wwPDB EM Validation Summary Report (i)

Apr 16, 2024 – 07:53 am BST

PDB ID	:	5LZD
EMDB ID	:	EMD-4124
Title	:	Structure of SelB-Sec-tRNASec bound to the 70S ribosome in the GTPase activated state (GA)
Authors	:	Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on	:	2016-09-29
Resolution	:	3.40 Å(reported)

This is a wwPDB EM Validation Summary 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:

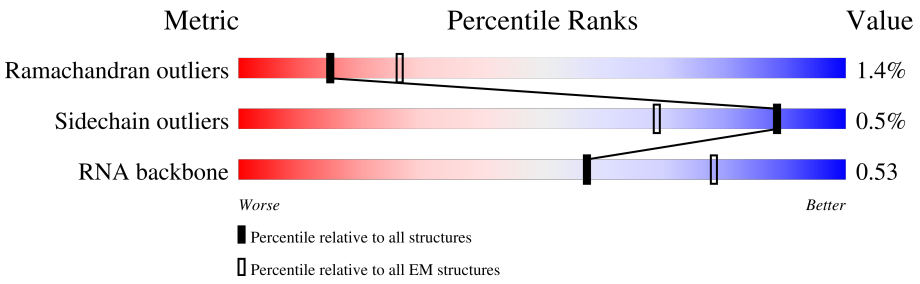
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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%

Mol	Chain	Length	Quality of chain
1	a	1539	80% 18% •
2	b	218	93% 6% •
3	c	206	98% •
4	d	205	95% 5%
5	e	157	96% •
6	f	100	94% 5% •
7	g	151	97% •
8	h	129	96% • •
9	i	127	94% 5% •

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Mol	Chain	Length	Quality of chain
10	j	98	93% 6%
11	k	116	96%
12	l	123	92% 7%
13	m	114	92% 8%
14	n	100	94% 6%
15	o	88	94% 6%
16	p	82	99%
17	q	80	90% 10%
18	r	65	94% 6%
19	s	86	93% 6%
20	t	85	98%
21	u	65	89% 11%
22	v	77	77% 19%
23	x	48	40% 38% 23%
24	y	95	65% 35%
25	z	614	96%
26	A	2903	76% 22%
27	B	120	74% 23%
28	C	271	97%
29	D	209	99%
30	E	201	97%
31	F	177	93% 6%
32	G	176	96%
33	I	141	99%
34	H	149	96%

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Mol	Chain	Length	Quality of chain
35	J	142	99%
36	K	122	97%
37	L	143	97%
38	M	136	99%
39	N	120	98%
40	O	116	99%
41	P	114	98%
42	Q	117	99%
43	R	103	99%
44	S	110	97%
45	T	93	99%
46	U	102	92% 7%
47	V	94	100%
48	W	75	100%
49	X	77	99%
50	Y	63	94% 6%
51	Z	58	98%
52	0	56	96%
53	1	50	94% 6%
54	2	46	100%
55	3	64	97%
56	4	38	92% 8%
57	6	66	94% 5%
58	w	3	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
26	G7M	A	2069	X	-	-	-

2 Entry composition (i)

There are 65 unique types of molecules in this entry. The entry contains 153177 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1539	33029	14738	6052	10700	1539	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	100	794	495	164	132	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	r	65	505	317	96	92	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	s	86	687	438	131	116	2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	u	65	496	307	100	88	1	0	0

- Molecule 22 is a RNA chain called fMet-tRNAfMet.

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

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	x	48	1025	457	183	337	48	0	0

- Molecule 24 is a RNA chain called Sec-tRNASec.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	y	95	2031	907	357	672	95	0	0

- Molecule 25 is a protein called Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	z	614	4853	3043	901	892	17	0	0

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	A	2903	62335	27815	11467	20150	2903	0	0

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	I	141	1032	651	179	196	6	0	0

- Molecule 34 is a protein called 50S ribosomal protein L9.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

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

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

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

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	0	56	444	269	94	80	1	0	0

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	1	50	410	263	75	72	0	0

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	2	46	377	228	90	57	2	0	0

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	3	64	504	323	105	74	2	0	0

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	4	38	302	185	65	48	4	0	0

- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	6	66	523	323	99	95	6	0	0

- Molecule 58 is a RNA chain called CCA 3' end of E-site tRNASec (low occupancy).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
58	w	3	62	28	11	20	3	0	0

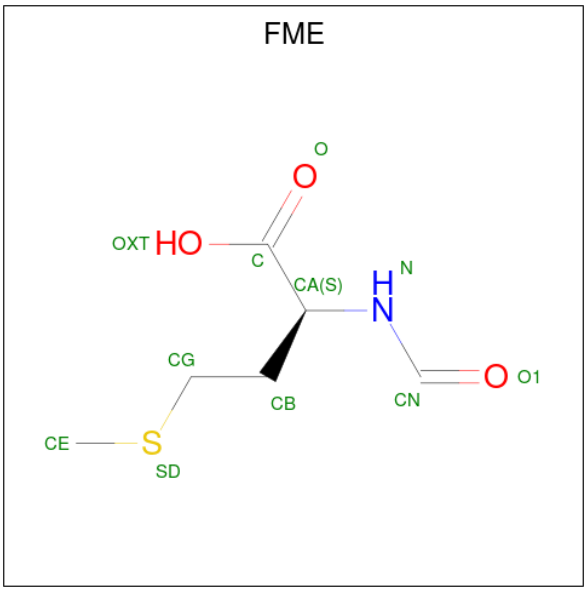
- Molecule 59 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
59	a	1	1	1	0

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

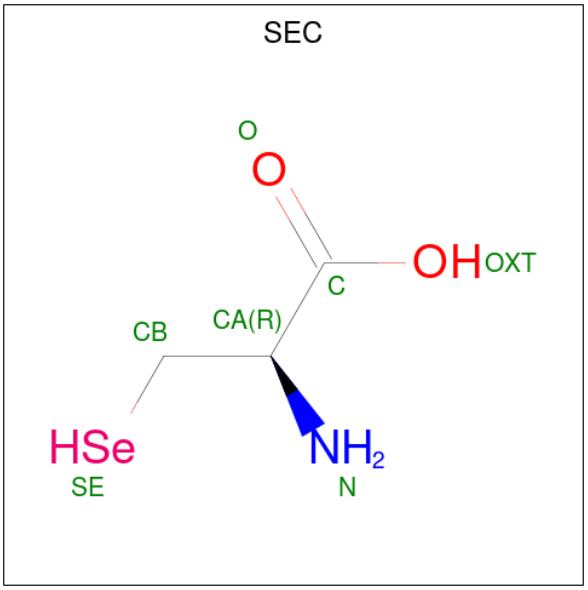
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	a	30	30	30	0
60	n	1	1	1	0
60	v	1	1	1	0
60	y	1	1	1	0
60	z	1	1	1	0
60	A	111	111	111	0
60	B	2	2	2	0

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



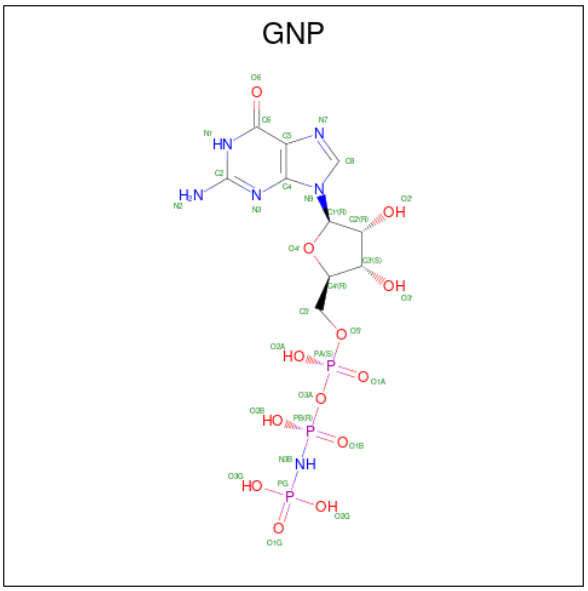
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
61	v	1	10	6	1	2	1	0

- Molecule 62 is SELENOCYSTEINE (three-letter code: SEC) (formula: $C_3H_7NO_2Se$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	Se	
62	y	1	6	3	1	1	1	0

- Molecule 63 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
63	z	1	32	10	6	13	3	0

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
64	4	1	1	1	0
64	6	1	1	1	0

- Molecule 65 is water.

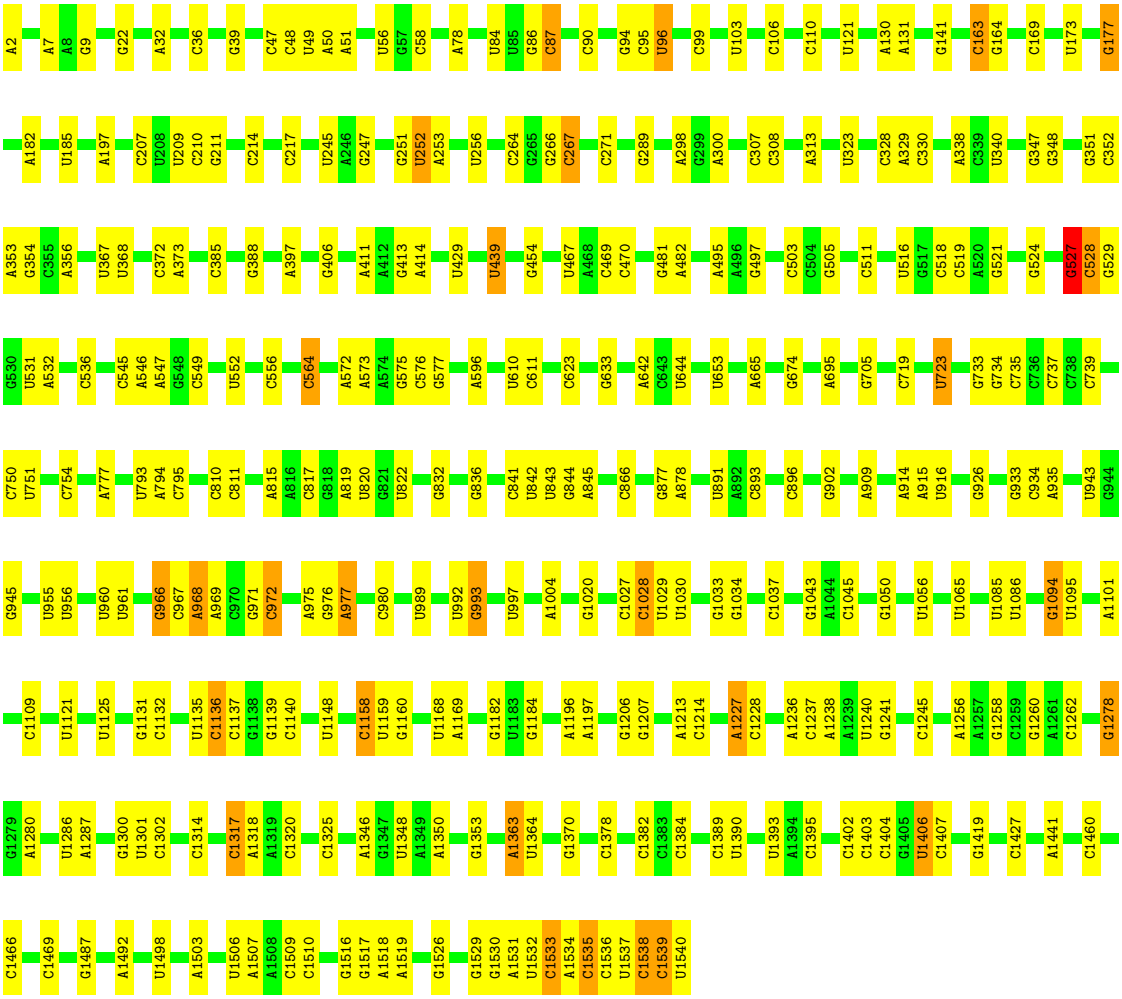
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
65	z	2	2	2	0

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. 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. 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.

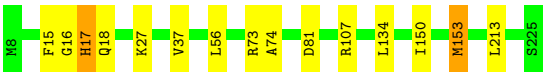
- Molecule 1: 16S ribosomal RNA

Chain a: 80% 18%



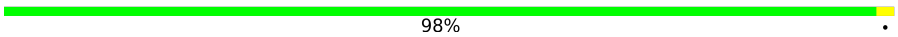
- Molecule 2: 30S ribosomal protein S2

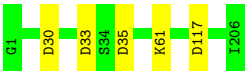
Chain b: 93% 6%



- Molecule 3: 30S ribosomal protein S3

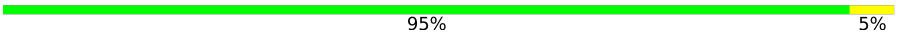
Chain c:

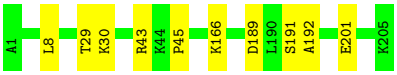




- Molecule 4: 30S ribosomal protein S4

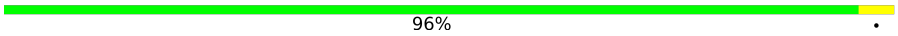
Chain d:

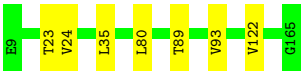




- Molecule 5: 30S ribosomal protein S5

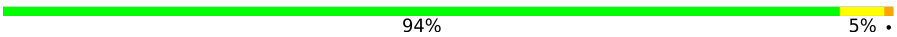
Chain e:

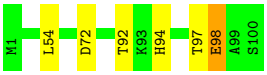




- Molecule 6: 30S ribosomal protein S6

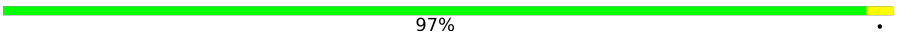
Chain f:





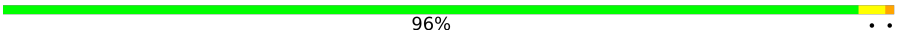
- Molecule 7: 30S ribosomal protein S7

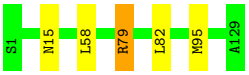
Chain g:



- Molecule 8: 30S ribosomal protein S8

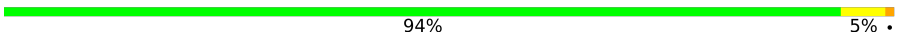
Chain h:





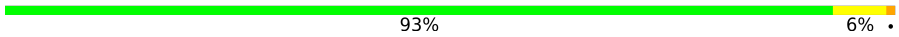
- Molecule 9: 30S ribosomal protein S9

Chain i:



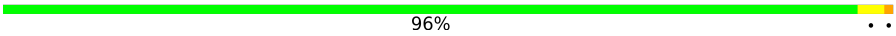
- Molecule 10: 30S ribosomal protein S10

Chain j:



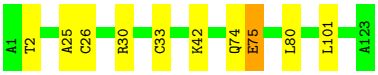
• Molecule 11: 30S ribosomal protein S11

Chain k:



• Molecule 12: 30S ribosomal protein S12

Chain l:

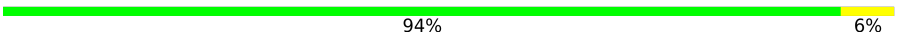


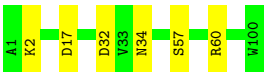
• Molecule 13: 30S ribosomal protein S13

Chain m:

• Molecule 14: 30S ribosomal protein S14

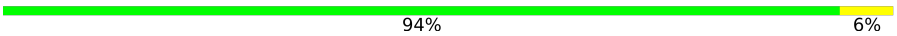
Chain n:





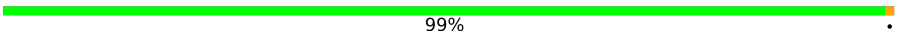
• Molecule 15: 30S ribosomal protein S15

Chain o:



• Molecule 16: 30S ribosomal protein S16

Chain p:



• Molecule 17: 30S ribosomal protein S17

Chain q: 90% 10%

• Molecule 18: 30S ribosomal protein S18

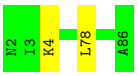
Chain r: 94% 6%

• Molecule 19: 30S ribosomal protein S19

Chain s: 93% 6%

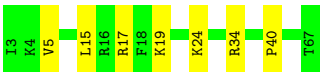
• Molecule 20: 30S ribosomal protein S20

Chain t: 98%



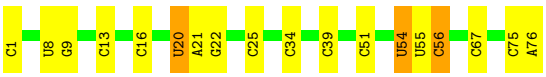
• Molecule 21: 30S ribosomal protein S21

Chain u: 89% 11%



• Molecule 22: fMet-tRNAfMet

Chain v: 77% 19%



• Molecule 23: SECIS mRNA

Chain x: 40% 38% 23%

• Molecule 24: Sec-tRNASec

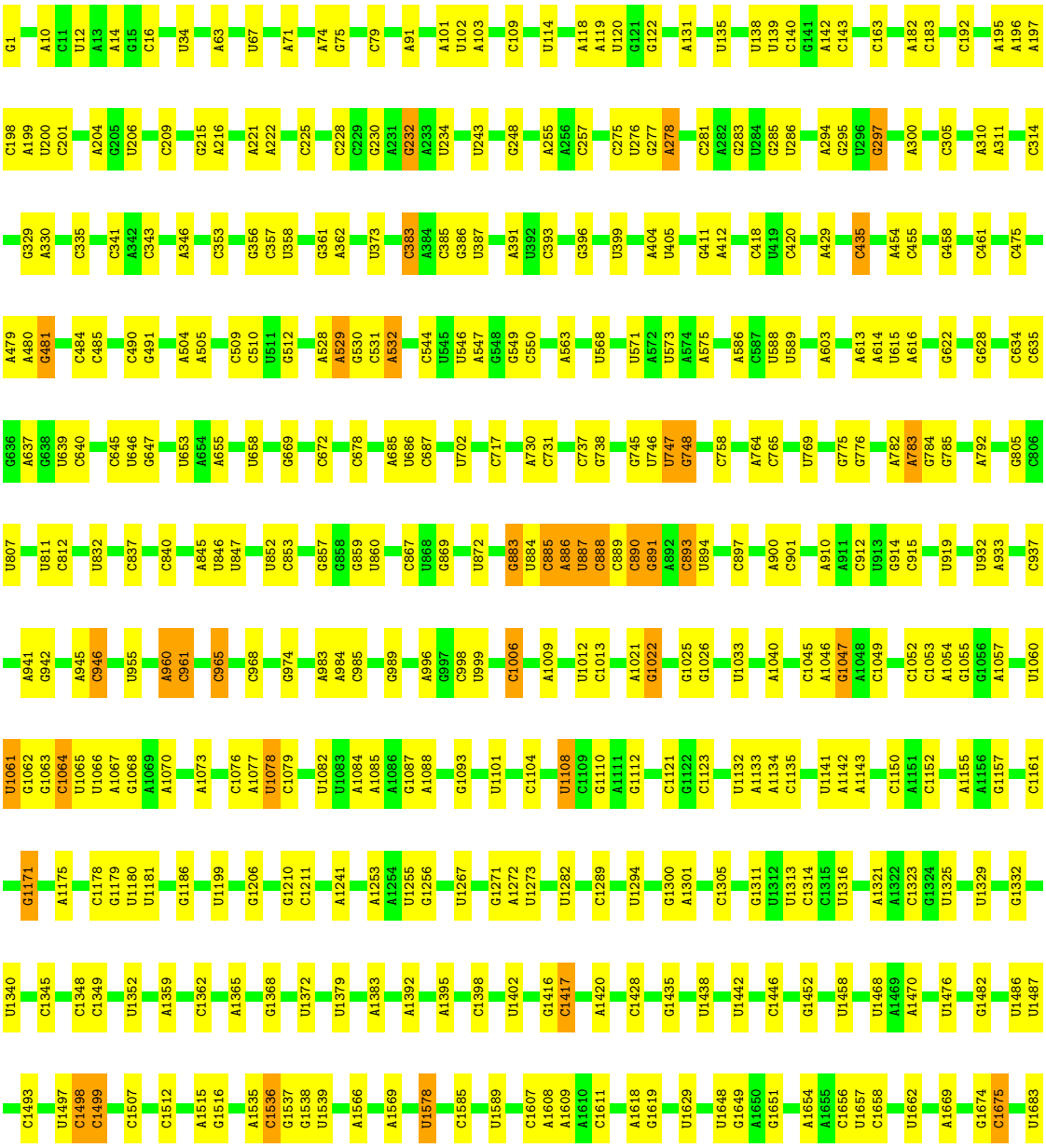
Chain y: 65% 35%

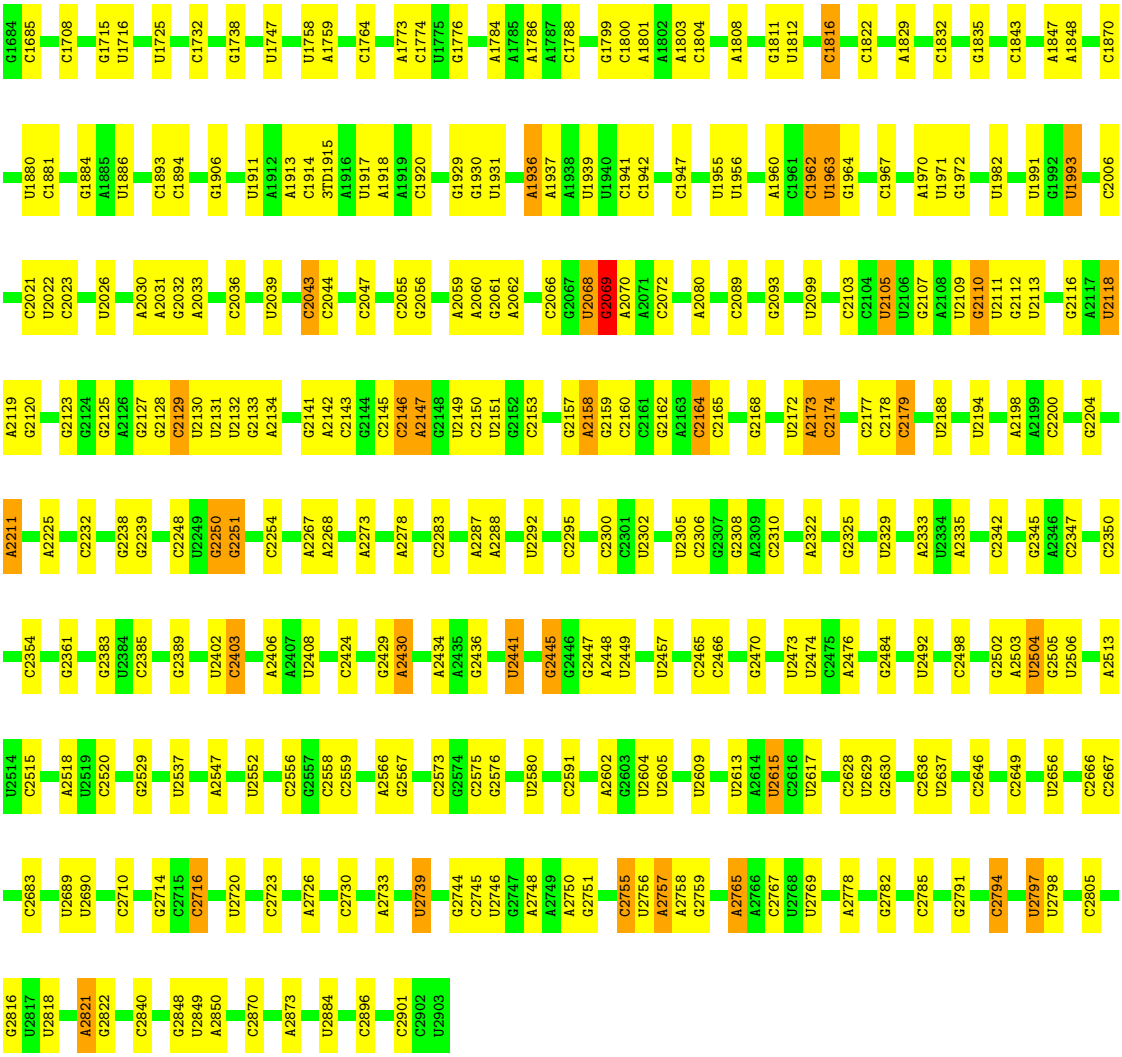
- Molecule 25: Selenocysteine-specific elongation factor

Chain z: 96%

- Molecule 26: 23S ribosomal RNA

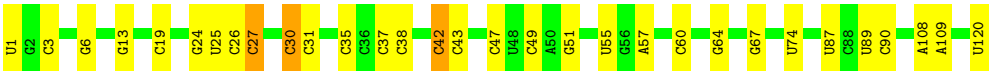
Chain A: 76% 22%





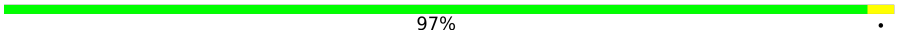
- Molecule 27: 5S ribosomal RNA

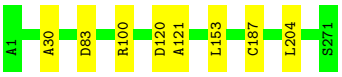
Chain B:



- Molecule 28: 50S ribosomal protein L2

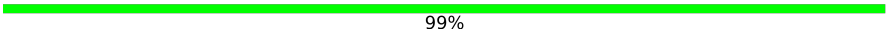
Chain C:

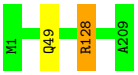




- Molecule 29: 50S ribosomal protein L3

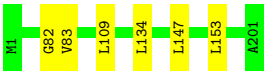
Chain D:





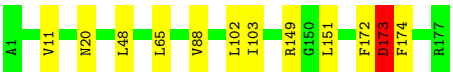
• Molecule 30: 50S ribosomal protein L4

Chain E: 97%



• Molecule 31: 50S ribosomal protein L5

Chain F: 93% 6%



• Molecule 32: 50S ribosomal protein L6

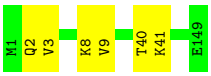
Chain G: 96%

• Molecule 33: 50S ribosomal protein L11

Chain I: 99%

• Molecule 34: 50S ribosomal protein L9

Chain H: 96%



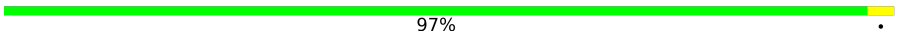
• Molecule 35: 50S ribosomal protein L13

Chain J: 99%

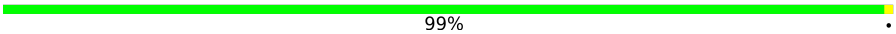
• Molecule 36: 50S ribosomal protein L14

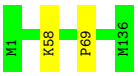
Chain K: 97%

• Molecule 37: 50S ribosomal protein L15

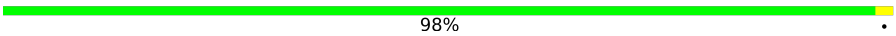
Chain L: 

• Molecule 38: 50S ribosomal protein L16

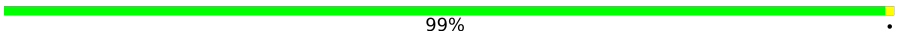
Chain M: 



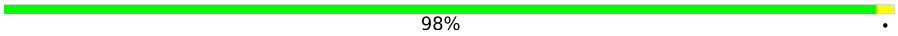
• Molecule 39: 50S ribosomal protein L17

Chain N: 

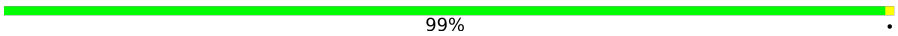
• Molecule 40: 50S ribosomal protein L18

Chain O: 

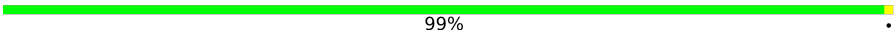
• Molecule 41: 50S ribosomal protein L19

Chain P: 

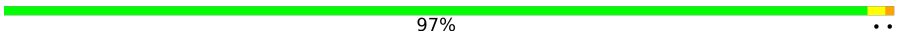
• Molecule 42: 50S ribosomal protein L20

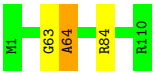
Chain Q: 

• Molecule 43: 50S ribosomal protein L21

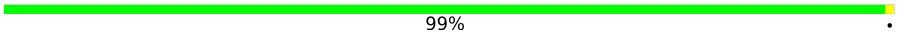
Chain R: 

• Molecule 44: 50S ribosomal protein L22

Chain S: 



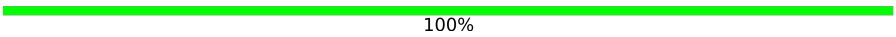
• Molecule 45: 50S ribosomal protein L23

Chain T: 

• Molecule 46: 50S ribosomal protein L24

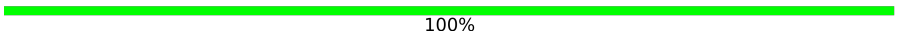
Chain U:

• Molecule 47: 50S ribosomal protein L25

Chain V: 

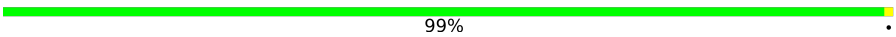
There are no outlier residues recorded for this chain.

• Molecule 48: 50S ribosomal protein L27

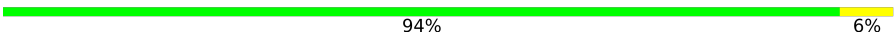
Chain W: 

There are no outlier residues recorded for this chain.

• Molecule 49: 50S ribosomal protein L28

Chain X: 

• Molecule 50: 50S ribosomal protein L29

Chain Y: 

• Molecule 51: 50S ribosomal protein L30

Chain Z: 98%

• Molecule 52: 50S ribosomal protein L32

Chain 0: 96%

• Molecule 53: 50S ribosomal protein L33

Chain 1: 94% 6%

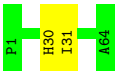
• Molecule 54: 50S ribosomal protein L34

Chain 2: 100%

There are no outlier residues recorded for this chain.

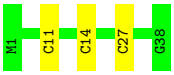
• Molecule 55: 50S ribosomal protein L35

Chain 3: 97%



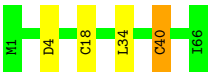
• Molecule 56: 50S ribosomal protein L36

Chain 4: 92% 8%



• Molecule 57: 50S ribosomal protein L31

Chain 6: 94% 5%



• Molecule 58: CCA 3' end of E-site tRNASec (low occupancy)

Chain w: 100%

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	159729	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	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: 5MU, GNP, CL, OMC, UR3, 1MG, 2MG, SEC, 6MZ, OMG, 4OC, MA6, 2MA, 4SU, H2U, ZN, OMU, PSU, 6IA, G7M, MG, 3TD, FME, 5MC

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	a	0.58	2/36701 (0.0%)	1.18	255/57246 (0.4%)
2	b	0.51	2/1736 (0.1%)	0.90	6/2338 (0.3%)
3	c	0.44	0/1652	0.82	4/2225 (0.2%)
4	d	0.49	0/1665	0.87	2/2227 (0.1%)
5	e	0.51	0/1170	0.88	2/1573 (0.1%)
6	f	0.56	0/836	0.87	2/1128 (0.2%)
7	g	0.48	0/1196	0.81	2/1602 (0.1%)
8	h	0.46	0/989	0.86	5/1326 (0.4%)
9	i	0.55	0/1034	0.97	4/1375 (0.3%)
10	j	0.50	0/797	0.95	1/1077 (0.1%)
11	k	0.53	0/886	0.88	2/1195 (0.2%)
12	l	0.64	2/969 (0.2%)	0.93	3/1300 (0.2%)
13	m	0.52	0/893	0.98	5/1193 (0.4%)
14	n	0.53	0/806	0.90	3/1074 (0.3%)
15	o	0.44	0/722	0.81	3/964 (0.3%)
16	p	0.49	0/659	0.77	0/884
17	q	0.60	0/658	1.07	3/881 (0.3%)
18	r	0.42	0/512	0.82	2/689 (0.3%)
19	s	0.45	0/703	0.89	2/944 (0.2%)
20	t	0.47	0/671	0.81	2/888 (0.2%)
21	u	0.53	0/501	1.06	2/668 (0.3%)
22	v	0.58	1/1745 (0.1%)	1.18	13/2716 (0.5%)
23	x	0.76	2/1145 (0.2%)	1.63	31/1781 (1.7%)
24	y	0.53	1/2168 (0.0%)	1.27	26/3375 (0.8%)
25	z	0.46	1/4952 (0.0%)	0.89	13/6712 (0.2%)
26	A	0.62	10/69240 (0.0%)	1.22	593/108014 (0.5%)
27	B	0.58	1/2873 (0.0%)	1.28	30/4478 (0.7%)
28	C	0.50	1/2122 (0.0%)	0.81	3/2852 (0.1%)
29	D	0.49	0/1586	0.81	2/2134 (0.1%)
30	E	0.47	0/1571	0.81	4/2113 (0.2%)
31	F	0.61	1/1435 (0.1%)	1.00	9/1926 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	G	0.45	0/1343	0.79	2/1816 (0.1%)
33	I	0.40	0/1046	0.73	1/1410 (0.1%)
34	H	0.41	0/1122	0.72	0/1515
35	J	0.46	0/1152	0.72	0/1551
36	K	0.53	1/948 (0.1%)	0.85	1/1268 (0.1%)
37	L	0.42	0/1054	0.78	1/1403 (0.1%)
38	M	0.44	0/1093	0.78	0/1460
39	N	0.50	0/974	0.78	1/1301 (0.1%)
40	O	0.48	0/902	0.75	1/1209 (0.1%)
41	P	0.45	0/929	0.82	3/1242 (0.2%)
42	Q	0.50	0/960	0.68	1/1278 (0.1%)
43	R	0.47	0/829	0.77	0/1107
44	S	0.46	0/864	0.80	2/1156 (0.2%)
45	T	0.45	0/745	0.73	0/994
46	U	0.52	0/788	0.90	3/1051 (0.3%)
47	V	0.47	0/766	0.71	0/1025
48	W	0.46	0/582	0.75	0/769
49	X	0.42	0/635	0.77	1/848 (0.1%)
50	Y	0.52	0/510	0.97	2/677 (0.3%)
51	Z	0.41	0/453	0.78	1/605 (0.2%)
52	0	0.51	1/450 (0.2%)	0.93	2/599 (0.3%)
53	1	0.42	0/417	0.85	1/554 (0.2%)
54	2	0.45	0/380	0.73	0/498
55	3	0.43	0/513	0.73	0/676
56	4	0.75	2/303 (0.7%)	0.93	2/397 (0.5%)
57	6	0.47	0/532	1.00	4/709 (0.6%)
58	w	0.39	0/68	0.94	0/103
All	All	0.57	28/164951 (0.0%)	1.12	1063/246119 (0.4%)

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
1	a	2	0
2	b	0	2
4	d	0	1
6	f	0	1
10	j	0	3
11	k	0	2
12	l	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	p	0	1
17	q	0	2
21	u	0	1
25	z	0	1
26	A	2	0
28	C	0	1
30	E	0	1
31	F	0	2
32	G	0	2
34	H	0	3
44	S	0	1
46	U	0	2
53	1	0	1
55	3	0	1
All	All	4	30

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	1	U	OP3-P	-10.85	1.48	1.61
24	y	1	G	OP3-P	-10.68	1.48	1.61
22	v	1	C	OP3-P	-10.68	1.48	1.61
26	A	1	G	OP3-P	-10.59	1.48	1.61
1	a	2	A	OP3-P	-10.59	1.48	1.61

The worst 5 of 1063 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	968	A	N1-C6-N6	-23.76	104.34	118.60
1	a	1158	C	N1-C2-O2	18.14	129.78	118.90
26	A	2059	A	N1-C2-N3	-17.84	120.38	129.30
1	a	1158	C	N3-C2-O2	-17.55	109.61	121.90
1	a	529	G	C5-C6-O6	-15.48	119.31	128.60

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3',C4'
26	A	2069	G7M	C3',C4'

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	b	16	GLY	Peptide
2	b	17	HIS	Mainchain
4	d	30	LYS	Mainchain
6	f	97	THR	Peptide
10	j	41	PRO	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (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	
2	b	216/218 (99%)	184 (85%)	26 (12%)	6 (3%)	5	24
3	c	204/206 (99%)	191 (94%)	12 (6%)	1 (0%)	29	61
4	d	203/205 (99%)	185 (91%)	13 (6%)	5 (2%)	5	26
5	e	155/157 (99%)	138 (89%)	12 (8%)	5 (3%)	4	22
6	f	98/100 (98%)	81 (83%)	14 (14%)	3 (3%)	4	23
7	g	149/151 (99%)	136 (91%)	11 (7%)	2 (1%)	12	39
8	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
9	i	125/127 (98%)	105 (84%)	16 (13%)	4 (3%)	4	22
10	j	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	3	18
11	k	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	17	49
12	l	121/123 (98%)	106 (88%)	12 (10%)	3 (2%)	5	26
13	m	112/114 (98%)	101 (90%)	8 (7%)	3 (3%)	5	26
14	n	98/100 (98%)	86 (88%)	9 (9%)	3 (3%)	4	23
15	o	86/88 (98%)	71 (83%)	12 (14%)	3 (4%)	3	21
16	p	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	12	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	q	78/80 (98%)	68 (87%)	7 (9%)	3 (4%)	3	19
18	r	63/65 (97%)	55 (87%)	6 (10%)	2 (3%)	4	22
19	s	84/86 (98%)	74 (88%)	5 (6%)	5 (6%)	1	10
20	t	83/85 (98%)	76 (92%)	7 (8%)	0	100	100
21	u	63/65 (97%)	51 (81%)	9 (14%)	3 (5%)	2	15
25	z	612/614 (100%)	581 (95%)	24 (4%)	7 (1%)	14	44
28	C	269/271 (99%)	247 (92%)	20 (7%)	2 (1%)	22	55
29	D	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
30	E	199/201 (99%)	186 (94%)	12 (6%)	1 (0%)	29	61
31	F	175/177 (99%)	162 (93%)	10 (6%)	3 (2%)	9	34
32	G	174/176 (99%)	159 (91%)	13 (8%)	2 (1%)	14	44
33	I	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	22	55
34	H	147/149 (99%)	129 (88%)	15 (10%)	3 (2%)	7	30
35	J	140/142 (99%)	134 (96%)	5 (4%)	1 (1%)	22	55
36	K	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	51
37	L	141/143 (99%)	128 (91%)	11 (8%)	2 (1%)	11	37
38	M	134/136 (98%)	119 (89%)	13 (10%)	2 (2%)	10	36
39	N	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
40	O	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
41	P	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
42	Q	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
43	R	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	15	46
44	S	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	17	49
45	T	91/93 (98%)	80 (88%)	11 (12%)	0	100	100
46	U	100/102 (98%)	88 (88%)	10 (10%)	2 (2%)	7	30
47	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
48	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
49	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
50	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	9	34
51	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
52	0	54/56 (96%)	48 (89%)	5 (9%)	1 (2%)	8	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	1	48/50 (96%)	46 (96%)	1 (2%)	1 (2%)	7	30
54	2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
55	3	62/64 (97%)	55 (89%)	6 (10%)	1 (2%)	9	34
56	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
57	6	64/66 (97%)	55 (86%)	8 (12%)	1 (2%)	9	34
All	All	6336/6438 (98%)	5763 (91%)	482 (8%)	91 (1%)	15	37

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
2	b	73	ARG
5	e	93	VAL
6	f	94	HIS
6	f	98	GLU

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	
2	b	180/180 (100%)	179 (99%)	1 (1%)	86	94
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	170 (99%)	2 (1%)	71	85
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	86 (99%)	1 (1%)	73	86
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	102 (98%)	2 (2%)	57	78
9	i	105/105 (100%)	104 (99%)	1 (1%)	76	88
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	88 (99%)	1 (1%)	73	86
12	l	103/103 (100%)	102 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	m	92/92 (100%)	91 (99%)	1 (1%)	73	86
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	74/74 (100%)	73 (99%)	1 (1%)	67	83
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	74/74 (100%)	74 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	43 (98%)	1 (2%)	50	74
25	z	501/501 (100%)	498 (99%)	3 (1%)	86	94
28	C	216/216 (100%)	215 (100%)	1 (0%)	88	94
29	D	164/164 (100%)	163 (99%)	1 (1%)	86	94
30	E	165/165 (100%)	165 (100%)	0	100	100
31	F	148/148 (100%)	147 (99%)	1 (1%)	84	92
32	G	137/137 (100%)	136 (99%)	1 (1%)	84	92
33	I	109/109 (100%)	109 (100%)	0	100	100
34	H	114/114 (100%)	114 (100%)	0	100	100
35	J	116/116 (100%)	116 (100%)	0	100	100
36	K	103/103 (100%)	102 (99%)	1 (1%)	76	88
37	L	102/102 (100%)	101 (99%)	1 (1%)	76	88
38	M	109/109 (100%)	109 (100%)	0	100	100
39	N	100/100 (100%)	98 (98%)	2 (2%)	55	77
40	O	86/86 (100%)	86 (100%)	0	100	100
41	P	99/99 (100%)	99 (100%)	0	100	100
42	Q	89/89 (100%)	89 (100%)	0	100	100
43	R	84/84 (100%)	84 (100%)	0	100	100
44	S	93/93 (100%)	93 (100%)	0	100	100
45	T	80/80 (100%)	79 (99%)	1 (1%)	69	84
46	U	83/83 (100%)	81 (98%)	2 (2%)	49	74
47	V	78/78 (100%)	78 (100%)	0	100	100
48	W	57/57 (100%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	X	67/67 (100%)	67 (100%)	0	100	100
50	Y	55/55 (100%)	54 (98%)	1 (2%)	59	79
51	Z	48/48 (100%)	48 (100%)	0	100	100
52	0	47/47 (100%)	47 (100%)	0	100	100
53	1	45/45 (100%)	45 (100%)	0	100	100
54	2	38/38 (100%)	38 (100%)	0	100	100
55	3	51/51 (100%)	51 (100%)	0	100	100
56	4	34/34 (100%)	34 (100%)	0	100	100
57	6	59/59 (100%)	59 (100%)	0	100	100
All	All	5233/5256 (100%)	5206 (100%)	27 (0%)	89	94

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	z	344	ARG
31	F	103	ILE
46	U	40	LEU
29	D	128	ARG
32	G	72	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
25	z	491	GLN
32	G	138	GLN
25	z	532	GLN
30	E	46	GLN
44	S	7	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	187 (12%)	0
22	v	76/77 (98%)	8 (10%)	0
23	x	47/48 (97%)	23 (48%)	0
24	y	93/95 (97%)	12 (12%)	0
26	A	2898/2903 (99%)	411 (14%)	8 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	B	119/120 (99%)	17 (14%)	0
58	w	2/3 (66%)	0	0
All	All	4770/4785 (99%)	658 (13%)	8 (0%)

5 of 658 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	7	A
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	2430	A
26	A	2250	G
26	A	1536	C
26	A	960	A
26	A	2211	A

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

43 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	4SU	v	8	22	18,21,22	1.73	4 (22%)	26,30,33	2.69	6 (23%)
26	5MU	A	1939	26	19,22,23	1.35	4 (21%)	28,32,35	2.30	6 (21%)
1	5MC	a	967	1	18,22,23	0.94	1 (5%)	26,32,35	1.14	2 (7%)
26	PSU	A	2604	26	18,21,22	1.43	3 (16%)	22,30,33	1.90	4 (18%)
26	PSU	A	1917	26	18,21,22	1.48	5 (27%)	22,30,33	1.95	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	H2U	A	2449	26	18,21,22	1.24	3 (16%)	21,30,33	2.25	1 (4%)
1	5MC	a	1407	1	18,22,23	0.85	2 (11%)	26,32,35	1.17	3 (11%)
24	PSU	y	55	24	18,21,22	1.47	3 (16%)	22,30,33	1.98	4 (18%)
1	PSU	a	516	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	5 (22%)
26	1MG	A	745	26	18,26,27	0.88	1 (5%)	19,39,42	1.06	2 (10%)
1	2MG	a	1516	1	18,26,27	0.94	1 (5%)	16,38,41	1.22	2 (12%)
1	2MG	a	966	1	18,26,27	1.05	1 (5%)	16,38,41	1.10	2 (12%)
26	OMG	A	2251	22,26	18,26,27	0.99	1 (5%)	19,38,41	1.14	2 (10%)
26	OMU	A	2552	26	19,22,23	1.23	2 (10%)	26,31,34	1.93	7 (26%)
26	PSU	A	2605	26	18,21,22	1.34	3 (16%)	22,30,33	1.88	4 (18%)
1	MA6	a	1518	1	18,26,27	0.93	1 (5%)	19,38,41	2.04	5 (26%)
26	PSU	A	955	26	18,21,22	1.49	4 (22%)	22,30,33	1.90	3 (13%)
26	PSU	A	1911	26	18,21,22	1.46	4 (22%)	22,30,33	2.05	4 (18%)
26	2MA	A	2503	26	17,25,26	1.04	1 (5%)	17,37,40	0.95	1 (5%)
26	PSU	A	2504	26	18,21,22	1.51	3 (16%)	22,30,33	1.85	4 (18%)
24	6IA	y	37	24	22,29,30	0.78	1 (4%)	22,41,44	1.69	3 (13%)
26	6MZ	A	1618	26	18,25,26	0.96	1 (5%)	16,36,39	2.28	4 (25%)
26	PSU	A	2457	26	18,21,22	1.47	3 (16%)	22,30,33	2.03	4 (18%)
26	G7M	A	2069	26	20,26,27	1.54	3 (15%)	17,39,42	1.60	4 (23%)
22	H2U	v	20	22	18,21,22	1.02	2 (11%)	21,30,33	1.91	2 (9%)
26	2MG	A	1835	26	18,26,27	0.93	1 (5%)	16,38,41	1.22	3 (18%)
22	5MU	v	54	22	19,22,23	1.48	6 (31%)	28,32,35	2.13	9 (32%)
26	3TD	A	1915	26	18,22,23	4.03	7 (38%)	22,32,35	1.87	3 (13%)
26	5MC	A	1962	26	18,22,23	1.03	2 (11%)	26,32,35	1.70	5 (19%)
24	H2U	y	19	24	18,21,22	1.03	2 (11%)	21,30,33	1.76	3 (14%)
26	PSU	A	2580	26	18,21,22	1.40	4 (22%)	22,30,33	1.95	4 (18%)
1	G7M	a	527	1	20,26,27	1.55	3 (15%)	17,39,42	1.62	3 (17%)
26	5MU	A	747	26	19,22,23	1.47	5 (26%)	28,32,35	2.03	7 (25%)
26	6MZ	A	2030	26	18,25,26	1.01	1 (5%)	16,36,39	1.91	4 (25%)
22	PSU	v	55	22	18,21,22	1.44	3 (16%)	22,30,33	1.87	4 (18%)
24	5MU	y	54	24	19,22,23	1.43	6 (31%)	28,32,35	1.92	7 (25%)
26	OMC	A	2498	26	19,22,23	0.88	0	26,31,34	1.22	3 (11%)
26	PSU	A	746	26	18,21,22	1.42	3 (16%)	22,30,33	1.85	4 (18%)
1	2MG	a	1207	1	18,26,27	1.03	1 (5%)	16,38,41	1.14	2 (12%)
1	MA6	a	1519	1	18,26,27	0.93	1 (5%)	19,38,41	1.73	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	2MG	A	2445	26	18,26,27	1.07	1 (5%)	16,38,41	1.26	3 (18%)
1	UR3	a	1498	1	19,22,23	0.95	1 (5%)	26,32,35	1.81	5 (19%)
1	4OC	a	1402	1	20,23,24	0.77	0	26,32,35	1.41	4 (15%)

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
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
26	PSU	A	1917	26	-	3/7/25/26	0/2/2/2
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
24	PSU	y	55	24	-	0/7/25/26	0/2/2/2
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
26	1MG	A	745	26	-	0/3/25/26	0/3/3/3
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	2MG	a	966	1	-	2/5/27/28	0/3/3/3
26	OMG	A	2251	22,26	-	1/5/27/28	0/3/3/3
26	OMU	A	2552	26	-	2/9/27/28	0/2/2/2
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	2/7/29/30	0/3/3/3
26	PSU	A	955	26	-	0/7/25/26	0/2/2/2
26	PSU	A	1911	26	-	2/7/25/26	0/2/2/2
26	2MA	A	2503	26	-	1/3/25/26	0/3/3/3
26	PSU	A	2504	26	-	2/7/25/26	0/2/2/2
24	6IA	y	37	24	-	3/9/31/32	0/3/3/3
26	6MZ	A	1618	26	-	2/5/27/28	0/3/3/3
26	PSU	A	2457	26	-	2/7/25/26	0/2/2/2
26	G7M	A	2069	26	2/2/5/5	2/3/25/26	0/3/3/3
22	H2U	v	20	22	-	1/7/38/39	0/2/2/2
26	2MG	A	1835	26	-	0/5/27/28	0/3/3/3
22	5MU	v	54	22	-	3/7/25/26	0/2/2/2
26	3TD	A	1915	26	-	4/7/25/26	0/2/2/2
26	5MC	A	1962	26	-	5/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	y	19	24	-	4/7/38/39	0/2/2/2
26	PSU	A	2580	26	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	1/3/25/26	0/3/3/3
26	5MU	A	747	26	-	0/7/25/26	0/2/2/2
26	6MZ	A	2030	26	-	3/5/27/28	0/3/3/3
22	PSU	v	55	22	-	2/7/25/26	0/2/2/2
24	5MU	y	54	24	-	0/7/25/26	0/2/2/2
26	OMC	A	2498	26	-	0/9/27/28	0/2/2/2
26	PSU	A	746	26	-	2/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1519	1	-	3/7/29/30	0/3/3/3
26	2MG	A	2445	26	-	2/5/27/28	0/3/3/3
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	4/9/29/30	0/2/2/2

The worst 5 of 106 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1915	3TD	C6-C5	11.98	1.49	1.35
26	A	1915	3TD	C2-N1	8.84	1.48	1.37
26	A	1915	3TD	C6-N1	5.60	1.45	1.36
22	v	8	4SU	C4-S4	-4.56	1.59	1.68
26	A	2069	G7M	C5-C4	4.25	1.47	1.39

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2449	H2U	C4-N3-C2	-9.42	117.98	125.79
22	v	20	H2U	C4-N3-C2	-7.55	119.53	125.79
22	v	8	4SU	C4-N3-C2	-7.47	120.09	127.34
22	v	8	4SU	C5-C4-S4	-6.78	115.74	124.47
26	A	2457	PSU	N1-C2-N3	6.66	122.68	115.13

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3'
1	a	527	G7M	C4'
26	A	2069	G7M	C3'
26	A	2069	G7M	C4'

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	966	2MG	N1-C2-N2-CM2
1	a	966	2MG	N3-C2-N2-CM2
1	a	1402	4OC	O4'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C1'-N1-C2
1	a	1518	MA6	C5-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 153 ligands modelled in this entry, 150 are 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	$\#\|Z\| > 2$
63	GNP	z	701	60	29,34,34	1.50	4 (13%)	33,54,54	2.08	10 (30%)
62	SEC	y	701	24	2,5,6	0.72	0	0,5,7	-	-
61	FME	v	101	22	8,9,10	0.93	0	7,9,11	1.47	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
63	GNP	z	701	60	-	5/14/38/38	0/3/3/3
62	SEC	y	701	24	-	0/0/4/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	FME	v	101	22	-	4/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	701	GNP	PB-N3B	3.83	1.73	1.63
63	z	701	GNP	C5-C6	3.81	1.47	1.41
63	z	701	GNP	PG-N3B	3.51	1.72	1.63
63	z	701	GNP	C5-C4	2.48	1.47	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	z	701	GNP	PB-O3A-PA	-5.05	114.82	132.62
63	z	701	GNP	C2-N3-C4	4.57	120.58	115.36
63	z	701	GNP	C5-C6-N1	-4.15	117.76	123.43
63	z	701	GNP	C2-N1-C6	3.99	122.26	115.93
63	z	701	GNP	C4-C5-C6	-3.27	117.68	120.80

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	v	101	FME	O1-CN-N-CA
61	v	101	FME	C-CA-CB-CG
63	z	701	GNP	PB-N3B-PG-O1G
63	z	701	GNP	PG-N3B-PB-O1B
63	z	701	GNP	C5'-O5'-PA-O3A

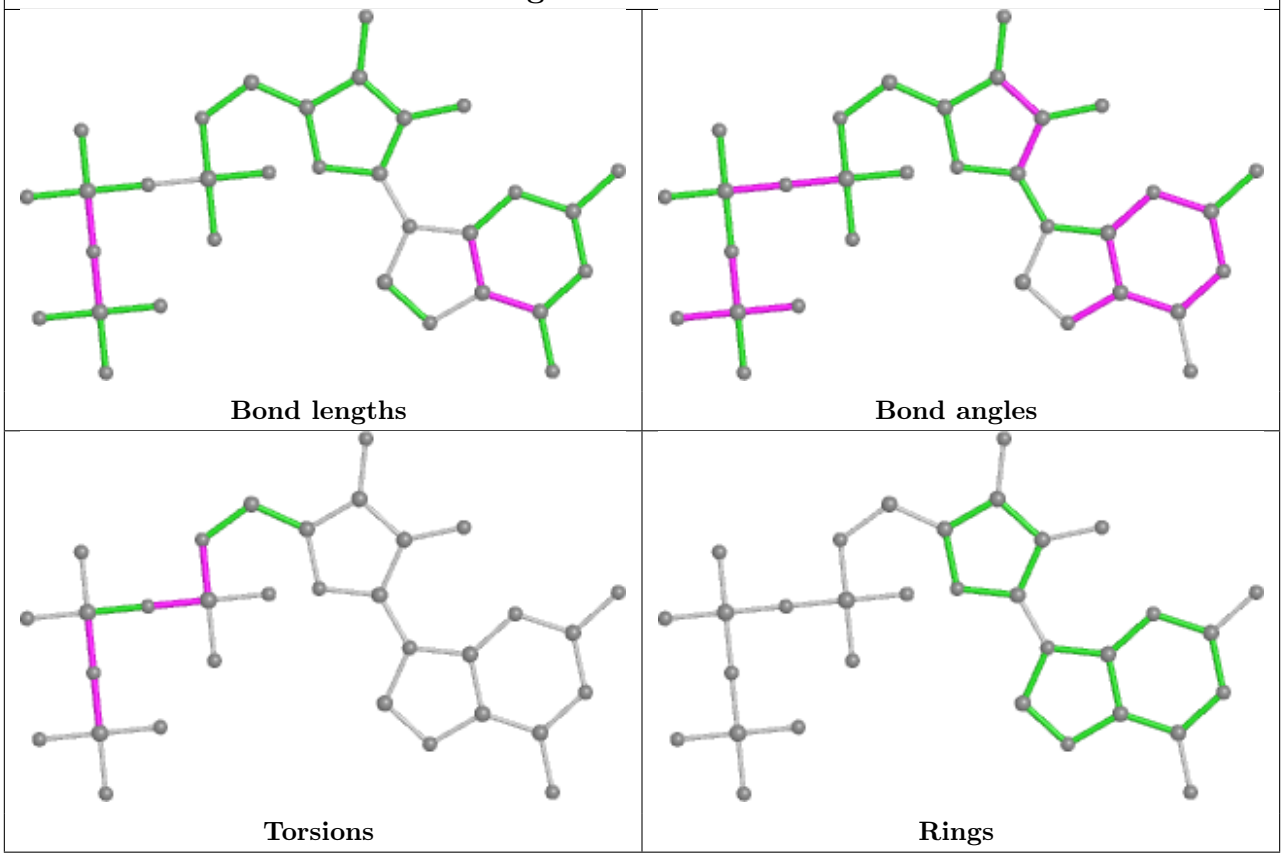
There are no ring outliers.

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 GNP z 701



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-4124. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

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

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

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)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit (i)

This section was not generated.