



## Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 09:58 AM EST

PDB ID : 7K54  
EMDB ID : EMD-22673  
Title : Mid-translocated +1-frameshifting(CCC-A) complex with EF-G and GDPCP (Structure II-FS)  
Authors : Demo, G.; Loveland, A.B.; Svidritskiy, E.; Gamper, H.B.; Hou, Y.M.; Korostelev, A.A.  
Deposited on : 2020-09-16  
Resolution : 3.20 Å (reported)  
Based on initial models : 4V9P, 6ENJ, 5UYM, 4V7D

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:

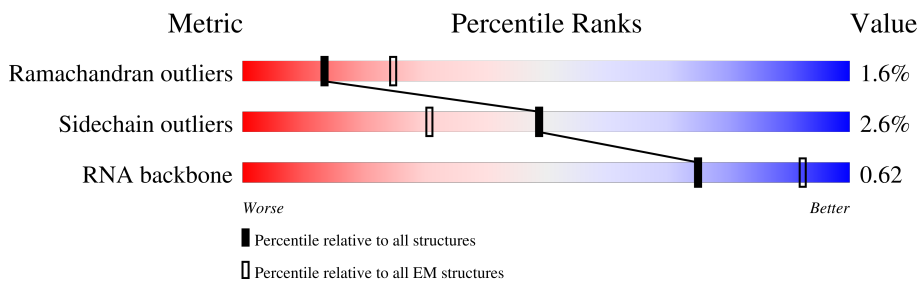
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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.



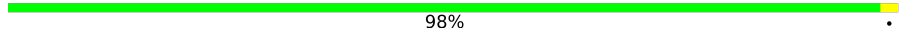
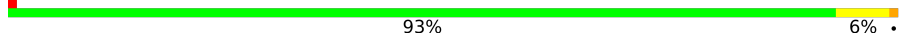
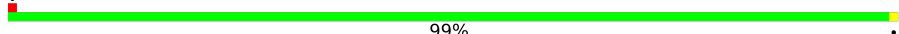
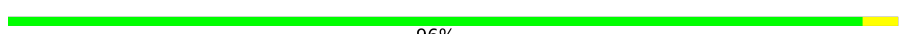


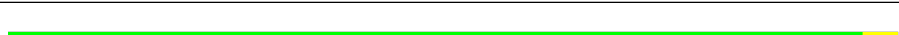
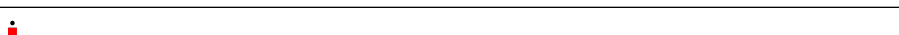
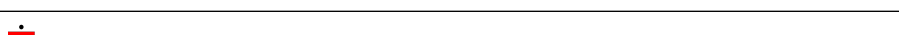
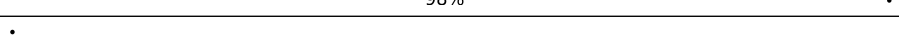
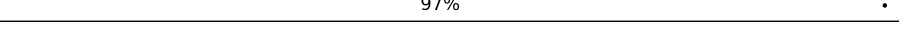
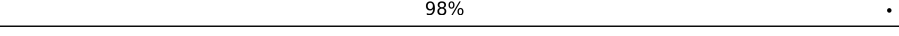
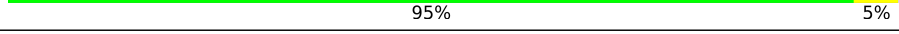
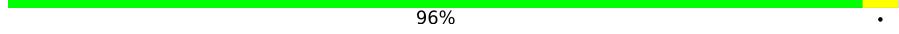
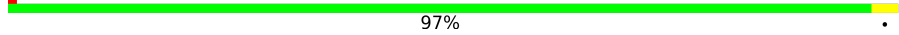
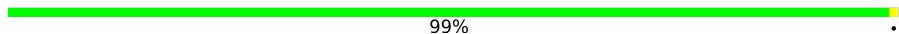

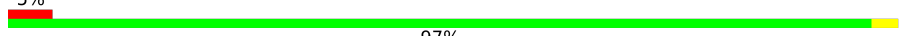






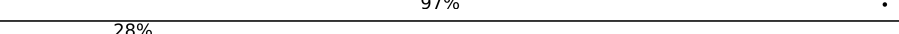
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	b	271	97%
2	c	209	98%
3	d	201	5%
4	e	177	96%
5	f	176	98%
6	g	149	58%
7	h	131	59%
8	i	141	47%

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Mol	Chain	Length	Quality of chain
9	j	142	 98%
10	k	122	 93% 6%
11	l	143	 99%
12	m	136	 96%
13	n	120	 97%
14	o	116	 95% 5%
15	p	114	 96%
16	q	117	 100%
17	r	103	 98%
18	s	110	 97%
19	t	93	 98%
20	u	102	 95% 5%
21	v	94	 96%
22	w	75	 97%
23	x	77	 99%
24	y	63	 89% 11% 6%
25	z	58	 97% 5%
26	A	66	 89% 11% 29%
27	B	56	 100%
28	C	50	 98% 6%
29	D	46	 98%
30	E	64	 89% 11%
31	F	38	 97%
32	G	225	 92% 5% 28%
33	H	206	 94% 6% 12%

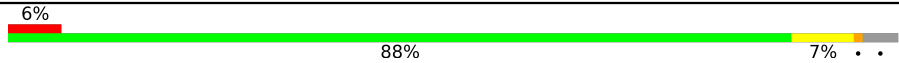
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Mol	Chain	Length	Quality of chain
34	I	205	5% 94% 6%
35	J	157	90% 9%
36	K	100	89% 10%
37	L	151	38% 95% 5%
38	M	129	98%
39	N	127	17% 87% 13%
40	O	98	31% 84% 11% 5%
41	P	116	91% 9%
42	Q	123	94% 6%
43	R	114	27% 85% 15%
44	S	100	6% 90% 10%
45	T	88	95% 5%
46	U	82	7% 98%
47	V	80	98%
48	W	65	8% 89% 11%
49	X	79	97%
50	Y	85	96%
51	Z	65	94% 6%
52	a	223	48% 50% 9% 40%
53	3	1539	84% 15%
54	1	2903	86% 14%
55	2	120	87% 12%
56	5	77	78% 21%
57	6	77	70% 30%
58	4	16	75% 25%

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Mol	Chain	Length	Quality of chain
59	8	711	 6% 88% 7% . .

## 2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 153368 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 L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	b	271	2083	1288	423	365	7	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	e	177	1411	899	249	257	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	g	125	936	590	166	179	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	h	84	633	397	114	118	4	0	0

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	i	74	551	358	91	99	3	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	k	122	939	587	180	166	6	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	n	120	961	593	196	167	5	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	t	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	u	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 21 is a protein called 50S ribosomal protein L25.



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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	C	50	Total	C	N	O	0	0
			410	263	75	72		

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

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

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

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

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

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

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	J	157	1157	719	218	214	6	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	K	100	818	515	148	149	6	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	L	151	1182	735	227	216	4	0	0

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	O	98	787	493	150	143	1	0	0

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	P	116	870	535	173	159	3	0	0

- Molecule 42 is a protein called 30S ribosomal protein S12.

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

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	R	114	884	546	178	157	3	0	0

- Molecule 44 is a protein called 30S ribosomal protein S14.

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

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	V	80	649	411	121	114	3	0	0

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	W	65	536	339	100	96	1	0	0

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	X	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

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

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	2	120	2568	1145	471	833	119	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 56 is a RNA chain called tRNAPro.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	5	77	1647	733	295	542	77	0	0

- Molecule 57 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	6	77	1640	732	297	535	76	0	0

- Molecule 58 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
58	4	16	346	155	68	107	16	0	0

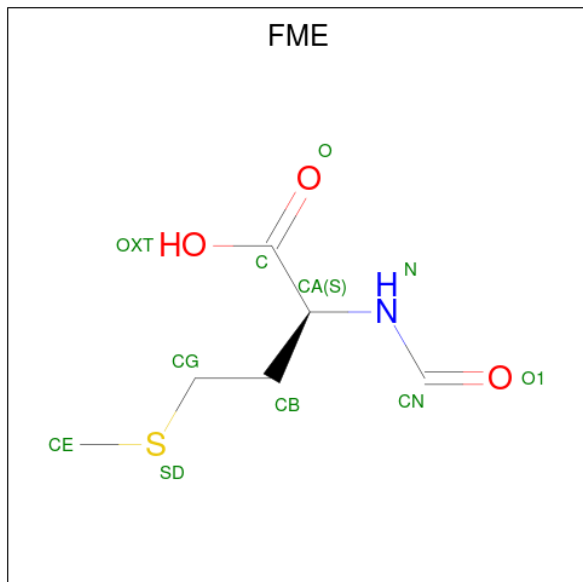
- Molecule 59 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	8	685	5312	3351	911	1025	25	0	0

There are 8 discrepancies between the modelled and reference sequences:

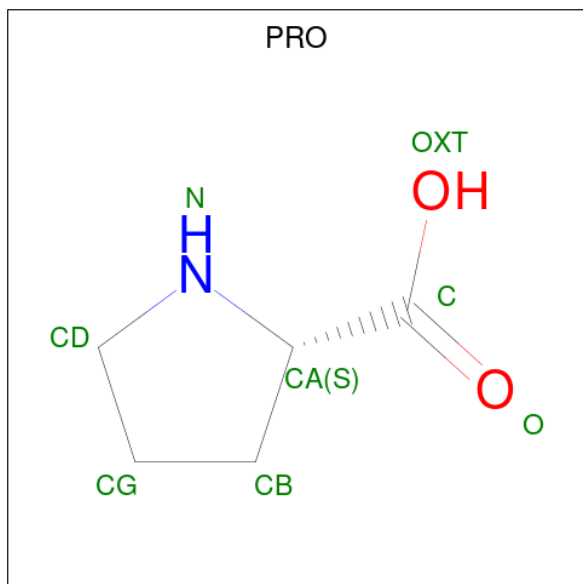
Chain	Residue	Modelled	Actual	Comment	Reference
8	705	LEU	-	expression tag	UNP U9XYS4
8	706	GLU	-	expression tag	UNP U9XYS4
8	707	HIS	-	expression tag	UNP U9XYS4
8	708	HIS	-	expression tag	UNP U9XYS4
8	709	HIS	-	expression tag	UNP U9XYS4
8	710	HIS	-	expression tag	UNP U9XYS4
8	711	HIS	-	expression tag	UNP U9XYS4
8	712	HIS	-	expression tag	UNP U9XYS4

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



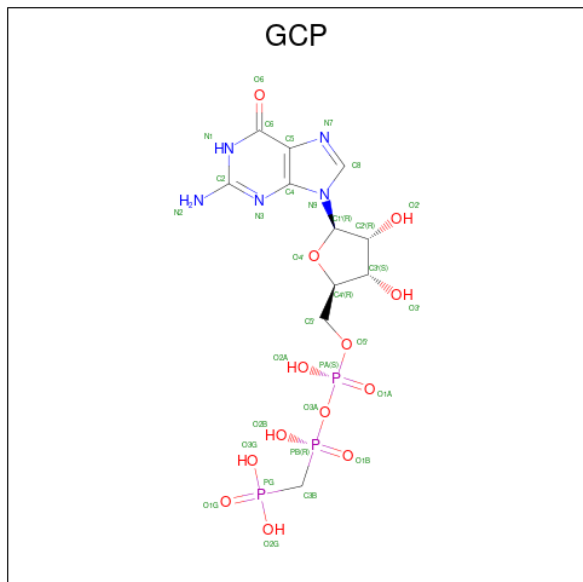
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	1	1	10	6	1	2	1	0

- Molecule 61 is PROLINE (three-letter code: PRO) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
61	5	1	7	5	1	1	0

- Molecule 62 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
62	8	1	32	11	5	13	3	0

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

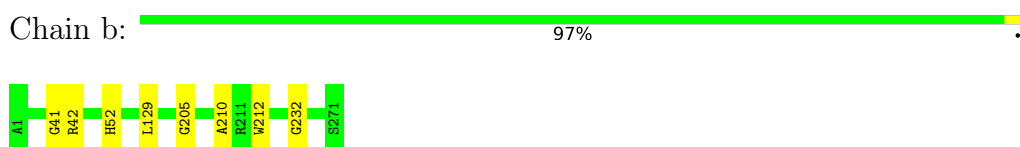
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
63	8	1	1	1	0



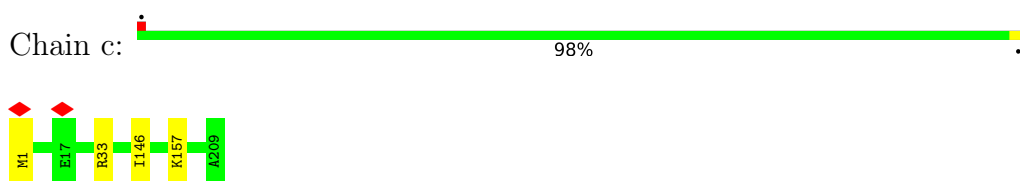
### 3 Residue-property plots [i](#)

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.

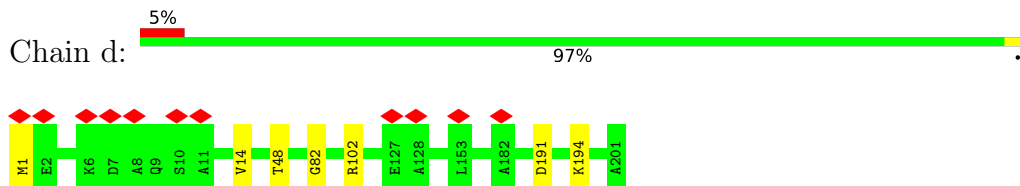
- Molecule 1: 50S ribosomal protein L2



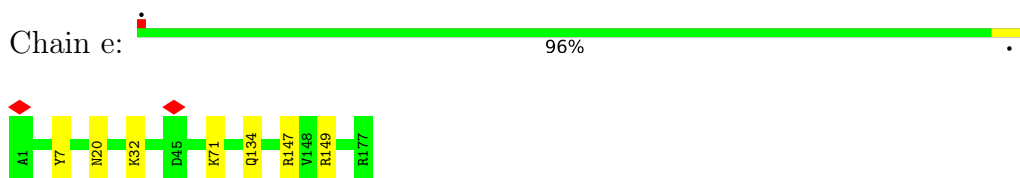
- Molecule 2: 50S ribosomal protein L3



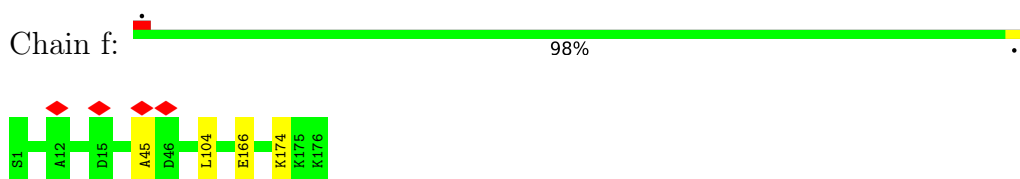
- Molecule 3: 50S ribosomal protein L4



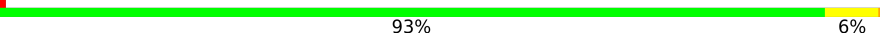
- Molecule 4: 50S ribosomal protein L5

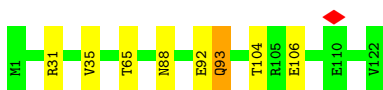


- Molecule 5: 50S ribosomal protein L6



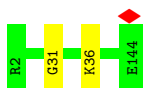


Chain k:  93% 6%



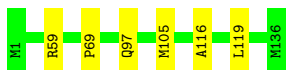
- Molecule 11: 50S ribosomal protein L15

Chain l:  99%



- Molecule 12: 50S ribosomal protein L16

Chain m:  96%



- Molecule 13: 50S ribosomal protein L17

Chain n:  97%



- Molecule 14: 50S ribosomal protein L18

Chain o:  95% 5%



- Molecule 15: 50S ribosomal protein L19

Chain p:  96%



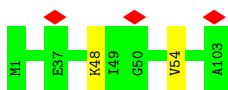
- Molecule 16: 50S ribosomal protein L20

Chain q:  100%



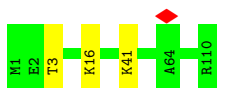
- Molecule 17: 50S ribosomal protein L21

Chain r:  98%



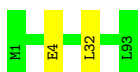
- Molecule 18: 50S ribosomal protein L22

Chain s:  97%



- Molecule 19: 50S ribosomal protein L23

Chain t:  98%



- Molecule 20: 50S ribosomal protein L24

Chain u:  95% 5%



- Molecule 21: 50S ribosomal protein L25

Chain v:  96%



- Molecule 22: 50S ribosomal protein L27

Chain w:  97%

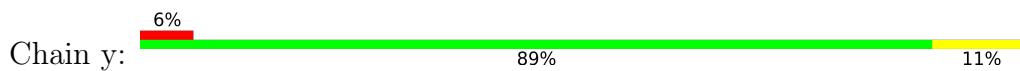


- Molecule 23: 50S ribosomal protein L28

Chain x:  99%



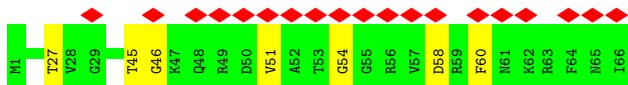
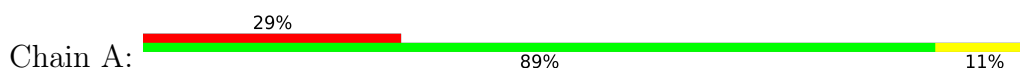
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



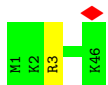
- Molecule 27: 50S ribosomal protein L32



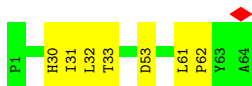
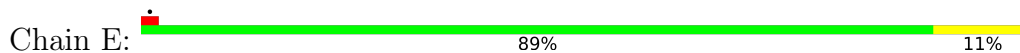
- Molecule 28: 50S ribosomal protein L33



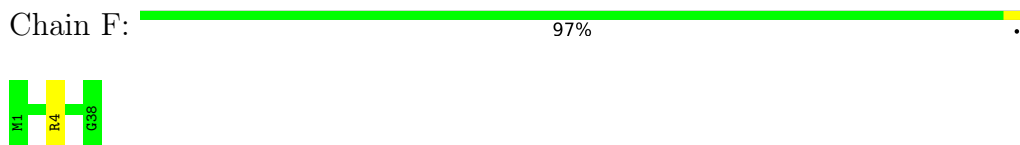
- Molecule 29: 50S ribosomal protein L34



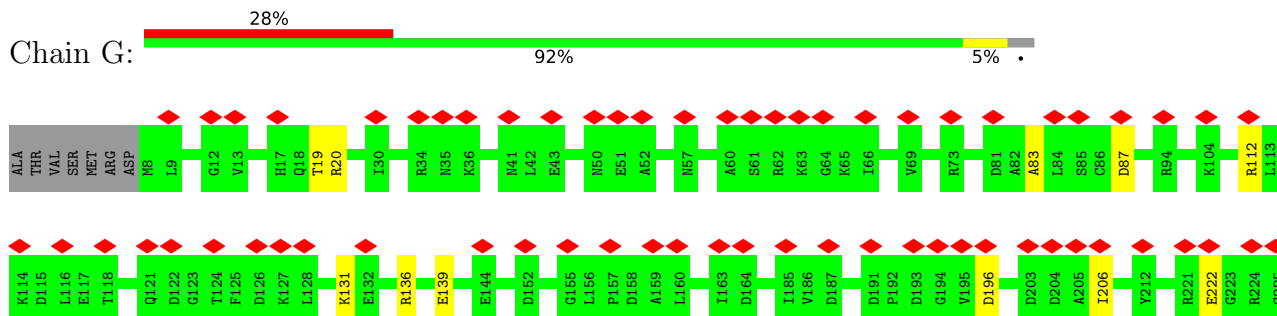
- Molecule 30: 50S ribosomal protein L35



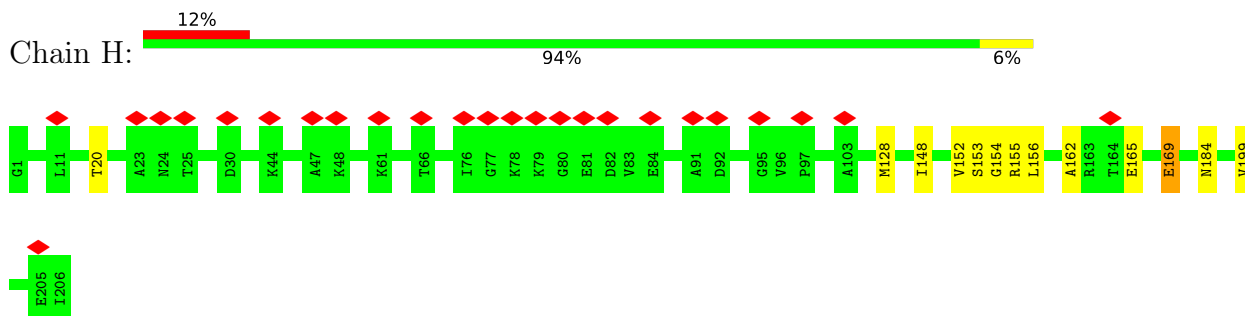
- Molecule 31: 50S ribosomal protein L36



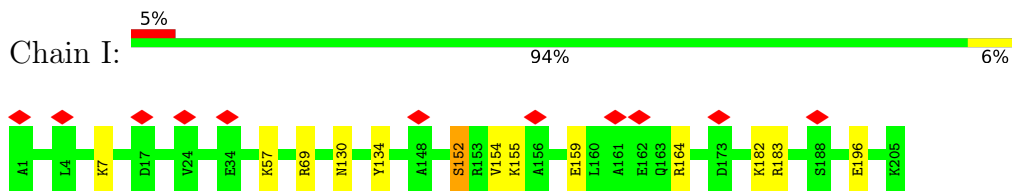
- Molecule 32: 30S ribosomal protein S2



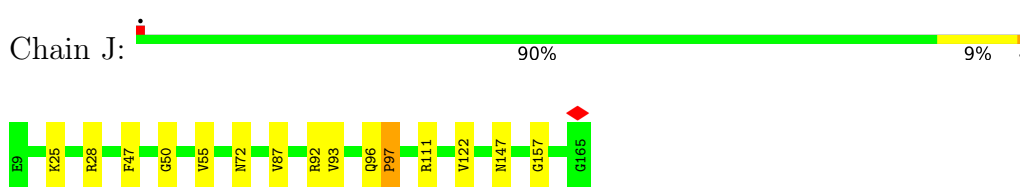
- Molecule 33: 30S ribosomal protein S3



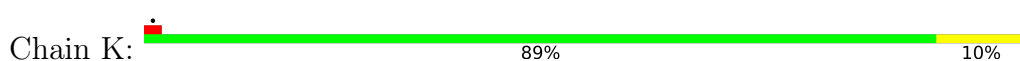
- Molecule 34: 30S ribosomal protein S4

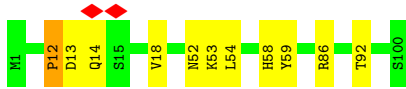


- Molecule 35: 30S ribosomal protein S5

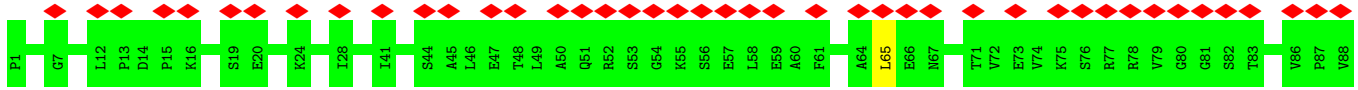


- Molecule 36: 30S ribosomal protein S6

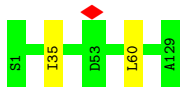




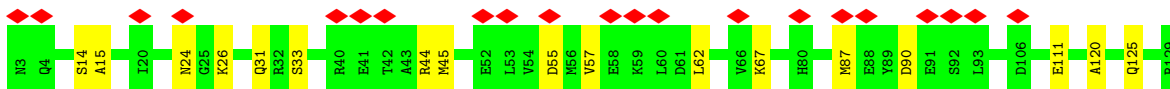
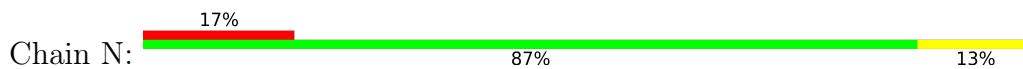
- Molecule 37: 30S ribosomal protein S7



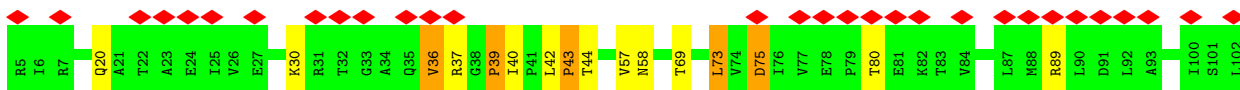
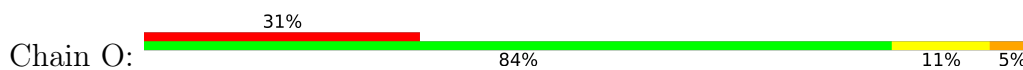
- Molecule 38: 30S ribosomal protein S8



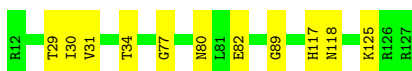
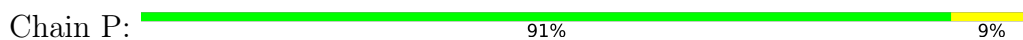
- Molecule 39: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S10

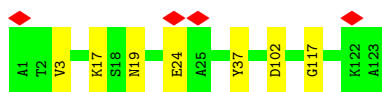


- Molecule 41: 30S ribosomal protein S11

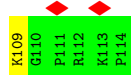
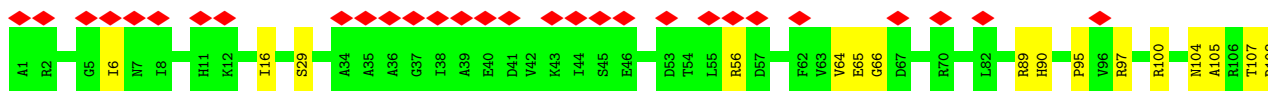
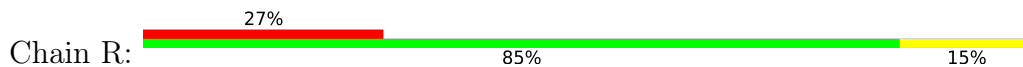


- Molecule 42: 30S ribosomal protein S12

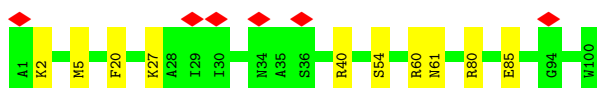
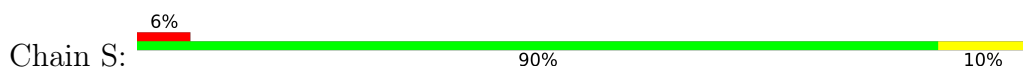




- Molecule 43: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S14



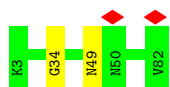
- Molecule 45: 30S ribosomal protein S15



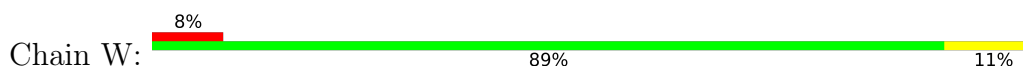
- Molecule 46: 30S ribosomal protein S16



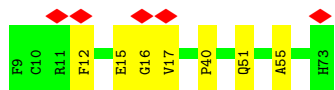
- Molecule 47: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S18







• Molecule 49: 30S ribosomal protein S19



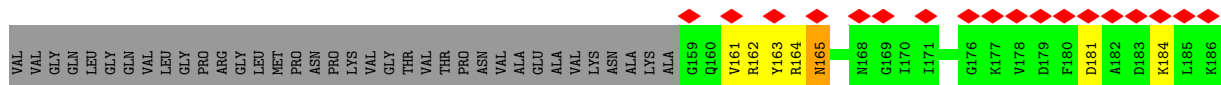
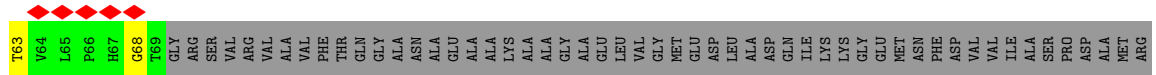
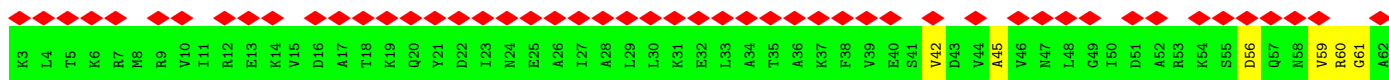
• Molecule 50: 30S ribosomal protein S20



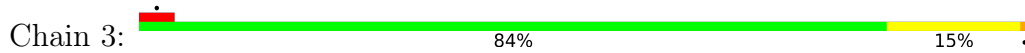
• Molecule 51: 30S ribosomal protein S21

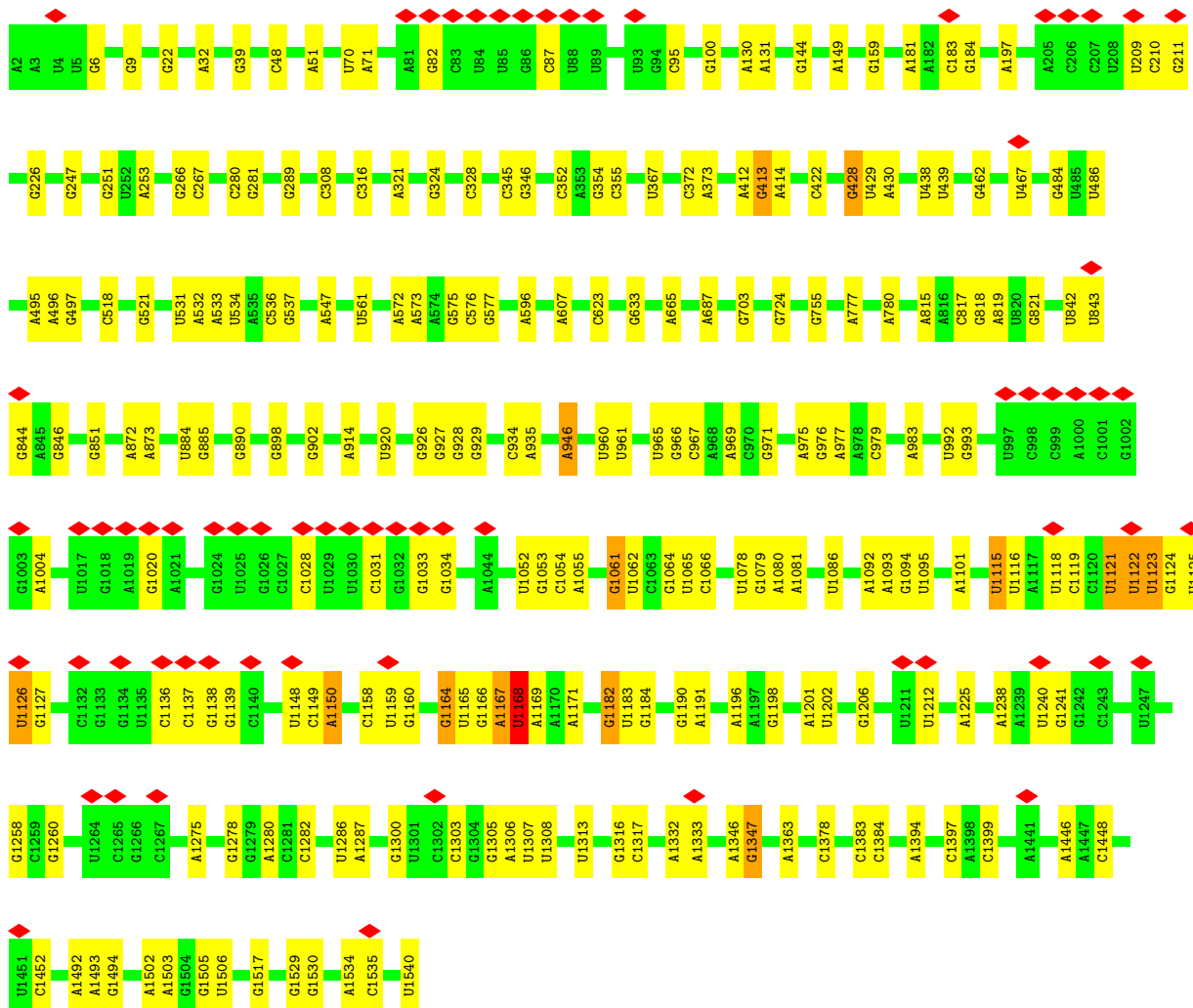


• Molecule 52: 50S ribosomal protein L1

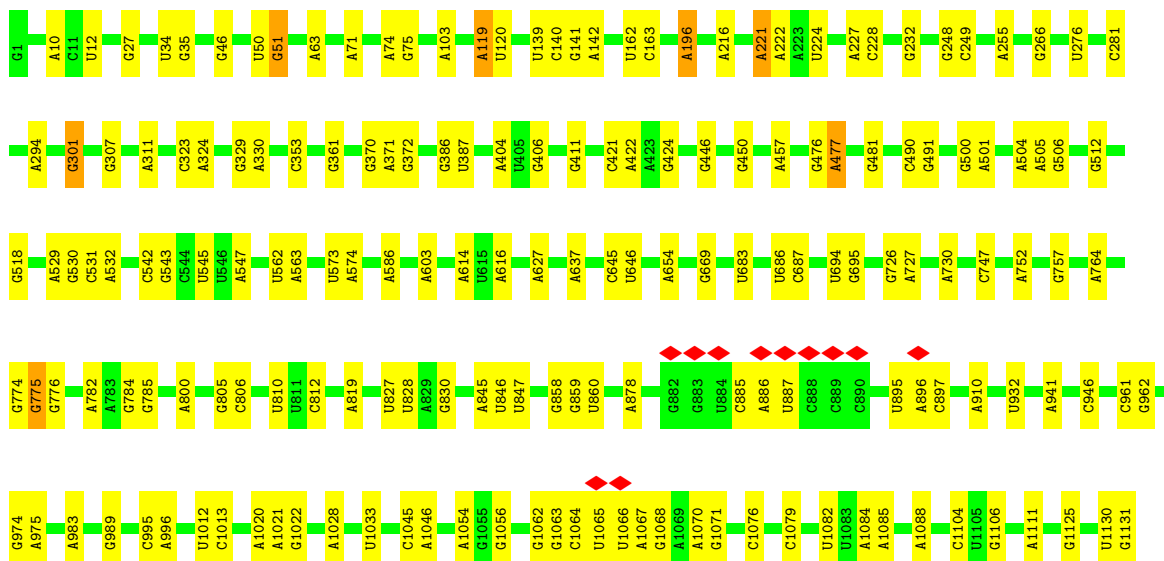
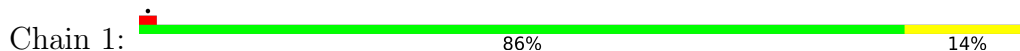


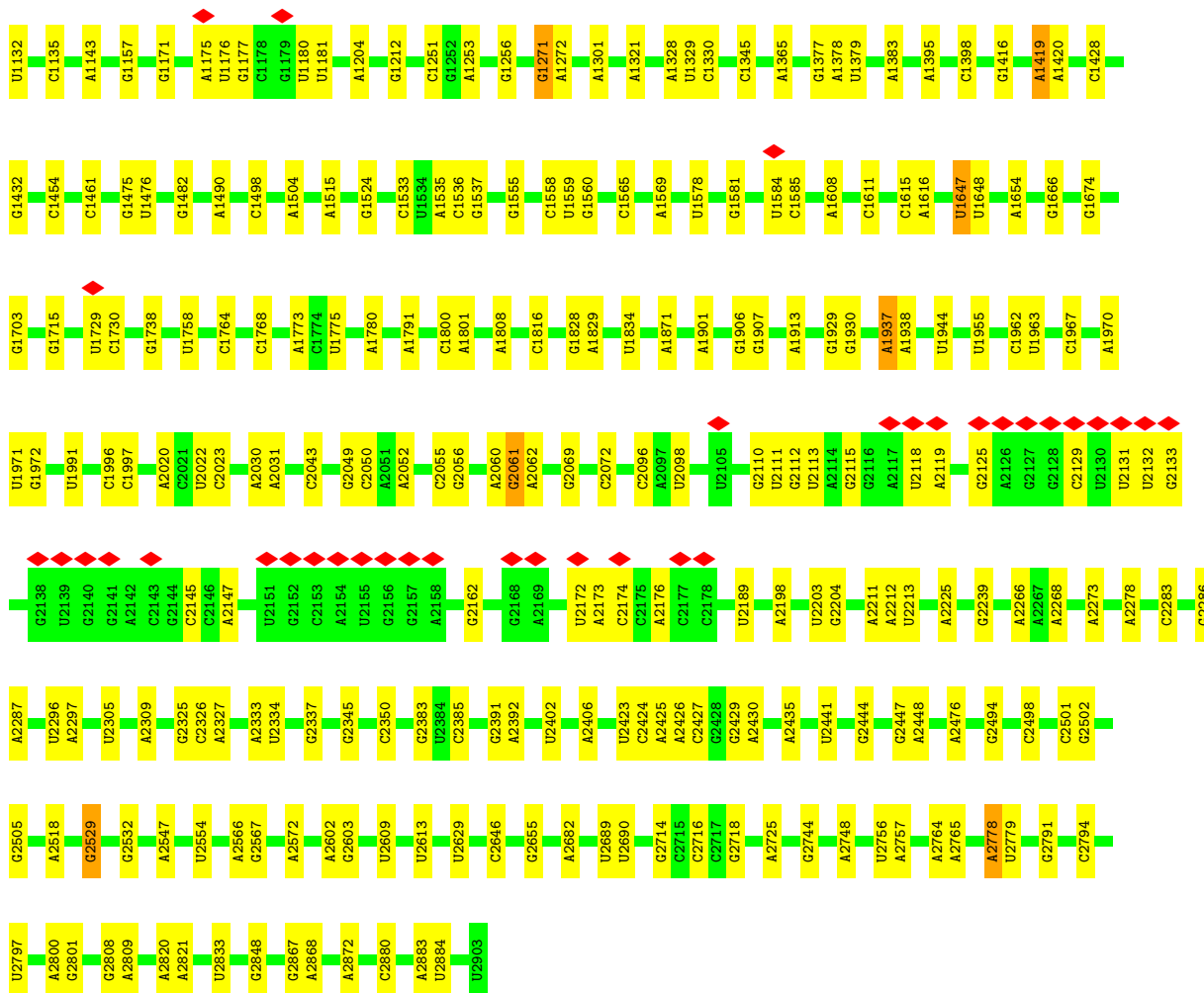
• Molecule 53: 16S ribosomal RNA



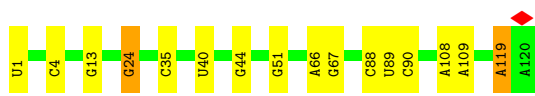
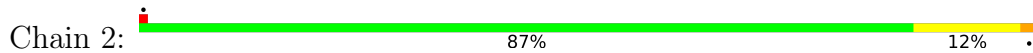


• Molecule 54: 23S ribosomal RNA

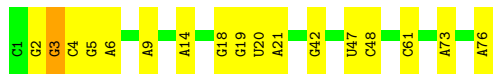
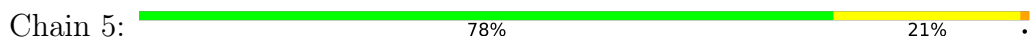




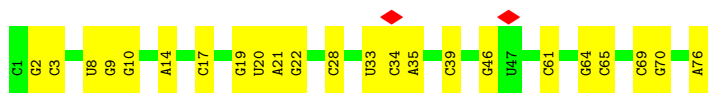
• Molecule 55: 5S ribosomal RNA




• Molecule 56: tRNA<sup>Pro</sup>



• Molecule 57: tRNA<sup>fMet</sup>




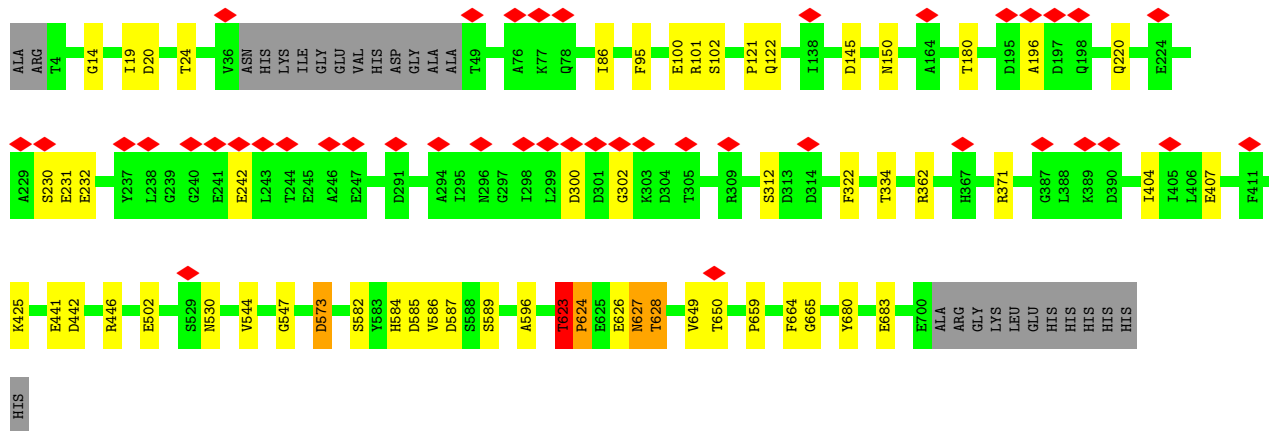
- Molecule 58: mRNA

Chain 4:  75% 25%



- Molecule 59: Elongation factor G

Chain 8:  6% 88% 7% . .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9059	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 ( $e^-/\text{\AA}^2$ )	47.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	23.041	Depositor
Minimum map value	-7.245	Depositor
Average map value	0.019	Depositor
Map value standard deviation	1.364	Depositor
Recommended contour level	3.7	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: GCP, MG, FME

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	b	0.64	2/2122 (0.1%)	0.74	0/2852
2	c	0.61	1/1586 (0.1%)	0.70	0/2134
3	d	0.71	4/1571 (0.3%)	0.68	0/2113
4	e	0.66	1/1435 (0.1%)	0.69	0/1926
5	f	0.62	1/1343 (0.1%)	0.68	0/1816
6	g	1.27	10/946 (1.1%)	0.96	6/1275 (0.5%)
7	h	1.04	5/638 (0.8%)	0.94	1/860 (0.1%)
8	i	1.56	11/564 (2.0%)	1.09	4/768 (0.5%)
9	j	0.58	2/1152 (0.2%)	0.62	1/1551 (0.1%)
10	k	0.68	0/948	0.81	0/1268
11	l	0.57	0/1054	0.70	0/1403
12	m	0.67	3/1093 (0.3%)	0.71	0/1460
13	n	0.57	1/974 (0.1%)	0.64	0/1301
14	o	0.77	4/902 (0.4%)	0.69	1/1209 (0.1%)
15	p	0.55	1/929 (0.1%)	0.64	0/1242
16	q	0.61	0/960	0.65	0/1278
17	r	0.55	0/829	0.73	0/1107
18	s	0.74	3/864 (0.3%)	0.76	0/1156
19	t	0.62	1/745 (0.1%)	0.64	0/994
20	u	0.52	0/788	0.63	0/1051
21	v	0.58	1/766 (0.1%)	0.70	1/1025 (0.1%)
22	w	0.59	1/582 (0.2%)	0.65	1/769 (0.1%)
23	x	0.67	1/635 (0.2%)	0.77	0/848
24	y	0.72	2/510 (0.4%)	0.69	0/677
25	z	0.54	1/453 (0.2%)	0.62	0/605
26	A	0.82	3/532 (0.6%)	0.75	0/709
27	B	0.45	0/450	0.59	0/599
28	C	0.61	1/417 (0.2%)	0.68	0/554
29	D	0.53	0/380	0.61	0/498
30	E	0.62	0/513	0.68	0/676
31	F	0.60	1/303 (0.3%)	0.71	0/397
32	G	0.72	3/1736 (0.2%)	0.72	0/2338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	H	0.88	9/1652 (0.5%)	0.75	0/2225
34	I	0.71	3/1665 (0.2%)	0.75	2/2227 (0.1%)
35	J	0.73	1/1170 (0.1%)	0.78	1/1573 (0.1%)
36	K	0.83	3/836 (0.4%)	0.80	0/1128
37	L	0.84	4/1196 (0.3%)	0.76	0/1602
38	M	0.67	1/989 (0.1%)	0.70	0/1326
39	N	0.70	5/1034 (0.5%)	0.74	2/1375 (0.1%)
40	O	1.06	5/797 (0.6%)	0.93	5/1077 (0.5%)
41	P	0.74	2/886 (0.2%)	0.78	2/1195 (0.2%)
42	Q	0.60	0/969	0.72	0/1300
43	R	0.94	5/893 (0.6%)	0.94	1/1193 (0.1%)
44	S	0.86	2/817 (0.2%)	0.74	0/1088
45	T	0.72	1/722 (0.1%)	0.73	0/964
46	U	0.56	0/659	0.62	0/884
47	V	0.46	0/658	0.65	0/881
48	W	0.88	4/545 (0.7%)	0.75	1/731 (0.1%)
49	X	0.74	1/653 (0.2%)	0.75	0/877
50	Y	0.75	2/671 (0.3%)	0.66	0/888
51	Z	0.70	0/551	0.81	0/728
52	a	1.42	17/1034 (1.6%)	1.00	7/1387 (0.5%)
53	3	0.64	2/36963 (0.0%)	0.71	13/57662 (0.0%)
54	1	0.51	0/69796	0.67	3/108888 (0.0%)
55	2	0.46	0/2872	0.67	1/4479 (0.0%)
56	5	0.46	0/1840	0.71	0/2868
57	6	0.47	0/1832	0.69	0/2855
58	4	0.87	1/388 (0.3%)	0.74	1/603 (0.2%)
59	8	0.74	16/5411 (0.3%)	0.77	6/7323 (0.1%)
All	All	0.62	148/166219 (0.1%)	0.70	60/247786 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	g	0	4
34	I	0	1
35	J	0	1
53	3	0	25
54	1	0	59
55	2	0	3
56	5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
59	8	0	2
All	All	0	96

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	g	8	LYS	C-O	-19.85	0.85	1.23
52	a	59	VAL	C-O	19.00	1.59	1.23
8	i	56	VAL	C-O	15.48	1.52	1.23
40	O	73	LEU	C-O	14.75	1.51	1.23
52	a	163	TYR	C-O	14.60	1.51	1.23
40	O	75	ASP	C-O	12.57	1.47	1.23
6	g	114	GLU	C-O	11.90	1.46	1.23
8	i	8	VAL	C-O	11.74	1.45	1.23
37	L	104	VAL	C-O	10.97	1.44	1.23
8	i	58	ILE	C-O	10.53	1.43	1.23
48	W	12	PHE	C-O	10.43	1.43	1.23
8	i	54	ILE	C-O	10.23	1.42	1.23
33	H	154	GLY	C-O	10.20	1.40	1.23
52	a	195	ALA	C-O	10.11	1.42	1.23
52	a	61	GLY	C-O	10.09	1.39	1.23
52	a	181	ASP	C-O	9.74	1.41	1.23
36	K	13	ASP	C-O	9.16	1.40	1.23
32	G	83	ALA	C-O	8.83	1.40	1.23
6	g	132	PHE	C-O	8.66	1.39	1.23
59	8	665	GLY	C-O	8.66	1.37	1.23
58	4	14	A	O3'-P	-8.62	1.50	1.61
6	g	126	GLY	C-O	8.58	1.37	1.23
33	H	169	GLU	C-O	8.44	1.39	1.23
8	i	57	VAL	C-O	8.43	1.39	1.23
14	o	77	ALA	C-O	8.41	1.39	1.23
2	c	157	LYS	C-O	8.22	1.39	1.23
49	X	66	VAL	C-O	8.12	1.38	1.23
3	d	48	THR	C-O	8.02	1.38	1.23
26	A	45	THR	C-O	7.95	1.38	1.23
59	8	650	THR	C-O	7.86	1.38	1.23
59	8	623	THR	C-O	7.80	1.38	1.23
6	g	43	ASN	C-O	7.75	1.38	1.23
14	o	76	LYS	C-O	7.66	1.37	1.23
59	8	14	GLY	C-O	7.62	1.35	1.23
43	R	16	ILE	C-O	7.62	1.37	1.23
52	a	161	VAL	C-O	7.55	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	213	SER	C-O	7.49	1.37	1.23
6	g	42	LYS	C-O	7.48	1.37	1.23
8	i	10	LEU	C-O	7.39	1.37	1.23
59	8	589	SER	C-O	7.29	1.37	1.23
32	G	206	ILE	C-O	7.26	1.37	1.23
40	O	80	THR	C-O	7.24	1.37	1.23
33	H	199	VAL	C-O	7.17	1.36	1.23
7	h	59	LEU	C-O	7.15	1.36	1.23
59	8	100	GLU	C-O	7.09	1.36	1.23
52	a	63	THR	C-O	7.04	1.36	1.23
8	i	27	LEU	C-O	7.02	1.36	1.23
59	8	95	PHE	C-O	6.98	1.36	1.23
38	M	35	ILE	C-O	6.98	1.36	1.23
24	y	40	SER	C-O	6.96	1.36	1.23
52	a	42	VAL	C-O	6.91	1.36	1.23
48	W	16	GLY	N-CA	6.85	1.56	1.46
5	f	104	LEU	C-O	6.83	1.36	1.23
43	R	89	ARG	C-O	6.83	1.36	1.23
34	I	69	ARG	C-O	6.79	1.36	1.23
3	d	191	ASP	C-O	6.75	1.36	1.23
39	N	24	ASN	C-O	6.65	1.35	1.23
43	R	56	ARG	C-O	6.62	1.35	1.23
8	i	40	ALA	C-O	6.62	1.35	1.23
35	J	96	GLN	C-O	6.62	1.35	1.23
31	F	4	ARG	C-O	6.61	1.35	1.23
4	e	7	TYR	C-O	6.59	1.35	1.23
52	a	45	ALA	C-O	6.56	1.35	1.23
6	g	101	ASP	C-O	6.56	1.35	1.23
34	I	155	LYS	N-CA	6.55	1.59	1.46
3	d	14	VAL	C-O	6.55	1.35	1.23
1	b	210	ALA	C-O	6.52	1.35	1.23
26	A	46	GLY	C-O	6.52	1.34	1.23
32	G	139	GLU	C-O	6.51	1.35	1.23
52	a	165	ASN	N-CA	6.51	1.59	1.46
21	v	92	VAL	N-CA	6.45	1.59	1.46
33	H	20	THR	C-O	6.41	1.35	1.23
6	g	13	GLY	C-O	-6.32	1.13	1.23
1	b	41	GLY	C-O	6.29	1.33	1.23
7	h	25	ALA	C-O	6.26	1.35	1.23
22	w	27	VAL	C-O	6.24	1.35	1.23
8	i	8	VAL	N-CA	6.18	1.58	1.46
59	8	180	THR	C-O	6.16	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	t	4	GLU	C-O	6.15	1.35	1.23
43	R	29	SER	C-O	6.14	1.35	1.23
14	o	58	ILE	C-O	6.14	1.35	1.23
15	p	6	GLN	C-O	6.14	1.35	1.23
18	s	41	LYS	C-O	6.11	1.34	1.23
48	W	55	ALA	C-O	6.10	1.34	1.23
43	R	66	GLY	C-O	6.07	1.33	1.23
52	a	184	LYS	C-O	6.03	1.34	1.23
59	8	101	ARG	C-O	6.02	1.34	1.23
40	O	37	ARG	N-CA	6.00	1.58	1.46
7	h	7	ASP	C-O	5.96	1.34	1.23
7	h	57	ASN	C-O	5.96	1.34	1.23
59	8	312	SER	C-O	5.92	1.34	1.23
33	H	128	MET	C-O	5.92	1.34	1.23
52	a	196	LEU	C-O	5.89	1.34	1.23
37	L	103	ILE	C-O	5.81	1.34	1.23
48	W	40	PRO	C-O	5.79	1.34	1.23
37	L	108	ARG	N-CA	5.77	1.57	1.46
59	8	544	VAL	C-O	5.77	1.34	1.23
59	8	659	PRO	C-O	5.75	1.34	1.23
12	m	116	ALA	C-O	5.75	1.34	1.23
52	a	212	VAL	C-O	5.73	1.34	1.23
18	s	16	LYS	C-O	5.73	1.34	1.23
44	S	80	ARG	C-O	5.71	1.34	1.23
12	m	119	LEU	C-O	5.68	1.34	1.23
26	A	60	PHE	C-O	5.68	1.34	1.23
52	a	164	ARG	C-N	5.67	1.47	1.34
24	y	19	LEU	C-O	5.66	1.34	1.23
53	3	1052	U	N1-C2	5.65	1.43	1.38
44	S	40	ARG	C-O	5.64	1.34	1.23
59	8	232	GLU	C-O	5.63	1.34	1.23
53	3	1115	U	N1-C2	5.60	1.43	1.38
50	Y	60	GLN	C-O	5.57	1.33	1.23
33	H	148	ILE	C-O	5.56	1.33	1.23
34	I	134	TYR	C-O	5.56	1.33	1.23
36	K	14	GLN	C-O	5.55	1.33	1.23
36	K	59	TYR	C-O	5.53	1.33	1.23
23	x	65	THR	C-O	5.52	1.33	1.23
59	8	230	SER	N-CA	5.49	1.57	1.46
59	8	628	THR	N-CA	5.46	1.57	1.46
39	N	33	SER	N-CA	5.45	1.57	1.46
41	P	31	VAL	N-CA	5.45	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	j	69	ARG	C-O	5.44	1.33	1.23
40	O	39	PRO	C-N	5.43	1.46	1.34
52	a	164	ARG	C-O	5.43	1.33	1.23
8	i	57	VAL	C-N	5.42	1.46	1.34
33	H	184	ASN	C-O	5.42	1.33	1.23
25	z	42	ALA	C-O	5.39	1.33	1.23
28	C	25	ASN	C-O	5.36	1.33	1.23
12	m	105	MET	C-O	5.35	1.33	1.23
6	g	100	ALA	C-O	5.32	1.33	1.23
14	o	75	GLY	C-O	5.32	1.32	1.23
41	P	80	ASN	C-O	5.30	1.33	1.23
3	d	194	LYS	C-O	5.29	1.33	1.23
59	8	150	ASN	C-O	5.29	1.33	1.23
9	j	7	LYS	C-O	5.28	1.33	1.23
13	n	17	ARG	C-O	5.28	1.33	1.23
8	i	42	ASN	C-O	5.27	1.33	1.23
7	h	57	ASN	N-CA	5.26	1.56	1.46
39	N	67	LYS	C-O	5.26	1.33	1.23
39	N	62	LEU	C-O	5.24	1.33	1.23
52	a	192	LEU	C-O	5.24	1.33	1.23
45	T	59	VAL	C-O	5.17	1.33	1.23
33	H	155	ARG	C-O	5.14	1.33	1.23
6	g	49	ALA	C-O	5.13	1.33	1.23
50	Y	58	ASP	C-O	5.13	1.33	1.23
37	L	65	LEU	C-O	5.10	1.33	1.23
39	N	15	ALA	N-CA	5.10	1.56	1.46
18	s	3	THR	C-O	5.09	1.33	1.23
33	H	152	VAL	C-O	5.07	1.32	1.23

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	3	1061	G	C2'-C3'-O3'	8.75	128.75	109.50
34	I	154	VAL	C-N-CA	-8.41	100.68	121.70
52	a	164	ARG	C-N-CA	-8.33	100.88	121.70
6	g	41	LYS	O-C-N	-8.24	109.51	122.70
40	O	39	PRO	C-N-CA	-7.69	102.48	121.70
34	I	152	SER	O-C-N	-7.59	110.56	122.70
40	O	39	PRO	N-CA-C	7.55	131.72	112.10
6	g	13	GLY	O-C-N	-7.52	110.67	122.70
40	O	73	LEU	O-C-N	7.20	134.22	122.70
55	2	119	A	N9-C1'-C2'	6.97	123.06	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	9	LYS	C-N-CA	-6.88	104.49	121.70
8	i	58	ILE	O-C-N	6.76	133.52	122.70
52	a	60	ARG	C-N-CA	-6.41	108.83	122.30
41	P	29	THR	O-C-N	-6.39	112.47	122.70
58	4	14	A	P-O3'-C3'	6.38	127.35	119.70
53	3	1061	G	C3'-C2'-C1'	-6.32	96.44	101.50
53	3	1126	U	N1-C1'-C2'	6.26	122.14	114.00
48	W	15	GLU	C-N-CA	-6.18	109.31	122.30
53	3	1150	A	O4'-C1'-N9	6.17	113.14	108.20
53	3	428	G	N9-C1'-C2'	6.14	121.99	114.00
54	1	477	A	N9-C1'-C2'	6.14	121.98	114.00
59	8	627	ASN	C-N-CA	-6.09	106.47	121.70
53	3	1206	G	C1'-O4'-C4'	-6.08	105.04	109.90
53	3	1347	G	C1'-O4'-C4'	-6.00	105.10	109.90
53	3	1168	U	O4'-C4'-C3'	-5.92	98.08	104.00
7	h	77	VAL	C-N-CA	-5.79	110.14	122.30
52	a	198	LYS	C-N-CA	-5.77	107.28	121.70
54	1	1558	C	N1-C1'-C2'	5.70	121.41	114.00
52	a	184	LYS	C-N-CA	-5.67	107.53	121.70
8	i	11	GLN	C-N-CA	5.66	135.85	121.70
59	8	584	HIS	O-C-N	-5.64	113.67	122.70
59	8	102	SER	C-N-CA	-5.61	107.67	121.70
53	3	1206	G	O4'-C1'-N9	5.58	112.66	108.20
39	N	31	GLN	O-C-N	-5.50	113.90	122.70
41	P	29	THR	CA-C-O	5.46	131.57	120.10
59	8	628	THR	N-CA-C	5.40	125.57	111.00
53	3	1061	G	P-O3'-C3'	-5.39	113.23	119.70
9	j	81	ILE	N-CA-C	5.38	125.53	111.00
6	g	44	ILE	C-N-CA	-5.37	108.27	121.70
53	3	1061	G	O4'-C4'-C3'	-5.36	98.64	104.00
52	a	162	ARG	C-N-CA	-5.35	108.32	121.70
54	1	301	G	N9-C1'-C2'	5.33	120.93	114.00
21	v	91	PHE	C-N-CA	-5.26	108.54	121.70
6	g	8	LYS	CA-C-O	-5.25	109.07	120.10
59	8	596	ALA	C-N-CA	-5.25	108.58	121.70
6	g	43	ASN	C-N-CA	-5.24	108.60	121.70
40	O	36	VAL	C-N-CA	-5.23	108.62	121.70
6	g	132	PHE	O-C-N	5.21	131.03	122.70
53	3	1158	C	N1-C1'-C2'	5.19	120.75	114.00
35	J	111	ARG	C-N-CA	-5.19	108.73	121.70
40	O	44	THR	N-CA-C	5.17	124.96	111.00
53	3	967	C	C1'-O4'-C4'	-5.17	105.77	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	57	VAL	O-C-N	5.12	130.90	122.70
52	a	56	ASP	C-N-CA	-5.11	108.93	121.70
43	R	109	LYS	C-N-CA	-5.10	111.60	122.30
22	w	60	ASP	C-N-CA	-5.09	111.62	122.30
59	8	86	ILE	N-CA-C	5.07	124.69	111.00
39	N	14	SER	C-N-CA	-5.06	109.05	121.70
14	o	79	ALA	C-N-CA	-5.05	109.08	121.70
52	a	164	ARG	O-C-N	5.04	130.76	122.70

There are no chirality outliers.

All (96) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	1	1028	A	Sidechain
54	1	1125	G	Sidechain
54	1	1171	G	Sidechain
54	1	119	A	Sidechain
54	1	1204	A	Sidechain
54	1	1271	G	Sidechain
54	1	1328	A	Sidechain
54	1	1377	G	Sidechain
54	1	1419	A	Sidechain
54	1	1432	G	Sidechain
54	1	1615	C	Sidechain
54	1	1647	U	Sidechain
54	1	1666	G	Sidechain
54	1	1768	C	Sidechain
54	1	1775	U	Sidechain
54	1	1828	G	Sidechain
54	1	1834	U	Sidechain
54	1	1937	A	Sidechain
54	1	196	A	Sidechain
54	1	1996	C	Sidechain
54	1	2050	C	Sidechain
54	1	2061	G	Sidechain
54	1	221	A	Sidechain
54	1	2266	A	Sidechain
54	1	2273	A	Sidechain
54	1	232	G	Sidechain
54	1	2444	G	Sidechain
54	1	2447	G	Sidechain
54	1	2501	C	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
54	1	2529	G	Sidechain
54	1	2532	G	Sidechain
54	1	27	G	Sidechain
54	1	2718	G	Sidechain
54	1	2725	A	Sidechain
54	1	2778	A	Sidechain
54	1	2848	G	Sidechain
54	1	307	G	Sidechain
54	1	370	G	Sidechain
54	1	446	G	Sidechain
54	1	450	G	Sidechain
54	1	476	G	Sidechain
54	1	477	A	Sidechain
54	1	500	G	Sidechain
54	1	501	A	Sidechain
54	1	506	G	Sidechain
54	1	51	G	Sidechain
54	1	512	G	Sidechain
54	1	562	U	Sidechain
54	1	586	A	Sidechain
54	1	683	U	Sidechain
54	1	726	G	Sidechain
54	1	727	A	Sidechain
54	1	757	G	Sidechain
54	1	775	G	Sidechain
54	1	800	A	Sidechain
54	1	810	U	Sidechain
54	1	895	U	Sidechain
54	1	975	A	Sidechain
54	1	989	G	Sidechain
55	2	1	U	Sidechain
55	2	119	A	Sidechain
55	2	24	G	Sidechain
53	3	1121	U	Sidechain
53	3	1122	U	Sidechain
53	3	1123	U	Sidechain
53	3	1150	A	Sidechain
53	3	1164	G	Sidechain
53	3	1167	A	Sidechain
53	3	1168	U	Sidechain
53	3	1171	A	Sidechain
53	3	1182	G	Sidechain

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Mol	Chain	Res	Type	Group
53	3	1307	U	Sidechain
53	3	1316	G	Sidechain
53	3	1332	A	Sidechain
53	3	1333	A	Sidechain
53	3	159	G	Sidechain
53	3	324	G	Sidechain
53	3	413	G	Sidechain
53	3	428	G	Sidechain
53	3	496	A	Sidechain
53	3	521	G	Sidechain
53	3	780	A	Sidechain
53	3	872	A	Sidechain
53	3	884	U	Sidechain
53	3	898	G	Sidechain
53	3	920	U	Sidechain
53	3	946	A	Sidechain
56	5	3	G	Sidechain
59	8	623	THR	Mainchain
59	8	627	ASN	Mainchain
34	I	152	SER	Mainchain
35	J	92	ARG	Mainchain
6	g	13	GLY	Mainchain,Peptide
6	g	41	LYS	Mainchain
6	g	8	LYS	Mainchain

## 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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	269/271 (99%)	232 (86%)	35 (13%)	2 (1%)	22	61
2	c	207/209 (99%)	187 (90%)	20 (10%)	0	100	100
3	d	199/201 (99%)	176 (88%)	22 (11%)	1 (0%)	29	67
4	e	175/177 (99%)	156 (89%)	17 (10%)	2 (1%)	14	51
5	f	174/176 (99%)	153 (88%)	19 (11%)	2 (1%)	14	51
6	g	121/149 (81%)	97 (80%)	19 (16%)	5 (4%)	3	21
7	h	82/131 (63%)	62 (76%)	16 (20%)	4 (5%)	2	17
8	i	72/141 (51%)	54 (75%)	17 (24%)	1 (1%)	11	46
9	j	140/142 (99%)	128 (91%)	12 (9%)	0	100	100
10	k	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	3	20
11	l	141/143 (99%)	116 (82%)	23 (16%)	2 (1%)	11	46
12	m	134/136 (98%)	120 (90%)	13 (10%)	1 (1%)	22	61
13	n	118/120 (98%)	101 (86%)	16 (14%)	1 (1%)	19	58
14	o	114/116 (98%)	99 (87%)	15 (13%)	0	100	100
15	p	112/114 (98%)	98 (88%)	13 (12%)	1 (1%)	17	56
16	q	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
17	r	101/103 (98%)	82 (81%)	18 (18%)	1 (1%)	15	54
18	s	108/110 (98%)	91 (84%)	17 (16%)	0	100	100
19	t	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
20	u	100/102 (98%)	82 (82%)	17 (17%)	1 (1%)	15	54
21	v	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	14	51
22	w	73/75 (97%)	64 (88%)	9 (12%)	0	100	100
23	x	75/77 (97%)	65 (87%)	10 (13%)	0	100	100
24	y	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
25	z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
26	A	64/66 (97%)	45 (70%)	17 (27%)	2 (3%)	4	26
27	B	54/56 (96%)	48 (89%)	6 (11%)	0	100	100
28	C	48/50 (96%)	40 (83%)	8 (17%)	0	100	100
29	D	44/46 (96%)	38 (86%)	6 (14%)	0	100	100
30	E	62/64 (97%)	50 (81%)	9 (14%)	3 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	F	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
32	G	216/225 (96%)	175 (81%)	39 (18%)	2 (1%)	17	56
33	H	204/206 (99%)	181 (89%)	22 (11%)	1 (0%)	29	67
34	I	203/205 (99%)	173 (85%)	28 (14%)	2 (1%)	15	54
35	J	155/157 (99%)	128 (83%)	20 (13%)	7 (4%)	2	18
36	K	98/100 (98%)	78 (80%)	14 (14%)	6 (6%)	1	12
37	L	149/151 (99%)	128 (86%)	20 (13%)	1 (1%)	22	61
38	M	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
39	N	125/127 (98%)	93 (74%)	26 (21%)	6 (5%)	2	17
40	O	96/98 (98%)	72 (75%)	19 (20%)	5 (5%)	2	15
41	P	114/116 (98%)	96 (84%)	15 (13%)	3 (3%)	5	31
42	Q	121/123 (98%)	95 (78%)	23 (19%)	3 (2%)	5	32
43	R	112/114 (98%)	89 (80%)	19 (17%)	4 (4%)	3	23
44	S	98/100 (98%)	81 (83%)	13 (13%)	4 (4%)	3	21
45	T	86/88 (98%)	69 (80%)	16 (19%)	1 (1%)	13	49
46	U	80/82 (98%)	66 (82%)	14 (18%)	0	100	100
47	V	78/80 (98%)	59 (76%)	17 (22%)	2 (3%)	5	31
48	W	63/65 (97%)	51 (81%)	11 (18%)	1 (2%)	9	43
49	X	77/79 (98%)	58 (75%)	19 (25%)	0	100	100
50	Y	83/85 (98%)	75 (90%)	8 (10%)	0	100	100
51	Z	63/65 (97%)	35 (56%)	25 (40%)	3 (5%)	2	17
52	a	130/223 (58%)	118 (91%)	10 (8%)	2 (2%)	10	44
59	8	681/711 (96%)	561 (82%)	103 (15%)	17 (2%)	5	32
All	All	6517/6889 (95%)	5493 (84%)	919 (14%)	105 (2%)	13	43

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	g	14	SER
10	k	92	GLU
17	r	54	VAL
20	u	99	SER
30	E	31	ILE
35	J	87	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	J	122	VAL
39	N	90	ASP
44	S	20	PHE
44	S	54	SER
45	T	46	LYS
47	V	49	ASN
51	Z	9	GLU
51	Z	37	TYR
59	8	122	GLN
59	8	586	VAL
59	8	624	PRO
59	8	628	THR
1	b	232	GLY
6	g	12	LEU
7	h	32	GLY
10	k	35	VAL
13	n	71	ARG
32	G	19	THR
32	G	87	ASP
35	J	93	VAL
39	N	57	VAL
40	O	58	ASN
40	O	89	ARG
41	P	89	GLY
43	R	105	ALA
47	V	34	GLY
48	W	17	VAL
59	8	121	PRO
59	8	302	GLY
59	8	425	LYS
59	8	649	VAL
59	8	664	PHE
3	d	82	GLY
5	f	45	ALA
5	f	174	LYS
6	g	9	VAL
6	g	89	LYS
7	h	81	LEU
10	k	106	GLU
11	l	31	GLY
35	J	25	LYS
36	K	52	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	K	54	LEU
41	P	125	LYS
42	Q	3	VAL
42	Q	24	GLU
43	R	100	ARG
52	a	165	ASN
59	8	196	ALA
59	8	242	GLU
59	8	582	SER
59	8	585	ASP
4	e	20	ASN
7	h	58	THR
10	k	104	THR
26	A	54	GLY
30	E	33	THR
35	J	97	PRO
37	L	111	GLY
39	N	120	ALA
39	N	125	GLN
43	R	65	GLU
44	S	61	ASN
59	8	300	ASP
59	8	573	ASP
4	e	149	ARG
11	l	36	LYS
12	m	69	PRO
33	H	162	ALA
34	I	7	LYS
36	K	53	LYS
36	K	92	THR
39	N	55	ASP
39	N	111	GLU
40	O	57	VAL
41	P	77	GLY
44	S	60	ARG
52	a	68	GLY
6	g	94	ILE
8	i	4	VAL
15	p	113	LEU
21	v	93	ARG
34	I	182	LYS
35	J	50	GLY

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Mol	Chain	Res	Type
40	O	43	PRO
7	h	79	PRO
36	K	12	PRO
42	Q	117	GLY
26	A	51	VAL
35	J	157	GLY
40	O	39	PRO
30	E	62	PRO
51	Z	10	PRO
1	b	205	GLY
43	R	6	ILE
59	8	404	ILE
59	8	547	GLY
10	k	93	GLN
36	K	18	VAL

### 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	b	216/216 (100%)	212 (98%)	4 (2%)	57	81
2	c	164/164 (100%)	161 (98%)	3 (2%)	59	82
3	d	165/165 (100%)	163 (99%)	2 (1%)	71	88
4	e	148/148 (100%)	144 (97%)	4 (3%)	44	75
5	f	137/137 (100%)	136 (99%)	1 (1%)	84	94
6	g	98/114 (86%)	98 (100%)	0	100	100
7	h	66/100 (66%)	66 (100%)	0	100	100
8	i	60/109 (55%)	60 (100%)	0	100	100
9	j	116/116 (100%)	116 (100%)	0	100	100
10	k	103/103 (100%)	99 (96%)	4 (4%)	32	67
11	l	102/102 (100%)	102 (100%)	0	100	100
12	m	109/109 (100%)	107 (98%)	2 (2%)	59	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	n	100/100 (100%)	98 (98%)	2 (2%)	55	80
14	o	86/86 (100%)	85 (99%)	1 (1%)	71	88
15	p	99/99 (100%)	97 (98%)	2 (2%)	55	80
16	q	89/89 (100%)	89 (100%)	0	100	100
17	r	84/84 (100%)	83 (99%)	1 (1%)	71	88
18	s	93/93 (100%)	93 (100%)	0	100	100
19	t	80/80 (100%)	79 (99%)	1 (1%)	69	87
20	u	83/83 (100%)	79 (95%)	4 (5%)	25	61
21	v	78/78 (100%)	77 (99%)	1 (1%)	69	87
22	w	57/57 (100%)	57 (100%)	0	100	100
23	x	67/67 (100%)	67 (100%)	0	100	100
24	y	55/55 (100%)	50 (91%)	5 (9%)	9	34
25	z	48/48 (100%)	47 (98%)	1 (2%)	53	79
26	A	59/59 (100%)	57 (97%)	2 (3%)	37	70
27	B	47/47 (100%)	47 (100%)	0	100	100
28	C	45/45 (100%)	45 (100%)	0	100	100
29	D	38/38 (100%)	37 (97%)	1 (3%)	46	76
30	E	51/51 (100%)	47 (92%)	4 (8%)	12	43
31	F	34/34 (100%)	34 (100%)	0	100	100
32	G	180/186 (97%)	174 (97%)	6 (3%)	38	71
33	H	170/170 (100%)	166 (98%)	4 (2%)	49	77
34	I	172/172 (100%)	166 (96%)	6 (4%)	36	69
35	J	119/119 (100%)	113 (95%)	6 (5%)	24	60
36	K	87/87 (100%)	84 (97%)	3 (3%)	37	70
37	L	124/124 (100%)	122 (98%)	2 (2%)	62	84
38	M	104/104 (100%)	103 (99%)	1 (1%)	76	90
39	N	105/105 (100%)	101 (96%)	4 (4%)	33	67
40	O	86/86 (100%)	77 (90%)	9 (10%)	7	28
41	P	89/89 (100%)	84 (94%)	5 (6%)	21	57
42	Q	103/103 (100%)	99 (96%)	4 (4%)	32	67
43	R	92/92 (100%)	85 (92%)	7 (8%)	13	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	S	83/83 (100%)	79 (95%)	4 (5%)	25	61
45	T	76/76 (100%)	74 (97%)	2 (3%)	46	76
46	U	65/65 (100%)	63 (97%)	2 (3%)	40	72
47	V	74/74 (100%)	74 (100%)	0	100	100
48	W	56/56 (100%)	55 (98%)	1 (2%)	59	82
49	X	70/70 (100%)	69 (99%)	1 (1%)	67	86
50	Y	65/65 (100%)	64 (98%)	1 (2%)	65	85
51	Z	55/55 (100%)	54 (98%)	1 (2%)	59	82
52	a	110/174 (63%)	109 (99%)	1 (1%)	78	91
59	8	566/585 (97%)	543 (96%)	23 (4%)	30	66
All	All	5428/5616 (97%)	5290 (98%)	138 (2%)	49	77

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	42	ARG
1	b	52	HIS
1	b	129	LEU
1	b	212	TRP
2	c	1	MET
2	c	33	ARG
2	c	146	ILE
3	d	1	MET
3	d	102	ARG
4	e	32	LYS
4	e	71	LYS
4	e	134	GLN
4	e	147	ARG
5	f	166	GLU
10	k	31	ARG
10	k	65	THR
10	k	88	ASN
10	k	93	GLN
12	m	59	ARG
12	m	97	GLN
13	n	12	ARG
13	n	37	THR
14	o	112	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	p	30	TRP
15	p	65	ASN
17	r	48	LYS
19	t	32	LEU
20	u	36	GLU
20	u	46	LYS
20	u	81	ARG
20	u	88	ASP
21	v	59	GLU
24	y	1	MET
24	y	4	LYS
24	y	12	GLU
24	y	17	GLU
24	y	23	ARG
25	z	16	LEU
26	A	27	THR
26	A	58	ASP
29	D	3	ARG
30	E	30	HIS
30	E	32	LEU
30	E	53	ASP
30	E	61	LEU
32	G	20	ARG
32	G	112	ARG
32	G	131	LYS
32	G	136	ARG
32	G	196	ASP
32	G	222	GLU
33	H	153	SER
33	H	156	LEU
33	H	165	GLU
33	H	169	GLU
34	I	57	LYS
34	I	130	ASN
34	I	159	GLU
34	I	164	ARG
34	I	183	ARG
34	I	196	GLU
35	J	28	ARG
35	J	47	PHE
35	J	55	VAL
35	J	72	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	J	97	PRO
35	J	147	ASN
36	K	12	PRO
36	K	58	HIS
36	K	86	ARG
37	L	91	ARG
37	L	118	ARG
38	M	60	LEU
39	N	26	LYS
39	N	44	ARG
39	N	45	MET
39	N	87	MET
40	O	20	GLN
40	O	30	LYS
40	O	36	VAL
40	O	40	ILE
40	O	42	LEU
40	O	43	PRO
40	O	69	THR
40	O	73	LEU
40	O	75	ASP
41	P	30	ILE
41	P	34	THR
41	P	82	GLU
41	P	117	HIS
41	P	118	ASN
42	Q	17	LYS
42	Q	19	ASN
42	Q	37	TYR
42	Q	102	ASP
43	R	64	VAL
43	R	90	HIS
43	R	95	PRO
43	R	97	ARG
43	R	104	ASN
43	R	107	THR
43	R	108	ARG
44	S	2	LYS
44	S	5	MET
44	S	27	LYS
44	S	85	GLU
45	T	86	LEU

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Mol	Chain	Res	Type
45	T	88	ARG
46	U	5	ARG
46	U	46	LYS
48	W	51	GLN
49	X	54	ARG
50	Y	84	LYS
51	Z	11	PHE
52	a	217	THR
59	8	19	ILE
59	8	20	ASP
59	8	24	THR
59	8	145	ASP
59	8	220	GLN
59	8	231	GLU
59	8	322	PHE
59	8	334	THR
59	8	362	ARG
59	8	371	ARG
59	8	407	GLU
59	8	441	GLU
59	8	442	ASP
59	8	446	ARG
59	8	502	GLU
59	8	530	ASN
59	8	573	ASP
59	8	587	ASP
59	8	623	THR
59	8	624	PRO
59	8	626	GLU
59	8	680	TYR
59	8	683	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	44	ASN
1	b	45	ASN
1	b	196	ASN
2	c	134	HIS
2	c	149	ASN
3	d	30	GLN
10	k	13	ASN

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Mol	Chain	Res	Type
10	k	88	ASN
12	m	17	ASN
13	n	62	ASN
17	r	6	GLN
17	r	11	GLN
17	r	87	GLN
20	u	39	ASN
20	u	73	ASN
23	x	16	ASN
26	A	20	ASN
28	C	45	HIS
32	G	119	GLN
32	G	145	ASN
34	I	195	ASN
35	J	96	GLN
37	L	67	ASN
37	L	129	ASN
37	L	147	ASN
43	R	7	ASN
44	S	3	GLN
45	T	34	GLN
46	U	9	HIS
49	X	52	ASN
50	Y	2	ASN
59	8	55	GLN
59	8	194	ASN
59	8	276	GLN
59	8	645	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	3	1538/1539 (99%)	214 (13%)	17 (1%)
54	1	2902/2903 (99%)	358 (12%)	15 (0%)
55	2	119/120 (99%)	12 (10%)	2 (1%)
56	5	76/77 (98%)	16 (21%)	2 (2%)
57	6	76/77 (98%)	23 (30%)	0
58	4	15/16 (93%)	3 (20%)	0
All	All	4726/4732 (99%)	626 (13%)	36 (0%)

All (626) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	3	6	G
53	3	9	G
53	3	22	G
53	3	32	A
53	3	39	G
53	3	48	C
53	3	51	A
53	3	71	A
53	3	82	G
53	3	87	C
53	3	95	C
53	3	100	G
53	3	130	A
53	3	131	A
53	3	144	G
53	3	149	A
53	3	181	A
53	3	183	C
53	3	184	G
53	3	197	A
53	3	209	U
53	3	210	C
53	3	211	G
53	3	226	G
53	3	247	G
53	3	251	G
53	3	253	A
53	3	266	G
53	3	267	C
53	3	281	G
53	3	289	G
53	3	308	C
53	3	316	C
53	3	321	A
53	3	328	C
53	3	345	C
53	3	346	G
53	3	352	C
53	3	354	G
53	3	355	C
53	3	367	U
53	3	372	C
53	3	373	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	3	412	A
53	3	413	G
53	3	414	A
53	3	422	C
53	3	429	U
53	3	430	A
53	3	439	U
53	3	462	G
53	3	467	U
53	3	484	G
53	3	486	U
53	3	495	A
53	3	497	G
53	3	518	C
53	3	531	U
53	3	532	A
53	3	533	A
53	3	534	U
53	3	536	C
53	3	537	G
53	3	547	A
53	3	561	U
53	3	572	A
53	3	573	A
53	3	575	G
53	3	576	C
53	3	577	G
53	3	596	A
53	3	607	A
53	3	623	C
53	3	633	G
53	3	665	A
53	3	687	A
53	3	703	G
53	3	724	G
53	3	755	G
53	3	777	A
53	3	815	A
53	3	817	C
53	3	818	G
53	3	819	A
53	3	821	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	3	842	U
53	3	843	U
53	3	844	G
53	3	846	G
53	3	851	G
53	3	873	A
53	3	885	G
53	3	890	G
53	3	902	G
53	3	914	A
53	3	926	G
53	3	927	G
53	3	928	G
53	3	929	G
53	3	934	C
53	3	935	A
53	3	946	A
53	3	960	U
53	3	961	U
53	3	966	G
53	3	969	A
53	3	971	G
53	3	975	A
53	3	976	G
53	3	977	A
53	3	979	C
53	3	983	A
53	3	992	U
53	3	993	G
53	3	1004	A
53	3	1020	G
53	3	1028	C
53	3	1031	C
53	3	1033	G
53	3	1034	G
53	3	1053	G
53	3	1054	C
53	3	1055	A
53	3	1061	G
53	3	1062	U
53	3	1064	G
53	3	1065	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	3	1066	C
53	3	1079	G
53	3	1080	A
53	3	1081	A
53	3	1086	U
53	3	1092	A
53	3	1093	A
53	3	1094	G
53	3	1095	U
53	3	1101	A
53	3	1115	U
53	3	1116	U
53	3	1118	U
53	3	1119	C
53	3	1121	U
53	3	1122	U
53	3	1123	U
53	3	1124	G
53	3	1125	U
53	3	1126	U
53	3	1127	G
53	3	1136	C
53	3	1137	C
53	3	1138	G
53	3	1139	G
53	3	1148	U
53	3	1149	C
53	3	1159	U
53	3	1160	G
53	3	1165	U
53	3	1166	G
53	3	1167	A
53	3	1168	U
53	3	1169	A
53	3	1182	G
53	3	1183	U
53	3	1184	G
53	3	1190	G
53	3	1191	A
53	3	1196	A
53	3	1198	G
53	3	1201	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	3	1202	U
53	3	1212	U
53	3	1225	A
53	3	1238	A
53	3	1240	U
53	3	1241	G
53	3	1258	G
53	3	1260	G
53	3	1275	A
53	3	1278	G
53	3	1280	A
53	3	1282	C
53	3	1286	U
53	3	1287	A
53	3	1300	G
53	3	1303	C
53	3	1305	G
53	3	1306	A
53	3	1308	U
53	3	1313	U
53	3	1317	C
53	3	1346	A
53	3	1347	G
53	3	1363	A
53	3	1378	C
53	3	1383	C
53	3	1384	C
53	3	1394	A
53	3	1397	C
53	3	1399	C
53	3	1446	A
53	3	1448	C
53	3	1452	C
53	3	1492	A
53	3	1494	G
53	3	1502	A
53	3	1503	A
53	3	1505	G
53	3	1506	U
53	3	1517	G
53	3	1529	G
53	3	1530	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	3	1534	A
53	3	1535	C
53	3	1540	U
54	1	10	A
54	1	12	U
54	1	34	U
54	1	35	G
54	1	46	G
54	1	50	U
54	1	51	G
54	1	63	A
54	1	71	A
54	1	74	A
54	1	75	G
54	1	103	A
54	1	119	A
54	1	120	U
54	1	139	U
54	1	140	C
54	1	141	G
54	1	142	A
54	1	162	U
54	1	163	C
54	1	196	A
54	1	216	A
54	1	221	A
54	1	222	A
54	1	224	U
54	1	228	C
54	1	248	G
54	1	249	C
54	1	255	A
54	1	266	G
54	1	276	U
54	1	281	C
54	1	294	A
54	1	301	G
54	1	311	A
54	1	323	C
54	1	324	A
54	1	329	G
54	1	330	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	1	353	C
54	1	361	G
54	1	371	A
54	1	372	G
54	1	386	G
54	1	387	U
54	1	404	A
54	1	406	G
54	1	411	G
54	1	422	A
54	1	424	G
54	1	457	A
54	1	481	G
54	1	491	G
54	1	504	A
54	1	505	A
54	1	518	G
54	1	529	A
54	1	530	G
54	1	531	C
54	1	532	A
54	1	542	C
54	1	543	G
54	1	545	U
54	1	547	A
54	1	563	A
54	1	573	U
54	1	574	A
54	1	603	A
54	1	614	A
54	1	616	A
54	1	627	A
54	1	637	A
54	1	645	C
54	1	646	U
54	1	654	A
54	1	669	G
54	1	686	U
54	1	687	C
54	1	694	U
54	1	695	G
54	1	730	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	1	747	C
54	1	752	A
54	1	764	A
54	1	775	G
54	1	776	G
54	1	782	A
54	1	784	G
54	1	785	G
54	1	805	G
54	1	806	C
54	1	812	C
54	1	819	A
54	1	827	U
54	1	828	U
54	1	830	G
54	1	845	A
54	1	846	U
54	1	847	U
54	1	858	G
54	1	859	G
54	1	860	U
54	1	878	A
54	1	885	C
54	1	886	A
54	1	887	U
54	1	896	A
54	1	897	C
54	1	910	A
54	1	932	U
54	1	941	A
54	1	946	C
54	1	961	C
54	1	962	G
54	1	974	G
54	1	983	A
54	1	995	C
54	1	996	A
54	1	1012	U
54	1	1013	C
54	1	1021	A
54	1	1022	G
54	1	1033	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	1	1045	C
54	1	1046	A
54	1	1054	A
54	1	1056	G
54	1	1062	G
54	1	1063	G
54	1	1064	C
54	1	1065	U
54	1	1066	U
54	1	1067	A
54	1	1068	G
54	1	1070	A
54	1	1071	G
54	1	1076	C
54	1	1079	C
54	1	1082	U
54	1	1084	A
54	1	1085	A
54	1	1088	A
54	1	1104	C
54	1	1106	G
54	1	1111	A
54	1	1131	G
54	1	1132	U
54	1	1135	C
54	1	1143	A
54	1	1157	G
54	1	1175	A
54	1	1176	U
54	1	1177	G
54	1	1180	U
54	1	1181	U
54	1	1212	G
54	1	1251	C
54	1	1253	A
54	1	1256	G
54	1	1271	G
54	1	1272	A
54	1	1301	A
54	1	1321	A
54	1	1329	U
54	1	1330	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	1	1345	C
54	1	1365	A
54	1	1378	A
54	1	1379	U
54	1	1383	A
54	1	1395	A
54	1	1398	C
54	1	1416	G
54	1	1419	A
54	1	1420	A
54	1	1428	C
54	1	1454	C
54	1	1461	C
54	1	1476	U
54	1	1482	G
54	1	1490	A
54	1	1498	C
54	1	1504	A
54	1	1515	A
54	1	1524	G
54	1	1533	C
54	1	1535	A
54	1	1536	C
54	1	1537	G
54	1	1555	G
54	1	1559	U
54	1	1560	G
54	1	1565	C
54	1	1569	A
54	1	1578	U
54	1	1581	G
54	1	1584	U
54	1	1585	C
54	1	1608	A
54	1	1611	C
54	1	1616	A
54	1	1647	U
54	1	1648	U
54	1	1654	A
54	1	1674	G
54	1	1703	G
54	1	1715	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	1	1729	U
54	1	1730	C
54	1	1738	G
54	1	1758	U
54	1	1764	C
54	1	1773	A
54	1	1780	A
54	1	1791	A
54	1	1800	C
54	1	1801	A
54	1	1808	A
54	1	1816	C
54	1	1829	A
54	1	1871	A
54	1	1901	A
54	1	1906	G
54	1	1907	G
54	1	1913	A
54	1	1929	G
54	1	1930	G
54	1	1937	A
54	1	1938	A
54	1	1944	U
54	1	1955	U
54	1	1962	C
54	1	1963	U
54	1	1967	C
54	1	1970	A
54	1	1971	U
54	1	1972	G
54	1	1991	U
54	1	1997	C
54	1	2020	A
54	1	2022	U
54	1	2023	C
54	1	2030	A
54	1	2031	A
54	1	2043	C
54	1	2049	G
54	1	2052	A
54	1	2055	C
54	1	2056	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	1	2060	A
54	1	2061	G
54	1	2062	A
54	1	2069	G
54	1	2072	C
54	1	2096	C
54	1	2098	U
54	1	2110	G
54	1	2111	U
54	1	2112	G
54	1	2113	U
54	1	2115	G
54	1	2118	U
54	1	2119	A
54	1	2125	G
54	1	2129	C
54	1	2131	U
54	1	2132	U
54	1	2133	G
54	1	2145	C
54	1	2147	A
54	1	2162	G
54	1	2172	U
54	1	2173	A
54	1	2174	C
54	1	2176	A
54	1	2189	U
54	1	2198	A
54	1	2203	U
54	1	2204	G
54	1	2211	A
54	1	2212	A
54	1	2213	U
54	1	2225	A
54	1	2239	G
54	1	2268	A
54	1	2278	A
54	1	2283	C
54	1	2287	A
54	1	2297	A
54	1	2305	U
54	1	2309	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	1	2325	G
54	1	2327	A
54	1	2334	U
54	1	2337	G
54	1	2345	G
54	1	2350	C
54	1	2383	G
54	1	2385	C
54	1	2392	A
54	1	2402	U
54	1	2406	A
54	1	2423	U
54	1	2424	C
54	1	2425	A
54	1	2426	A
54	1	2427	C
54	1	2429	G
54	1	2430	A
54	1	2435	A
54	1	2441	U
54	1	2448	A
54	1	2476	A
54	1	2494	G
54	1	2498	C
54	1	2502	G
54	1	2505	G
54	1	2518	A
54	1	2529	G
54	1	2547	A
54	1	2554	U
54	1	2566	A
54	1	2567	G
54	1	2572	A
54	1	2602	A
54	1	2603	G
54	1	2609	U
54	1	2613	U
54	1	2629	U
54	1	2646	C
54	1	2655	G
54	1	2682	A
54	1	2689	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	1	2690	U
54	1	2714	G
54	1	2716	C
54	1	2744	G
54	1	2748	A
54	1	2757	A
54	1	2764	A
54	1	2765	A
54	1	2778	A
54	1	2779	U
54	1	2791	G
54	1	2794	C
54	1	2797	U
54	1	2800	A
54	1	2801	G
54	1	2809	A
54	1	2820	A
54	1	2821	A
54	1	2833	U
54	1	2867	G
54	1	2868	A
54	1	2872	A
54	1	2880	C
54	1	2883	A
54	1	2884	U
55	2	4	C
55	2	13	G
55	2	24	G
55	2	35	C
55	2	40	U
55	2	44	G
55	2	51	G
55	2	67	G
55	2	89	U
55	2	90	C
55	2	108	A
55	2	109	A
56	5	3	G
56	5	4	C
56	5	5	G
56	5	6	A
56	5	9	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
56	5	14	A
56	5	18	G
56	5	19	G
56	5	20	U
56	5	21	A
56	5	42	G
56	5	47	U
56	5	48	C
56	5	61	C
56	5	73	A
56	5	76	A
57	6	2	G
57	6	3	C
57	6	8	U
57	6	9	G
57	6	10	G
57	6	14	A
57	6	17	C
57	6	19	G
57	6	20	U
57	6	21	A
57	6	22	G
57	6	28	C
57	6	33	U
57	6	34	C
57	6	35	A
57	6	39	C
57	6	46	G
57	6	61	C
57	6	64	G
57	6	65	C
57	6	69	C
57	6	70	G
57	6	76	A
58	4	16	A
58	4	20	C
58	4	21	C

All (36) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	3	70	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	3	280	C
53	3	328	C
53	3	413	G
53	3	438	U
53	3	928	G
53	3	965	U
53	3	1061	G
53	3	1078	U
53	3	1164	G
53	3	1168	U
53	3	1183	U
53	3	1201	A
53	3	1280	A
53	3	1305	G
53	3	1347	G
53	3	1493	A
54	1	227	A
54	1	421	C
54	1	490	C
54	1	774	G
54	1	859	G
54	1	1020	A
54	1	1130	U
54	1	1475	G
54	1	2286	G
54	1	2296	U
54	1	2326	C
54	1	2333	A
54	1	2391	G
54	1	2756	U
54	1	2808	G
55	2	66	A
55	2	88	C
56	5	2	G
56	5	3	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
61	PRO	5	101	56,60	5,7,8	0.56	0	7,8,10	1.20	1 (14%)
60	FME	1	3001	61	8,9,10	0.72	0	7,9,11	1.22	1 (14%)
62	GCP	8	801	63	27,34,34	2.27	7 (25%)	34,54,54	3.83	19 (55%)

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
61	PRO	5	101	56,60	-	0/0/9/11	0/1/1/1
60	FME	1	3001	61	-	1/7/9/11	-
62	GCP	8	801	63	-	9/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	8	801	GCP	PB-O3A	-8.17	1.49	1.58
62	8	801	GCP	O4'-C1'	3.81	1.46	1.41
62	8	801	GCP	C6-N1	3.38	1.38	1.33
62	8	801	GCP	PB-O2B	-3.04	1.49	1.56
62	8	801	GCP	PG-O2G	-2.51	1.49	1.54
62	8	801	GCP	C2-N1	2.48	1.39	1.35
62	8	801	GCP	PG-O3G	-2.44	1.49	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	8	801	GCP	C1'-N9-C4	13.76	150.81	126.64
62	8	801	GCP	C5-C6-N1	-8.68	111.56	123.43
62	8	801	GCP	C2-N1-C6	6.58	126.38	115.93
62	8	801	GCP	O4'-C1'-C2'	-4.50	100.35	106.93
62	8	801	GCP	O2G-PG-C3B	-4.47	95.54	106.40
62	8	801	GCP	C2-N3-C4	-4.35	110.39	115.36
62	8	801	GCP	O3G-PG-O2G	4.14	120.16	108.08
62	8	801	GCP	C4-C5-C6	-3.73	117.23	120.80
62	8	801	GCP	O2B-PB-O1B	3.71	122.45	110.07
62	8	801	GCP	O3'-C3'-C4'	-3.48	100.98	111.05
62	8	801	GCP	C4-C5-N7	3.44	112.98	109.40
62	8	801	GCP	O1B-PB-C3B	2.84	116.58	109.07
62	8	801	GCP	PB-O3A-PA	2.82	141.52	132.56
62	8	801	GCP	O2A-PA-O5'	-2.70	95.19	107.75
62	8	801	GCP	N3-C2-N1	-2.58	123.79	127.22
62	8	801	GCP	O3G-PG-O1G	-2.49	105.80	112.39
62	8	801	GCP	O4'-C4'-C5'	2.30	116.95	109.37
62	8	801	GCP	O2A-PA-O1A	2.27	123.47	112.24
60	1	3001	FME	CA-N-CN	-2.23	119.39	122.82
61	5	101	PRO	O-C-CA	-2.20	119.01	124.78
62	8	801	GCP	C3'-C2'-C1'	-2.02	97.94	100.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

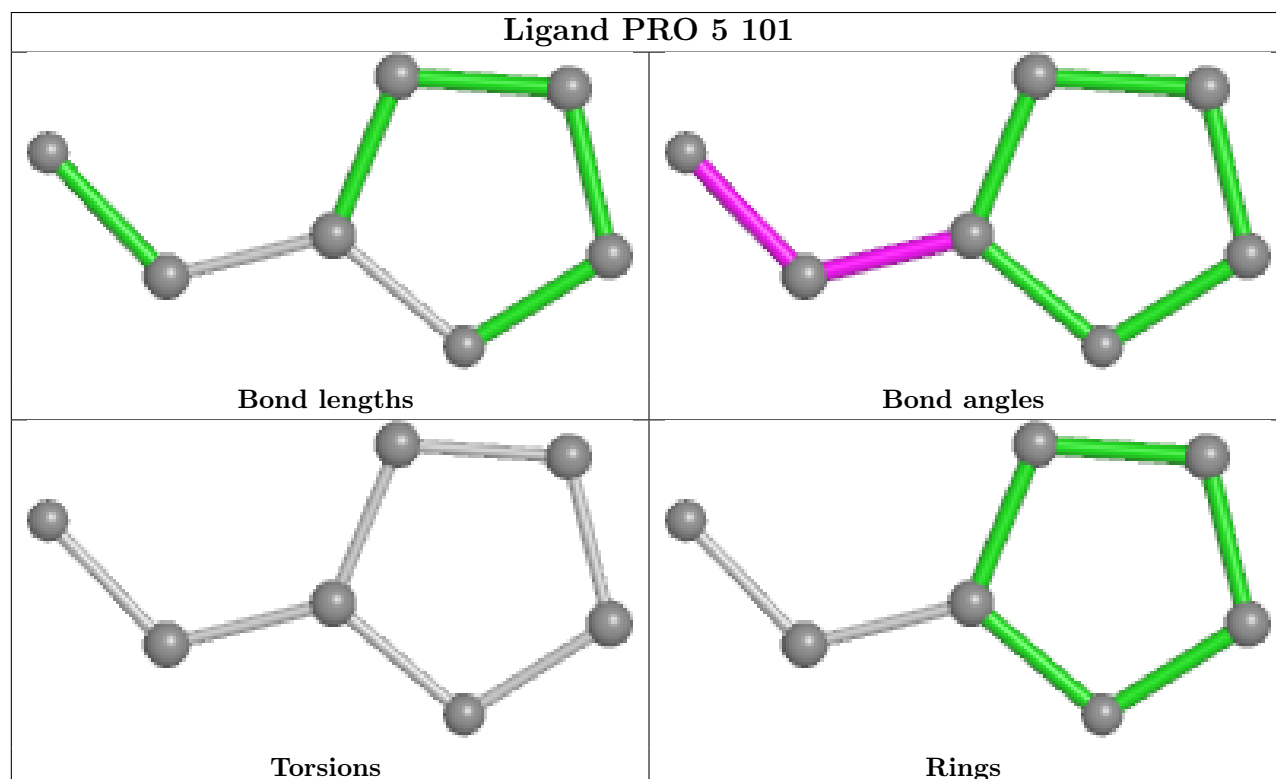
Mol	Chain	Res	Type	Atoms
60	1	3001	FME	O1-CN-N-CA
62	8	801	GCP	PB-C3B-PG-O1G
62	8	801	GCP	PG-C3B-PB-O1B
62	8	801	GCP	C5'-O5'-PA-O3A
62	8	801	GCP	C5'-O5'-PA-O1A
62	8	801	GCP	O4'-C4'-C5'-O5'
62	8	801	GCP	C5'-O5'-PA-O2A
62	8	801	GCP	PB-C3B-PG-O2G
62	8	801	GCP	PB-C3B-PG-O3G
62	8	801	GCP	C3'-C4'-C5'-O5'

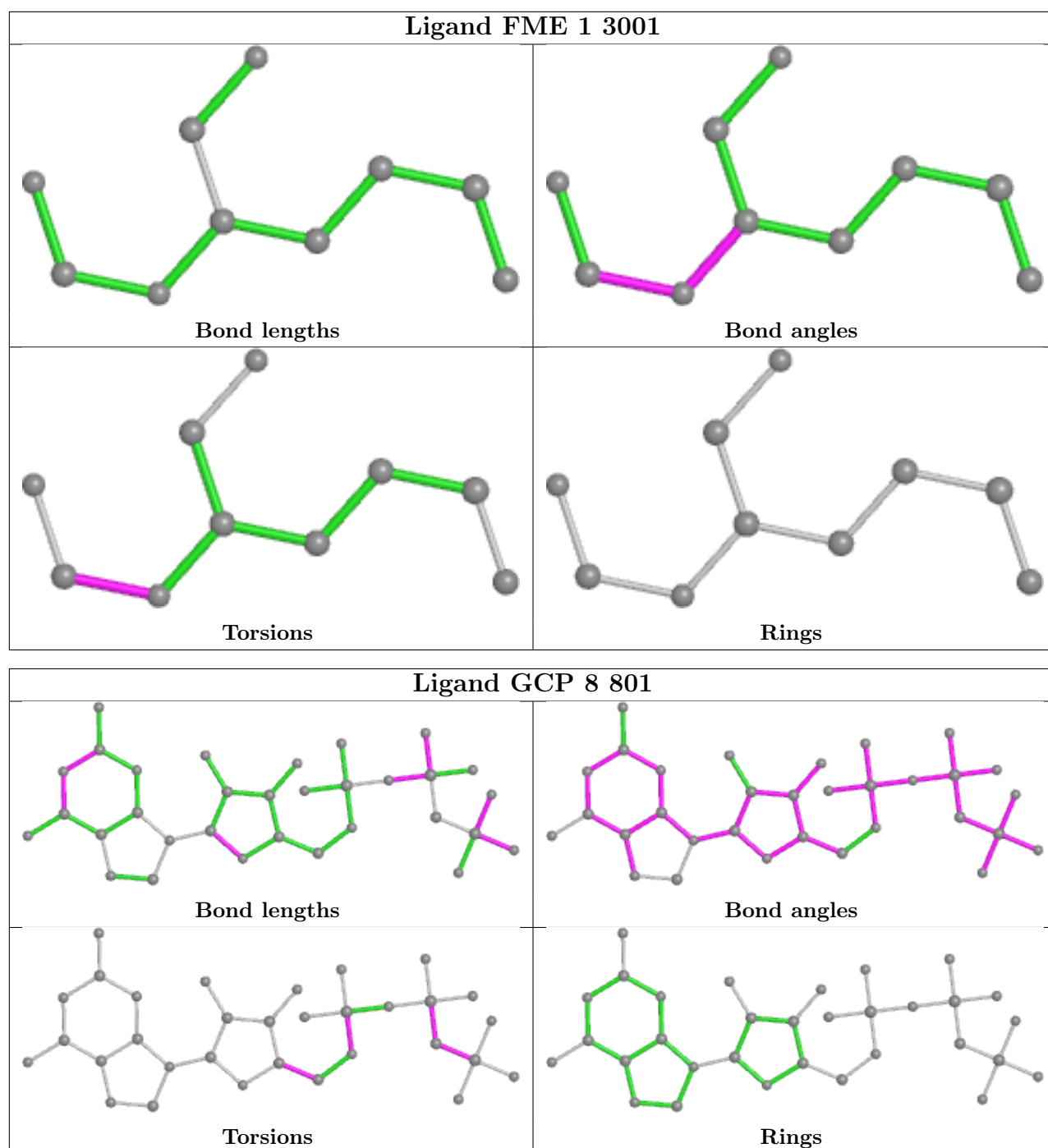
There are no ring outliers.

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.

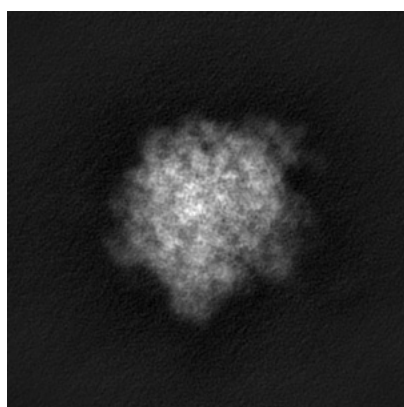
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22673. These allow visual inspection of the internal detail of the map and identification of artifacts.

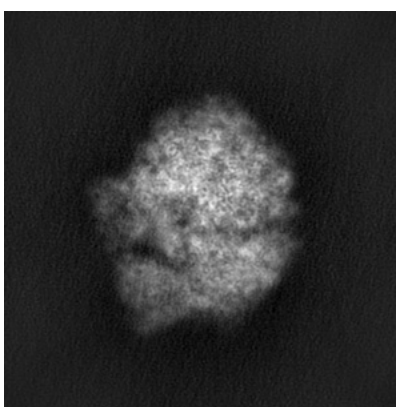
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

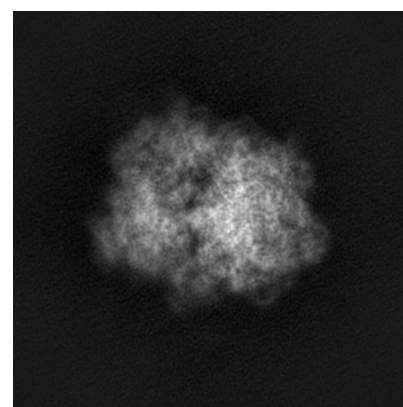
#### 6.1.1 Primary map



X



Y

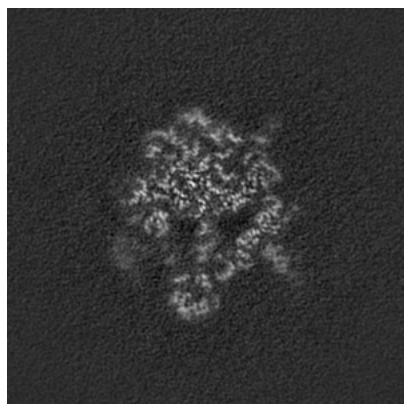


Z

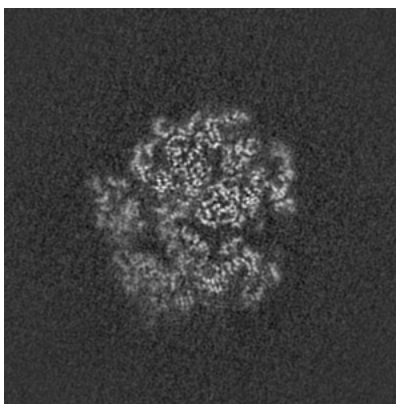
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

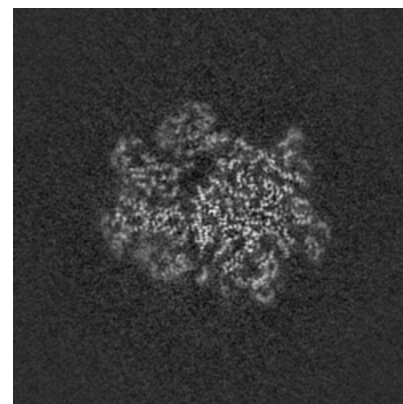
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

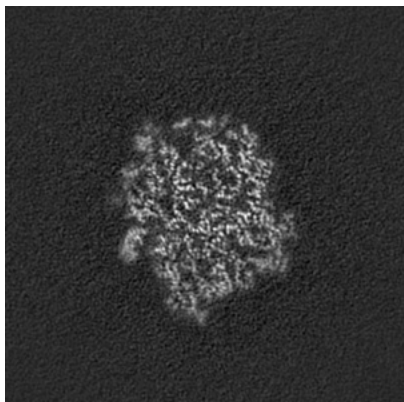


Z Index: 200

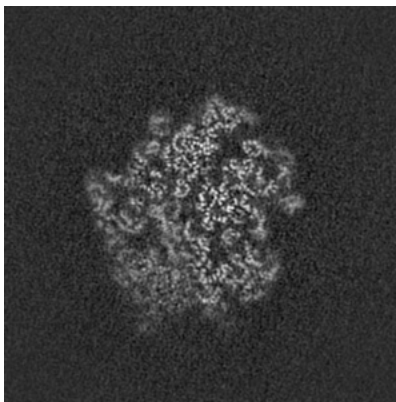
The images above show central slices of the map in three orthogonal directions.

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

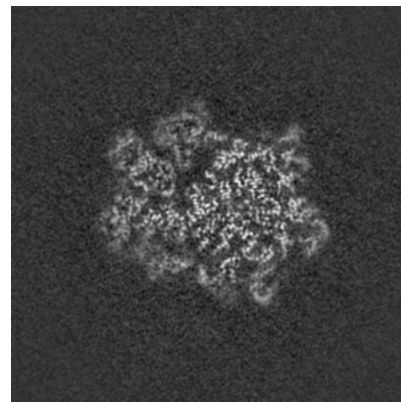
### 6.3.1 Primary map



X Index: 222



Y Index: 193



Z Index: 203

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



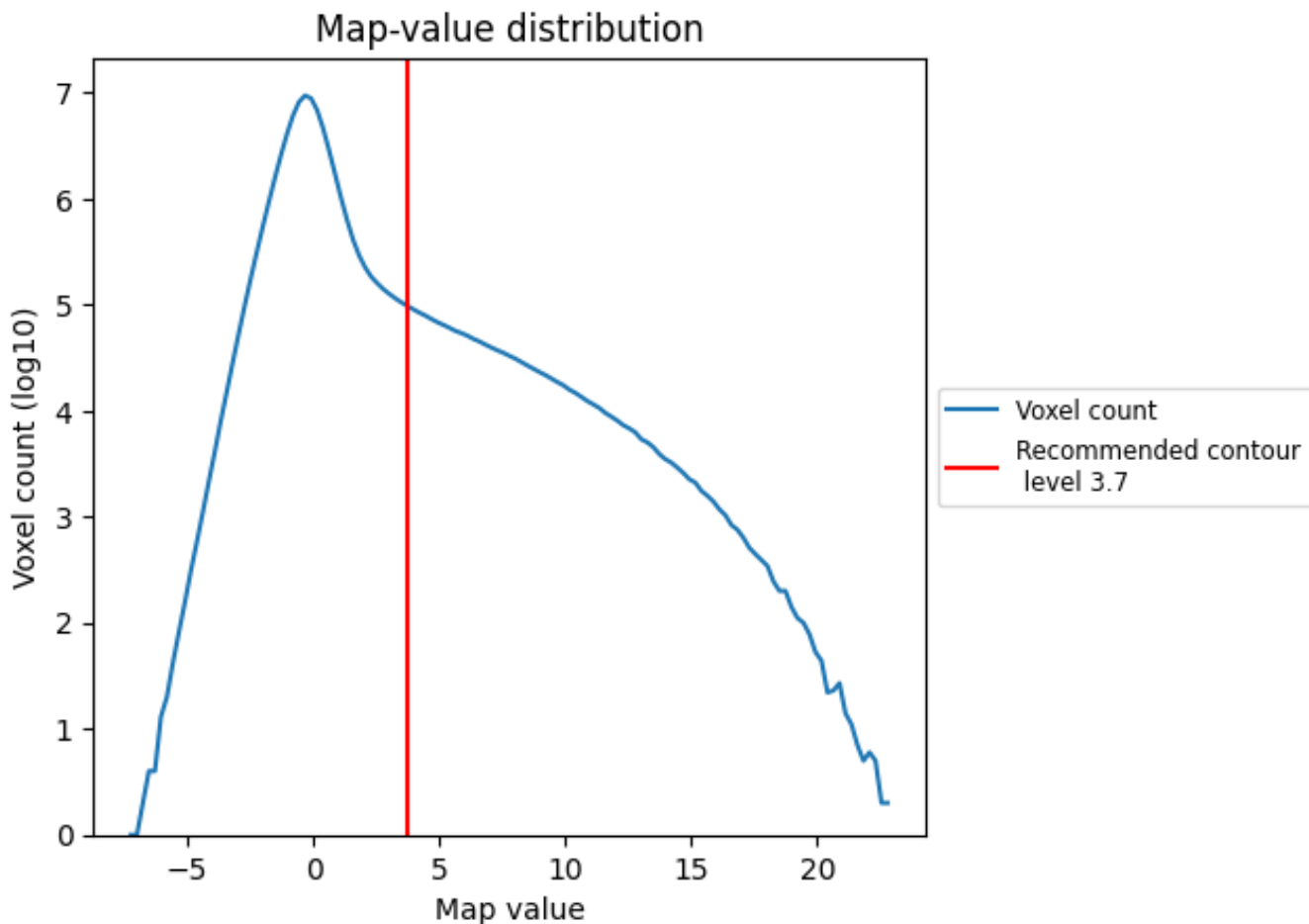
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

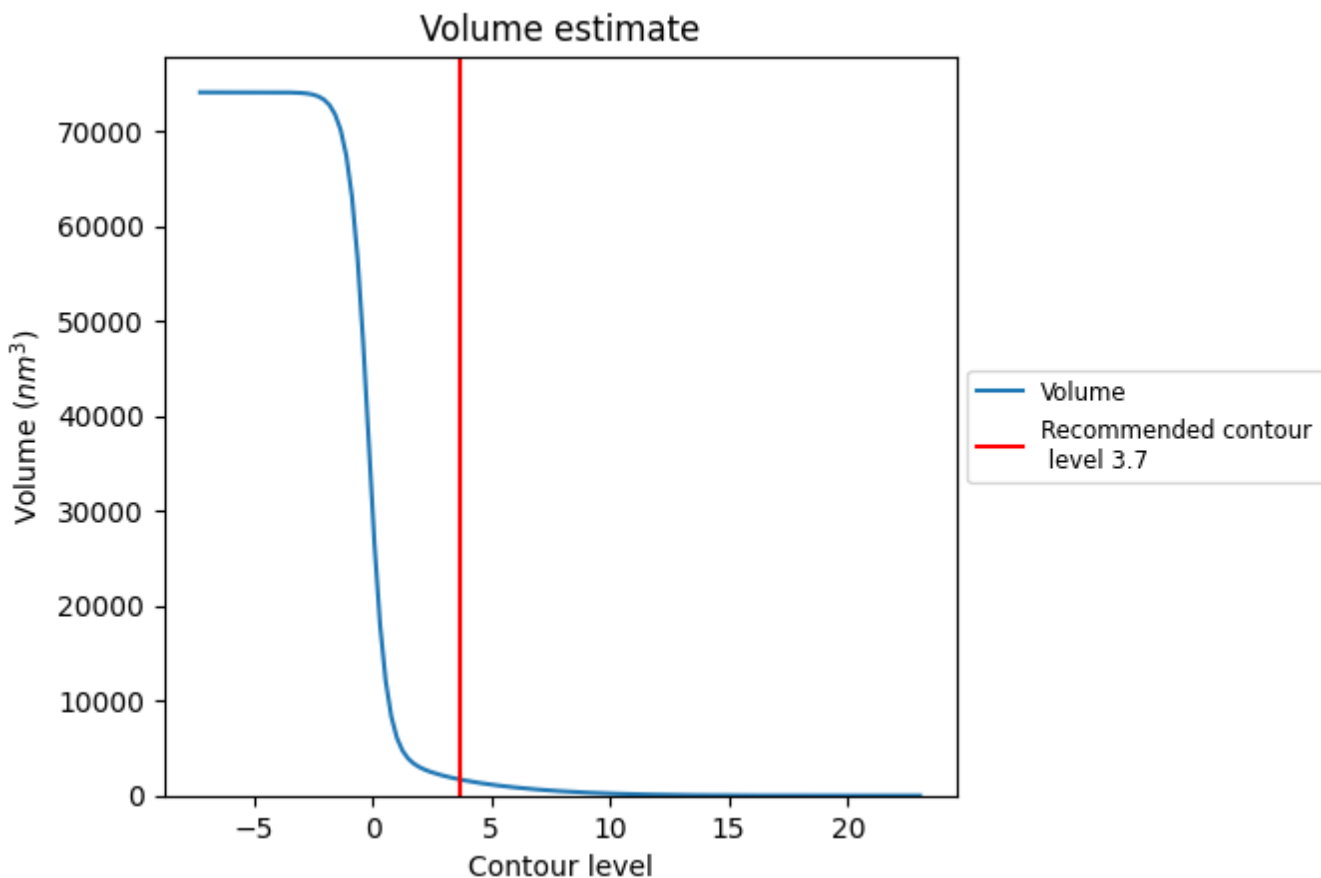
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

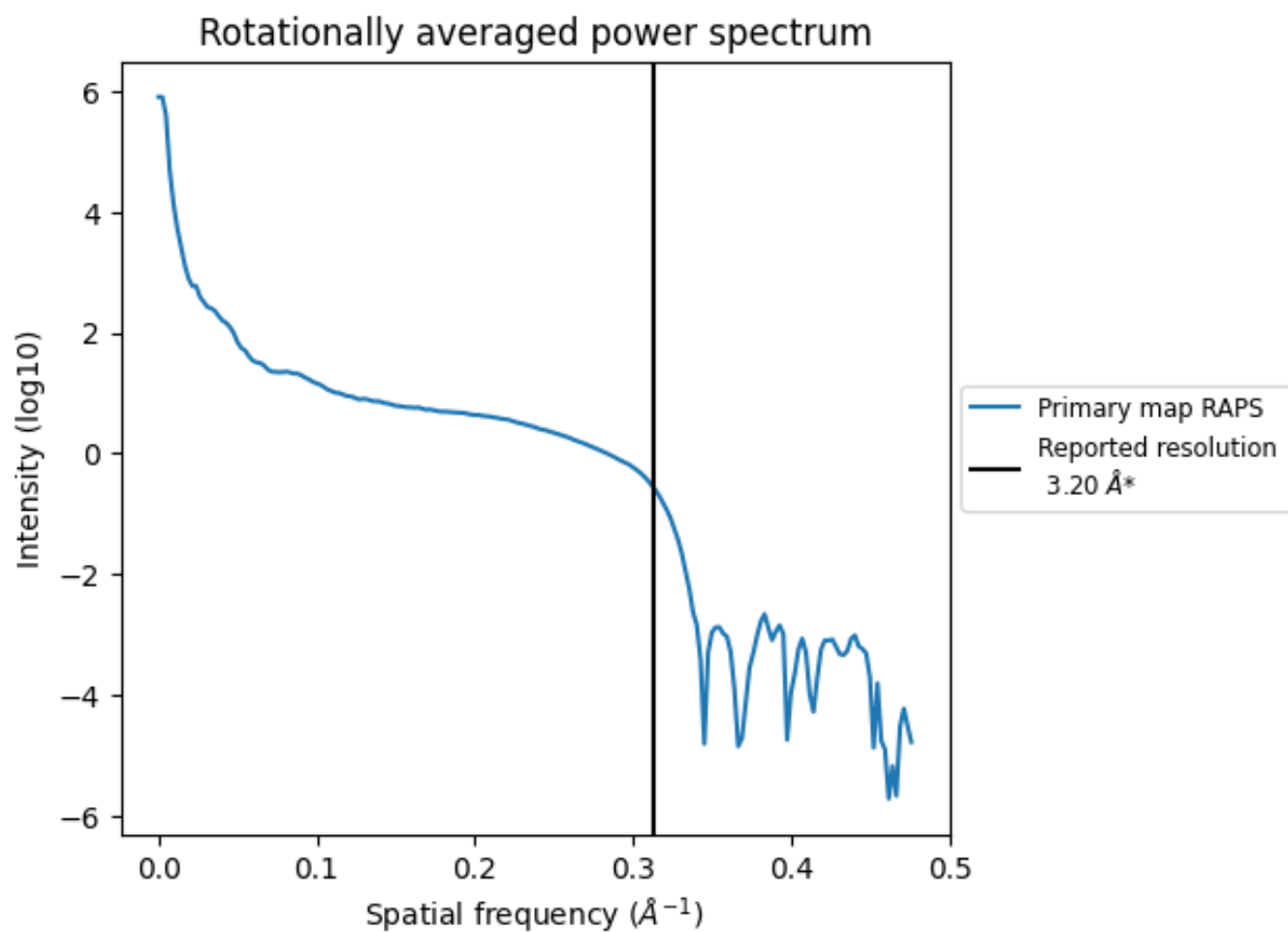
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1689 nm<sup>3</sup>; this corresponds to an approximate mass of 1525 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 0.312 Å<sup>-1</sup>

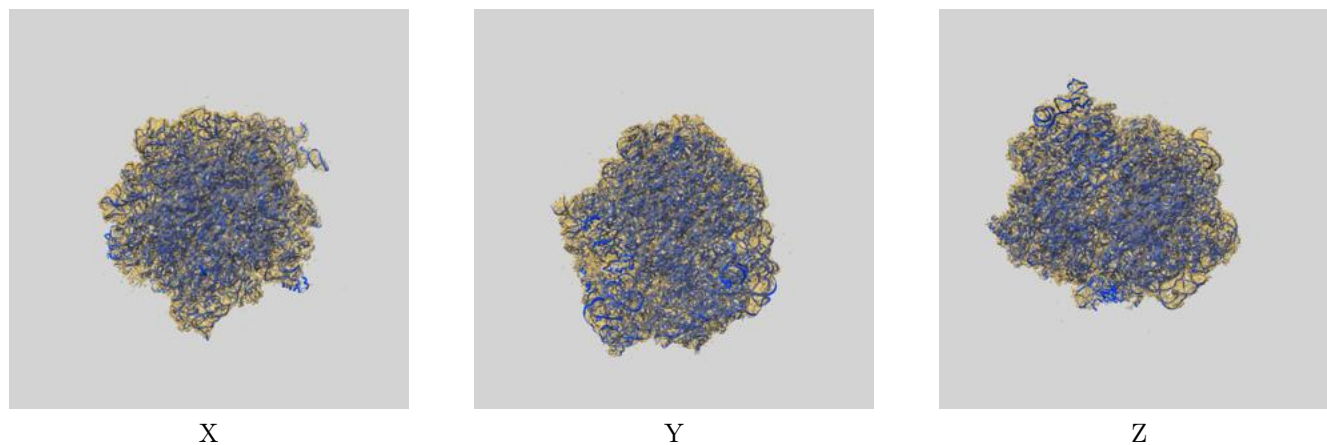
## 8 Fourier-Shell correlation

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

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

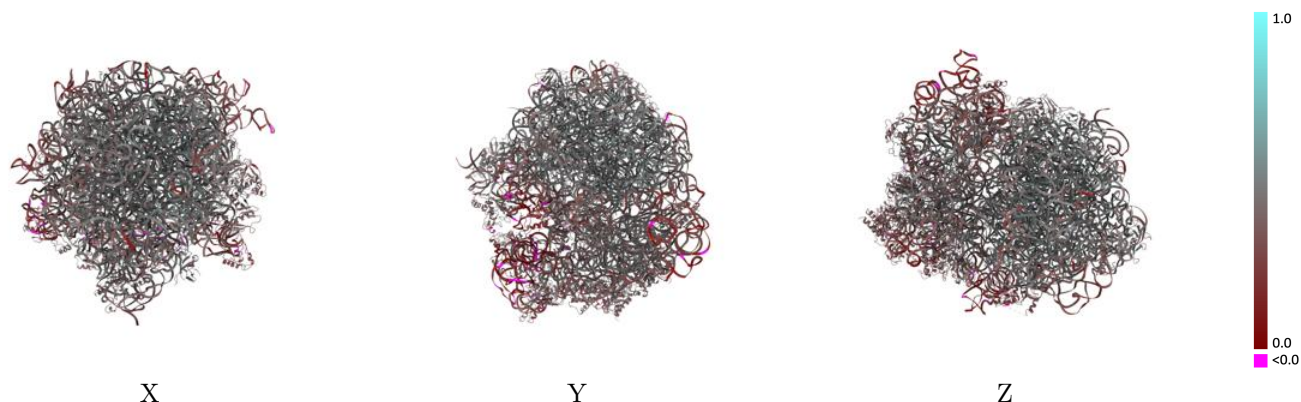
This section contains information regarding the fit between EMDB map EMD-22673 and PDB model 7K54. Per-residue inclusion information can be found in section 3 on page 17.

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



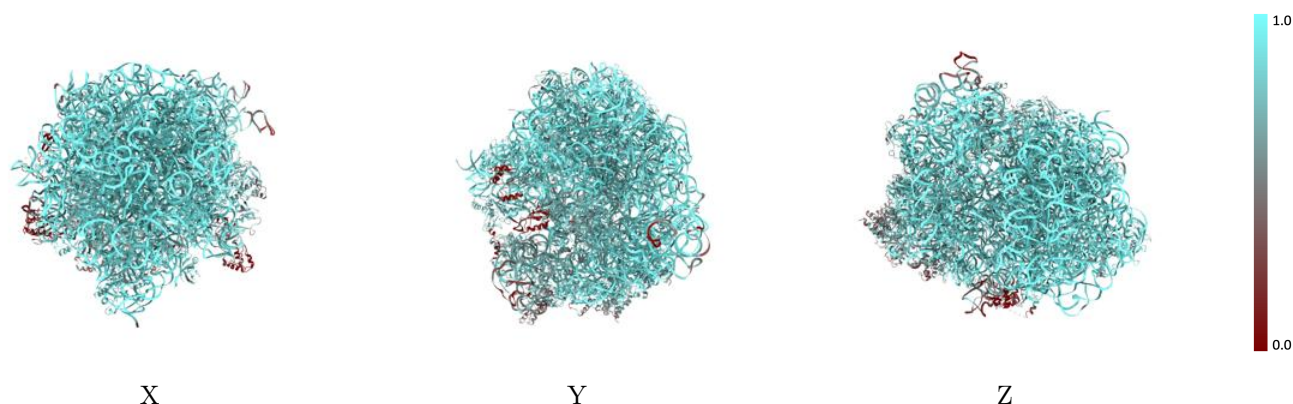
The images above show the 3D surface view of the map at the recommended contour level 3.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



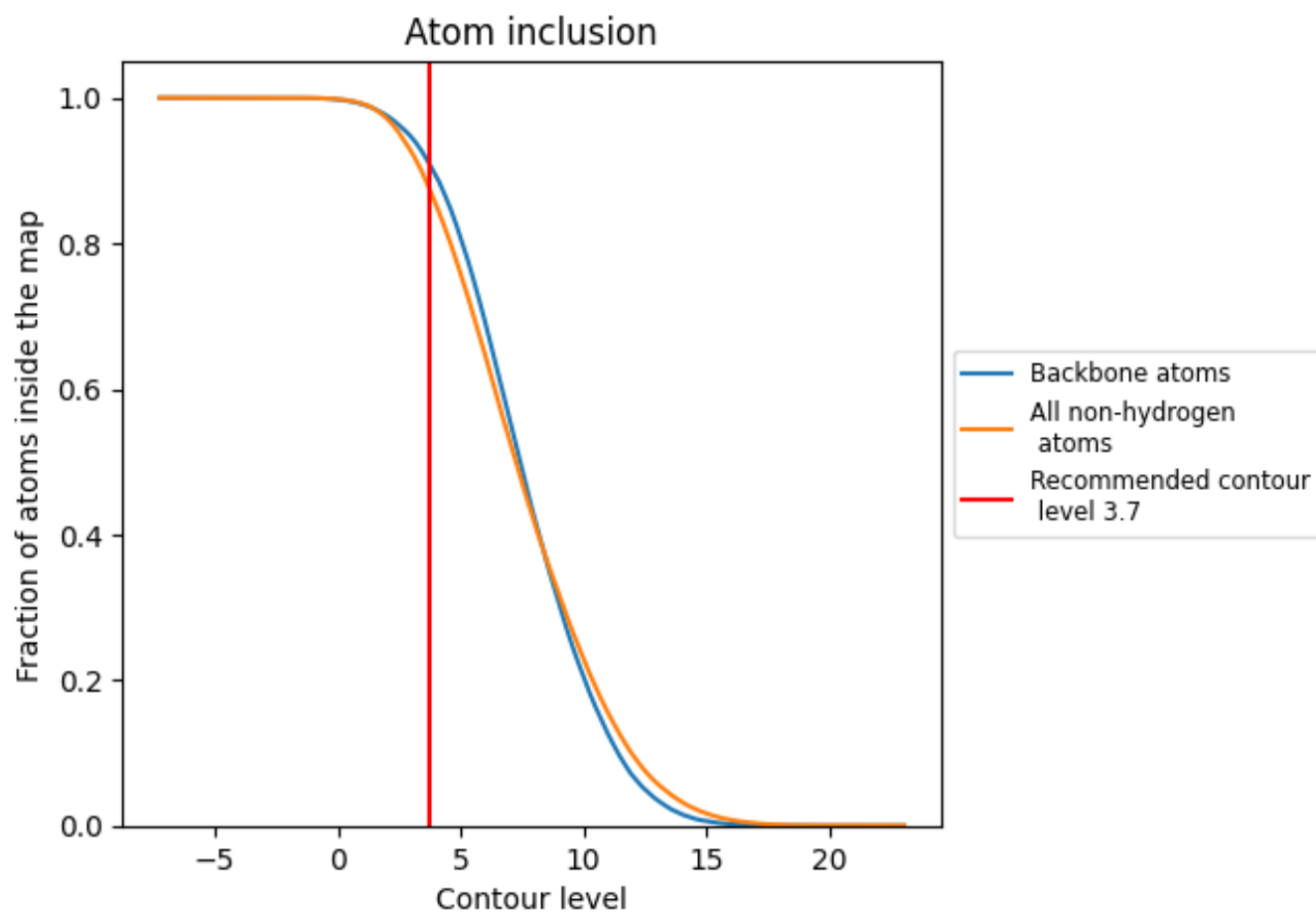
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.7).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 91% of all backbone atoms, 88% 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 (3.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8774	 0.4060
1	 0.9622	 0.4380
2	 0.9611	 0.4100
3	 0.8840	 0.3450
4	 0.7254	 0.3410
5	 0.9395	 0.3580
6	 0.9006	 0.3430
8	 0.7548	 0.3830
A	 0.5938	 0.2860
B	 0.9112	 0.4640
C	 0.7090	 0.4330
D	 0.9155	 0.4900
E	 0.9267	 0.4920
F	 0.9144	 0.4770
G	 0.5406	 0.3570
H	 0.6947	 0.4040
I	 0.7597	 0.3970
J	 0.8414	 0.4310
K	 0.8281	 0.3880
L	 0.4952	 0.3060
M	 0.8406	 0.4260
N	 0.6537	 0.3620
O	 0.5315	 0.3510
P	 0.8735	 0.4050
Q	 0.8393	 0.4580
R	 0.6045	 0.3240
S	 0.7907	 0.3810
T	 0.8507	 0.4080
U	 0.8086	 0.4220
V	 0.8641	 0.4190
W	 0.8369	 0.4010
X	 0.7637	 0.3280
Y	 0.8262	 0.3950
Z	 0.7317	 0.3320
a	 0.2020	 0.2340



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Chain	Atom inclusion	Q-score
b	 0.9192	 0.4940
c	 0.8999	 0.4780
d	 0.7921	 0.4420
e	 0.8115	 0.3850
f	 0.8219	 0.4250
g	 0.2384	 0.3080
h	 0.1118	 0.2330
i	 0.1316	 0.2020
j	 0.9000	 0.4660
k	 0.8807	 0.4820
l	 0.8848	 0.4720
m	 0.9107	 0.4820
n	 0.9133	 0.4690
o	 0.8621	 0.4220
p	 0.8818	 0.4710
q	 0.9141	 0.4790
r	 0.8532	 0.4650
s	 0.8768	 0.4680
t	 0.8492	 0.4550
u	 0.8307	 0.4200
v	 0.8482	 0.4540
w	 0.9070	 0.4890
x	 0.9035	 0.4690
y	 0.7545	 0.3880
z	 0.8741	 0.4560