Full wwPDB EM Validation Report (i)

May 18, 2024 – 09:28 AM EDT

PDB ID	:	7K51
EMDB ID	:	EMD-22670
Title	:	Mid-translocated non-frameshifting(CCA-A) complex with EF-G and GDPCP (Structure II)
Authors	:	Demo, G.; Loveland, A.B.; Svidritskiy, E.; Gamper, H.B.; Hou, Y.M.; Korostelev, A.A.
Deposited on	:	2020-09-16
Resolution	:	3.50 Å(reported)
Based on initial models	:	4V9P, 4V7D, 6ENJ, 5UYM

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

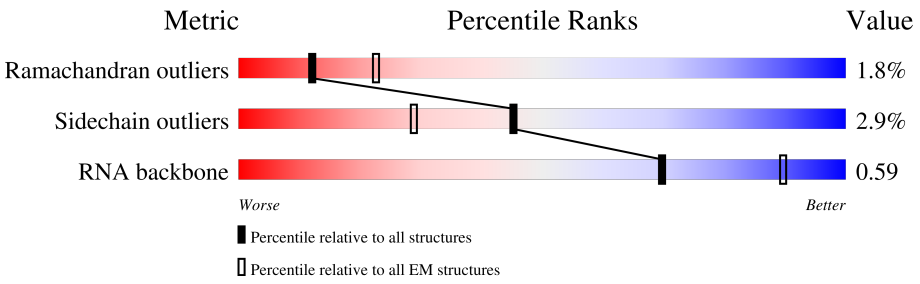
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	b	271	94% 6%
2	c	209	98% •
3	d	201	5% 94% 6%
4	e	177	6% 90% 10% •
5	f	176	• 97% •
6	g	149	60% 72% 11% 16%
7	h	131	52% 53% 11% 36%
8	i	141	38% 38% 12% • 48%

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Mol	Chain	Length	Quality of chain
9	j	142	96%
10	k	122	94% 6%
11	l	143	93% 7%
12	m	136	94% 6%
13	n	120	98%
14	o	116	96%
15	p	114	97%
16	q	117	97%
17	r	103	5% 96%
18	s	110	95% 5%
19	t	93	97%
20	u	102	98%
21	v	94	98%
22	w	75	93% 7%
23	x	77	97%
24	y	63	5% 97%
25	z	58	95% 5%
26	A	66	32% 91% 9%
27	B	56	96%
28	C	50	16% 96%
29	D	46	96%
30	E	64	95% 5%
31	F	38	89% 11%
32	G	225	21% 88% 9%
33	H	206	31% 93% 7%

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Mol	Chain	Length	Quality of chain
34	I	205	8% 90% 8%
35	J	157	86% 13%
36	K	100	78% 20%
37	L	151	55% 93% 7%
38	M	129	95% 5%
39	N	127	35% 88% 11%
40	O	98	51% 83% 17%
41	P	116	89% 11%
42	Q	123	6% 93% 7%
43	R	114	41% 88% 11%
44	S	100	6% 87% 13%
45	T	88	88% 11%
46	U	82	5% 91% 7%
47	V	80	6% 95% 5%
48	W	65	8% 89% 11%
49	X	79	14% 82% 16%
50	Y	85	5% 94% 6%
51	Z	65	20% 83% 12% 5%
52	a	223	47% 49% 11% 40%
53	3	1539	83% 17%
54	1	2903	85% 15%
55	2	120	86% 12%
56	5	77	79% 21%
57	6	77	75% 23%
58	4	16	31% 81% 19%

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Mol	Chain	Length	Quality of chain
59	8	711	9% 85% 11%

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 153370 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 56 is a RNA chain called tRNAPro.

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

- Molecule 57 is a RNA chain called tRNAfMet.

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

- Molecule 58 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
58	4	16	348	156	70	106	16	0	0

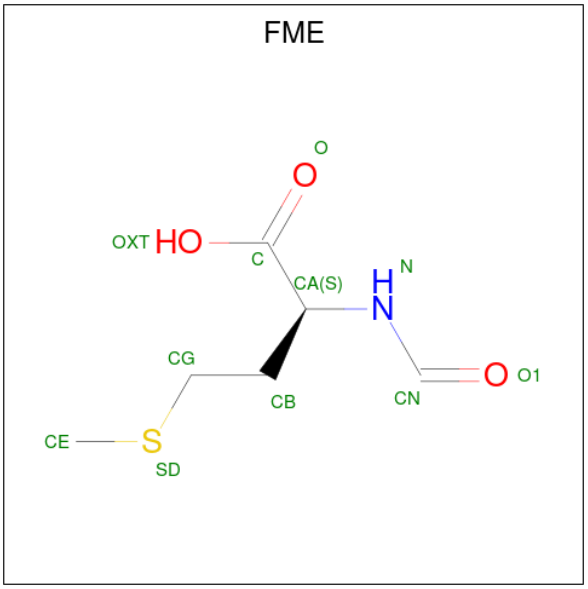
- Molecule 59 is a protein called Elongation factor G.

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

There are 8 discrepancies between the modelled and reference sequences:

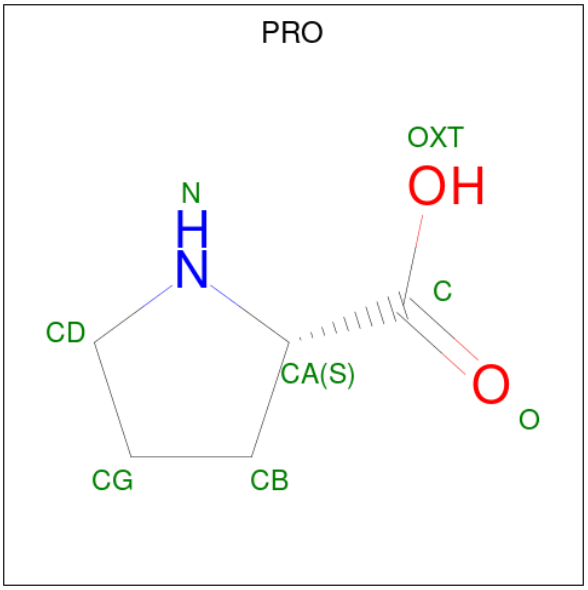
Chain	Residue	Modelled	Actual	Comment	Reference
8	705	LEU	-	expression tag	UNP H4UQ46
8	706	GLU	-	expression tag	UNP H4UQ46
8	707	HIS	-	expression tag	UNP H4UQ46
8	708	HIS	-	expression tag	UNP H4UQ46
8	709	HIS	-	expression tag	UNP H4UQ46
8	710	HIS	-	expression tag	UNP H4UQ46
8	711	HIS	-	expression tag	UNP H4UQ46
8	712	HIS	-	expression tag	UNP H4UQ46

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



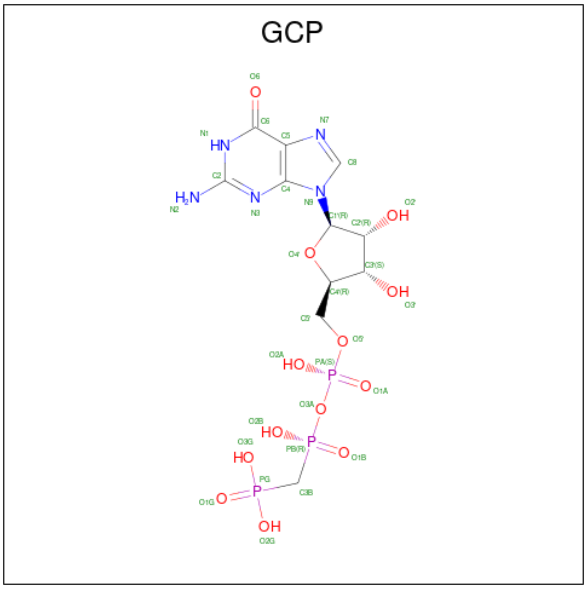
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	1	1	10	6	1	2	1	0

- 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: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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

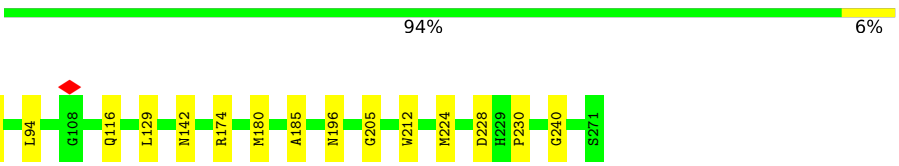
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
63	8	1	1	1	0

3 Residue-property plots (i)

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

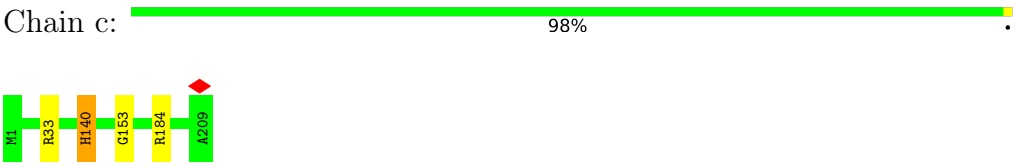
• Molecule 1: 50S ribosomal protein L2

Chain b:



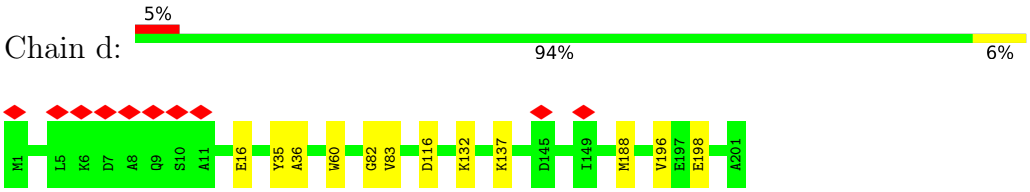
• Molecule 2: 50S ribosomal protein L3

Chain c:



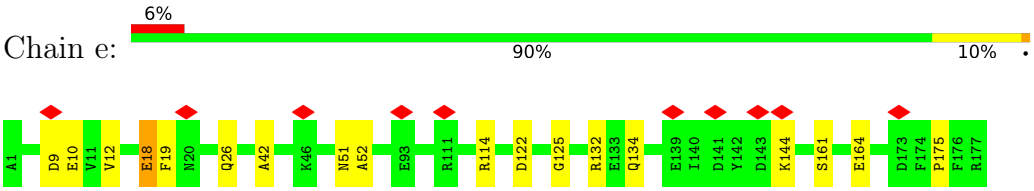
• Molecule 3: 50S ribosomal protein L4

Chain d:



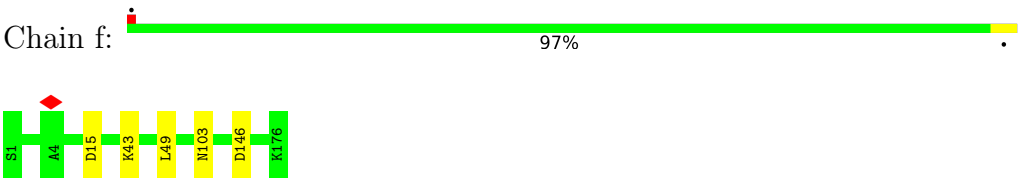
• Molecule 4: 50S ribosomal protein L5

Chain e:



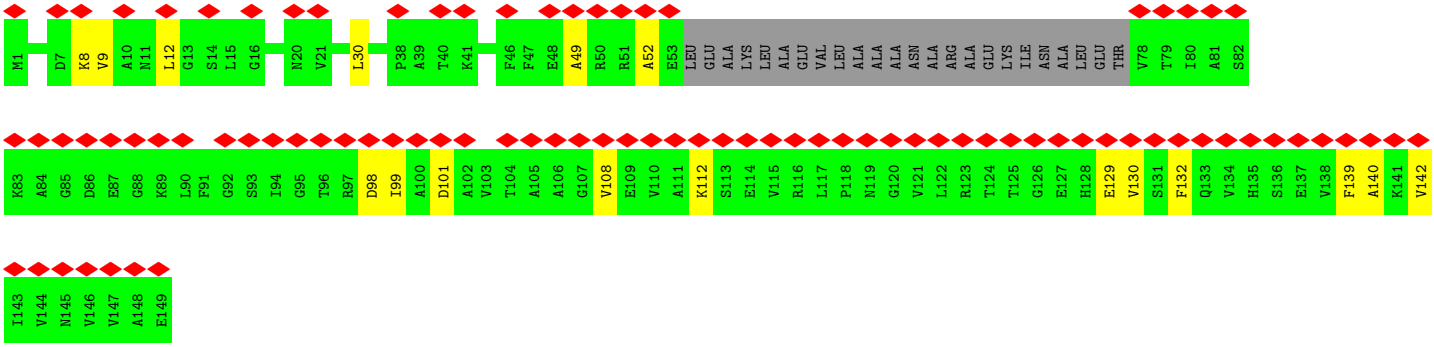
• Molecule 5: 50S ribosomal protein L6

Chain f:



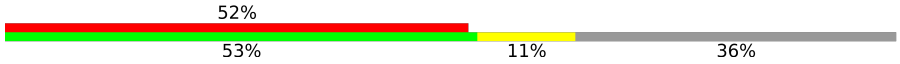
- Molecule 6: 50S ribosomal protein L9

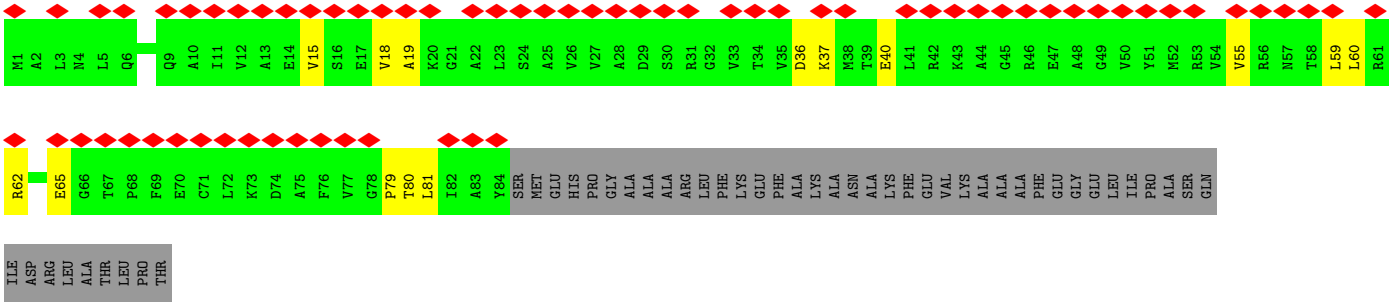
Chain g:



- Molecule 7: 50S ribosomal protein L10

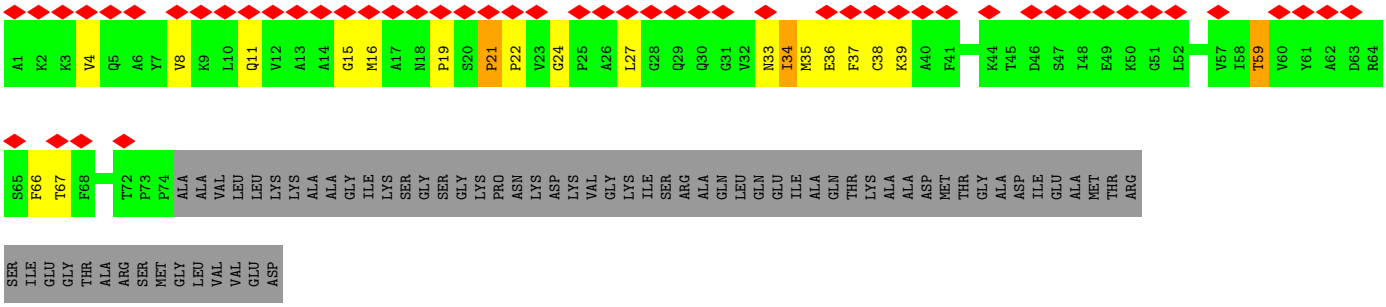
Chain h:





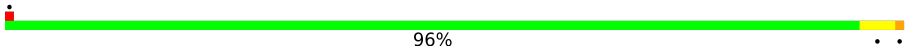
- Molecule 8: 50S ribosomal protein L11

Chain i:



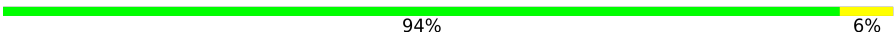
- Molecule 9: 50S ribosomal protein L13

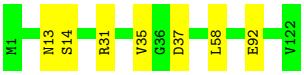
Chain j:



- Molecule 10: 50S ribosomal protein L14

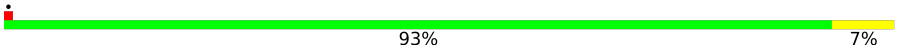
Chain k:





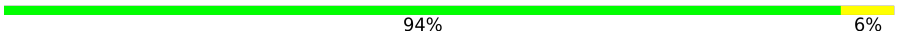
- Molecule 11: 50S ribosomal protein L15

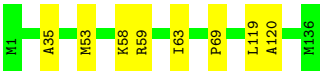
Chain l:



- Molecule 12: 50S ribosomal protein L16

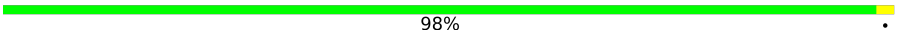
Chain m:

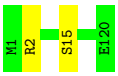




- Molecule 13: 50S ribosomal protein L17

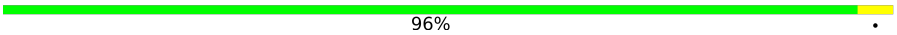
Chain n:

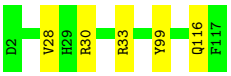




- Molecule 14: 50S ribosomal protein L18

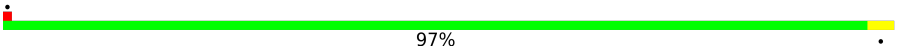
Chain o:

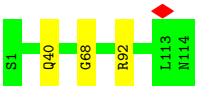




- Molecule 15: 50S ribosomal protein L19

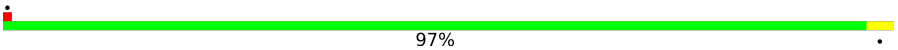
Chain p:

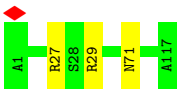




- Molecule 16: 50S ribosomal protein L20

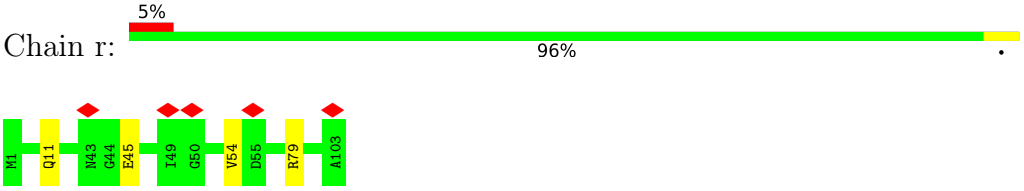
Chain q:





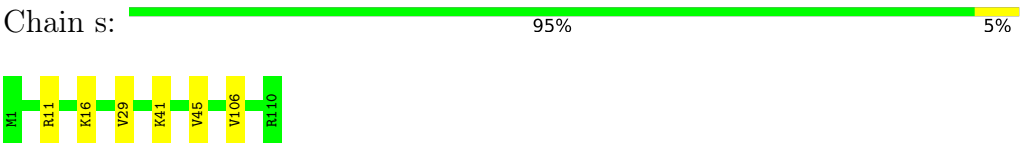
• Molecule 17: 50S ribosomal protein L21

Chain r:



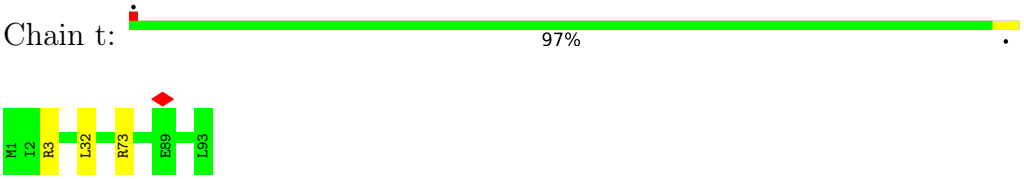
• Molecule 18: 50S ribosomal protein L22

Chain s:



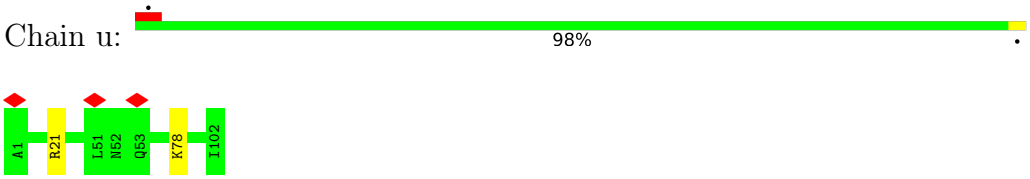
• Molecule 19: 50S ribosomal protein L23

Chain t:



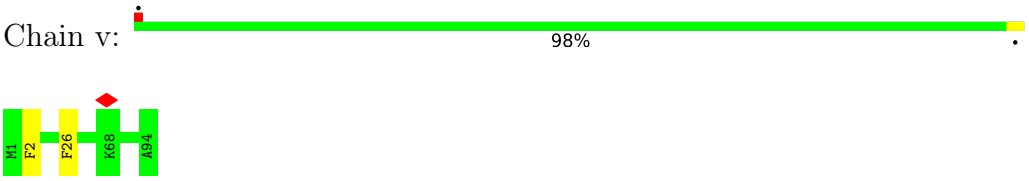
• Molecule 20: 50S ribosomal protein L24

Chain u:



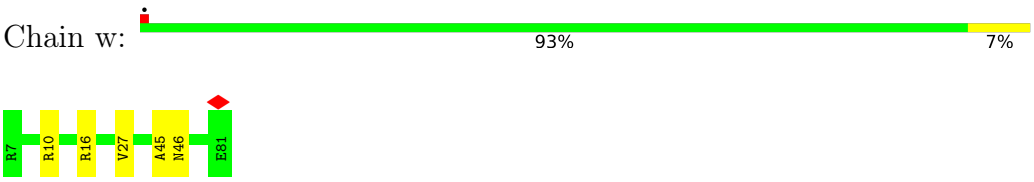
• Molecule 21: 50S ribosomal protein L25

Chain v:



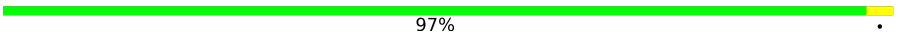
• Molecule 22: 50S ribosomal protein L27

Chain w:



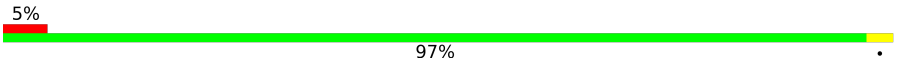
• Molecule 23: 50S ribosomal protein L28

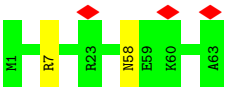
Chain x:



• Molecule 24: 50S ribosomal protein L29

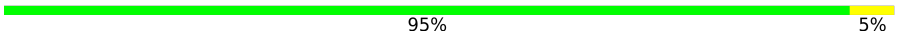
Chain y:

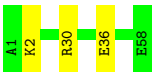




• Molecule 25: 50S ribosomal protein L30

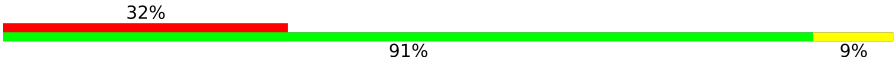
Chain z:

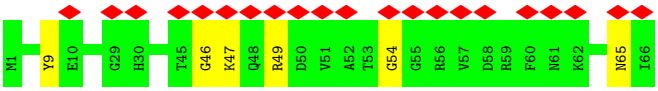




• Molecule 26: 50S ribosomal protein L31

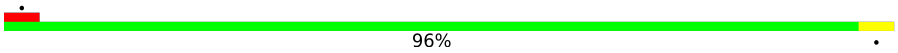
Chain A:

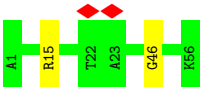




• Molecule 27: 50S ribosomal protein L32

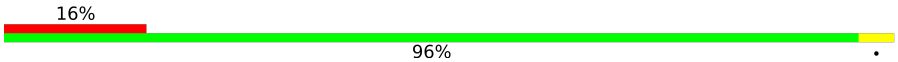
Chain B:

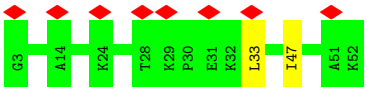




• Molecule 28: 50S ribosomal protein L33

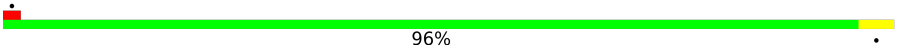
Chain C:

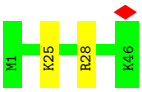




• Molecule 29: 50S ribosomal protein L34

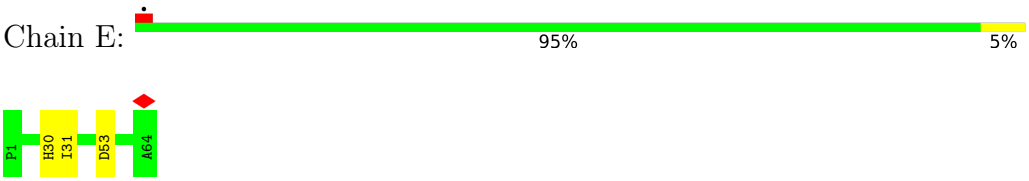
Chain D:





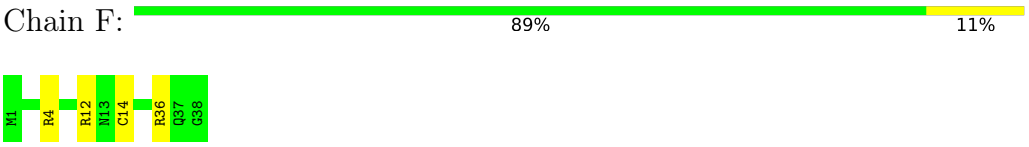
• Molecule 30: 50S ribosomal protein L35

Chain E:



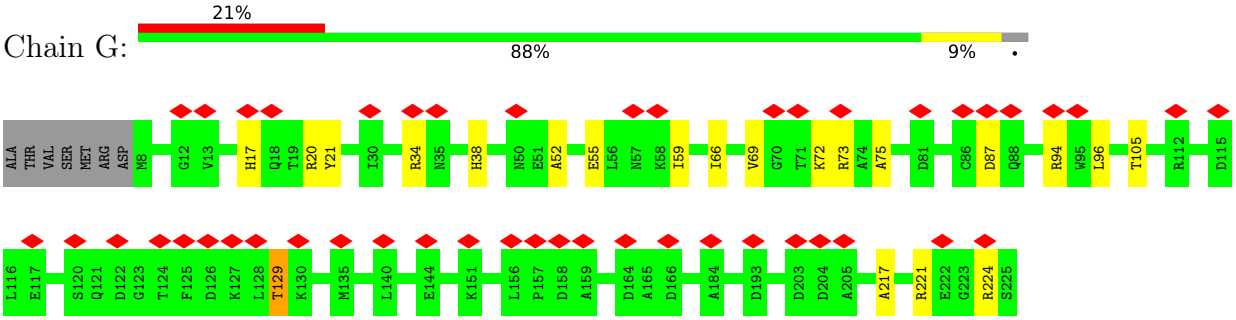
• Molecule 31: 50S ribosomal protein L36

Chain F:



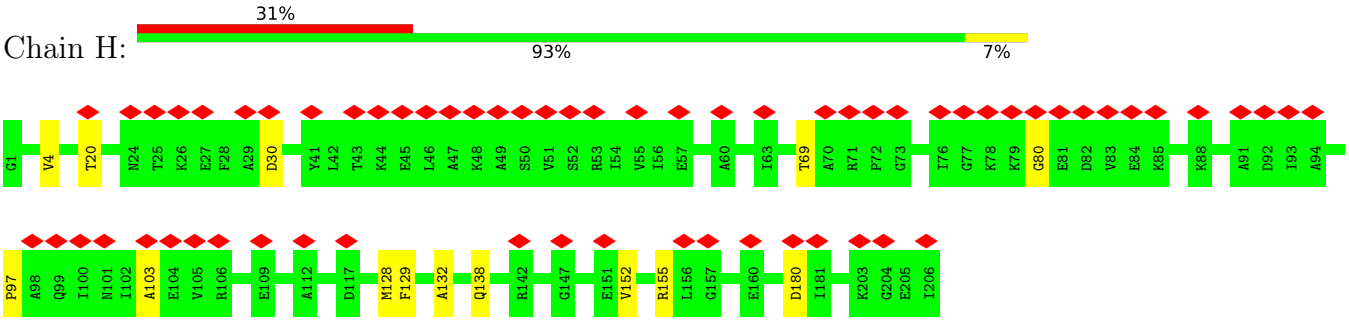
• Molecule 32: 30S ribosomal protein S2

Chain G:



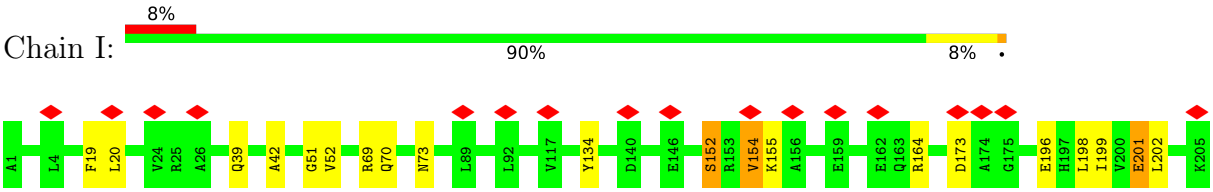
• Molecule 33: 30S ribosomal protein S3

Chain H:



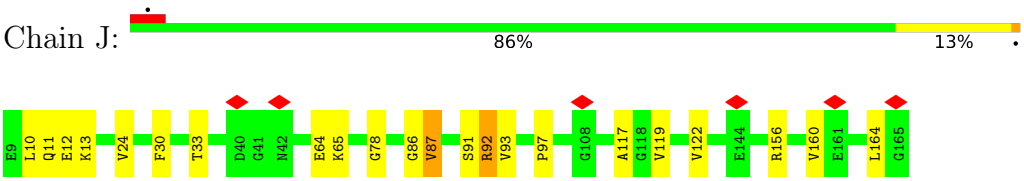
• Molecule 34: 30S ribosomal protein S4

Chain I:



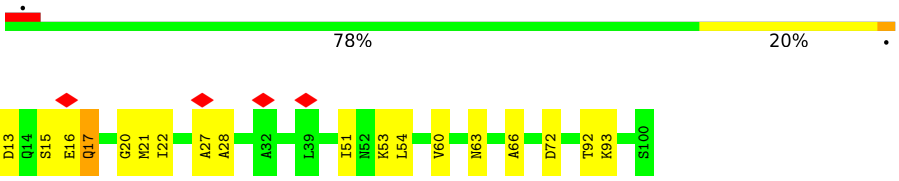
• Molecule 35: 30S ribosomal protein S5

Chain J:



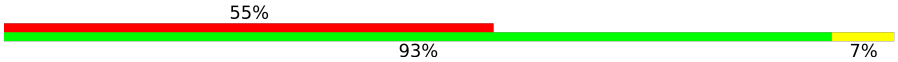
- Molecule 36: 30S ribosomal protein S6

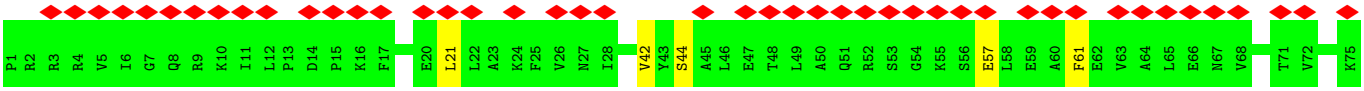
Chain K:

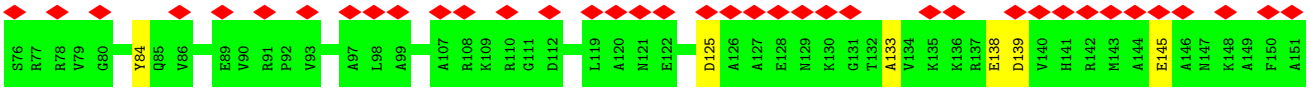


- Molecule 37: 30S ribosomal protein S7

Chain L:

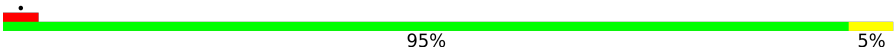


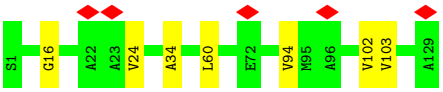




- Molecule 38: 30S ribosomal protein S8

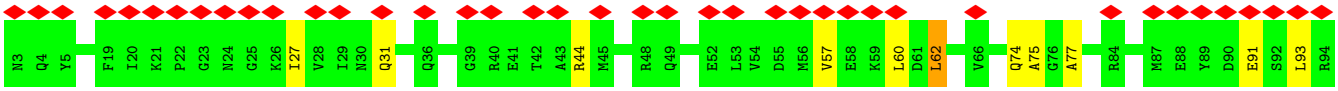
Chain M:

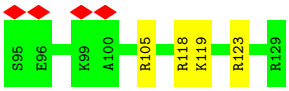




- Molecule 39: 30S ribosomal protein S9

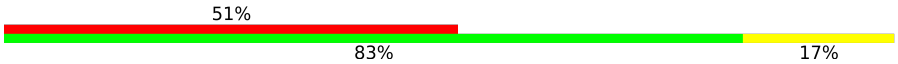
Chain N:

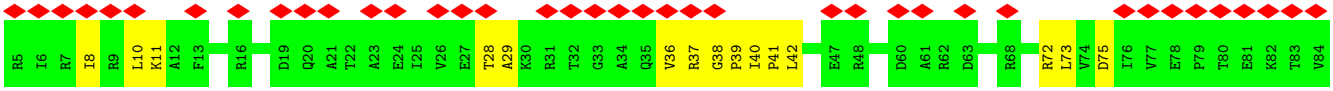


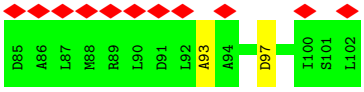


- Molecule 40: 30S ribosomal protein S10

Chain O:







- Molecule 41: 30S ribosomal protein S11

Chain P: 89% 11%

R12 K13 Q14 T29 I30 V31 E67 A70 D71 V85 P88 G89 A102 G103 I109 T110 D111 N118 K124 R127

• Molecule 42: 30S ribosomal protein S12

Chain Q: 6% 93% 7%

A1 N4 V32 C33 T40 A47 G70 H71 N72 E75 R93 L101 K107 D108 R113 K122 A123

• Molecule 43: 30S ribosomal protein S13

Chain R: 41% 88% 11%

A1 R2 I3 A4 G5 I6 N7 I8 P9 D10 A14 V15 I16 A17 L18 Y22 K30 A31 I32 L33 A34 A35 A36 G37 I38 A39 E40 D41 V42 K43 I44 S45 E46 L47 S48 E49 G50 Q51 I52 D53 T54 L55 R56 D57 E58 V59 A60 K61 F62 E65 S75 I76 K77 D81

R89 H90 R91 V96 R97 G98 Q99 R100 T101 G110 K113 P114

• Molecule 44: 30S ribosomal protein S14

Chain S: 6% 87% 13%

A1 M5 K6 A7 R8 K27 A28 I29 D32 V33 N34 E38 D39 R40 W41 L45 R52 R62 G77 K82 V83 R84 W100

• Molecule 45: 30S ribosomal protein S15

Chain T: 88% 11%

S1 A6 T7 T21 T24 E44 H45 K46 K64 K70 V74 A75 R76 Y77 R88

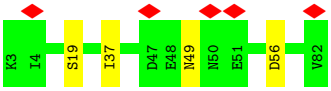
• Molecule 46: 30S ribosomal protein S16

Chain U: 5% 91% 7%

M1 G37 A43 S44 E45 G49 I75 V78 N79 K80 A81 A82

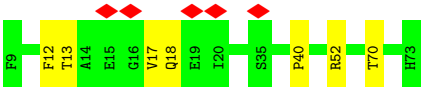
• Molecule 47: 30S ribosomal protein S17

Chain V: 6% 95% 5%



• Molecule 48: 30S ribosomal protein S18

Chain W:

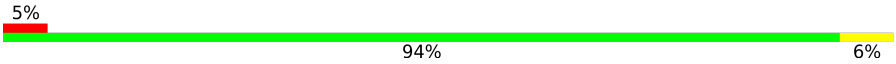


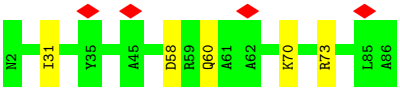
• Molecule 49: 30S ribosomal protein S19

Chain X:

• Molecule 50: 30S ribosomal protein S20

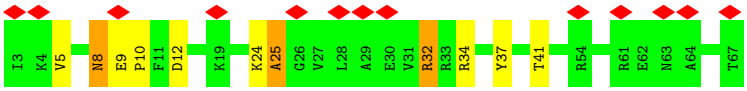
Chain Y:





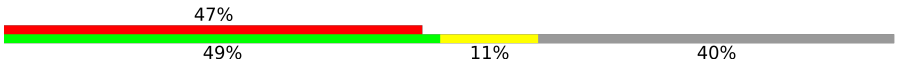
• Molecule 51: 30S ribosomal protein S21

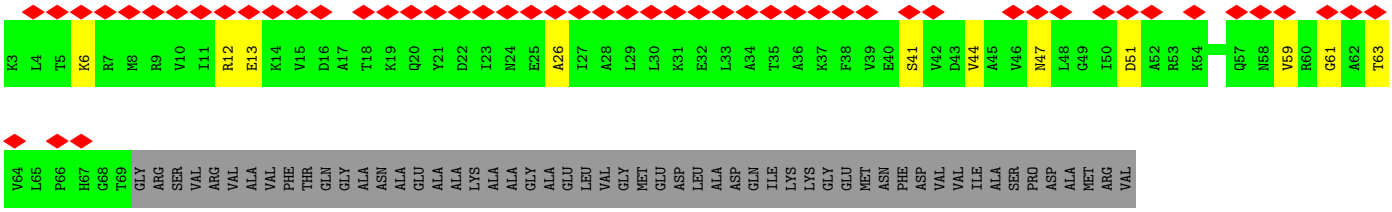
Chain Z:

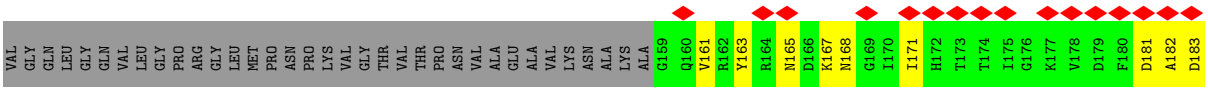


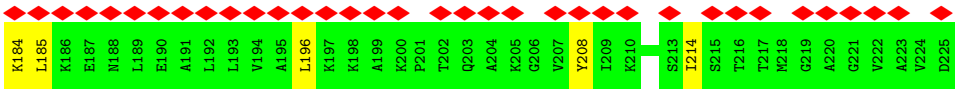
• Molecule 52: 50S ribosomal protein L1

Chain a:



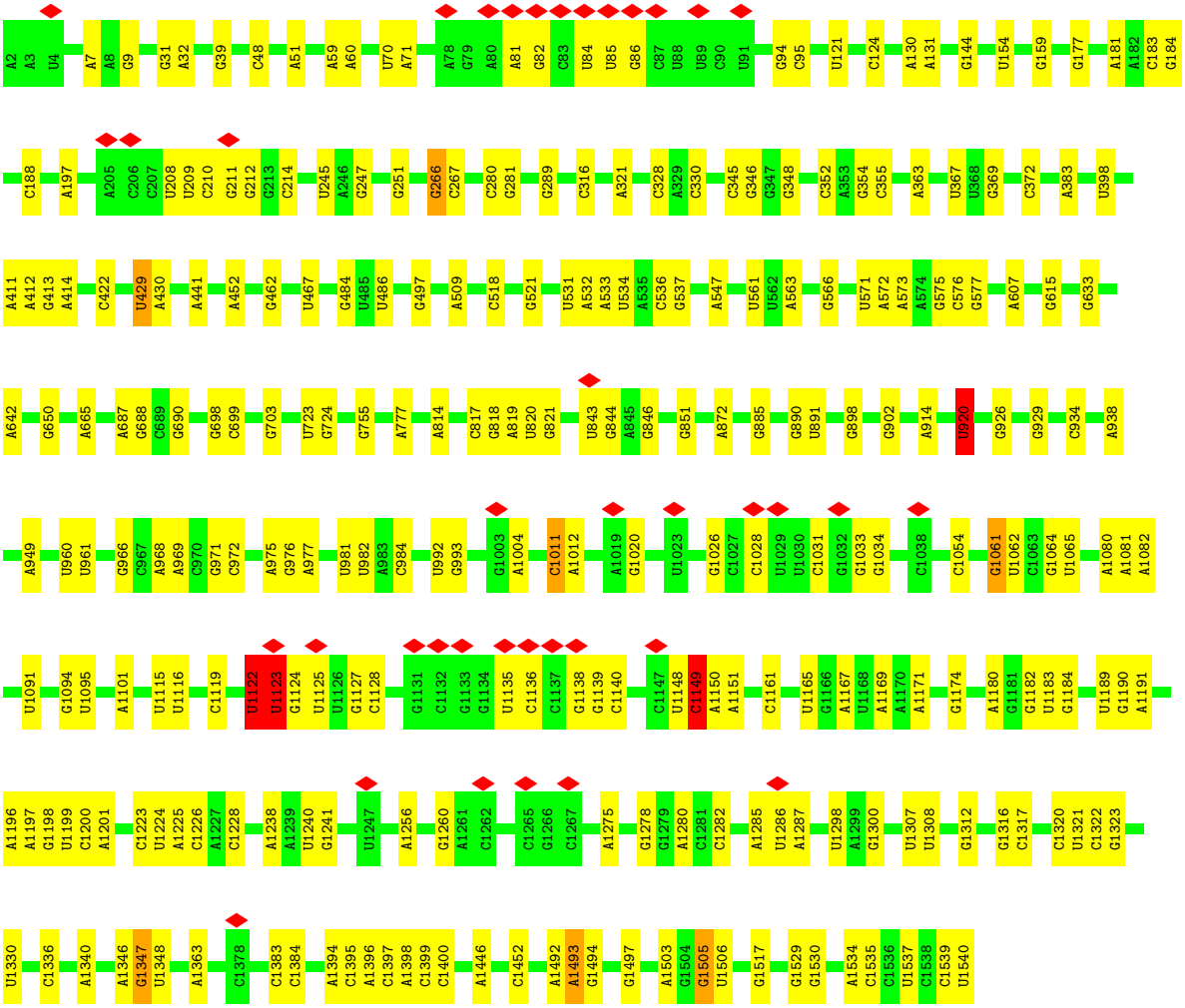






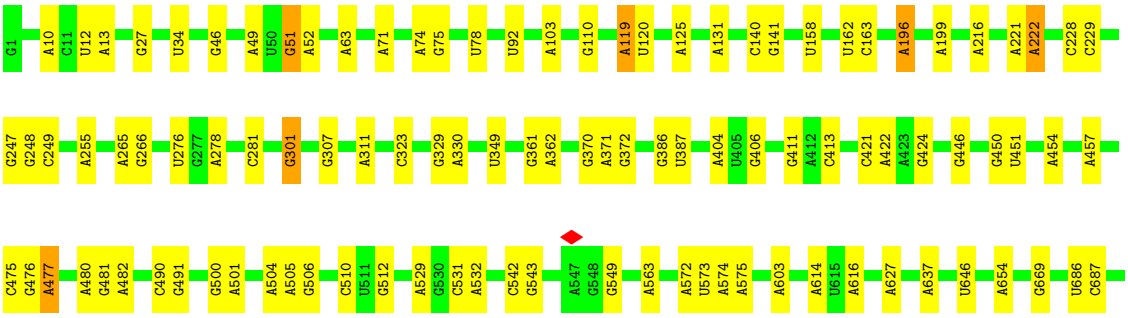
• Molecule 53: 16S ribosomal RNA

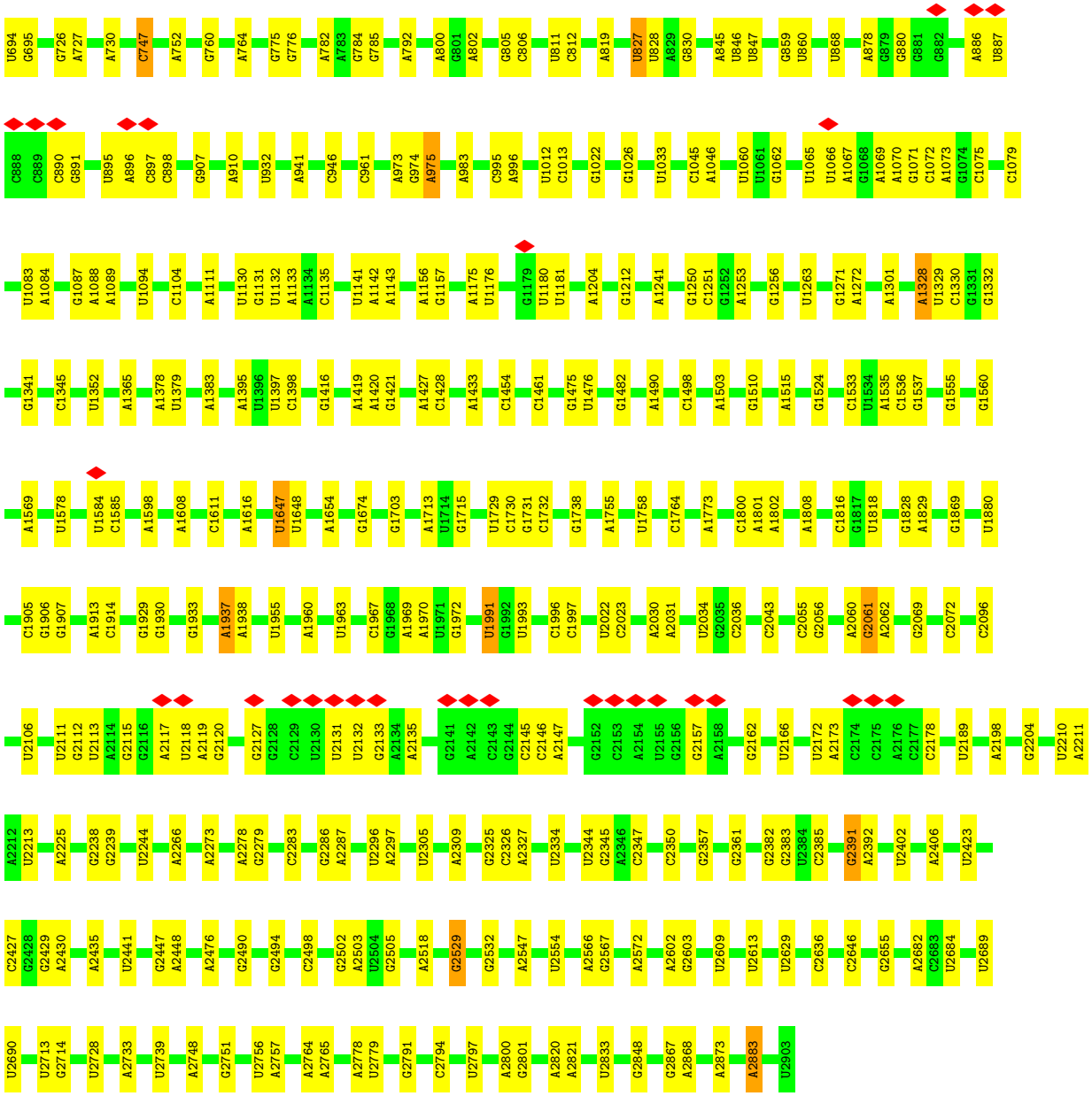
Chain 3:



• Molecule 54: 23S ribosomal RNA

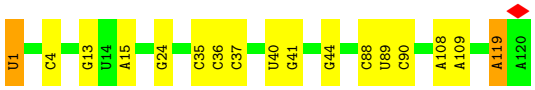
Chain 1:





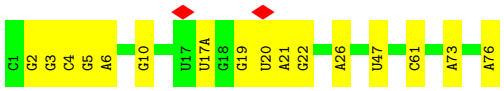
- Molecule 55: 5S ribosomal RNA

Chain 2:



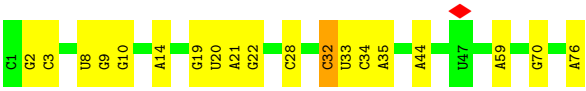
- Molecule 56: tRNAPro

Chain 5:



- Molecule 57: tRNAfMet

Chain 6:

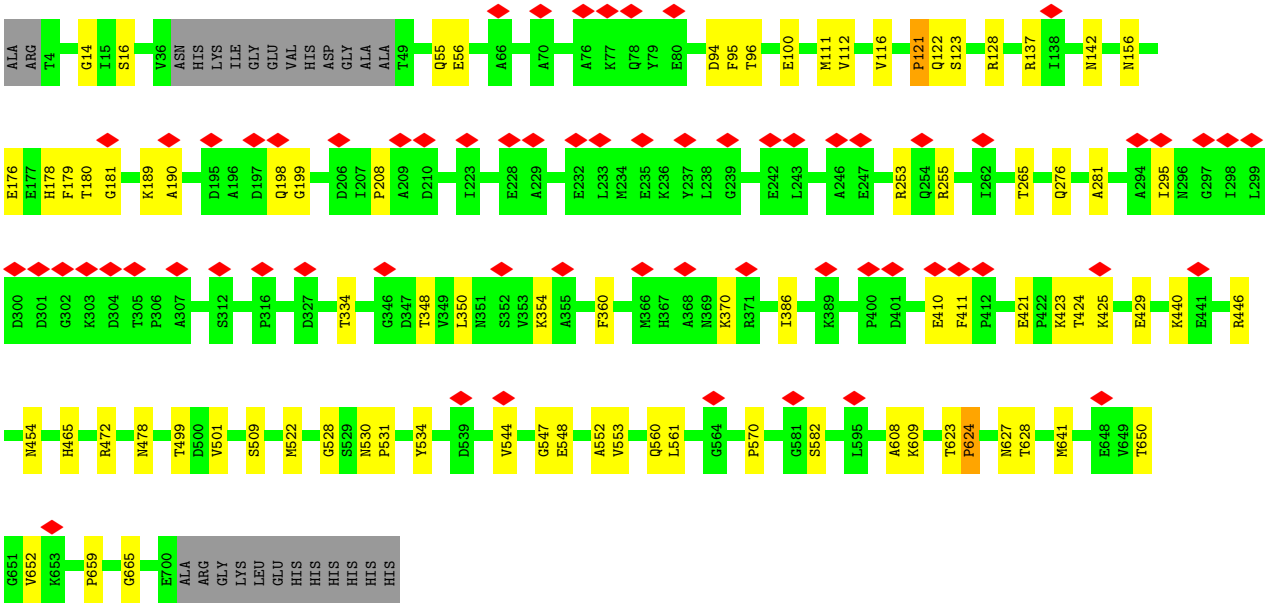


- Molecule 58: mRNA

Chain 4:

- Molecule 59: Elongation factor G

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3179	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 ($e^-/Å^2$)	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	21.906	Depositor
Minimum map value	-8.364	Depositor
Average map value	0.019	Depositor
Map value standard deviation	1.404	Depositor
Recommended contour level	3.7	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.70	3/2122 (0.1%)	0.77	1/2852 (0.0%)
2	c	0.67	1/1586 (0.1%)	0.80	0/2134
3	d	0.80	6/1571 (0.4%)	0.82	1/2113 (0.0%)
4	e	0.83	4/1435 (0.3%)	0.84	4/1926 (0.2%)
5	f	0.70	2/1343 (0.1%)	0.73	2/1816 (0.1%)
6	g	1.25	11/946 (1.2%)	0.92	3/1275 (0.2%)
7	h	1.12	7/638 (1.1%)	0.95	2/860 (0.2%)
8	i	1.52	11/564 (2.0%)	1.20	8/768 (1.0%)
9	j	0.70	2/1152 (0.2%)	0.74	2/1551 (0.1%)
10	k	0.71	2/948 (0.2%)	0.81	0/1268
11	l	0.55	0/1054	0.70	0/1403
12	m	0.81	4/1093 (0.4%)	0.80	1/1460 (0.1%)
13	n	0.67	1/974 (0.1%)	0.69	0/1301
14	o	0.67	2/902 (0.2%)	0.71	1/1209 (0.1%)
15	p	0.59	1/929 (0.1%)	0.67	0/1242
16	q	0.78	0/960	0.72	0/1278
17	r	0.53	0/829	0.70	0/1107
18	s	0.81	4/864 (0.5%)	0.77	0/1156
19	t	0.59	0/745	0.69	0/994
20	u	0.49	0/788	0.65	0/1051
21	v	0.64	1/766 (0.1%)	0.71	0/1025
22	w	0.78	3/582 (0.5%)	0.74	0/769
23	x	0.57	0/635	0.66	0/848
24	y	0.72	0/510	0.72	0/677
25	z	0.72	1/453 (0.2%)	0.65	0/605
26	A	0.92	2/532 (0.4%)	0.84	1/709 (0.1%)
27	B	0.61	1/450 (0.2%)	0.67	0/599
28	C	0.80	2/417 (0.5%)	0.71	0/554
29	D	0.66	1/380 (0.3%)	0.70	0/498
30	E	0.62	1/513 (0.2%)	0.65	0/676
31	F	0.75	1/303 (0.3%)	0.72	0/397
32	G	0.93	10/1736 (0.6%)	0.86	0/2338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	H	1.01	11/1652 (0.7%)	0.83	0/2225
34	I	0.88	13/1665 (0.8%)	0.84	4/2227 (0.2%)
35	J	0.91	7/1170 (0.6%)	0.87	3/1573 (0.2%)
36	K	1.43	17/836 (2.0%)	1.09	5/1128 (0.4%)
37	L	1.03	10/1196 (0.8%)	0.88	1/1602 (0.1%)
38	M	0.85	5/989 (0.5%)	0.83	0/1326
39	N	0.77	5/1034 (0.5%)	0.82	2/1375 (0.1%)
40	O	1.50	13/797 (1.6%)	1.12	10/1077 (0.9%)
41	P	0.90	6/886 (0.7%)	0.91	3/1195 (0.3%)
42	Q	0.64	0/969	0.75	0/1300
43	R	1.04	9/893 (1.0%)	0.99	4/1193 (0.3%)
44	S	1.03	8/817 (1.0%)	0.83	1/1088 (0.1%)
45	T	1.10	8/722 (1.1%)	0.85	0/964
46	U	0.71	2/659 (0.3%)	0.76	1/884 (0.1%)
47	V	0.59	1/658 (0.2%)	0.68	0/881
48	W	0.76	2/545 (0.4%)	0.81	0/731
49	X	1.01	5/653 (0.8%)	0.96	5/877 (0.6%)
50	Y	1.02	4/671 (0.6%)	0.84	0/888
51	Z	0.88	2/551 (0.4%)	0.97	2/728 (0.3%)
52	a	1.18	17/1034 (1.6%)	1.01	3/1387 (0.2%)
53	3	0.70	8/36963 (0.0%)	0.71	11/57662 (0.0%)
54	1	0.51	0/69796	0.67	7/108888 (0.0%)
55	2	0.43	0/2872	0.70	2/4479 (0.0%)
56	5	0.48	0/1840	0.73	0/2868
57	6	0.49	0/1832	0.73	2/2855 (0.1%)
58	4	0.65	0/391	0.79	0/608
59	8	0.90	39/5411 (0.7%)	0.88	10/7323 (0.1%)
All	All	0.68	276/166222 (0.2%)	0.73	102/247791 (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
34	I	0	2
35	J	0	2
46	U	0	1
53	3	0	22
54	1	0	49
55	2	0	3
56	5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
57	6	0	1
59	8	0	1
All	All	0	82

All (276) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	3	1123	U	N3-C4	27.67	1.63	1.38
53	3	1123	U	N1-C6	25.64	1.61	1.38
53	3	1123	U	N1-C2	25.54	1.61	1.38
53	3	1123	U	C4-C5	23.89	1.65	1.43
53	3	1123	U	C2-N3	23.87	1.54	1.37
53	3	1123	U	C5-C6	22.26	1.54	1.34
6	g	132	PHE	C-O	15.40	1.52	1.23
36	K	13	ASP	C-O	14.83	1.51	1.23
40	O	73	LEU	C-O	14.21	1.50	1.23
40	O	40	ILE	N-CA	13.90	1.74	1.46
6	g	142	VAL	C-O	12.84	1.47	1.23
8	i	19	PRO	C-O	12.55	1.48	1.23
8	i	35	MET	C-O	12.48	1.47	1.23
40	O	75	ASP	C-O	12.10	1.46	1.23
32	G	59	ILE	C-O	11.82	1.45	1.23
36	K	12	PRO	C-O	11.80	1.46	1.23
40	O	40	ILE	C-O	10.91	1.44	1.23
40	O	72	ARG	C-O	10.91	1.44	1.23
6	g	130	VAL	C-O	10.75	1.43	1.23
8	i	36	GLU	C-O	10.69	1.43	1.23
26	A	46	GLY	C-O	10.63	1.40	1.23
40	O	39	PRO	C-N	10.35	1.57	1.34
45	T	70	LYS	C-O	10.15	1.42	1.23
40	O	11	LYS	C-O	10.14	1.42	1.23
50	Y	60	GLN	C-O	9.77	1.42	1.23
6	g	98	ASP	C-O	9.77	1.42	1.23
59	8	181	GLY	C-O	9.75	1.39	1.23
36	K	17	GLN	N-CA	9.68	1.65	1.46
59	8	386	ILE	C-O	9.57	1.41	1.23
44	S	6	LYS	C-O	9.52	1.41	1.23
28	C	33	LEU	C-O	9.46	1.41	1.23
26	A	47	LYS	C-O	9.35	1.41	1.23
37	L	125	ASP	C-O	9.35	1.41	1.23
31	F	4	ARG	C-O	9.25	1.41	1.23
35	J	78	GLY	C-O	9.14	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	f	43	LYS	C-O	9.11	1.40	1.23
7	h	19	ALA	N-CA	9.05	1.64	1.46
8	i	34	ILE	C-O	9.02	1.40	1.23
59	8	665	GLY	C-O	9.02	1.38	1.23
36	K	20	GLY	C-O	9.00	1.38	1.23
4	e	51	ASN	C-O	8.89	1.40	1.23
7	h	15	VAL	C-O	8.86	1.40	1.23
32	G	105	THR	C-O	8.85	1.40	1.23
40	O	97	ASP	C-O	8.81	1.40	1.23
34	I	198	LEU	C-O	8.78	1.40	1.23
8	i	37	PHE	C-O	8.74	1.40	1.23
39	N	75	ALA	C-O	8.73	1.40	1.23
52	a	59	VAL	C-O	8.70	1.39	1.23
44	S	77	GLY	C-O	8.57	1.37	1.23
41	P	85	VAL	C-O	8.55	1.39	1.23
36	K	16	GLU	N-CA	8.49	1.63	1.46
33	H	128	MET	C-O	8.46	1.39	1.23
3	d	36	ALA	C-O	8.38	1.39	1.23
37	L	21	LEU	C-O	8.34	1.39	1.23
43	R	56	ARG	C-O	8.33	1.39	1.23
10	k	14	SER	C-O	8.20	1.39	1.23
1	b	116	GLN	C-O	8.13	1.38	1.23
59	8	429	GLU	C-O	8.11	1.38	1.23
45	T	76	ARG	C-O	8.03	1.38	1.23
59	8	112	VAL	N-CA	8.02	1.62	1.46
36	K	21	MET	C-O	8.01	1.38	1.23
34	I	69	ARG	C-O	7.99	1.38	1.23
59	8	276	GLN	C-O	7.97	1.38	1.23
37	L	139	ASP	C-O	7.87	1.38	1.23
37	L	57	GLU	C-O	7.84	1.38	1.23
8	i	38	CYS	N-CA	7.82	1.61	1.46
22	w	27	VAL	C-O	7.82	1.38	1.23
59	8	156	ASN	C-O	7.78	1.38	1.23
8	i	67	THR	C-O	7.78	1.38	1.23
7	h	36	ASP	C-O	7.75	1.38	1.23
3	d	35	TYR	C-O	7.71	1.38	1.23
18	s	41	LYS	C-O	7.71	1.38	1.23
33	H	132	ALA	C-O	7.69	1.38	1.23
52	a	61	GLY	C-O	7.67	1.35	1.23
34	I	199	ILE	C-O	7.65	1.37	1.23
27	B	46	GLY	C-O	7.64	1.35	1.23
59	8	561	LEU	C-O	7.61	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	38	HIS	C-O	7.60	1.37	1.23
45	T	7	THR	C-O	7.60	1.37	1.23
36	K	72	ASP	C-O	7.56	1.37	1.23
33	H	180	ASP	C-O	7.56	1.37	1.23
41	P	67	GLU	C-O	7.54	1.37	1.23
49	X	19	GLU	C-O	7.48	1.37	1.23
18	s	106	VAL	C-O	7.47	1.37	1.23
52	a	214	ILE	C-O	7.47	1.37	1.23
18	s	16	LYS	C-O	7.44	1.37	1.23
7	h	37	LYS	C-O	7.42	1.37	1.23
52	a	47	ASN	C-O	7.42	1.37	1.23
52	a	185	LEU	N-CA	7.39	1.61	1.46
59	8	472	ARG	C-O	7.36	1.37	1.23
6	g	101	ASP	C-O	7.34	1.37	1.23
52	a	181	ASP	C-O	7.31	1.37	1.23
59	8	650	THR	C-O	7.29	1.37	1.23
4	e	9	ASP	C-O	7.27	1.37	1.23
33	H	129	PHE	C-O	7.24	1.37	1.23
12	m	119	LEU	C-O	7.22	1.37	1.23
6	g	108	VAL	C-O	7.20	1.37	1.23
32	G	129	THR	C-O	7.19	1.37	1.23
35	J	92	ARG	C-O	-7.17	1.09	1.23
6	g	140	ALA	N-CA	7.16	1.60	1.46
33	H	103	ALA	C-O	7.16	1.36	1.23
44	S	82	LYS	C-O	7.16	1.36	1.23
46	U	75	ILE	C-O	7.15	1.36	1.23
59	8	176	GLU	C-O	-7.12	1.09	1.23
36	K	11	HIS	C-O	7.11	1.36	1.23
7	h	59	LEU	C-O	7.07	1.36	1.23
37	L	42	VAL	C-O	7.07	1.36	1.23
59	8	553	VAL	N-CA	-7.00	1.32	1.46
12	m	35	ALA	C-O	6.97	1.36	1.23
50	Y	73	ARG	C-O	6.94	1.36	1.23
9	j	27	ARG	C-O	6.93	1.36	1.23
40	O	29	ALA	C-O	6.93	1.36	1.23
10	k	37	ASP	C-O	6.88	1.36	1.23
43	R	101	THR	N-CA	6.86	1.60	1.46
36	K	8	PHE	C-O	6.85	1.36	1.23
44	S	7	ALA	C-O	6.78	1.36	1.23
34	I	155	LYS	N-CA	6.76	1.59	1.46
36	K	66	ALA	C-O	6.75	1.36	1.23
25	z	2	LYS	C-O	6.73	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	161	VAL	C-O	6.72	1.36	1.23
59	8	544	VAL	C-O	6.70	1.36	1.23
15	p	68	GLY	C-O	6.65	1.34	1.23
36	K	51	ILE	N-CA	6.65	1.59	1.46
32	G	75	ALA	C-O	6.64	1.35	1.23
59	8	641	MET	C-O	6.63	1.35	1.23
44	S	39	ASP	C-O	6.62	1.35	1.23
33	H	30	ASP	C-O	6.62	1.35	1.23
34	I	51	GLY	C-O	6.61	1.34	1.23
41	P	109	ILE	C-O	6.59	1.35	1.23
6	g	30	LEU	C-O	6.58	1.35	1.23
43	R	76	ILE	C-O	6.57	1.35	1.23
45	T	77	TYR	C-O	6.55	1.35	1.23
43	R	22	TYR	C-O	6.54	1.35	1.23
43	R	75	SER	C-O	6.53	1.35	1.23
30	E	53	ASP	C-O	6.51	1.35	1.23
45	T	74	VAL	C-O	6.47	1.35	1.23
49	X	9	PHE	C-O	6.46	1.35	1.23
12	m	120	ALA	C-O	6.45	1.35	1.23
49	X	20	LYS	C-O	6.42	1.35	1.23
52	a	44	VAL	C-O	6.42	1.35	1.23
39	N	74	GLN	C-O	6.42	1.35	1.23
59	8	295	ILE	C-O	6.40	1.35	1.23
59	8	16	SER	N-CA	6.38	1.59	1.46
52	a	163	TYR	C-O	6.37	1.35	1.23
44	S	5	MET	C-O	6.37	1.35	1.23
4	e	161	SER	C-O	6.37	1.35	1.23
59	8	552	ALA	C-O	6.36	1.35	1.23
40	O	10	LEU	C-O	6.34	1.35	1.23
36	K	60	VAL	C-O	6.34	1.35	1.23
59	8	96	THR	N-CA	6.33	1.59	1.46
34	I	19	PHE	C-O	6.33	1.35	1.23
14	o	30	ARG	N-CA	6.32	1.58	1.46
21	v	2	PHE	C-O	6.30	1.35	1.23
35	J	64	GLU	C-O	6.28	1.35	1.23
7	h	62	ARG	C-O	6.25	1.35	1.23
59	8	553	VAL	C-O	6.25	1.35	1.23
3	d	132	LYS	C-O	6.24	1.35	1.23
34	I	52	VAL	C-O	6.24	1.35	1.23
35	J	91	SER	C-O	6.22	1.35	1.23
38	M	16	GLY	C-O	6.21	1.33	1.23
49	X	66	VAL	C-O	6.13	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	L	145	GLU	C-O	6.12	1.34	1.23
59	8	608	ALA	C-O	6.12	1.34	1.23
35	J	65	LYS	C-O	6.11	1.34	1.23
8	i	59	THR	C-O	6.10	1.34	1.23
40	O	72	ARG	C-N	6.08	1.48	1.34
59	8	100	GLU	C-O	6.08	1.34	1.23
37	L	44	SER	C-O	6.05	1.34	1.23
3	d	188	MET	N-CA	6.04	1.58	1.46
34	I	73	ASN	C-O	6.04	1.34	1.23
52	a	183	ASP	C-O	6.04	1.34	1.23
9	j	98	GLU	C-O	6.03	1.34	1.23
41	P	31	VAL	N-CA	6.03	1.58	1.46
59	8	627	ASN	C-N	6.02	1.48	1.34
38	M	24	VAL	C-O	6.02	1.34	1.23
35	J	117	ALA	C-O	6.00	1.34	1.23
13	n	15	SER	C-O	6.00	1.34	1.23
52	a	196	LEU	C-O	5.99	1.34	1.23
59	8	652	VAL	N-CA	5.96	1.58	1.46
43	R	89	ARG	C-O	5.94	1.34	1.23
59	8	94	ASP	C-O	-5.93	1.12	1.23
4	e	52	ALA	C-O	5.92	1.34	1.23
8	i	33	ASN	C-O	5.92	1.34	1.23
45	T	75	ALA	C-O	5.91	1.34	1.23
36	K	22	ILE	C-O	5.88	1.34	1.23
34	I	70	GLN	C-O	5.87	1.34	1.23
50	Y	31	ILE	C-O	5.87	1.34	1.23
33	H	69	THR	C-O	5.86	1.34	1.23
48	W	40	PRO	C-O	5.85	1.34	1.23
52	a	41	SER	C-O	5.85	1.34	1.23
33	H	80	GLY	C-O	5.85	1.33	1.23
59	8	253	ARG	C-O	5.84	1.34	1.23
39	N	27	ILE	C-O	5.84	1.34	1.23
33	H	138	GLN	C-O	5.84	1.34	1.23
32	G	52	ALA	C-O	5.82	1.34	1.23
50	Y	58	ASP	C-O	5.82	1.34	1.23
52	a	208	TYR	C-O	5.82	1.34	1.23
28	C	47	ILE	C-O	5.80	1.34	1.23
34	I	152	SER	C-O	-5.79	1.12	1.23
33	H	20	THR	C-O	5.78	1.34	1.23
59	8	659	PRO	C-O	5.78	1.34	1.23
38	M	102	VAL	C-O	5.78	1.34	1.23
6	g	99	ILE	C-O	5.75	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	M	34	ALA	C-O	5.71	1.34	1.23
59	8	95	PHE	C-O	5.71	1.34	1.23
59	8	208	PRO	C-O	5.70	1.34	1.23
33	H	97	PRO	C-O	5.69	1.34	1.23
43	R	59	VAL	C-O	5.68	1.34	1.23
43	R	49	GLU	C-O	5.65	1.34	1.23
40	O	37	ARG	N-CA	5.64	1.57	1.46
1	b	32	LEU	C-O	5.62	1.34	1.23
59	8	370	LYS	C-O	5.61	1.34	1.23
59	8	190	ALA	C-O	5.60	1.33	1.23
38	M	60	LEU	C-O	5.60	1.33	1.23
8	i	39	LYS	C-O	5.59	1.33	1.23
37	L	133	ALA	C-O	5.59	1.33	1.23
32	G	66	ILE	C-O	5.59	1.33	1.23
59	8	180	THR	C-O	5.58	1.33	1.23
44	S	84	ARG	C-O	5.57	1.33	1.23
59	8	55	GLN	C-O	5.55	1.33	1.23
36	K	16	GLU	C-O	5.54	1.33	1.23
22	w	46	ASN	C-O	5.53	1.33	1.23
52	a	165	ASN	N-CA	5.49	1.57	1.46
46	U	79	ASN	N-CA	5.48	1.57	1.46
51	Z	5	VAL	C-O	5.46	1.33	1.23
51	Z	41	THR	C-O	5.46	1.33	1.23
59	8	128	ARG	C-O	5.46	1.33	1.23
32	G	69	VAL	C-O	5.42	1.33	1.23
59	8	360	PHE	C-N	5.42	1.42	1.33
35	J	87	VAL	N-CA	5.40	1.57	1.46
41	P	71	ASP	N-CA	5.39	1.57	1.46
34	I	202	LEU	N-CA	5.39	1.57	1.46
52	a	171	ILE	C-O	5.36	1.33	1.23
59	8	360	PHE	C-O	5.36	1.33	1.23
48	W	52	ARG	C-O	5.34	1.33	1.23
44	S	41	TRP	C-O	5.34	1.33	1.23
34	I	196	GLU	C-O	5.34	1.33	1.23
39	N	93	LEU	C-O	5.33	1.33	1.23
32	G	217	ALA	C-O	5.33	1.33	1.23
49	X	43	MET	C-O	5.31	1.33	1.23
14	o	116	GLN	C-O	5.30	1.33	1.23
36	K	27	ALA	C-O	5.28	1.33	1.23
2	c	140	HIS	C-O	5.28	1.33	1.23
3	d	196	VAL	C-O	5.28	1.33	1.23
32	G	96	LEU	C-O	5.27	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	w	45	ALA	C-O	5.26	1.33	1.23
34	I	134	TYR	C-O	5.25	1.33	1.23
36	K	2	ARG	C-O	5.24	1.33	1.23
8	i	27	LEU	C-O	5.24	1.33	1.23
59	8	178	HIS	C-O	5.22	1.33	1.23
5	f	146	ASP	C-O	5.21	1.33	1.23
37	L	138	GLU	C-O	5.20	1.33	1.23
52	a	63	THR	C-O	5.20	1.33	1.23
36	K	28	ALA	C-O	5.19	1.33	1.23
59	8	255	ARG	C-O	5.17	1.33	1.23
3	d	137	LYS	C-O	5.17	1.33	1.23
59	8	465	HIS	C-O	5.14	1.33	1.23
6	g	49	ALA	C-O	5.12	1.33	1.23
45	T	24	THR	C-O	5.12	1.33	1.23
59	8	281	ALA	C-O	5.12	1.33	1.23
43	R	51	GLN	C-O	5.12	1.33	1.23
53	3	1115	U	N1-C2	5.12	1.43	1.38
1	b	174	ARG	C-O	5.10	1.33	1.23
52	a	26	ALA	C-O	5.09	1.33	1.23
47	V	37	ILE	C-O	5.08	1.33	1.23
29	D	28	ARG	C-O	5.07	1.32	1.23
45	T	64	LYS	C-O	5.06	1.32	1.23
12	m	53	MET	C-O	5.05	1.32	1.23
18	s	45	VAL	N-CA	5.04	1.56	1.46
53	3	1123	U	C2-O2	5.04	1.26	1.22
40	O	8	ILE	C-O	5.03	1.32	1.23
39	N	62	LEU	C-O	5.02	1.32	1.23
7	h	40	GLU	C-O	5.02	1.32	1.23
41	P	103	GLY	N-CA	5.02	1.53	1.46
6	g	129	GLU	C-N	5.01	1.45	1.34
37	L	61	PHE	N-CA	5.01	1.56	1.46

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2	1	U	N1-C1'-C2'	9.95	126.93	114.00
8	i	37	PHE	C-N-CA	-8.84	99.60	121.70
7	h	18	VAL	C-N-CA	-8.51	100.43	121.70
36	K	13	ASP	CA-C-O	8.14	137.20	120.10
59	8	178	HIS	C-N-CA	-7.82	102.15	121.70
36	K	16	GLU	C-N-CA	-7.80	102.20	121.70
40	O	72	ARG	C-N-CA	-7.72	102.39	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	I	154	VAL	C-N-CA	-7.56	102.81	121.70
59	8	176	GLU	O-C-N	-7.55	110.62	122.70
41	P	102	ALA	C-N-CA	-7.51	106.52	122.30
40	O	39	PRO	N-CA-C	7.41	131.36	112.10
4	e	12	VAL	C-N-CA	-7.28	103.50	121.70
59	8	627	ASN	C-N-CA	-7.18	103.74	121.70
39	N	77	ALA	C-N-CA	-6.73	104.86	121.70
36	K	13	ASP	O-C-N	-6.73	111.93	122.70
34	I	152	SER	O-C-N	-6.69	111.99	122.70
49	X	24	SER	C-N-CA	-6.68	108.26	122.30
57	6	32	C	C2'-C3'-O3'	6.68	124.39	113.70
53	3	920	U	O4'-C1'-N1	6.65	113.52	108.20
43	R	96	VAL	N-CA-C	6.65	128.95	111.00
53	3	1122	U	N1-C1'-C2'	6.54	122.51	114.00
52	a	184	LYS	C-N-CA	-6.53	105.38	121.70
6	g	139	PHE	C-N-CA	-6.50	105.46	121.70
57	6	32	C	OP2-P-O3'	6.47	119.44	105.20
36	K	15	SER	C-N-CA	-6.46	105.54	121.70
49	X	25	GLY	N-CA-C	6.46	129.26	113.10
53	3	1149	C	N1-C1'-C2'	6.43	122.36	114.00
43	R	99	GLN	O-C-N	-6.41	112.44	122.70
8	i	38	CYS	C-N-CA	-6.34	105.84	121.70
40	O	39	PRO	O-C-N	6.33	132.82	122.70
7	h	65	GLU	C-N-CA	-6.31	109.06	122.30
40	O	39	PRO	CA-C-O	-6.30	105.07	120.20
53	3	1128	C	N1-C1'-C2'	6.26	122.13	114.00
40	O	40	ILE	CB-CA-C	-6.19	99.22	111.60
34	I	201	GLU	C-N-CA	-6.17	106.27	121.70
41	P	29	THR	O-C-N	-6.15	112.86	122.70
6	g	129	GLU	C-N-CA	-6.11	106.44	121.70
6	g	52	ALA	C-N-CA	-6.10	106.45	121.70
1	b	94	LEU	C-N-CA	-6.04	106.59	121.70
40	O	10	LEU	C-N-CA	-6.03	106.62	121.70
43	R	101	THR	N-CA-C	5.98	127.16	111.00
46	U	79	ASN	N-CA-C	5.97	127.12	111.00
59	8	123	SER	C-N-CA	-5.96	106.80	121.70
37	L	21	LEU	C-N-CA	-5.94	106.84	121.70
51	Z	10	PRO	N-CA-C	5.92	127.48	112.10
40	O	36	VAL	C-N-CA	-5.91	106.92	121.70
59	8	628	THR	N-CA-C	5.89	126.91	111.00
14	o	28	VAL	O-C-N	-5.89	113.28	122.70
8	i	16	MET	N-CA-C	-5.88	95.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1	1328	A	N9-C1'-C2'	5.88	121.65	114.00
8	i	15	GLY	C-N-CA	-5.88	107.00	121.70
52	a	13	GLU	C-N-CA	-5.88	107.00	121.70
9	j	30	THR	C-N-CA	-5.84	107.09	121.70
36	K	13	ASP	C-N-CA	-5.79	107.22	121.70
49	X	36	ARG	C-N-CA	-5.79	107.22	121.70
55	2	119	A	N9-C1'-C2'	-5.75	105.67	112.00
53	3	1493	A	C2'-C3'-O3'	5.73	122.86	113.70
52	a	181	ASP	CA-C-O	5.70	132.07	120.10
53	3	1115	U	N1-C1'-C2'	5.68	121.38	114.00
59	8	14	GLY	O-C-N	-5.64	113.68	122.70
39	N	75	ALA	C-N-CA	-5.56	110.62	122.30
40	O	38	GLY	CA-C-O	5.53	130.55	120.60
4	e	164	GLU	C-N-CA	-5.51	110.72	122.30
59	8	116	VAL	C-N-CA	-5.47	110.80	122.30
26	A	49	ARG	C-N-CA	-5.47	108.03	121.70
8	i	21	PRO	N-CA-C	5.43	126.23	112.10
35	J	164	LEU	C-N-CA	-5.43	110.91	122.30
54	1	1060	U	N1-C1'-C2'	5.38	121.00	114.00
5	f	43	LYS	O-C-N	5.38	131.31	122.70
3	d	82	GLY	N-CA-C	5.37	126.53	113.10
41	P	70	ALA	C-N-CA	-5.35	108.33	121.70
8	i	39	LYS	C-N-CA	-5.34	108.35	121.70
51	Z	25	ALA	C-N-CA	-5.34	111.09	122.30
59	8	14	GLY	CA-C-O	5.34	130.21	120.60
4	e	9	ASP	CA-C-O	5.32	131.28	120.10
49	X	23	GLU	C-N-CA	-5.32	108.39	121.70
4	e	144	LYS	C-N-CA	-5.31	108.43	121.70
40	O	37	ARG	N-CA-C	5.31	125.33	111.00
59	8	360	PHE	C-N-CA	-5.30	111.18	122.30
34	I	52	VAL	C-N-CA	-5.29	108.48	121.70
9	j	81	ILE	N-CA-C	5.27	125.23	111.00
59	8	111	MET	C-N-CA	-5.26	108.56	121.70
54	1	1818	U	N1-C1'-C2'	5.24	120.81	114.00
53	3	1347	G	N9-C1'-C2'	5.24	120.81	114.00
40	O	72	ARG	O-C-N	5.22	131.06	122.70
53	3	563	A	N9-C1'-C2'	5.22	120.78	114.00
35	J	87	VAL	N-CA-C	5.20	125.05	111.00
54	1	477	A	N9-C1'-C2'	5.18	120.74	114.00
54	1	747	C	N1-C1'-C2'	5.18	120.74	114.00
43	R	99	GLN	CA-C-O	5.17	130.96	120.10
53	3	1011	C	N1-C1'-C2'	5.16	120.70	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1	301	G	N9-C1'-C2'	5.15	120.69	114.00
8	i	22	PRO	C-N-CA	-5.10	108.96	121.70
53	3	1312	G	N9-C1'-C2'	5.07	120.60	114.00
35	J	119	VAL	C-N-CA	-5.04	109.09	121.70
53	3	1505	G	N9-C1'-C2'	5.04	120.55	114.00
44	S	8	ARG	C-N-CA	-5.04	109.11	121.70
5	f	49	LEU	C-N-CA	-5.03	109.12	121.70
49	X	22	VAL	C-N-CA	-5.02	109.14	121.70
8	i	67	THR	N-CA-C	-5.02	97.45	111.00
54	1	158	U	N1-C1'-C2'	5.01	120.51	114.00
12	m	35	ALA	O-C-N	5.01	130.71	122.70

There are no chirality outliers.

All (82) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	1	119	A	Sidechain
54	1	1204	A	Sidechain
54	1	1241	A	Sidechain
54	1	1263	U	Sidechain
54	1	1328	A	Sidechain
54	1	1433	A	Sidechain
54	1	1647	U	Sidechain
54	1	1755	A	Sidechain
54	1	1828	G	Sidechain
54	1	1905	C	Sidechain
54	1	1937	A	Sidechain
54	1	196	A	Sidechain
54	1	1991	U	Sidechain
54	1	1996	C	Sidechain
54	1	2061	G	Sidechain
54	1	222	A	Sidechain
54	1	2244	U	Sidechain
54	1	2266	A	Sidechain
54	1	2273	A	Sidechain
54	1	2344	U	Sidechain
54	1	2391	G	Sidechain
54	1	2447	G	Sidechain
54	1	247	G	Sidechain
54	1	2529	G	Sidechain
54	1	2532	G	Sidechain
54	1	27	G	Sidechain

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Mol	Chain	Res	Type	Group
54	1	2848	G	Sidechain
54	1	2883	A	Sidechain
54	1	307	G	Sidechain
54	1	370	G	Sidechain
54	1	446	G	Sidechain
54	1	450	G	Sidechain
54	1	454	A	Sidechain
54	1	476	G	Sidechain
54	1	477	A	Sidechain
54	1	500	G	Sidechain
54	1	501	A	Sidechain
54	1	506	G	Sidechain
54	1	51	G	Sidechain
54	1	512	G	Sidechain
54	1	52	A	Sidechain
54	1	726	G	Sidechain
54	1	727	A	Sidechain
54	1	775	G	Sidechain
54	1	827	U	Sidechain
54	1	868	U	Sidechain
54	1	895	U	Sidechain
54	1	973	A	Sidechain
54	1	975	A	Sidechain
55	2	1	U	Sidechain
55	2	119	A	Sidechain
55	2	24	G	Sidechain
53	3	1020	G	Sidechain
53	3	1061	G	Sidechain
53	3	1082	A	Sidechain
53	3	1122	U	Sidechain
53	3	1123	U	Sidechain
53	3	1149	C	Sidechain
53	3	1150	A	Sidechain
53	3	1171	A	Sidechain
53	3	124	C	Sidechain
53	3	1316	G	Sidechain
53	3	1330	U	Sidechain
53	3	1363	A	Sidechain
53	3	159	G	Sidechain
53	3	266	G	Sidechain
53	3	383	A	Sidechain
53	3	429	U	Sidechain

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Mol	Chain	Res	Type	Group
53	3	566	G	Sidechain
53	3	820	U	Sidechain
53	3	872	A	Sidechain
53	3	898	G	Sidechain
53	3	920	U	Sidechain
53	3	938	A	Sidechain
56	5	26	A	Sidechain
57	6	44	A	Sidechain
59	8	623	THR	Mainchain
34	I	152	SER	Mainchain
34	I	154	VAL	Mainchain
35	J	86	GLY	Mainchain
35	J	92	ARG	Mainchain
46	U	78	VAL	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%)	42 (16%)	4 (2%)	10	45
2	c	207/209 (99%)	174 (84%)	31 (15%)	2 (1%)	15	54
3	d	199/201 (99%)	165 (83%)	32 (16%)	2 (1%)	15	54
4	e	175/177 (99%)	143 (82%)	26 (15%)	6 (3%)	3	28
5	f	174/176 (99%)	150 (86%)	24 (14%)	0	100	100
6	g	121/149 (81%)	92 (76%)	26 (22%)	3 (2%)	5	34
7	h	82/131 (63%)	57 (70%)	20 (24%)	5 (6%)	1	15
8	i	72/141 (51%)	49 (68%)	18 (25%)	5 (7%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	140/142 (99%)	121 (86%)	18 (13%)	1 (1%)	22	61
10	k	120/122 (98%)	96 (80%)	22 (18%)	2 (2%)	9	42
11	l	141/143 (99%)	106 (75%)	29 (21%)	6 (4%)	2	22
12	m	134/136 (98%)	113 (84%)	19 (14%)	2 (2%)	10	45
13	n	118/120 (98%)	92 (78%)	26 (22%)	0	100	100
14	o	114/116 (98%)	98 (86%)	15 (13%)	1 (1%)	17	56
15	p	112/114 (98%)	96 (86%)	16 (14%)	0	100	100
16	q	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
17	r	101/103 (98%)	84 (83%)	16 (16%)	1 (1%)	15	54
18	s	108/110 (98%)	94 (87%)	13 (12%)	1 (1%)	17	56
19	t	91/93 (98%)	79 (87%)	12 (13%)	0	100	100
20	u	100/102 (98%)	82 (82%)	18 (18%)	0	100	100
21	v	92/94 (98%)	78 (85%)	14 (15%)	0	100	100
22	w	73/75 (97%)	62 (85%)	11 (15%)	0	100	100
23	x	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
24	y	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
25	z	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
26	A	64/66 (97%)	54 (84%)	8 (12%)	2 (3%)	4	30
27	B	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
28	C	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
29	D	44/46 (96%)	33 (75%)	11 (25%)	0	100	100
30	E	62/64 (97%)	52 (84%)	9 (14%)	1 (2%)	9	43
31	F	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	G	216/225 (96%)	175 (81%)	36 (17%)	5 (2%)	6	36
33	H	204/206 (99%)	177 (87%)	26 (13%)	1 (0%)	29	68
34	I	203/205 (99%)	161 (79%)	40 (20%)	2 (1%)	15	54
35	J	155/157 (99%)	123 (79%)	24 (16%)	8 (5%)	2	18
36	K	98/100 (98%)	84 (86%)	10 (10%)	4 (4%)	3	23
37	L	149/151 (99%)	121 (81%)	28 (19%)	0	100	100
38	M	127/129 (98%)	109 (86%)	17 (13%)	1 (1%)	19	58
39	N	125/127 (98%)	97 (78%)	25 (20%)	3 (2%)	6	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	O	96/98 (98%)	80 (83%)	14 (15%)	2 (2%)	7	38
41	P	114/116 (98%)	84 (74%)	27 (24%)	3 (3%)	5	33
42	Q	121/123 (98%)	89 (74%)	28 (23%)	4 (3%)	4	28
43	R	112/114 (98%)	90 (80%)	20 (18%)	2 (2%)	8	41
44	S	98/100 (98%)	72 (74%)	24 (24%)	2 (2%)	7	39
45	T	86/88 (98%)	78 (91%)	6 (7%)	2 (2%)	6	36
46	U	80/82 (98%)	63 (79%)	12 (15%)	5 (6%)	1	14
47	V	78/80 (98%)	59 (76%)	18 (23%)	1 (1%)	12	48
48	W	63/65 (97%)	53 (84%)	8 (13%)	2 (3%)	4	29
49	X	77/79 (98%)	56 (73%)	18 (23%)	3 (4%)	3	25
50	Y	83/85 (98%)	75 (90%)	8 (10%)	0	100	100
51	Z	63/65 (97%)	37 (59%)	19 (30%)	7 (11%)	0	6
52	a	130/223 (58%)	104 (80%)	24 (18%)	2 (2%)	10	45
59	8	681/711 (96%)	541 (79%)	125 (18%)	15 (2%)	6	37
All	All	6517/6889 (95%)	5319 (82%)	1080 (17%)	118 (2%)	12	41

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	205	GLY
3	d	83	VAL
4	e	19	PHE
4	e	122	ASP
6	g	9	VAL
7	h	80	THR
8	i	11	GLN
10	k	35	VAL
11	l	85	VAL
12	m	58	LYS
14	o	99	TYR
17	r	54	VAL
26	A	65	ASN
30	E	31	ILE
32	G	73	ARG
35	J	87	VAL
35	J	93	VAL
36	K	54	LEU

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Mol	Chain	Res	Type
36	K	92	THR
36	K	93	LYS
39	N	57	VAL
42	Q	32	VAL
43	R	65	GLU
46	U	43	ALA
46	U	45	GLU
46	U	79	ASN
47	V	49	ASN
51	Z	8	ASN
51	Z	25	ALA
59	8	121	PRO
59	8	425	LYS
59	8	582	SER
59	8	624	PRO
11	l	31	GLY
32	G	34	ARG
33	H	4	VAL
35	J	13	LYS
35	J	160	VAL
39	N	91	GLU
39	N	118	ARG
41	P	89	GLY
44	S	62	ARG
48	W	17	VAL
49	X	4	LEU
51	Z	32	ARG
52	a	6	LYS
52	a	182	ALA
59	8	199	GLY
59	8	423	LYS
59	8	501	VAL
1	b	185	ALA
2	c	140	HIS
3	d	16	GLU
4	e	42	ALA
4	e	125	GLY
6	g	8	LYS
7	h	60	LEU
7	h	81	LEU
10	k	92	GLU
11	l	86	GLU

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Mol	Chain	Res	Type
32	G	87	ASP
35	J	12	GLU
36	K	53	LYS
42	Q	33	CYS
42	Q	101	LEU
44	S	52	ARG
49	X	77	ARG
51	Z	24	LYS
51	Z	34	ARG
59	8	509	SER
1	b	240	GLY
11	l	54	GLN
32	G	17	HIS
32	G	72	LYS
34	I	42	ALA
40	O	93	ALA
41	P	14	GLN
51	Z	37	TYR
59	8	424	THR
1	b	24	HIS
2	c	153	GLY
4	e	18	GLU
6	g	12	LEU
8	i	34	ILE
9	j	81	ILE
18	s	29	VAL
34	I	20	LEU
35	J	11	GLN
35	J	122	VAL
43	R	97	ARG
45	T	46	LYS
48	W	12	PHE
49	X	26	ASP
51	Z	12	ASP
59	8	198	GLN
59	8	548	GLU
8	i	24	GLY
11	l	16	GLY
41	P	88	PRO
42	Q	75	GLU
45	T	24	THR
59	8	528	GLY

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Mol	Chain	Res	Type
7	h	55	VAL
12	m	69	PRO
38	M	94	VAL
4	e	175	PRO
8	i	21	PRO
11	l	56	PRO
46	U	49	GLY
26	A	54	GLY
35	J	97	PRO
40	O	41	PRO
46	U	37	GLY
59	8	547	GLY
8	i	4	VAL
7	h	79	PRO
59	8	531	PRO
59	8	570	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	216/216 (100%)	207 (96%)	9 (4%)	30	63
2	c	164/164 (100%)	162 (99%)	2 (1%)	71	87
3	d	165/165 (100%)	162 (98%)	3 (2%)	59	81
4	e	148/148 (100%)	142 (96%)	6 (4%)	30	63
5	f	137/137 (100%)	135 (98%)	2 (2%)	65	84
6	g	98/114 (86%)	97 (99%)	1 (1%)	76	88
7	h	66/100 (66%)	66 (100%)	0	100	100
8	i	60/109 (55%)	57 (95%)	3 (5%)	24	58
9	j	116/116 (100%)	114 (98%)	2 (2%)	60	82
10	k	103/103 (100%)	100 (97%)	3 (3%)	42	71
11	l	102/102 (100%)	98 (96%)	4 (4%)	32	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	m	109/109 (100%)	107 (98%)	2 (2%)	59	81
13	n	100/100 (100%)	99 (99%)	1 (1%)	76	88
14	o	86/86 (100%)	85 (99%)	1 (1%)	71	87
15	p	99/99 (100%)	97 (98%)	2 (2%)	55	79
16	q	89/89 (100%)	86 (97%)	3 (3%)	37	68
17	r	84/84 (100%)	81 (96%)	3 (4%)	35	66
18	s	93/93 (100%)	92 (99%)	1 (1%)	73	88
19	t	80/80 (100%)	77 (96%)	3 (4%)	33	65
20	u	83/83 (100%)	81 (98%)	2 (2%)	49	76
21	v	78/78 (100%)	77 (99%)	1 (1%)	69	86
22	w	57/57 (100%)	55 (96%)	2 (4%)	36	67
23	x	67/67 (100%)	65 (97%)	2 (3%)	41	71
24	y	55/55 (100%)	53 (96%)	2 (4%)	35	66
25	z	48/48 (100%)	46 (96%)	2 (4%)	30	63
26	A	59/59 (100%)	58 (98%)	1 (2%)	60	82
27	B	47/47 (100%)	46 (98%)	1 (2%)	53	79
28	C	45/45 (100%)	45 (100%)	0	100	100
29	D	38/38 (100%)	37 (97%)	1 (3%)	46	74
30	E	51/51 (100%)	50 (98%)	1 (2%)	55	79
31	F	34/34 (100%)	31 (91%)	3 (9%)	10	38
32	G	180/186 (97%)	173 (96%)	7 (4%)	32	64
33	H	170/170 (100%)	168 (99%)	2 (1%)	71	87
34	I	172/172 (100%)	168 (98%)	4 (2%)	50	77
35	J	119/119 (100%)	114 (96%)	5 (4%)	30	63
36	K	87/87 (100%)	84 (97%)	3 (3%)	37	68
37	L	124/124 (100%)	123 (99%)	1 (1%)	81	91
38	M	104/104 (100%)	103 (99%)	1 (1%)	76	88
39	N	105/105 (100%)	98 (93%)	7 (7%)	16	48
40	O	86/86 (100%)	84 (98%)	2 (2%)	50	77
41	P	89/89 (100%)	88 (99%)	1 (1%)	73	88
42	Q	103/103 (100%)	99 (96%)	4 (4%)	32	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	R	92/92 (100%)	89 (97%)	3 (3%)	38	68
44	S	83/83 (100%)	81 (98%)	2 (2%)	49	76
45	T	76/76 (100%)	74 (97%)	2 (3%)	46	74
46	U	65/65 (100%)	64 (98%)	1 (2%)	65	84
47	V	74/74 (100%)	72 (97%)	2 (3%)	44	73
48	W	56/56 (100%)	53 (95%)	3 (5%)	22	55
49	X	70/70 (100%)	68 (97%)	2 (3%)	42	71
50	Y	65/65 (100%)	64 (98%)	1 (2%)	65	84
51	Z	55/55 (100%)	52 (94%)	3 (6%)	21	54
52	a	110/174 (63%)	106 (96%)	4 (4%)	35	66
59	8	566/585 (97%)	540 (95%)	26 (5%)	27	61
All	All	5428/5616 (97%)	5273 (97%)	155 (3%)	45	71

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	42	ARG
1	b	129	LEU
1	b	142	ASN
1	b	180	MET
1	b	196	ASN
1	b	212	TRP
1	b	224	MET
1	b	228	ASP
1	b	230	PRO
2	c	33	ARG
2	c	184	ARG
3	d	60	TRP
3	d	116	ASP
3	d	198	GLU
4	e	10	GLU
4	e	18	GLU
4	e	26	GLN
4	e	114	ARG
4	e	132	ARG
4	e	134	GLN
5	f	15	ASP
5	f	103	ASN

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Mol	Chain	Res	Type
6	g	112	LYS
8	i	8	VAL
8	i	59	THR
8	i	66	PHE
9	j	31	GLU
9	j	128	ASN
10	k	13	ASN
10	k	31	ARG
10	k	58	LEU
11	l	4	ASN
11	l	47	ARG
11	l	57	LEU
11	l	104	GLN
12	m	59	ARG
12	m	63	ILE
13	n	2	ARG
14	o	33	ARG
15	p	40	GLN
15	p	92	ARG
16	q	27	ARG
16	q	29	ARG
16	q	71	ASN
17	r	11	GLN
17	r	45	GLU
17	r	79	ARG
18	s	11	ARG
19	t	3	ARG
19	t	32	LEU
19	t	73	ARG
20	u	21	ARG
20	u	78	LYS
21	v	26	PHE
22	w	10	ARG
22	w	16	ARG
23	x	21	LEU
23	x	47	THR
24	y	7	ARG
24	y	58	ASN
25	z	30	ARG
25	z	36	GLU
26	A	9	TYR
27	B	15	ARG

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Mol	Chain	Res	Type
29	D	25	LYS
30	E	30	HIS
31	F	12	ARG
31	F	14	CYS
31	F	36	ARG
32	G	20	ARG
32	G	21	TYR
32	G	55	GLU
32	G	94	ARG
32	G	129	THR
32	G	221	ARG
32	G	224	ARG
33	H	152	VAL
33	H	155	ARG
34	I	39	GLN
34	I	164	ARG
34	I	173	ASP
34	I	201	GLU
35	J	10	LEU
35	J	24	VAL
35	J	30	PHE
35	J	33	THR
35	J	156	ARG
36	K	8	PHE
36	K	17	GLN
36	K	63	ASN
37	L	84	TYR
38	M	103	VAL
39	N	31	GLN
39	N	44	ARG
39	N	60	LEU
39	N	62	LEU
39	N	105	ARG
39	N	119	LYS
39	N	123	ARG
40	O	28	THR
40	O	42	LEU
41	P	124	LYS
42	Q	4	ASN
42	Q	40	THR
42	Q	93	ARG
42	Q	113	ARG

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Mol	Chain	Res	Type
43	R	77	LYS
43	R	97	ARG
43	R	99	GLN
44	S	27	LYS
44	S	32	ASP
45	T	21	THR
45	T	88	ARG
46	U	79	ASN
47	V	19	SER
47	V	56	ASP
48	W	13	THR
48	W	18	GLN
48	W	70	THR
49	X	4	LEU
49	X	11	ASP
50	Y	70	LYS
51	Z	8	ASN
51	Z	9	GLU
51	Z	32	ARG
52	a	12	ARG
52	a	51	ASP
52	a	167	LYS
52	a	168	ASN
59	8	56	GLU
59	8	121	PRO
59	8	122	GLN
59	8	137	ARG
59	8	142	ASN
59	8	179	PHE
59	8	189	LYS
59	8	265	THR
59	8	334	THR
59	8	348	THR
59	8	350	LEU
59	8	354	LYS
59	8	410	GLU
59	8	411	PHE
59	8	421	GLU
59	8	440	LYS
59	8	446	ARG
59	8	454	ASN
59	8	478	ASN

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Mol	Chain	Res	Type
59	8	499	THR
59	8	522	MET
59	8	530	ASN
59	8	534	TYR
59	8	560	GLN
59	8	609	LYS
59	8	624	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	127	ASN
2	c	32	ASN
2	c	134	HIS
5	f	21	GLN
5	f	142	GLN
6	g	11	ASN
8	i	11	GLN
10	k	93	GLN
13	n	107	ASN
16	q	80	ASN
17	r	11	GLN
18	s	9	HIS
19	t	28	ASN
20	u	65	GLN
20	u	73	ASN
27	B	18	HIS
32	G	41	ASN
32	G	145	ASN
37	L	67	ASN
37	L	85	GLN
37	L	129	ASN
37	L	147	ASN
38	M	3	GLN
41	P	118	ASN
45	T	34	GLN
49	X	52	ASN
50	Y	74	HIS
59	8	18	HIS
59	8	142	ASN
59	8	496	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	3	1538/1539 (99%)	245 (15%)	6 (0%)
54	1	2902/2903 (99%)	392 (13%)	12 (0%)
55	2	119/120 (99%)	14 (11%)	1 (0%)
56	5	76/77 (98%)	14 (18%)	1 (1%)
57	6	76/77 (98%)	17 (22%)	1 (1%)
58	4	15/16 (93%)	3 (20%)	0
All	All	4726/4732 (99%)	685 (14%)	21 (0%)

All (685) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	3	7	A
53	3	9	G
53	3	31	G
53	3	32	A
53	3	39	G
53	3	48	C
53	3	51	A
53	3	59	A
53	3	60	A
53	3	71	A
53	3	81	A
53	3	82	G
53	3	84	U
53	3	85	U
53	3	86	G
53	3	94	G
53	3	95	C
53	3	121	U
53	3	130	A
53	3	131	A
53	3	144	G
53	3	154	U
53	3	177	G
53	3	181	A
53	3	183	C
53	3	184	G
53	3	188	C
53	3	197	A
53	3	208	U
53	3	209	U

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Mol	Chain	Res	Type
53	3	210	C
53	3	211	G
53	3	212	G
53	3	214	C
53	3	245	U
53	3	247	G
53	3	251	G
53	3	266	G
53	3	267	C
53	3	280	C
53	3	281	G
53	3	289	G
53	3	316	C
53	3	321	A
53	3	328	C
53	3	330	C
53	3	345	C
53	3	346	G
53	3	348	G
53	3	352	C
53	3	354	G
53	3	355	C
53	3	363	A
53	3	367	U
53	3	369	G
53	3	372	C
53	3	398	U
53	3	411	A
53	3	412	A
53	3	413	G
53	3	414	A
53	3	422	C
53	3	429	U
53	3	430	A
53	3	441	A
53	3	452	A
53	3	462	G
53	3	467	U
53	3	484	G
53	3	486	U
53	3	497	G
53	3	509	A

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Mol	Chain	Res	Type
53	3	518	C
53	3	521	G
53	3	531	U
53	3	532	A
53	3	533	A
53	3	534	U
53	3	536	C
53	3	537	G
53	3	547	A
53	3	561	U
53	3	571	U
53	3	572	A
53	3	573	A
53	3	575	G
53	3	576	C
53	3	577	G
53	3	607	A
53	3	615	G
53	3	633	G
53	3	642	A
53	3	650	G
53	3	665	A
53	3	687	A
53	3	688	G
53	3	690	G
53	3	698	G
53	3	699	C
53	3	703	G
53	3	723	U
53	3	724	G
53	3	755	G
53	3	777	A
53	3	814	A
53	3	817	C
53	3	818	G
53	3	819	A
53	3	821	G
53	3	843	U
53	3	844	G
53	3	846	G
53	3	851	G
53	3	885	G

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Mol	Chain	Res	Type
53	3	890	G
53	3	891	U
53	3	902	G
53	3	914	A
53	3	920	U
53	3	926	G
53	3	929	G
53	3	934	C
53	3	949	A
53	3	960	U
53	3	961	U
53	3	966	G
53	3	968	A
53	3	969	A
53	3	971	G
53	3	972	C
53	3	975	A
53	3	976	G
53	3	977	A
53	3	981	U
53	3	982	U
53	3	984	C
53	3	992	U
53	3	993	G
53	3	1004	A
53	3	1011	C
53	3	1012	A
53	3	1026	G
53	3	1028	C
53	3	1031	C
53	3	1033	G
53	3	1034	G
53	3	1054	C
53	3	1061	G
53	3	1062	U
53	3	1064	G
53	3	1065	U
53	3	1080	A
53	3	1081	A
53	3	1091	U
53	3	1094	G
53	3	1095	U

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Mol	Chain	Res	Type
53	3	1101	A
53	3	1116	U
53	3	1119	C
53	3	1122	U
53	3	1123	U
53	3	1124	G
53	3	1125	U
53	3	1127	G
53	3	1135	U
53	3	1136	C
53	3	1138	G
53	3	1139	G
53	3	1140	C
53	3	1148	U
53	3	1149	C
53	3	1151	A
53	3	1161	C
53	3	1165	U
53	3	1167	A
53	3	1169	A
53	3	1174	G
53	3	1180	A
53	3	1182	G
53	3	1183	U
53	3	1184	G
53	3	1189	U
53	3	1190	G
53	3	1191	A
53	3	1196	A
53	3	1197	A
53	3	1198	G
53	3	1199	U
53	3	1200	C
53	3	1201	A
53	3	1223	C
53	3	1224	U
53	3	1225	A
53	3	1226	C
53	3	1228	C
53	3	1238	A
53	3	1240	U
53	3	1241	G

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Mol	Chain	Res	Type
53	3	1256	A
53	3	1260	G
53	3	1275	A
53	3	1278	G
53	3	1280	A
53	3	1282	C
53	3	1285	A
53	3	1286	U
53	3	1287	A
53	3	1298	U
53	3	1300	G
53	3	1307	U
53	3	1308	U
53	3	1317	C
53	3	1320	C
53	3	1321	U
53	3	1322	C
53	3	1323	G
53	3	1336	C
53	3	1340	A
53	3	1346	A
53	3	1347	G
53	3	1348	U
53	3	1383	C
53	3	1384	C
53	3	1394	A
53	3	1395	C
53	3	1397	C
53	3	1398	A
53	3	1399	C
53	3	1400	C
53	3	1446	A
53	3	1452	C
53	3	1492	A
53	3	1494	G
53	3	1497	G
53	3	1503	A
53	3	1505	G
53	3	1506	U
53	3	1517	G
53	3	1529	G
53	3	1530	G

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Mol	Chain	Res	Type
53	3	1534	A
53	3	1535	C
53	3	1537	U
53	3	1539	C
53	3	1540	U
54	1	10	A
54	1	12	U
54	1	13	A
54	1	34	U
54	1	46	G
54	1	49	A
54	1	51	G
54	1	63	A
54	1	71	A
54	1	74	A
54	1	75	G
54	1	78	U
54	1	92	U
54	1	103	A
54	1	110	G
54	1	119	A
54	1	120	U
54	1	125	A
54	1	131	A
54	1	140	C
54	1	141	G
54	1	162	U
54	1	163	C
54	1	196	A
54	1	199	A
54	1	216	A
54	1	221	A
54	1	222	A
54	1	228	C
54	1	229	C
54	1	248	G
54	1	249	C
54	1	255	A
54	1	265	A
54	1	266	G
54	1	276	U
54	1	278	A

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Mol	Chain	Res	Type
54	1	281	C
54	1	301	G
54	1	311	A
54	1	323	C
54	1	329	G
54	1	330	A
54	1	349	U
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	406	G
54	1	411	G
54	1	413	C
54	1	422	A
54	1	424	G
54	1	451	U
54	1	457	A
54	1	475	C
54	1	480	A
54	1	481	G
54	1	482	A
54	1	491	G
54	1	504	A
54	1	505	A
54	1	510	C
54	1	529	A
54	1	531	C
54	1	532	A
54	1	542	C
54	1	543	G
54	1	549	G
54	1	563	A
54	1	572	A
54	1	573	U
54	1	574	A
54	1	575	A
54	1	603	A
54	1	614	A

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Mol	Chain	Res	Type
54	1	616	A
54	1	627	A
54	1	637	A
54	1	646	U
54	1	654	A
54	1	669	G
54	1	686	U
54	1	687	C
54	1	694	U
54	1	695	G
54	1	730	A
54	1	747	C
54	1	752	A
54	1	760	G
54	1	764	A
54	1	776	G
54	1	782	A
54	1	784	G
54	1	785	G
54	1	792	A
54	1	800	A
54	1	802	A
54	1	805	G
54	1	806	C
54	1	811	U
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	859	G
54	1	860	U
54	1	878	A
54	1	880	G
54	1	886	A
54	1	887	U
54	1	890	C
54	1	891	G
54	1	896	A

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Mol	Chain	Res	Type
54	1	897	C
54	1	898	C
54	1	907	G
54	1	910	A
54	1	932	U
54	1	941	A
54	1	946	C
54	1	961	C
54	1	974	G
54	1	975	A
54	1	983	A
54	1	995	C
54	1	996	A
54	1	1012	U
54	1	1013	C
54	1	1022	G
54	1	1026	G
54	1	1033	U
54	1	1045	C
54	1	1046	A
54	1	1062	G
54	1	1065	U
54	1	1066	U
54	1	1067	A
54	1	1069	A
54	1	1070	A
54	1	1071	G
54	1	1072	C
54	1	1073	A
54	1	1075	C
54	1	1079	C
54	1	1083	U
54	1	1084	A
54	1	1087	G
54	1	1088	A
54	1	1089	A
54	1	1094	U
54	1	1104	C
54	1	1111	A
54	1	1131	G
54	1	1132	U
54	1	1133	A

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Mol	Chain	Res	Type
54	1	1135	C
54	1	1141	U
54	1	1142	A
54	1	1143	A
54	1	1156	A
54	1	1157	G
54	1	1175	A
54	1	1176	U
54	1	1180	U
54	1	1181	U
54	1	1212	G
54	1	1250	G
54	1	1251	C
54	1	1253	A
54	1	1256	G
54	1	1271	G
54	1	1272	A
54	1	1301	A
54	1	1329	U
54	1	1330	C
54	1	1332	G
54	1	1341	G
54	1	1345	C
54	1	1352	U
54	1	1365	A
54	1	1378	A
54	1	1379	U
54	1	1383	A
54	1	1395	A
54	1	1397	U
54	1	1398	C
54	1	1416	G
54	1	1419	A
54	1	1420	A
54	1	1421	G
54	1	1427	A
54	1	1428	C
54	1	1454	C
54	1	1461	C
54	1	1476	U
54	1	1482	G
54	1	1490	A

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Mol	Chain	Res	Type
54	1	1498	C
54	1	1503	A
54	1	1510	G
54	1	1515	A
54	1	1524	G
54	1	1533	C
54	1	1535	A
54	1	1536	C
54	1	1537	G
54	1	1555	G
54	1	1560	G
54	1	1569	A
54	1	1578	U
54	1	1584	U
54	1	1585	C
54	1	1598	A
54	1	1608	A
54	1	1611	C
54	1	1616	A
54	1	1647	U
54	1	1648	U
54	1	1654	A
54	1	1674	G
54	1	1703	G
54	1	1713	A
54	1	1715	G
54	1	1729	U
54	1	1730	C
54	1	1731	G
54	1	1732	C
54	1	1738	G
54	1	1758	U
54	1	1764	C
54	1	1773	A
54	1	1800	C
54	1	1801	A
54	1	1802	A
54	1	1808	A
54	1	1816	C
54	1	1829	A
54	1	1869	G
54	1	1880	U

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Mol	Chain	Res	Type
54	1	1906	G
54	1	1907	G
54	1	1913	A
54	1	1914	C
54	1	1929	G
54	1	1930	G
54	1	1933	G
54	1	1937	A
54	1	1938	A
54	1	1955	U
54	1	1960	A
54	1	1963	U
54	1	1967	C
54	1	1969	A
54	1	1970	A
54	1	1972	G
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	2034	U
54	1	2036	C
54	1	2043	C
54	1	2055	C
54	1	2056	G
54	1	2060	A
54	1	2061	G
54	1	2062	A
54	1	2069	G
54	1	2072	C
54	1	2096	C
54	1	2106	U
54	1	2111	U
54	1	2112	G
54	1	2113	U
54	1	2115	G
54	1	2117	A
54	1	2118	U
54	1	2119	A

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Mol	Chain	Res	Type
54	1	2120	G
54	1	2127	G
54	1	2131	U
54	1	2132	U
54	1	2133	G
54	1	2135	A
54	1	2145	C
54	1	2146	C
54	1	2147	A
54	1	2157	G
54	1	2162	G
54	1	2166	U
54	1	2172	U
54	1	2173	A
54	1	2178	C
54	1	2189	U
54	1	2198	A
54	1	2204	G
54	1	2210	U
54	1	2211	A
54	1	2213	U
54	1	2225	A
54	1	2238	G
54	1	2239	G
54	1	2278	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	2345	G
54	1	2347	C
54	1	2350	C
54	1	2357	G
54	1	2361	G
54	1	2382	G
54	1	2383	G
54	1	2385	C

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Mol	Chain	Res	Type
54	1	2391	G
54	1	2392	A
54	1	2402	U
54	1	2406	A
54	1	2423	U
54	1	2427	C
54	1	2429	G
54	1	2430	A
54	1	2435	A
54	1	2441	U
54	1	2448	A
54	1	2476	A
54	1	2490	G
54	1	2494	G
54	1	2498	C
54	1	2502	G
54	1	2503	A
54	1	2505	G
54	1	2518	A
54	1	2529	G
54	1	2547	A
54	1	2554	U
54	1	2566	A
54	1	2567	G
54	1	2572	A
54	1	2602	A
54	1	2603	G
54	1	2609	U
54	1	2613	U
54	1	2629	U
54	1	2636	C
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	2713	U
54	1	2714	G
54	1	2728	U
54	1	2733	A
54	1	2739	U

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Mol	Chain	Res	Type
54	1	2748	A
54	1	2751	G
54	1	2757	A
54	1	2764	A
54	1	2765	A
54	1	2778	A
54	1	2779	U
54	1	2791	G
54	1	2794	C
54	1	2797	U
54	1	2800	A
54	1	2801	G
54	1	2820	A
54	1	2821	A
54	1	2833	U
54	1	2867	G
54	1	2868	A
54	1	2873	A
54	1	2883	A
55	2	4	C
55	2	13	G
55	2	15	A
55	2	35	C
55	2	36	C
55	2	37	C
55	2	40	U
55	2	41	G
55	2	44	G
55	2	88	C
55	2	89	U
55	2	90	C
55	2	108	A
55	2	109	A
56	5	3	G
56	5	4	C
56	5	5	G
56	5	6	A
56	5	10	G
56	5	17(A)	U
56	5	19	G
56	5	20	U
56	5	21	A

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Mol	Chain	Res	Type
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	10	G
57	6	14	A
57	6	19	G
57	6	20	U
57	6	21	A
57	6	22	G
57	6	28	C
57	6	33	U
57	6	34	C
57	6	35	A
57	6	59	A
57	6	70	G
57	6	76	A
58	4	12	A
58	4	15	A
58	4	16	A

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	3	70	U
53	3	890	G
53	3	1183	U
53	3	1396	A
53	3	1493	A
53	3	1534	A
54	1	421	C
54	1	481	G
54	1	490	C
54	1	859	G
54	1	1130	U
54	1	1475	G
54	1	1730	C

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Mol	Chain	Res	Type
54	1	2286	G
54	1	2296	U
54	1	2326	C
54	1	2391	G
54	1	2756	U
55	2	88	C
56	5	2	G
57	6	32	C

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	1.15	0	7,9,11	0.89	0
62	GCP	8	801	63	27,34,34	2.09	8 (29%)	34,54,54	3.70	19 (55%)
61	PRO	5	101	56,60	5,7,8	0.47	0	7,8,10	1.28	1 (14%)

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	-	2/7/9/11	-
62	GCP	8	801	63	-	9/15/38/38	0/3/3/3
61	PRO	5	101	56,60	-	0/0/9/11	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	8	801	GCP	PB-O3A	-6.55	1.51	1.58
62	8	801	GCP	O4'-C1'	3.72	1.46	1.41
62	8	801	GCP	C6-N1	3.24	1.38	1.33
62	8	801	GCP	C2-N1	3.22	1.41	1.35
62	8	801	GCP	PB-O2B	-2.63	1.50	1.56
62	8	801	GCP	PG-O3G	-2.52	1.49	1.54
62	8	801	GCP	C2'-C1'	2.11	1.57	1.53
62	8	801	GCP	PG-O2G	-2.04	1.50	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	8	801	GCP	C1'-N9-C4	12.26	148.18	126.64
62	8	801	GCP	C5-C6-N1	-8.60	111.67	123.43
62	8	801	GCP	C2-N1-C6	6.67	126.53	115.93
62	8	801	GCP	O4'-C1'-C2'	-5.70	98.60	106.93
62	8	801	GCP	C4-C5-C6	-4.56	116.44	120.80
62	8	801	GCP	O3G-PG-O2G	4.23	120.42	108.08
62	8	801	GCP	C2-N3-C4	-4.17	110.60	115.36
62	8	801	GCP	O2G-PG-C3B	-3.83	97.11	106.40
62	8	801	GCP	O2B-PB-O1B	3.58	122.02	110.07
62	8	801	GCP	C4-C5-N7	3.40	112.95	109.40
62	8	801	GCP	O3'-C3'-C4'	-3.25	101.65	111.05
62	8	801	GCP	N3-C2-N1	-3.15	123.03	127.22
62	8	801	GCP	O2A-PA-O5'	-2.88	94.39	107.75
62	8	801	GCP	O1B-PB-C3B	2.41	115.43	109.07
61	5	101	PRO	O-C-CA	-2.37	118.57	124.78
62	8	801	GCP	PB-O3A-PA	2.32	139.92	132.56
62	8	801	GCP	O3G-PG-O1G	-2.27	106.38	112.39
62	8	801	GCP	O2A-PA-O1A	2.25	123.38	112.24
62	8	801	GCP	O4'-C4'-C5'	2.16	116.47	109.37
62	8	801	GCP	C3'-C2'-C1'	-2.07	97.87	100.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

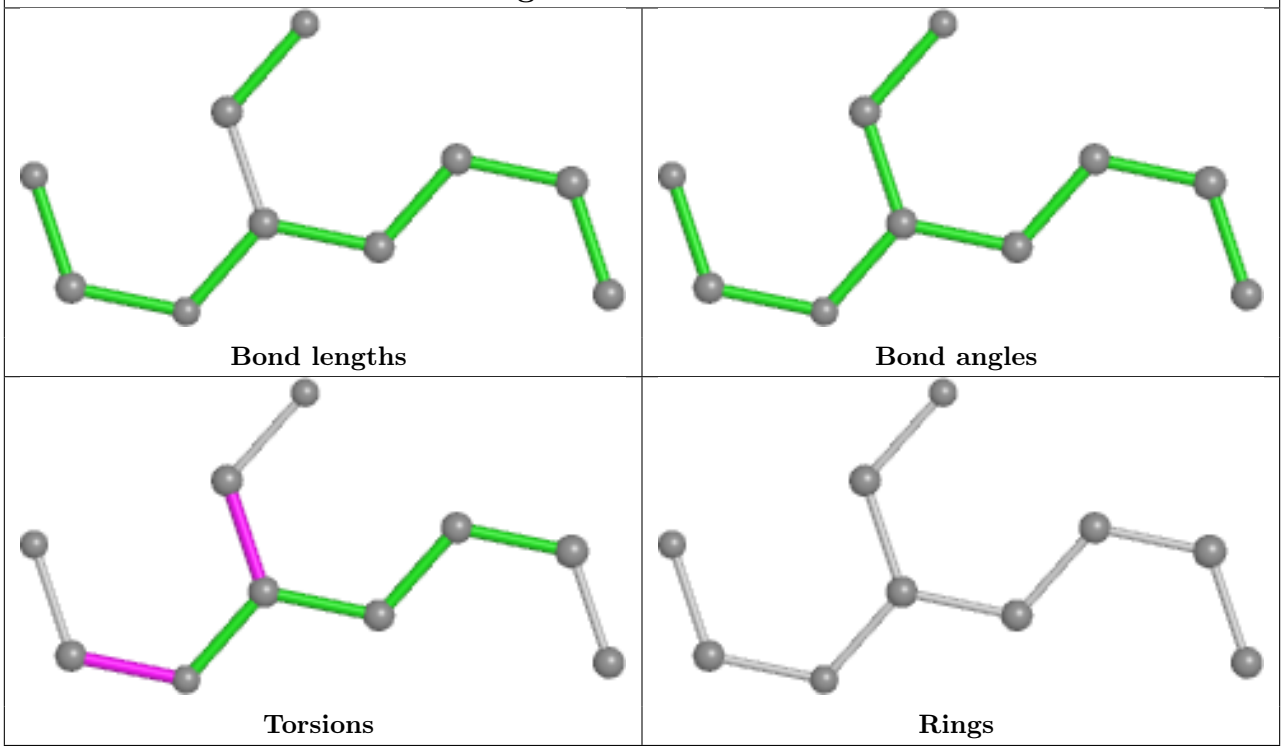
Mol	Chain	Res	Type	Atoms
60	1	3001	FME	O1-CN-N-CA
60	1	3001	FME	O-C-CA-CB
62	8	801	GCP	PB-C3B-PG-O1G
62	8	801	GCP	PB-C3B-PG-O2G
62	8	801	GCP	PG-C3B-PB-O1B
62	8	801	GCP	C5'-O5'-PA-O3A
62	8	801	GCP	C5'-O5'-PA-O1A
62	8	801	GCP	O4'-C4'-C5'-O5'
62	8	801	GCP	C3'-C4'-C5'-O5'
62	8	801	GCP	PB-C3B-PG-O3G
62	8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

There are no ring outliers.

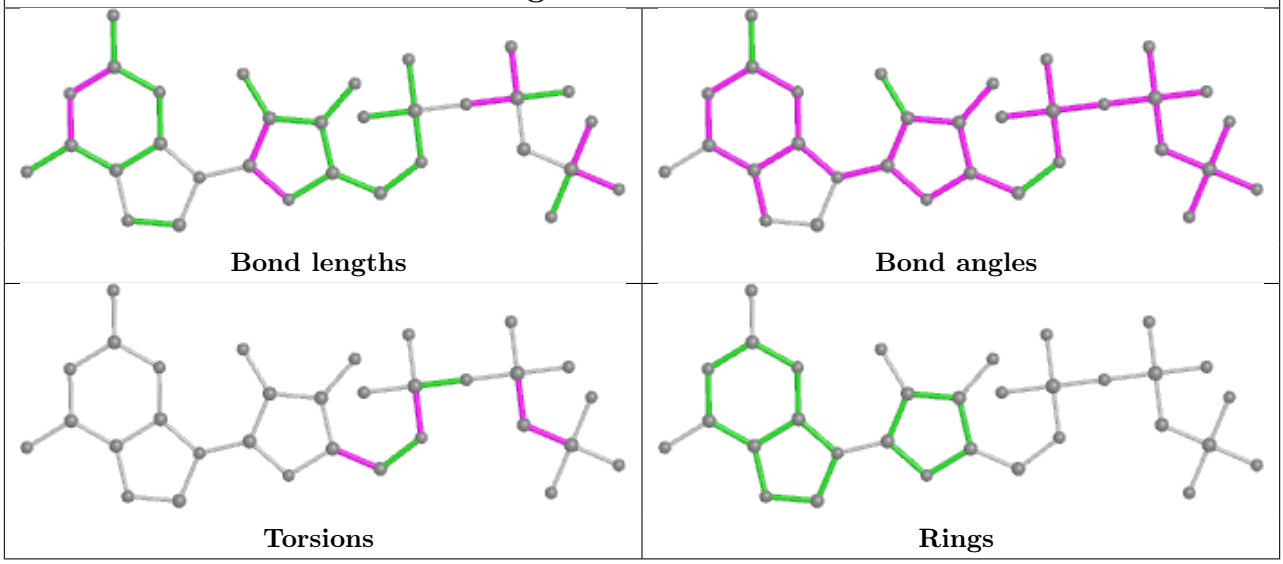
No monomer is involved in short contacts.

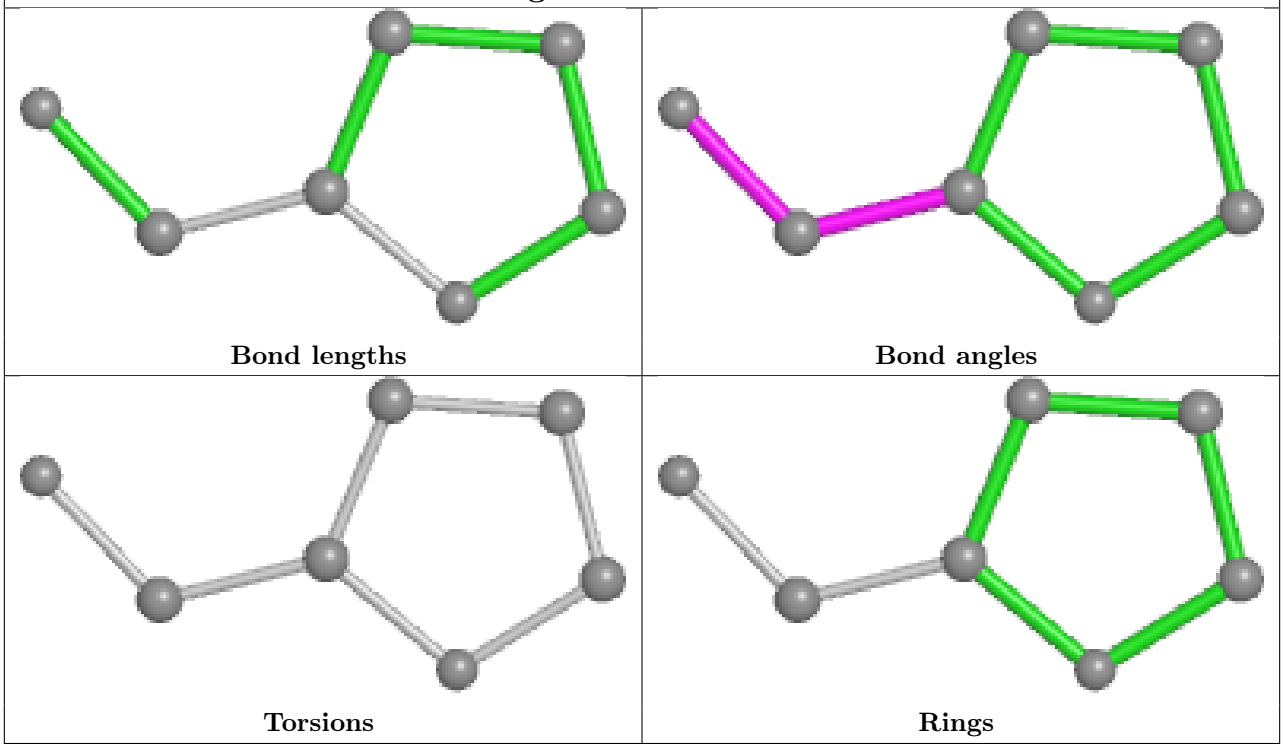
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FME 1 3001



Ligand GCP 8 801



Ligand PRO 5 101	
	
Bond lengths	Bond angles
Torsions	Rings

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.

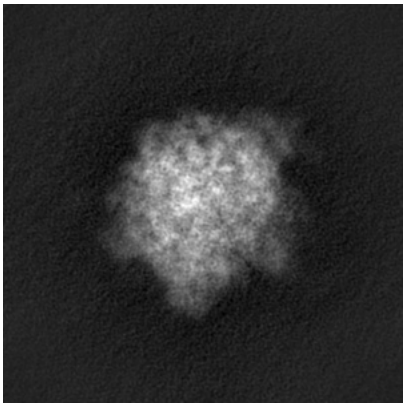
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22670. These allow visual inspection of the internal detail of the map and identification of artifacts.

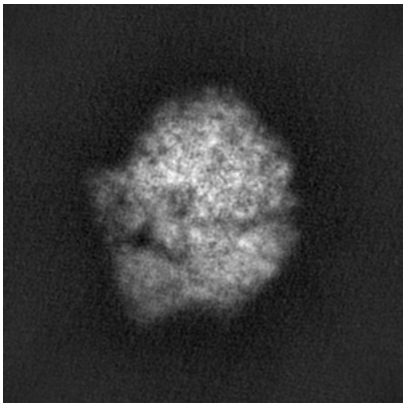
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

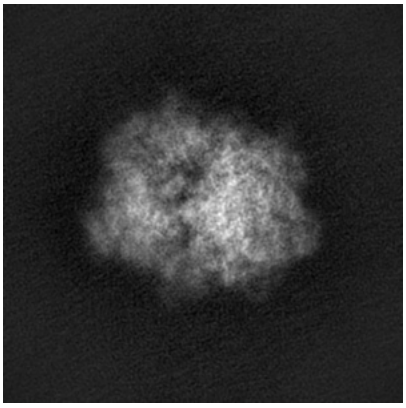
6.1.1 Primary map



X



Y

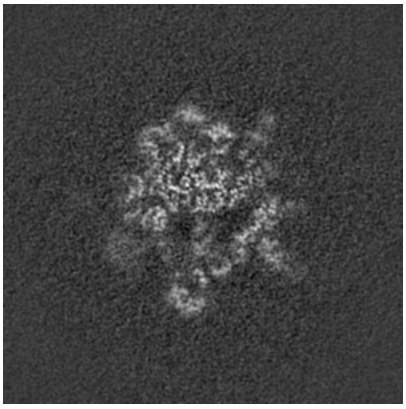


Z

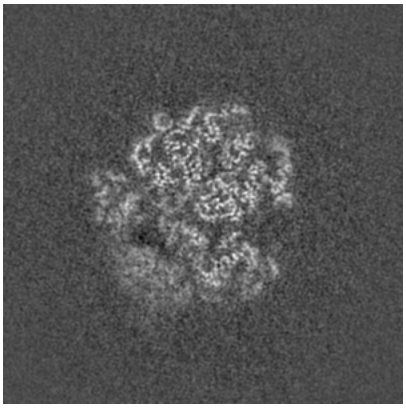
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

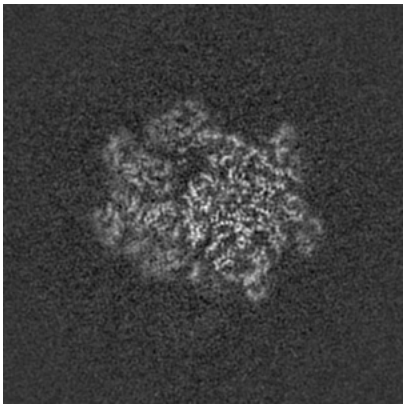
6.2.1 Primary map



X Index: 200



Y Index: 200

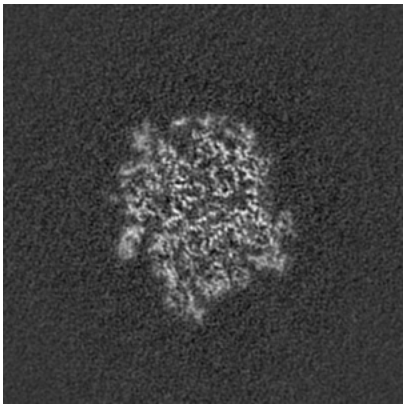


Z Index: 200

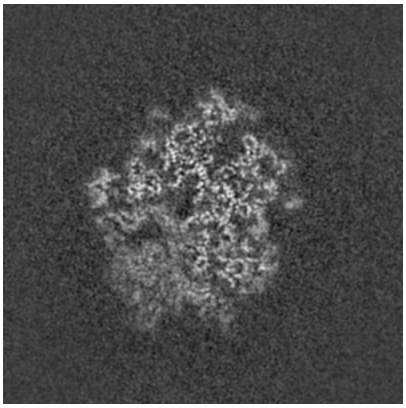
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

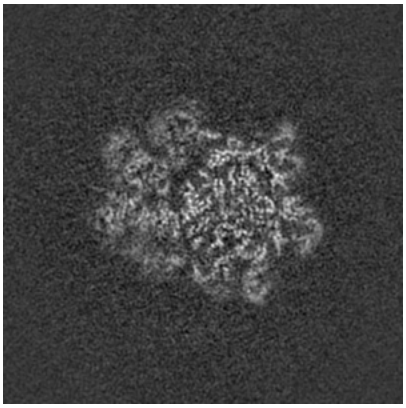
6.3.1 Primary map



X Index: 223



Y Index: 189

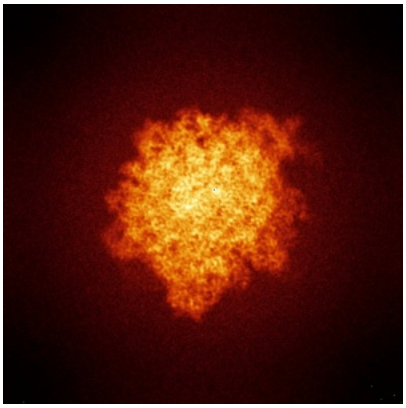


Z Index: 203

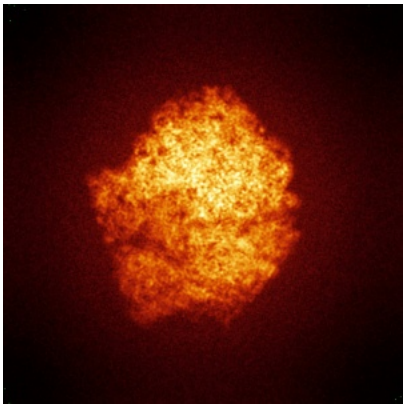
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

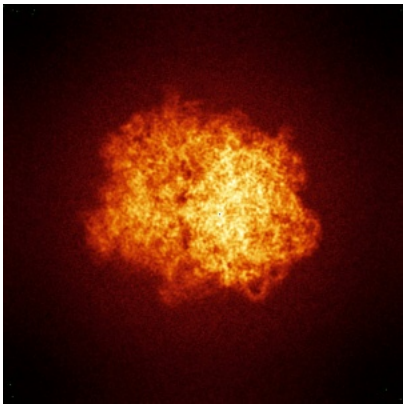
6.4.1 Primary map



X



Y

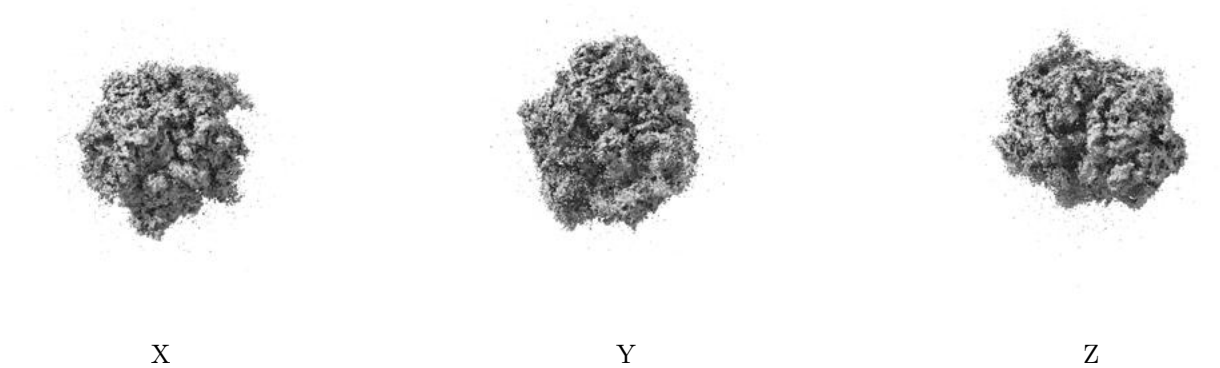


Z

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



X Y Z

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

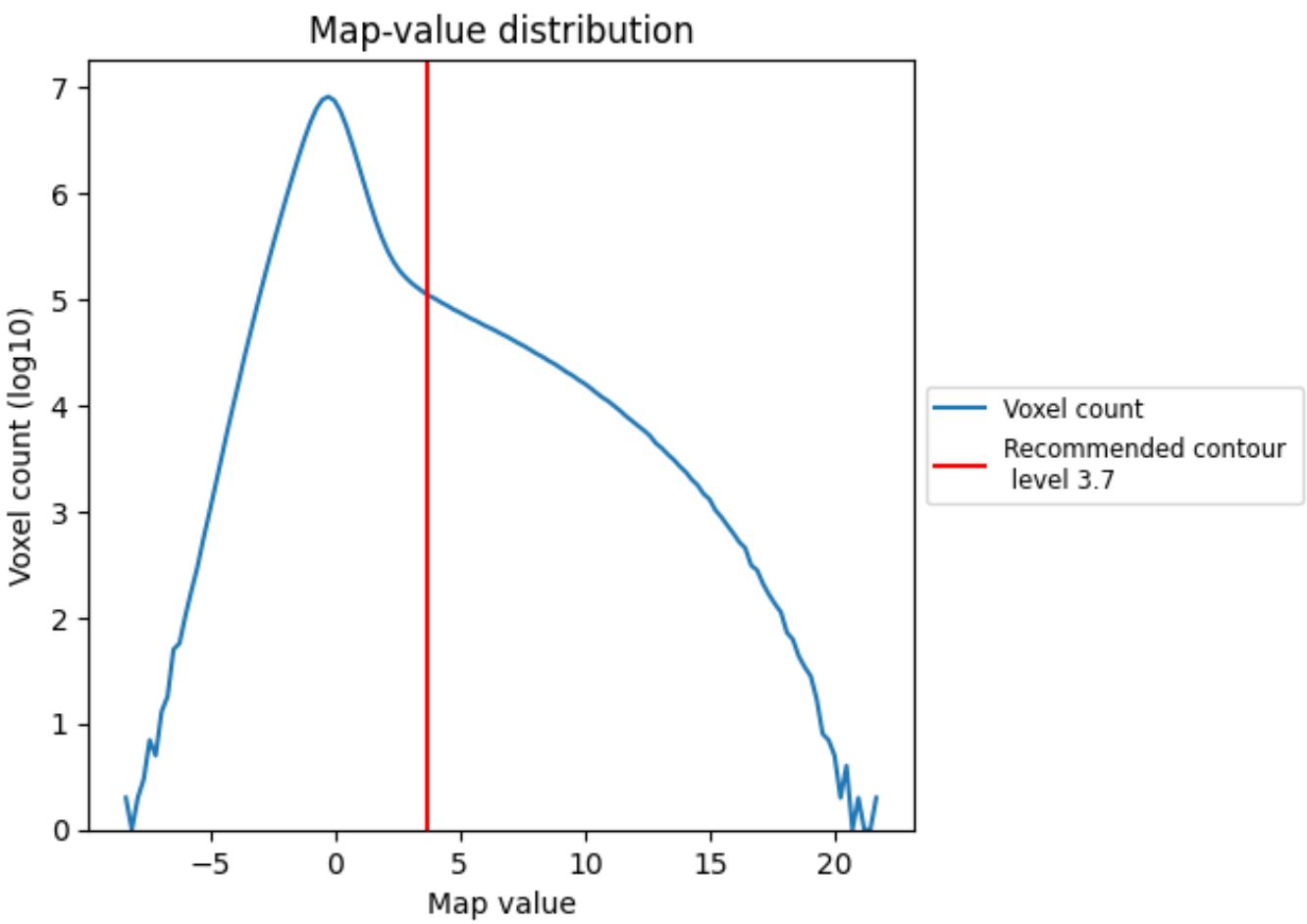
6.6 Mask visualisation (i)

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

7 Map analysis (i)

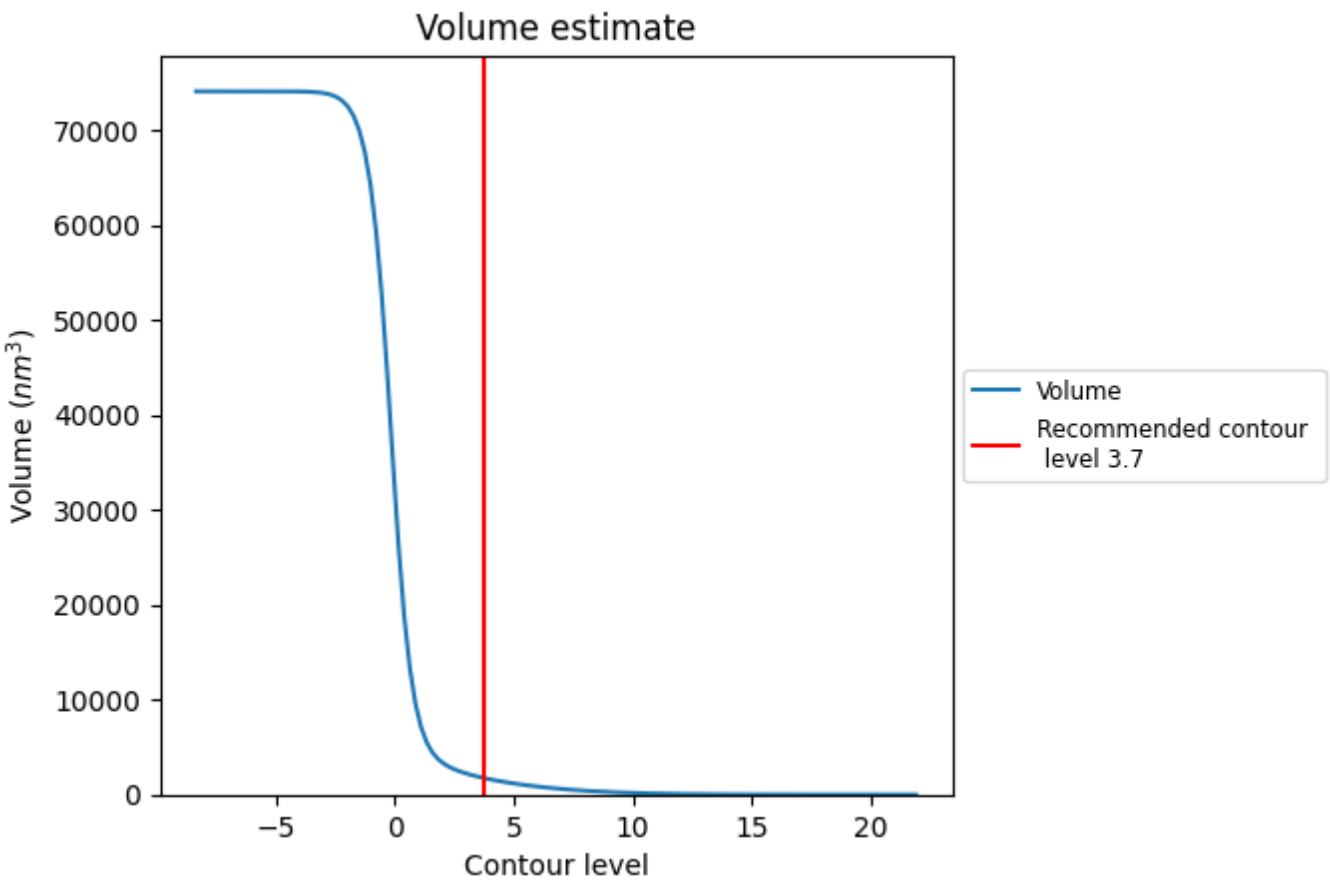
This section contains the results of statistical analysis of the map.

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.

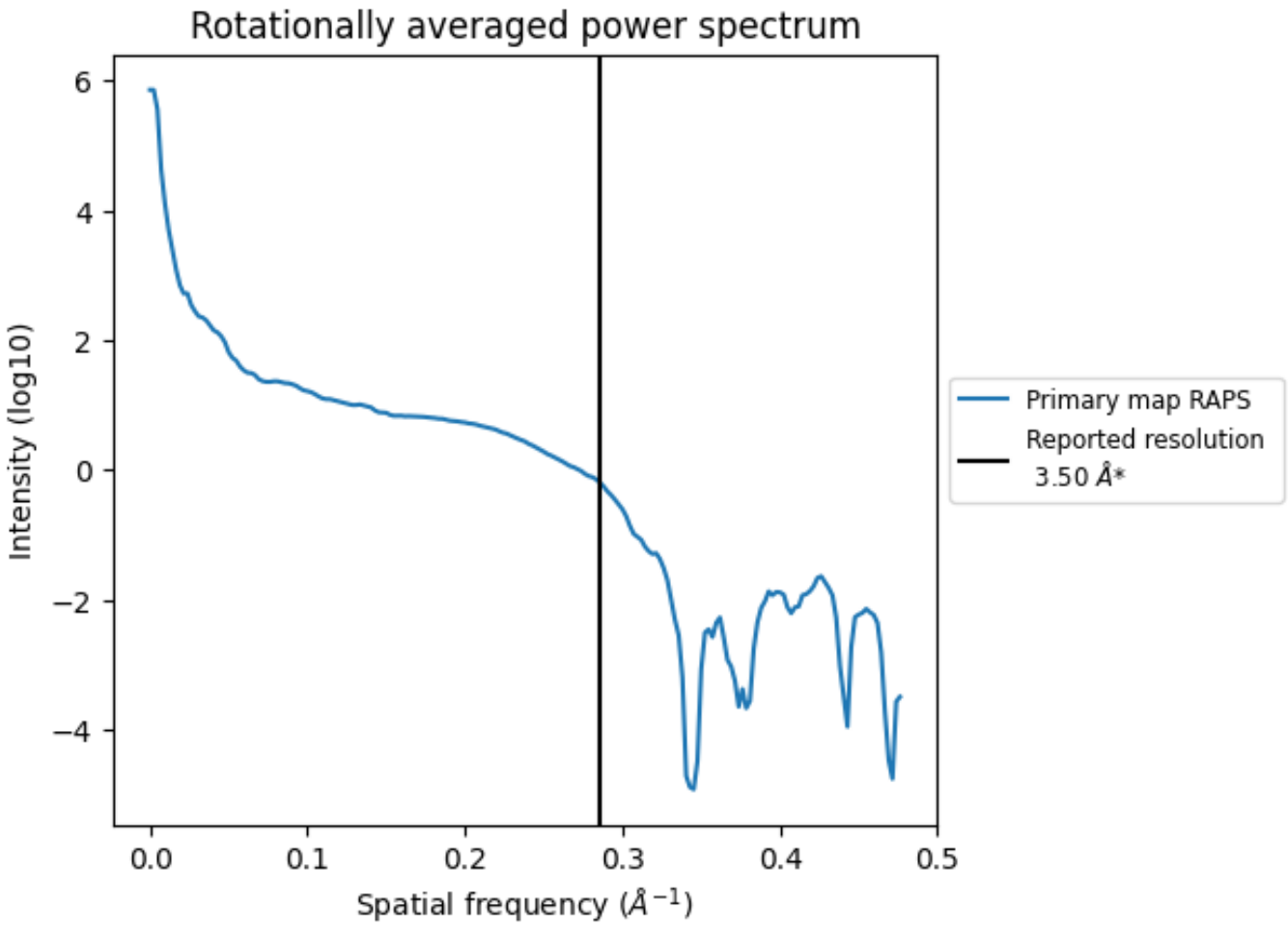
7.2 Volume estimate (i)



The volume at the recommended contour level is 1761 nm^3; this corresponds to an approximate mass of 1590 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

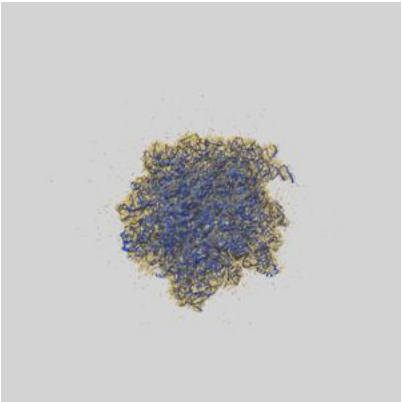
8 Fourier-Shell correlation (i)

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

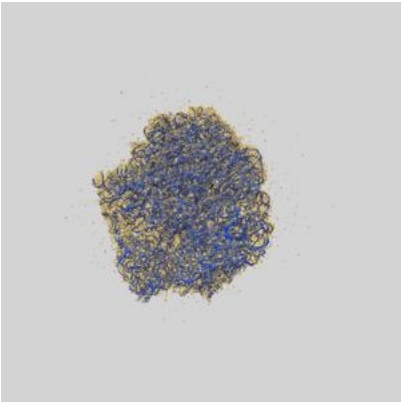
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22670 and PDB model 7K51. Per-residue inclusion information can be found in section 3 on page 17.

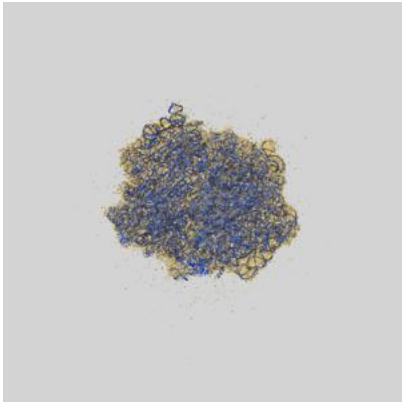
9.1 Map-model overlay (i)



X



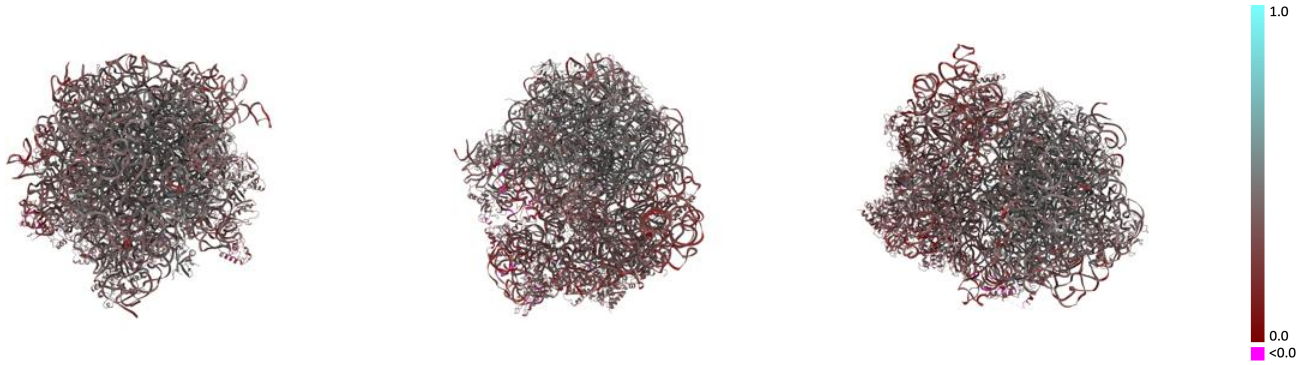
Y



Z

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

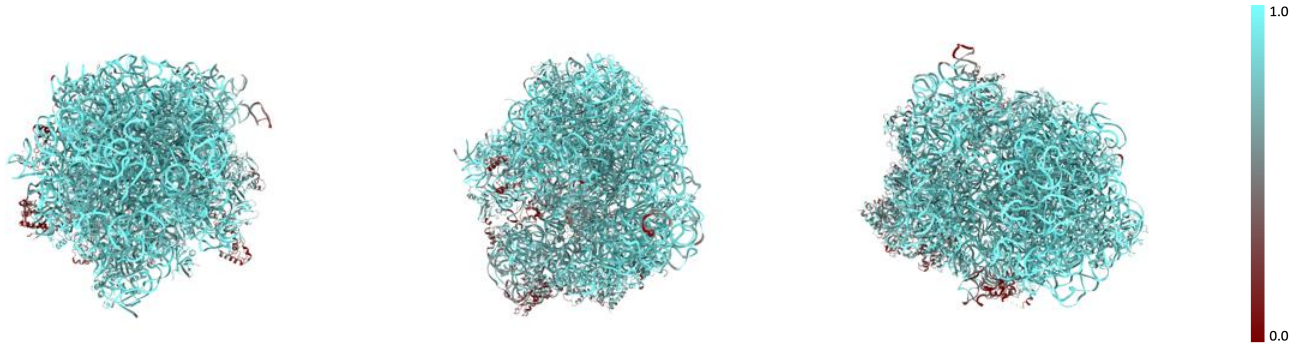
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

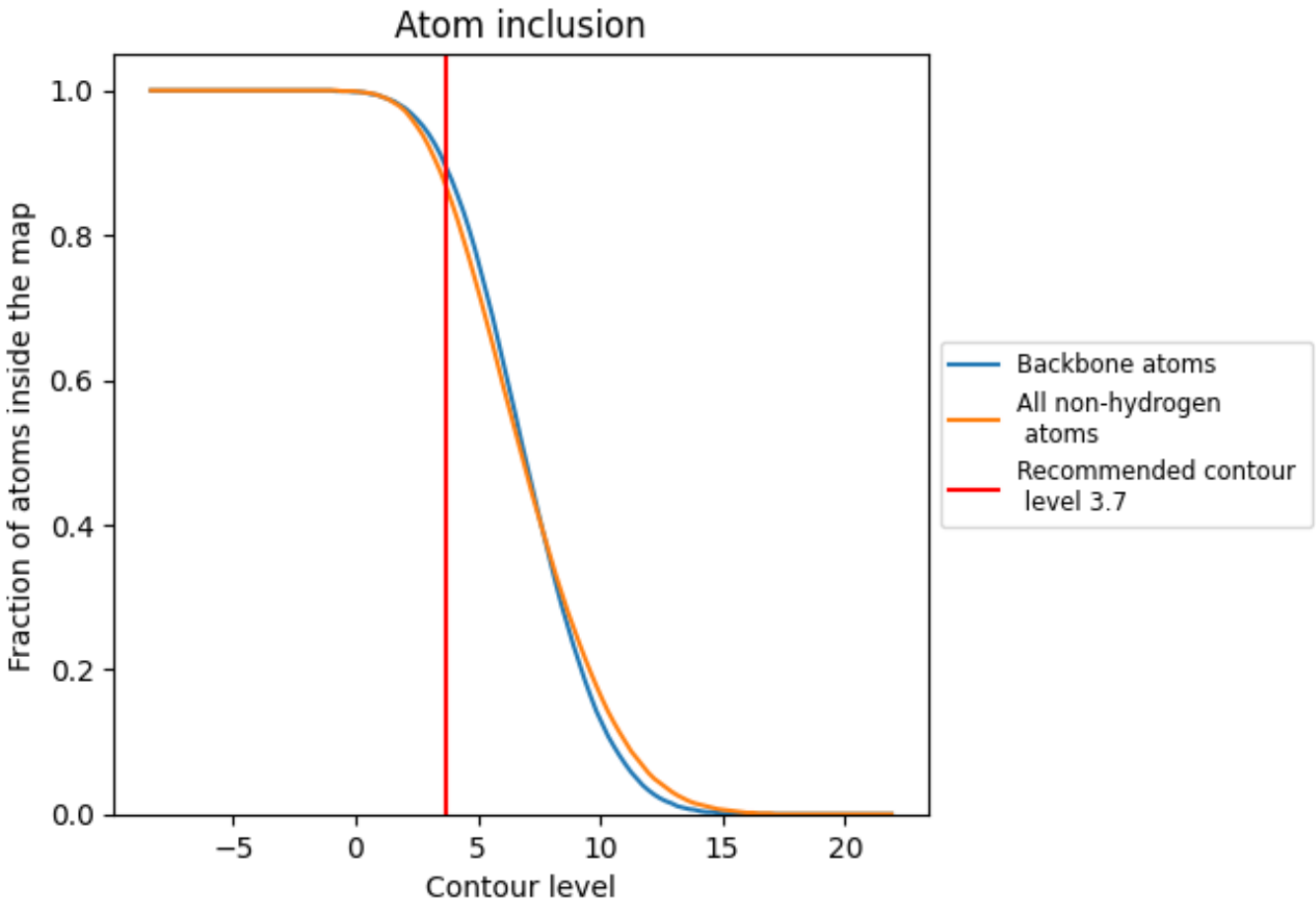
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.7).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8670	0.3690
1	0.9600	0.4030
2	0.9510	0.3720
3	0.8870	0.3140
4	0.6520	0.2280
5	0.8080	0.2890
6	0.8420	0.2660
8	0.7170	0.3480
A	0.6130	0.2710
B	0.8970	0.4310
C	0.6320	0.3830
D	0.9070	0.4600
E	0.8720	0.4550
F	0.8730	0.4570
G	0.5820	0.3250
H	0.5880	0.3240
I	0.7540	0.3240
J	0.8330	0.3820
K	0.7840	0.3490
L	0.3720	0.2830
M	0.8290	0.3810
N	0.5530	0.2890
O	0.4070	0.2980
P	0.8250	0.3530
Q	0.8140	0.3820
R	0.5070	0.2930
S	0.7420	0.3140
T	0.8350	0.3440
U	0.8010	0.3660
V	0.7950	0.3460
W	0.8020	0.3390
X	0.6980	0.3040
Y	0.7780	0.3160
Z	0.6200	0.3060
a	0.2230	0.2200

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	0.9020	0.4470
c	0.8800	0.4440
d	0.7820	0.4080
e	0.7850	0.3540
f	0.8420	0.3980
g	0.2730	0.2880
h	0.2270	0.2420
i	0.2630	0.2480
j	0.8790	0.4450
k	0.8610	0.4460
l	0.8810	0.4330
m	0.8870	0.4510
n	0.9060	0.4370
o	0.8440	0.3980
p	0.8940	0.4390
q	0.8820	0.4370
r	0.8220	0.4180
s	0.8680	0.4340
t	0.8290	0.4110
u	0.8150	0.3930
v	0.8420	0.4320
w	0.8870	0.4550
x	0.8970	0.4300
y	0.7560	0.3580
z	0.8720	0.4430