



## Full wwPDB EM Validation Report ⓘ

May 18, 2024 – 10:40 AM EDT

PDB ID : 7K55  
EMDB ID : EMD-22674  
Title : Near post-translocated +1-frameshifting(CCC-A) complex with EF-G and GDPCP (Structure III-FS)  
Authors : Demo, G.; Loveland, A.B.; Svidritskiy, E.; Gamper, H.B.; Hou, Y.M.; Korostelev, A.A.  
Deposited on : 2020-09-16  
Resolution : 3.30 Å(reported)  
Based on initial models : 4V7D, 5UYM, 4V9P, 6ENJ

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 : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

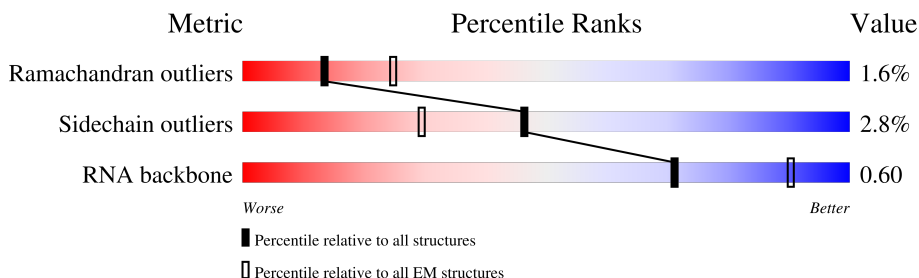
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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.



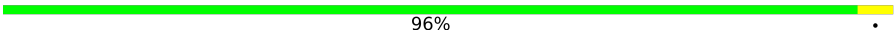
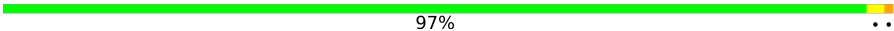
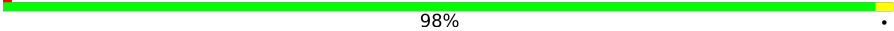
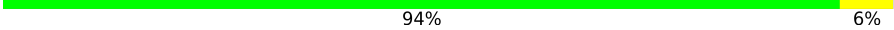


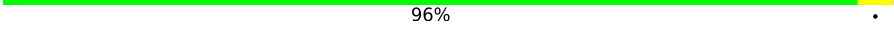
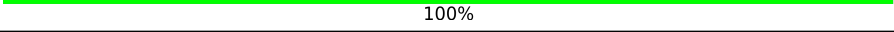
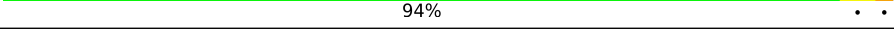
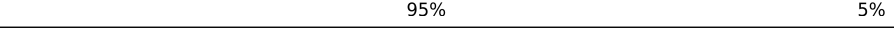
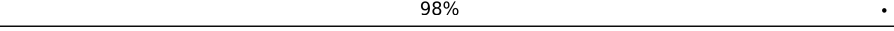
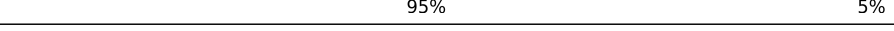
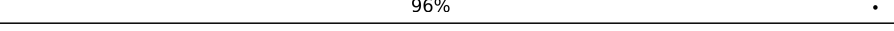
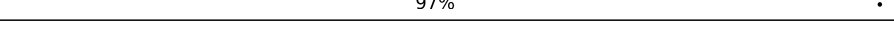
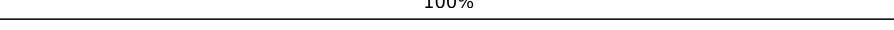
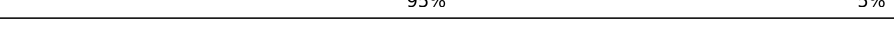
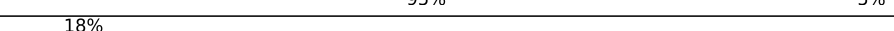

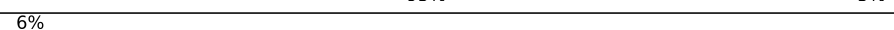
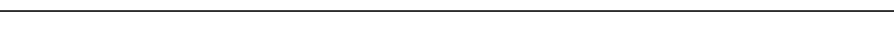

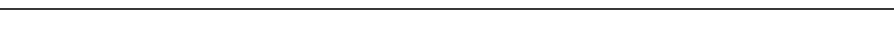
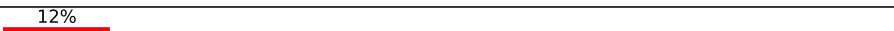


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	
2	c	209	
3	d	201	
4	e	177	
5	f	176	
6	g	149	
7	h	131	
8	i	141	



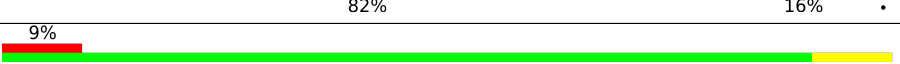
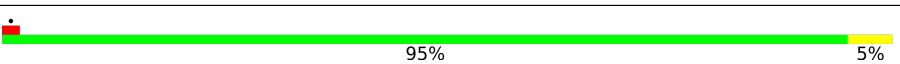
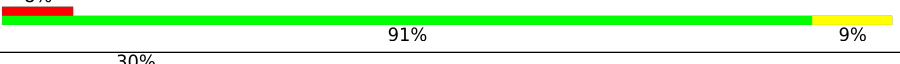

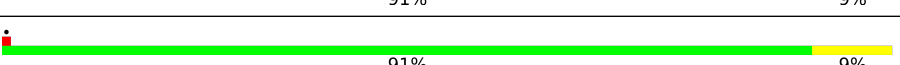

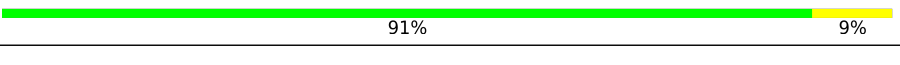
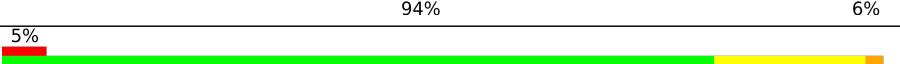
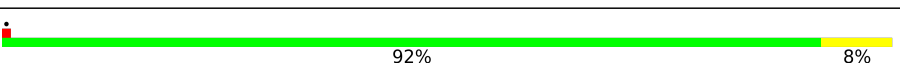
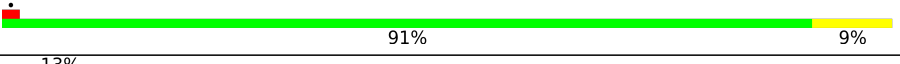

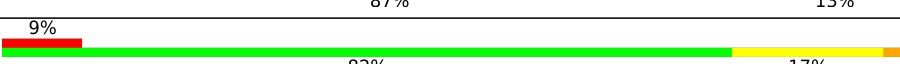

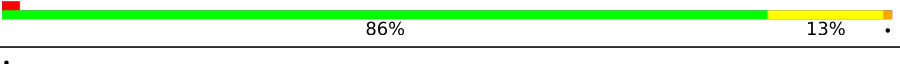

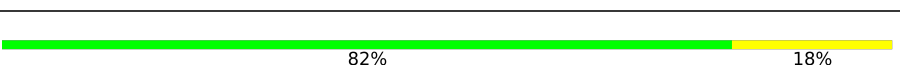





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Mol	Chain	Length	Quality of chain
9	j	142	 96% .
10	k	122	 97% ..
11	l	143	 98% .
12	m	136	 94% 6%
13	n	120	 92% 8% .
14	o	116	 92% 8%
15	p	114	 96% .
16	q	117	 100%
17	r	103	 94% . .
18	s	110	 95% 5%
19	t	93	 98% .
20	u	102	 95% 5%
21	v	94	 96% .
22	w	75	 97% .
23	x	77	 100%
24	y	63	 95% 5%
25	z	58	 95% 5%
26	A	66	 18% 89% 11%
27	B	56	 95% 5%
28	C	50	 6% 98% .
29	D	46	 96% .
30	E	64	 84% 16%
31	F	38	 87% 13%
32	G	225	 12% 87% 9% .
33	H	206	 10% 90% 10%

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Mol	Chain	Length	Quality of chain
34	I	205	
35	J	157	
36	K	100	
37	L	151	
38	M	129	
39	N	127	
40	O	98	
41	P	116	
42	Q	123	
43	R	114	
44	S	100	
45	T	88	
46	U	82	
47	V	80	
48	W	65	
49	X	79	
50	Y	85	
51	Z	65	
52	a	223	
53	3	1539	
54	1	2903	
55	2	120	
56	5	77	
57	6	77	
58	4	16	

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Mol	Chain	Length	Quality of chain
59	8	711	<div><div></div><div>20%</div><div></div><div>84%</div><div></div><div>12%</div><div></div></div>

## 2 Entry composition

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
1	b	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			917	574	179	163	1	0

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

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

- 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
			816	516	153	145	2	0

- 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
			857	532	166	156	3	0

- 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
			739	466	139	132	2	0

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

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

- 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
35	J	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
55	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

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
56	5	77	Total	C	N	O	P	0	0
			1647	733	295	542	77		

- Molecule 57 is a RNA chain called tRNAfMet.

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

- Molecule 58 is a RNA chain called mRNA.

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

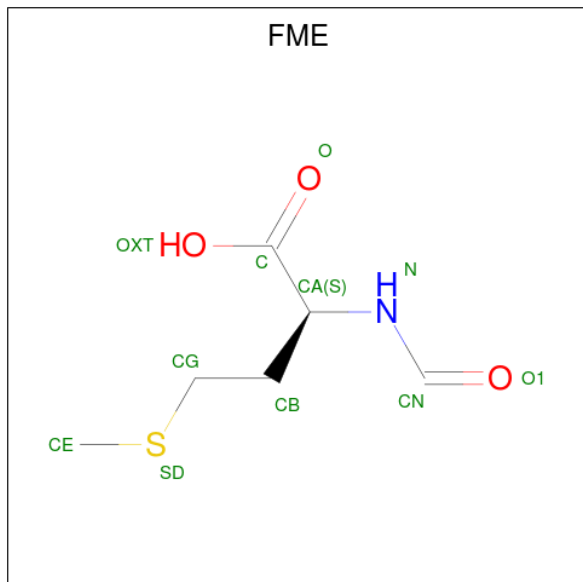
- Molecule 59 is a protein called Elongation factor G.

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

There are 8 discrepancies between the modelled and reference sequences:

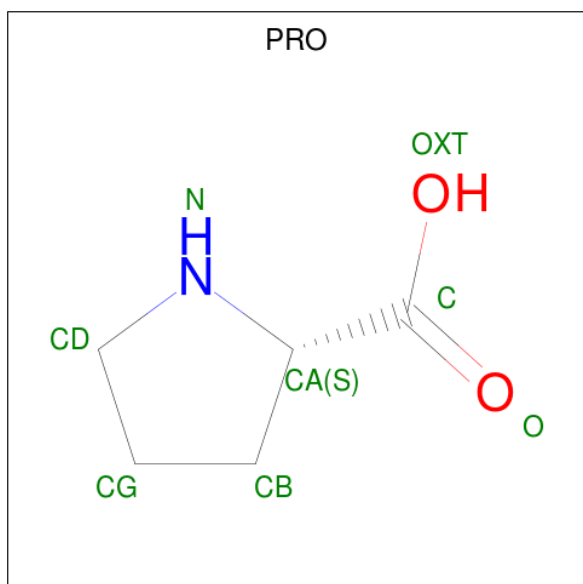
Chain	Residue	Modelled	Actual	Comment	Reference
8	705	LEU	-	expression tag	UNP U9XYS4
8	706	GLU	-	expression tag	UNP U9XYS4
8	707	HIS	-	expression tag	UNP U9XYS4
8	708	HIS	-	expression tag	UNP U9XYS4
8	709	HIS	-	expression tag	UNP U9XYS4
8	710	HIS	-	expression tag	UNP U9XYS4
8	711	HIS	-	expression tag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

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $C_6H_{11}NO_3S$ ) (labeled as "Ligand of Interest" by depositor).



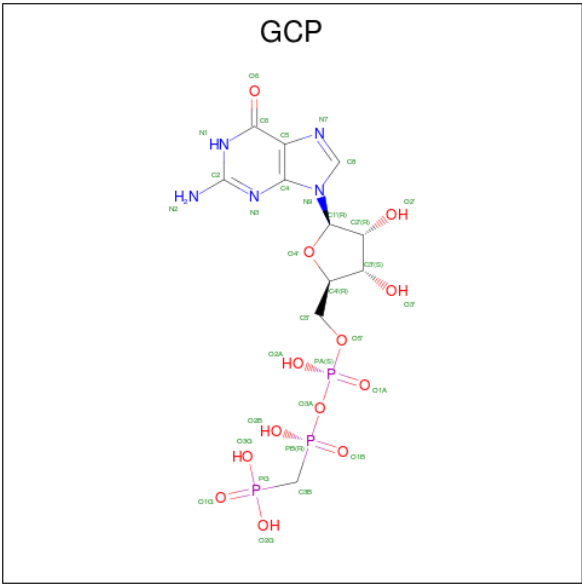
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	1	1	10	6	1	2	1	0

- Molecule 61 is PROLINE (three-letter code: PRO) (formula:  $C_5H_9NO_2$ ) (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<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



### 3 Residue-property plots

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

- Molecule 1: 50S ribosomal protein L2

Chain b:  92% 8%



- Molecule 2: 50S ribosomal protein L3

Chain c:  97% .



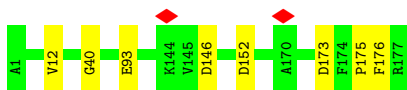
- Molecule 3: 50S ribosomal protein L4

Chain d:  95% 5%




- Molecule 4: 50S ribosomal protein L5

Chain e:  95% 5%




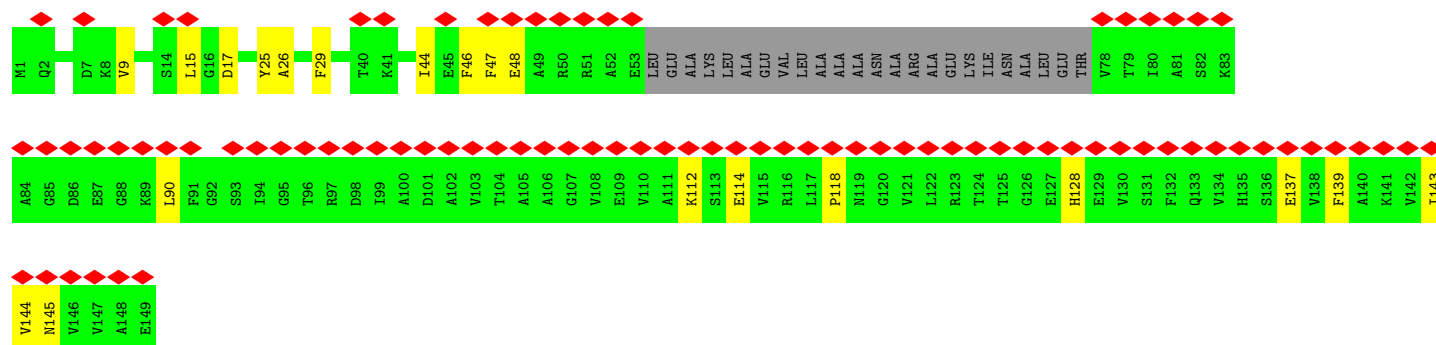
- Molecule 5: 50S ribosomal protein L6

Chain f:  91% 9%



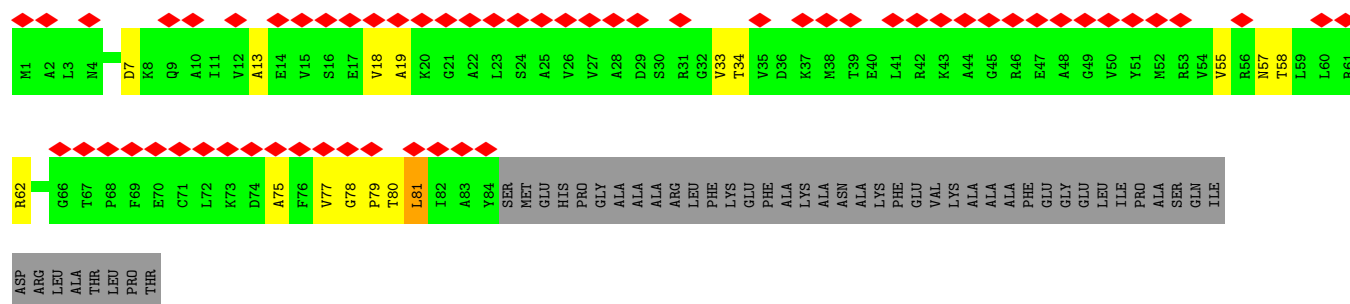
- Molecule 6: 50S ribosomal protein L9

Chain g: 

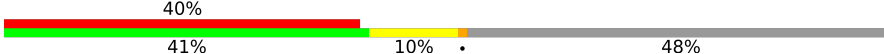


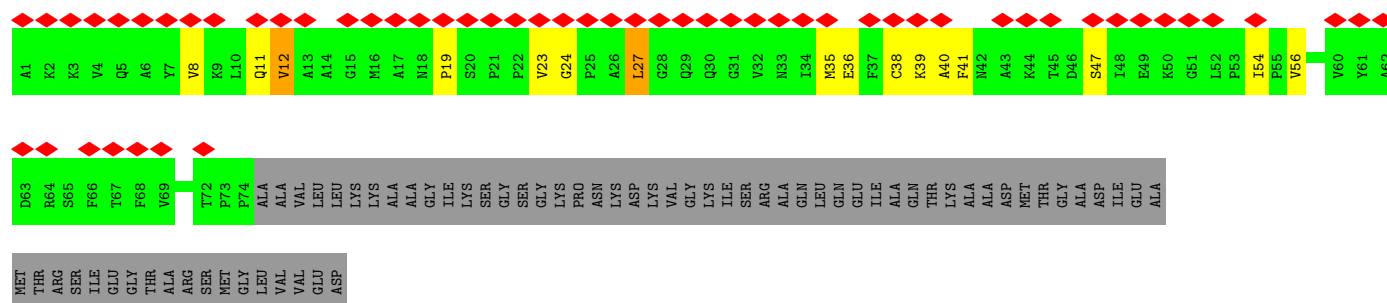
• Molecule 7: 50S ribosomal protein L10

Chain h: 



• Molecule 8: 50S ribosomal protein L11

Chain i: 



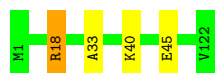
• Molecule 9: 50S ribosomal protein L13

Chain j: 



• Molecule 10: 50S ribosomal protein L14

Chain k:  97% ..



- Molecule 11: 50S ribosomal protein L15

Chain l:  98% .



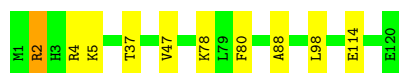
- Molecule 12: 50S ribosomal protein L16

Chain m:  94% 6%



- Molecule 13: 50S ribosomal protein L17

Chain n:  92% 8% .



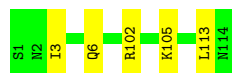
- Molecule 14: 50S ribosomal protein L18

Chain o:  92% 8%



- Molecule 15: 50S ribosomal protein L19

Chain p:  96% .




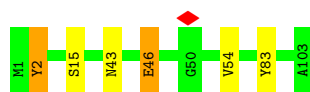
- Molecule 16: 50S ribosomal protein L20

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 50S ribosomal protein L21

Chain r:  94% . .



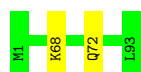
- Molecule 18: 50S ribosomal protein L22

Chain s: 95% 5%



- Molecule 19: 50S ribosomal protein L23

Chain t: 98% .



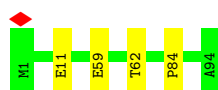
- Molecule 20: 50S ribosomal protein L24

Chain u: 95% 5%



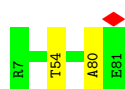
- Molecule 21: 50S ribosomal protein L25

Chain v: 96% .



- Molecule 22: 50S ribosomal protein L27

Chain w: 97% .



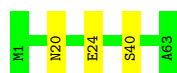
- Molecule 23: 50S ribosomal protein L28

Chain x: 100%

There are no outlier residues recorded for this chain.

- Molecule 24: 50S ribosomal protein L29

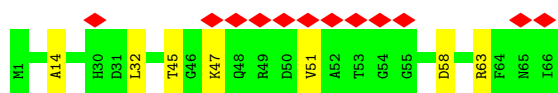
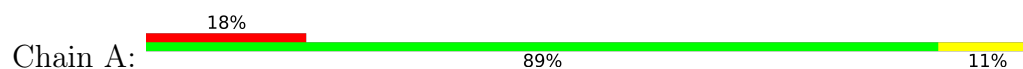
Chain y: 95% 5%



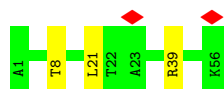
- Molecule 25: 50S ribosomal protein L30



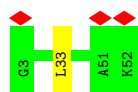
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



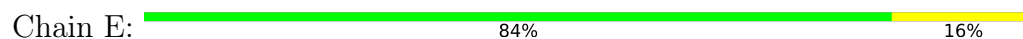
- Molecule 28: 50S ribosomal protein L33




- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35




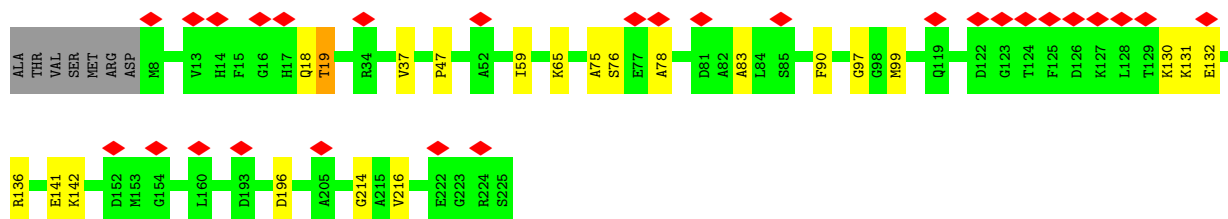
- Molecule 31: 50S ribosomal protein L36

Chain F:  87% 13%

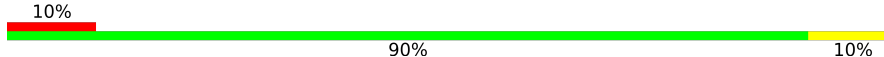


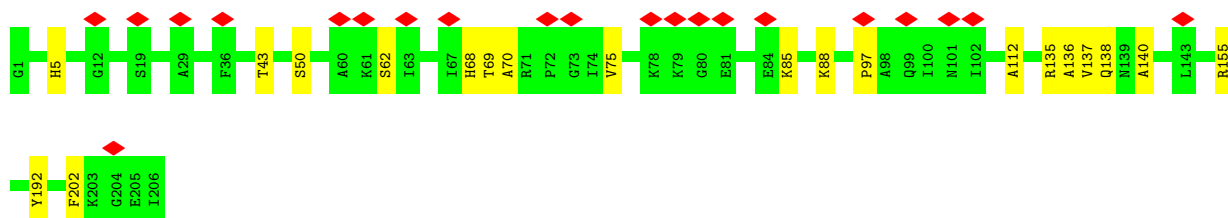
- Molecule 32: 30S ribosomal protein S2

Chain G:  12% 87% 9%




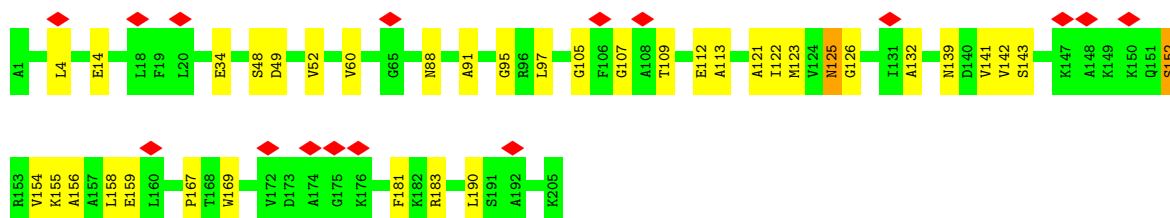
- Molecule 33: 30S ribosomal protein S3

Chain H:  10% 90% 10%




- Molecule 34: 30S ribosomal protein S4

Chain I:  8% 82% 17%




- Molecule 35: 30S ribosomal protein S5

Chain J:  88% 12%

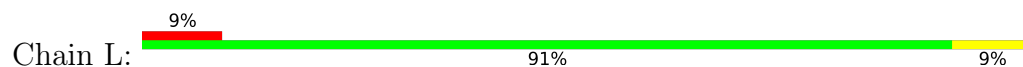


- Molecule 36: 30S ribosomal protein S6

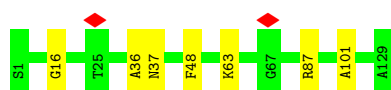
Chain K:  82% 16%



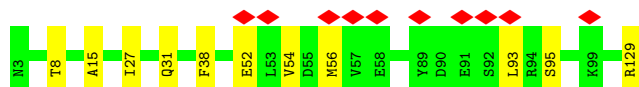
- Molecule 37: 30S ribosomal protein S7



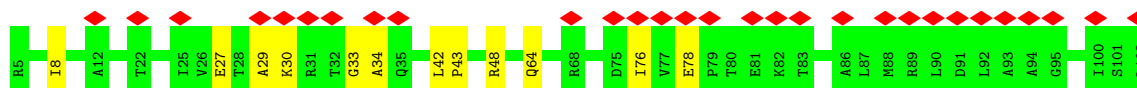
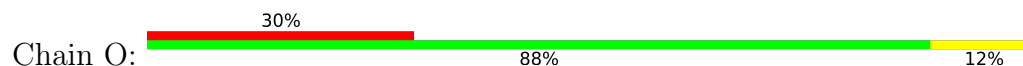
- Molecule 38: 30S ribosomal protein S8



- Molecule 39: 30S ribosomal protein S9



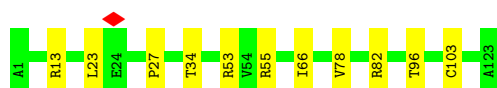
- Molecule 40: 30S ribosomal protein S10



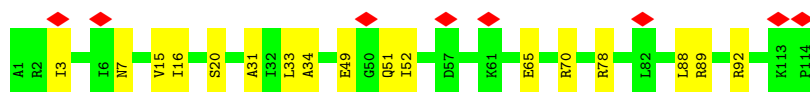
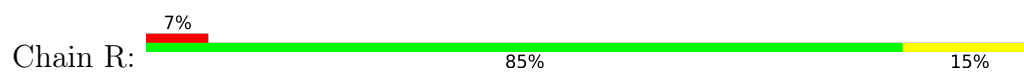
- Molecule 41: 30S ribosomal protein S11



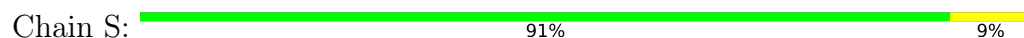
- Molecule 42: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S13



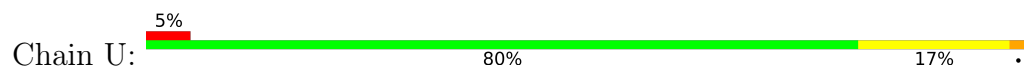
- Molecule 44: 30S ribosomal protein S14



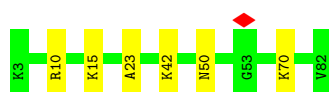
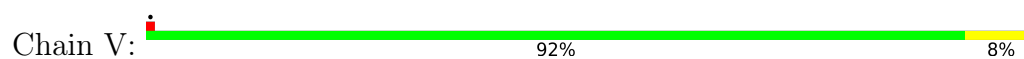
- Molecule 45: 30S ribosomal protein S15



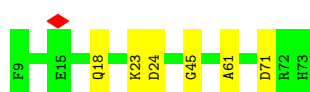
- Molecule 46: 30S ribosomal protein S16



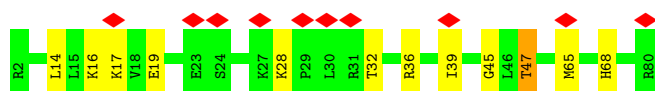
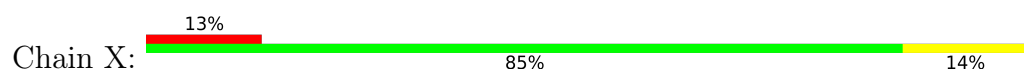
- Molecule 47: 30S ribosomal protein S17



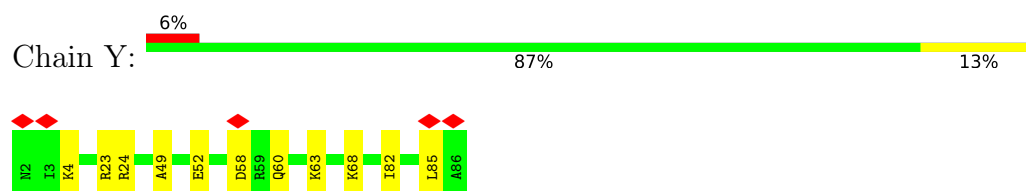
- Molecule 48: 30S ribosomal protein S18



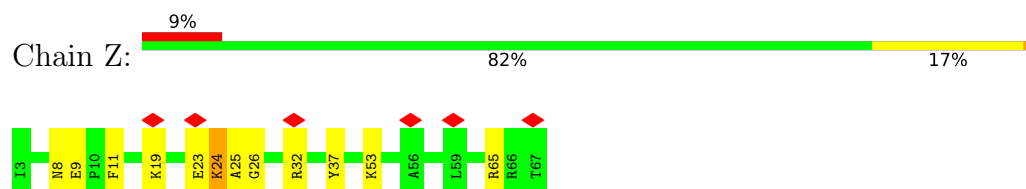
- Molecule 49: 30S ribosomal protein S19



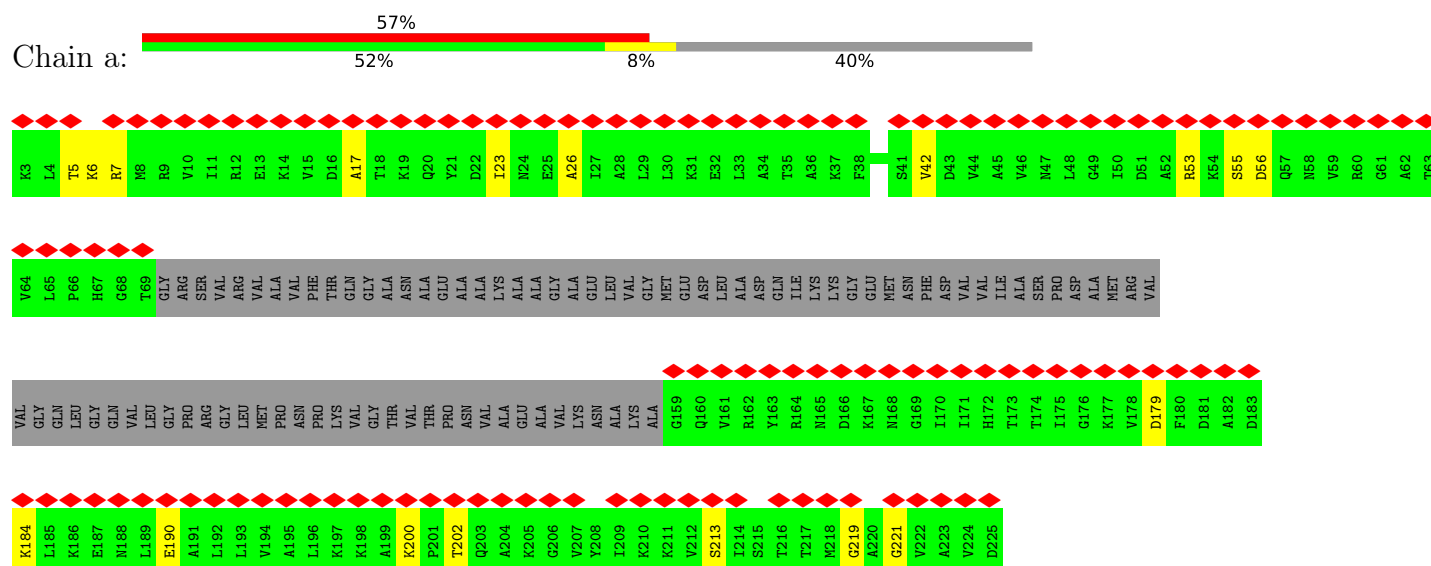
- Molecule 50: 30S ribosomal protein S20



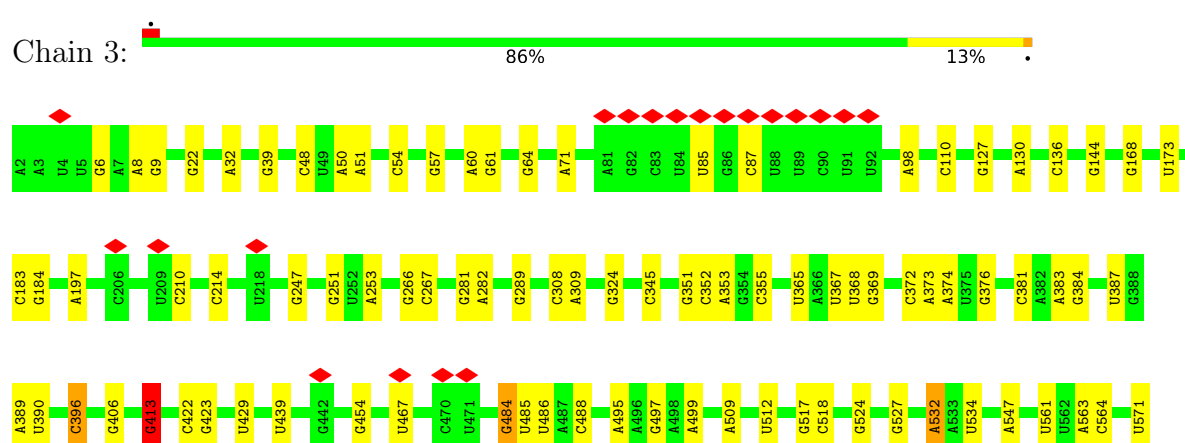
- Molecule 51: 30S ribosomal protein S21

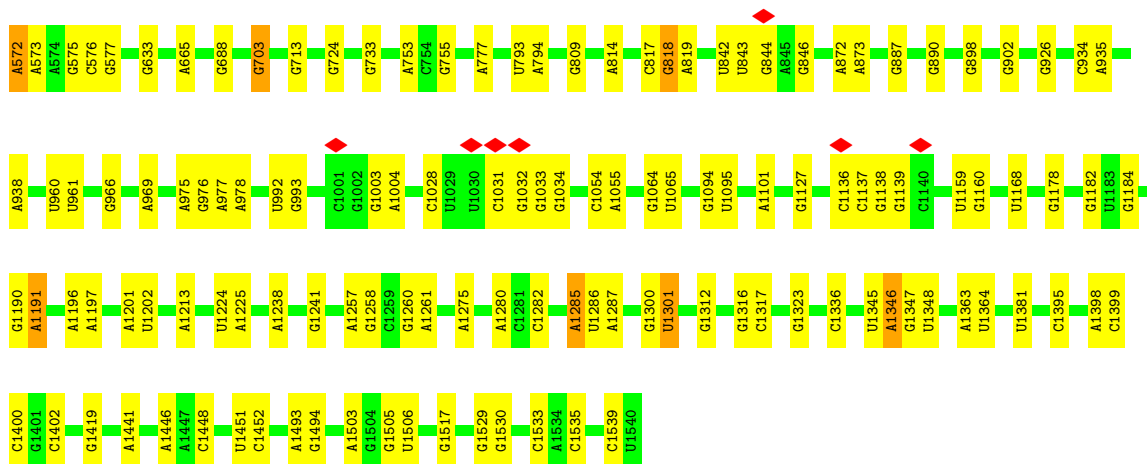


- Molecule 52: 50S ribosomal protein L1

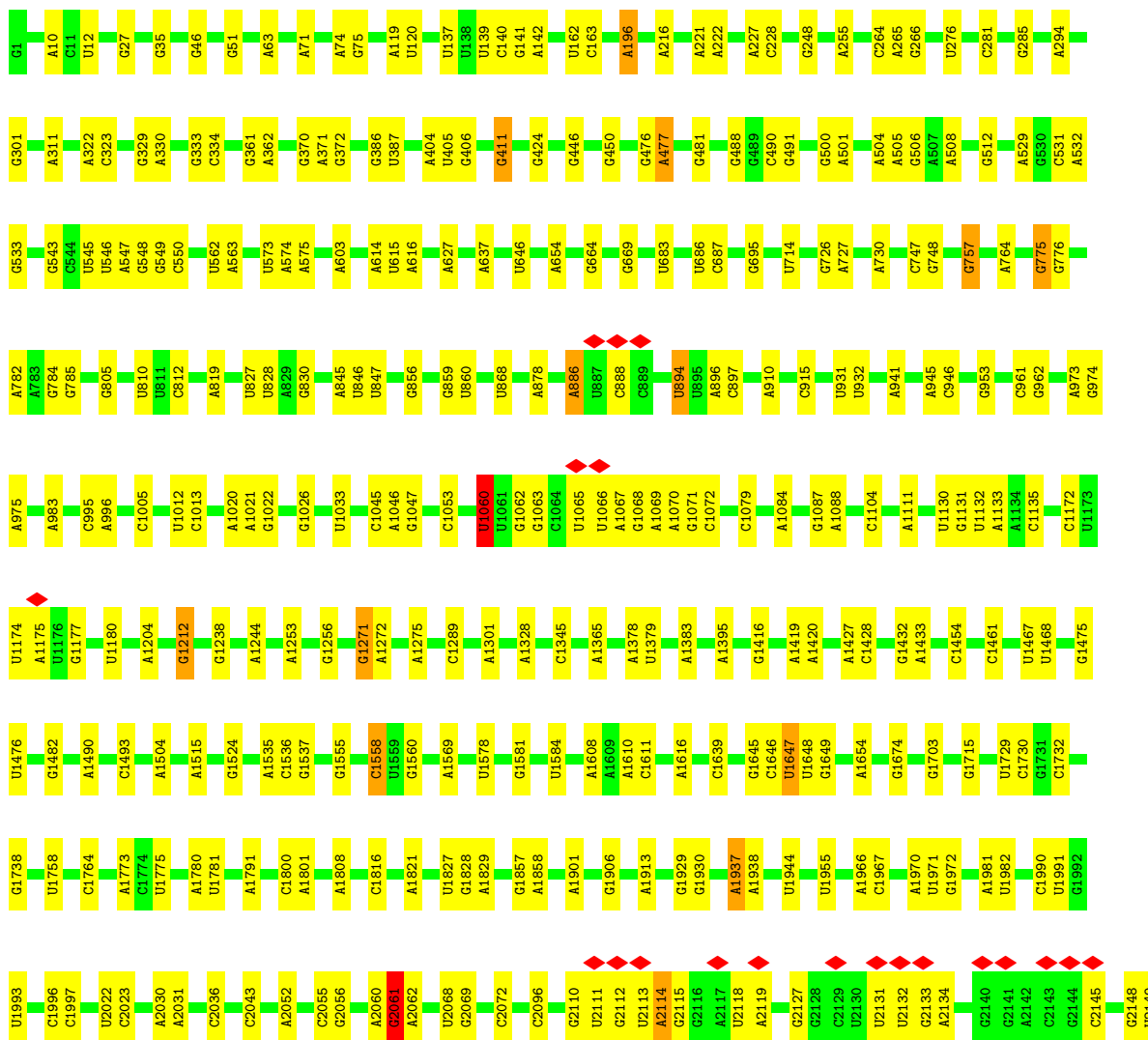
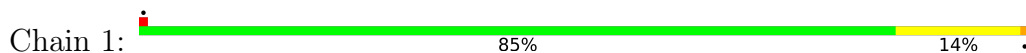


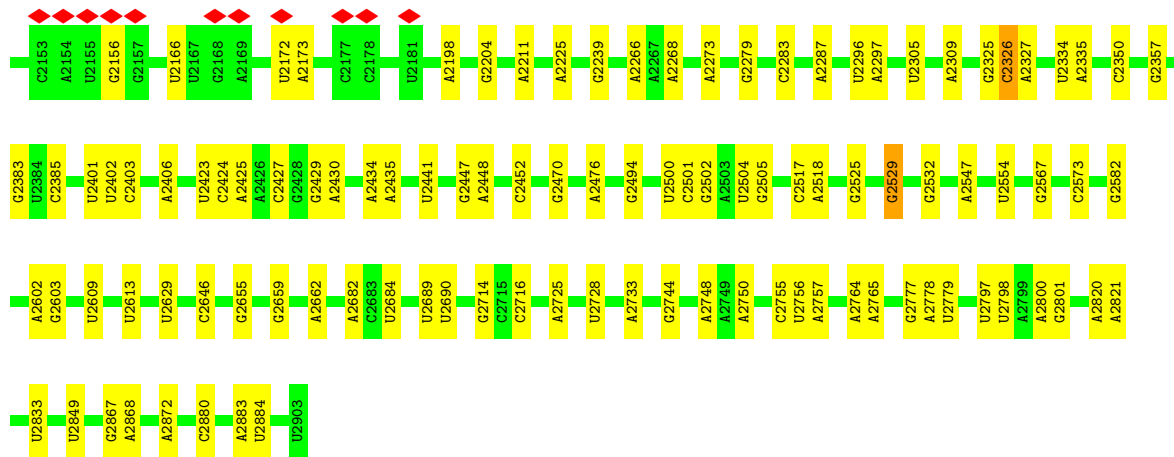
- Molecule 53: 16S ribosomal RNA





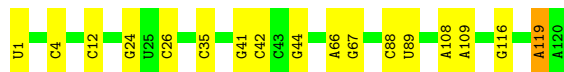
• Molecule 54: 23S ribosomal RNA





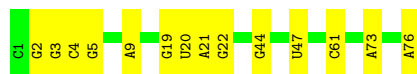
• Molecule 55: 5S ribosomal RNA

Chain 2: 86% 13%



• Molecule 56: tRNA<sup>Pro</sup>

Chain 5: 82% 18%



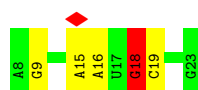
• Molecule 57: tRNA<sup>fMet</sup>

Chain 6: 36% 70% 27%



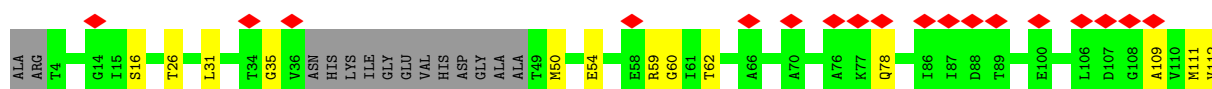
• Molecule 58: mRNA

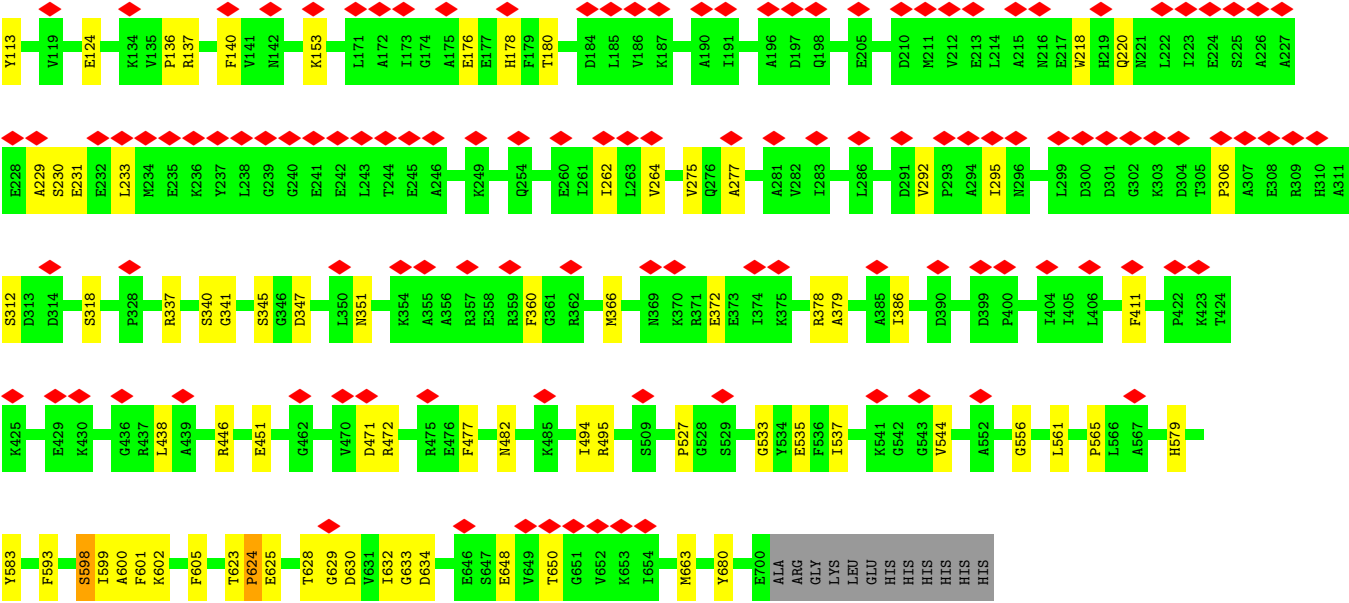
Chain 4: 6% 69% 25% 6%



• Molecule 59: Elongation factor G

Chain 8: 20% 84% 12%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	6029	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	25.366	Depositor
Minimum map value	-7.465	Depositor
Average map value	0.018	Depositor
Map value standard deviation	1.395	Depositor
Recommended contour level	3.3	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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, MG, GCP

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	0.73	6/2122 (0.3%)	0.81	3/2852 (0.1%)
2	c	0.67	3/1586 (0.2%)	0.76	0/2134
3	d	0.70	5/1571 (0.3%)	0.75	2/2113 (0.1%)
4	e	0.66	1/1435 (0.1%)	0.75	0/1926
5	f	0.91	8/1343 (0.6%)	0.85	0/1816
6	g	1.21	13/946 (1.4%)	1.00	4/1275 (0.3%)
7	h	1.13	8/638 (1.3%)	1.02	3/860 (0.3%)
8	i	1.82	13/564 (2.3%)	1.28	5/768 (0.7%)
9	j	0.67	2/1152 (0.2%)	0.74	0/1551
10	k	0.71	2/948 (0.2%)	0.80	0/1268
11	l	0.63	2/1054 (0.2%)	0.73	0/1403
12	m	0.73	3/1093 (0.3%)	0.78	0/1460
13	n	0.74	3/974 (0.3%)	0.80	2/1301 (0.2%)
14	o	0.80	4/902 (0.4%)	0.78	0/1209
15	p	0.70	2/929 (0.2%)	0.76	1/1242 (0.1%)
16	q	0.70	0/960	0.72	0/1278
17	r	0.70	3/829 (0.4%)	0.79	0/1107
18	s	0.73	2/864 (0.2%)	0.77	0/1156
19	t	0.70	1/745 (0.1%)	0.73	0/994
20	u	0.58	1/788 (0.1%)	0.67	0/1051
21	v	0.59	0/766	0.72	1/1025 (0.1%)
22	w	0.73	1/582 (0.2%)	0.74	0/769
23	x	0.65	0/635	0.80	0/848
24	y	0.81	2/510 (0.4%)	0.72	0/677
25	z	0.72	2/453 (0.4%)	0.72	0/605
26	A	1.02	5/532 (0.9%)	0.83	2/709 (0.3%)
27	B	0.71	0/450	0.79	0/599
28	C	0.71	1/417 (0.2%)	0.71	0/554
29	D	0.67	1/380 (0.3%)	0.73	0/498
30	E	0.83	4/513 (0.8%)	0.83	0/676
31	F	0.95	2/303 (0.7%)	0.90	2/397 (0.5%)
32	G	0.95	15/1736 (0.9%)	0.84	1/2338 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	H	1.10	14/1652 (0.8%)	0.88	5/2225 (0.2%)
34	I	1.24	21/1665 (1.3%)	1.08	14/2227 (0.6%)
35	J	0.87	6/1170 (0.5%)	0.89	4/1573 (0.3%)
36	K	1.33	11/836 (1.3%)	1.01	8/1128 (0.7%)
37	L	0.98	10/1196 (0.8%)	0.84	2/1602 (0.1%)
38	M	0.85	5/989 (0.5%)	0.83	0/1326
39	N	0.73	3/1034 (0.3%)	0.80	1/1375 (0.1%)
40	O	1.03	5/797 (0.6%)	0.88	2/1077 (0.2%)
41	P	0.77	4/886 (0.5%)	0.79	2/1195 (0.2%)
42	Q	0.75	2/969 (0.2%)	0.81	0/1300
43	R	1.15	12/893 (1.3%)	0.96	2/1193 (0.2%)
44	S	0.92	7/817 (0.9%)	0.81	0/1088
45	T	0.90	5/722 (0.7%)	0.80	0/964
46	U	1.12	8/659 (1.2%)	1.03	5/884 (0.6%)
47	V	0.71	2/658 (0.3%)	0.76	0/881
48	W	0.71	1/545 (0.2%)	0.67	0/731
49	X	1.08	7/653 (1.1%)	0.94	2/877 (0.2%)
50	Y	1.16	6/671 (0.9%)	0.96	2/888 (0.2%)
51	Z	1.03	5/551 (0.9%)	1.22	6/728 (0.8%)
52	a	0.94	6/1034 (0.6%)	0.93	1/1387 (0.1%)
53	3	0.64	0/36963	0.70	9/57662 (0.0%)
54	1	0.54	0/69796	0.68	9/108888 (0.0%)
55	2	0.47	0/2872	0.66	1/4479 (0.0%)
56	5	0.46	0/1840	0.69	0/2868
57	6	0.55	0/1832	0.73	3/2855 (0.1%)
58	4	0.54	0/388	0.79	1/603 (0.2%)
59	8	1.07	49/5411 (0.9%)	0.94	18/7323 (0.2%)
All	All	0.69	304/166219 (0.2%)	0.74	123/247786 (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
18	s	0	1
34	I	0	1
36	K	0	1
46	U	0	1
53	3	0	20
54	1	0	59
55	2	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
56	5	0	1
57	6	0	1
58	4	0	1
59	8	0	1
All	All	0	90

All (304) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	8	312	SER	C-O	16.80	1.55	1.23
8	i	19	PRO	C-O	16.15	1.55	1.23
36	K	13	ASP	C-O	15.49	1.52	1.23
8	i	27	LEU	C-O	14.52	1.50	1.23
36	K	53	LYS	C-O	-14.36	0.96	1.23
33	H	50	SER	C-O	14.15	1.50	1.23
8	i	54	ILE	C-O	14.13	1.50	1.23
34	I	169	TRP	C-O	13.34	1.48	1.23
6	g	114	GLU	C-O	12.61	1.47	1.23
59	8	630	ASP	C-O	12.14	1.46	1.23
8	i	24	GLY	C-O	11.93	1.42	1.23
59	8	472	ARG	C-O	11.44	1.45	1.23
34	I	156	ALA	C-O	11.39	1.45	1.23
34	I	132	ALA	C-O	11.24	1.44	1.23
59	8	629	GLY	C-O	11.12	1.41	1.23
33	H	97	PRO	C-O	10.64	1.44	1.23
34	I	141	VAL	C-O	10.44	1.43	1.23
52	a	26	ALA	C-O	10.30	1.43	1.23
59	8	318	SER	C-O	10.14	1.42	1.23
36	K	17	GLN	N-CA	10.09	1.66	1.46
36	K	14	GLN	C-O	10.06	1.42	1.23
59	8	180	THR	C-O	10.01	1.42	1.23
40	O	27	GLU	C-O	9.98	1.42	1.23
26	A	14	ALA	C-O	9.97	1.42	1.23
8	i	12	VAL	C-O	9.96	1.42	1.23
43	R	16	ILE	C-O	9.86	1.42	1.23
37	L	98	LEU	C-O	9.83	1.42	1.23
6	g	44	ILE	C-O	9.81	1.42	1.23
59	8	386	ILE	C-O	9.75	1.41	1.23
36	K	12	PRO	C-O	9.60	1.42	1.23
59	8	598	SER	C-O	9.60	1.41	1.23
31	F	4	ARG	C-O	9.58	1.41	1.23
33	H	68	HIS	C-O	9.56	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	O	30	LYS	C-O	9.55	1.41	1.23
43	R	7	ASN	C-O	9.39	1.41	1.23
6	g	144	VAL	C-O	9.35	1.41	1.23
34	I	49	ASP	C-O	9.25	1.41	1.23
32	G	130	LYS	C-O	9.13	1.40	1.23
59	8	176	GLU	C-O	-9.11	1.06	1.23
33	H	138	GLN	C-O	9.01	1.40	1.23
24	y	40	SER	C-O	8.99	1.40	1.23
49	X	19	GLU	C-O	8.87	1.40	1.23
47	V	23	ALA	C-O	8.73	1.40	1.23
34	I	113	ALA	C-O	8.70	1.39	1.23
50	Y	60	GLN	C-O	8.70	1.39	1.23
8	i	56	VAL	C-O	8.63	1.39	1.23
43	R	52	ILE	C-O	8.62	1.39	1.23
45	T	67	ASP	C-O	8.62	1.39	1.23
26	A	45	THR	C-O	8.61	1.39	1.23
33	H	85	LYS	C-O	8.57	1.39	1.23
34	I	155	LYS	N-CA	8.50	1.63	1.46
43	R	51	GLN	C-O	8.37	1.39	1.23
12	m	106	ASP	C-O	8.24	1.39	1.23
32	G	131	LYS	C-O	8.20	1.39	1.23
8	i	38	CYS	C-O	8.18	1.38	1.23
50	Y	49	ALA	C-O	8.16	1.38	1.23
40	O	76	ILE	C-O	8.11	1.38	1.23
59	8	341	GLY	N-CA	8.10	1.58	1.46
46	U	73	ALA	C-O	8.05	1.38	1.23
59	8	650	THR	C-O	8.03	1.38	1.23
51	Z	25	ALA	C-N	8.02	1.47	1.33
26	A	47	LYS	C-O	8.01	1.38	1.23
44	S	24	ALA	C-O	8.01	1.38	1.23
34	I	109	THR	C-O	8.00	1.38	1.23
14	o	75	GLY	C-O	7.99	1.36	1.23
59	8	556	GLY	C-O	7.91	1.36	1.23
6	g	128	HIS	C-O	7.90	1.38	1.23
5	f	133	LYS	C-O	7.88	1.38	1.23
50	Y	23	ARG	C-O	7.87	1.38	1.23
38	M	16	GLY	C-O	7.84	1.36	1.23
34	I	121	ALA	C-O	7.84	1.38	1.23
59	8	231	GLU	C-O	7.79	1.38	1.23
59	8	599	ILE	C-O	7.79	1.38	1.23
5	f	49	LEU	C-O	7.76	1.38	1.23
8	i	39	LYS	C-O	7.74	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	H	43	THR	C-O	7.73	1.38	1.23
34	I	60	VAL	C-O	7.68	1.38	1.23
59	8	124	GLU	C-O	7.65	1.37	1.23
12	m	119	LEU	C-O	7.61	1.37	1.23
36	K	51	ILE	N-CA	7.58	1.61	1.46
34	I	143	SER	C-O	7.55	1.37	1.23
6	g	29	PHE	C-O	7.54	1.37	1.23
32	G	37	VAL	C-O	7.46	1.37	1.23
49	X	47	THR	N-CA	7.46	1.61	1.46
37	L	125	ASP	C-O	7.43	1.37	1.23
37	L	95	ARG	C-O	7.43	1.37	1.23
15	p	6	GLN	C-O	7.40	1.37	1.23
36	K	20	GLY	C-O	7.39	1.35	1.23
9	j	90	GLU	C-O	7.38	1.37	1.23
52	a	5	THR	C-O	7.38	1.37	1.23
2	c	157	LYS	C-O	7.38	1.37	1.23
59	8	537	ILE	C-O	7.37	1.37	1.23
59	8	600	ALA	C-O	7.36	1.37	1.23
46	U	38	PHE	C-O	7.30	1.37	1.23
59	8	109	ALA	C-O	7.30	1.37	1.23
40	O	8	ILE	C-O	7.29	1.37	1.23
13	n	78	LYS	C-O	7.26	1.37	1.23
47	V	10	ARG	C-O	7.24	1.37	1.23
59	8	113	TYR	C-O	7.22	1.37	1.23
59	8	634	ASP	N-CA	7.20	1.60	1.46
38	M	101	ALA	C-O	7.19	1.37	1.23
59	8	264	VAL	N-CA	7.19	1.60	1.46
59	8	593	PHE	C-O	7.19	1.37	1.23
59	8	544	VAL	C-O	7.16	1.36	1.23
33	H	70	ALA	N-CA	7.16	1.60	1.46
46	U	4	ILE	C-O	7.11	1.36	1.23
1	b	117	SER	C-O	7.08	1.36	1.23
33	H	202	PHE	C-O	7.05	1.36	1.23
37	L	96	ASN	C-O	7.04	1.36	1.23
42	Q	53	ARG	C-O	7.02	1.36	1.23
51	Z	26	GLY	N-CA	7.02	1.56	1.46
35	J	77	ASN	N-CA	7.02	1.60	1.46
33	H	5	HIS	C-O	6.98	1.36	1.23
26	A	32	LEU	C-O	6.97	1.36	1.23
33	H	88	LYS	C-O	6.95	1.36	1.23
32	G	132	GLU	C-O	6.92	1.36	1.23
32	G	216	VAL	C-O	6.91	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	Y	82	ILE	C-O	6.91	1.36	1.23
43	R	3	ILE	C-O	6.85	1.36	1.23
28	C	33	LEU	C-O	6.81	1.36	1.23
43	R	31	ALA	C-O	6.81	1.36	1.23
59	8	233	LEU	C-O	6.75	1.36	1.23
39	N	95	SER	C-O	6.71	1.36	1.23
49	X	16	LYS	C-O	6.68	1.36	1.23
59	8	602	LYS	N-CA	6.67	1.59	1.46
33	H	136	ALA	C-O	6.67	1.36	1.23
7	h	7	ASP	C-O	6.66	1.36	1.23
7	h	33	VAL	C-O	6.65	1.35	1.23
59	8	112	VAL	N-CA	6.60	1.59	1.46
34	I	48	SER	C-O	6.58	1.35	1.23
48	W	61	ALA	C-O	6.58	1.35	1.23
59	8	561	LEU	C-O	6.56	1.35	1.23
43	R	88	LEU	C-O	6.56	1.35	1.23
52	a	184	LYS	C-O	6.55	1.35	1.23
35	J	120	HIS	C-O	6.54	1.35	1.23
59	8	471	ASP	C-O	6.54	1.35	1.23
25	z	42	ALA	C-O	6.51	1.35	1.23
8	i	40	ALA	C-O	6.49	1.35	1.23
59	8	16	SER	C-O	6.48	1.35	1.23
34	I	91	ALA	C-O	6.47	1.35	1.23
30	E	53	ASP	C-O	6.46	1.35	1.23
1	b	188	ARG	C-O	6.44	1.35	1.23
24	y	20	ASN	C-O	6.44	1.35	1.23
59	8	378	ARG	C-O	6.41	1.35	1.23
3	d	177	PRO	C-O	6.39	1.36	1.23
8	i	36	GLU	C-O	6.39	1.35	1.23
46	U	53	ASP	C-O	6.38	1.35	1.23
34	I	181	PHE	C-O	6.36	1.35	1.23
32	G	214	GLY	C-O	6.33	1.33	1.23
34	I	105	GLY	C-O	-6.33	1.13	1.23
59	8	26	THR	C-O	6.29	1.35	1.23
50	Y	58	ASP	C-O	6.28	1.35	1.23
45	T	68	TYR	C-O	6.24	1.35	1.23
7	h	57	ASN	C-O	6.23	1.35	1.23
11	l	134	ALA	C-O	6.22	1.35	1.23
36	K	8	PHE	C-O	6.18	1.35	1.23
32	G	59	ILE	C-O	6.17	1.35	1.23
44	S	43	ALA	C-O	6.17	1.35	1.23
43	R	89	ARG	C-O	6.14	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	H	140	ALA	C-O	6.12	1.34	1.23
36	K	16	GLU	N-CA	6.12	1.58	1.46
6	g	48	GLU	N-CA	6.10	1.58	1.46
9	j	20	ALA	N-CA	6.10	1.58	1.46
6	g	26	ALA	C-O	6.10	1.34	1.23
20	u	95	PHE	C-O	6.09	1.34	1.23
59	8	230	SER	C-O	6.08	1.34	1.23
30	E	50	SER	C-O	6.07	1.34	1.23
17	r	83	TYR	C-O	6.07	1.34	1.23
32	G	78	ALA	C-O	6.06	1.34	1.23
43	R	15	VAL	C-O	6.06	1.34	1.23
34	I	107	GLY	N-CA	6.05	1.55	1.46
2	c	121	THR	C-O	6.04	1.34	1.23
43	R	49	GLU	C-O	6.04	1.34	1.23
32	G	76	SER	C-O	6.04	1.34	1.23
6	g	139	PHE	N-CA	6.04	1.58	1.46
7	h	19	ALA	N-CA	6.03	1.58	1.46
6	g	17	ASP	C-O	6.03	1.34	1.23
10	k	33	ALA	C-O	6.03	1.34	1.23
59	8	601	PHE	C-O	6.02	1.34	1.23
32	G	47	PRO	C-O	6.01	1.35	1.23
59	8	275	VAL	C-O	6.00	1.34	1.23
3	d	190	ALA	C-O	6.00	1.34	1.23
37	L	44	SER	C-O	5.99	1.34	1.23
49	X	32	THR	C-O	5.97	1.34	1.23
13	n	47	VAL	C-O	5.97	1.34	1.23
34	I	122	ILE	C-O	5.97	1.34	1.23
29	D	19	ARG	C-O	5.96	1.34	1.23
39	N	15	ALA	N-CA	5.95	1.58	1.46
59	8	351	ASN	C-O	5.93	1.34	1.23
8	i	35	MET	C-O	5.93	1.34	1.23
5	f	74	MET	C-O	5.87	1.34	1.23
32	G	75	ALA	C-O	5.86	1.34	1.23
46	U	58	ALA	C-O	5.86	1.34	1.23
35	J	120	HIS	N-CA	5.85	1.58	1.46
7	h	75	ALA	C-O	5.84	1.34	1.23
5	f	8	VAL	C-O	5.84	1.34	1.23
7	h	62	ARG	C-O	5.83	1.34	1.23
34	I	123	MET	C-O	5.83	1.34	1.23
35	J	138	ALA	C-O	5.83	1.34	1.23
59	8	438	LEU	C-O	5.82	1.34	1.23
49	X	14	LEU	C-O	5.81	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	Z	11	PHE	N-CA	5.80	1.57	1.46
14	o	30	ARG	N-CA	5.77	1.57	1.46
33	H	137	VAL	C-O	5.77	1.34	1.23
59	8	663	MET	C-O	5.77	1.34	1.23
14	o	69	ASP	C-O	5.76	1.34	1.23
52	a	42	VAL	C-O	5.75	1.34	1.23
59	8	31	LEU	C-O	5.74	1.34	1.23
1	b	225	ASN	C-O	5.73	1.34	1.23
26	A	58	ASP	C-O	5.73	1.34	1.23
49	X	68	HIS	C-O	5.73	1.34	1.23
43	R	20	SER	N-CA	5.72	1.57	1.46
19	t	68	LYS	C-O	5.71	1.34	1.23
8	i	8	VAL	C-O	5.71	1.34	1.23
35	J	109	ALA	C-O	5.70	1.34	1.23
18	s	106	VAL	C-O	5.69	1.34	1.23
59	8	347	ASP	C-O	5.69	1.34	1.23
46	U	76	LYS	C-O	5.69	1.34	1.23
44	S	19	TYR	C-O	5.68	1.34	1.23
10	k	18	ARG	C-O	5.67	1.34	1.23
3	d	136	GLN	C-O	5.67	1.34	1.23
43	R	33	LEU	C-O	5.67	1.34	1.23
31	F	23	ILE	N-CA	5.67	1.57	1.46
44	S	2	LYS	C-O	5.66	1.34	1.23
40	O	29	ALA	C-O	5.66	1.34	1.23
7	h	34	THR	C-O	5.66	1.34	1.23
59	8	477	PHE	N-CA	5.62	1.57	1.46
32	G	65	LYS	C-O	5.62	1.34	1.23
17	r	2	TYR	C-O	5.62	1.34	1.23
18	s	16	LYS	C-O	5.62	1.34	1.23
17	r	15	SER	C-O	5.60	1.33	1.23
30	E	55	GLY	C-O	5.60	1.32	1.23
1	b	185	ALA	C-O	5.59	1.33	1.23
6	g	143	ILE	C-O	5.59	1.33	1.23
59	8	295	ILE	C-O	5.59	1.33	1.23
59	8	360	PHE	C-N	5.59	1.43	1.33
6	g	25	TYR	C-O	5.58	1.33	1.23
34	I	154	VAL	C-O	5.55	1.33	1.23
59	8	277	ALA	C-O	5.53	1.33	1.23
37	L	92	PRO	C-O	5.53	1.34	1.23
1	b	210	ALA	C-O	5.52	1.33	1.23
3	d	137	LYS	C-O	5.52	1.33	1.23
5	f	82	PHE	C-O	5.52	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	Z	19	LYS	C-O	5.51	1.33	1.23
32	G	83	ALA	C-O	5.51	1.33	1.23
59	8	136	PRO	C-O	5.50	1.34	1.23
44	S	36	SER	N-CA	5.50	1.57	1.46
37	L	117	LEU	C-O	5.48	1.33	1.23
41	P	73	VAL	C-O	5.48	1.33	1.23
41	P	111	ASP	N-CA	5.48	1.57	1.46
42	Q	34	THR	C-O	5.47	1.33	1.23
6	g	46	PHE	C-O	5.47	1.33	1.23
37	L	133	ALA	C-O	5.46	1.33	1.23
6	g	112	LYS	C-O	5.46	1.33	1.23
44	S	80	ARG	C-O	5.45	1.33	1.23
49	X	17	LYS	C-O	5.45	1.33	1.23
7	h	13	ALA	C-O	5.43	1.33	1.23
3	d	121	VAL	N-CA	5.42	1.57	1.46
15	p	3	ILE	C-O	5.41	1.33	1.23
44	S	13	VAL	C-O	5.41	1.33	1.23
22	w	54	THR	C-O	5.39	1.33	1.23
38	M	36	ALA	C-O	5.39	1.33	1.23
37	L	71	THR	C-O	5.38	1.33	1.23
52	a	23	ILE	C-O	5.38	1.33	1.23
38	M	63	LYS	C-O	5.38	1.33	1.23
30	E	57	VAL	C-O	5.37	1.33	1.23
14	o	82	ALA	C-O	5.34	1.33	1.23
37	L	5	VAL	N-CA	5.34	1.57	1.46
8	i	41	PHE	C-O	5.29	1.33	1.23
35	J	64	GLU	C-O	5.29	1.33	1.23
41	P	59	PRO	C-O	5.27	1.33	1.23
2	c	203	VAL	N-CA	5.25	1.56	1.46
41	P	60	PHE	C-O	5.24	1.33	1.23
32	G	141	GLU	C-O	5.24	1.33	1.23
51	Z	25	ALA	C-O	5.24	1.33	1.23
59	8	633	GLY	N-CA	5.23	1.53	1.46
45	T	79	GLN	C-O	5.20	1.33	1.23
25	z	43	ILE	C-O	5.20	1.33	1.23
36	K	16	GLU	C-O	5.20	1.33	1.23
50	Y	24	ARG	C-O	5.19	1.33	1.23
59	8	153	LYS	C-O	5.18	1.33	1.23
59	8	605	PHE	C-O	5.17	1.33	1.23
34	I	158	LEU	C-O	5.17	1.33	1.23
59	8	533	GLY	N-CA	5.15	1.53	1.46
52	a	190	GLU	C-O	5.15	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	62	LYS	C-O	5.15	1.33	1.23
46	U	77	GLU	N-CA	5.15	1.56	1.46
5	f	73	SER	C-O	5.14	1.33	1.23
39	N	27	ILE	C-O	5.13	1.33	1.23
11	l	108	ALA	C-O	5.13	1.33	1.23
13	n	5	LYS	N-CA	5.12	1.56	1.46
45	T	70	LYS	C-O	5.08	1.33	1.23
46	U	67	ILE	N-CA	5.07	1.56	1.46
59	8	140	PHE	C-O	5.07	1.32	1.23
4	e	12	VAL	C-O	5.06	1.32	1.23
5	f	90	GLY	N-CA	5.06	1.53	1.46
5	f	134	GLY	C-O	5.05	1.31	1.23
38	M	87	ARG	C-O	5.05	1.32	1.23
45	T	78	THR	C-O	5.04	1.32	1.23
33	H	135	ARG	C-O	5.04	1.32	1.23
36	K	69	GLU	C-O	5.03	1.32	1.23
1	b	16	VAL	C-O	5.03	1.32	1.23
32	G	142	LYS	C-O	5.01	1.32	1.23
34	I	95	GLY	CA-C	5.01	1.59	1.51

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	Z	25	ALA	C-N-CA	-11.78	97.57	122.30
8	i	27	LEU	C-N-CA	-11.62	97.89	122.30
51	Z	23	GLU	O-C-N	-11.32	104.58	122.70
34	I	152	SER	O-C-N	-9.94	106.80	122.70
51	Z	23	GLU	CA-C-O	9.83	140.75	120.10
34	I	154	VAL	C-N-CA	-9.40	98.20	121.70
59	8	340	SER	C-N-CA	-8.34	104.78	122.30
36	K	16	GLU	C-N-CA	-7.89	101.97	121.70
59	8	178	HIS	C-N-CA	-7.80	102.19	121.70
36	K	13	ASP	CA-C-O	7.73	136.34	120.10
40	O	33	GLY	C-N-CA	-7.47	103.03	121.70
50	Y	63	LYS	C-N-CA	-7.47	106.61	122.30
49	X	45	GLY	CA-C-O	7.45	134.01	120.60
36	K	50	PRO	C-N-CA	-7.34	103.36	121.70
59	8	601	PHE	C-N-CA	-7.26	103.56	121.70
59	8	262	ILE	O-C-N	-7.12	111.31	122.70
46	U	76	LYS	C-N-CA	-7.12	103.90	121.70
35	J	75	LEU	O-C-N	-7.00	111.50	122.70
13	n	4	ARG	C-N-CA	-7.00	104.21	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	H	69	THR	C-N-CA	-6.95	104.33	121.70
8	i	38	CYS	C-N-CA	-6.94	104.36	121.70
58	4	18	G	N9-C1'-C2'	6.91	122.98	114.00
46	U	73	ALA	O-C-N	-6.89	111.67	122.70
6	g	29	PHE	C-N-CA	-6.88	104.49	121.70
53	3	439	U	N1-C1'-C2'	6.81	122.85	114.00
36	K	53	LYS	O-C-N	-6.59	112.16	122.70
13	n	2	ARG	O-C-N	-6.49	112.32	122.70
53	3	1346	A	N9-C1'-C2'	6.48	122.42	114.00
8	i	23	VAL	C-N-CA	-6.42	108.81	122.30
1	b	262	THR	C-N-CA	-6.41	105.69	121.70
57	6	69	C	N1-C1'-C2'	6.35	122.25	114.00
49	X	45	GLY	O-C-N	-6.33	112.56	122.70
53	3	484	G	N9-C1'-C2'	6.32	122.22	114.00
54	1	2501	C	N1-C1'-C2'	6.31	122.21	114.00
54	1	1060	U	N1-C1'-C2'	6.31	122.21	114.00
50	Y	85	LEU	C-N-CA	-6.31	105.93	121.70
59	8	176	GLU	O-C-N	-6.26	112.69	122.70
57	6	56	C	N1-C1'-C2'	6.25	122.12	114.00
31	F	21	GLY	O-C-N	-6.18	112.81	122.70
59	8	262	ILE	CA-C-O	6.17	133.06	120.10
40	O	30	LYS	O-C-N	6.16	132.55	122.70
59	8	472	ARG	C-N-CA	-6.10	106.45	121.70
35	J	102	THR	C-N-CA	-6.10	109.50	122.30
46	U	75	ILE	C-N-CA	-6.10	106.45	121.70
6	g	47	PHE	C-N-CA	-6.07	106.53	121.70
7	h	18	VAL	C-N-CA	-6.06	106.54	121.70
32	G	132	GLU	C-N-CA	-6.06	106.56	121.70
34	I	181	PHE	C-N-CA	-6.01	106.66	121.70
59	8	632	ILE	C-N-CA	-6.00	109.69	122.30
53	3	413	G	N9-C1'-C2'	5.99	121.78	114.00
35	J	121	ASN	N-CA-C	5.97	127.11	111.00
43	R	92	ARG	C-N-CA	-5.97	109.77	122.30
43	R	34	ALA	C-N-CA	-5.94	106.84	121.70
59	8	472	ARG	CA-C-O	5.94	132.57	120.10
31	F	21	GLY	CA-C-O	5.93	131.27	120.60
7	h	78	GLY	N-CA-C	5.83	127.67	113.10
53	3	1301	U	N1-C1'-C2'	5.80	121.55	114.00
59	8	633	GLY	C-N-CA	-5.78	107.26	121.70
54	1	2061	G	C5'-C4'-O4'	5.74	115.99	109.10
34	I	125	ASN	N-CA-C	5.74	126.50	111.00
59	8	318	SER	O-C-N	5.71	131.84	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	K	13	ASP	O-C-N	-5.70	113.58	122.70
53	3	1539	C	N1-C1'-C2'	5.69	121.39	114.00
6	g	137	GLU	O-C-N	-5.68	113.61	122.70
1	b	213	ARG	C-N-CA	-5.64	110.45	122.30
59	8	124	GLU	C-N-CA	-5.62	107.66	121.70
46	U	73	ALA	CA-C-O	5.58	131.82	120.10
54	1	886	A	N9-C1'-C2'	5.58	121.25	114.00
37	L	3	ARG	O-C-N	-5.57	113.79	122.70
41	P	102	ALA	C-N-CA	-5.56	110.62	122.30
53	3	572	A	N9-C1'-C2'	5.56	121.22	114.00
39	N	31	GLN	O-C-N	-5.53	113.85	122.70
34	I	152	SER	CA-C-O	5.50	131.65	120.10
53	3	818	G	N9-C1'-C2'	5.50	121.14	114.00
36	K	18	VAL	N-CA-C	5.49	125.83	111.00
26	A	45	THR	C-N-CA	-5.49	110.78	122.30
54	1	1558	C	N1-C1'-C2'	5.48	121.12	114.00
54	1	2061	G	C1'-O4'-C4'	-5.47	105.53	109.90
34	I	181	PHE	O-C-N	5.46	131.43	122.70
34	I	159	GLU	C-N-CA	-5.45	108.07	121.70
34	I	105	GLY	O-C-N	-5.45	113.98	122.70
37	L	98	LEU	C-N-CA	-5.44	108.11	121.70
52	a	200	LYS	N-CA-C	5.43	125.65	111.00
34	I	95	GLY	O-C-N	-5.42	114.03	122.70
54	1	477	A	N9-C1'-C2'	5.41	121.03	114.00
8	i	12	VAL	N-CA-C	-5.40	96.42	111.00
35	J	120	HIS	CA-C-N	-5.40	105.32	117.20
3	d	82	GLY	N-CA-C	5.39	126.59	113.10
7	h	77	VAL	C-N-CA	-5.38	111.01	122.30
34	I	95	GLY	CA-C-O	5.37	130.27	120.60
51	Z	53	LYS	C-N-CA	-5.37	108.28	121.70
6	g	114	GLU	C-N-CA	-5.35	108.32	121.70
54	1	2529	G	N9-C1'-C2'	5.35	120.96	114.00
59	8	625	GLU	N-CA-C	5.35	125.44	111.00
33	H	75	VAL	C-N-CA	-5.31	108.42	121.70
59	8	341	GLY	O-C-N	-5.30	114.22	122.70
54	1	894	U	N1-C1'-C2'	5.26	120.83	114.00
59	8	111	MET	C-N-CA	-5.25	108.58	121.70
1	b	203	VAL	O-C-N	-5.24	114.31	122.70
3	d	119	ILE	O-C-N	-5.24	114.32	122.70
51	Z	8	ASN	N-CA-C	5.23	125.13	111.00
55	2	119	A	N9-C1'-C2'	5.20	120.76	114.00
34	I	132	ALA	CA-C-O	5.20	131.01	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	I	52	VAL	C-N-CA	-5.18	108.75	121.70
41	P	19	VAL	O-C-N	-5.18	114.41	122.70
33	H	202	PHE	O-C-N	5.17	130.97	122.70
59	8	494	ILE	C-N-CA	-5.16	108.80	121.70
26	A	14	ALA	O-C-N	5.13	130.91	122.70
15	p	3	ILE	C-N-CA	-5.12	108.89	121.70
21	v	62	THR	C-N-CA	-5.10	108.95	121.70
8	i	47	SER	C-N-CA	-5.09	108.96	121.70
34	I	14	GLU	C-N-CA	-5.08	111.62	122.30
53	3	374	A	N9-C1'-C2'	5.08	120.61	114.00
57	6	34	C	N1-C1'-C2'	5.08	120.60	114.00
36	K	15	SER	C-N-CA	-5.07	109.02	121.70
51	Z	25	ALA	N-CA-C	-5.07	97.31	111.00
59	8	312	SER	CA-C-N	-5.06	106.07	117.20
46	U	65	ALA	O-C-N	-5.06	114.61	122.70
36	K	16	GLU	O-C-N	5.05	130.78	122.70
59	8	218	TRP	C-N-CA	-5.05	109.07	121.70
33	H	62	SER	C-N-CA	-5.04	109.10	121.70
34	I	142	VAL	O-C-N	5.04	130.77	122.70
33	H	68	HIS	O-C-N	5.02	130.73	122.70

There are no chirality outliers.

All (90) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	1	1060	U	Sidechain
54	1	1087	G	Sidechain
54	1	1204	A	Sidechain
54	1	1212	G	Sidechain
54	1	1271	G	Sidechain
54	1	1328	A	Sidechain
54	1	1432	G	Sidechain
54	1	1433	A	Sidechain
54	1	1558	C	Sidechain
54	1	1645	G	Sidechain
54	1	1647	U	Sidechain
54	1	1775	U	Sidechain
54	1	1827	U	Sidechain
54	1	1828	G	Sidechain
54	1	1937	A	Sidechain
54	1	196	A	Sidechain
54	1	1981	A	Sidechain

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Mol	Chain	Res	Type	Group
54	1	1990	C	Sidechain
54	1	1996	C	Sidechain
54	1	2061	G	Sidechain
54	1	2114	A	Sidechain
54	1	2266	A	Sidechain
54	1	2273	A	Sidechain
54	1	2326	C	Sidechain
54	1	2401	U	Sidechain
54	1	2424	C	Sidechain
54	1	2447	G	Sidechain
54	1	2452	C	Sidechain
54	1	2500	U	Sidechain
54	1	2517	C	Sidechain
54	1	2529	G	Sidechain
54	1	2532	G	Sidechain
54	1	2659	G	Sidechain
54	1	2662	A	Sidechain
54	1	27	G	Sidechain
54	1	2725	A	Sidechain
54	1	2728	U	Sidechain
54	1	2883	A	Sidechain
54	1	370	G	Sidechain
54	1	411	G	Sidechain
54	1	446	G	Sidechain
54	1	450	G	Sidechain
54	1	476	G	Sidechain
54	1	477	A	Sidechain
54	1	488	G	Sidechain
54	1	500	G	Sidechain
54	1	501	A	Sidechain
54	1	506	G	Sidechain
54	1	512	G	Sidechain
54	1	562	U	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	810	U	Sidechain
54	1	868	U	Sidechain
54	1	894	U	Sidechain
54	1	973	A	Sidechain

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Mol	Chain	Res	Type	Group
55	2	1	U	Sidechain
55	2	119	A	Sidechain
55	2	24	G	Sidechain
53	3	1064	G	Sidechain
53	3	1178	G	Sidechain
53	3	1191	A	Sidechain
53	3	1285	A	Sidechain
53	3	1301	U	Sidechain
53	3	1316	G	Sidechain
53	3	1323	G	Sidechain
53	3	308	C	Sidechain
53	3	324	G	Sidechain
53	3	383	A	Sidechain
53	3	384	G	Sidechain
53	3	396	C	Sidechain
53	3	413	G	Sidechain
53	3	484	G	Sidechain
53	3	532	A	Sidechain
53	3	57	G	Sidechain
53	3	703	G	Sidechain
53	3	872	A	Sidechain
53	3	898	G	Sidechain
53	3	938	A	Sidechain
58	4	18	G	Sidechain
56	5	44	G	Sidechain
57	6	3	C	Sidechain
59	8	598	SER	Mainchain
34	I	152	SER	Mainchain
36	K	53	LYS	Mainchain
46	U	73	ALA	Mainchain
18	s	58	ALA	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.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	269/271 (99%)	223 (83%)	40 (15%)	6 (2%)	6	30
2	c	207/209 (99%)	179 (86%)	28 (14%)	0	100	100
3	d	199/201 (99%)	168 (84%)	30 (15%)	1 (0%)	29	61
4	e	175/177 (99%)	143 (82%)	28 (16%)	4 (2%)	6	29
5	f	174/176 (99%)	145 (83%)	27 (16%)	2 (1%)	14	45
6	g	121/149 (81%)	93 (77%)	24 (20%)	4 (3%)	4	22
7	h	82/131 (63%)	59 (72%)	18 (22%)	5 (6%)	1	10
8	i	72/141 (51%)	60 (83%)	11 (15%)	1 (1%)	11	38
9	j	140/142 (99%)	119 (85%)	20 (14%)	1 (1%)	22	54
10	k	120/122 (98%)	101 (84%)	19 (16%)	0	100	100
11	l	141/143 (99%)	124 (88%)	16 (11%)	1 (1%)	22	54
12	m	134/136 (98%)	120 (90%)	12 (9%)	2 (2%)	10	38
13	n	118/120 (98%)	98 (83%)	18 (15%)	2 (2%)	9	35
14	o	114/116 (98%)	101 (89%)	13 (11%)	0	100	100
15	p	112/114 (98%)	96 (86%)	16 (14%)	0	100	100
16	q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
17	r	101/103 (98%)	83 (82%)	16 (16%)	2 (2%)	7	32
18	s	108/110 (98%)	93 (86%)	14 (13%)	1 (1%)	17	48
19	t	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
20	u	100/102 (98%)	78 (78%)	21 (21%)	1 (1%)	15	46
21	v	92/94 (98%)	83 (90%)	8 (9%)	1 (1%)	14	45
22	w	73/75 (97%)	63 (86%)	9 (12%)	1 (1%)	11	38
23	x	75/77 (97%)	66 (88%)	9 (12%)	0	100	100
24	y	61/63 (97%)	54 (88%)	6 (10%)	1 (2%)	9	36
25	z	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
26	A	64/66 (97%)	54 (84%)	10 (16%)	0	100	100
27	B	54/56 (96%)	42 (78%)	12 (22%)	0	100	100
28	C	48/50 (96%)	39 (81%)	9 (19%)	0	100	100
29	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	E	62/64 (97%)	48 (77%)	9 (14%)	5 (8%)	1	6
31	F	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	5	25
32	G	216/225 (96%)	177 (82%)	35 (16%)	4 (2%)	8	34
33	H	204/206 (99%)	183 (90%)	20 (10%)	1 (0%)	29	61
34	I	203/205 (99%)	151 (74%)	48 (24%)	4 (2%)	7	32
35	J	155/157 (99%)	122 (79%)	26 (17%)	7 (4%)	2	15
36	K	98/100 (98%)	81 (83%)	15 (15%)	2 (2%)	7	32
37	L	149/151 (99%)	124 (83%)	24 (16%)	1 (1%)	22	54
38	M	127/129 (98%)	109 (86%)	18 (14%)	0	100	100
39	N	125/127 (98%)	97 (78%)	28 (22%)	0	100	100
40	O	96/98 (98%)	75 (78%)	18 (19%)	3 (3%)	4	23
41	P	114/116 (98%)	92 (81%)	20 (18%)	2 (2%)	8	35
42	Q	121/123 (98%)	95 (78%)	24 (20%)	2 (2%)	9	35
43	R	112/114 (98%)	94 (84%)	17 (15%)	1 (1%)	17	48
44	S	98/100 (98%)	77 (79%)	20 (20%)	1 (1%)	15	46
45	T	86/88 (98%)	73 (85%)	13 (15%)	0	100	100
46	U	80/82 (98%)	53 (66%)	24 (30%)	3 (4%)	3	19
47	V	78/80 (98%)	54 (69%)	21 (27%)	3 (4%)	3	19
48	W	63/65 (97%)	49 (78%)	11 (18%)	3 (5%)	2	14
49	X	77/79 (98%)	60 (78%)	17 (22%)	0	100	100
50	Y	83/85 (98%)	73 (88%)	9 (11%)	1 (1%)	13	42
51	Z	63/65 (97%)	41 (65%)	18 (29%)	4 (6%)	1	9
52	a	130/223 (58%)	104 (80%)	19 (15%)	7 (5%)	2	12
59	8	681/711 (96%)	558 (82%)	108 (16%)	15 (2%)	6	30
All	All	6517/6889 (95%)	5386 (83%)	1025 (16%)	106 (2%)	13	36

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	107	LYS
3	d	83	VAL
4	e	176	PHE
7	h	80	THR
8	i	11	GLN

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Mol	Chain	Res	Type
13	n	88	ALA
17	r	54	VAL
30	E	31	ILE
32	G	19	THR
34	I	125	ASN
35	J	26	GLY
37	L	6	ILE
41	P	92	ARG
46	U	79	ASN
47	V	15	LYS
47	V	70	LYS
51	Z	24	LYS
51	Z	65	ARG
52	a	6	LYS
52	a	7	ARG
59	8	379	ALA
59	8	624	PRO
1	b	205	GLY
1	b	206	LYS
4	e	173	ASP
5	f	174	LYS
9	j	81	ILE
24	y	24	GLU
30	E	33	THR
31	F	27	CYS
32	G	18	GLN
35	J	93	VAL
35	J	101	GLY
35	J	122	VAL
43	R	65	GLU
44	S	3	GLN
51	Z	37	TYR
59	8	35	GLY
59	8	50	MET
59	8	78	GLN
59	8	628	THR
4	e	40	GLY
4	e	175	PRO
7	h	58	THR
7	h	81	LEU
12	m	59	ARG
30	E	27	ASN

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Mol	Chain	Res	Type
32	G	99	MET
33	H	112	ALA
40	O	34	ALA
46	U	69	ASP
51	Z	9	GLU
52	a	17	ALA
52	a	55	SER
52	a	202	THR
52	a	221	GLY
59	8	345	SER
59	8	527	PRO
1	b	232	GLY
6	g	90	LEU
7	h	79	PRO
11	l	80	SER
12	m	70	ASP
21	v	84	PRO
22	w	80	ALA
30	E	32	LEU
35	J	25	LYS
36	K	95	ALA
48	W	71	ASP
50	Y	68	LYS
59	8	60	GLY
59	8	482	ASN
1	b	119	VAL
1	b	207	ALA
5	f	175	LYS
6	g	15	LEU
13	n	80	PHE
30	E	18	LYS
34	I	4	LEU
36	K	92	THR
41	P	89	GLY
46	U	13	LYS
47	V	50	ASN
48	W	24	ASP
52	a	219	GLY
59	8	54	GLU
59	8	229	ALA
59	8	306	PRO
6	g	9	VAL

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Mol	Chain	Res	Type
17	r	46	GLU
18	s	3	THR
35	J	87	VAL
40	O	43	PRO
42	Q	23	LEU
59	8	451	GLU
34	I	167	PRO
48	W	45	GLY
6	g	118	PRO
20	u	54	PRO
34	I	126	GLY
42	Q	27	PRO
59	8	565	PRO
7	h	55	VAL
32	G	97	GLY
35	J	83	PRO
40	O	42	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	216/216 (100%)	208 (96%)	8 (4%)	34	63
2	c	164/164 (100%)	161 (98%)	3 (2%)	59	78
3	d	165/165 (100%)	162 (98%)	3 (2%)	59	78
4	e	148/148 (100%)	145 (98%)	3 (2%)	55	76
5	f	137/137 (100%)	132 (96%)	5 (4%)	35	63
6	g	98/114 (86%)	97 (99%)	1 (1%)	76	86
7	h	66/100 (66%)	65 (98%)	1 (2%)	65	81
8	i	60/109 (55%)	58 (97%)	2 (3%)	38	66
9	j	116/116 (100%)	114 (98%)	2 (2%)	60	78
10	k	103/103 (100%)	100 (97%)	3 (3%)	42	69
11	l	102/102 (100%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	m	109/109 (100%)	106 (97%)	3 (3%)	43	70
13	n	100/100 (100%)	96 (96%)	4 (4%)	31	61
14	o	86/86 (100%)	81 (94%)	5 (6%)	20	50
15	p	99/99 (100%)	96 (97%)	3 (3%)	41	68
16	q	89/89 (100%)	89 (100%)	0	100	100
17	r	84/84 (100%)	81 (96%)	3 (4%)	35	63
18	s	93/93 (100%)	92 (99%)	1 (1%)	73	85
19	t	80/80 (100%)	79 (99%)	1 (1%)	69	82
20	u	83/83 (100%)	80 (96%)	3 (4%)	35	63
21	v	78/78 (100%)	76 (97%)	2 (3%)	46	71
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%)	55 (100%)	0	100	100
25	z	48/48 (100%)	47 (98%)	1 (2%)	53	75
26	A	59/59 (100%)	57 (97%)	2 (3%)	37	65
27	B	47/47 (100%)	44 (94%)	3 (6%)	17	46
28	C	45/45 (100%)	45 (100%)	0	100	100
29	D	38/38 (100%)	37 (97%)	1 (3%)	46	71
30	E	51/51 (100%)	50 (98%)	1 (2%)	55	76
31	F	34/34 (100%)	33 (97%)	1 (3%)	42	69
32	G	180/186 (97%)	176 (98%)	4 (2%)	52	74
33	H	170/170 (100%)	168 (99%)	2 (1%)	71	83
34	I	172/172 (100%)	165 (96%)	7 (4%)	30	61
35	J	119/119 (100%)	115 (97%)	4 (3%)	37	65
36	K	87/87 (100%)	83 (95%)	4 (5%)	27	58
37	L	124/124 (100%)	122 (98%)	2 (2%)	62	79
38	M	104/104 (100%)	102 (98%)	2 (2%)	57	77
39	N	105/105 (100%)	98 (93%)	7 (7%)	16	45
40	O	86/86 (100%)	83 (96%)	3 (4%)	36	64
41	P	89/89 (100%)	86 (97%)	3 (3%)	37	65
42	Q	103/103 (100%)	96 (93%)	7 (7%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	R	92/92 (100%)	90 (98%)	2 (2%)	52	74
44	S	83/83 (100%)	82 (99%)	1 (1%)	71	83
45	T	76/76 (100%)	76 (100%)	0	100	100
46	U	65/65 (100%)	61 (94%)	4 (6%)	18	47
47	V	74/74 (100%)	73 (99%)	1 (1%)	67	82
48	W	56/56 (100%)	54 (96%)	2 (4%)	35	63
49	X	70/70 (100%)	65 (93%)	5 (7%)	14	42
50	Y	65/65 (100%)	63 (97%)	2 (3%)	40	67
51	Z	55/55 (100%)	53 (96%)	2 (4%)	35	63
52	a	110/174 (63%)	106 (96%)	4 (4%)	35	63
59	8	566/585 (97%)	548 (97%)	18 (3%)	39	67
All	All	5428/5616 (97%)	5277 (97%)	151 (3%)	46	70

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	42	ARG
1	b	45	ASN
1	b	86	ARG
1	b	142	ASN
1	b	173	LEU
1	b	202	ARG
1	b	219	VAL
1	b	237	ARG
2	c	77	ARG
2	c	88	GLU
2	c	197	THR
3	d	46	GLN
3	d	60	TRP
3	d	102	ARG
4	e	93	GLU
4	e	146	ASP
4	e	152	ASP
5	f	68	ARG
5	f	94	ARG
5	f	151	ARG
5	f	154	GLU
5	f	166	GLU

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Mol	Chain	Res	Type
6	g	145	ASN
7	h	81	LEU
8	i	12	VAL
8	i	27	LEU
9	j	128	ASN
9	j	138	GLN
10	k	18	ARG
10	k	40	LYS
10	k	45	GLU
12	m	42	THR
12	m	91	TYR
12	m	136	MET
13	n	2	ARG
13	n	37	THR
13	n	98	LEU
13	n	114	GLU
14	o	24	THR
14	o	31	THR
14	o	46	GLU
14	o	56	LYS
14	o	95	SER
15	p	102	ARG
15	p	105	LYS
15	p	113	LEU
17	r	2	TYR
17	r	43	ASN
17	r	46	GLU
18	s	11	ARG
19	t	72	GLN
20	u	36	GLU
20	u	44	HIS
20	u	87	GLU
21	v	11	GLU
21	v	59	GLU
25	z	36	GLU
26	A	51	VAL
26	A	63	ARG
27	B	8	THR
27	B	21	LEU
27	B	39	ARG
29	D	13	ASN
30	E	61	LEU

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Mol	Chain	Res	Type
31	F	24	ARG
32	G	19	THR
32	G	90	PHE
32	G	136	ARG
32	G	196	ASP
33	H	155	ARG
33	H	192	TYR
34	I	34	GLU
34	I	88	ASN
34	I	97	LEU
34	I	112	GLU
34	I	139	ASN
34	I	183	ARG
34	I	190	LEU
35	J	18	ASN
35	J	37	VAL
35	J	95	MET
35	J	162	GLU
36	K	6	ILE
36	K	8	PHE
36	K	52	ASN
36	K	97	THR
37	L	141	HIS
37	L	147	ASN
38	M	37	ASN
38	M	48	PHE
39	N	8	THR
39	N	38	PHE
39	N	52	GLU
39	N	54	VAL
39	N	56	MET
39	N	93	LEU
39	N	129	ARG
40	O	48	ARG
40	O	64	GLN
40	O	78	GLU
41	P	55	ARG
41	P	105	ARG
41	P	124	LYS
42	Q	13	ARG
42	Q	55	ARG
42	Q	66	ILE

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Mol	Chain	Res	Type
42	Q	78	VAL
42	Q	82	ARG
42	Q	96	THR
42	Q	103	CYS
43	R	70	ARG
43	R	78	ARG
44	S	34	ASN
46	U	21	VAL
46	U	40	ASN
46	U	51	ARG
46	U	76	LYS
47	V	42	LYS
48	W	18	GLN
48	W	23	LYS
49	X	28	LYS
49	X	36	ARG
49	X	39	ILE
49	X	47	THR
49	X	65	MET
50	Y	4	LYS
50	Y	52	GLU
51	Z	24	LYS
51	Z	32	ARG
52	a	53	ARG
52	a	56	ASP
52	a	179	ASP
52	a	213	SER
59	8	59	ARG
59	8	62	THR
59	8	137	ARG
59	8	220	GLN
59	8	292	VAL
59	8	337	ARG
59	8	366	MET
59	8	372	GLU
59	8	411	PHE
59	8	446	ARG
59	8	495	ARG
59	8	535	GLU
59	8	579	HIS
59	8	583	TYR
59	8	623	THR

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Mol	Chain	Res	Type
59	8	624	PRO
59	8	648	GLU
59	8	680	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	69	ASN
1	b	127	ASN
1	b	250	GLN
2	c	130	GLN
2	c	150	GLN
3	d	24	ASN
3	d	94	GLN
4	e	134	GLN
8	i	5	GLN
10	k	93	GLN
17	r	89	HIS
19	t	28	ASN
20	u	68	ASN
23	x	15	ASN
23	x	33	HIS
24	y	41	HIS
26	A	61	ASN
27	B	4	GLN
28	C	44	GLN
32	G	17	HIS
33	H	31	ASN
33	H	184	ASN
34	I	135	GLN
35	J	69	ASN
35	J	145	ASN
36	K	3	HIS
37	L	51	GLN
39	N	3	ASN
39	N	125	GLN
40	O	64	GLN
43	R	7	ASN
44	S	59	GLN
45	T	27	GLN
47	V	30	HIS
49	X	55	GLN

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Mol	Chain	Res	Type
59	8	272	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	3	1538/1539 (99%)	198 (12%)	5 (0%)
54	1	2902/2903 (99%)	368 (12%)	12 (0%)
55	2	119/120 (99%)	13 (10%)	2 (1%)
56	5	76/77 (98%)	12 (15%)	1 (1%)
57	6	76/77 (98%)	21 (27%)	0
58	4	15/16 (93%)	5 (33%)	0
All	All	4726/4732 (99%)	617 (13%)	20 (0%)

All (617) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	3	6	G
53	3	8	A
53	3	9	G
53	3	22	G
53	3	32	A
53	3	39	G
53	3	48	C
53	3	50	A
53	3	51	A
53	3	54	C
53	3	60	A
53	3	61	G
53	3	64	G
53	3	71	A
53	3	85	U
53	3	87	C
53	3	98	A
53	3	110	C
53	3	127	G
53	3	130	A
53	3	136	C
53	3	144	G
53	3	168	G
53	3	173	U
53	3	183	C

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Mol	Chain	Res	Type
53	3	184	G
53	3	197	A
53	3	210	C
53	3	214	C
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	282	A
53	3	289	G
53	3	309	A
53	3	345	C
53	3	351	G
53	3	352	C
53	3	353	A
53	3	355	C
53	3	365	U
53	3	367	U
53	3	368	U
53	3	369	G
53	3	372	C
53	3	373	A
53	3	376	G
53	3	381	C
53	3	387	U
53	3	389	A
53	3	390	U
53	3	396	C
53	3	406	G
53	3	413	G
53	3	422	C
53	3	423	G
53	3	429	U
53	3	454	G
53	3	467	U
53	3	485	U
53	3	486	U
53	3	488	C
53	3	495	A
53	3	497	G

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Mol	Chain	Res	Type
53	3	499	A
53	3	509	A
53	3	512	U
53	3	517	G
53	3	518	C
53	3	524	G
53	3	527	G
53	3	532	A
53	3	534	U
53	3	547	A
53	3	561	U
53	3	563	A
53	3	564	C
53	3	571	U
53	3	572	A
53	3	573	A
53	3	575	G
53	3	576	C
53	3	577	G
53	3	633	G
53	3	665	A
53	3	688	G
53	3	703	G
53	3	713	G
53	3	724	G
53	3	733	G
53	3	753	A
53	3	755	G
53	3	777	A
53	3	793	U
53	3	794	A
53	3	809	G
53	3	814	A
53	3	817	C
53	3	818	G
53	3	819	A
53	3	842	U
53	3	843	U
53	3	844	G
53	3	846	G
53	3	873	A
53	3	887	G

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Mol	Chain	Res	Type
53	3	890	G
53	3	902	G
53	3	926	G
53	3	934	C
53	3	935	A
53	3	960	U
53	3	961	U
53	3	966	G
53	3	969	A
53	3	975	A
53	3	976	G
53	3	977	A
53	3	978	A
53	3	992	U
53	3	993	G
53	3	1003	G
53	3	1004	A
53	3	1028	C
53	3	1031	C
53	3	1032	G
53	3	1033	G
53	3	1034	G
53	3	1054	C
53	3	1055	A
53	3	1065	U
53	3	1094	G
53	3	1095	U
53	3	1101	A
53	3	1127	G
53	3	1136	C
53	3	1137	C
53	3	1138	G
53	3	1139	G
53	3	1159	U
53	3	1160	G
53	3	1168	U
53	3	1182	G
53	3	1184	G
53	3	1191	A
53	3	1196	A
53	3	1197	A
53	3	1201	A

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Mol	Chain	Res	Type
53	3	1202	U
53	3	1213	A
53	3	1224	U
53	3	1225	A
53	3	1238	A
53	3	1241	G
53	3	1257	A
53	3	1258	G
53	3	1260	G
53	3	1261	A
53	3	1275	A
53	3	1280	A
53	3	1282	C
53	3	1285	A
53	3	1286	U
53	3	1287	A
53	3	1300	G
53	3	1312	G
53	3	1317	C
53	3	1336	C
53	3	1345	U
53	3	1346	A
53	3	1348	U
53	3	1363	A
53	3	1364	U
53	3	1381	U
53	3	1395	C
53	3	1398	A
53	3	1399	C
53	3	1400	C
53	3	1402	C
53	3	1419	G
53	3	1441	A
53	3	1446	A
53	3	1448	C
53	3	1451	U
53	3	1452	C
53	3	1493	A
53	3	1494	G
53	3	1503	A
53	3	1505	G
53	3	1506	U

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Mol	Chain	Res	Type
53	3	1517	G
53	3	1529	G
53	3	1530	G
53	3	1533	C
53	3	1535	C
54	1	10	A
54	1	12	U
54	1	35	G
54	1	46	G
54	1	51	G
54	1	63	A
54	1	71	A
54	1	74	A
54	1	75	G
54	1	119	A
54	1	120	U
54	1	137	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	228	C
54	1	248	G
54	1	255	A
54	1	264	C
54	1	265	A
54	1	266	G
54	1	276	U
54	1	281	C
54	1	285	G
54	1	294	A
54	1	301	G
54	1	311	A
54	1	322	A
54	1	323	C
54	1	329	G

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Mol	Chain	Res	Type
54	1	330	A
54	1	333	G
54	1	334	C
54	1	361	G
54	1	362	A
54	1	371	A
54	1	372	G
54	1	386	G
54	1	387	U
54	1	404	A
54	1	405	U
54	1	406	G
54	1	411	G
54	1	424	G
54	1	481	G
54	1	491	G
54	1	504	A
54	1	505	A
54	1	508	A
54	1	529	A
54	1	531	C
54	1	532	A
54	1	533	G
54	1	543	G
54	1	545	U
54	1	547	A
54	1	548	G
54	1	549	G
54	1	550	C
54	1	563	A
54	1	573	U
54	1	574	A
54	1	575	A
54	1	603	A
54	1	614	A
54	1	615	U
54	1	616	A
54	1	627	A
54	1	637	A
54	1	646	U
54	1	654	A
54	1	664	G

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Mol	Chain	Res	Type
54	1	669	G
54	1	686	U
54	1	687	C
54	1	695	G
54	1	714	U
54	1	730	A
54	1	747	C
54	1	748	G
54	1	757	G
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	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	856	G
54	1	860	U
54	1	878	A
54	1	886	A
54	1	888	C
54	1	896	A
54	1	897	C
54	1	910	A
54	1	915	C
54	1	931	U
54	1	932	U
54	1	941	A
54	1	945	A
54	1	946	C
54	1	953	G
54	1	961	C
54	1	962	G
54	1	974	G

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Mol	Chain	Res	Type
54	1	975	A
54	1	983	A
54	1	995	C
54	1	996	A
54	1	1005	C
54	1	1012	U
54	1	1013	C
54	1	1021	A
54	1	1022	G
54	1	1026	G
54	1	1033	U
54	1	1045	C
54	1	1046	A
54	1	1047	G
54	1	1053	C
54	1	1060	U
54	1	1062	G
54	1	1063	G
54	1	1065	U
54	1	1066	U
54	1	1067	A
54	1	1068	G
54	1	1069	A
54	1	1070	A
54	1	1071	G
54	1	1072	C
54	1	1079	C
54	1	1084	A
54	1	1088	A
54	1	1104	C
54	1	1111	A
54	1	1131	G
54	1	1132	U
54	1	1133	A
54	1	1135	C
54	1	1172	C
54	1	1174	U
54	1	1175	A
54	1	1177	G
54	1	1180	U
54	1	1212	G
54	1	1238	G

*Continued on next page...*

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Mol	Chain	Res	Type
54	1	1244	A
54	1	1253	A
54	1	1256	G
54	1	1271	G
54	1	1272	A
54	1	1275	A
54	1	1289	C
54	1	1301	A
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	1416	G
54	1	1419	A
54	1	1420	A
54	1	1427	A
54	1	1428	C
54	1	1454	C
54	1	1461	C
54	1	1467	U
54	1	1468	U
54	1	1476	U
54	1	1482	G
54	1	1490	A
54	1	1493	C
54	1	1504	A
54	1	1515	A
54	1	1524	G
54	1	1535	A
54	1	1536	C
54	1	1537	G
54	1	1555	G
54	1	1560	G
54	1	1569	A
54	1	1578	U
54	1	1581	G
54	1	1584	U
54	1	1608	A
54	1	1610	A
54	1	1611	C

*Continued on next page...*

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Mol	Chain	Res	Type
54	1	1616	A
54	1	1639	C
54	1	1646	C
54	1	1647	U
54	1	1648	U
54	1	1649	G
54	1	1654	A
54	1	1674	G
54	1	1703	G
54	1	1715	G
54	1	1729	U
54	1	1730	C
54	1	1732	C
54	1	1738	G
54	1	1758	U
54	1	1764	C
54	1	1773	A
54	1	1780	A
54	1	1781	U
54	1	1791	A
54	1	1800	C
54	1	1801	A
54	1	1808	A
54	1	1816	C
54	1	1821	A
54	1	1829	A
54	1	1858	A
54	1	1901	A
54	1	1906	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	1966	A
54	1	1967	C
54	1	1970	A
54	1	1971	U
54	1	1972	G
54	1	1982	U

*Continued on next page...*

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Mol	Chain	Res	Type
54	1	1991	U
54	1	1993	U
54	1	1997	C
54	1	2022	U
54	1	2023	C
54	1	2030	A
54	1	2031	A
54	1	2036	C
54	1	2043	C
54	1	2052	A
54	1	2055	C
54	1	2056	G
54	1	2060	A
54	1	2061	G
54	1	2062	A
54	1	2068	U
54	1	2069	G
54	1	2072	C
54	1	2096	C
54	1	2110	G
54	1	2111	U
54	1	2112	G
54	1	2113	U
54	1	2114	A
54	1	2115	G
54	1	2118	U
54	1	2119	A
54	1	2127	G
54	1	2131	U
54	1	2132	U
54	1	2133	G
54	1	2134	A
54	1	2145	C
54	1	2148	G
54	1	2149	U
54	1	2156	G
54	1	2166	U
54	1	2172	U
54	1	2173	A
54	1	2198	A
54	1	2204	G
54	1	2211	A

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Mol	Chain	Res	Type
54	1	2225	A
54	1	2239	G
54	1	2268	A
54	1	2279	G
54	1	2283	C
54	1	2287	A
54	1	2297	A
54	1	2305	U
54	1	2309	A
54	1	2325	G
54	1	2327	A
54	1	2334	U
54	1	2335	A
54	1	2350	C
54	1	2357	G
54	1	2383	G
54	1	2385	C
54	1	2402	U
54	1	2403	C
54	1	2406	A
54	1	2423	U
54	1	2425	A
54	1	2427	C
54	1	2429	G
54	1	2430	A
54	1	2434	A
54	1	2435	A
54	1	2441	U
54	1	2448	A
54	1	2470	G
54	1	2476	A
54	1	2494	G
54	1	2502	G
54	1	2504	U
54	1	2505	G
54	1	2518	A
54	1	2525	G
54	1	2547	A
54	1	2554	U
54	1	2567	G
54	1	2573	C
54	1	2582	G

*Continued on next page...*

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Mol	Chain	Res	Type
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	2684	U
54	1	2689	U
54	1	2690	U
54	1	2714	G
54	1	2716	C
54	1	2733	A
54	1	2744	G
54	1	2748	A
54	1	2750	A
54	1	2755	C
54	1	2757	A
54	1	2764	A
54	1	2765	A
54	1	2777	G
54	1	2778	A
54	1	2779	U
54	1	2797	U
54	1	2798	U
54	1	2800	A
54	1	2801	G
54	1	2820	A
54	1	2821	A
54	1	2833	U
54	1	2849	U
54	1	2867	G
54	1	2868	A
54	1	2872	A
54	1	2880	C
54	1	2884	U
55	2	4	C
55	2	12	C
55	2	26	C
55	2	35	C
55	2	41	G

*Continued on next page...*

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Mol	Chain	Res	Type
55	2	42	C
55	2	44	G
55	2	67	G
55	2	88	C
55	2	89	U
55	2	108	A
55	2	109	A
55	2	116	G
56	5	3	G
56	5	4	C
56	5	5	G
56	5	9	A
56	5	19	G
56	5	20	U
56	5	21	A
56	5	22	G
56	5	47	U
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	14	A
57	6	18	G
57	6	19	G
57	6	21	A
57	6	22	G
57	6	28	C
57	6	33	U
57	6	35	A
57	6	37	A
57	6	48	C
57	6	56	C
57	6	61	C
57	6	64	G
57	6	70	G
57	6	71	C
57	6	72	A
57	6	76	A
58	4	9	G

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Mol	Chain	Res	Type
58	4	15	A
58	4	16	A
58	4	18	G
58	4	19	C

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	3	413	G
53	3	890	G
53	3	1190	G
53	3	1201	A
53	3	1347	G
54	1	227	A
54	1	490	C
54	1	546	U
54	1	784	G
54	1	859	G
54	1	1020	A
54	1	1130	U
54	1	1475	G
54	1	1857	G
54	1	2296	U
54	1	2326	C
54	1	2756	U
55	2	66	A
55	2	88	C
56	5	2	G

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

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	$\# Z  > 2$
60	FME	1	3001	61	8,9,10	0.66	0	7,9,11	0.78	0
61	PRO	5	101	60,56	5,7,8	0.52	0	7,8,10	1.17	1 (14%)
62	GCP	8	801	63	27,34,34	2.12	9 (33%)	34,54,54	3.86	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
60	FME	1	3001	61	-	1/7/9/11	-
61	PRO	5	101	60,56	-	0/0/9/11	0/1/1/1
62	GCP	8	801	63	-	9/15/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	8	801	GCP	PB-O3A	-5.75	1.51	1.58
62	8	801	GCP	O4'-C1'	4.18	1.46	1.41
62	8	801	GCP	C6-N1	3.64	1.39	1.33
62	8	801	GCP	PB-O2B	-3.30	1.48	1.56
62	8	801	GCP	C2-N1	2.76	1.40	1.35
62	8	801	GCP	C5-C6	2.64	1.45	1.41
62	8	801	GCP	C2'-C1'	2.41	1.57	1.53
62	8	801	GCP	PG-O3G	-2.19	1.49	1.54
62	8	801	GCP	PG-O2G	-2.18	1.49	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	8	801	GCP	C1'-N9-C4	13.51	150.38	126.64
62	8	801	GCP	C5-C6-N1	-9.06	111.04	123.43
62	8	801	GCP	C2-N1-C6	6.99	127.03	115.93
62	8	801	GCP	O4'-C1'-C2'	-5.47	98.94	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	8	801	GCP	O2G-PG-C3B	-4.29	95.99	106.40
62	8	801	GCP	C2-N3-C4	-4.29	110.46	115.36
62	8	801	GCP	O3G-PG-O2G	4.17	120.25	108.08
62	8	801	GCP	C4-C5-C6	-3.68	117.28	120.80
62	8	801	GCP	O2B-PB-O1B	3.67	122.31	110.07
62	8	801	GCP	O3'-C3'-C4'	-3.30	101.52	111.05
62	8	801	GCP	C4-C5-N7	3.17	112.70	109.40
62	8	801	GCP	O2A-PA-O5'	-3.13	93.21	107.75
62	8	801	GCP	PB-O3A-PA	2.93	141.85	132.56
62	8	801	GCP	C3'-C2'-C1'	-2.73	96.87	100.98
62	8	801	GCP	N3-C2-N1	-2.60	123.76	127.22
61	5	101	PRO	O-C-CA	-2.31	118.73	124.78
62	8	801	GCP	O2A-PA-O1A	2.26	123.44	112.24
62	8	801	GCP	O3G-PG-O1G	-2.22	106.53	112.39
62	8	801	GCP	O4'-C4'-C5'	2.15	116.44	109.37
62	8	801	GCP	O1B-PB-C3B	2.02	114.42	109.07

There are no chirality outliers.

All (10) torsion outliers are listed below:

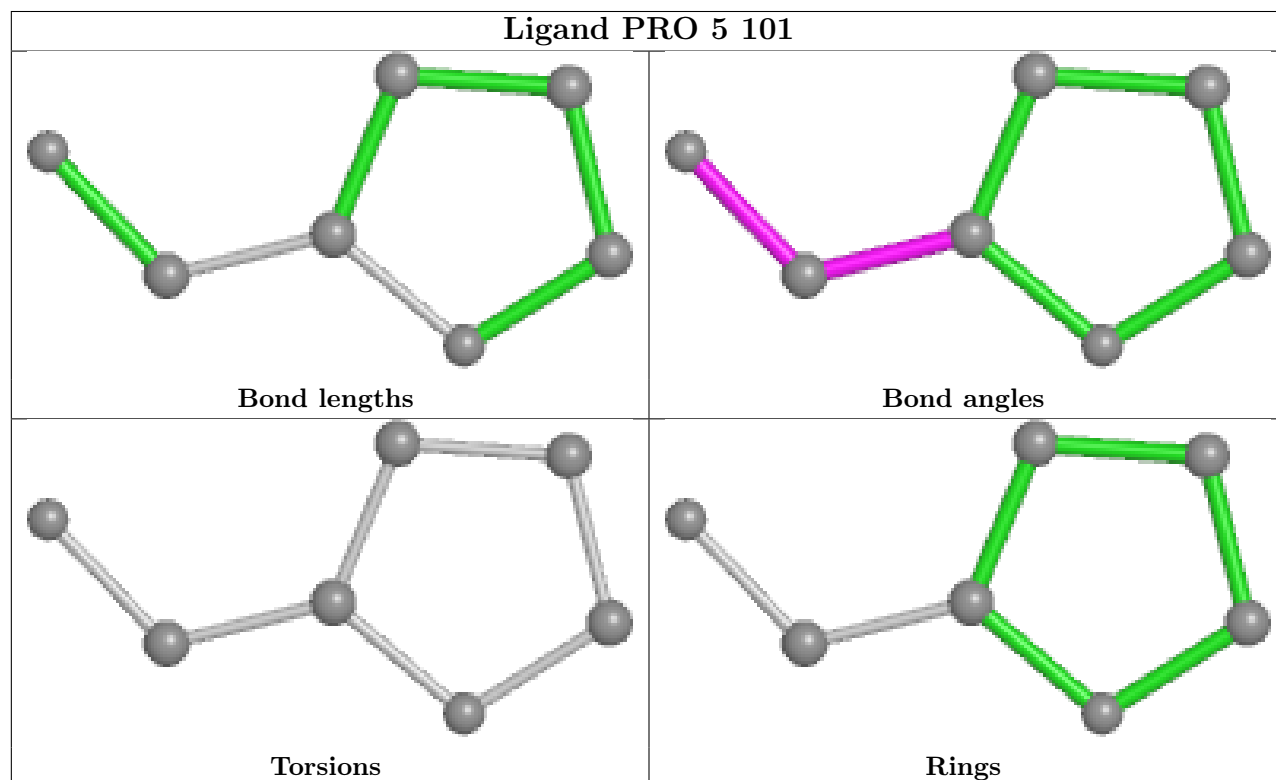
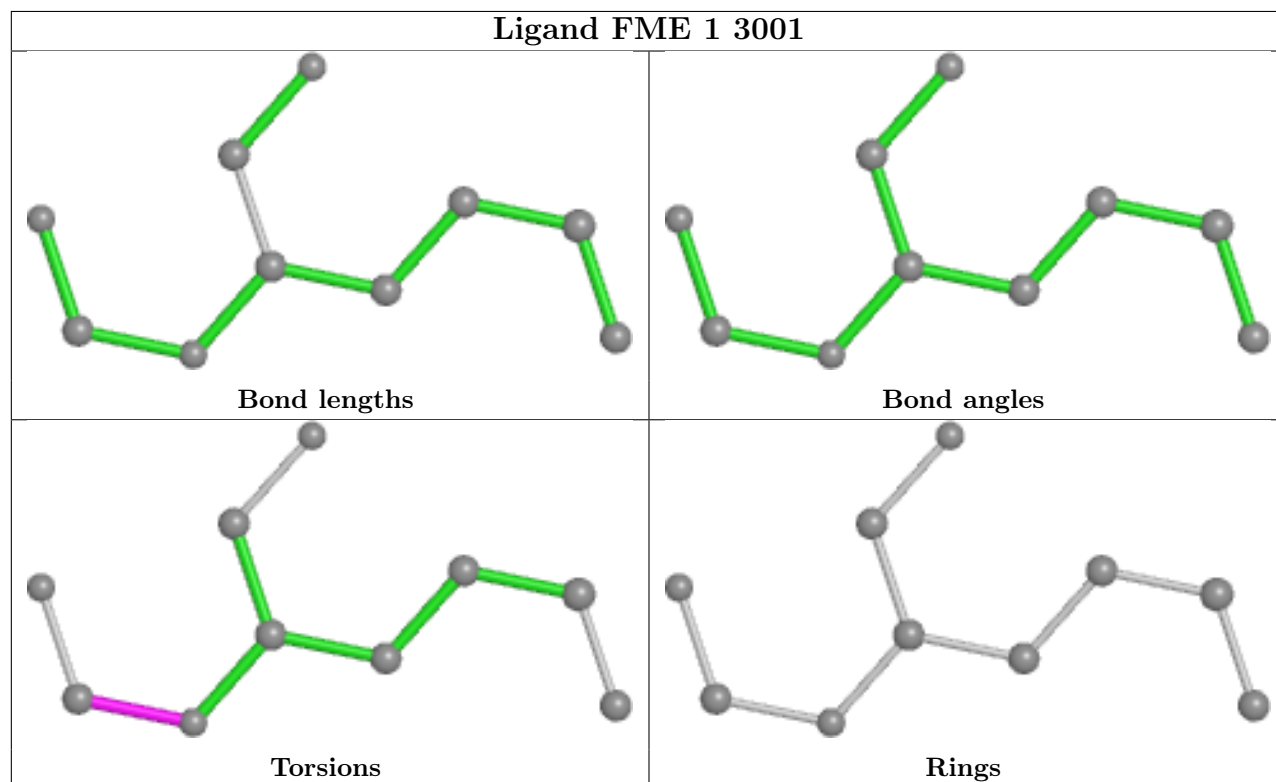
Mol	Chain	Res	Type	Atoms
60	1	3001	FME	O1-CN-N-CA
62	8	801	GCP	PB-C3B-PG-O1G
62	8	801	GCP	PB-C3B-PG-O2G
62	8	801	GCP	PG-C3B-PB-O1B
62	8	801	GCP	C5'-O5'-PA-O3A
62	8	801	GCP	C5'-O5'-PA-O1A
62	8	801	GCP	O4'-C4'-C5'-O5'
62	8	801	GCP	C5'-O5'-PA-O2A
62	8	801	GCP	PB-C3B-PG-O3G
62	8	801	GCP	C3'-C4'-C5'-O5'

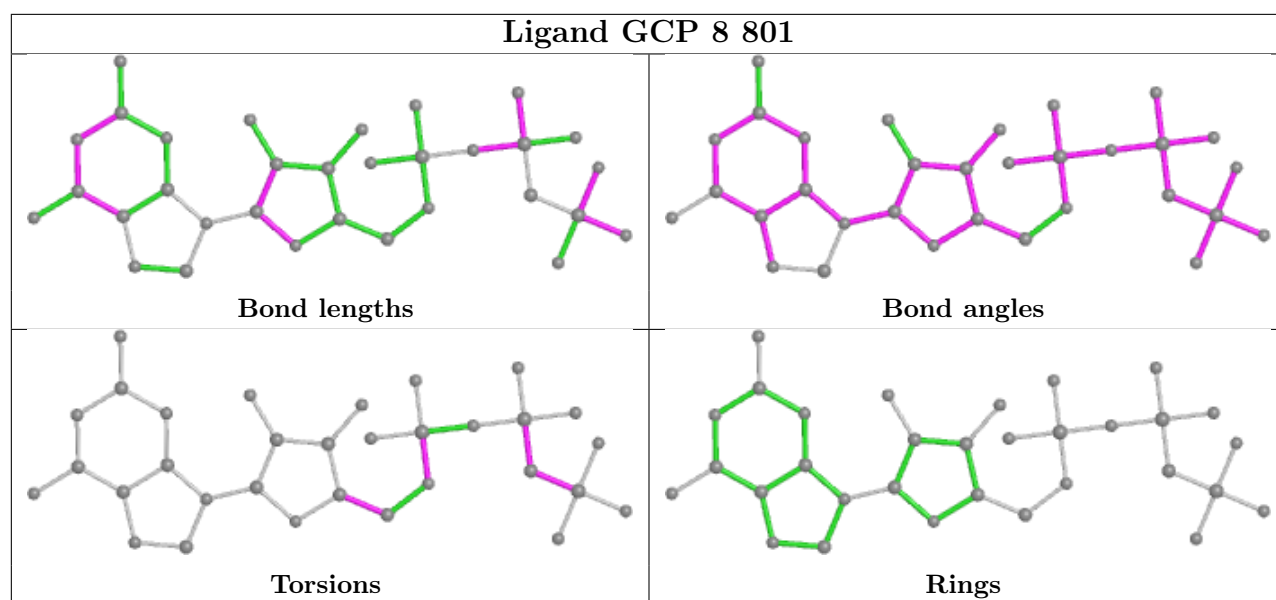
There are no ring outliers.

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.

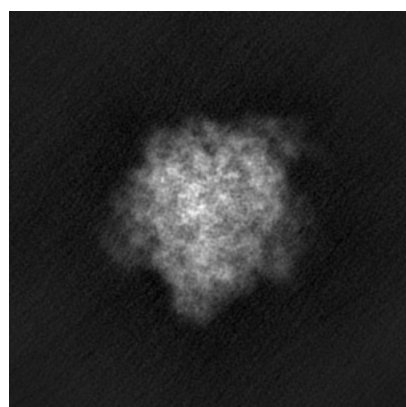
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22674. These allow visual inspection of the internal detail of the map and identification of artifacts.

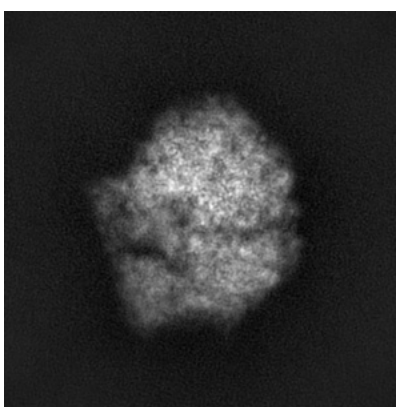
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

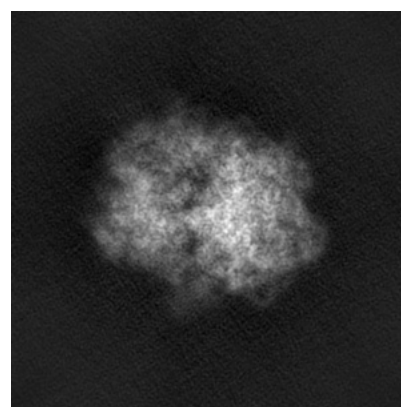
#### 6.1.1 Primary map



X



Y

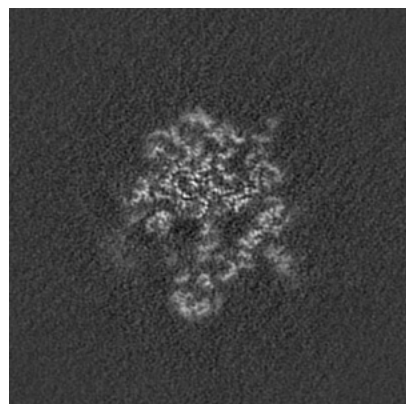


Z

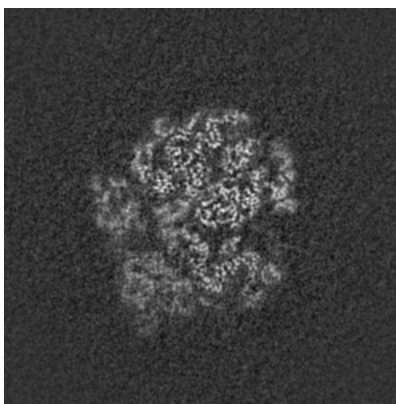
The images above show the map projected in three orthogonal directions.

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

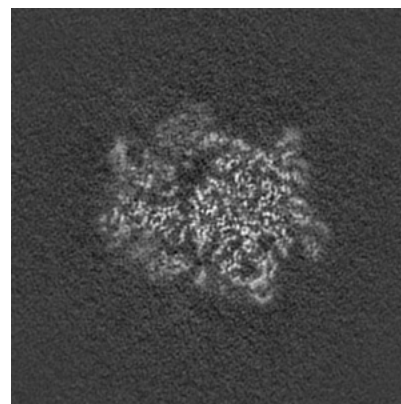
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

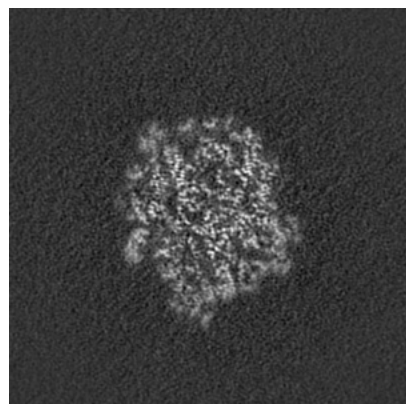


Z Index: 200

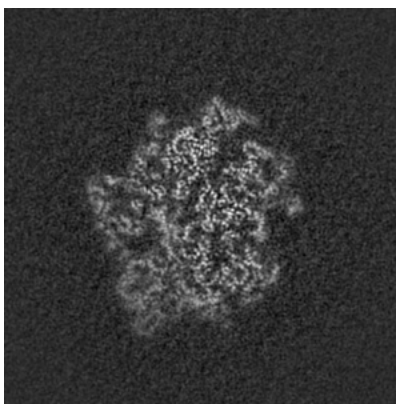
The images above show central slices of the map in three orthogonal directions.

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

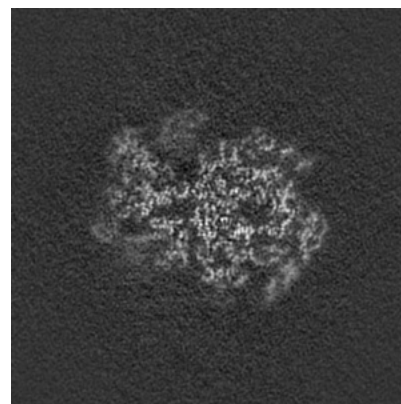
### 6.3.1 Primary map



X Index: 223



Y Index: 192

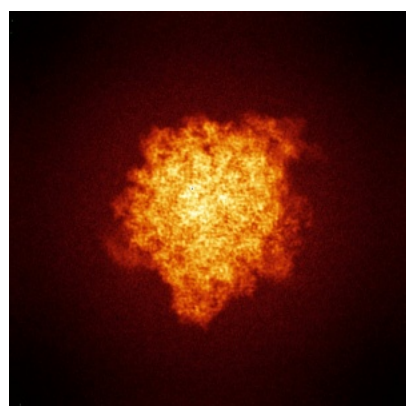


Z Index: 214

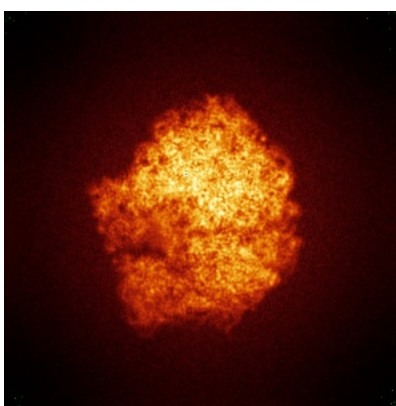
The images above show the largest variance slices of the map in three orthogonal directions.

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

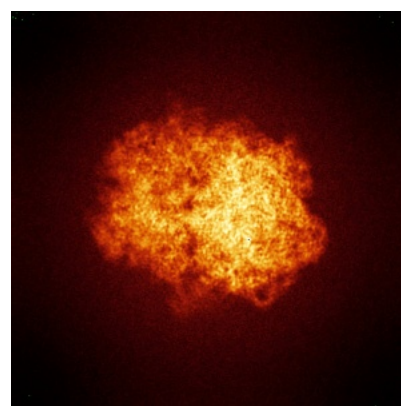
### 6.4.1 Primary map



X



Y



Z

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 3.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

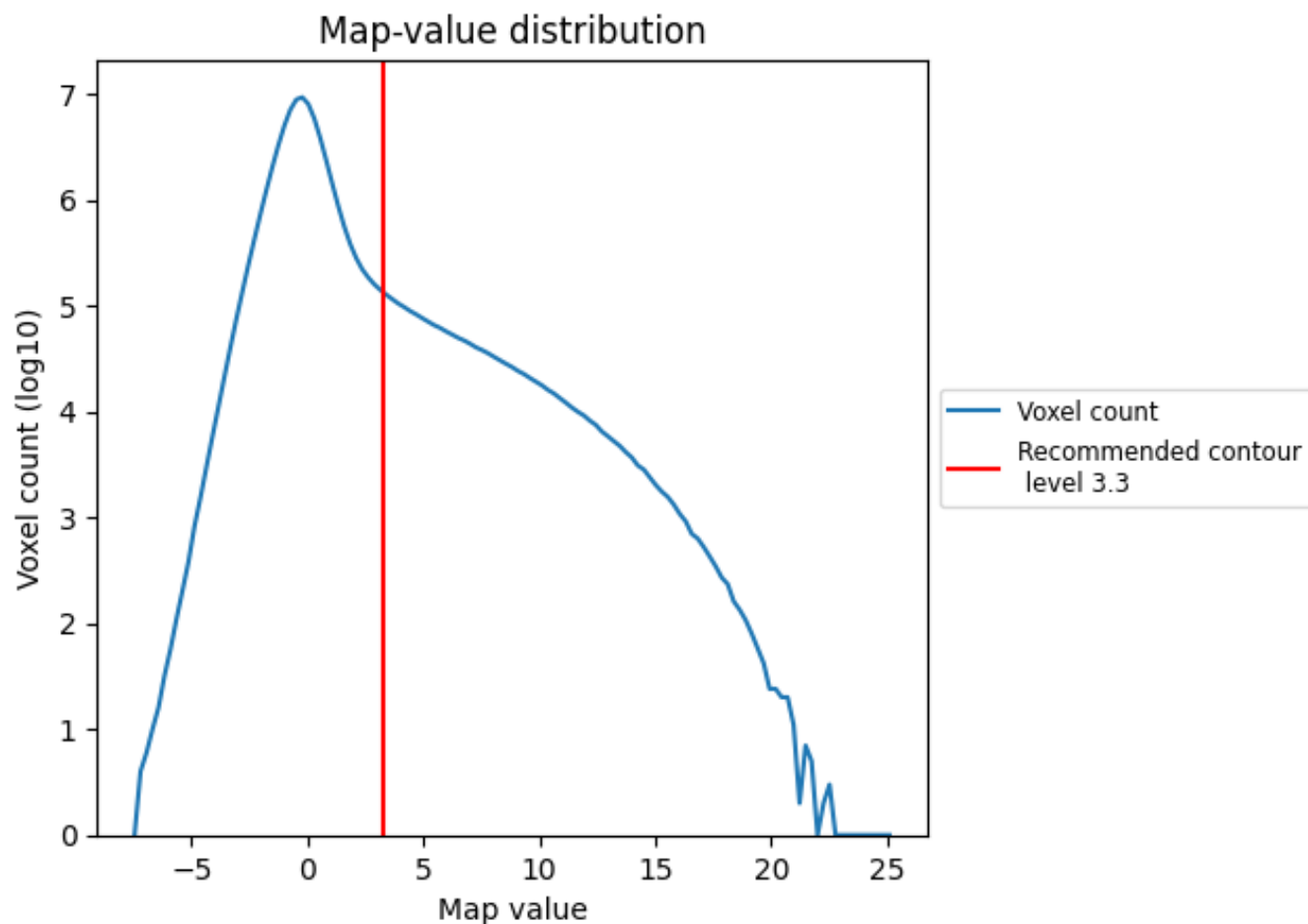
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

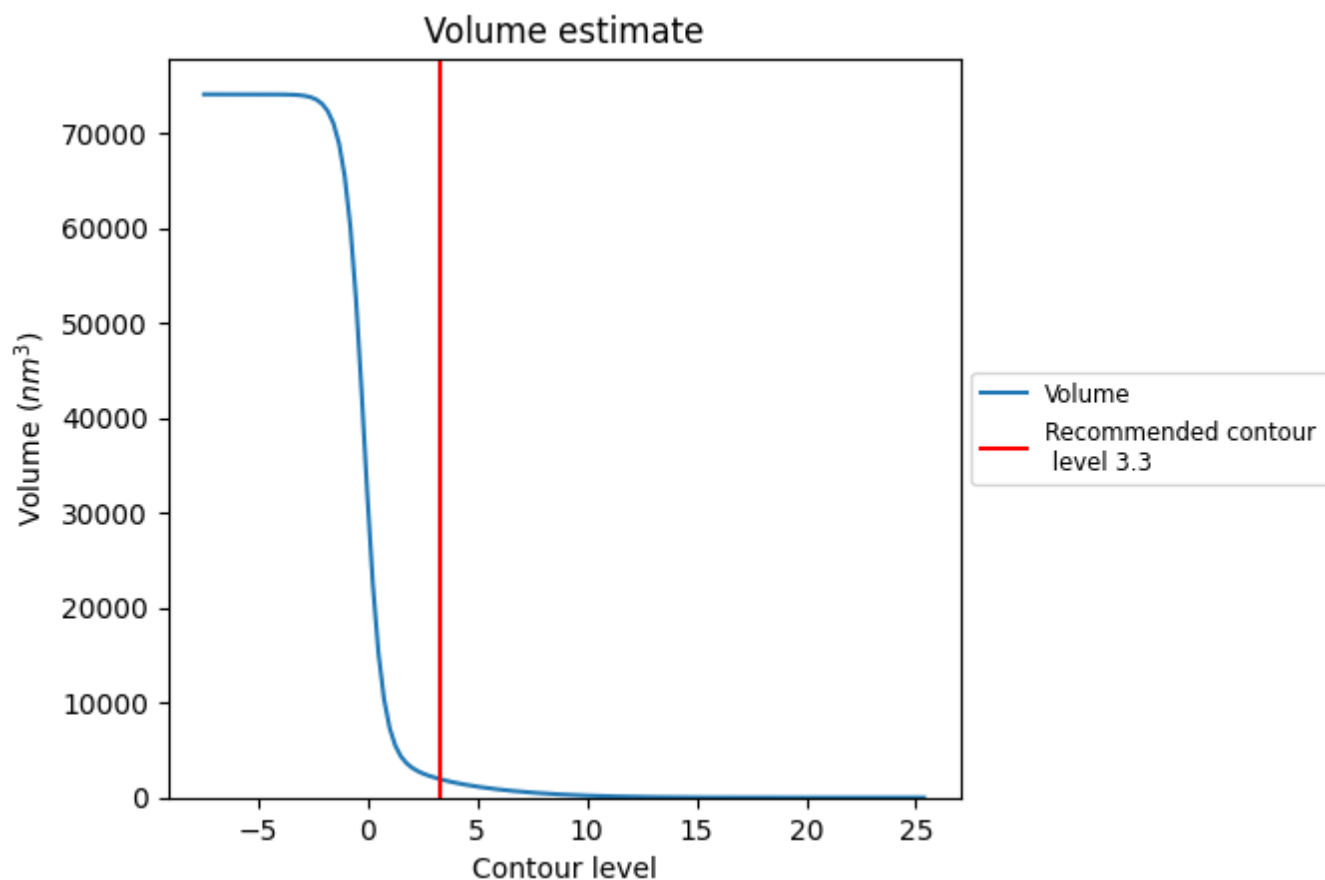
This section contains the results of statistical analysis of the map.

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



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

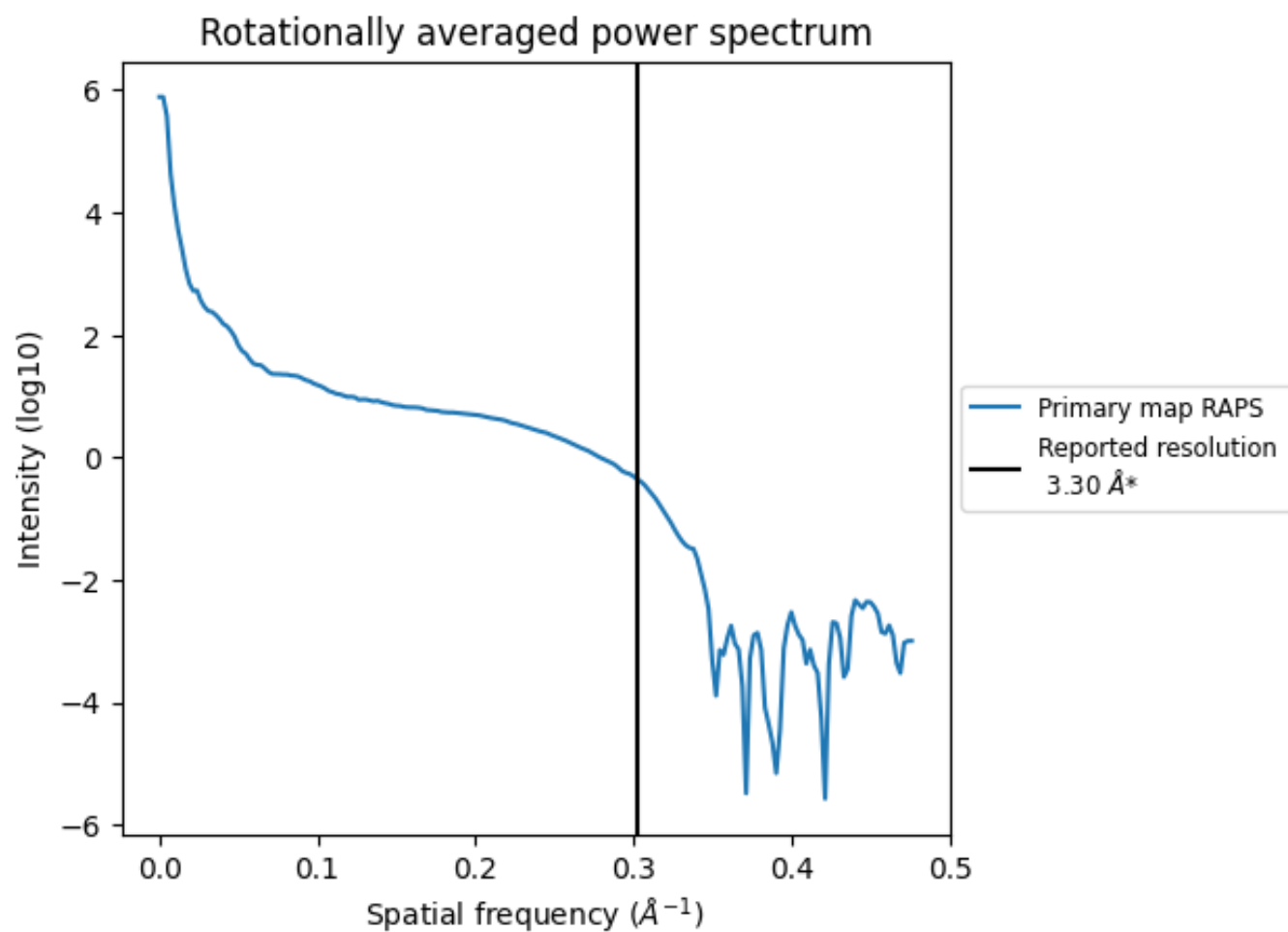
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1936 nm<sup>3</sup>; this corresponds to an approximate mass of 1749 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

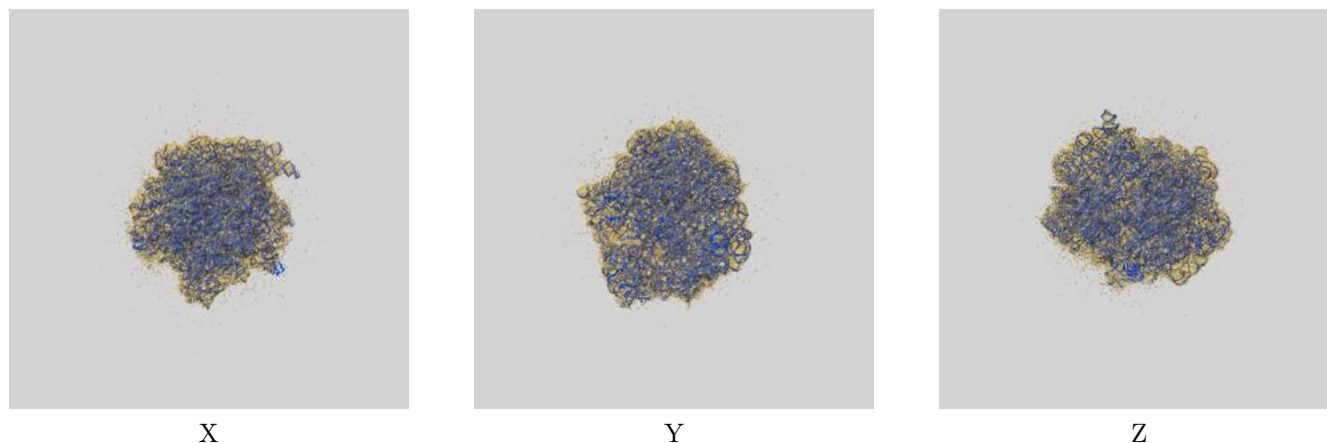
## 8 Fourier-Shell correlation ⓘ

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

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

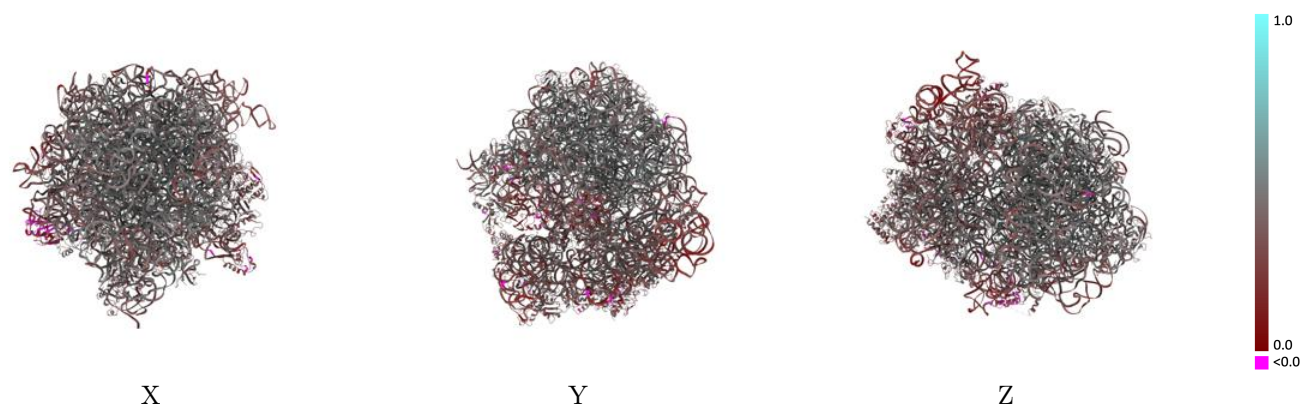
This section contains information regarding the fit between EMDB map EMD-22674 and PDB model 7K55. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



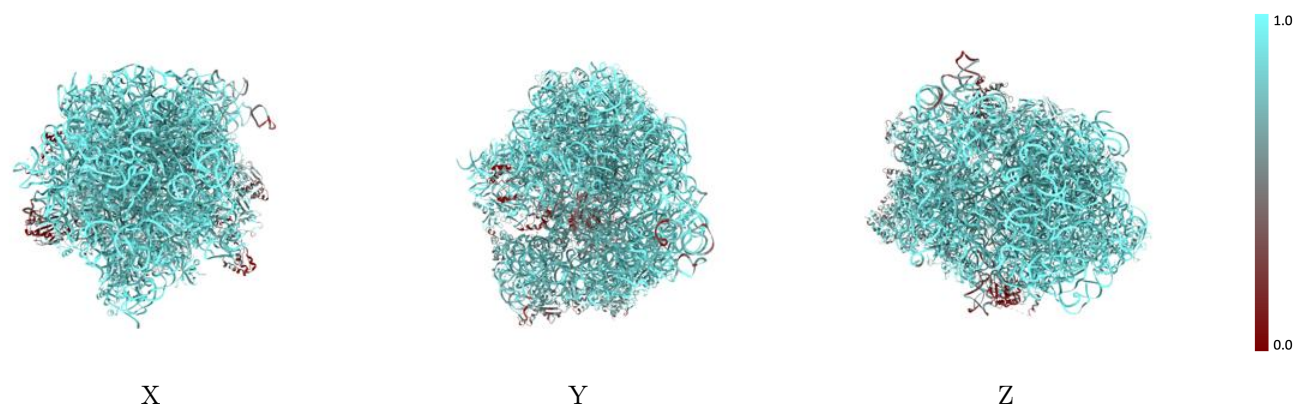
The images above show the 3D surface view of the map at the recommended contour level 3.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



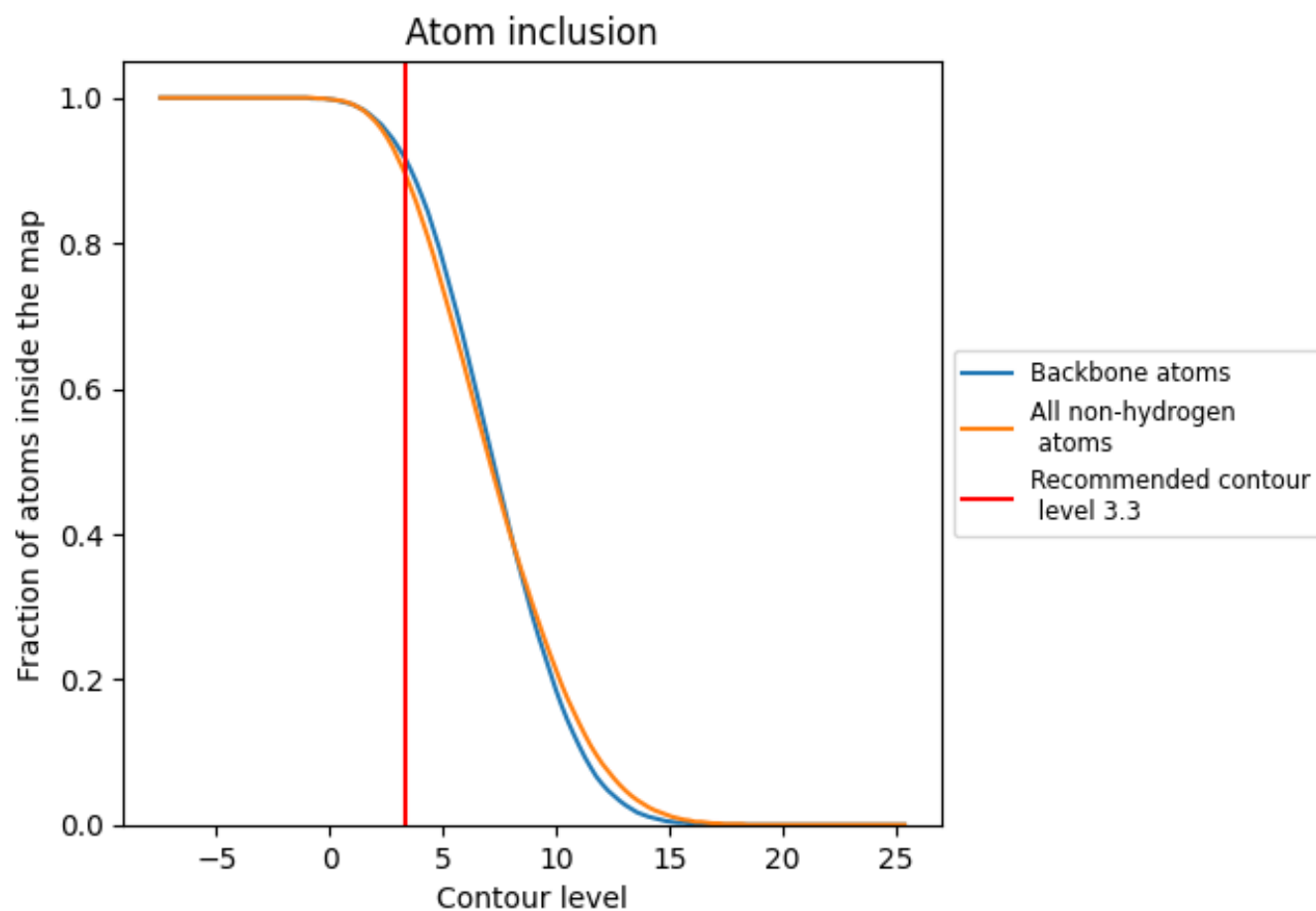
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.3).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 90% 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 (3.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8980	 0.3940
1	 0.9720	 0.4270
2	 0.9790	 0.4050
3	 0.9270	 0.3600
4	 0.7490	 0.2820
5	 0.9760	 0.3440
6	 0.4840	 0.1950
8	 0.6460	 0.3170
A	 0.7210	 0.3380
B	 0.8950	 0.4420
C	 0.7710	 0.4190
D	 0.9440	 0.4800
E	 0.9590	 0.4870
F	 0.8840	 0.4600
G	 0.6780	 0.3610
H	 0.7040	 0.3840
I	 0.7650	 0.2950
J	 0.8930	 0.4190
K	 0.8760	 0.3790
L	 0.7060	 0.3390
M	 0.8840	 0.4080
N	 0.7910	 0.3440
O	 0.6170	 0.3330
P	 0.9070	 0.4160
Q	 0.8780	 0.4030
R	 0.8040	 0.3370
S	 0.8440	 0.3560
T	 0.9220	 0.4050
U	 0.8500	 0.3650
V	 0.8960	 0.3680
W	 0.9220	 0.4050
X	 0.7120	 0.3320
Y	 0.8280	 0.3630
Z	 0.7280	 0.3170
a	 0.1060	 0.0370



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Chain	Atom inclusion	Q-score
b	 0.9440	 0.4720
c	 0.9230	 0.4590
d	 0.8200	 0.4300
e	 0.8930	 0.3720
f	 0.8570	 0.3950
g	 0.3050	 0.3150
h	 0.2240	 0.2420
i	 0.2430	 0.2320
j	 0.9380	 0.4560
k	 0.9120	 0.4700
l	 0.9280	 0.4580
m	 0.9230	 0.4500
n	 0.9370	 0.4490
o	 0.9150	 0.4170
p	 0.9100	 0.4580
q	 0.9390	 0.4600
r	 0.9070	 0.4550
s	 0.9020	 0.4570
t	 0.9070	 0.4480
u	 0.8850	 0.4210
v	 0.9000	 0.4260
w	 0.9210	 0.4750
x	 0.9150	 0.4440
y	 0.8830	 0.3940
z	 0.9130	 0.4430