wwPDB EM Validation Summary Report (i)

Mar 15, 2025 – 06:36 pm GMT

PDB ID	:	9GHC
EMDB ID	:	EMD-51352
Title	:	Pre-release fusidic acid-locked Escherichia coli 70S ribosome with Staphylococcus aureus EF-G and FusB (FusB-EF-G-70S)
Authors	:	Gonzalez-Lopez, A.; Selmer, M.
Deposited on	:	2024-08-15
Resolution	:	2.79 Å(reported)
Based on initial models	:	9GHE, 8P2H

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:

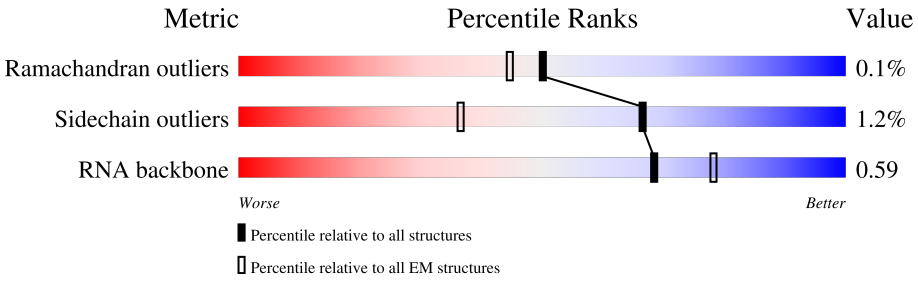
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 2.79 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	0	55	91% 9%
2	1	46	98% .
3	2	65	97% . .
4	3	38	100%
5	4	70	83% . 14%
6	9	24	25% 17% 58%
7	A	1554	83% 15% .
8	B	241	90% . 8%
9	C	233	88% . 12%

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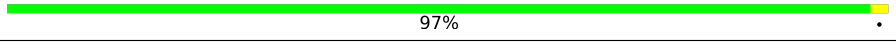
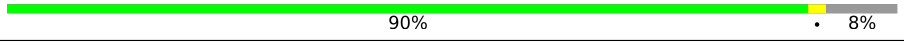
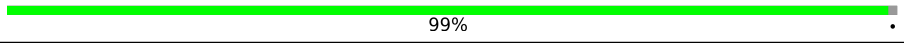
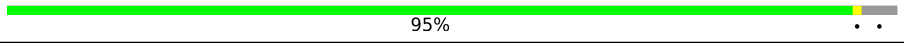
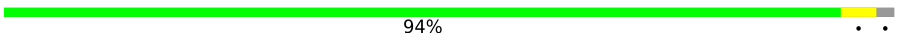
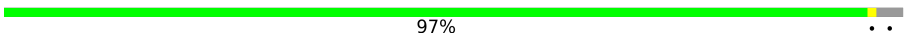
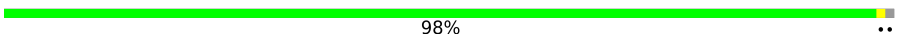
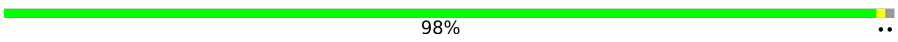
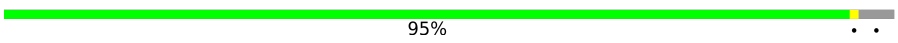
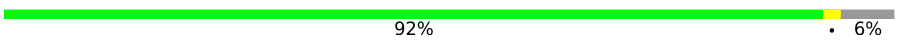
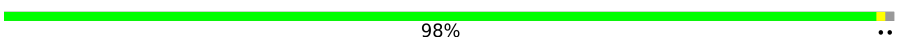
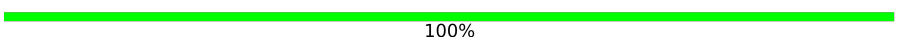
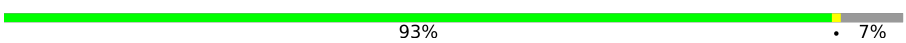
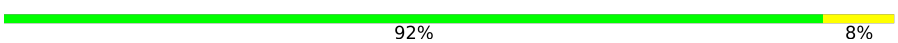
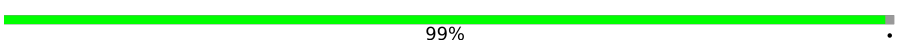
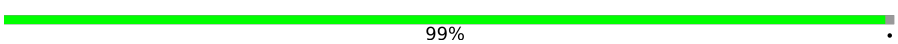
Mol	Chain	Length	Quality of chain
10	D	206	
11	E	167	
12	F	135	
13	G	179	
14	H	130	
15	I	130	
16	J	103	
17	K	129	
18	L	124	
19	M	118	
20	N	101	
21	O	89	
22	P	82	
23	Q	84	
24	R	75	
25	S	92	
26	T	87	
27	U	71	
28	V	213	
29	W	693	
30	Z	77	
31	a	2930	
32	b	119	
33	c	273	
34	d	209	

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Mol	Chain	Length	Quality of chain
35	e	201	100%
36	f	179	97%
37	g	177	93% 5%
38	h	149	28% 72%
39	i	142	99%
40	j	123	100%
41	k	144	99%
42	l	136	99%
43	m	127	93% 7%
44	n	117	96%
45	o	115	97%
46	p	118	98%
47	q	103	98%
48	r	110	98%
49	s	100	89% 7%
50	t	104	88% 11%
51	u	94	97%
52	v	85	87% 12%
53	w	78	99%
54	x	63	95% 5%
55	y	59	98%
56	z	57	95% 5%

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 147172 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 L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	50	Total	C	N	O	0	0
			413	267	75	71		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	10	Total	C	N	O	P	0	0
			218	98	45	65	10		

- Molecule 7 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1514	Total	C	N	O	P	0	0
			32500	14503	5963	10520	1514		

- Molecule 8 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	222	Total	C	N	O	S	0	0
			1737	1099	312	318	8		

- Molecule 9 is a protein called 30S ribosomal protein S3.

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

- Molecule 10 is a protein called 30S ribosomal protein S4.

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

- Molecule 11 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	154	Total	C	N	O	S	0	0
			1135	706	215	208	6		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	150	Total	C	N	O	S	0	0
			1176	732	226	214	4		

- Molecule 14 is a protein called 30S ribosomal protein S8.

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

- Molecule 15 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	125	Total	C	N	O	S	0	0
			1001	622	200	176	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	96	Total	C	N	O	S	0	0
			775	487	148	139	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 18 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 19 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 20 is a protein called 30S ribosomal protein S14.

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

- Molecule 21 is a protein called 30S ribosomal protein S15.

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

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	79	Total	C	N	O	S	0	0
			629	394	124	110	1		

- Molecule 23 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 24 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	64	Total	C	N	O	S	0	0
			524	330	99	94	1		

- Molecule 25 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 26 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 28 is a protein called Far1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	213	Total	C	N	O	S	0	0
			1773	1143	291	331	8		

- Molecule 29 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	647	Total	C	N	O	S	0	0
			5020	3156	833	1003	28		

- Molecule 30 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	2782	Total	C	N	O	P	0	0
			59756	26665	11017	19292	2782		

- Molecule 32 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 33 is a protein called 50S ribosomal protein L2.

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

- Molecule 34 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1552	972	286	291	3		

- Molecule 35 is a protein called 50S ribosomal protein L4.

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	168	Total	C	N	O	S	0	0
			1255	791	228	234	2		

- Molecule 38 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 39 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	141	Total	C	N	O	S	0	0
			1121	709	211	198	3		

- Molecule 40 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 41 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	modified residue	UNP P0ADY7

- Molecule 43 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

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

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	t	93	Total	C	N	O	0	0
			717	452	135	130		

- Molecule 51 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

- Molecule 52 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 53 is a protein called 50S ribosomal protein L28.

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

- Molecule 54 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 55 is a protein called 50S ribosomal protein L30.

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

- Molecule 56 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	
57	V	1	Total	Zn	0
			1	1	

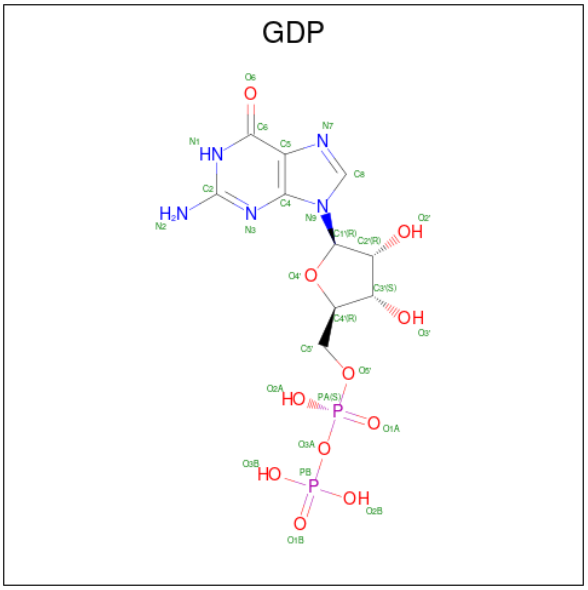
- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	A	29	Total	K	0
			29	29	
58	F	1	Total	K	0
			1	1	
58	a	76	Total	K	0
			76	76	
58	c	2	Total	K	0
			2	2	
58	e	1	Total	K	0
			1	1	

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

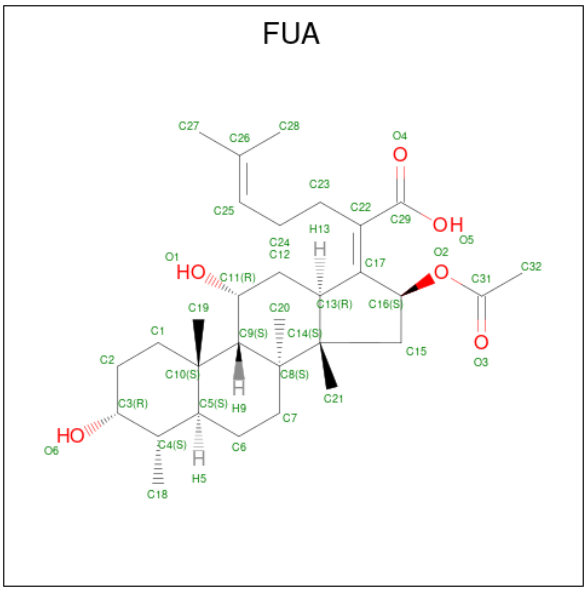
Mol	Chain	Residues	Atoms	AltConf
59	A	55	Total Mg 55 55	0
59	W	1	Total Mg 1 1	0
59	a	236	Total Mg 236 236	0
59	b	3	Total Mg 3 3	0
59	c	3	Total Mg 3 3	0
59	m	1	Total Mg 1 1	0
59	p	1	Total Mg 1 1	0
59	z	1	Total Mg 1 1	0

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 61 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by depositor).



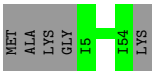
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
61	W	1	37	31	6	0

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.

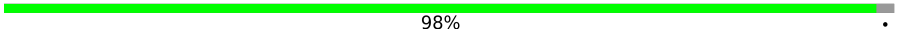
- Molecule 1: 50S ribosomal protein L33

Chain 0:



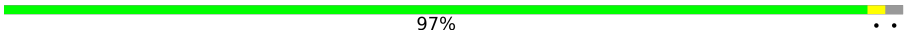
- Molecule 2: 50S ribosomal protein L34

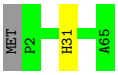
Chain 1:



- Molecule 3: 50S ribosomal protein L35

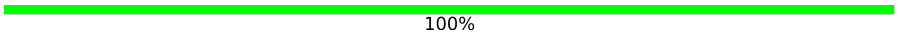
Chain 2:





- Molecule 4: 50S ribosomal protein L36

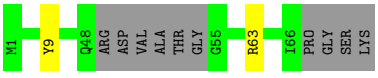
Chain 3:



There are no outlier residues recorded for this chain.

- Molecule 5: 50S ribosomal protein L31

Chain 4:

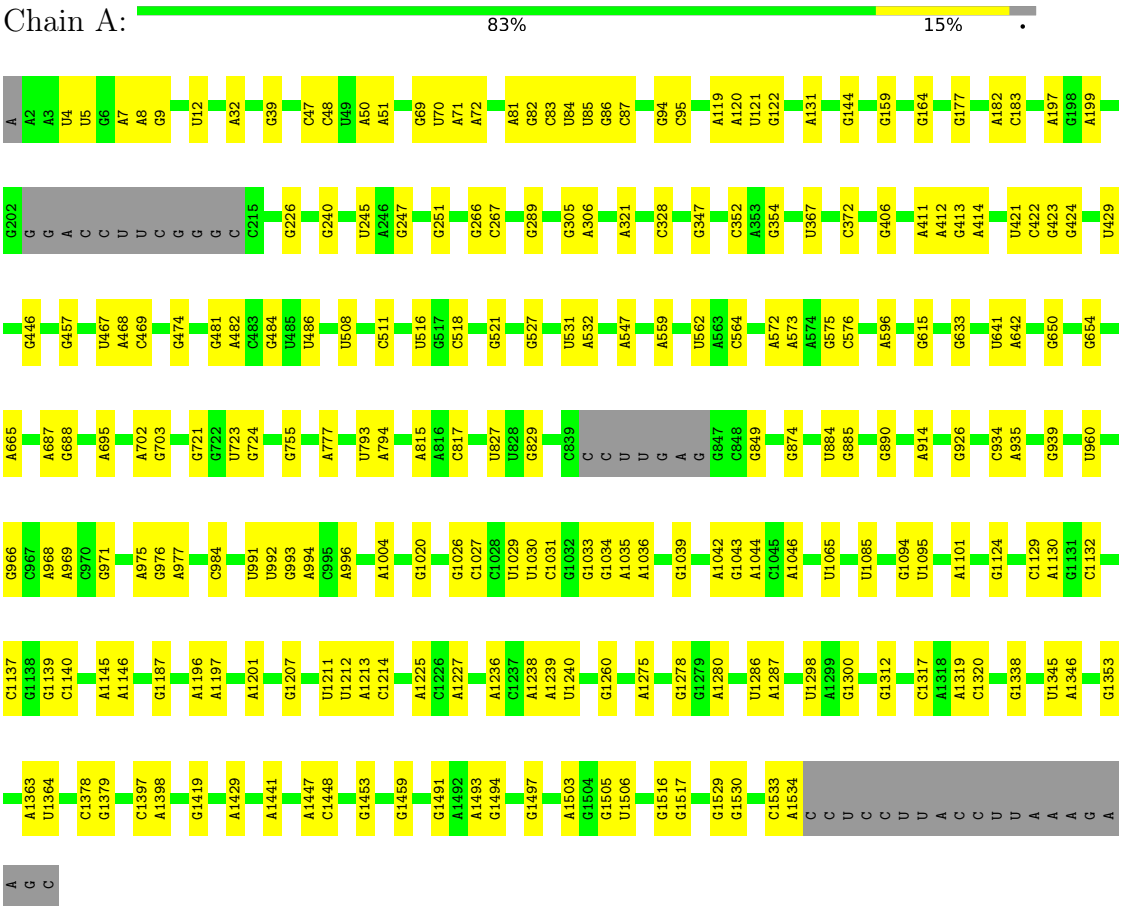


- Molecule 6: mRNA

Chain 9:

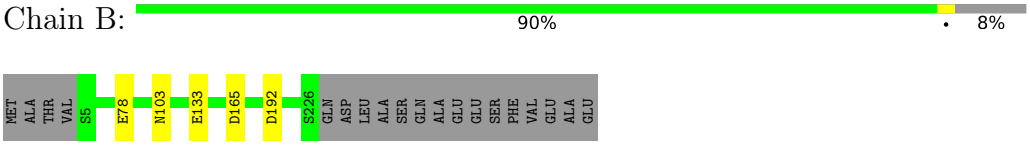
• Molecule 7: 16S rRNA

Chain A:



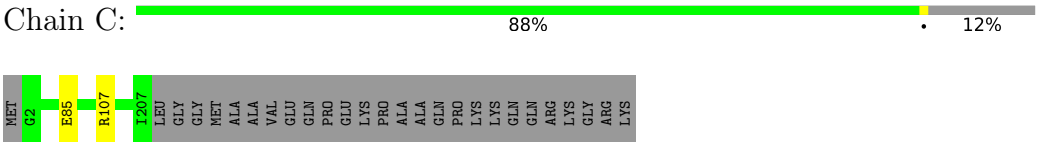
• Molecule 8: 30S ribosomal protein S2

Chain B:



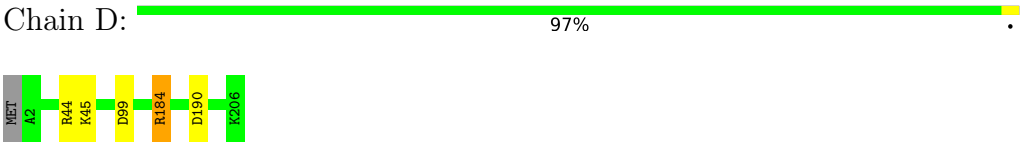
• Molecule 9: 30S ribosomal protein S3

Chain C:



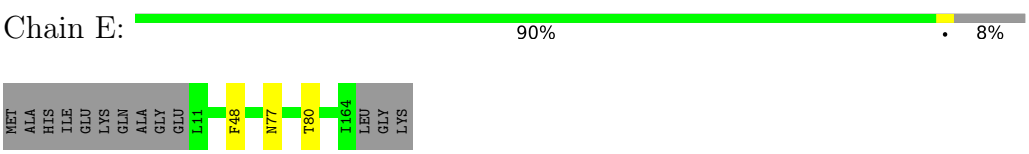
• Molecule 10: 30S ribosomal protein S4

Chain D:



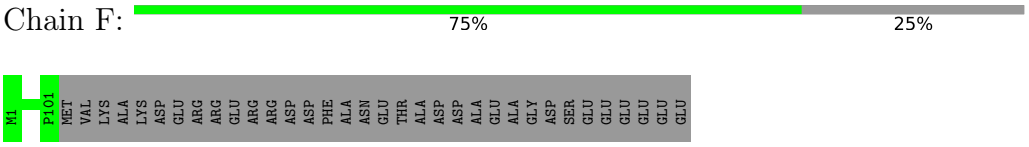
• Molecule 11: 30S ribosomal protein S5

Chain E:



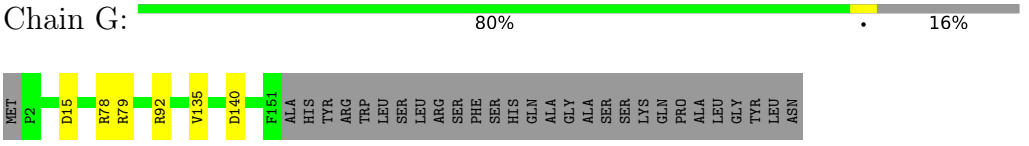
• Molecule 12: 30S ribosomal protein S6

Chain F:



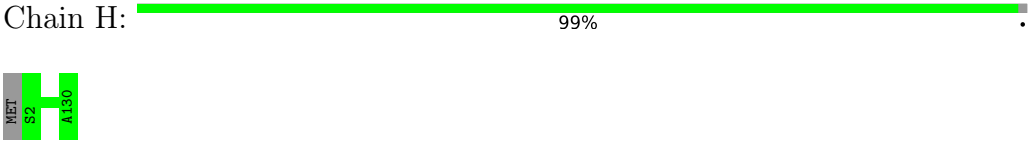
• Molecule 13: 30S ribosomal protein S7

Chain G:



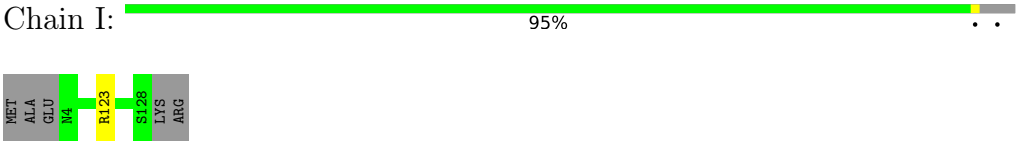
• Molecule 14: 30S ribosomal protein S8

Chain H:



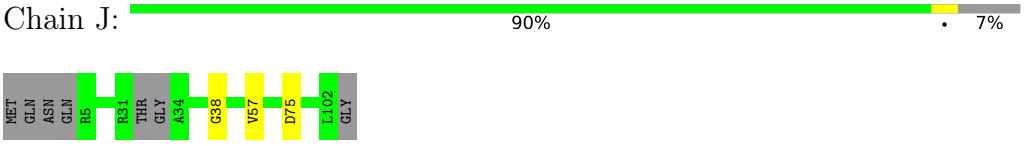
• Molecule 15: 30S ribosomal protein S9

Chain I:



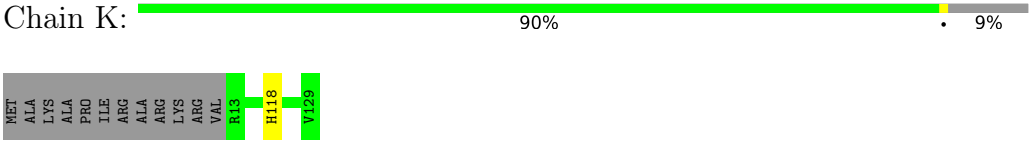
• Molecule 16: 30S ribosomal protein S10

Chain J:



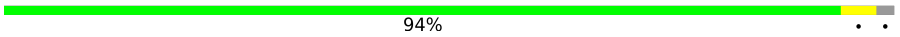
• Molecule 17: Small ribosomal subunit protein uS11

Chain K:



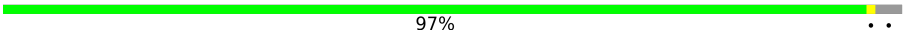
• Molecule 18: 30S ribosomal protein S12

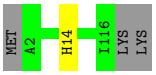
Chain L:



• Molecule 19: 30S ribosomal protein S13

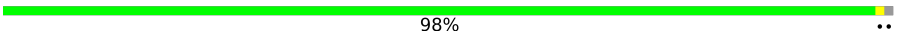
Chain M:

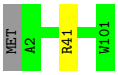




• Molecule 20: 30S ribosomal protein S14

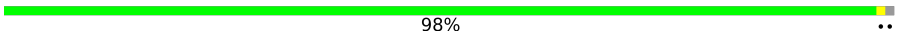
Chain N:





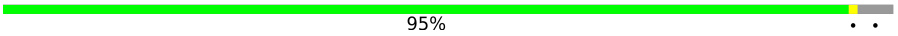
• Molecule 21: 30S ribosomal protein S15

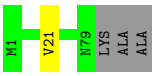
Chain O:



• Molecule 22: 30S ribosomal protein S16

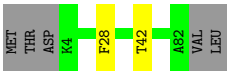
Chain P:





• Molecule 23: 30S ribosomal protein S17

Chain Q:

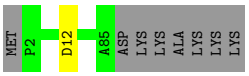


• Molecule 24: 30S ribosomal protein S18

Chain R:

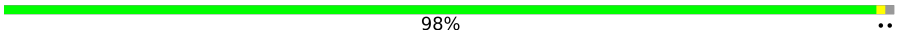
• Molecule 25: 30S ribosomal protein S19

Chain S:



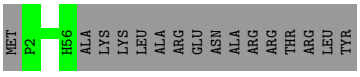
• Molecule 26: 30S ribosomal protein S20

Chain T:



• Molecule 27: 30S ribosomal protein S21

Chain U:

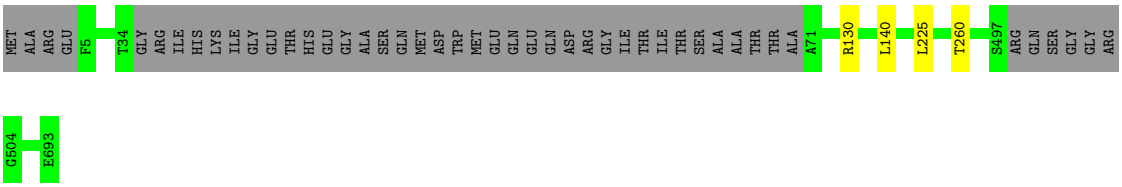


• Molecule 28: Far1

Chain V:

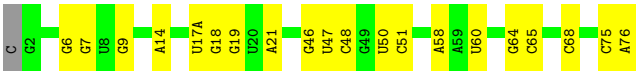
• Molecule 29: Elongation factor G

Chain W:



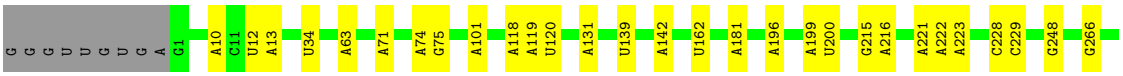
• Molecule 30: tRNA

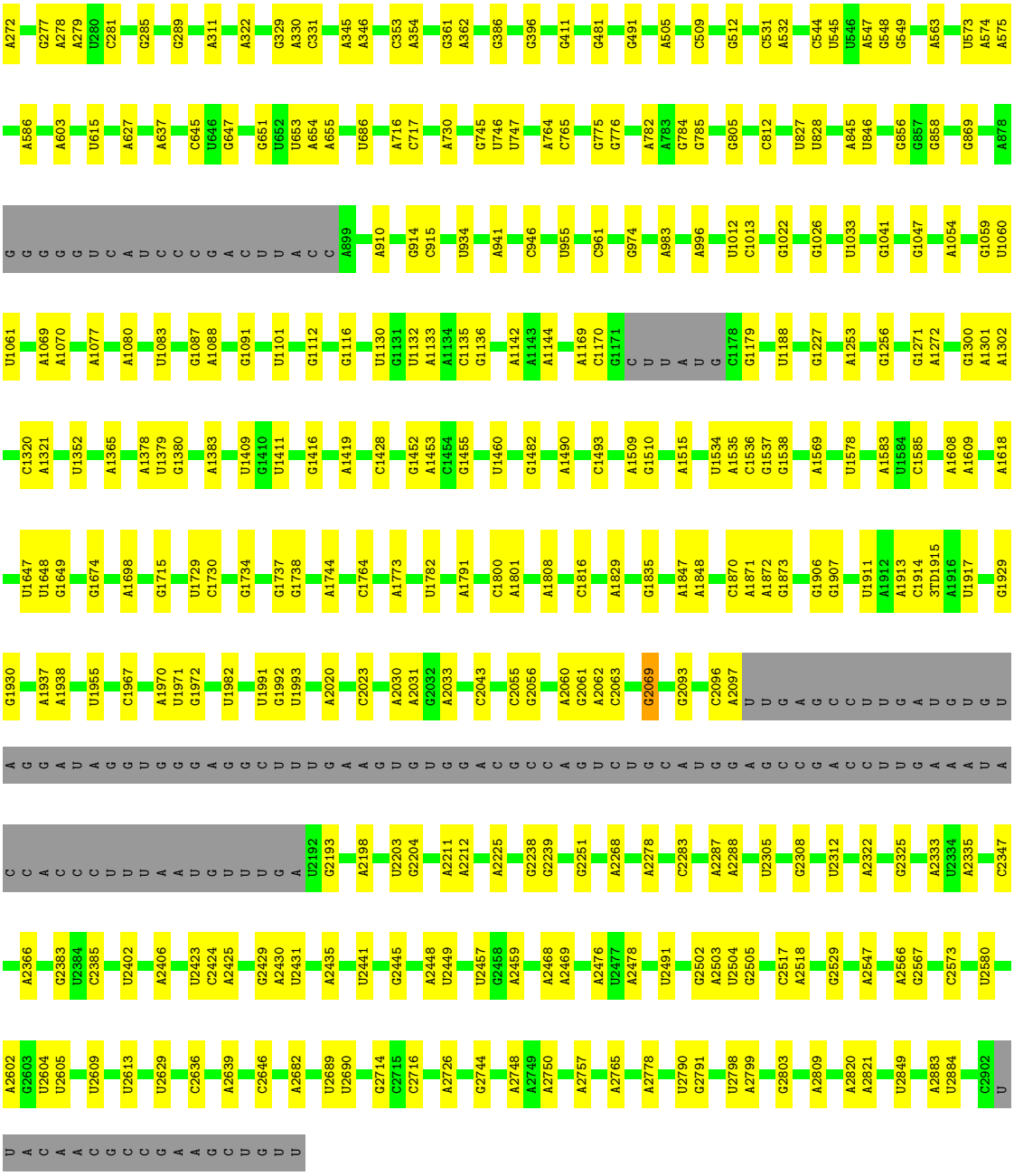
Chain Z:



• Molecule 31: 23S rRNA

Chain a:



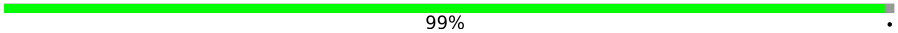


• Molecule 32: 5S rRNA

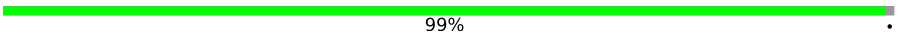
Chain b:

• Molecule 33: 50S ribosomal protein L2

Chain c:



• Molecule 34: 50S ribosomal protein L3

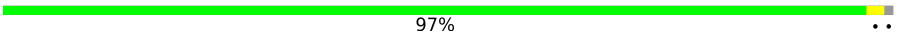
Chain d: 

• Molecule 35: 50S ribosomal protein L4

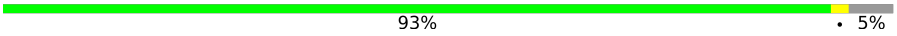
Chain e: 

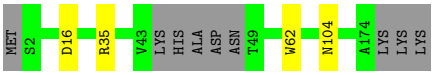
There are no outlier residues recorded for this chain.

• Molecule 36: 50S ribosomal protein L5

Chain f: 

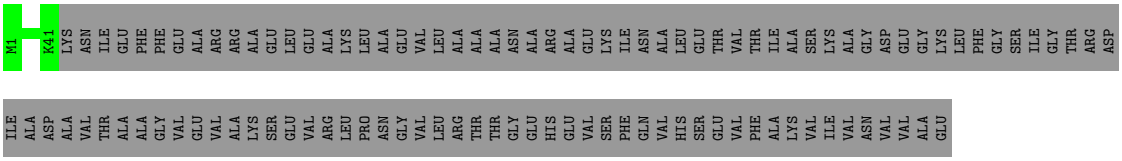
• Molecule 37: 50S ribosomal protein L6

Chain g: 

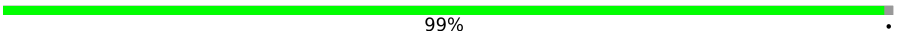


• Molecule 38: 50S ribosomal protein L9

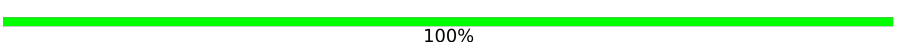
Chain h: 



• Molecule 39: 50S ribosomal protein L13

Chain i: 

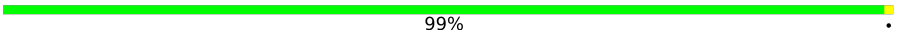
• Molecule 40: 50S ribosomal protein L14

Chain j: 

There are no outlier residues recorded for this chain.

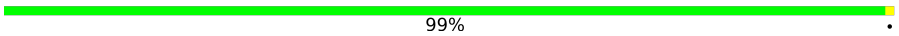
• Molecule 41: Large ribosomal subunit protein uL15

Chain k:



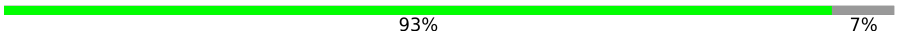
• Molecule 42: 50S ribosomal protein L16

Chain l:



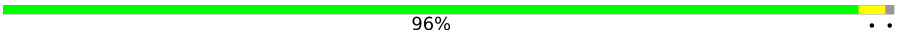
• Molecule 43: 50S ribosomal protein L17

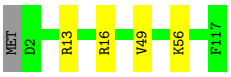
Chain m:



• Molecule 44: 50S ribosomal protein L18

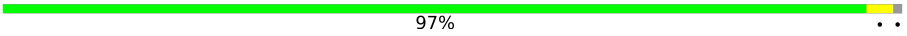
Chain n:





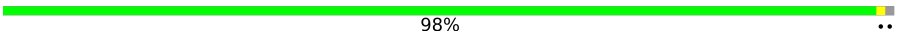
• Molecule 45: 50S ribosomal protein L19

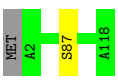
Chain o:



• Molecule 46: 50S ribosomal protein L20

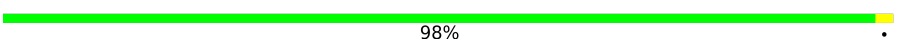
Chain p:





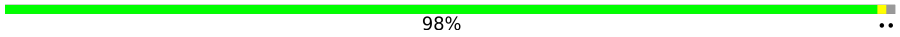
• Molecule 47: 50S ribosomal protein L21

Chain q:



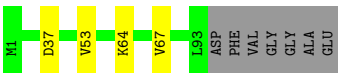
• Molecule 48: 50S ribosomal protein L22

Chain r:



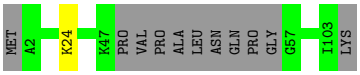
• Molecule 49: 50S ribosomal protein L23

Chain s:



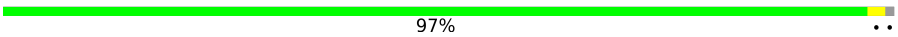
• Molecule 50: 50S ribosomal protein L24

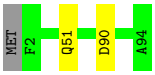
Chain t:



• Molecule 51: 50S ribosomal protein L25

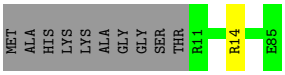
Chain u:





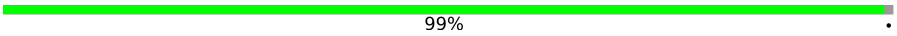
• Molecule 52: 50S ribosomal protein L27

Chain v:



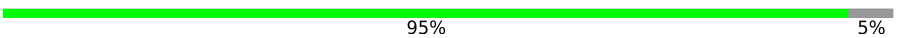
• Molecule 53: 50S ribosomal protein L28

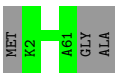
Chain w:



• Molecule 54: Large ribosomal subunit protein uL29

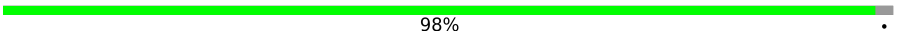
Chain x:





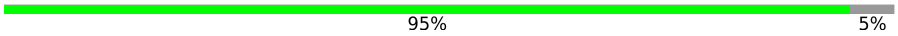
• Molecule 55: 50S ribosomal protein L30

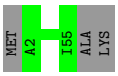
Chain y:



• Molecule 56: 50S ribosomal protein L32

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34617	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k 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: H2U, 4OC, MS6, 3TD, G7M, ZN, 4D4, D2T, MA6, 5MC, IAS, PSU, K, 5MU, 2MA, OMC, 2MG, OMG, MG, OMU, 1MG, 6MZ, GDP, MEQ, UR3, FUA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	0	0.31	0/420	0.56	0/560
2	1	0.30	0/370	0.61	0/487
3	2	0.33	0/513	0.55	0/676
4	3	0.29	0/303	0.58	0/397
5	4	0.32	0/488	0.56	0/649
6	9	0.47	0/245	0.91	0/380
7	A	0.43	0/36110	0.89	0/56322
8	B	0.29	0/1768	0.54	0/2381
9	C	0.28	0/1651	0.54	0/2225
10	D	0.29	0/1665	0.55	0/2227
11	E	0.29	0/1148	0.54	0/1545
12	F	0.28	0/843	0.51	0/1140
13	G	0.29	0/1190	0.54	0/1595
14	H	0.29	0/989	0.55	0/1326
15	I	0.29	0/1013	0.57	0/1350
16	J	0.28	0/784	0.60	0/1059
17	K	0.30	0/884	0.53	0/1191
18	L	0.29	0/945	0.60	0/1268
19	M	0.29	0/900	0.54	0/1204
20	N	0.30	0/817	0.53	0/1088
21	O	0.29	0/722	0.51	0/964
22	P	0.28	0/639	0.57	0/859
23	Q	0.28	0/650	0.54	0/871
24	R	0.28	0/532	0.53	0/715
25	S	0.32	0/685	0.55	0/922
26	T	0.28	0/676	0.49	0/895
27	U	0.31	0/467	0.58	0/620
28	V	0.29	0/1806	0.48	0/2426
29	W	0.29	0/5109	0.48	0/6910
30	Z	0.47	0/1813	0.89	0/2825
31	a	0.42	0/66355	0.88	1/103511 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	b	0.44	0/2850	0.88	0/4444
33	c	0.29	0/2121	0.56	0/2852
34	d	0.29	0/1562	0.53	0/2102
35	e	0.29	0/1571	0.52	0/2113
36	f	0.29	0/1434	0.53	0/1926
37	g	0.29	0/1273	0.54	0/1725
38	h	0.30	0/306	0.55	0/413
39	i	0.28	0/1144	0.53	0/1541
40	j	0.29	0/955	0.55	0/1279
41	k	0.31	0/1062	0.55	0/1413
42	l	0.29	0/1073	0.54	0/1433
43	m	0.28	0/958	0.54	0/1281
44	n	0.29	0/902	0.55	0/1209
45	o	0.29	0/929	0.54	0/1242
46	p	0.29	0/960	0.56	0/1278
47	q	0.30	0/829	0.55	0/1107
48	r	0.28	0/852	0.55	0/1142
49	s	0.27	0/744	0.53	0/994
50	t	0.30	0/721	0.54	0/956
51	u	0.29	0/758	0.55	0/1015
52	v	0.32	0/576	0.54	0/762
53	w	0.30	0/635	0.54	0/848
54	x	0.27	0/492	0.49	0/655
55	y	0.29	0/453	0.51	0/605
56	z	0.30	0/435	0.56	0/581
All	All	0.39	0/158095	0.80	1/235504 (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
10	D	0	1
13	G	0	1
16	J	0	1
17	K	0	1
26	T	0	1
29	W	0	1
36	f	0	1
37	g	0	1
44	n	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
52	v	0	1
All	All	0	10

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	512	G	O4'-C1'-N9	5.04	112.23	108.20

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	D	184	ARG	Sidechain
13	G	79	ARG	Sidechain
16	J	38	GLY	Peptide
17	K	118	HIS	Peptide
26	T	24	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	48/55 (87%)	48 (100%)	0	0	100	100
2	1	43/46 (94%)	43 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	56/70 (80%)	55 (98%)	1 (2%)	0	100	100
8	B	220/241 (91%)	213 (97%)	6 (3%)	1 (0%)	25	56
9	C	204/233 (88%)	200 (98%)	4 (2%)	0	100	100
10	D	203/206 (98%)	202 (100%)	1 (0%)	0	100	100
11	E	152/167 (91%)	151 (99%)	1 (1%)	0	100	100
12	F	99/135 (73%)	98 (99%)	1 (1%)	0	100	100
13	G	148/179 (83%)	147 (99%)	1 (1%)	0	100	100
14	H	127/130 (98%)	127 (100%)	0	0	100	100
15	I	123/130 (95%)	121 (98%)	2 (2%)	0	100	100
16	J	92/103 (89%)	87 (95%)	4 (4%)	1 (1%)	12	37
17	K	113/129 (88%)	112 (99%)	1 (1%)	0	100	100
18	L	118/124 (95%)	114 (97%)	4 (3%)	0	100	100
19	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
20	N	98/101 (97%)	98 (100%)	0	0	100	100
21	O	86/89 (97%)	86 (100%)	0	0	100	100
22	P	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
23	Q	77/84 (92%)	77 (100%)	0	0	100	100
24	R	62/75 (83%)	62 (100%)	0	0	100	100
25	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
26	T	84/87 (97%)	84 (100%)	0	0	100	100
27	U	53/71 (75%)	53 (100%)	0	0	100	100
28	V	211/213 (99%)	208 (99%)	3 (1%)	0	100	100
29	W	641/693 (92%)	633 (99%)	8 (1%)	0	100	100
33	c	269/273 (98%)	265 (98%)	3 (1%)	1 (0%)	30	61
34	d	204/209 (98%)	200 (98%)	4 (2%)	0	100	100
35	e	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
36	f	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
37	g	164/177 (93%)	162 (99%)	2 (1%)	0	100	100
38	h	39/149 (26%)	37 (95%)	2 (5%)	0	100	100
39	i	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
40	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
42	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
43	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
44	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
45	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
46	p	115/118 (98%)	114 (99%)	0	1 (1%)	14	42
47	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
48	r	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
49	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
50	t	89/104 (86%)	88 (99%)	1 (1%)	0	100	100
51	u	91/94 (97%)	89 (98%)	2 (2%)	0	100	100
52	v	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
53	w	75/78 (96%)	75 (100%)	0	0	100	100
54	x	58/63 (92%)	58 (100%)	0	0	100	100
55	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
56	z	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
All	All	6262/6819 (92%)	6167 (98%)	91 (2%)	4 (0%)	50	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	J	57	VAL
33	c	240	PHE
46	p	87	SER
8	B	165	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	37/38 (97%)	37 (100%)	0	100	100
3	2	51/52 (98%)	50 (98%)	1 (2%)	50	81
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	53 (96%)	2 (4%)	30	64
8	B	184/199 (92%)	180 (98%)	4 (2%)	47	79
9	C	170/190 (90%)	168 (99%)	2 (1%)	67	89
10	D	172/173 (99%)	167 (97%)	5 (3%)	37	71
11	E	117/126 (93%)	114 (97%)	3 (3%)	41	75
12	F	88/116 (76%)	88 (100%)	0	100	100
13	G	124/147 (84%)	119 (96%)	5 (4%)	27	60
14	H	104/105 (99%)	104 (100%)	0	100	100
15	I	103/107 (96%)	102 (99%)	1 (1%)	73	91
16	J	85/90 (94%)	84 (99%)	1 (1%)	67	89
17	K	89/98 (91%)	89 (100%)	0	100	100
18	L	101/103 (98%)	97 (96%)	4 (4%)	27	60
19	M	93/96 (97%)	92 (99%)	1 (1%)	70	90
20	N	83/84 (99%)	82 (99%)	1 (1%)	67	89
21	O	76/77 (99%)	75 (99%)	1 (1%)	65	88
22	P	64/65 (98%)	63 (98%)	1 (2%)	58	85
23	Q	73/78 (94%)	71 (97%)	2 (3%)	40	74
24	R	55/65 (85%)	54 (98%)	1 (2%)	54	83
25	S	72/79 (91%)	71 (99%)	1 (1%)	62	87
26	T	65/66 (98%)	65 (100%)	0	100	100
27	U	48/61 (79%)	48 (100%)	0	100	100
28	V	204/204 (100%)	203 (100%)	1 (0%)	86	95
29	W	544/579 (94%)	541 (99%)	3 (1%)	84	95
33	c	216/218 (99%)	216 (100%)	0	100	100
34	d	162/163 (99%)	162 (100%)	0	100	100
35	e	165/165 (100%)	165 (100%)	0	100	100
36	f	148/150 (99%)	145 (98%)	3 (2%)	50	81
37	g	130/138 (94%)	127 (98%)	3 (2%)	45	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	h	32/114 (28%)	32 (100%)	0	100	100
39	i	115/116 (99%)	115 (100%)	0	100	100
40	j	104/104 (100%)	104 (100%)	0	100	100
41	k	103/103 (100%)	102 (99%)	1 (1%)	73	91
42	l	107/107 (100%)	105 (98%)	2 (2%)	52	82
43	m	98/103 (95%)	98 (100%)	0	100	100
44	n	86/87 (99%)	83 (96%)	3 (4%)	31	65
45	o	99/100 (99%)	96 (97%)	3 (3%)	36	70
46	p	89/90 (99%)	89 (100%)	0	100	100
47	q	84/84 (100%)	82 (98%)	2 (2%)	44	77
48	r	92/93 (99%)	91 (99%)	1 (1%)	70	90
49	s	80/84 (95%)	76 (95%)	4 (5%)	20	51
50	t	76/85 (89%)	75 (99%)	1 (1%)	65	88
51	u	77/78 (99%)	75 (97%)	2 (3%)	41	75
52	v	56/63 (89%)	56 (100%)	0	100	100
53	w	67/68 (98%)	67 (100%)	0	100	100
54	x	54/55 (98%)	54 (100%)	0	100	100
55	y	48/49 (98%)	48 (100%)	0	100	100
56	z	46/48 (96%)	46 (100%)	0	100	100
All	All	5271/5608 (94%)	5206 (99%)	65 (1%)	66	89

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	r	109	ASP
49	s	53	VAL
18	L	14	ARG
16	J	75	ASP
49	s	64	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
25	S	83	HIS

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Mol	Chain	Res	Type
29	W	163	GLN
54	x	58	ASN
26	T	68	HIS
28	V	77	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	Z	75/77 (97%)	18 (24%)	4 (5%)
31	a	2774/2930 (94%)	322 (11%)	0
32	b	118/119 (99%)	9 (7%)	0
6	9	9/24 (37%)	4 (44%)	1 (11%)
7	A	1508/1554 (97%)	197 (13%)	47 (3%)
All	All	4484/4704 (95%)	550 (12%)	52 (1%)

5 of 550 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	9	19	G
6	9	20	C
6	9	21	A
6	9	22	A
7	A	4	U

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	1042	A
7	A	1201	A
30	Z	17(A)	U
7	A	1043	G
7	A	1129	C

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

39 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	$\#\|Z\| > 2$
31	PSU	a	2605	31	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
7	G7M	A	527	7	20,26,27	1.14	2 (10%)	17,39,42	0.46	0
42	4D4	l	81	42	9,11,12	0.55	0	8,13,15	0.67	0
7	2MG	A	1516	7	18,26,27	1.03	2 (11%)	16,38,41	0.75	0
31	PSU	a	2504	31	18,21,22	0.91	1 (5%)	22,30,33	0.66	0
7	2MG	A	1207	7,58	18,26,27	1.01	2 (11%)	16,38,41	0.74	0
7	PSU	A	516	7,59	18,21,22	0.91	1 (5%)	22,30,33	0.59	0
31	OMU	a	2552	31	19,22,23	0.21	0	26,31,34	0.42	0
31	PSU	a	2604	31	18,21,22	0.91	1 (5%)	22,30,33	0.79	1 (4%)
31	6MZ	a	1618	31	18,25,26	0.67	0	16,36,39	0.70	1 (6%)
31	OMG	a	2251	30,31,58	18,26,27	1.00	2 (11%)	19,38,41	0.68	0
31	PSU	a	746	31,59	18,21,22	0.90	1 (5%)	22,30,33	0.63	0
31	5MC	a	1962	31	18,22,23	0.34	0	26,32,35	0.47	0
31	PSU	a	955	31	18,21,22	0.89	1 (5%)	22,30,33	0.58	0
31	5MU	a	747	31	19,22,23	0.26	0	28,32,35	0.28	0
31	2MG	a	1835	31	18,26,27	1.02	2 (11%)	16,38,41	0.70	0
31	H2U	a	2449	31	18,21,22	0.56	0	21,30,33	0.75	1 (4%)
7	MA6	A	1518	7	18,26,27	0.75	0	19,38,41	0.45	0
31	PSU	a	1917	31	18,21,22	0.91	1 (5%)	22,30,33	0.55	0
17	IAS	K	119	17	6,7,8	0.92	0	6,8,10	0.99	0
31	2MG	a	2445	31	18,26,27	1.02	2 (11%)	16,38,41	0.71	0
7	5MC	A	967	7	18,22,23	0.33	0	26,32,35	0.48	0
7	2MG	A	966	7	18,26,27	1.01	2 (11%)	16,38,41	0.77	0
31	PSU	a	1911	31	18,21,22	0.90	1 (5%)	22,30,33	0.65	0
31	G7M	a	2069	31	20,26,27	1.12	3 (15%)	17,39,42	0.47	0
7	5MC	A	1407	7	18,22,23	0.32	0	26,32,35	0.58	0
7	4OC	A	1402	7	20,23,24	0.37	0	26,32,35	0.44	0
18	D2T	L	89	18	7,9,10	0.97	0	6,11,13	1.67	3 (50%)
31	PSU	a	2580	31	18,21,22	0.88	1 (5%)	22,30,33	0.76	1 (4%)
7	UR3	A	1498	7	19,22,23	0.27	0	26,32,35	0.64	0
31	PSU	a	2457	31	18,21,22	0.92	1 (5%)	22,30,33	0.61	0
31	5MU	a	1939	31,58	19,22,23	0.29	0	28,32,35	0.34	0
31	3TD	a	1915	31	18,22,23	0.97	1 (5%)	22,32,35	0.62	0
31	6MZ	a	2030	31	18,25,26	0.68	0	16,36,39	0.71	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	OMC	a	2498	31,59	19,22,23	0.26	0	26,31,34	0.49	0
31	2MA	a	2503	31,58,59	19,25,26	1.01	1 (5%)	21,37,40	1.82	5 (23%)
31	1MG	a	745	31	18,26,27	0.95	1 (5%)	19,39,42	0.54	0
7	MA6	A	1519	7	18,26,27	0.76	0	19,38,41	0.55	0
34	MEQ	d	150	34	8,9,10	0.43	0	5,10,12	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	a	2605	31	-	0/7/25/26	0/2/2/2
7	G7M	A	527	7	-	1/3/25/26	0/3/3/3
42	4D4	l	81	42	-	1/11/12/14	-
7	2MG	A	1516	7	-	0/5/27/28	0/3/3/3
31	PSU	a	2504	31	-	0/7/25/26	0/2/2/2
7	2MG	A	1207	7,58	-	0/5/27/28	0/3/3/3
7	PSU	A	516	7,59	-	0/7/25/26	0/2/2/2
31	OMU	a	2552	31	-	0/9/27/28	0/2/2/2
31	PSU	a	2604	31	-	0/7/25/26	0/2/2/2
31	6MZ	a	1618	31	-	0/5/27/28	0/3/3/3
31	OMG	a	2251	30,31,58	-	0/5/27/28	0/3/3/3
31	PSU	a	746	31,59	-	3/7/25/26	0/2/2/2
31	5MC	a	1962	31	-	0/7/25/26	0/2/2/2
31	PSU	a	955	31	-	0/7/25/26	0/2/2/2
31	5MU	a	747	31	-	1/7/25/26	0/2/2/2
31	2MG	a	1835	31	-	0/5/27/28	0/3/3/3
31	H2U	a	2449	31	-	0/7/38/39	0/2/2/2
7	MA6	A	1518	7	-	0/7/29/30	0/3/3/3
31	PSU	a	1917	31	-	0/7/25/26	0/2/2/2
17	IAS	K	119	17	-	3/7/7/8	-
31	2MG	a	2445	31	-	1/5/27/28	0/3/3/3
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
7	2MG	A	966	7	-	0/5/27/28	0/3/3/3
31	PSU	a	1911	31	-	2/7/25/26	0/2/2/2
31	G7M	a	2069	31	-	2/3/25/26	0/3/3/3
7	5MC	A	1407	7	-	0/7/25/26	0/2/2/2
7	4OC	A	1402	7	-	0/9/29/30	0/2/2/2
18	D2T	L	89	18	-	4/7/12/14	-
31	PSU	a	2580	31	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	UR3	A	1498	7	-	0/7/25/26	0/2/2/2
31	PSU	a	2457	31	-	0/7/25/26	0/2/2/2
31	5MU	a	1939	31,58	-	0/7/25/26	0/2/2/2
31	3TD	a	1915	31	-	2/7/25/26	0/2/2/2
31	6MZ	a	2030	31	-	2/5/27/28	0/3/3/3
31	OMC	a	2498	31,59	-	0/9/27/28	0/2/2/2
31	2MA	a	2503	31,58,59	-	2/3/25/26	0/3/3/3
31	1MG	a	745	31	-	0/3/25/26	0/3/3/3
7	MA6	A	1519	7	-	1/7/29/30	0/3/3/3
34	MEQ	d	150	34	-	2/8/9/11	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1915	3TD	C6-C5	3.67	1.39	1.35
31	a	2457	PSU	C6-C5	3.63	1.39	1.35
7	A	516	PSU	C6-C5	3.60	1.39	1.35
31	a	1917	PSU	C6-C5	3.60	1.39	1.35
31	a	2504	PSU	C6-C5	3.58	1.39	1.35

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	2503	2MA	C5-C6-N1	-5.38	117.48	121.01
31	a	2503	2MA	C5-C6-N6	4.39	127.02	120.35
31	a	2503	2MA	CM2-C2-N1	2.80	121.52	117.15
18	L	89	D2T	OD1-CG-CB	-2.55	117.10	122.44
31	a	2580	PSU	C3'-C2'-C1'	2.39	104.42	101.64

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	L	89	D2T	O-C-CA-CB
31	a	746	PSU	C2'-C1'-C5-C4
31	a	746	PSU	O4'-C1'-C5-C6
31	a	1911	PSU	O4'-C1'-C5-C4
31	a	1911	PSU	O4'-C1'-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 415 ligands modelled in this entry, 413 are monoatomic - leaving 2 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	GDP	W	701	59	24,30,30	0.94	2 (8%)	30,47,47	0.65	0
61	FUA	W	703	-	39,40,40	1.47	2 (5%)	49,64,64	0.91	2 (4%)

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	GDP	W	701	59	-	1/12/32/32	0/3/3/3
61	FUA	W	703	-	-	6/15/92/92	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	W	703	FUA	C29-C22	-8.45	1.35	1.47
60	W	701	GDP	C5-C6	-2.51	1.42	1.47
61	W	703	FUA	O5-C29	-2.34	1.23	1.30
60	W	701	GDP	C8-N7	-2.06	1.31	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	W	703	FUA	C16-O2-C31	2.20	120.41	117.06
61	W	703	FUA	C14-C8-C9	-2.19	105.11	109.40

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

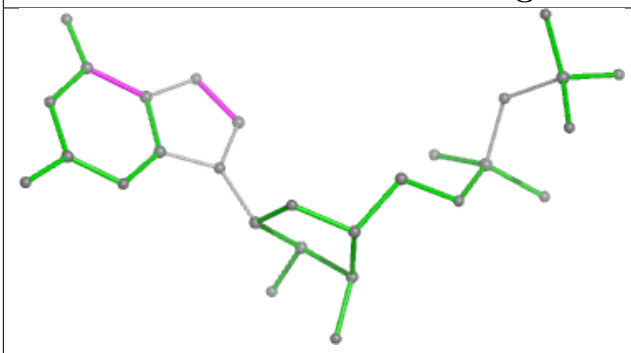
Mol	Chain	Res	Type	Atoms
61	W	703	FUA	C13-C17-C22-C29
61	W	703	FUA	C17-C22-C29-O5
61	W	703	FUA	C32-C31-O2-C16
61	W	703	FUA	O3-C31-O2-C16
60	W	701	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

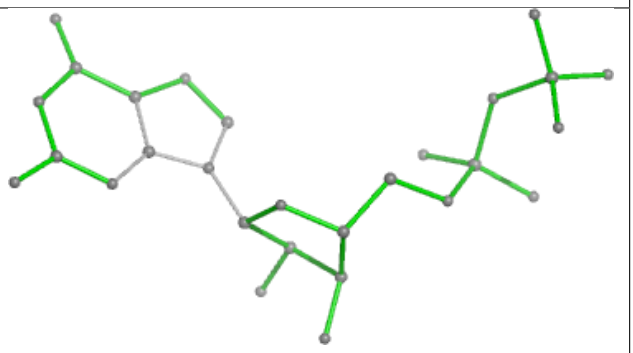
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

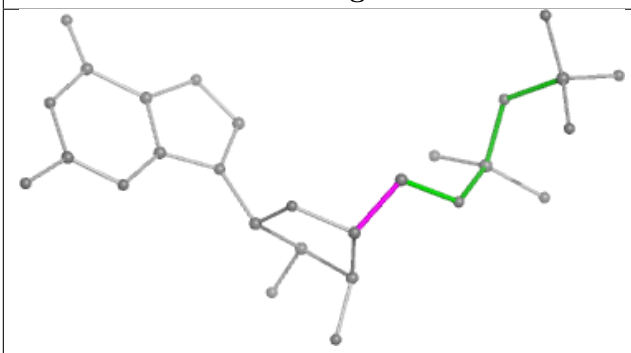
Ligand GDP W 701



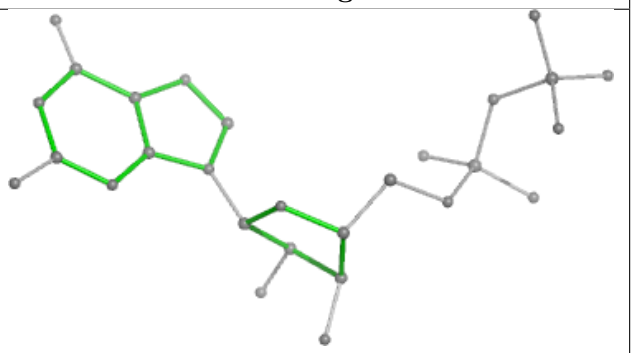
Bond lengths



Bond angles

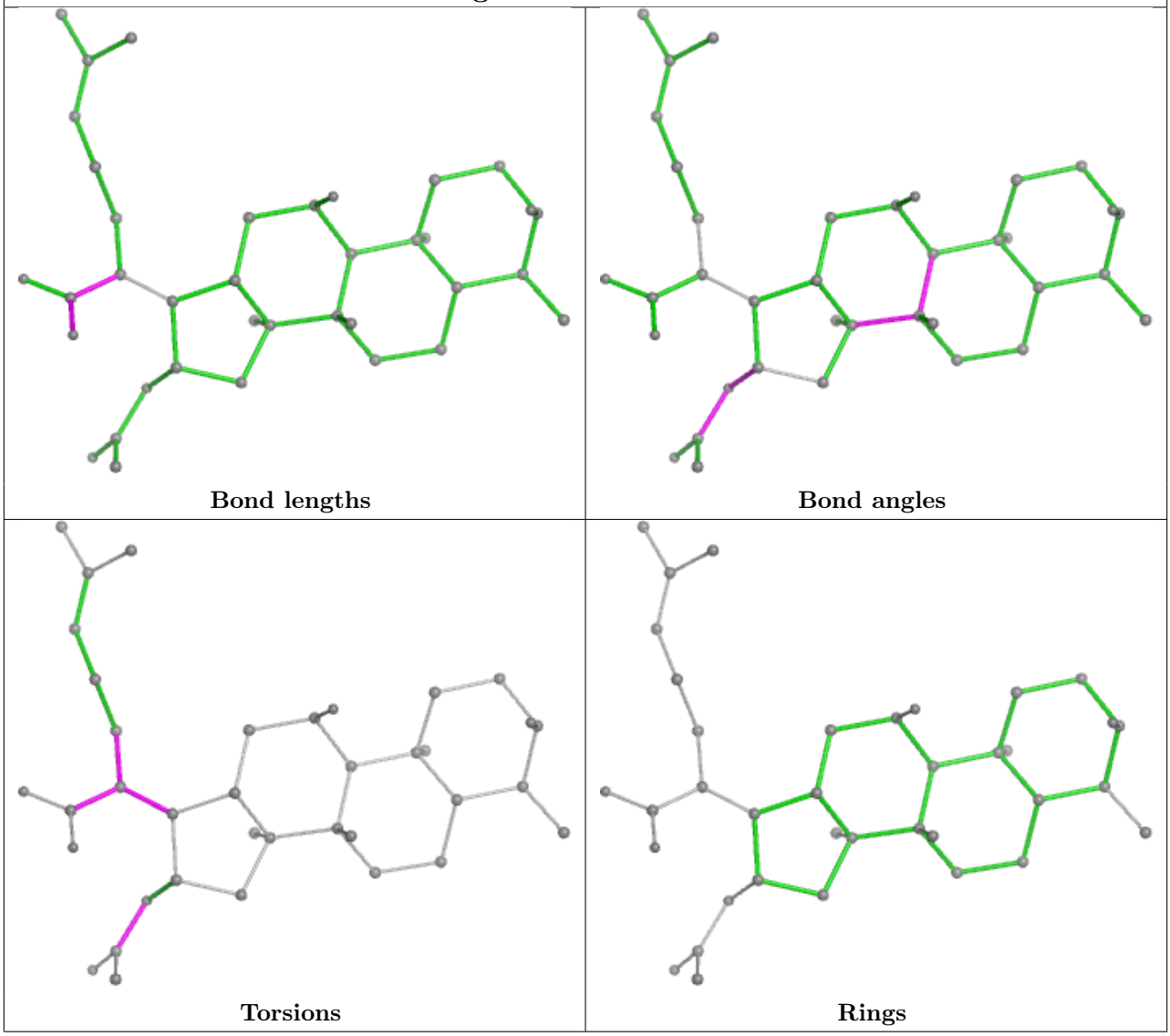


Torsions



Rings

Ligand FUA W 703



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.