-N1	-3.19	119.27	122.79
8	A	1939	5MU	C5M-C5-C4	3.17	122.26	118.77
55	v	20	H2U	N3-C2-N1	3.16	120.00	116.65
56	w	37	MIA	O4'-C4'-C5'	-3.11	99.15	109.37
8	A	2504	PSU	O2-C2-N1	-3.01	119.48	122.79
56	w	46	G7M	C2-N1-C6	-2.97	119.63	125.10
56	w	37	MIA	O4'-C1'-C2'	-2.96	102.60	106.93
8	A	2552	OMU	O4-C4-C5	-2.96	119.95	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	55	PSU	O2-C2-N1	-2.91	119.58	122.79
8	A	2580	PSU	C6-N1-C2	-2.89	119.72	122.68
8	A	2445	2MG	O5'-C5'-C4'	-2.89	99.16	108.99
8	A	2069	G7M	O4'-C1'-C2'	-2.88	102.72	106.93
8	A	2503	2MA	C8-N7-C5	2.86	108.44	102.99
8	A	1917	PSU	O2-C2-N1	-2.86	119.64	122.79
56	w	32	PSU	O2-C2-N1	-2.85	119.65	122.79
8	A	2251	OMG	C5-C6-N1	2.84	118.96	113.95
56	w	39	PSU	C6-N1-C2	-2.82	119.80	122.68
8	A	1618	6MZ	C1'-N9-C4	-2.78	121.76	126.64
8	A	2069	G7M	C2-N1-C6	-2.76	120.01	125.10
34	a	1407	5MC	C5-C6-N1	-2.74	120.52	123.34
55	v	20	H2U	C5-C4-N3	2.73	119.72	116.65
55	v	54	5MU	O2-C2-N1	-2.73	119.15	122.79
8	A	955	PSU	C6-N1-C2	-2.72	119.90	122.68
55	v	20	H2U	C5-C6-N1	2.71	120.55	111.61
34	a	1207	2MG	CM2-N2-C2	-2.70	117.89	123.86
8	A	1917	PSU	C6-N1-C2	-2.68	119.94	122.68
34	a	527	G7M	C2-N1-C6	-2.67	120.18	125.10
34	a	516	PSU	O2-C2-N1	-2.66	119.86	122.79
56	w	37	MIA	C2'-C3'-C4'	-2.66	97.47	102.64
34	a	1516	2MG	CM2-N2-C2	-2.64	118.02	123.86
34	a	1516	2MG	C8-N7-C5	2.64	108.02	102.99
34	a	966	2MG	O6-C6-C5	-2.63	119.23	124.37
34	a	1498	UR3	C1'-N1-C2	2.60	121.37	116.99
8	A	2457	PSU	O2-C2-N1	-2.55	119.98	122.79
8	A	2580	PSU	O4'-C1'-C2'	2.55	108.74	105.14
55	v	54	5MU	O4-C4-N3	-2.55	115.23	120.12
8	A	1835	2MG	C8-N7-C5	2.54	107.82	102.99
8	A	2552	OMU	C1'-N1-C2	2.53	122.15	117.57
34	a	1207	2MG	C8-N7-C5	2.52	107.80	102.99
8	A	2604	PSU	O2-C2-N1	-2.52	120.02	122.79
8	A	2251	OMG	CM2-O2'-C2'	-2.48	108.01	114.52
56	w	32	PSU	C6-N1-C2	-2.46	120.16	122.68
8	A	745	1MG	C8-N7-C5	2.46	107.67	102.99
8	A	1835	2MG	O6-C6-C5	-2.46	119.58	124.37
8	A	2445	2MG	CM2-N2-C2	-2.45	118.45	123.86
8	A	746	PSU	O2-C2-N1	-2.44	120.10	122.79
8	A	1835	2MG	CM2-N2-C2	-2.44	118.47	123.86
8	A	2251	OMG	O6-C6-C5	-2.43	119.63	124.37
8	A	2457	PSU	C6-N1-C2	-2.43	120.20	122.68
8	A	2445	2MG	C5-C6-N1	2.42	118.22	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2504	PSU	C6-N1-C2	-2.42	120.21	122.68
56	w	54	5MU	O2-C2-N1	-2.37	119.64	122.79
56	w	46	G7M	C3'-C2'-C1'	2.33	104.48	100.98
8	A	1939	5MU	O4-C4-N3	-2.32	115.66	120.12
8	A	1911	PSU	C6-C5-C4	2.32	119.82	118.20
56	w	54	5MU	C5M-C5-C4	2.31	121.31	118.77
8	A	1911	PSU	O2-C2-N1	-2.31	120.25	122.79
34	a	966	2MG	C8-N7-C5	2.28	107.34	102.99
34	a	516	PSU	C6-N1-C2	-2.28	120.36	122.68
56	w	37	MIA	C11-S10-C2	-2.27	100.57	102.27
8	A	2251	OMG	O4'-C4'-C3'	-2.27	100.62	105.11
55	v	20	H2U	O2-C2-N1	-2.27	120.26	123.11
8	A	2251	OMG	C8-N7-C5	2.25	107.28	102.99
55	v	55	PSU	O2-C2-N1	-2.23	120.33	122.79
8	A	746	PSU	C6-C5-C4	2.23	119.76	118.20
34	a	1207	2MG	O6-C6-C5	-2.21	120.05	124.37
8	A	2445	2MG	C8-N7-C5	2.21	107.20	102.99
8	A	1962	5MC	O4'-C1'-N1	2.20	113.40	108.36
8	A	1962	5MC	C5-C4-N3	-2.20	119.30	121.67
8	A	1911	PSU	O4-C4-C5	-2.18	118.36	124.05
8	A	2498	OMC	O2-C2-N3	-2.17	118.81	122.33
55	v	55	PSU	C6-N1-C2	-2.16	120.48	122.68
8	A	747	5MC	C5-C4-N3	-2.12	119.39	121.67
8	A	2457	PSU	O4'-C1'-C2'	2.12	108.13	105.14
34	a	1498	UR3	C6-N1-C2	-2.09	119.91	121.79
8	A	1915	3TD	O4'-C1'-C2'	2.09	108.09	105.14
8	A	745	1MG	O6-C6-C5	-2.08	120.51	124.19
8	A	2580	PSU	C6-C5-C4	2.08	119.65	118.20
8	A	1911	PSU	C6-N1-C2	-2.07	120.56	122.68
8	A	2605	PSU	C6-C5-C4	2.05	119.63	118.20
34	a	516	PSU	O4'-C1'-C2'	2.05	108.03	105.14
34	a	1402	4OC	CM4-N4-C4	-2.05	118.45	122.45
56	w	39	PSU	O4'-C1'-C2'	2.04	108.03	105.14
8	A	2445	2MG	O6-C6-C5	-2.03	120.41	124.37
56	w	54	5MU	C5M-C5-C6	-2.02	120.16	122.85
34	a	1516	2MG	O6-C6-C5	-2.01	120.44	124.37
56	w	54	5MU	C3'-C2'-C1'	2.01	105.24	101.43
34	a	1402	4OC	C6-C5-C4	2.01	119.42	116.96

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	966	2MG	O4'-C4'-C5'-O5'
34	a	966	2MG	C3'-C4'-C5'-O5'
34	a	1498	UR3	O4'-C1'-N1-C2
55	v	20	H2U	O4'-C4'-C5'-O5'
55	v	20	H2U	O4'-C1'-N1-C6
8	A	746	PSU	C2'-C1'-C5-C4
8	A	746	PSU	C2'-C1'-C5-C6
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C6
8	A	1917	PSU	C3'-C4'-C5'-O5'
8	A	2030	6MZ	O4'-C4'-C5'-O5'
8	A	2030	6MZ	C3'-C4'-C5'-O5'
8	A	2251	OMG	C1'-C2'-O2'-CM2
8	A	2552	OMU	O4'-C1'-N1-C2
8	A	2552	OMU	O4'-C1'-N1-C6
8	A	2552	OMU	C1'-C2'-O2'-CM2
56	w	32	PSU	O4'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C6
56	w	37	MIA	C12-C13-C14-C15
56	w	37	MIA	C12-C13-C14-C16
56	w	39	PSU	C2'-C1'-C5-C4
56	w	39	PSU	O4'-C1'-C5-C4
56	w	39	PSU	O4'-C1'-C5-C6
58	y	101	FME	O1-CN-N-CA
58	y	101	FME	O-C-CA-CB
34	a	1498	UR3	O4'-C1'-N1-C6
55	v	20	H2U	C3'-C4'-C5'-O5'
8	A	1917	PSU	O4'-C4'-C5'-O5'
8	A	1939	5MU	O4'-C4'-C5'-O5'
8	A	2069	G7M	O4'-C4'-C5'-O5'
56	w	37	MIA	O4'-C4'-C5'-O5'
58	y	101	FME	CA-CB-CG-SD
8	A	1835	2MG	O4'-C4'-C5'-O5'
8	A	1835	2MG	C3'-C4'-C5'-O5'
8	A	1939	5MU	C3'-C4'-C5'-O5'
55	v	20	H2U	C2'-C1'-N1-C6
58	y	101	FME	N-CA-CB-CG
55	v	20	H2U	C2'-C1'-N1-C2
8	A	2069	G7M	C3'-C4'-C5'-O5'
8	A	2503	2MA	O4'-C4'-C5'-O5'
58	y	101	FME	CB-CG-SD-CE
55	v	20	H2U	O4'-C1'-N1-C2
55	v	55	PSU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
56	w	46	G7M	C4'-C5'-O5'-P
34	a	1519	MA6	C3'-C4'-C5'-O5'
34	a	527	G7M	C4'-C5'-O5'-P
34	a	1519	MA6	C5-C6-N6-C10
34	a	1402	4OC	O4'-C4'-C5'-O5'
58	y	101	FME	C-CA-CB-CG
34	a	1519	MA6	C4'-C5'-O5'-P
8	A	746	PSU	O4'-C1'-C5-C4
8	A	1917	PSU	O4'-C1'-C5-C4
8	A	747	5MC	C4'-C5'-O5'-P
8	A	746	PSU	O4'-C1'-C5-C6
56	w	32	PSU	O4'-C4'-C5'-O5'
8	A	2498	OMC	C2'-C1'-N1-C2
55	v	20	H2U	C4'-C5'-O5'-P
8	A	2251	OMG	C3'-C4'-C5'-O5'
58	y	101	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 378 ligands modelled in this entry, 373 are monoatomic - leaving 5 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	AM2	a	1648	-	40,40,40	0.54	0	53,60,60	0.93	1 (1%)
64	GDP	x	801	60	24,30,30	1.28	2 (8%)	30,47,47	1.83	10 (33%)
63	AM2	a	1652	-	40,40,40	0.52	0	53,60,60	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
63	AM2	a	1657	-	40,40,40	0.51	0	53,60,60	0.87	2 (3%)
65	PO4	x	802	60	4,4,4	4.81	2 (50%)	6,6,6	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	AM2	a	1652	-	-	2/12/84/84	0/4/4/4
63	AM2	a	1657	-	-	2/12/84/84	0/4/4/4
64	GDP	x	801	60	-	0/12/32/32	0/3/3/3
63	AM2	a	1648	-	-	0/12/84/84	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	x	802	PO4	P-O1	9.16	1.72	1.50
64	x	801	GDP	C6-N1	-3.79	1.32	1.37
64	x	801	GDP	C2'-C1'	-2.54	1.49	1.53
65	x	802	PO4	P-O3	-2.07	1.48	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	x	801	GDP	PA-O3A-PB	-4.50	117.39	132.83
64	x	801	GDP	O3'-C3'-C4'	-4.25	98.75	111.05
63	a	1648	AM2	CA9-NA7-CA7	3.70	119.77	114.38
63	a	1652	AM2	CA9-NA7-CA7	3.60	119.63	114.38
63	a	1657	AM2	CA9-NA7-CA7	3.52	119.51	114.38
64	x	801	GDP	C5-C6-N1	2.92	119.10	113.95
63	a	1657	AM2	CB1-OA8-CA8	-2.71	109.58	114.42
64	x	801	GDP	C5'-C4'-C3'	-2.54	105.66	115.18
64	x	801	GDP	O2A-PA-O1A	2.47	124.43	112.24
64	x	801	GDP	O3A-PB-O1B	-2.43	97.68	111.19
63	a	1652	AM2	CA1-OA4-CA5	2.43	116.98	113.06
64	x	801	GDP	O3B-PB-O2B	2.33	116.55	107.64
64	x	801	GDP	C8-N7-C5	2.25	107.28	102.99
64	x	801	GDP	O3'-C3'-C2'	-2.20	104.71	111.82
64	x	801	GDP	O6-C6-C5	-2.03	120.41	124.37
63	a	1652	AM2	OA4-CA5-CA4	2.03	111.95	108.88

There are no chirality outliers.

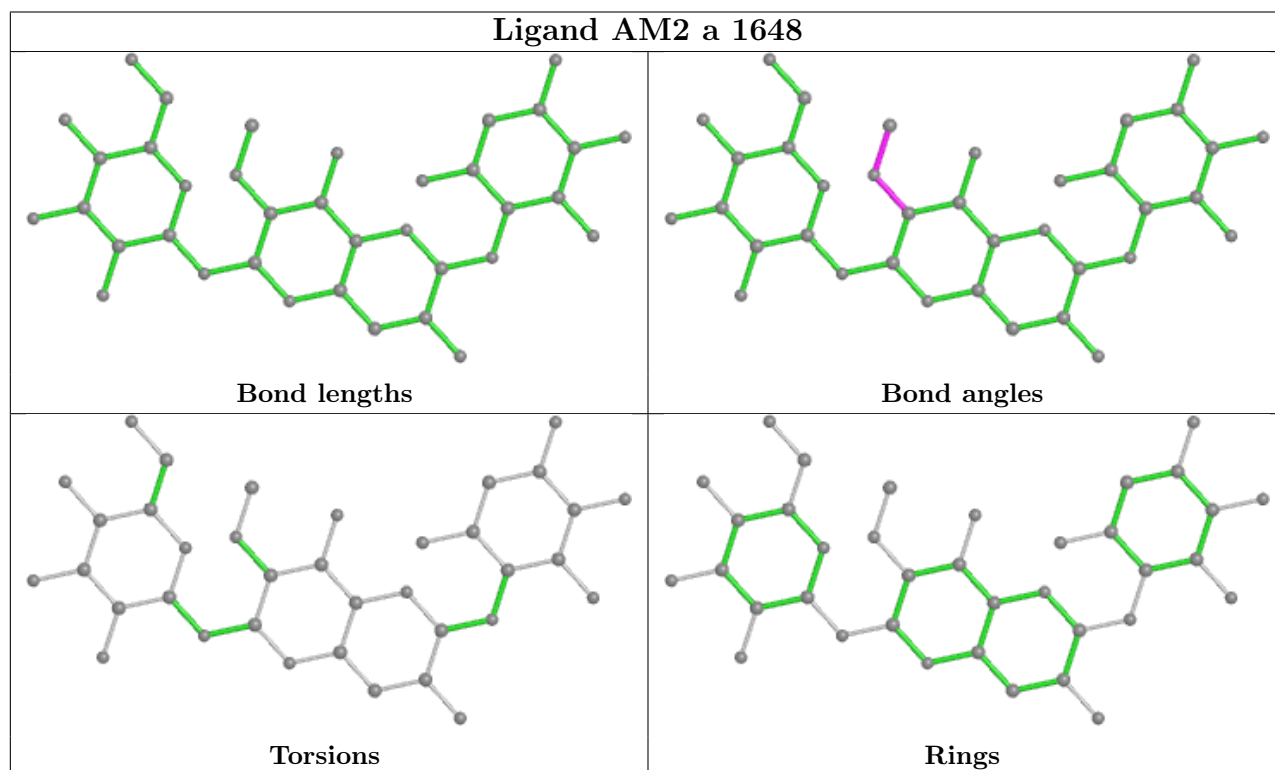
All (4) torsion outliers are listed below:

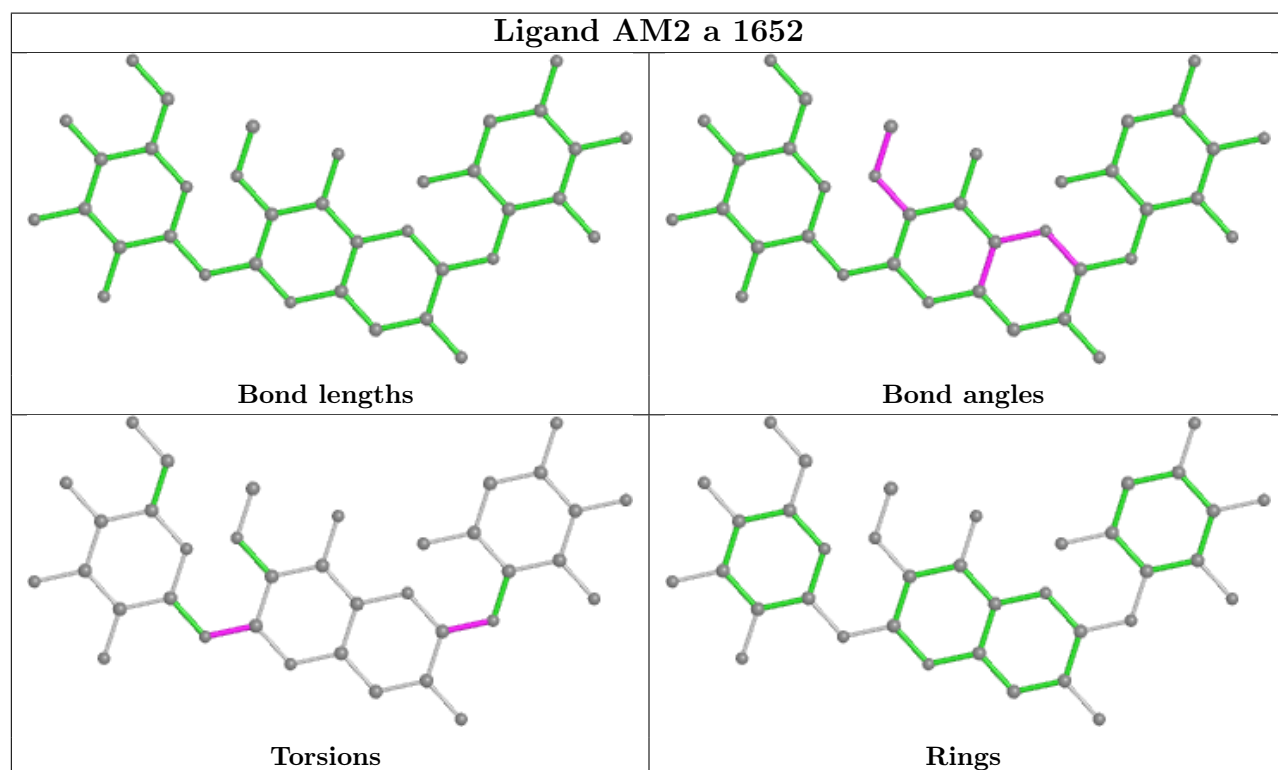
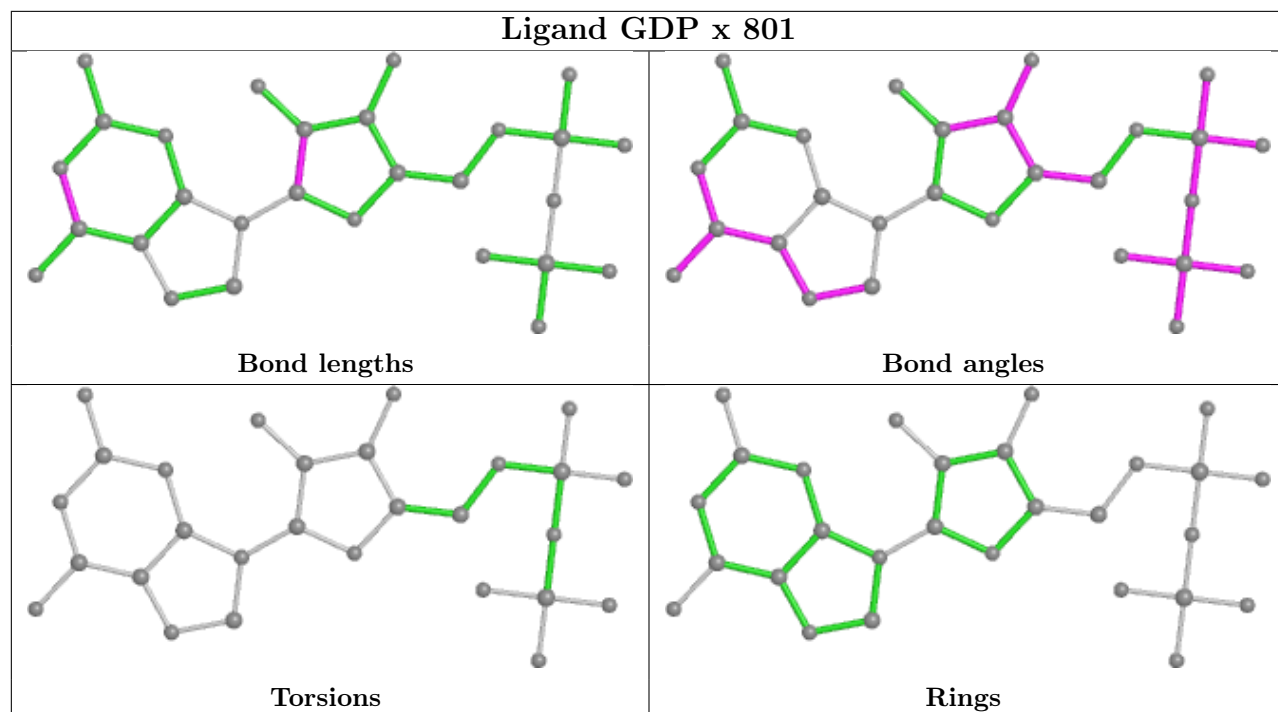
Mol	Chain	Res	Type	Atoms
63	a	1652	AM2	OA5-CA8-OA8-CB1
63	a	1657	AM2	CA6-CA7-NA7-CA9
63	a	1657	AM2	OB1-CB5-CB6-OB6
63	a	1652	AM2	OA4-CA1-OA1-CC1

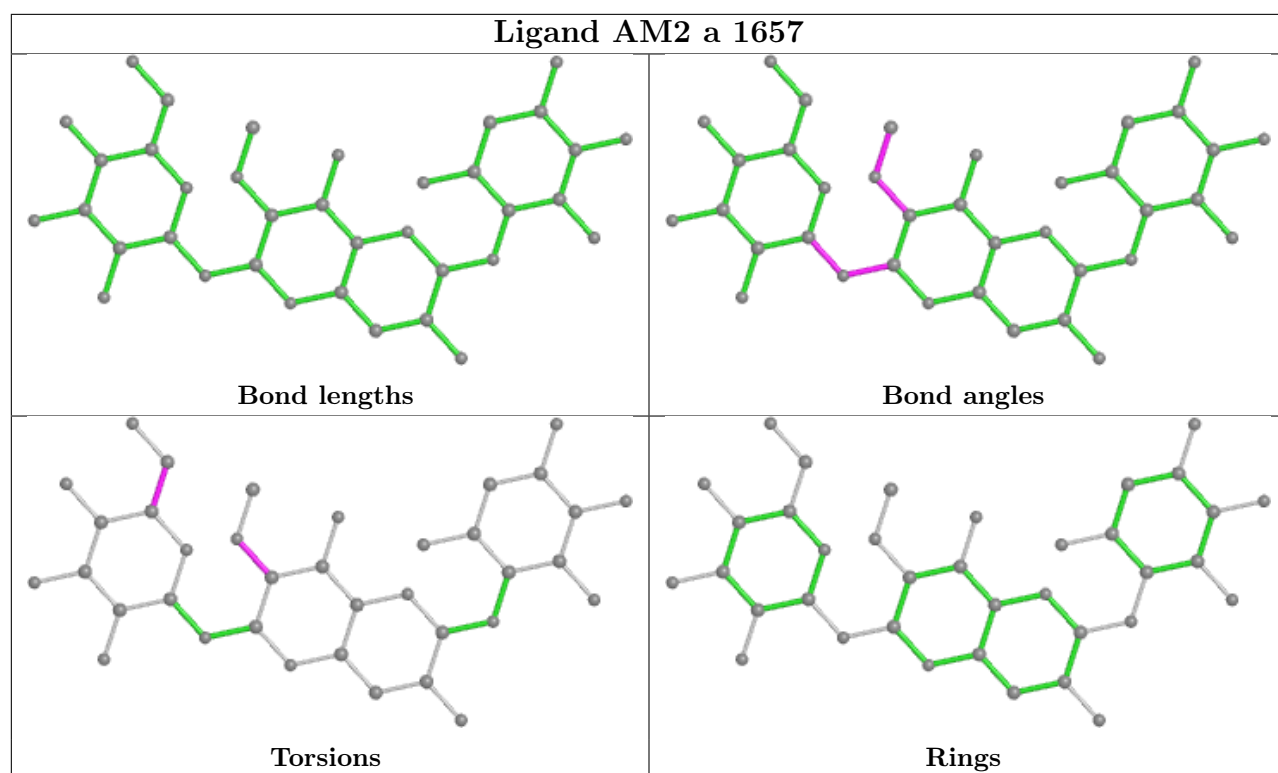
There are no ring outliers.

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.

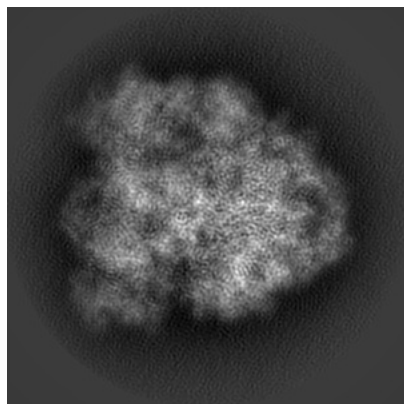
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13461. These allow visual inspection of the internal detail of the map and identification of artifacts.

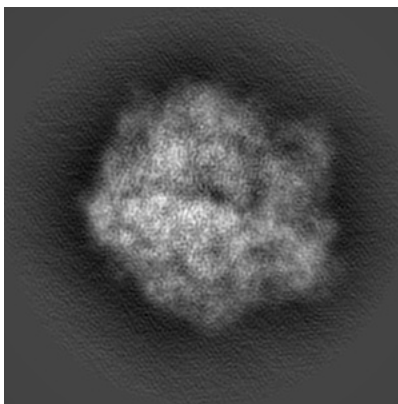
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

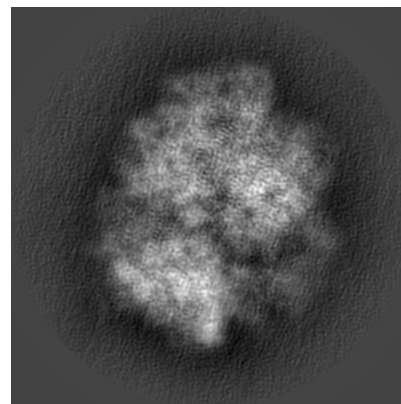
#### 6.1.1 Primary map



X

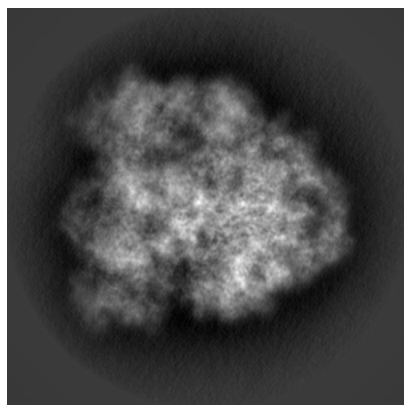


Y

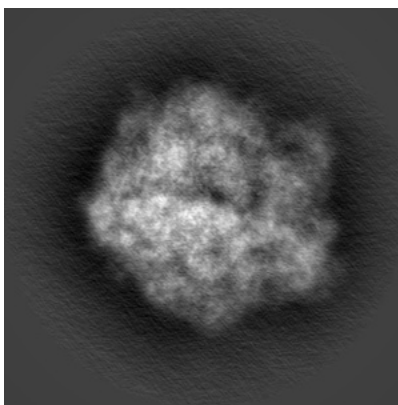


Z

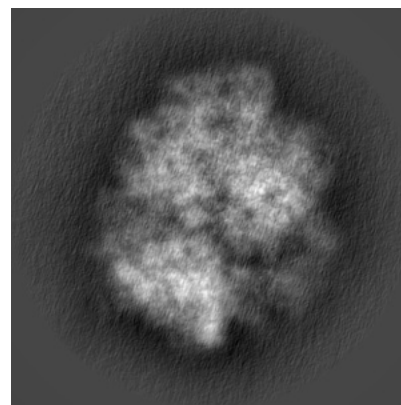
#### 6.1.2 Raw map



X



Y



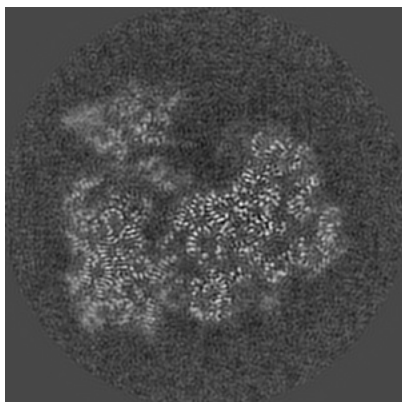
Z

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

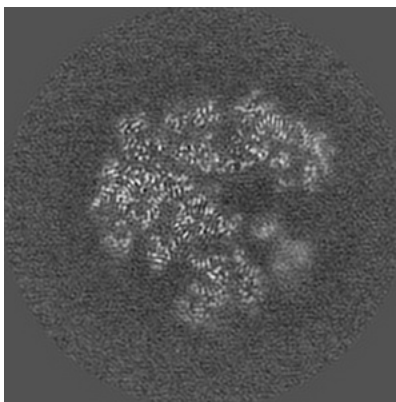


## 6.2 Central slices [i](#)

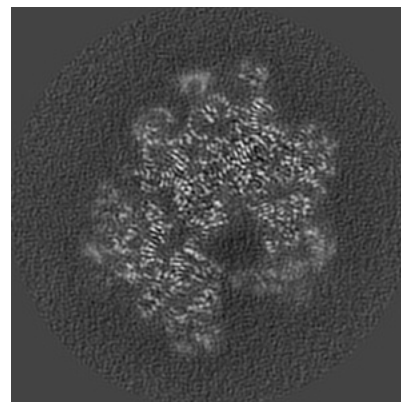
### 6.2.1 Primary map



X Index: 256

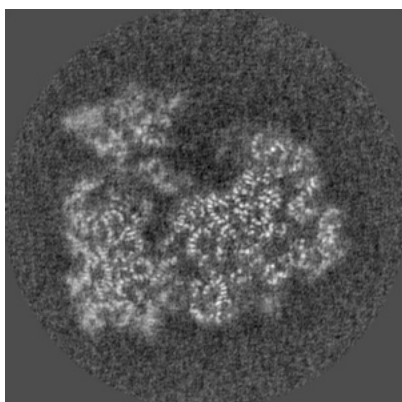


Y Index: 256

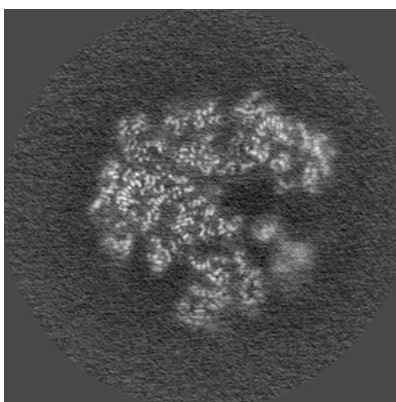


Z Index: 256

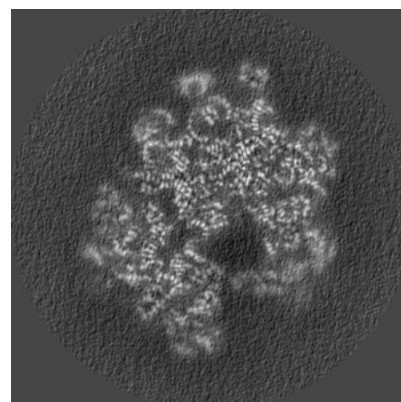
### 6.2.2 Raw map



X Index: 144



Y Index: 144

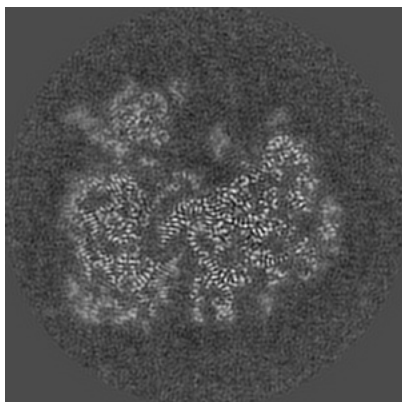


Z Index: 144

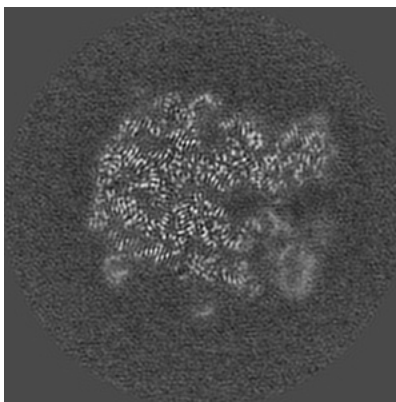
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

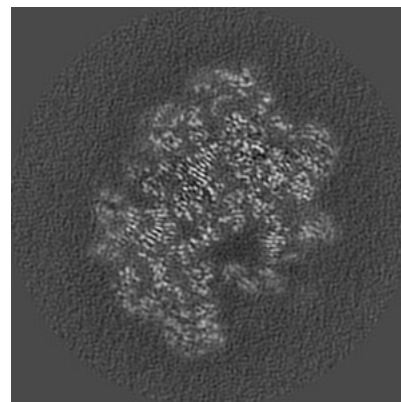
### 6.3.1 Primary map



X Index: 248

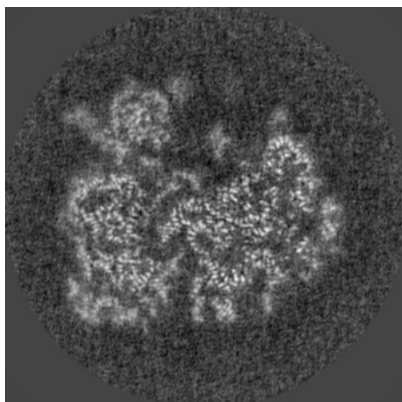


Y Index: 280

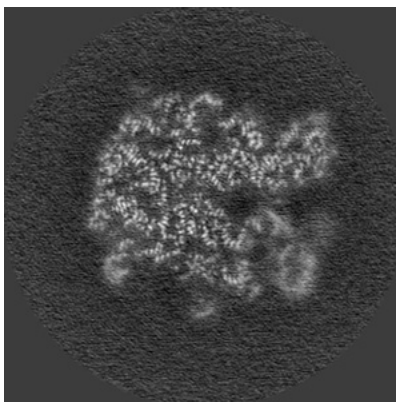


Z Index: 239

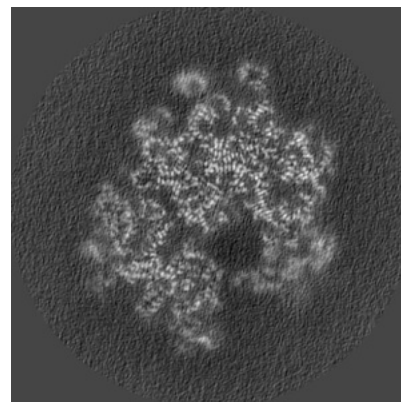
### 6.3.2 Raw map



X Index: 139



Y Index: 157

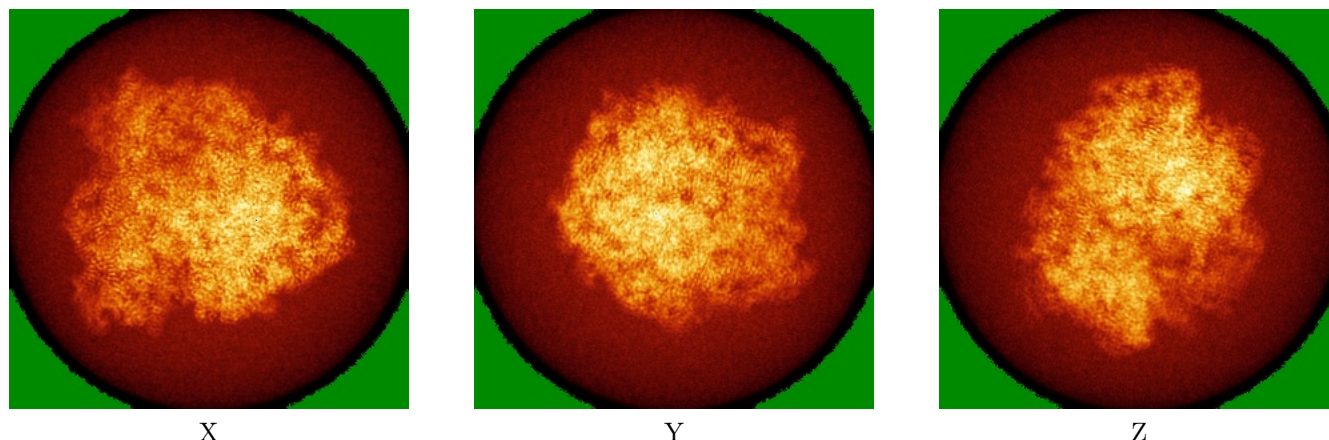


Z Index: 146

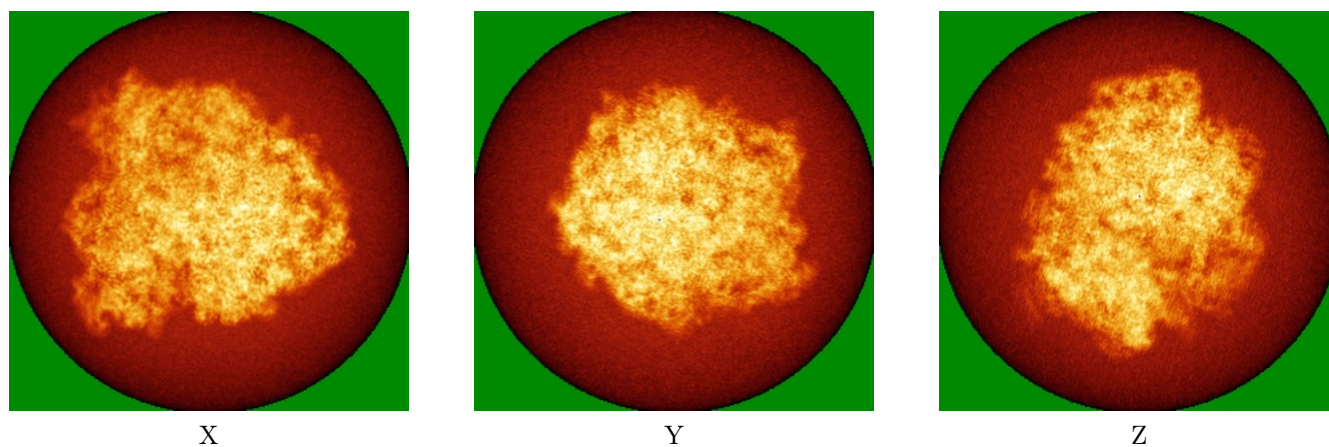
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



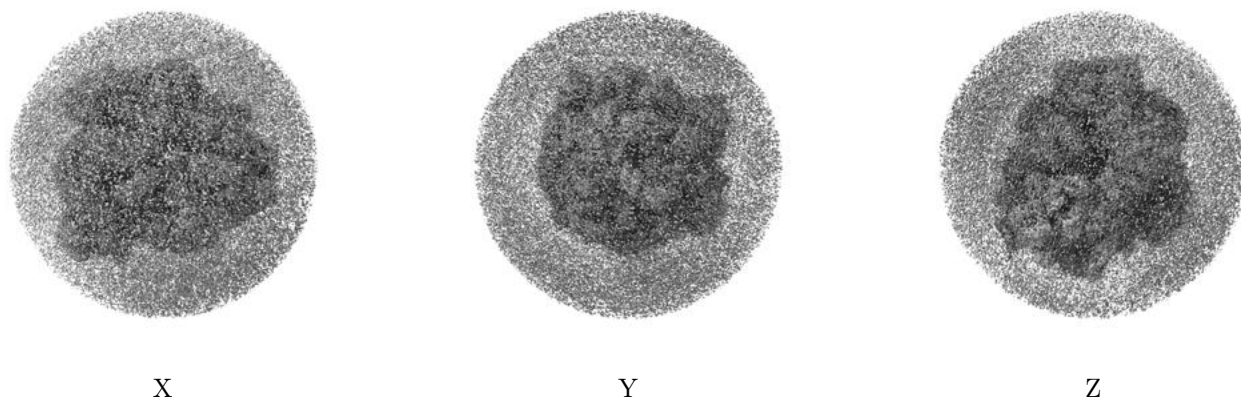
### 6.4.2 Raw map



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

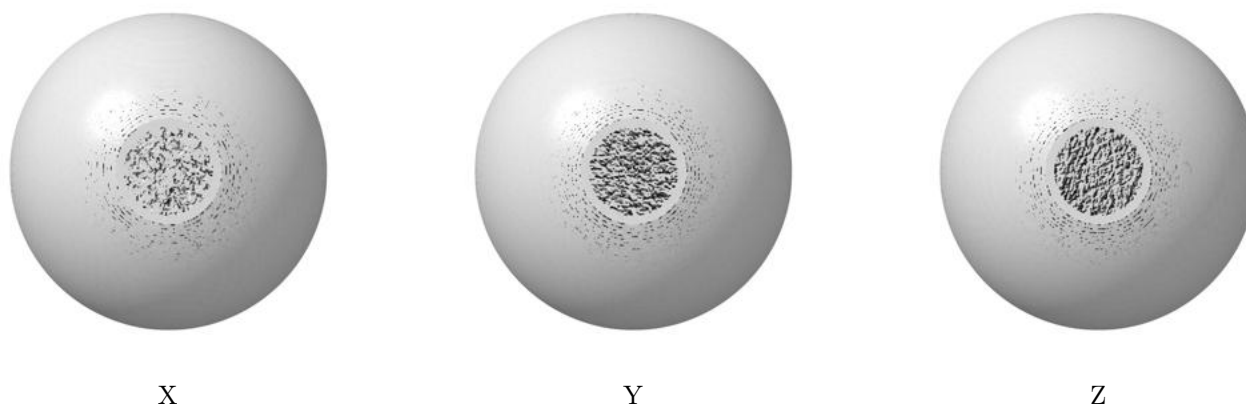
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. 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.

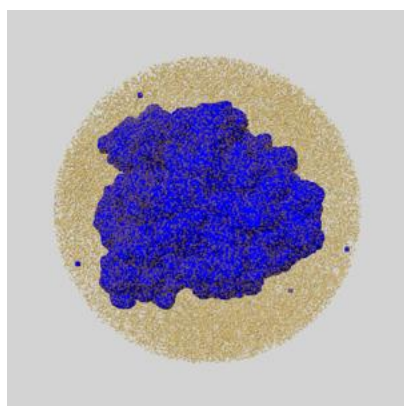
## 6.6 Mask visualisation [i](#)

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

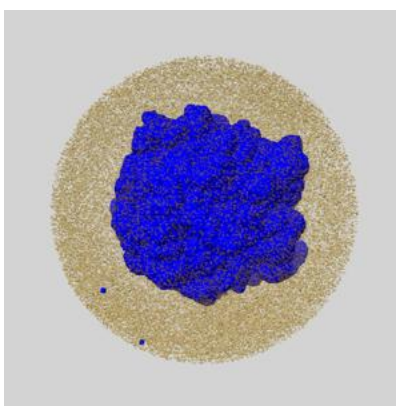
A mask typically either:

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

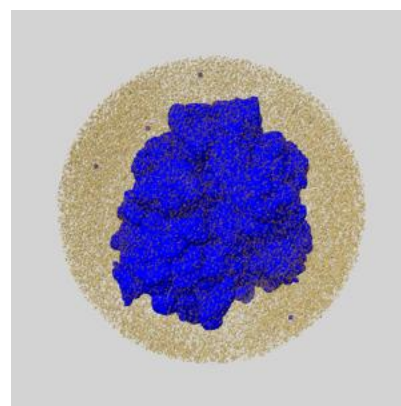
### 6.6.1 emd\_13461\_msk\_1.map [i](#)



X



Y

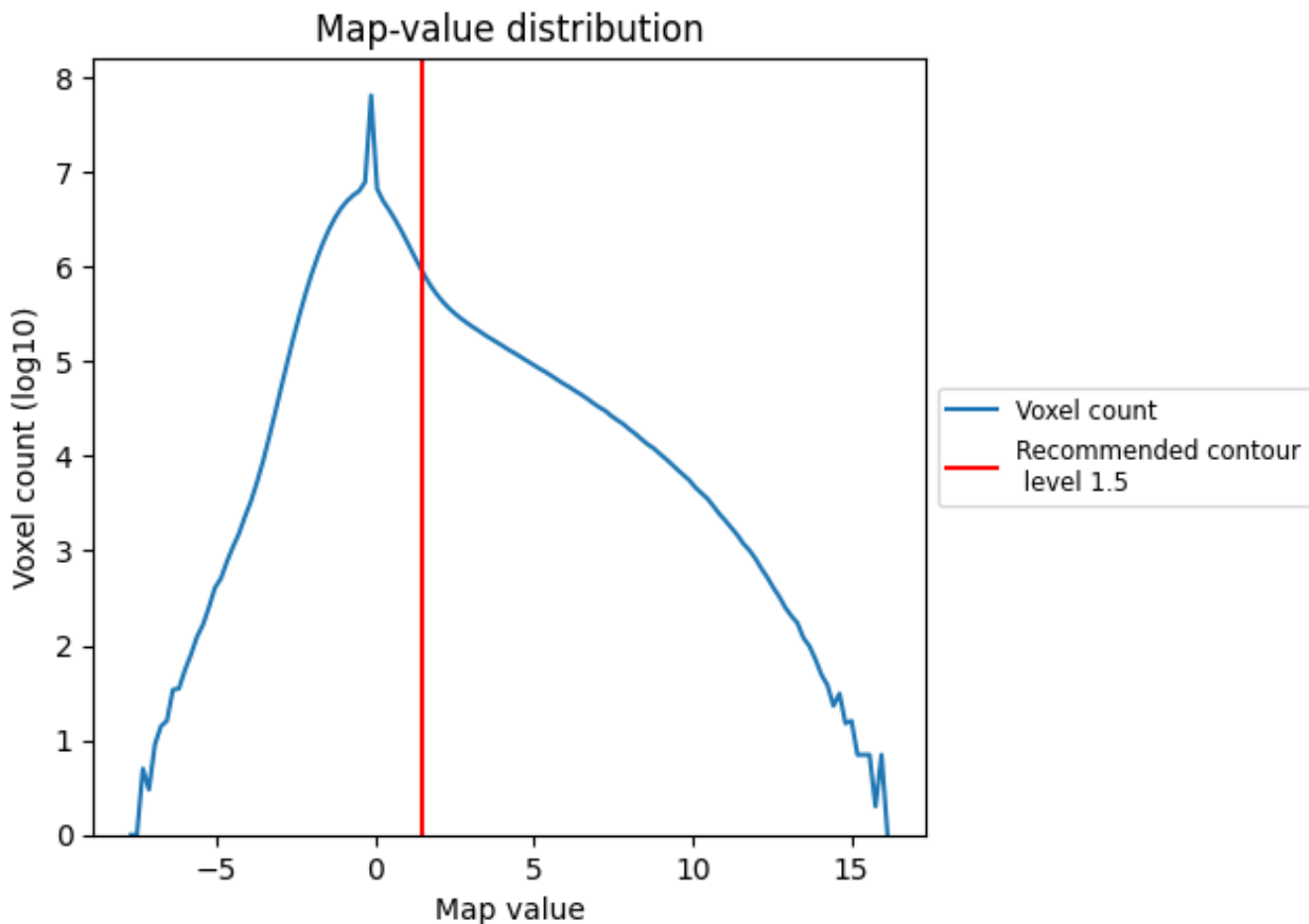


Z

## 7 Map analysis [i](#)

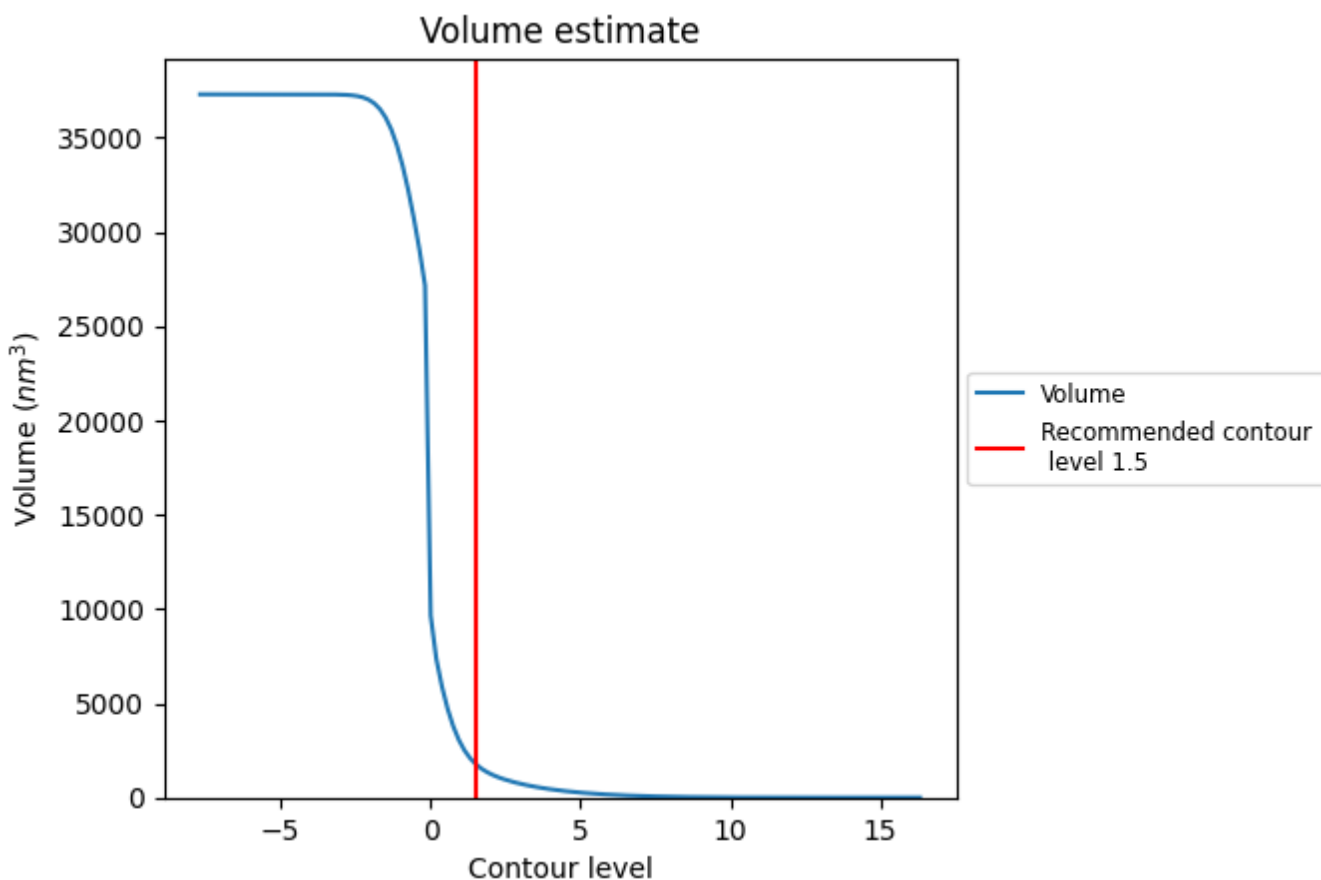
This section contains the results of statistical analysis of the map.

### 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.

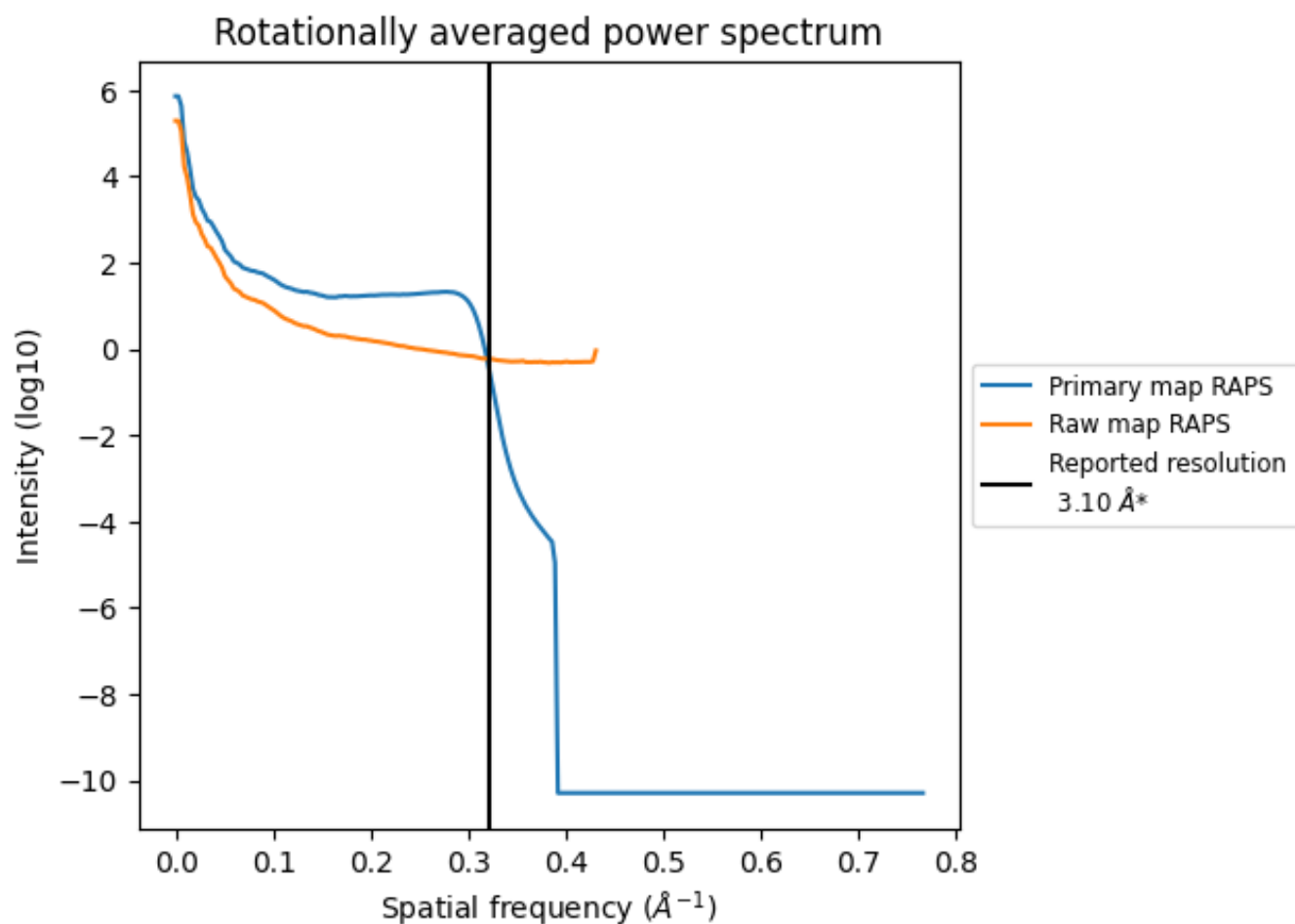
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1787  $\text{nm}^3$ ; this corresponds to an approximate mass of 1614 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



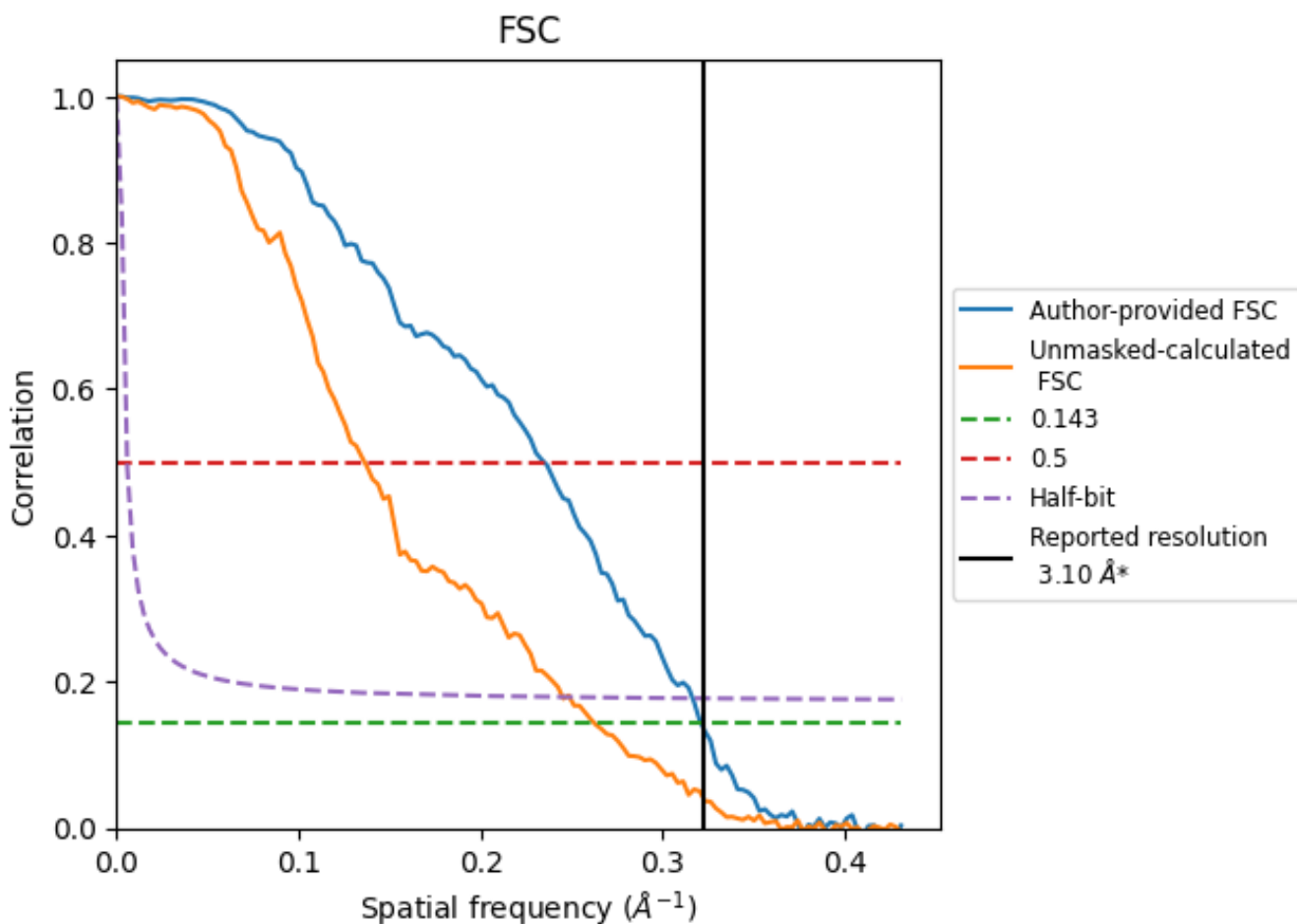
\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

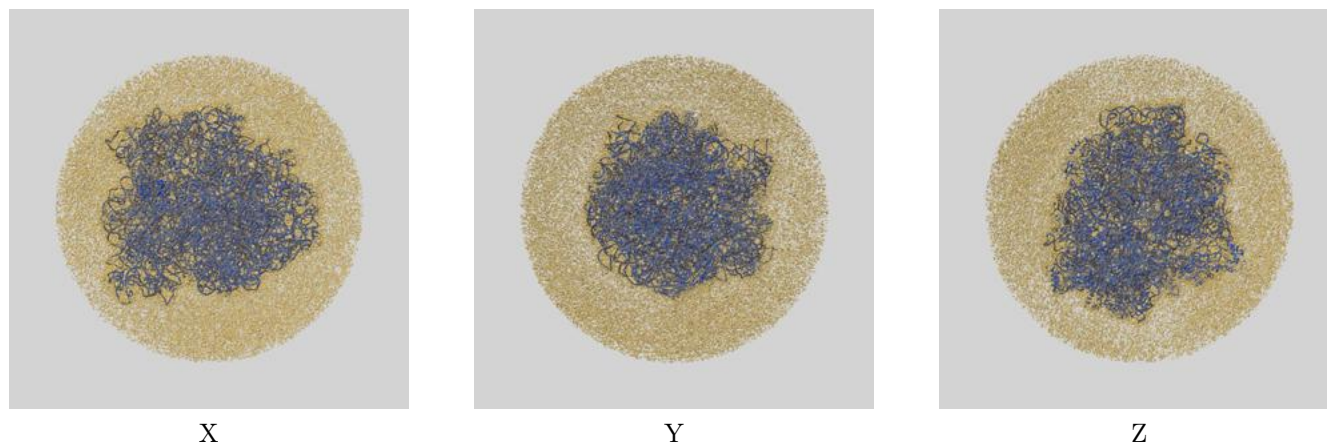
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	4.26	3.16
Unmasked-calculated*	3.81	7.34	4.08

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.81 differs from the reported value 3.1 by more than 10 %

## 9 Map-model fit [i](#)

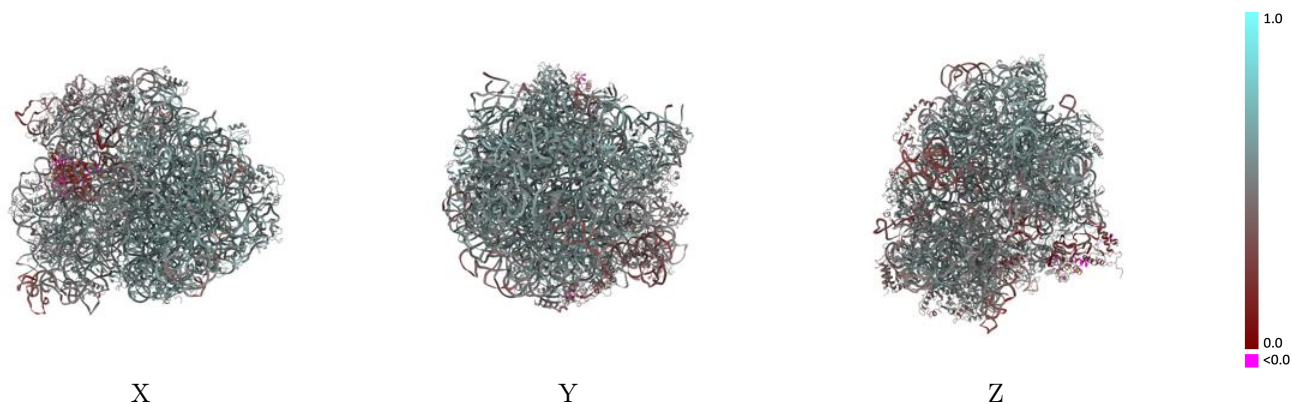
This section contains information regarding the fit between EMDB map EMD-13461 and PDB model 7PJV. Per-residue inclusion information can be found in section 3 on page 18.

### 9.1 Map-model overlay [i](#)



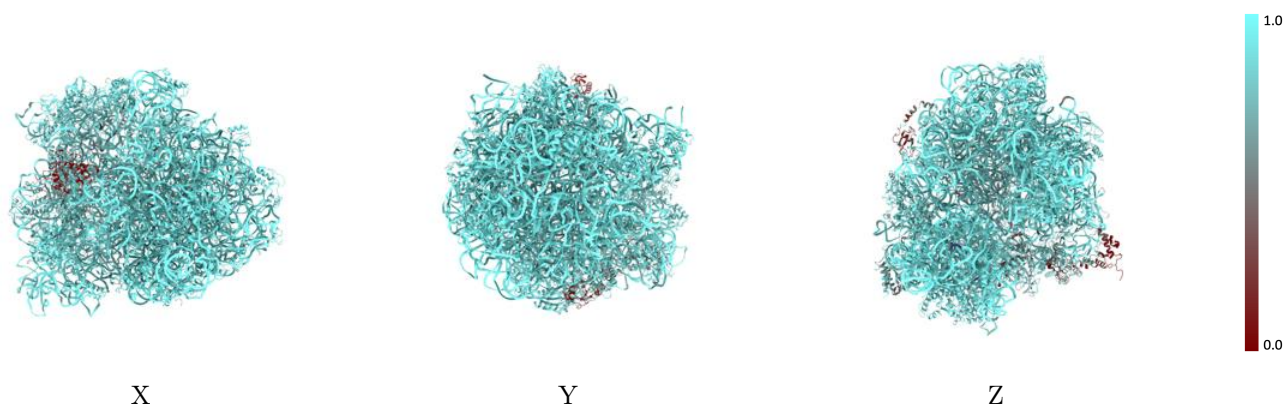
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



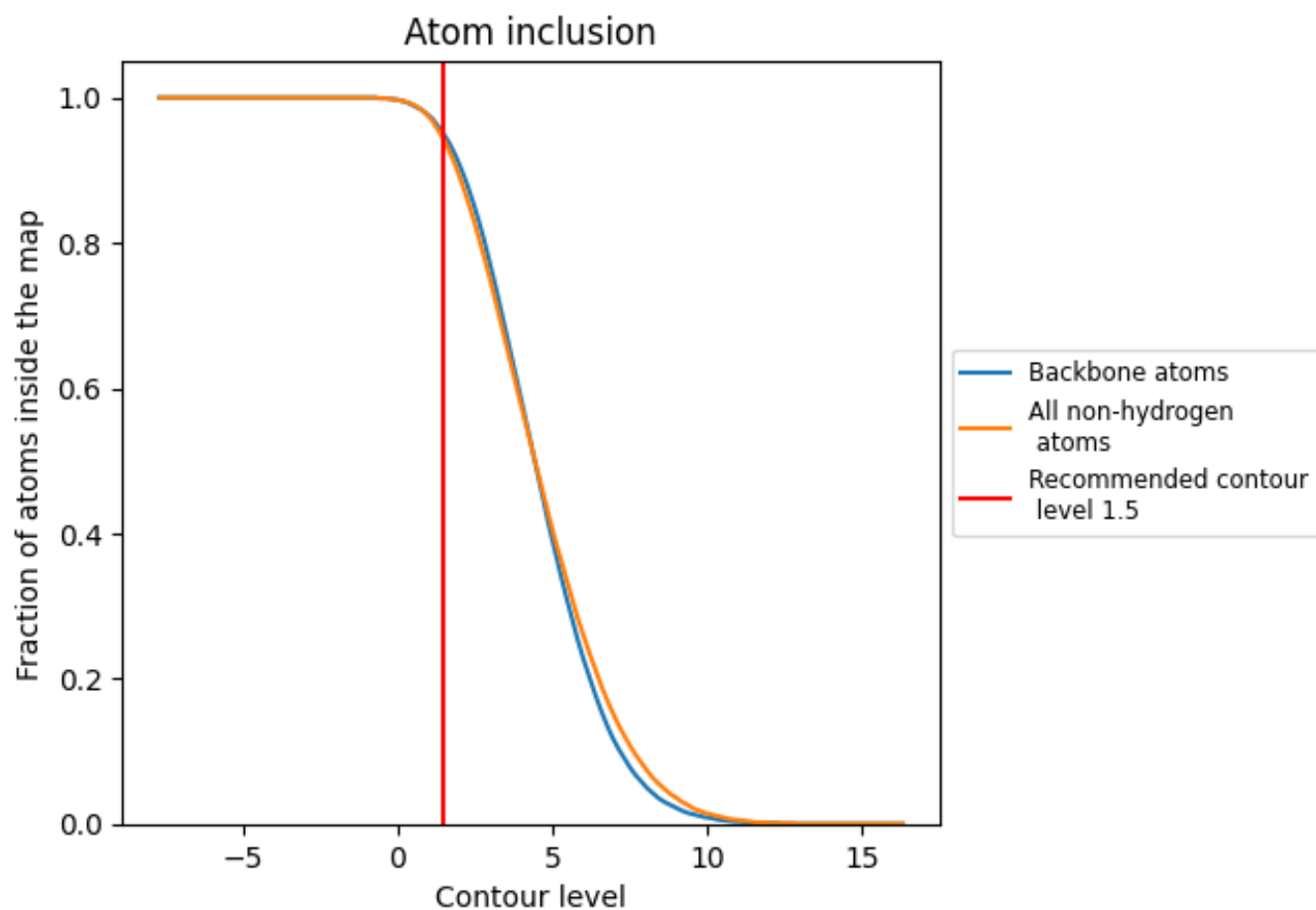
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9420	 0.5140
0	 0.9440	 0.5580
1	 0.9080	 0.5550
2	 0.9490	 0.5850
3	 0.9630	 0.5910
4	 0.9590	 0.5540
5	 0.3090	 0.2560
6	 0.8630	 0.4130
A	 0.9770	 0.5320
B	 0.9810	 0.5230
C	 0.9350	 0.5620
D	 0.9440	 0.5640
E	 0.9370	 0.5430
F	 0.8910	 0.4740
G	 0.8980	 0.4980
H	 0.4570	 0.3710
I	 0.4560	 0.2230
J	 0.9580	 0.5680
K	 0.9100	 0.5550
L	 0.9400	 0.5510
M	 0.9420	 0.5600
N	 0.9570	 0.5630
O	 0.9540	 0.5240
P	 0.9100	 0.5560
Q	 0.9740	 0.5680
R	 0.9250	 0.5330
S	 0.9340	 0.5610
T	 0.9420	 0.5310
U	 0.9320	 0.5130
V	 0.9390	 0.5300
W	 0.9610	 0.5760
X	 0.9280	 0.5560
Y	 0.9210	 0.5020
Z	 0.9380	 0.5690
a	 0.9760	 0.5070



*Continued on next page...*

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Chain	Atom inclusion	Q-score
b	 0.7380	 0.4420
c	 0.9120	 0.5020
d	 0.9010	 0.4830
e	 0.9390	 0.5380
f	 0.8840	 0.4600
g	 0.7770	 0.4170
h	 0.9270	 0.5350
i	 0.9220	 0.4800
j	 0.8760	 0.4390
k	 0.9090	 0.5120
l	 0.9010	 0.5370
m	 0.9080	 0.4610
n	 0.9400	 0.4970
o	 0.9350	 0.5170
p	 0.9200	 0.5160
q	 0.9220	 0.5160
r	 0.9100	 0.5110
s	 0.8880	 0.4540
t	 0.9310	 0.5060
u	 0.8330	 0.4820
v	 0.9340	 0.4530
w	 0.8620	 0.4000
x	 0.8090	 0.4470
y	 0.8090	 0.5250
z	 0.9350	 0.5320