Full wwPDB EM Validation Report (i)

Sep 16, 2026 – 09:34 PM EDT

PDB ID	:	7M4Y / pdb_00007m4y
EMDB ID	:	EMD-23670
Title	:	A. baumannii Ribosome-Eravacycline complex: E-site tRNA 70S
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2021-03-22
Resolution	:	2.50 Å(reported)

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

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

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

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

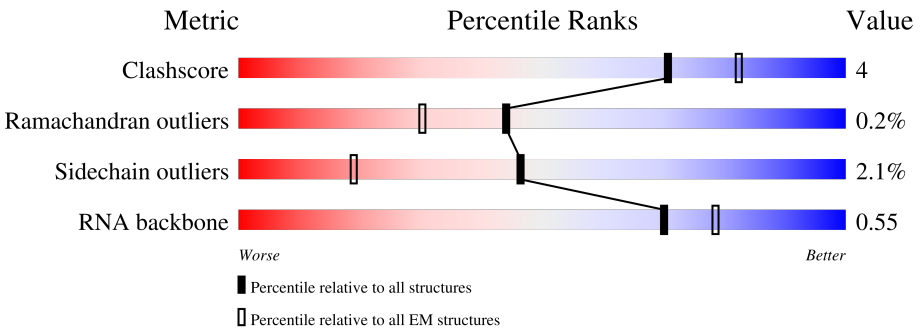
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

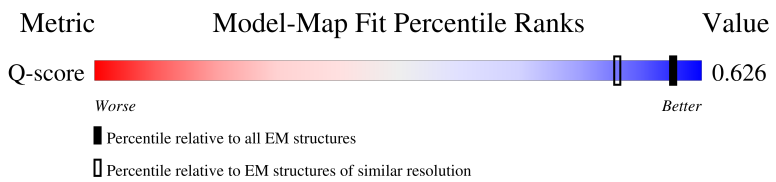
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	0	51	94% 6%
2	1	44	93% 7%
3	2	64	92% 6%

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Mol	Chain	Length	Quality of chain
4	3	38	89% 8%
5	A	2918	6% 69% 21% 6%
6	B	115	11% 70% 23% 7%
7	C	274	89% 10%
8	D	212	90% 9%
9	E	200	90% 10%
10	F	178	87% 63% 33%
11	G	177	19% 88% 11%
12	H	148	26% 36% 59%
13	I	142	92% 8%
14	J	122	89% 11%
15	K	146	96%
16	L	137	88% 12%
17	M	125	89% 6% 5%
18	N	116	12% 93% 5%
19	O	122	84% 11% 5%
20	P	119	91% 8%
21	Q	103	94% 6%
22	R	109	94% 5%
23	S	106	6% 80% 6% 14%
24	T	105	13% 91% 6%
25	U	98	7% 92% 7%
26	V	85	84% 7% 9%
27	W	78	95%
28	X	65	17% 83% 8% 8%

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Mol	Chain	Length	Quality of chain
29	Y	58	93% 7%
30	Z	61	84% 11%
31	a	1544	73% 22%
32	b	250	60% 69% 18% 10%
33	c	250	74% 11% 14%
34	d	208	87% 12%
35	e	165	79% 14% 6%
36	f	127	5% 66% 13% 18%
37	g	156	6% 76% 12% 13%
38	h	131	92% 7%
39	i	128	89% 9%
40	j	103	84% 12%
41	k	128	7% 75% 16% 9%
42	l	124	81% 17%
43	m	118	84% 14%
44	n	101	88% 11%
45	o	89	92% 7%
46	p	101	76% 19%
47	q	85	78% 14% 7%
48	r	75	60% 8% 31%
49	s	91	84% 7% 10%
50	t	88	95%
51	u	71	52% 69% 18% 11%
52	v	77	45% 64% 25% 10%
53	w	3	33% 67%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 139817 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
			Total	C	N	O	S		
1	0	51	427	274	77	73	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	44	363	222	85	54	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	63	509	319	110	76	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	38	295	179	64	48	4	0	0

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	A	2730	58566	26143	10721	18972	2730	0	0

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	B	115	2450	1095	440	800	115	0	0

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	272	2111	1302	436	365	8	0	0

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	211	1572	972	297	300	3	0	0

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	200	1516	952	281	278	5	0	0

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	174	1370	871	243	248	8	0	0

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	174	1318	832	236	249	1	0	0

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	60	458	287	84	86	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	142	1125	718	200	203	4	0	0

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	J	122	946	592	180	169	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	K	144	1071	663	213	195	0	0

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	L	137	1087	687	210	185	5	0	0

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	M	119	942	590	186	163	3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N	114	857	528	173	155	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	O	116	913	575	176	162	0	0

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	P	117	934	589	197	146	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	103	807	506	155	143	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	109	826	514	158	150	4	0	0

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	S	91	710	452	128	129	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	T	103	766	476	142	148	0	0

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	U	97	760	477	143	139	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	V	77	581	360	112	107	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	W	77	632	395	130	105	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	X	60	486	302	93	90	1	0	0

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	58	463	286	88	85	4	0	0

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Z	54	447	265	100	81	1	0	0

- Molecule 31 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	a	1528	32782	14631	5994	10630	1527	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1007	U	C	conflict	GB 1211343212
a	1034	C	U	conflict	GB 1211343212

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	b	225	1769	1110	328	325	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	215	1690	1065	318	299	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	d	207	1631	1017	313	299	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	e	155	1129	700	217	207	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	f	104	867	546	158	159	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	g	136	1073	671	201	194	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	h	130	985	615	177	187	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	i	126	991	618	197	175	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	j	100	801	500	150	148	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	k	117	862	535	167	159	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	l	122	945	580	193	167	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	m	115	903	558	184	158	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	n	100	792	493	158	137	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	o	88	705	434	144	126	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	p	82	644	403	128	112	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	q	79	621	390	116	114	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	r	52	426	273	74	79	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	s	82	646	412	125	107	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	t	86	663	409	139	113	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	u	63	522	327	105	89	1	0	0

- Molecule 52 is a RNA chain called tRNA-met.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
52	v	77	1636	733	291	535	76	1	0	0

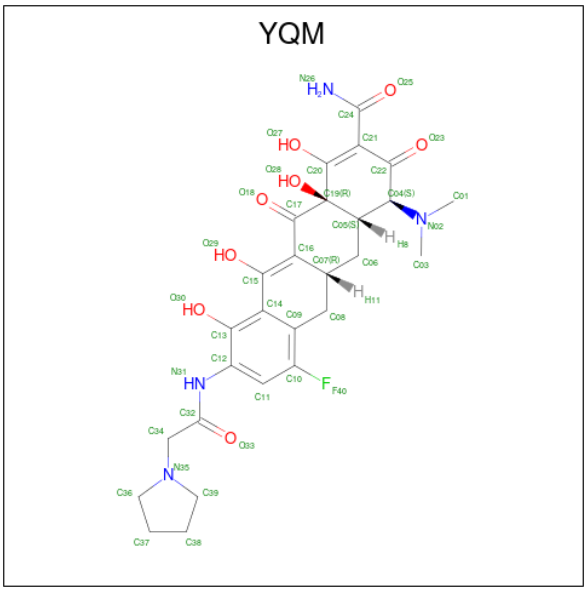
- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	w	3	65	29	12	21	3	0	0

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
54	3	1	1	1	0

- Molecule 55 is Eravacycline (CCD ID: YQM) (formula: $C_{27}H_{31}FN_4O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
55	A	1	40	27	1	4	8	0
			Total	C	F	N	O	
55	A	1	40	27	1	4	8	0
			Total	C	F	N	O	
55	a	1	40	27	1	4	8	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	A	138	138	138	0
			Total	Mg	
56	B	1	1	1	0
			Total	Mg	
56	D	1	1	1	0
			Total	Mg	
56	K	1	1	1	0
			Total	Mg	
56	a	54	54	54	0
			Total	Mg	
56	t	1	1	1	0

- Molecule 57 is water.

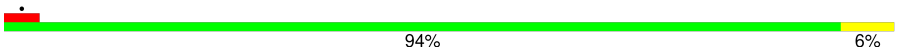
Mol	Chain	Residues	Atoms	AltConf
57	2	1	Total O 1 1	0
57	A	707	Total O 707 707	0
57	B	4	Total O 4 4	0
57	C	7	Total O 7 7	0
57	D	5	Total O 5 5	0
57	E	4	Total O 4 4	0
57	K	7	Total O 7 7	0
57	R	1	Total O 1 1	0
57	S	1	Total O 1 1	0
57	U	1	Total O 1 1	0
57	Z	7	Total O 7 7	0
57	a	283	Total O 283 283	0
57	j	3	Total O 3 3	0
57	l	1	Total O 1 1	0
57	m	1	Total O 1 1	0
57	n	5	Total O 5 5	0
57	q	1	Total O 1 1	0
57	s	1	Total O 1 1	0
57	t	3	Total O 3 3	0
57	u	1	Total O 1 1	0

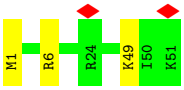
3 Residue-property plots (i)

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

- Molecule 1: 50S ribosomal protein L33

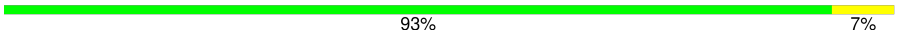
Chain 0:

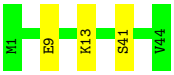




- Molecule 2: 50S ribosomal protein L34

Chain 1:





- Molecule 3: 50S ribosomal protein L35

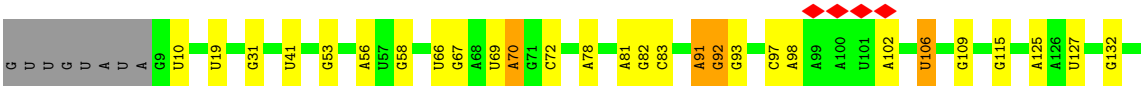
Chain 2:

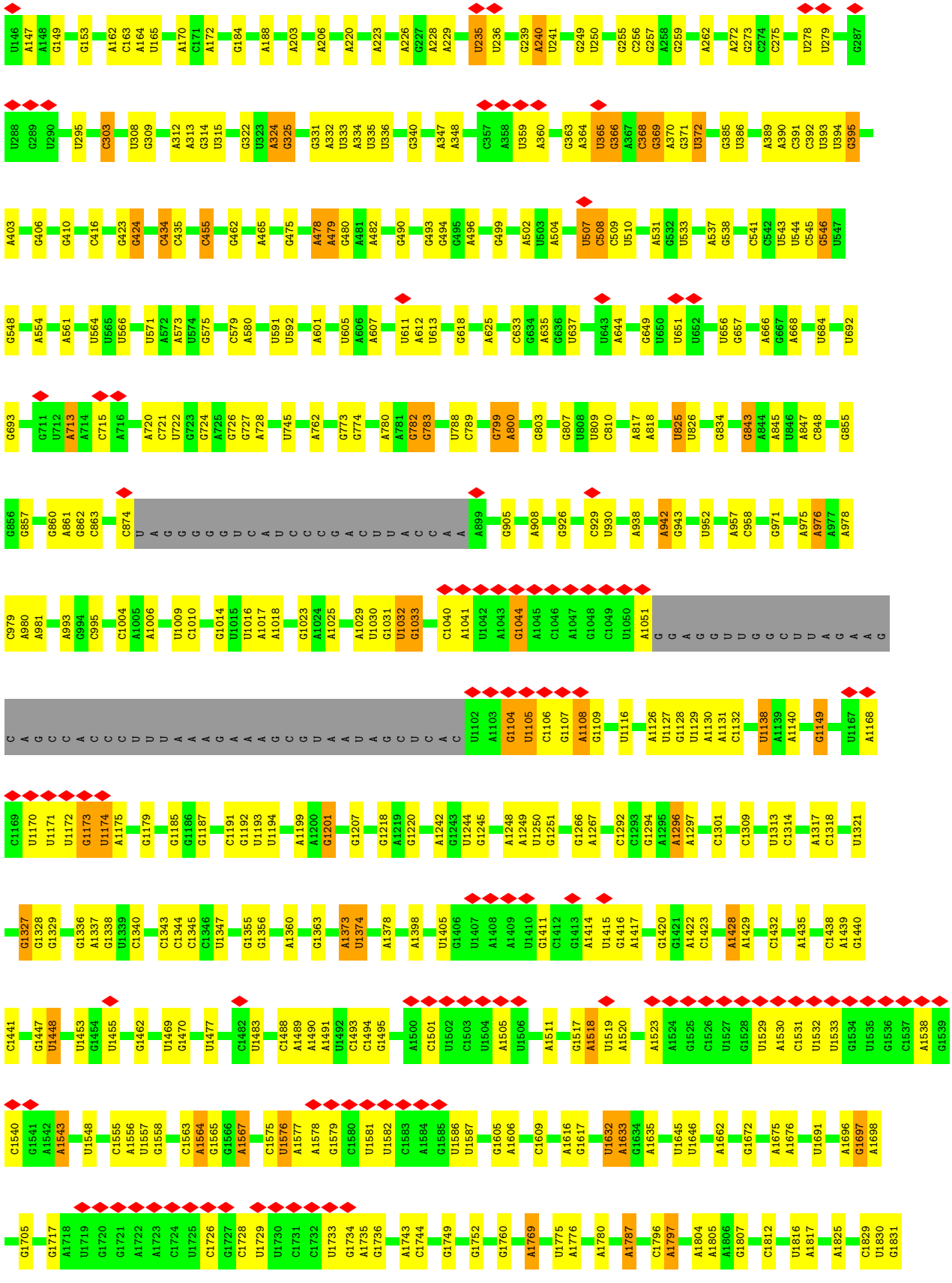
- Molecule 4: 50S ribosomal protein L36

Chain 3:

- Molecule 5: 23s ribosomal RNA

Chain A:




U146 A147 A148 G149 G153 A162 C163 A164 U165 A170 C171 A172 G184 A188 A203 A206 A220 A223 A226 G227 A228 A229 U235 U236 G239 A240 U241 G249 U250 G255 C256 G257 A258 G259 A262 A272 G273 C274 C275 U278 U279 G287
U288 G289 U290 U295 C303 U308 G309 A312 A313 G314 U315 G322 U323 A324 G325 G331 A332 U333 A334 U335 U336 G340 A347 A348 C357 A358 U359 A360 G363 A364 U365 G366 A367 C368 G369 A370 G371 U372 G385 U386 A389 A390 C391 C392 U393 U394 G395
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G693 G711 U712 A713 A714 C715 A716 A720 C721 U722 G723 G724 A725 G726 G727 A728 U745 A762 G773 G774 A780 A781 G782 G783 U788 C789 G799 A800 G803 G807 U808 U809 C810 A817 A818 U825 U826 G834 G843 A844 A845 U846 A847 C848 G855
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C1441 G1447 U1448 U1453 G1454 U1455 G1462 U1469 G1470 U1477 C1482 U1483 C1488 A1489 A1490 A1491 U1492 G1493 C1494 G1495 A1500 C1501 U1502 C1503 U1504 A1505 U1506 A1511 G1517 A1518 U1519 A1520 A1523 A1524 G1525 C1526 U1527 G1528 U1529 A1530 C1531 U1532 U1533 G1534 U1535 C1536 C1537 A1538 G1539
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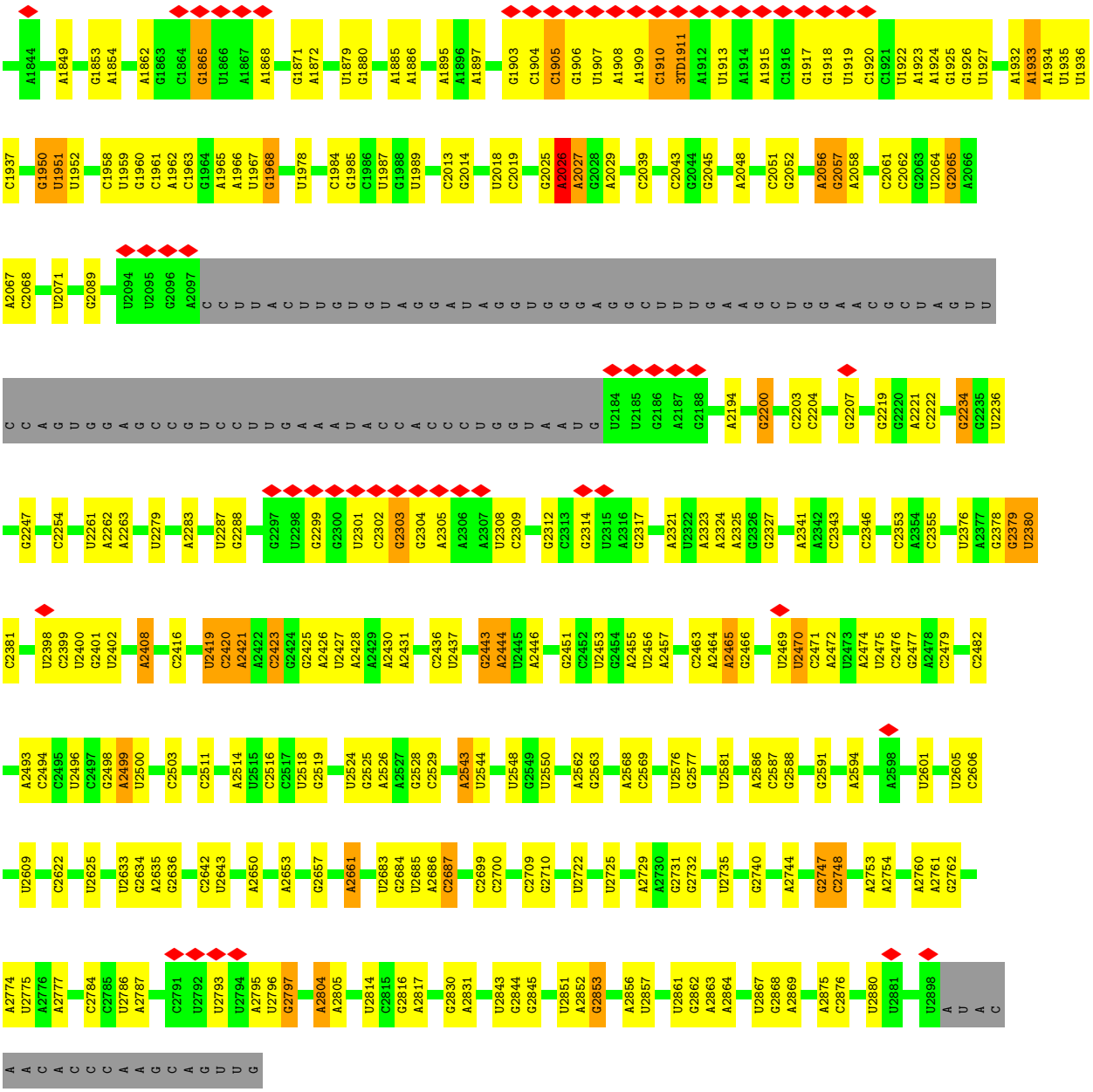
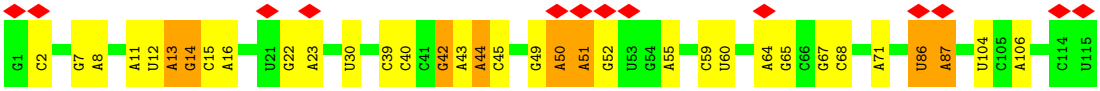
G1705 G1717 A1718 U1719 G1720 G1721 A1722 A1723 C1724 U1725 C1726 G1727 C1728 U1729 U1730 C1731 C1732 U1733 G1734 A1735 G1736 A1743 C1744 G1749 G1752 G1760 A1769 U1775 A1776 A1780 A1787 C1796 A1797 A1804 A1805 A1806 G1807 C1812 U1816 A1817 A1825 C1829 U1830 G1831



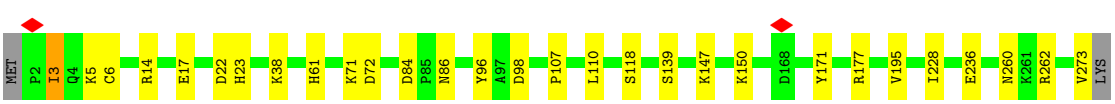
• Molecule 6: 5s ribosomal RNA

Chain B:



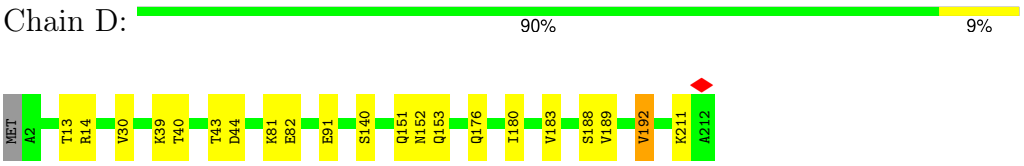
• Molecule 7: 50S ribosomal protein L2

Chain C:



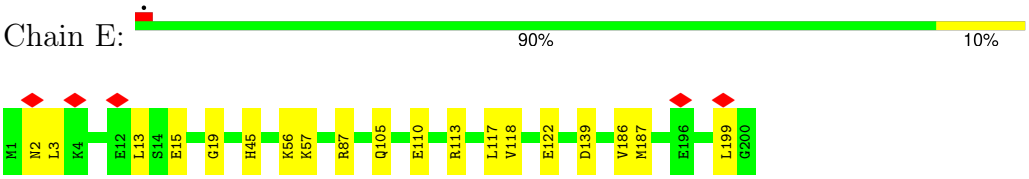
- Molecule 8: 50S ribosomal protein L3

Chain D:



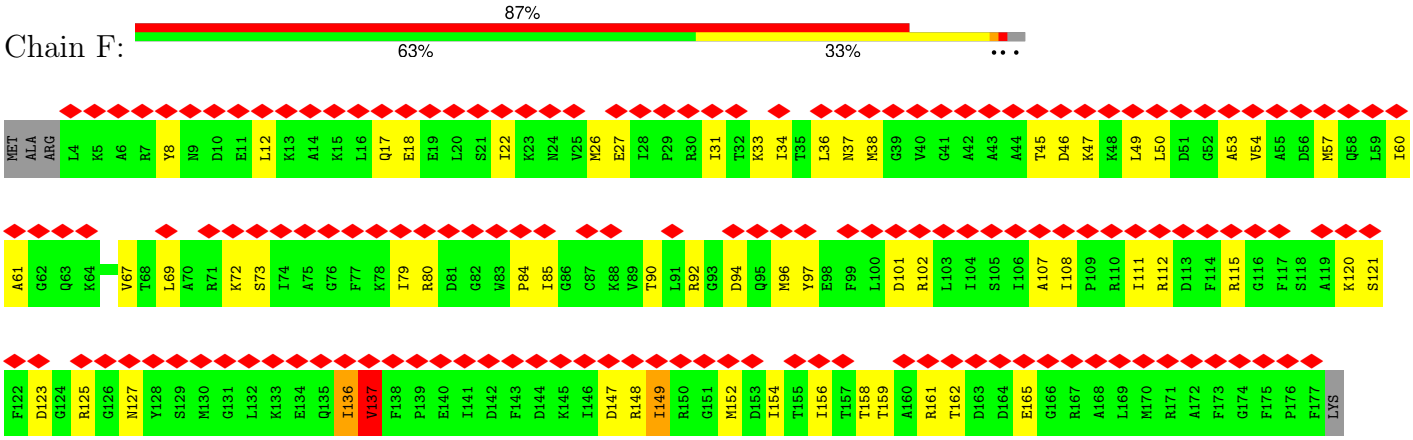
- Molecule 9: 50S ribosomal protein L4

Chain E:



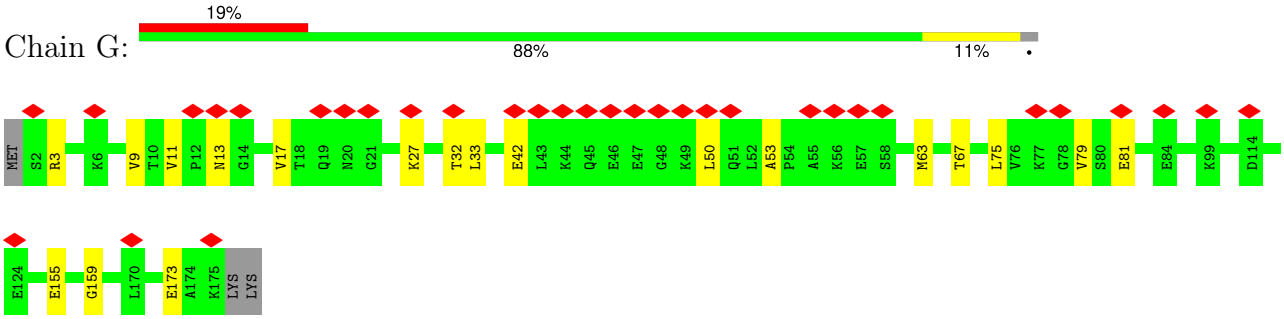
- Molecule 10: 50S ribosomal protein L5

Chain F:



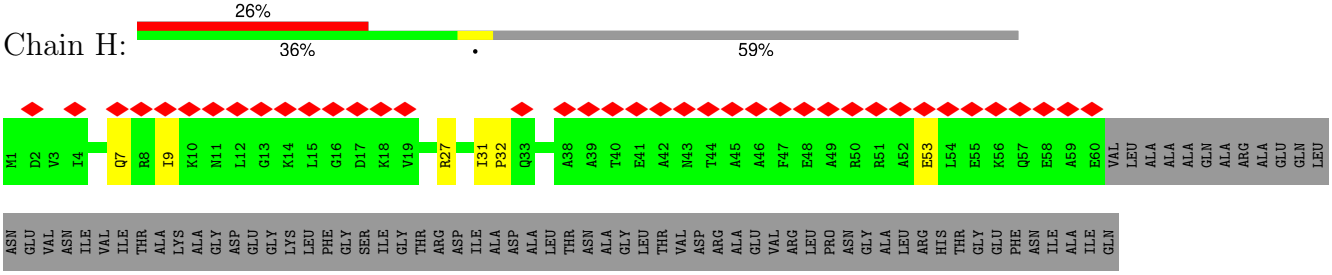
- Molecule 11: 50S ribosomal protein L6

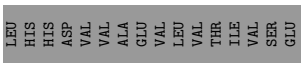
Chain G:



- Molecule 12: 50S ribosomal protein L9

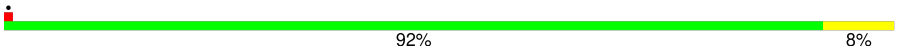
Chain H:

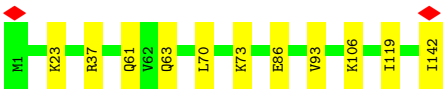




• Molecule 13: 50S ribosomal protein L13

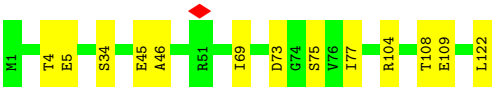
Chain I:





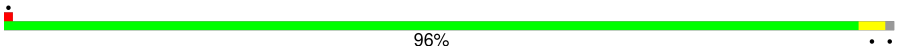
• Molecule 14: 50S ribosomal protein L14

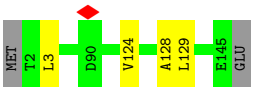
Chain J:



• Molecule 15: 50S ribosomal protein L15

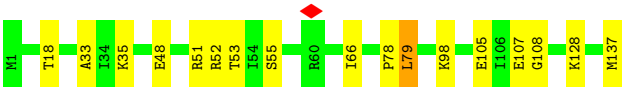
Chain K:





• Molecule 16: 50S ribosomal protein L16

Chain L:

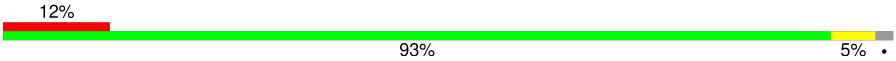


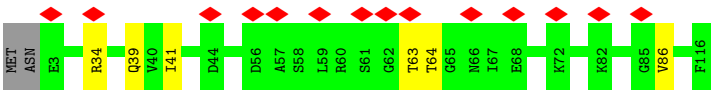
• Molecule 17: 50S ribosomal protein L17

Chain M:

• Molecule 18: 50S ribosomal protein L18

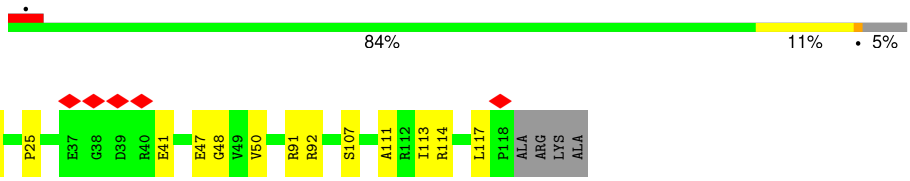
Chain N:





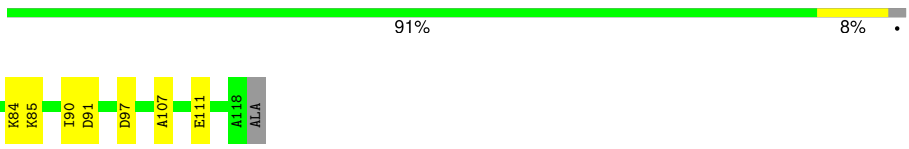
• Molecule 19: 50S ribosomal protein L19

Chain O:



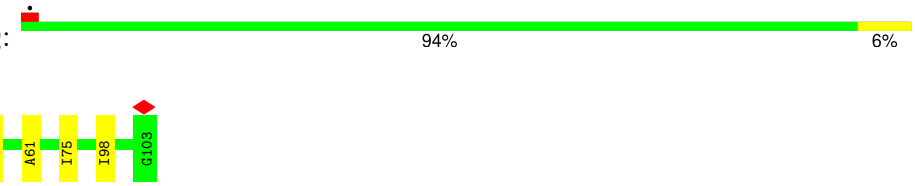
• Molecule 20: 50S ribosomal protein L20

Chain P:



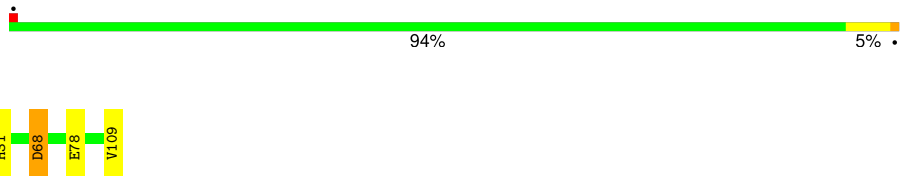
• Molecule 21: 50S ribosomal protein L21

Chain Q:



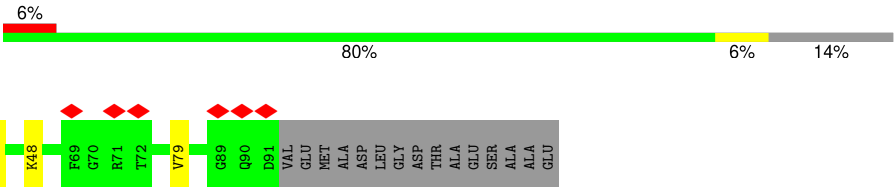
• Molecule 22: 50S ribosomal protein L22

Chain R:



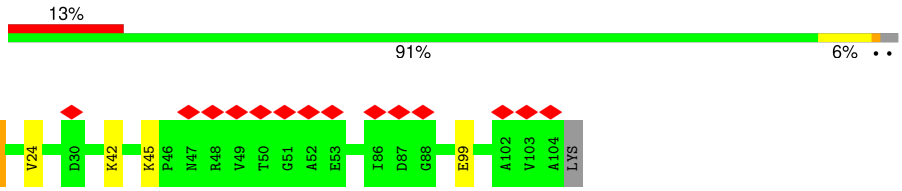
• Molecule 23: 50S ribosomal protein L23

Chain S:



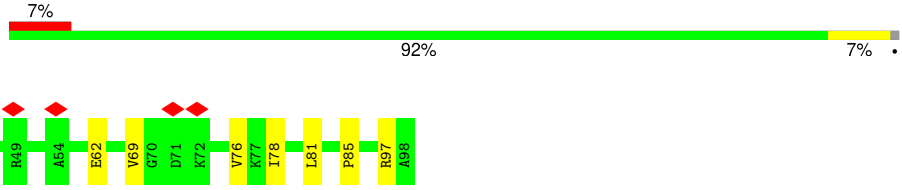
• Molecule 24: 50S ribosomal protein L24

Chain T:



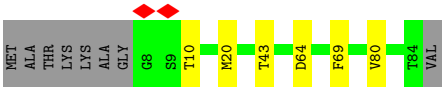
• Molecule 25: 50S ribosomal protein L25

Chain U:



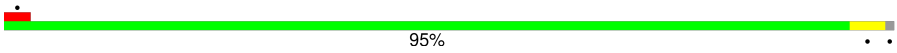
• Molecule 26: 50S ribosomal protein L27

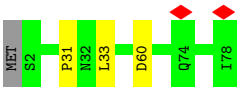
Chain V:



• Molecule 27: 50S ribosomal protein L28

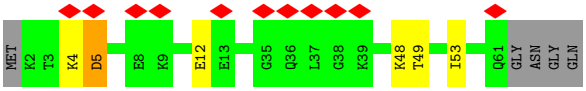
Chain W:





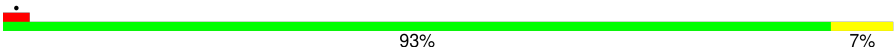
• Molecule 28: 50S ribosomal protein L29

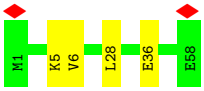
Chain X:



• Molecule 29: 50S ribosomal protein L30

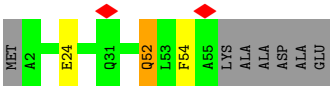
Chain Y:





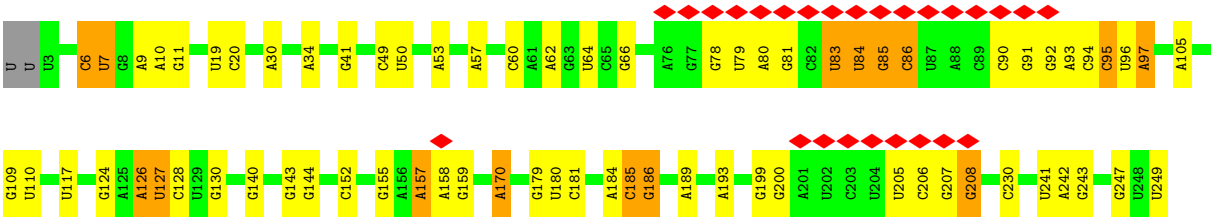
• Molecule 30: 50S ribosomal protein L32

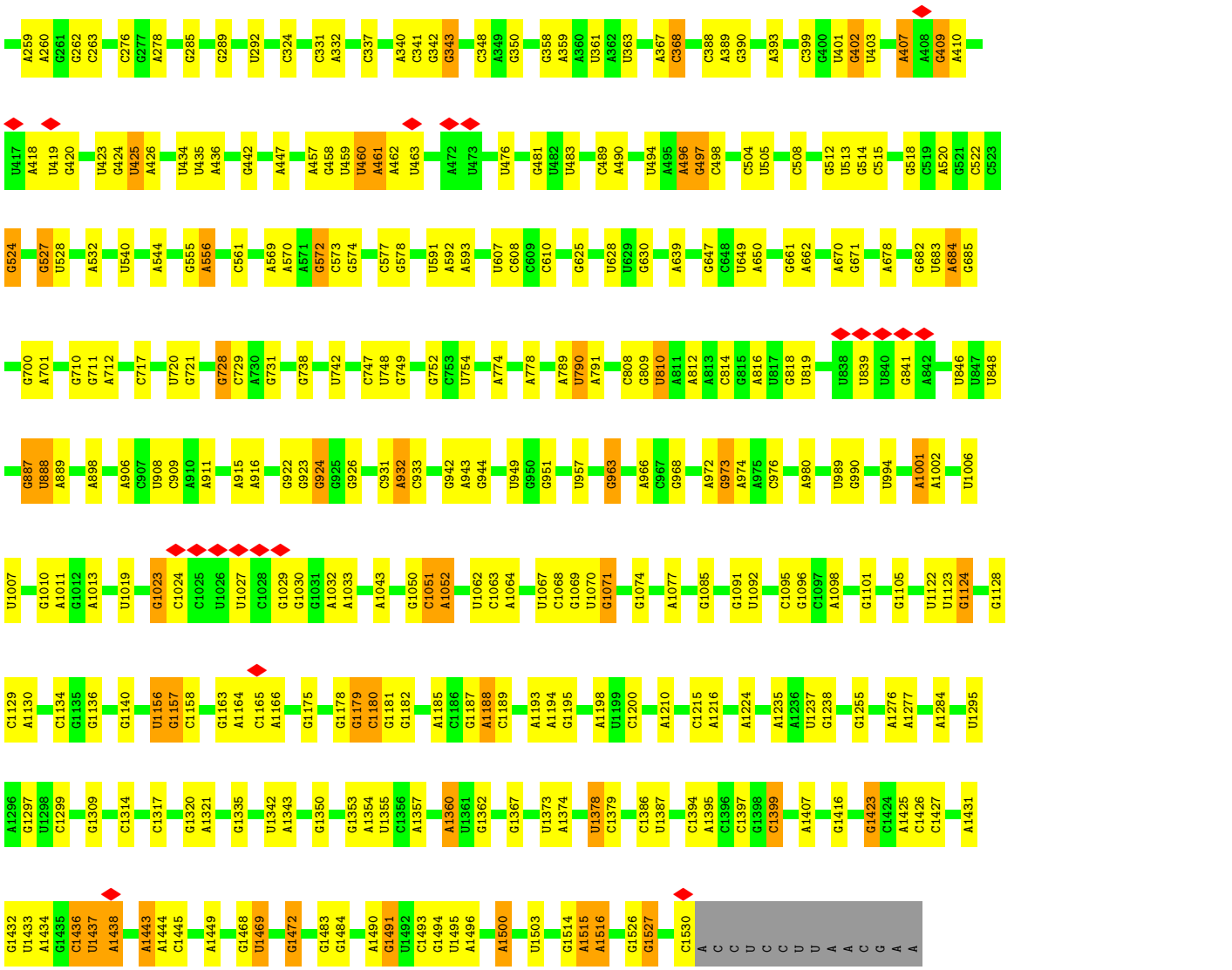
Chain Z:



• Molecule 31: 16s Ribosomal RNA

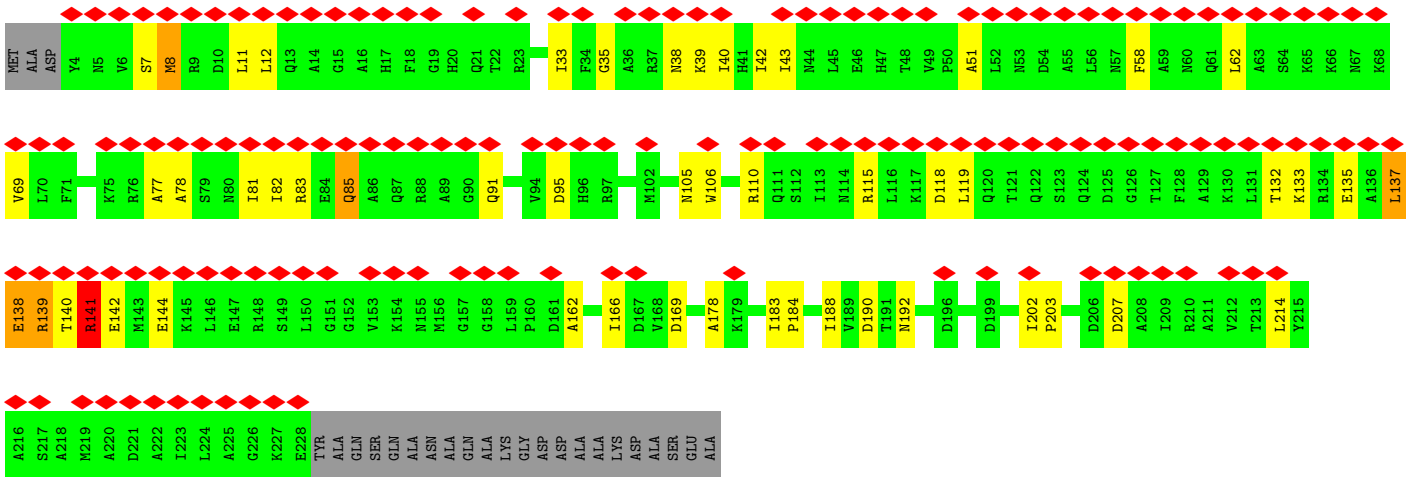
Chain a:





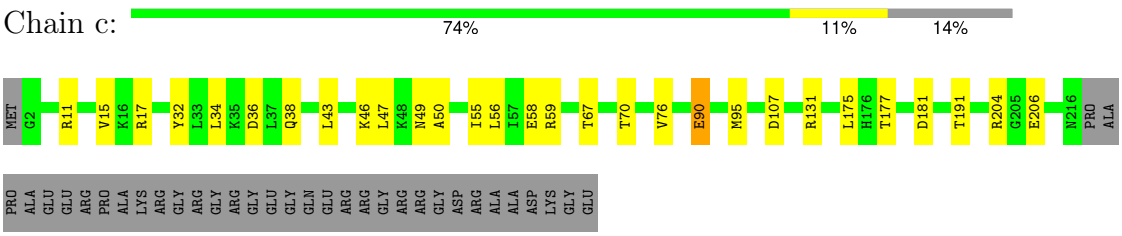
• Molecule 32: 30S ribosomal protein S2

Chain b:



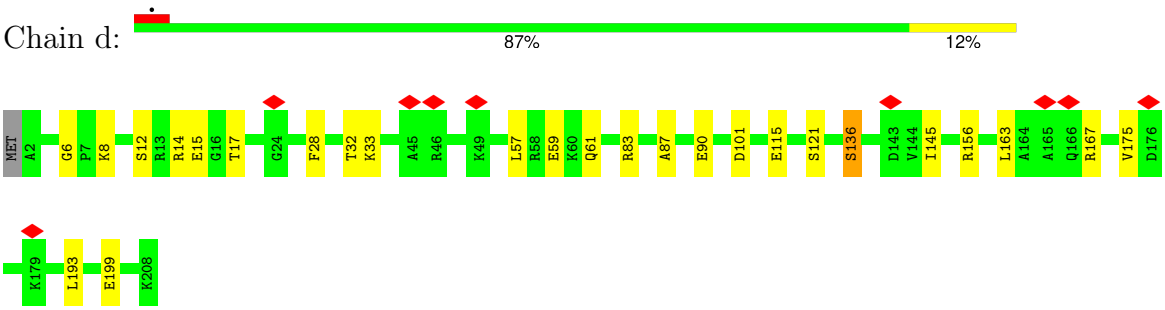
• Molecule 33: 30S ribosomal protein S3

Chain c:



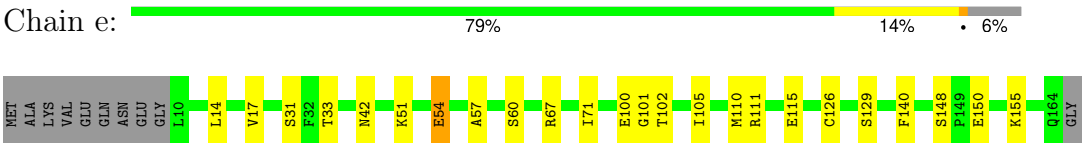
• Molecule 34: 30S ribosomal protein S4

Chain d:



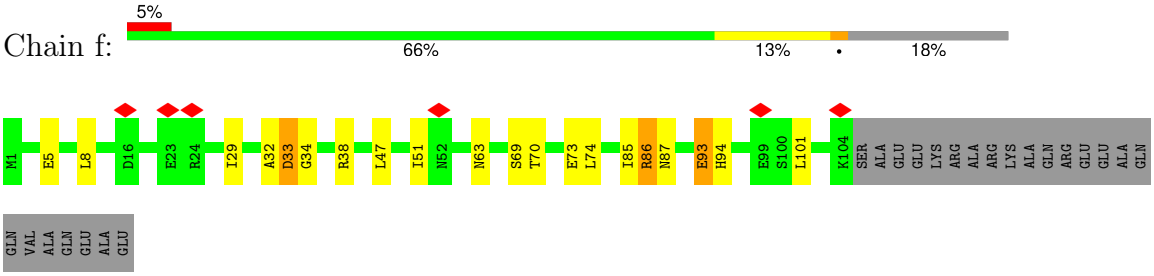
• Molecule 35: 30S ribosomal protein S5

Chain e:



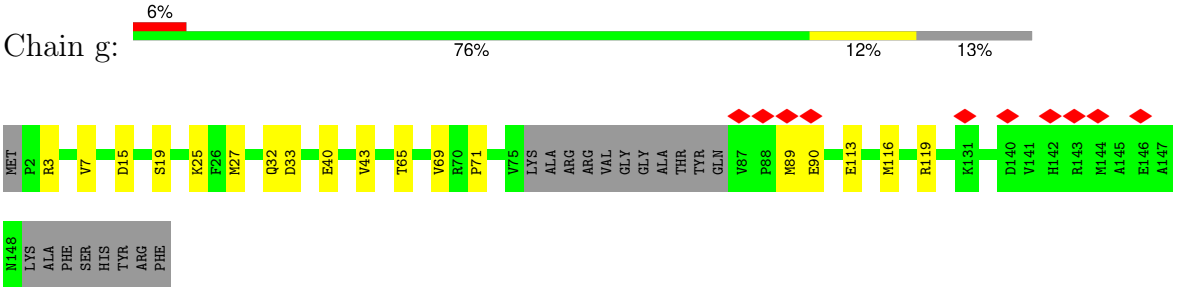
• Molecule 36: 30S ribosomal protein S6

Chain f:



• Molecule 37: 30S ribosomal protein S7

Chain g:

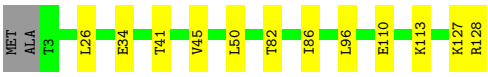


• Molecule 38: 30S ribosomal protein S8

Chain h:

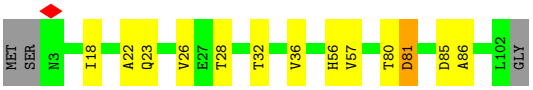
• Molecule 39: 30S ribosomal protein S9

Chain i:



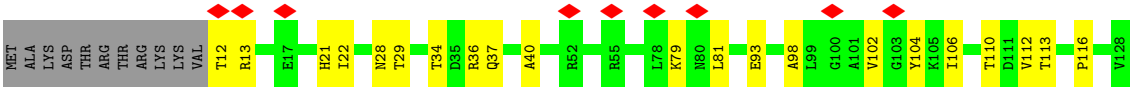
• Molecule 40: 30S ribosomal protein S10

Chain j:



• Molecule 41: 30S ribosomal protein S11

Chain k:

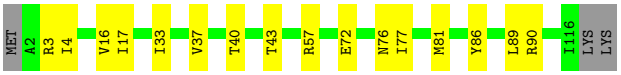


• Molecule 42: 30S ribosomal protein S12

Chain l:

• Molecule 43: 30S ribosomal protein S13

Chain m:

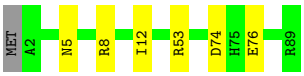


• Molecule 44: 30S ribosomal protein S14

Chain n:

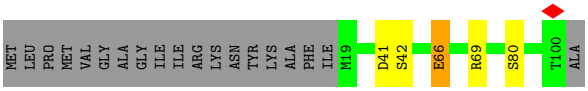
• Molecule 45: 30S ribosomal protein S15

Chain o:



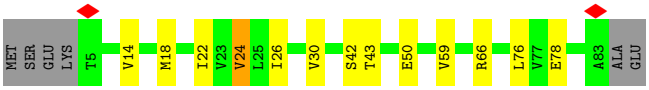
• Molecule 46: 30S ribosomal protein S16

Chain p:



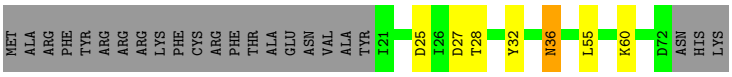
• Molecule 47: 30S ribosomal protein S17

Chain q:



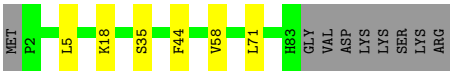
• Molecule 48: 30S ribosomal protein S18

Chain r:



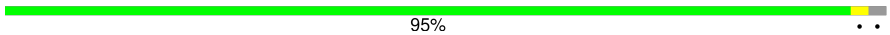
• Molecule 49: 30S ribosomal protein S19

Chain s:



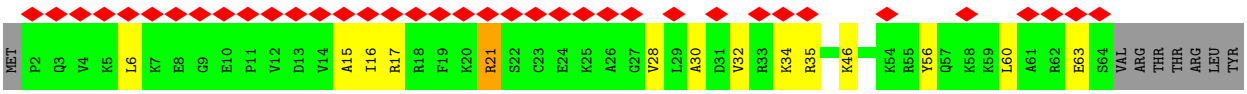
• Molecule 50: 30S ribosomal protein S20

Chain t:



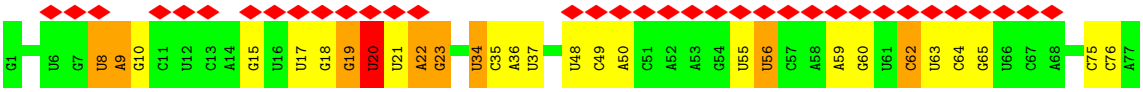
• Molecule 51: 30S ribosomal protein S21

Chain u:

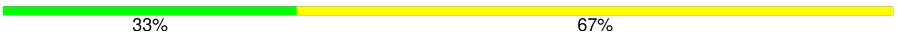


• Molecule 52: tRNA-met

Chain v:



- Molecule 53: mRNA

Chain w: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109599	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.682	Depositor
Minimum map value	-0.209	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	434.176, 434.176, 434.176	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.848, 0.848, 0.848	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: PSU, 4SU, 2MG, 5MC, MG, OMU, H2U, 3TD, UR3, OMG, 2MA, 6MZ, YQM, 5MU, 7MG, MA6, 4OC, ZN

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	0.15	0/434	0.34	0/573
2	1	0.14	0/367	0.31	0/481
3	2	0.14	0/515	0.35	0/678
4	3	0.17	0/296	0.35	0/389
5	A	0.10	0/65229	0.27	0/101736
6	B	0.09	0/2739	0.28	0/4266
7	C	0.12	0/2152	0.32	0/2891
8	D	0.12	0/1590	0.30	0/2142
9	E	0.12	0/1537	0.27	0/2073
10	F	0.18	0/1390	0.47	0/1863
11	G	0.13	0/1337	0.35	0/1807
12	H	0.13	0/461	0.35	0/616
13	I	0.13	0/1151	0.29	0/1551
14	J	0.13	0/956	0.31	0/1286
15	K	0.10	0/1079	0.26	0/1439
16	L	0.13	0/1104	0.31	0/1475
17	M	0.14	0/956	0.34	0/1282
18	N	0.09	0/865	0.26	0/1156
19	O	0.15	0/925	0.33	0/1241
20	P	0.13	0/947	0.29	0/1262
21	Q	0.12	0/818	0.29	0/1094
22	R	0.12	0/831	0.28	0/1113
23	S	0.13	0/716	0.28	0/957
24	T	0.09	0/770	0.25	0/1034
25	U	0.10	0/770	0.27	0/1036
26	V	0.10	0/589	0.30	0/788
27	W	0.11	0/642	0.27	0/856
28	X	0.10	0/487	0.23	0/646
29	Y	0.13	0/468	0.27	0/624
30	Z	0.10	0/453	0.26	0/604
31	a	0.12	0/36476	0.28	0/56895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	b	0.28	1/1799 (0.1%)	0.72	10/2429 (0.4%)
33	c	0.14	0/1714	0.33	0/2304
34	d	0.13	0/1653	0.35	0/2213
35	e	0.13	0/1141	0.34	0/1537
36	f	0.15	0/882	0.35	0/1189
37	g	0.47	2/1087 (0.2%)	0.68	4/1456 (0.3%)
38	h	0.12	0/993	0.30	0/1331
39	i	0.13	0/1002	0.34	0/1339
40	j	0.14	0/811	0.39	0/1096
41	k	0.12	0/878	0.30	0/1189
42	l	0.15	0/958	0.39	0/1284
43	m	0.13	0/913	0.37	0/1226
44	n	0.14	0/803	0.33	0/1071
45	o	0.14	0/715	0.29	0/958
46	p	0.11	0/655	0.31	0/879
47	q	0.12	0/628	0.32	0/847
48	r	0.11	0/432	0.28	0/583
49	s	0.14	0/664	0.30	0/897
50	t	0.14	0/669	0.27	0/892
51	u	0.14	0/528	0.33	0/697
52	v	0.16	1/1739 (0.1%)	0.28	0/2709
53	w	0.08	0/72	0.18	0/110
All	All	0.12	4/149786 (0.0%)	0.30	14/224090 (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
32	b	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	g	71	PRO	CG-CD	-13.36	1.05	1.50
37	g	71	PRO	N-CD	6.20	1.56	1.47
52	v	8	4SU	O3'-P	5.34	1.61	1.56
32	b	141	ARG	CB-CG	5.00	1.67	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	g	71	PRO	N-CD-CG	-15.71	79.63	103.20
32	b	138	GLU	CB-CG-CD	12.32	133.54	112.60
32	b	141	ARG	CB-CG-CD	11.98	138.84	111.30
37	g	71	PRO	CA-N-CD	-10.49	97.32	112.00
32	b	141	ARG	CG-CD-NE	8.75	131.26	112.00
37	g	71	PRO	CA-CB-CG	-8.62	88.12	104.50
32	b	137	LEU	CA-C-N	-7.68	108.64	121.92
32	b	137	LEU	C-N-CA	-7.68	108.64	121.92
32	b	141	ARG	CA-CB-CG	7.43	128.97	114.10
32	b	141	ARG	N-CA-CB	7.33	120.96	109.82
32	b	138	GLU	CB-CA-C	6.36	120.86	109.29
37	g	71	PRO	N-CA-CB	-5.42	98.63	103.35
32	b	141	ARG	CB-CA-C	-5.33	102.45	110.92
32	b	138	GLU	CA-CB-CG	5.24	124.59	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	b	141	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	427	0	462	3	0
2	1	363	0	401	1	0
3	2	509	0	566	2	0
4	3	295	0	326	2	0
5	A	58566	0	29452	233	0
6	B	2450	0	1241	17	0
7	C	2111	0	2176	18	0
8	D	1572	0	1610	11	0
9	E	1516	0	1569	10	0
10	F	1370	0	1420	55	0
11	G	1318	0	1373	14	0
12	H	458	0	480	3	0
13	I	1125	0	1148	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	J	946	0	1007	13	0
15	K	1071	0	1141	3	0
16	L	1087	0	1162	13	0
17	M	942	0	987	4	0
18	N	857	0	899	2	0
19	O	913	0	968	8	0
20	P	934	0	997	7	0
21	Q	807	0	842	6	0
22	R	826	0	894	4	0
23	S	710	0	768	3	0
24	T	766	0	816	6	0
25	U	760	0	783	6	0
26	V	581	0	583	7	0
27	W	632	0	667	2	0
28	X	486	0	528	3	0
29	Y	463	0	488	2	0
30	Z	447	0	435	2	0
31	a	32782	0	16508	149	0
32	b	1769	0	1787	57	0
33	c	1690	0	1774	14	0
34	d	1631	0	1691	18	0
35	e	1129	0	1174	13	0
36	f	867	0	868	16	0
37	g	1073	0	1118	15	0
38	h	985	0	1047	5	0
39	i	991	0	1048	9	0
40	j	801	0	832	9	0
41	k	862	0	877	14	0
42	l	945	0	998	14	0
43	m	903	0	962	8	0
44	n	792	0	833	7	0
45	o	705	0	712	6	0
46	p	644	0	655	2	0
47	q	621	0	665	6	0
48	r	426	0	447	5	0
49	s	646	0	663	3	0
50	t	663	0	715	2	0
51	u	522	0	565	10	0
52	v	1636	0	835	21	0
53	w	65	0	33	2	0
54	3	1	0	0	0	0
55	A	80	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	a	40	0	0	0	0
56	A	138	0	0	0	0
56	B	1	0	0	0	0
56	D	1	0	0	0	0
56	K	1	0	0	0	0
56	a	54	0	0	0	0
56	t	1	0	0	0	0
57	2	1	0	0	0	0
57	A	707	0	0	33	0
57	B	4	0	0	0	0
57	C	7	0	0	1	0
57	D	5	0	0	1	0
57	E	4	0	0	0	0
57	K	7	0	0	0	0
57	R	1	0	0	0	0
57	S	1	0	0	0	0
57	U	1	0	0	0	0
57	Z	7	0	0	0	0
57	a	283	0	0	9	0
57	j	3	0	0	0	0
57	l	1	0	0	0	0
57	m	1	0	0	0	0
57	n	5	0	0	0	0
57	q	1	0	0	0	0
57	s	1	0	0	0	0
57	t	3	0	0	0	0
57	u	1	0	0	0	0
All	All	139817	0	92996	798	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (798) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:38:MET:HE1	10:F:53:ALA:HB1	1.41	1.01
32:b:137:LEU:O	32:b:140:THR:OG1	1.78	1.00
31:a:403:U:O2'	34:d:115:GLU:OE1	1.82	0.98
5:A:1563:C:O2	5:A:1564:A:O2'	1.84	0.94
5:A:1172:U:O2'	5:A:1173:G:O4'	1.87	0.92
32:b:138:GLU:O	32:b:141:ARG:N	2.02	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1865:G:N2	5:A:1868:A:OP2	2.04	0.90
10:F:36:LEU:HD12	10:F:152:MET:HE3	1.55	0.89
10:F:27:GLU:OE1	10:F:161:ARG:NH2	2.07	0.86
16:L:18:THR:O	16:L:98:LYS:NZ	2.08	0.86
17:M:77:GLY:O	17:M:81:THR:OG1	1.93	0.86
32:b:138:GLU:C	32:b:141:ARG:HE	1.82	0.86
5:A:2747:G:O2'	5:A:2748:C:OP1	1.93	0.86
11:G:27:LYS:NZ	11:G:32:THR:OG1	2.10	0.85
5:A:1816:U:OP1	7:C:177:ARG:NH1	2.09	0.85
5:A:799:G:O2'	5:A:800:A:OP1	1.94	0.84
52:v:15:G:OP2	52:v:15:G:N2	2.10	0.84
38:h:43:GLU:OE2	38:h:115:ARG:NH2	2.12	0.83
5:A:1185:G:OP2	57:A:3401:HOH:O	1.96	0.82
5:A:1749:G:N2	5:A:1752:G:OP2	2.13	0.82
1:0:6:ARG:NH1	1:0:49:LYS:O	2.12	0.82
31:a:728:G:OP2	57:a:1701:HOH:O	1.97	0.81
5:A:363:G:OP2	5:A:364:A:O2'	1.97	0.81
25:U:62:GLU:N	25:U:62:GLU:OE1	2.12	0.81
5:A:2861:U:OP2	5:A:2862:G:O2'	1.99	0.81
31:a:85:G:O2'	31:a:86:C:OP2	1.99	0.80
5:A:1327:G:OP2	57:A:3404:HOH:O	1.99	0.80
5:A:1321:U:OP1	57:A:3402:HOH:O	1.98	0.80
32:b:138:GLU:OE1	32:b:141:ARG:CZ	2.29	0.80
31:a:1490:A:O2'	31:a:1491:G:O5'	2.00	0.80
5:A:942:A:OP1	57:A:3403:HOH:O	1.99	0.80
31:a:496:A:O2'	31:a:497:G:OP2	2.00	0.79
5:A:607:A:OP2	57:A:3406:HOH:O	2.00	0.79
3:2:33:THR:OG1	5:A:2416:C:OP1	1.99	0.79
5:A:2254:C:O2'	5:A:2423:C:OP2	2.00	0.79
31:a:1437:U:O2'	31:a:1438:A:O5'	1.99	0.78
5:A:1633:A:OP2	57:A:3405:HOH:O	2.00	0.78
5:A:1933:A:H1'	5:A:1935:5MU:H72	1.66	0.77
5:A:1635:A:OP2	57:A:3408:HOH:O	2.03	0.77
10:F:38:MET:CE	10:F:53:ALA:HB1	2.14	0.77
5:A:324:A:O2'	5:A:325:G:OP1	2.03	0.77
5:A:533:U:O2'	20:P:49:ASP:OD2	2.00	0.77
5:A:2443:G:O2'	5:A:2496:U:OP2	2.02	0.76
5:A:807:G:OP2	57:A:3410:HOH:O	2.03	0.76
5:A:2869:A:OP2	57:A:3407:HOH:O	2.03	0.76
6:B:55:A:O2'	10:F:27:GLU:OE2	2.01	0.76
5:A:184:G:N2	5:A:184:G:OP2	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:649:U:O4	31:a:749:G:O2'	2.03	0.75
31:a:1195:G:OP2	57:a:1702:HOH:O	2.03	0.75
32:b:138:GLU:OE1	32:b:141:ARG:NH1	2.19	0.75
32:b:115:ARG:O	32:b:119:LEU:HD12	1.86	0.75
5:A:1448:U:OP1	57:A:3411:HOH:O	2.05	0.75
5:A:1717:G:O2'	5:A:1735:A:N6	2.20	0.75
5:A:2775:U:OP2	57:A:3409:HOH:O	2.03	0.75
5:A:340:G:N7	57:A:3429:HOH:O	2.19	0.75
41:k:34:THR:HG22	41:k:40:ALA:HA	1.67	0.74
40:j:22:ALA:O	40:j:26:VAL:HG23	1.87	0.74
32:b:137:LEU:HD12	32:b:138:GLU:HB2	1.70	0.74
32:b:138:GLU:C	32:b:141:ARG:NE	2.45	0.74
5:A:1517:G:OP2	5:A:1518:A:O2'	2.03	0.73
5:A:789:C:OP2	57:A:3412:HOH:O	2.06	0.73
40:j:85:ASP:OD1	40:j:86:ALA:N	2.21	0.73
31:a:808:C:OP2	57:a:1704:HOH:O	2.07	0.72
6:B:42:G:O2'	6:B:45:C:N4	2.23	0.72
51:u:6:LEU:HD11	51:u:15:ALA:HB2	1.70	0.72
31:a:628:U:O2	57:a:1705:HOH:O	2.07	0.72
32:b:83:ARG:NH1	32:b:95:ASP:OD2	2.23	0.72
52:v:8:4SU:O2'	52:v:9:A:OP1	2.08	0.72
31:a:189:A:O2'	50:t:59:ASP:OD2	2.08	0.71
37:g:15:ASP:OD1	37:g:19:SER:N	2.23	0.71
5:A:2064:U:OP2	57:A:3415:HOH:O	2.09	0.71
31:a:170:A:OP1	57:a:1703:HOH:O	2.06	0.71
7:C:72:ASP:OD1	7:C:118:SER:OG	2.08	0.71
32:b:139:ARG:NH2	32:b:141:ARG:NH2	2.38	0.71
10:F:136:ILE:O	10:F:137:VAL:HG22	1.91	0.71
10:F:60:ILE:CD1	10:F:152:MET:HE1	2.22	0.70
5:A:2219:G:OP1	7:C:171:TYR:OH	2.10	0.70
26:V:43:THR:HG23	26:V:43:THR:O	1.91	0.70
31:a:924:G:O2'	31:a:1500:A:N7	2.22	0.70
5:A:2436:C:OP2	57:A:3413:HOH:O	2.08	0.70
43:m:40:THR:OG1	43:m:43:THR:OG1	2.10	0.70
5:A:1937:C:N4	5:A:1961:C:O4'	2.25	0.69
7:C:236:GLU:OE2	57:C:301:HOH:O	2.09	0.69
11:G:27:LYS:HE3	11:G:27:LYS:HA	1.74	0.69
35:e:155:LYS:NZ	38:h:72:VAL:O	2.22	0.69
32:b:115:ARG:NH2	32:b:142:GLU:OE2	2.24	0.69
3:2:31:ILE:O	3:2:35:LYS:NZ	2.24	0.69
31:a:84:U:O5'	31:a:85:G:N2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1095:C:O2'	31:a:1164:A:N1	2.25	0.69
5:A:2528:G:O2'	5:A:2653:A:N1	2.26	0.69
5:A:1004:C:OP2	57:A:3417:HOH:O	2.11	0.69
8:D:140:SER:O	57:D:401:HOH:O	2.10	0.69
5:A:2401:G:O2'	5:A:2408:A:N6	2.24	0.68
10:F:8:TYR:HA	10:F:12:LEU:HD23	1.73	0.68
11:G:155:GLU:OE2	11:G:159:GLY:N	2.27	0.68
5:A:2014:G:OP2	57:A:3416:HOH:O	2.09	0.68
5:A:1804:A:OP2	57:A:3418:HOH:O	2.11	0.68
5:A:2026:6MZ:O2'	5:A:2027:A:OP2	2.12	0.68
5:A:2577:G:OP2	5:A:2577:G:N2	2.25	0.68
31:a:647:G:O6	57:a:1706:HOH:O	2.09	0.68
52:v:55:5MU:O2'	52:v:56:PSU:O4'	2.08	0.68
41:k:116:PRO:O	51:u:35:ARG:NH2	2.27	0.67
32:b:139:ARG:N	32:b:141:ARG:HE	1.90	0.67
5:A:2494:C:OP1	57:A:3420:HOH:O	2.11	0.67
5:A:566:U:OP1	57:A:3419:HOH:O	2.11	0.67
9:E:110:GLU:HB3	15:K:3:LEU:HD22	1.76	0.67
5:A:1016:U:OP1	5:A:1032:U:O2'	2.10	0.66
5:A:1104:G:O2'	5:A:1105:U:O4'	2.12	0.66
31:a:520:A:N6	42:l:89:ASP:OD2	2.23	0.66
5:A:91:A:O2'	5:A:92:G:OP2	2.13	0.66
31:a:407:A:O2'	31:a:409:G:OP2	2.14	0.66
41:k:113:THR:HG21	51:u:32:VAL:HG21	1.77	0.66
32:b:85:GLN:N	32:b:85:GLN:OE1	2.29	0.66
32:b:135:GLU:HA	32:b:139:ARG:HH21	1.60	0.66
5:A:1769:A:OP2	57:A:3423:HOH:O	2.14	0.65
5:A:2013:C:OP1	57:A:3421:HOH:O	2.13	0.65
45:o:5:ASN:OD1	45:o:8:ARG:NH1	2.28	0.65
5:A:2309:C:O4'	10:F:37:ASN:ND2	2.30	0.65
5:A:2687:C:HO2'	5:A:2867:U:HO2'	1.45	0.65
10:F:60:ILE:HD13	10:F:152:MET:HE1	1.78	0.65
19:O:91:ARG:NH2	19:O:113:ILE:O	2.28	0.65
32:b:138:GLU:C	32:b:141:ARG:H	2.04	0.65
5:A:69:U:O4	5:A:70:A:N6	2.29	0.65
5:A:605:U:OP1	57:A:3422:HOH:O	2.14	0.65
6:B:50:A:O2'	6:B:51:A:N7	2.30	0.65
5:A:1787:A:OP2	57:A:3424:HOH:O	2.15	0.65
5:A:1950:G:O2'	5:A:1952:U:O4	2.10	0.64
1:0:1:MET:HA	1:0:1:MET:HE2	1.79	0.64
29:Y:5:LYS:NZ	29:Y:36:GLU:OE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:81:LEU:HD22	41:k:104:TYR:HB3	1.80	0.64
32:b:138:GLU:O	32:b:141:ARG:CD	2.46	0.64
5:A:2529:C:OP1	5:A:2661:A:O2'	2.16	0.64
31:a:610:C:OP1	34:d:83:ARG:NH1	2.27	0.64
31:a:1157:G:O6	31:a:1179:G:O6	2.16	0.63
14:J:108:THR:OG1	14:J:109:GLU:OE2	2.16	0.63
14:J:73:ASP:OD1	14:J:75:SER:OG	2.12	0.62
5:A:843:G:O2'	5:A:845:A:N7	2.32	0.62
10:F:34:ILE:HD12	10:F:156:ILE:HG22	1.81	0.62
31:a:1237:U:OP1	37:g:119:ARG:NH2	2.31	0.62
9:E:110:GLU:OE1	9:E:113:ARG:NH2	2.32	0.62
5:A:479:A:OP2	24:T:42:LYS:NZ	2.27	0.62
41:k:28:ASN:OD1	41:k:29:THR:N	2.33	0.62
8:D:30:VAL:O	8:D:188:SER:OG	2.09	0.62
52:v:22:A:O2'	52:v:23:G:O5'	2.17	0.62
31:a:808:C:O2'	31:a:898:A:N1	2.33	0.61
5:A:1962:A:N3	5:A:2588:G:O2'	2.32	0.61
10:F:90:THR:OG1	10:F:92:ARG:NH1	2.33	0.61
32:b:81:ILE:H	32:b:81:ILE:HD12	1.66	0.61
5:A:364:A:OP2	5:A:424:G:O2'	2.18	0.61
10:F:36:LEU:CD1	10:F:152:MET:HE3	2.28	0.61
9:E:56:LYS:NZ	9:E:57:LYS:O	2.31	0.61
42:l:68:GLY:O	42:l:99:ARG:NH1	2.32	0.61
35:e:33:THR:HG22	35:e:51:LYS:HG2	1.83	0.61
5:A:1441:C:HO2'	5:A:1543:A:HO2'	1.45	0.60
5:A:2795:A:O2'	5:A:2797:G:OP2	2.17	0.60
9:E:45:HIS:O	9:E:87:ARG:NH1	2.34	0.60
5:A:499:G:N1	5:A:502:A:OP2	2.35	0.60
33:c:36:ASP:OD1	33:c:59:ARG:NH2	2.34	0.60
5:A:97:C:OP2	5:A:98:A:O2'	2.16	0.60
8:D:176:GLN:OE1	8:D:211:LYS:NZ	2.35	0.60
10:F:31:ILE:HD12	10:F:158:THR:HG22	1.83	0.59
20:P:81:ASP:OD1	20:P:85:LYS:NZ	2.32	0.59
31:a:157:A:N6	31:a:343:G:O2'	2.33	0.59
51:u:6:LEU:HD11	51:u:15:ALA:CB	2.32	0.59
5:A:2496:U:O2	57:A:3425:HOH:O	2.15	0.59
24:T:8:ASP:N	24:T:8:ASP:OD1	2.33	0.59
13:I:23:LYS:NZ	13:I:142:ILE:O	2.35	0.59
34:d:12:SER:OG	34:d:17:THR:O	2.18	0.59
5:A:978:A:OP2	5:A:979:C:N4	2.33	0.58
32:b:138:GLU:HB3	32:b:141:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:A:3201:YQM:O30	55:A:3201:YQM:O33	2.20	0.58
19:O:117:LEU:O	19:O:117:LEU:HD12	2.03	0.58
11:G:33:LEU:HD12	11:G:79:VAL:HG13	1.85	0.58
30:Z:52:GLN:NE2	30:Z:54:PHE:O	2.37	0.58
48:r:27:ASP:N	48:r:27:ASP:OD1	2.35	0.58
31:a:230:C:OP1	57:a:1708:HOH:O	2.17	0.58
40:j:26:VAL:HG13	40:j:36:VAL:HG21	1.85	0.58
5:A:2327:G:O2'	26:V:43:THR:HG22	2.04	0.58
10:F:31:ILE:HG23	10:F:31:ILE:O	2.04	0.58
31:a:1200:C:OP1	44:n:2:ALA:N	2.37	0.57
16:L:33:ALA:HB2	16:L:105:GLU:HG2	1.85	0.57
5:A:1016:U:O2'	5:A:1018:A:N7	2.36	0.57
16:L:35:LYS:NZ	25:U:85:PRO:O	2.37	0.57
31:a:932:A:N1	37:g:3:ARG:NH1	2.52	0.57
5:A:1775:U:OP2	5:A:1780:A:N6	2.29	0.57
5:A:2519:G:HO2'	5:A:2760:A:HO2'	1.44	0.57
28:X:5:ASP:OD1	28:X:5:ASP:N	2.37	0.57
32:b:58:PHE:O	32:b:62:LEU:HD23	2.04	0.57
31:a:572:G:O2'	31:a:818:G:OP2	2.22	0.56
35:e:111:ARG:O	35:e:115:GLU:HG3	2.05	0.56
43:m:77:ILE:HG22	43:m:81:MET:HE2	1.87	0.56
24:T:5:LYS:O	24:T:24:VAL:HG21	2.05	0.56
13:I:106:LYS:HD2	13:I:119:ILE:HD13	1.86	0.56
33:c:50:ALA:O	33:c:70:THR:OG1	2.23	0.56
31:a:670:A:H2'	31:a:671:G:C8	2.40	0.56
5:A:1044:G:H2'	5:A:1108:A:H61	1.69	0.56
10:F:120:LYS:HG2	10:F:121:SER:H	1.71	0.56
32:b:138:GLU:O	32:b:141:ARG:CG	2.54	0.56
5:A:2853:G:N2	5:A:2856:A:OP2	2.35	0.56
5:A:809:U:OP1	57:A:3428:HOH:O	2.18	0.55
5:A:1965:A:HO2'	5:A:1968:G:HO2'	1.53	0.55
5:A:462:G:N2	5:A:465:A:OP2	2.35	0.55
15:K:124:VAL:HG11	15:K:129:LEU:HD11	1.86	0.55
52:v:19:G:OP1	52:v:20:H2U:H5"	2.06	0.55
5:A:2027:A:N3	5:A:2451:G:O2'	2.37	0.55
6:B:12:U:O3'	6:B:104:U:O2'	2.25	0.55
32:b:51:ALA:HB1	32:b:202:ILE:HG22	1.89	0.55
16:L:78:PRO:O	16:L:79:LEU:CB	2.56	0.54
32:b:138:GLU:O	32:b:141:ARG:CB	2.55	0.54
5:A:2747:G:O2'	5:A:2748:C:P	2.66	0.54
5:A:322:G:O2'	5:A:324:A:OP2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:33:LYS:O	10:F:34:ILE:HD13	2.08	0.54
16:L:137:MET:HE1	25:U:78:ILE:HG13	1.90	0.54
31:a:754:U:OP1	31:a:819:U:O2'	2.26	0.54
21:Q:51:ALA:HB3	21:Q:52:PRO:CD	2.37	0.54
35:e:110:MET:HE2	35:e:126:CYS:SG	2.48	0.54
5:A:2312:G:O2'	10:F:125:ARG:NH1	2.40	0.54
10:F:38:MET:SD	10:F:57:MET:HE1	2.47	0.54
42:l:62:GLU:OE2	42:l:62:GLU:HA	2.08	0.54
11:G:17:VAL:HG21	11:G:50:LEU:HD21	1.90	0.53
31:a:423:U:OP2	31:a:424:G:O2'	2.11	0.53
31:a:661:G:H22	31:a:738:G:H1	1.55	0.53
52:v:35:C:H42	53:w:3:G:H22	1.55	0.53
5:A:2379:G:O2'	5:A:2380:U:OP1	2.23	0.53
31:a:949:U:OP2	57:a:1709:HOH:O	2.18	0.53
39:i:127:LYS:NZ	52:v:35:C:OP2	2.28	0.53
43:m:72:GLU:OE2	43:m:76:ASN:ND2	2.41	0.53
32:b:138:GLU:O	32:b:141:ARG:CA	2.57	0.53
6:B:11:A:O2'	6:B:13:A:OP2	2.24	0.53
5:A:226:A:N3	5:A:241:U:O2'	2.39	0.53
16:L:137:MET:HE3	25:U:81:LEU:HB2	1.90	0.53
42:l:15:LEU:H	42:l:15:LEU:HD23	1.74	0.53
32:b:81:ILE:HD12	32:b:81:ILE:N	2.23	0.53
5:A:1292:C:OP2	57:A:3427:HOH:O	2.18	0.52
10:F:149:ILE:HD12	10:F:149:ILE:O	2.08	0.52
39:i:128:ARG:NH2	52:v:34:U:OP2	2.42	0.52
5:A:1567:A:OP1	7:C:61:HIS:NE2	2.37	0.52
50:t:34:ARG:HG2	50:t:34:ARG:HH11	1.74	0.52
36:f:5:GLU:OE1	36:f:63:ASN:ND2	2.32	0.52
19:O:114:ARG:NH1	19:O:114:ARG:HB2	2.25	0.52
40:j:56:HIS:CD2	40:j:57:VAL:HG13	2.45	0.52
43:m:4:ILE:HG23	43:m:57:ARG:HG2	1.92	0.52
10:F:136:ILE:O	10:F:137:VAL:HG13	2.10	0.52
33:c:107:ASP:OD1	33:c:107:ASP:N	2.43	0.52
7:C:17:GLU:OE1	7:C:17:GLU:HA	2.08	0.52
31:a:1156:U:O4'	31:a:1179:G:N2	2.42	0.52
31:a:1437:U:HO2'	31:a:1438:A:P	2.31	0.52
42:l:87:VAL:HG11	42:l:90:LEU:HD12	1.91	0.52
10:F:22:ILE:HD12	10:F:22:ILE:C	2.35	0.52
32:b:132:THR:OG1	32:b:133:LYS:N	2.42	0.52
5:A:2071:U:OP2	5:A:2234:G:O2'	2.29	0.51
5:A:2784:C:O2'	5:A:2805:A:N3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:242:A:C2	31:a:278:A:C5	2.99	0.51
32:b:140:THR:O	32:b:141:ARG:C	2.53	0.51
5:A:2379:G:O2'	5:A:2380:U:P	2.68	0.51
31:a:83:U:OP2	31:a:84:U:N3	2.43	0.51
5:A:303:C:H5"	5:A:336:U:H2'	1.93	0.51
52:v:20:H2U:H1'	52:v:22:A:OP1	2.11	0.51
31:a:1010:G:N2	31:a:1013:A:OP2	2.34	0.51
5:A:975:A:H2'	5:A:976:A:H5'	1.93	0.51
11:G:42:GLU:OE2	11:G:53:ALA:HB3	2.11	0.51
36:f:93:GLU:O	36:f:94:HIS:CG	2.64	0.51
11:G:173:GLU:N	11:G:173:GLU:OE1	2.44	0.50
5:A:2463:C:H2'	5:A:2464:A:O4'	2.11	0.50
10:F:17:GLN:OE1	10:F:22:ILE:HD11	2.10	0.50
31:a:1314:C:OP1	44:n:56:SER:OG	2.23	0.50
32:b:78:ALA:O	32:b:82:ILE:HG22	2.11	0.50
33:c:90:GLU:N	33:c:90:GLU:OE2	2.44	0.50
32:b:43:ILE:HD11	32:b:203:PRO:HB2	1.93	0.50
47:q:26:ILE:N	47:q:26:ILE:HD12	2.27	0.50
5:A:713:A:N1	45:o:53:ARG:NH1	2.59	0.50
5:A:1149:G:H4'	20:P:81:ASP:OD2	2.11	0.50
16:L:107:GLU:OE1	16:L:108:GLY:N	2.43	0.50
31:a:1050:G:H4'	31:a:1051:C:H3'	1.94	0.50
52:v:19:G:P	52:v:20:H2U:H5"	2.52	0.50
7:C:107:PRO:HD2	7:C:110:LEU:HD22	1.94	0.50
7:C:98:ASP:N	7:C:98:ASP:OD2	2.44	0.50
5:A:1033:G:O6	5:A:1116:U:O2	2.30	0.50
21:Q:51:ALA:HB3	21:Q:52:PRO:HD3	1.94	0.50
5:A:115:G:OP1	5:A:295:U:O2'	2.30	0.50
6:B:50:A:O2'	6:B:51:A:C8	2.64	0.50
31:a:1001:A:C6	31:a:1023:G:H1'	2.47	0.50
36:f:70:THR:O	36:f:74:LEU:HD12	2.11	0.50
5:A:1106:C:H2'	5:A:1107:G:C5	2.47	0.49
6:B:11:A:N1	6:B:67:G:O2'	2.34	0.49
8:D:81:LYS:NZ	8:D:82:GLU:O	2.45	0.49
31:a:30:A:O2'	31:a:292:U:OP1	2.28	0.49
31:a:424:G:H1'	31:a:425:U:OP2	2.12	0.49
31:a:1070:U:O2'	32:b:105:ASN:OD1	2.28	0.49
35:e:71:ILE:HD13	35:e:140:PHE:CZ	2.47	0.49
52:v:22:A:HO2'	52:v:23:G:P	2.35	0.49
10:F:136:ILE:C	10:F:137:VAL:HG13	2.36	0.49
13:I:73:LYS:NZ	13:I:86:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:5:LYS:N	24:T:8:ASP:OD2	2.43	0.49
31:a:922:G:C2	31:a:924:G:C8	3.00	0.49
10:F:154:ILE:HD12	10:F:154:ILE:N	2.27	0.49
11:G:11:VAL:HG23	11:G:50:LEU:HD11	1.94	0.49
17:M:95:LEU:HD23	17:M:115:LEU:HD23	1.94	0.49
7:C:5:LYS:NZ	7:C:6:CYS:O	2.45	0.49
28:X:49:THR:O	28:X:53:ILE:HG13	2.13	0.49
34:d:59:GLU:OE1	34:d:59:GLU:HA	2.13	0.49
5:A:92:G:N1	5:A:106:U:C2	2.81	0.49
41:k:112:VAL:HG12	41:k:112:VAL:O	2.12	0.49
5:A:2753:A:N1	11:G:67:THR:HG21	2.27	0.49
7:C:260:ASN:OD1	7:C:262:ARG:N	2.45	0.49
14:J:109:GLU:OE2	14:J:109:GLU:N	2.45	0.49
31:a:1374:A:C6	37:g:7:VAL:HG21	2.48	0.49
36:f:29:ILE:HG22	36:f:34:GLY:HA3	1.93	0.49
5:A:1025:A:N3	5:A:2482:C:O2'	2.40	0.49
13:I:61:GLN:O	13:I:63:GLN:NE2	2.46	0.49
31:a:84:U:O4'	31:a:85:G:N2	2.46	0.49
45:o:74:ASP:OD1	45:o:74:ASP:C	2.56	0.49
5:A:1548:U:OP1	5:A:1736:G:N2	2.45	0.48
10:F:46:ASP:HB2	10:F:49:LEU:HD22	1.95	0.48
16:L:52:ARG:HE	16:L:53:THR:N	2.10	0.48
22:R:31:HIS:NE2	30:Z:24:GLU:OE1	2.45	0.48
5:A:2465:A:N6	5:A:2477:G:O2'	2.46	0.48
6:B:86:U:O2'	6:B:87:A:OP2	2.23	0.48
7:C:3:ILE:HD12	7:C:3:ILE:N	2.28	0.48
31:a:1483:G:H2'	31:a:1484:G:O4'	2.13	0.48
32:b:58:PHE:CZ	32:b:62:LEU:HD21	2.48	0.48
37:g:89:MET:HE3	37:g:90:GLU:H	1.77	0.48
5:A:391:C:C2	5:A:392:C:C5	3.01	0.48
8:D:189:VAL:HG21	19:O:7:LEU:HD21	1.94	0.48
31:a:943:A:H2'	31:a:944:G:C8	2.49	0.48
31:a:1357:A:OP2	44:n:75:ARG:NH2	2.46	0.48
2:1:9:GLU:OE2	2:1:13:LYS:HG2	2.13	0.48
5:A:2048:A:H4'	8:D:151:GLN:O	2.12	0.48
12:H:7:GLN:O	12:H:9:ILE:HD12	2.13	0.48
44:n:73:TYR:O	44:n:79:LEU:O	2.32	0.48
5:A:475:G:N1	5:A:478:A:OP2	2.43	0.48
32:b:190:ASP:OD1	32:b:190:ASP:C	2.56	0.48
5:A:1172:U:HO2'	5:A:1173:G:C1'	2.21	0.48
5:A:782:G:H5'	5:A:783:G:OP1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2287:U:H2'	5:A:2288:G:C8	2.49	0.48
31:a:809:G:H1'	31:a:810:U:OP2	2.13	0.48
35:e:102:THR:HG22	35:e:105:ILE:CD1	2.43	0.48
35:e:150:GLU:OE1	35:e:150:GLU:N	2.43	0.48
36:f:8:LEU:HD23	36:f:87:ASN:HB3	1.96	0.48
52:v:59:A:O2'	52:v:62:C:N4	2.46	0.48
5:A:72:C:O2'	5:A:455:C:N3	2.45	0.48
5:A:1126:A:O2'	5:A:2511:C:O2'	2.32	0.48
5:A:2518:U:O2'	5:A:2643:U:OP1	2.15	0.48
36:f:101:LEU:H	36:f:101:LEU:HD12	1.79	0.48
41:k:98:ALA:O	41:k:102:VAL:HG23	2.14	0.48
19:O:107:SER:O	19:O:111:ALA:N	2.47	0.48
31:a:527:G:N3	31:a:527:G:H2'	2.29	0.48
31:a:126:A:N3	31:a:259:A:O2'	2.35	0.47
31:a:973:G:OP2	31:a:1355:U:O2'	2.32	0.47
42:l:86:ARG:HD2	42:l:88:LYS:N	2.28	0.47
5:A:31:G:O2'	22:R:78:GLU:O	2.32	0.47
5:A:726:G:H3'	5:A:727:G:H5'	1.95	0.47
5:A:2844:G:O2'	5:A:2864:A:N6	2.47	0.47
10:F:46:ASP:CB	10:F:49:LEU:HD22	2.45	0.47
31:a:1069:G:H2'	31:a:1070:U:O4'	2.14	0.47
5:A:309:G:N1	5:A:312:A:OP2	2.43	0.47
31:a:185:C:H1'	31:a:186:G:OP2	2.15	0.47
44:n:72:GLY:O	44:n:80:SER:HA	2.14	0.47
6:B:7:G:C2	6:B:8:A:C8	3.03	0.47
33:c:177:THR:HG21	33:c:206:GLU:OE1	2.13	0.47
34:d:28:PHE:O	34:d:32:THR:HG22	2.14	0.47
47:q:22:ILE:HD13	47:q:76:LEU:HD12	1.95	0.47
10:F:49:LEU:HD23	10:F:50:LEU:H	1.79	0.47
10:F:96:MET:HG3	10:F:97:TYR:N	2.30	0.47
31:a:367:A:H2'	31:a:368:C:O4'	2.14	0.47
31:a:789:A:O2'	31:a:790:U:OP2	2.24	0.47
31:a:1515:MA6:O5'	31:a:1515:MA6:H8	2.14	0.47
45:o:76:GLU:OE2	45:o:76:GLU:N	2.39	0.47
5:A:666:A:H2'	5:A:668:A:H62	1.78	0.47
34:d:87:ALA:HB3	34:d:90:GLU:HG2	1.95	0.47
4:3:23:ILE:HD13	5:A:1029:A:H1'	1.96	0.47
5:A:228:A:O4'	5:A:240:A:O2'	2.31	0.47
5:A:1004:C:OP1	13:I:37:ARG:NH1	2.47	0.47
5:A:2633:U:H2'	5:A:2634:G:O4'	2.15	0.47
6:B:52:G:H21	10:F:26:MET:CE	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:76:VAL:HG12	25:U:97:ARG:HA	1.96	0.47
31:a:358:G:N1	31:a:361:U:OP2	2.47	0.47
32:b:106:TRP:CD1	32:b:110:ARG:HE	2.32	0.47
34:d:115:GLU:OE2	34:d:156:ARG:NE	2.46	0.47
36:f:69:SER:O	36:f:73:GLU:HG2	2.14	0.47
41:k:34:THR:HG22	41:k:40:ALA:CA	2.43	0.47
43:m:3:ARG:O	43:m:3:ARG:HG3	2.14	0.47
5:A:1932:A:OP2	5:A:1958:C:N4	2.44	0.47
8:D:180:ILE:HD13	8:D:192:VAL:HG23	1.96	0.47
32:b:190:ASP:OD2	32:b:192:ASN:ND2	2.47	0.47
23:S:1:MET:HE3	23:S:6:ILE:HG13	1.97	0.47
31:a:207:G:O2'	31:a:208:G:O4'	2.29	0.47
31:a:1527:G:O6	51:u:46:LYS:NZ	2.48	0.47
10:F:107:ALA:O	10:F:111:ILE:HG23	2.15	0.47
14:J:4:THR:HG22	14:J:5:GLU:HG2	1.97	0.47
31:a:1320:G:H2'	31:a:1321:A:C8	2.50	0.47
51:u:17:ARG:HG2	51:u:21:ARG:NH2	2.30	0.47
5:A:2852:A:H2'	5:A:2853:G:O4'	2.15	0.46
10:F:67:VAL:HG12	10:F:84:PRO:HB3	1.97	0.46
32:b:77:ALA:O	32:b:81:ILE:HD13	2.15	0.46
5:A:392:C:C2	5:A:393:U:C5	3.03	0.46
5:A:482:A:OP1	24:T:45:LYS:NZ	2.39	0.46
5:A:2591:G:N2	5:A:2594:A:OP2	2.34	0.46
5:A:2683:U:H2'	5:A:2684:G:O4'	2.15	0.46
18:N:63:THR:O	18:N:64:THR:OG1	2.20	0.46
20:P:97:ASP:OD2	21:Q:13:ARG:NH1	2.48	0.46
32:b:91:GLN:HA	32:b:91:GLN:OE1	2.15	0.46
34:d:32:THR:HG23	34:d:33:LYS:N	2.29	0.46
41:k:36:ARG:O	41:k:37:GLN:HB2	2.15	0.46
5:A:1344:C:C2	5:A:1345:C:C5	3.04	0.46
5:A:2287:U:OP1	5:A:2376:U:O2'	2.31	0.46
5:A:2747:G:C2'	5:A:2748:C:OP1	2.63	0.46
7:C:84:ASP:OD1	7:C:86:ASN:ND2	2.46	0.46
43:m:16:VAL:HG13	43:m:17:ILE:HD12	1.97	0.46
51:u:17:ARG:HA	51:u:21:ARG:HH21	1.81	0.46
5:A:860:G:H2'	5:A:861:A:O4'	2.15	0.46
7:C:3:ILE:O	7:C:3:ILE:HG22	2.15	0.46
22:R:68:ASP:HB2	22:R:109:VAL:HG23	1.97	0.46
31:a:933:C:HO2'	31:a:1379:C:H5	1.63	0.46
5:A:2524:U:O2'	5:A:2526:A:OP1	2.13	0.46
31:a:577:C:H2'	31:a:578:G:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:101:ASP:N	34:d:101:ASP:OD1	2.49	0.46
39:i:34:GLU:H	39:i:34:GLU:CD	2.23	0.46
5:A:494:G:OP1	22:R:6:LYS:NZ	2.48	0.46
5:A:1696:A:H4'	5:A:1697:G:H3'	1.97	0.46
19:O:22:GLU:OE2	19:O:92:ARG:NH1	2.49	0.46
31:a:607:U:N3	31:a:608:C:C5	2.83	0.46
6:B:30:U:C2	6:B:49:G:N2	2.84	0.46
8:D:43:THR:HG23	8:D:44:ASP:OD1	2.16	0.46
37:g:40:GLU:OE2	39:i:41:THR:HG21	2.15	0.46
43:m:33:ILE:O	43:m:37:VAL:HG22	2.14	0.46
44:n:64:CYS:O	44:n:78:GLY:O	2.34	0.46
48:r:25:ASP:OD2	48:r:28:THR:HB	2.16	0.46
5:A:1491:A:N3	5:A:1575:C:O2'	2.36	0.46
5:A:2400:U:H2'	5:A:2401:G:O4'	2.16	0.46
10:F:57:MET:HA	10:F:60:ILE:HG12	1.98	0.46
32:b:138:GLU:HB3	32:b:141:ARG:HH21	1.80	0.46
5:A:1294:G:HO2'	5:A:1296:A:N6	2.13	0.46
5:A:1555:C:OP2	5:A:1556:A:O2'	2.21	0.46
31:a:1237:U:C5	37:g:116:MET:HE2	2.51	0.46
40:j:85:ASP:OD1	40:j:85:ASP:C	2.59	0.46
31:a:127:U:H2'	31:a:128:C:C6	2.51	0.46
31:a:389:A:C2	31:a:390:G:C8	3.04	0.46
31:a:748:U:H2'	31:a:749:G:O4'	2.16	0.46
31:a:1353:G:H2'	31:a:1354:A:C8	2.50	0.46
32:b:138:GLU:HG2	32:b:141:ARG:HB3	1.98	0.46
5:A:390:A:C5	5:A:391:C:C5	3.05	0.45
5:A:799:G:C2'	5:A:800:A:OP1	2.63	0.45
35:e:33:THR:HG22	35:e:51:LYS:CG	2.44	0.45
5:A:1199:A:O4'	5:A:1201:G:C8	2.68	0.45
5:A:1343:C:C5	5:A:1344:C:C5	3.04	0.45
5:A:2379:G:HO2'	5:A:2380:U:P	2.37	0.45
5:A:2843:U:H2'	5:A:2844:G:O4'	2.16	0.45
19:O:47:GLU:OE1	19:O:48:GLY:N	2.50	0.45
31:a:143:G:H2'	31:a:144:G:C8	2.51	0.45
32:b:8:MET:HG3	32:b:12:LEU:CD1	2.46	0.45
32:b:11:LEU:HD23	32:b:214:LEU:HD13	1.98	0.45
24:T:6:LYS:O	24:T:24:VAL:HG23	2.17	0.45
51:u:30:ALA:O	51:u:34:LYS:HG2	2.16	0.45
5:A:2061:C:C2	5:A:2062:C:C5	3.04	0.45
5:A:2067:A:H2'	5:A:2068:C:C6	2.52	0.45
31:a:179:G:C5	31:a:180:U:C6	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1074:G:N2	31:a:1077:A:OP2	2.41	0.45
32:b:42:ILE:HD12	32:b:42:ILE:C	2.41	0.45
5:A:1373:A:O2'	5:A:1374:U:OP2	2.25	0.45
5:A:2200:G:OP2	7:C:147:LYS:NZ	2.48	0.45
10:F:31:ILE:CD1	10:F:158:THR:HG22	2.47	0.45
10:F:123:ASP:OD2	10:F:127:ASN:ND2	2.50	0.45
21:Q:75:ILE:N	21:Q:75:ILE:HD12	2.31	0.45
26:V:43:THR:O	26:V:43:THR:CG2	2.62	0.45
31:a:180:U:C2	31:a:181:C:C5	3.04	0.45
42:l:87:VAL:O	42:l:88:LYS:HB3	2.16	0.45
5:A:92:G:C2	5:A:106:U:O2	2.69	0.45
5:A:2479:C:H1'	16:L:52:ARG:HH12	1.81	0.45
26:V:20:MET:SD	26:V:20:MET:N	2.89	0.45
31:a:742:U:OP1	31:a:848:U:O2'	2.35	0.45
31:a:810:U:OP2	31:a:810:U:H6	1.98	0.45
40:j:28:THR:O	40:j:32:THR:HG22	2.17	0.45
5:A:368:C:O2	5:A:368:C:O4'	2.34	0.45
5:A:1329:G:OP2	57:A:3434:HOH:O	2.21	0.45
5:A:1438:C:C2	5:A:1439:A:C8	3.05	0.45
5:A:1903:G:O6	5:A:1920:C:N4	2.49	0.45
5:A:2302:C:H3'	5:A:2303:G:H5"	1.98	0.45
8:D:39:LYS:NZ	8:D:82:GLU:OE1	2.47	0.45
9:E:3:LEU:HD12	9:E:13:LEU:HD12	1.98	0.45
10:F:36:LEU:HD11	10:F:154:ILE:HG13	1.99	0.45
14:J:104:ARG:NH1	14:J:104:ARG:HG3	2.31	0.45
31:a:1023:G:N3	31:a:1023:G:H2'	2.31	0.45
41:k:22:ILE:HD12	41:k:22:ILE:N	2.31	0.45
5:A:2324:A:H2'	5:A:2325:A:C8	2.52	0.45
32:b:132:THR:HG22	32:b:135:GLU:OE1	2.17	0.45
32:b:202:ILE:O	32:b:202:ILE:CG1	2.65	0.45
39:i:110:GLU:OE2	39:i:113:LYS:NZ	2.35	0.45
31:a:199:G:O2'	31:a:461:A:N1	2.50	0.45
38:h:60:LEU:HD23	38:h:61:THR:N	2.32	0.45
10:F:45:THR:O	10:F:47:LYS:NZ	2.49	0.44
31:a:96:U:O2'	31:a:97:A:N7	2.46	0.44
31:a:906:A:OP1	42:l:18:LYS:NZ	2.50	0.44
33:c:49:ASN:OD1	33:c:49:ASN:N	2.50	0.44
5:A:434:C:O2	5:A:434:C:O4'	2.34	0.44
5:A:1853:G:N2	5:A:1880:G:N3	2.66	0.44
10:F:72:LYS:HG2	10:F:73:SER:N	2.32	0.44
14:J:104:ARG:HG3	14:J:104:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:331:C:C2	31:a:332:A:C8	3.06	0.44
31:a:1436:C:H2'	31:a:1437:U:O4'	2.17	0.44
32:b:33:ILE:O	32:b:35:GLY:N	2.50	0.44
32:b:178:ALA:HB1	32:b:183:ILE:HD11	1.99	0.44
34:d:199:GLU:H	34:d:199:GLU:CD	2.25	0.44
52:v:63:U:H2'	52:v:64:C:O4'	2.17	0.44
4:3:2:LYS:NZ	5:A:2474:A:OP2	2.35	0.44
10:F:38:MET:CE	10:F:57:MET:CE	2.95	0.44
10:F:108:ILE:HD12	10:F:108:ILE:N	2.33	0.44
20:P:107:ALA:O	20:P:111:GLU:HG2	2.17	0.44
31:a:1070:U:O2'	32:b:105:ASN:ND2	2.50	0.44
34:d:199:GLU:OE1	34:d:199:GLU:N	2.50	0.44
26:V:69:PHE:CD2	26:V:80:VAL:HG12	2.52	0.44
36:f:85:ILE:O	36:f:85:ILE:CG1	2.65	0.44
5:A:19:U:O2	5:A:2622:C:H4'	2.17	0.44
5:A:546:G:N3	5:A:546:G:H2'	2.32	0.44
5:A:818:A:H4'	5:A:834:G:H22	1.82	0.44
5:A:1441:C:O2'	5:A:1543:A:O2'	2.20	0.44
5:A:1984:C:N4	5:A:1985:G:O6	2.50	0.44
5:A:2419:U:H4'	5:A:2420:C:O5'	2.16	0.44
31:a:710:G:H2'	31:a:711:G:C8	2.52	0.44
52:v:34:U:O2'	52:v:36:A:N7	2.44	0.44
5:A:365:U:H1'	5:A:366:G:OP2	2.18	0.44
5:A:1494:C:C2	5:A:1495:G:C8	3.05	0.44
5:A:2543:A:H2'	5:A:2544:U:C6	2.52	0.44
9:E:117:LEU:HD11	9:E:187:MET:HE3	2.00	0.44
31:a:489:C:H2'	31:a:490:A:C8	2.52	0.44
31:a:1001:A:H2'	31:a:1002:A:O4'	2.18	0.44
34:d:163:LEU:O	34:d:167:ARG:HG3	2.18	0.44
42:l:23:ALA:HB1	42:l:57:LEU:HD12	1.99	0.44
5:A:1317:A:C5	5:A:1318:C:C5	3.06	0.44
5:A:2804:A:H5'	5:A:2805:A:OP1	2.18	0.44
10:F:34:ILE:HG23	10:F:156:ILE:HG22	2.00	0.44
21:Q:61:ALA:HB2	21:Q:98:ILE:HD13	2.00	0.44
31:a:963:2MG:HM22	52:v:35:C:C5'	2.48	0.44
31:a:1051:C:H1'	31:a:1052:A:OP2	2.18	0.44
31:a:1373:U:OP2	37:g:25:LYS:NZ	2.42	0.44
33:c:32:TYR:O	33:c:59:ARG:NH2	2.50	0.44
5:A:537:A:H2'	5:A:538:G:O4'	2.18	0.44
10:F:162:THR:HG22	10:F:165:GLU:CD	2.43	0.44
31:a:711:G:H2'	31:a:712:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1175:G:N2	31:a:1178:G:OP2	2.50	0.44
31:a:1309:G:H5'	49:s:5:LEU:HD11	1.99	0.44
31:a:1437:U:O2'	31:a:1438:A:P	2.76	0.44
32:b:166:ILE:O	32:b:188:ILE:HB	2.18	0.44
36:f:85:ILE:O	36:f:86:ARG:CB	2.66	0.44
5:A:2043:C:OP2	57:A:3430:HOH:O	2.20	0.44
9:E:15:GLU:O	9:E:19:GLY:N	2.46	0.44
10:F:79:ILE:HG22	10:F:85:ILE:HG21	2.00	0.44
16:L:128:LYS:HE2	16:L:128:LYS:N	2.32	0.44
31:a:1378:U:O2	31:a:1378:U:O4'	2.36	0.44
31:a:1494:G:H1'	31:a:1515:MA6:H2	1.99	0.44
5:A:591:U:H2'	5:A:592:U:C6	2.53	0.43
5:A:1191:C:C2	5:A:1192:G:C8	3.06	0.43
14:J:45:GLU:OE1	14:J:46:ALA:N	2.50	0.43
20:P:91:ASP:OD1	20:P:91:ASP:C	2.60	0.43
31:a:963:2MG:HM22	52:v:35:C:H5'	1.99	0.43
32:b:7:SER:O	32:b:8:MET:CB	2.65	0.43
33:c:43:LEU:HD13	33:c:55:ILE:HD12	2.00	0.43
34:d:57:LEU:O	34:d:61:GLN:HG2	2.18	0.43
39:i:82:THR:O	39:i:86:ILE:HG12	2.18	0.43
42:l:87:VAL:HG11	42:l:90:LEU:CD1	2.48	0.43
5:A:394:U:O2'	5:A:395:G:N7	2.47	0.43
5:A:1355:G:N7	5:A:1356:G:C8	2.86	0.43
5:A:1879:U:H2'	5:A:1880:G:O4'	2.18	0.43
5:A:1951:U:OP2	57:A:3431:HOH:O	2.20	0.43
31:a:555:G:OP2	31:a:556:A:O2'	2.32	0.43
5:A:825:U:OP2	57:A:3433:HOH:O	2.21	0.43
5:A:975:A:H2'	5:A:976:A:C5'	2.48	0.43
31:a:249:U:O2'	47:q:18:MET:SD	2.68	0.43
31:a:976:C:O2	44:n:59:ARG:NH1	2.51	0.43
48:r:36:ASN:O	48:r:36:ASN:ND2	2.38	0.43
5:A:1193:U:C2	5:A:1194:U:C5	3.07	0.43
14:J:69:ILE:C	14:J:69:ILE:HD12	2.43	0.43
16:L:137:MET:HE1	25:U:78:ILE:CG1	2.49	0.43
23:S:20:GLN:NE2	23:S:24:ASP:OD2	2.51	0.43
31:a:457:A:C2	31:a:458:G:C8	3.07	0.43
31:a:889:A:OP2	57:a:1710:HOH:O	2.21	0.43
41:k:93:GLU:OE1	51:u:16:ILE:HG21	2.18	0.43
49:s:44:PHE:N	49:s:44:PHE:CD1	2.85	0.43
5:A:1428:A:H2'	5:A:1429:A:C8	2.54	0.43
5:A:2026:6MZ:O2'	5:A:2027:A:P	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:159:THR:O	10:F:159:THR:HG22	2.19	0.43
31:a:399:C:OP1	34:d:136:SER:OG	2.32	0.43
31:a:747:C:C2	31:a:748:U:C5	3.06	0.43
32:b:40:ILE:HD12	32:b:40:ILE:C	2.43	0.43
33:c:34:LEU:O	33:c:38:GLN:HG3	2.17	0.43
5:A:162:A:H2'	5:A:163:C:O4'	2.17	0.43
5:A:2420:C:OP2	5:A:2421:A:H2'	2.18	0.43
51:u:56:TYR:CE1	51:u:60:LEU:HD11	2.54	0.43
5:A:314:G:C2	5:A:315:U:C6	3.07	0.43
5:A:509:C:N3	5:A:510:U:C5	2.86	0.43
5:A:2747:G:OP2	11:G:3:ARG:NH1	2.51	0.43
46:p:41:ASP:OD1	46:p:42:SER:N	2.52	0.43
5:A:715:C:O2	5:A:715:C:O4'	2.36	0.43
5:A:995:C:OP1	20:P:84:LYS:NZ	2.52	0.43
5:A:2247:OMG:HM23	5:A:2247:OMG:H1'	1.66	0.43
32:b:183:ILE:HD12	32:b:184:PRO:O	2.19	0.43
34:d:15:GLU:OE1	34:d:15:GLU:HA	2.19	0.43
43:m:86:TYR:O	43:m:90:ARG:HG2	2.19	0.43
5:A:1218:G:C4	5:A:1220:G:OP2	2.71	0.42
6:B:12:U:OP2	6:B:68:C:O2'	2.32	0.42
11:G:9:VAL:HG13	11:G:50:LEU:HD13	2.01	0.42
17:M:103:ARG:O	17:M:107:ALA:N	2.51	0.42
31:a:260:A:H4'	47:q:66:ARG:NH1	2.34	0.42
41:k:106:ILE:HD12	41:k:106:ILE:O	2.19	0.42
48:r:32:TYR:CG	48:r:55:LEU:HD11	2.54	0.42
5:A:308:U:H2'	5:A:309:G:O4'	2.19	0.42
5:A:579:C:H2'	5:A:580:A:H8	1.83	0.42
5:A:1676:A:OP1	57:A:3436:HOH:O	2.22	0.42
9:E:105:GLN:NE2	9:E:199:LEU:O	2.49	0.42
10:F:115:ARG:O	10:F:115:ARG:HG2	2.18	0.42
31:a:1070:U:H2'	31:a:1071:G:O4'	2.18	0.42
45:o:8:ARG:O	45:o:12:ILE:HG13	2.19	0.42
5:A:235:U:O2	5:A:235:U:O4'	2.36	0.42
5:A:1469:U:H2'	5:A:1470:G:O4'	2.20	0.42
5:A:1743:A:H2'	5:A:1744:C:O4'	2.19	0.42
16:L:48:GLU:OE1	16:L:48:GLU:HA	2.19	0.42
31:a:1023:G:C2	31:a:1024:C:C6	3.07	0.42
52:v:55:5MU:C3'	52:v:55:5MU:C6	3.03	0.42
5:A:507:U:C4'	5:A:508:C:OP2	2.67	0.42
5:A:1797:A:OP2	7:C:150:LYS:NZ	2.50	0.42
5:A:2456:U:C2	5:A:2457:A:C8	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:13:A:O3'	6:B:14:G:H8	2.02	0.42
14:J:69:ILE:HD11	14:J:77:ILE:HD12	2.02	0.42
14:J:122:LEU:HD12	14:J:122:LEU:C	2.44	0.42
31:a:199:G:H1'	31:a:461:A:H61	1.83	0.42
31:a:1433:U:C2	31:a:1434:A:C8	3.07	0.42
32:b:207:ASP:OD1	32:b:207:ASP:N	2.52	0.42
33:c:11:ARG:NH2	33:c:175:LEU:O	2.52	0.42
36:f:85:ILE:O	36:f:85:ILE:HG13	2.19	0.42
37:g:15:ASP:OD1	37:g:15:ASP:C	2.62	0.42
52:v:20:H2U:O2	52:v:20:H2U:C2'	2.68	0.42
5:A:1173:G:H1'	5:A:1174:U:O5'	2.20	0.42
23:S:6:ILE:HD13	23:S:48:LYS:HD2	2.01	0.42
31:a:887:G:H4'	31:a:888:U:O5'	2.18	0.42
32:b:69:VAL:HG22	32:b:162:ALA:HB3	2.00	0.42
36:f:32:ALA:O	36:f:33:ASP:HB2	2.18	0.42
10:F:102:ARG:HA	10:F:102:ARG:NE	2.34	0.42
31:a:1123:U:H1'	31:a:1124:G:OP1	2.20	0.42
5:A:981:A:N3	5:A:981:A:H2'	2.35	0.42
31:a:504:C:OP2	31:a:505:U:O2'	2.12	0.42
35:e:54:GLU:OE1	35:e:57:ALA:HB2	2.20	0.42
39:i:26:LEU:C	39:i:26:LEU:HD23	2.45	0.42
5:A:368:C:C4'	5:A:369:G:OP2	2.67	0.42
5:A:1922:U:O2	5:A:1925:G:N1	2.53	0.42
7:C:71:LYS:HD3	7:C:96:TYR:CD2	2.55	0.42
36:f:47:LEU:HD13	36:f:51:ILE:HD12	2.02	0.42
52:v:35:C:N4	53:w:3:G:H22	2.17	0.42
5:A:1017:A:N1	5:A:1138:U:O2'	2.43	0.42
5:A:1439:A:C4	5:A:1440:G:C8	3.08	0.42
5:A:1910:C:O2	5:A:1910:C:H2'	2.19	0.42
5:A:2470:U:O2	5:A:2470:U:H2'	2.19	0.42
7:C:5:LYS:NZ	7:C:14:ARG:O	2.46	0.42
10:F:80:ARG:HD3	10:F:80:ARG:N	2.34	0.42
17:M:43:GLU:OE1	17:M:43:GLU:HA	2.19	0.42
31:a:78:G:H2'	31:a:79:U:O4'	2.19	0.42
31:a:540:U:OP1	34:d:14:ARG:NE	2.53	0.42
31:a:591:U:H2'	31:a:592:A:O4'	2.20	0.42
31:a:682:G:H2'	31:a:683:U:C6	2.55	0.42
31:a:1157:G:C2	31:a:1158:C:C6	3.07	0.42
5:A:164:A:H2'	5:A:165:U:O4'	2.19	0.42
5:A:575:G:O2'	5:A:1249:A:OP1	2.38	0.42
10:F:162:THR:HG22	10:F:165:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:94:C:C2	31:a:95:C:C5	3.07	0.42
31:a:717:C:O2	48:r:60:LYS:NZ	2.52	0.42
31:a:1397:C:O2	31:a:1397:C:O4'	2.37	0.42
32:b:190:ASP:OD1	32:b:192:ASN:N	2.53	0.42
35:e:42:ASN:OD1	35:e:42:ASN:O	2.38	0.42
36:f:94:HIS:CD2	36:f:94:HIS:C	2.98	0.42
37:g:27:MET:HE2	37:g:43:VAL:HB	2.02	0.42
5:A:2262:A:H4'	5:A:2263:A:N3	2.35	0.41
31:a:93:A:C6	31:a:94:C:C5	3.08	0.41
31:a:155:G:N2	31:a:158:A:OP2	2.52	0.41
31:a:942:G:C2	31:a:943:A:C8	3.07	0.41
34:d:145:ILE:HD12	34:d:145:ILE:N	2.35	0.41
40:j:23:GLN:OE1	40:j:23:GLN:HA	2.19	0.41
5:A:1313:U:C2	5:A:1314:C:C5	3.08	0.41
12:H:27:ARG:NH1	27:W:60:ASP:OD2	2.53	0.41
14:J:122:LEU:HD12	14:J:122:LEU:OXT	2.20	0.41
26:V:69:PHE:CE2	26:V:80:VAL:HG12	2.55	0.41
42:l:41:THR:HG22	42:l:49:MET:HE1	2.01	0.41
45:o:76:GLU:N	45:o:76:GLU:CD	2.78	0.41
47:q:50:GLU:HA	47:q:50:GLU:OE2	2.20	0.41
5:A:2443:G:H1'	5:A:2444:A:OP2	2.21	0.41
6:B:59:C:C2	6:B:60:U:C5	3.08	0.41
31:a:809:G:C1'	31:a:810:U:OP2	2.67	0.41
31:a:1423:G:C6	31:a:1472:G:C6	3.08	0.41
31:a:1443:A:O2'	31:a:1444:A:H5'	2.20	0.41
35:e:67:ARG:CZ	35:e:67:ARG:HB2	2.50	0.41
35:e:100:GLU:OE2	35:e:101:GLY:N	2.53	0.41
10:F:159:THR:O	10:F:159:THR:CG2	2.68	0.41
12:H:31:ILE:HB	12:H:32:PRO:HD3	2.02	0.41
14:J:5:GLU:OE1	14:J:5:GLU:HA	2.20	0.41
14:J:69:ILE:HD12	14:J:69:ILE:O	2.20	0.41
42:l:116:LYS:O	42:l:117:TYR:HB2	2.20	0.41
5:A:2045:G:O6	57:A:3432:HOH:O	2.21	0.41
5:A:2056:A:O2'	5:A:2057:G:OP2	2.35	0.41
11:G:63:MET:O	11:G:67:THR:HG23	2.21	0.41
19:O:25:PRO:O	19:O:50:VAL:O	2.38	0.41
31:a:6:C:C4'	31:a:7:U:OP1	2.67	0.41
31:a:684:A:C2	31:a:701:A:C5	3.08	0.41
33:c:46:LYS:HB3	33:c:47:LEU:HD22	2.03	0.41
32:b:38:ASN:CG	32:b:39:LYS:H	2.29	0.41
34:d:6:GLY:O	34:d:8:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:391:C:N3	5:A:392:C:C5	2.89	0.41
5:A:720:A:H2'	5:A:721:C:O4'	2.21	0.41
5:A:1586:U:C2	5:A:1587:U:C5	3.09	0.41
6:B:15:C:C2	6:B:16:A:C8	3.09	0.41
31:a:401:U:H3'	31:a:402:G:H5'	2.02	0.41
36:f:74:LEU:HD12	36:f:74:LEU:H	1.85	0.41
46:p:66:GLU:OE1	46:p:69:ARG:NH1	2.53	0.41
5:A:1577:A:C4	5:A:1578:A:C8	3.09	0.41
11:G:17:VAL:O	11:G:17:VAL:HG23	2.20	0.41
31:a:19:U:H2'	31:a:20:C:C6	2.56	0.41
31:a:458:G:C5	31:a:459:U:C4	3.09	0.41
31:a:1064:A:N1	31:a:1105:G:O2'	2.47	0.41
31:a:1431:A:H2'	31:a:1432:G:O4'	2.20	0.41
52:v:20:H2U:O2'	52:v:60:G:N7	2.53	0.41
5:A:83:C:OP1	28:X:48:LYS:NZ	2.49	0.41
5:A:478:A:H4'	5:A:479:A:OP1	2.19	0.41
5:A:1632:U:H4'	5:A:1633:A:OP2	2.20	0.41
5:A:1904:C:H3'	5:A:1905:C:H5"	2.02	0.41
5:A:2428:A:H1'	52:v:76:C:O4'	2.21	0.41
7:C:22:ASP:OD1	7:C:23:HIS:N	2.54	0.41
8:D:152:ASN:O	8:D:153:GLN:C	2.63	0.41
10:F:137:VAL:O	10:F:137:VAL:HG23	2.21	0.41
21:Q:51:ALA:CB	21:Q:52:PRO:HD3	2.50	0.41
26:V:64:ASP:N	26:V:64:ASP:OD1	2.53	0.41
31:a:60:C:O2	31:a:60:C:H2'	2.21	0.41
31:a:109:G:H2'	31:a:110:U:C6	2.56	0.41
31:a:459:U:H5"	31:a:460:U:OP1	2.20	0.41
31:a:497:G:H2'	31:a:498:C:C6	2.56	0.41
31:a:1011:A:OP2	49:s:18:LYS:NZ	2.45	0.41
31:a:1386:C:H2'	31:a:1387:U:O4'	2.21	0.41
31:a:1468:G:C2'	31:a:1469:U:H5'	2.50	0.41
33:c:131:ARG:HG3	33:c:131:ARG:HH11	1.86	0.41
35:e:14:LEU:HD11	35:e:17:VAL:HG23	2.01	0.41
36:f:70:THR:O	36:f:74:LEU:CD1	2.69	0.41
37:g:32:GLN:O	37:g:33:ASP:OD1	2.39	0.41
37:g:32:GLN:C	37:g:33:ASP:OD1	2.64	0.41
37:g:69:VAL:HG12	37:g:69:VAL:O	2.21	0.41
41:k:21:HIS:C	41:k:22:ILE:HD12	2.45	0.41
1:0:6:ARG:HG3	1:0:6:ARG:HH11	1.86	0.41
5:A:92:G:H2'	5:A:93:G:O4'	2.21	0.41
5:A:2699:C:C2	5:A:2700:C:C5	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:112:ARG:HA	10:F:112:ARG:NE	2.36	0.41
13:I:70:LEU:O	13:I:70:LEU:HD23	2.20	0.41
31:a:908:U:H2'	31:a:909:C:C6	2.56	0.41
31:a:915:A:H2'	31:a:916:A:O4'	2.21	0.41
5:A:372:U:C6	5:A:372:U:OP2	2.74	0.40
5:A:605:U:C5	5:A:618:G:C5	3.09	0.40
5:A:847:A:H2'	5:A:848:C:C6	2.56	0.40
5:A:862:G:H2'	5:A:863:C:C6	2.56	0.40
5:A:1493:C:O4'	5:A:1575:C:H4'	2.20	0.40
5:A:2586:A:H2'	5:A:2587:C:H6	1.86	0.40
6:B:50:A:H62	18:N:34:ARG:CG	2.35	0.40
33:c:56:LEU:HG	33:c:58:GLU:OE1	2.20	0.40
40:j:56:HIS:CG	40:j:57:VAL:HG13	2.56	0.40
40:j:80:THR:HG22	40:j:81:ASP:H	1.85	0.40
5:A:799:G:H1'	5:A:800:A:OP1	2.21	0.40
9:E:2:ASN:OD1	9:E:2:ASN:N	2.54	0.40
15:K:128:ALA:C	15:K:129:LEU:HD12	2.46	0.40
27:W:31:PRO:HG2	27:W:33:LEU:HD12	2.03	0.40
31:a:157:A:N6	31:a:343:G:HO2'	2.19	0.40
31:a:1360:A:O2'	31:a:1362:G:N7	2.49	0.40
32:b:81:ILE:H	32:b:81:ILE:CD1	2.33	0.40
32:b:139:ARG:HH22	32:b:141:ARG:NH2	2.17	0.40
38:h:49:VAL:HG13	38:h:60:LEU:HD21	2.02	0.40
5:A:1575:C:H2'	5:A:1576:U:C1'	2.51	0.40
6:B:44:A:C5	6:B:45:C:C5	3.10	0.40
11:G:33:LEU:HD13	11:G:75:LEU:HD23	2.03	0.40
29:Y:6:VAL:HG12	29:Y:28:LEU:HD11	2.03	0.40
31:a:1128:G:C6	31:a:1129:C:C5	3.09	0.40
31:a:1179:G:C4'	31:a:1180:C:OP2	2.69	0.40
32:b:51:ALA:CB	32:b:202:ILE:HG22	2.51	0.40
38:h:10:MET:HG3	38:h:27:MET:SD	2.61	0.40
42:l:74:LEU:HD11	42:l:104:CYS:SG	2.61	0.40
42:l:74:LEU:HD12	42:l:74:LEU:N	2.36	0.40
8:D:13:THR:HG23	8:D:14:ARG:N	2.36	0.40
9:E:118:VAL:HG13	9:E:186:VAL:HA	2.03	0.40
10:F:60:ILE:HG13	10:F:61:ALA:N	2.36	0.40
10:F:136:ILE:O	10:F:137:VAL:CG2	2.66	0.40
10:F:147:ASP:O	10:F:148:ARG:C	2.65	0.40
16:L:51:ARG:HH11	16:L:51:ARG:HG2	1.87	0.40
31:a:1215:C:H2'	31:a:1216:A:C8	2.56	0.40
31:a:1490:A:O2'	31:a:1491:G:C8	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:214:LEU:HD23	32:b:214:LEU:O	2.20	0.40
37:g:40:GLU:CD	39:i:41:THR:HG21	2.46	0.40
37:g:113:GLU:HB2	37:g:119:ARG:HB3	2.02	0.40
47:q:24:VAL:HG22	47:q:26:ILE:HD11	2.02	0.40
5:A:1922:U:C2	5:A:1924:A:OP2	2.74	0.40
5:A:2234:G:N3	5:A:2234:G:H2'	2.37	0.40
10:F:94:ASP:OD1	10:F:94:ASP:N	2.54	0.40
31:a:435:U:C2	31:a:436:A:C8	3.10	0.40
31:a:1187:G:C4'	31:a:1188:A:OP2	2.70	0.40
33:c:181:ASP:OD2	33:c:204:ARG:NH1	2.53	0.40
36:f:38:ARG:HB3	36:f:63:ASN:HB2	2.04	0.40
39:i:82:THR:HG23	39:i:96:LEU:HD22	2.04	0.40
41:k:12:THR:OG1	41:k:13:ARG:N	2.55	0.40

There are no symmetry-related clashes.

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	49/51 (96%)	49 (100%)	0	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	35 (97%)	0	1 (3%)	4	6
7	C	270/274 (98%)	265 (98%)	4 (2%)	1 (0%)	30	49
8	D	209/212 (99%)	200 (96%)	9 (4%)	0	100	100
9	E	198/200 (99%)	198 (100%)	0	0	100	100
10	F	172/178 (97%)	155 (90%)	16 (9%)	1 (1%)	21	38
11	G	172/177 (97%)	164 (95%)	6 (4%)	2 (1%)	10	20
12	H	58/148 (39%)	57 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
14	J	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
15	K	142/146 (97%)	138 (97%)	4 (3%)	0	100	100
16	L	135/137 (98%)	133 (98%)	1 (1%)	1 (1%)	18	34
17	M	117/125 (94%)	116 (99%)	1 (1%)	0	100	100
18	N	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
19	O	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
22	R	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
23	S	89/106 (84%)	88 (99%)	1 (1%)	0	100	100
24	T	101/105 (96%)	98 (97%)	3 (3%)	0	100	100
25	U	95/98 (97%)	95 (100%)	0	0	100	100
26	V	75/85 (88%)	75 (100%)	0	0	100	100
27	W	75/78 (96%)	75 (100%)	0	0	100	100
28	X	58/65 (89%)	58 (100%)	0	0	100	100
29	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	Z	52/61 (85%)	50 (96%)	2 (4%)	0	100	100
32	b	223/250 (89%)	212 (95%)	10 (4%)	1 (0%)	30	49
33	c	213/250 (85%)	206 (97%)	7 (3%)	0	100	100
34	d	205/208 (99%)	195 (95%)	10 (5%)	0	100	100
35	e	153/165 (93%)	152 (99%)	1 (1%)	0	100	100
36	f	102/127 (80%)	98 (96%)	2 (2%)	2 (2%)	6	10
37	g	132/156 (85%)	125 (95%)	7 (5%)	0	100	100
38	h	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
39	i	124/128 (97%)	119 (96%)	5 (4%)	0	100	100
40	j	98/103 (95%)	96 (98%)	2 (2%)	0	100	100
41	k	115/128 (90%)	112 (97%)	3 (3%)	0	100	100
42	l	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	95 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	o	86/89 (97%)	86 (100%)	0	0	100	100
46	p	80/101 (79%)	79 (99%)	1 (1%)	0	100	100
47	q	77/85 (91%)	77 (100%)	0	0	100	100
48	r	50/75 (67%)	49 (98%)	1 (2%)	0	100	100
49	s	80/91 (88%)	80 (100%)	0	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	61/71 (86%)	60 (98%)	1 (2%)	0	100	100
All	All	5413/5872 (92%)	5269 (97%)	135 (2%)	9 (0%)	44	63

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	137	VAL
16	L	79	LEU
32	b	8	MET
36	f	33	ASP
11	G	13	ASN
11	G	81	GLU
4	3	37	GLN
36	f	86	ARG
7	C	3	ILE

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	47/47 (100%)	47 (100%)	0	100	100
2	1	36/36 (100%)	35 (97%)	1 (3%)	38	66
3	2	52/53 (98%)	51 (98%)	1 (2%)	50	76
4	3	33/33 (100%)	31 (94%)	2 (6%)	17	35
7	C	218/220 (99%)	213 (98%)	5 (2%)	44	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	D	166/167 (99%)	162 (98%)	4 (2%)	43	70
9	E	155/155 (100%)	153 (99%)	2 (1%)	61	82
10	F	144/147 (98%)	137 (95%)	7 (5%)	22	45
11	G	139/142 (98%)	139 (100%)	0	100	100
12	H	45/112 (40%)	44 (98%)	1 (2%)	45	73
13	I	118/118 (100%)	117 (99%)	1 (1%)	73	88
14	J	103/103 (100%)	102 (99%)	1 (1%)	68	86
15	K	106/108 (98%)	106 (100%)	0	100	100
16	L	113/113 (100%)	111 (98%)	2 (2%)	51	77
17	M	96/101 (95%)	95 (99%)	1 (1%)	68	86
18	N	83/85 (98%)	80 (96%)	3 (4%)	31	58
19	O	98/102 (96%)	96 (98%)	2 (2%)	48	75
20	P	85/86 (99%)	84 (99%)	1 (1%)	63	83
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	86 (98%)	2 (2%)	44	72
23	S	77/87 (88%)	76 (99%)	1 (1%)	61	82
24	T	83/85 (98%)	81 (98%)	2 (2%)	43	70
25	U	79/80 (99%)	78 (99%)	1 (1%)	61	82
26	V	59/64 (92%)	58 (98%)	1 (2%)	53	78
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	53/56 (95%)	50 (94%)	3 (6%)	18	39
29	Y	54/54 (100%)	54 (100%)	0	100	100
30	Z	46/50 (92%)	45 (98%)	1 (2%)	45	73
32	b	185/200 (92%)	180 (97%)	5 (3%)	39	67
33	c	175/198 (88%)	168 (96%)	7 (4%)	28	54
34	d	170/171 (99%)	166 (98%)	4 (2%)	43	70
35	e	113/120 (94%)	108 (96%)	5 (4%)	25	50
36	f	94/111 (85%)	93 (99%)	1 (1%)	65	84
37	g	113/128 (88%)	112 (99%)	1 (1%)	70	87
38	h	108/109 (99%)	107 (99%)	1 (1%)	70	87
39	i	99/100 (99%)	97 (98%)	2 (2%)	48	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	j	89/91 (98%)	87 (98%)	2 (2%)	45	73
41	k	88/98 (90%)	86 (98%)	2 (2%)	44	72
42	l	104/106 (98%)	101 (97%)	3 (3%)	37	65
43	m	95/98 (97%)	94 (99%)	1 (1%)	65	84
44	n	81/82 (99%)	80 (99%)	1 (1%)	63	83
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	61 (97%)	2 (3%)	34	62
47	q	71/76 (93%)	64 (90%)	7 (10%)	7	16
48	r	46/66 (70%)	45 (98%)	1 (2%)	45	73
49	s	70/78 (90%)	67 (96%)	3 (4%)	26	51
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	54/62 (87%)	51 (94%)	3 (6%)	19	39
All	All	4483/4756 (94%)	4387 (98%)	96 (2%)	46	74

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	41	SER
3	2	64	ILE
4	3	10	ILE
4	3	37	GLN
7	C	38	LYS
7	C	139	SER
7	C	195	VAL
7	C	228	ILE
7	C	273	VAL
8	D	40	THR
8	D	91	GLU
8	D	183	VAL
8	D	192	VAL
9	E	122	GLU
9	E	139	ASP
10	F	18	GLU
10	F	54	VAL
10	F	69	LEU
10	F	101	ASP
10	F	136	ILE
10	F	137	VAL

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Mol	Chain	Res	Type
10	F	149	ILE
12	H	53	GLU
13	I	93	VAL
14	J	34	SER
16	L	55	SER
16	L	66	ILE
17	M	82	VAL
18	N	39	GLN
18	N	41	ILE
18	N	86	VAL
19	O	7	LEU
19	O	41	GLU
20	P	90	ILE
22	R	13	SER
22	R	68	ASP
23	S	79	VAL
24	T	8	ASP
24	T	99	GLU
25	U	69	VAL
26	V	10	THR
28	X	4	LYS
28	X	5	ASP
28	X	12	GLU
30	Z	52	GLN
32	b	85	GLN
32	b	118	ASP
32	b	139	ARG
32	b	144	GLU
32	b	169	ASP
33	c	15	VAL
33	c	17	ARG
33	c	67	THR
33	c	76	VAL
33	c	90	GLU
33	c	95	MET
33	c	191	THR
34	d	121	SER
34	d	136	SER
34	d	175	VAL
34	d	193	LEU
35	e	31	SER
35	e	54	GLU

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Mol	Chain	Res	Type
35	e	60	SER
35	e	129	SER
35	e	148	SER
36	f	93	GLU
37	g	65	THR
38	h	54	GLU
39	i	45	VAL
39	i	50	LEU
40	j	18	ILE
40	j	81	ASP
41	k	79	LYS
41	k	110	THR
42	l	14	THR
42	l	55	VAL
42	l	98	VAL
43	m	89	LEU
44	n	7	ILE
46	p	66	GLU
46	p	80	SER
47	q	14	VAL
47	q	24	VAL
47	q	30	VAL
47	q	42	SER
47	q	43	THR
47	q	59	VAL
47	q	78	GLU
48	r	36	ASN
49	s	35	SER
49	s	58	VAL
49	s	71	LEU
51	u	21	ARG
51	u	28	VAL
51	u	63	GLU

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

Mol	Chain	Res	Type
7	C	25	HIS
8	D	108	GLN
8	D	133	GLN
9	E	40	GLN
9	E	114	GLN

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Mol	Chain	Res	Type
9	E	165	HIS
10	F	37	ASN
10	F	58	GLN
11	G	104	ASN
11	G	106	ASN
13	I	135	GLN
22	R	62	ASN
28	X	24	ASN
29	Y	8	GLN
30	Z	4	GLN
32	b	20	HIS
32	b	111	GLN
33	c	3	GLN
33	c	38	GLN
33	c	176	HIS
34	d	61	GLN
36	f	81	ASN
38	h	4	GLN
39	i	35	GLN
40	j	50	ASN
41	k	118	ASN
42	l	96	HIS
44	n	82	ASN
45	o	75	HIS
50	t	20	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1527/1544 (98%)	243 (15%)	0
5	A	2726/2918 (93%)	449 (16%)	33 (1%)
52	v	76/77 (98%)	17 (22%)	0
53	w	2/3 (66%)	1 (50%)	0
6	B	114/115 (99%)	18 (15%)	2 (1%)
All	All	4445/4657 (95%)	728 (16%)	35 (0%)

All (728) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	U
5	A	41	U

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Mol	Chain	Res	Type
5	A	53	G
5	A	56	A
5	A	58	G
5	A	66	U
5	A	67	G
5	A	70	A
5	A	78	A
5	A	81	A
5	A	82	G
5	A	92	G
5	A	102	A
5	A	106	U
5	A	109	G
5	A	125	A
5	A	127	U
5	A	132	G
5	A	147	A
5	A	149	G
5	A	153	G
5	A	170	A
5	A	172	A
5	A	188	A
5	A	203	A
5	A	206	A
5	A	220	A
5	A	223	A
5	A	229	A
5	A	235	U
5	A	236	U
5	A	239	G
5	A	240	A
5	A	250	U
5	A	255	G
5	A	257	G
5	A	259	G
5	A	262	A
5	A	272	A
5	A	273	G
5	A	275	C
5	A	278	U
5	A	279	U
5	A	303	C

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Mol	Chain	Res	Type
5	A	313	A
5	A	324	A
5	A	325	G
5	A	331	G
5	A	332	A
5	A	333	U
5	A	335	U
5	A	347	A
5	A	348	A
5	A	359	U
5	A	360	A
5	A	365	U
5	A	366	G
5	A	368	C
5	A	369	G
5	A	370	A
5	A	371	G
5	A	372	U
5	A	385	G
5	A	386	U
5	A	389	A
5	A	395	G
5	A	403	A
5	A	410	G
5	A	416	C
5	A	423	G
5	A	434	C
5	A	435	C
5	A	455	C
5	A	479	A
5	A	480	G
5	A	490	G
5	A	493	G
5	A	504	A
5	A	507	U
5	A	508	C
5	A	531	A
5	A	541	C
5	A	543	U
5	A	544	U
5	A	545	C
5	A	546	G

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Mol	Chain	Res	Type
5	A	548	G
5	A	554	A
5	A	561	A
5	A	564	U
5	A	571	U
5	A	573	A
5	A	601	A
5	A	611	U
5	A	612	A
5	A	613	U
5	A	625	A
5	A	633	C
5	A	635	A
5	A	637	U
5	A	644	A
5	A	649	G
5	A	651	U
5	A	656	U
5	A	657	G
5	A	684	U
5	A	692	U
5	A	693	G
5	A	713	A
5	A	722	U
5	A	724	G
5	A	728	A
5	A	745	U
5	A	762	A
5	A	773	G
5	A	774	G
5	A	780	A
5	A	782	G
5	A	783	G
5	A	788	U
5	A	800	A
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U
5	A	826	U
5	A	843	G
5	A	855	G

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Mol	Chain	Res	Type
5	A	857	G
5	A	874	C
5	A	905	G
5	A	908	A
5	A	926	G
5	A	929	C
5	A	930	U
5	A	938	A
5	A	942	A
5	A	943	G
5	A	958	C
5	A	971	G
5	A	976	A
5	A	980	A
5	A	993	A
5	A	1006	A
5	A	1009	U
5	A	1010	C
5	A	1014	G
5	A	1023	G
5	A	1030	U
5	A	1031	G
5	A	1032	U
5	A	1033	G
5	A	1040	C
5	A	1041	A
5	A	1044	G
5	A	1051	A
5	A	1104	G
5	A	1105	U
5	A	1108	A
5	A	1109	G
5	A	1128	G
5	A	1129	U
5	A	1130	A
5	A	1131	A
5	A	1132	C
5	A	1138	U
5	A	1140	A
5	A	1149	G
5	A	1168	A
5	A	1170	U

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Mol	Chain	Res	Type
5	A	1171	U
5	A	1173	G
5	A	1174	U
5	A	1175	A
5	A	1201	G
5	A	1207	G
5	A	1242	A
5	A	1244	U
5	A	1245	G
5	A	1248	A
5	A	1250	U
5	A	1251	G
5	A	1266	G
5	A	1267	A
5	A	1296	A
5	A	1297	A
5	A	1301	C
5	A	1309	C
5	A	1327	G
5	A	1328	G
5	A	1336	G
5	A	1337	A
5	A	1338	G
5	A	1340	C
5	A	1347	U
5	A	1360	A
5	A	1363	G
5	A	1373	A
5	A	1374	U
5	A	1378	A
5	A	1398	A
5	A	1405	U
5	A	1411	G
5	A	1414	A
5	A	1415	U
5	A	1416	G
5	A	1417	A
5	A	1420	G
5	A	1422	A
5	A	1423	C
5	A	1428	A
5	A	1432	C

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Mol	Chain	Res	Type
5	A	1435	A
5	A	1447	G
5	A	1448	U
5	A	1453	U
5	A	1455	U
5	A	1462	G
5	A	1477	U
5	A	1483	U
5	A	1488	C
5	A	1489	A
5	A	1501	C
5	A	1505	A
5	A	1511	A
5	A	1518	A
5	A	1520	A
5	A	1523	A
5	A	1529	U
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1538	A
5	A	1540	C
5	A	1543	A
5	A	1557	U
5	A	1558	G
5	A	1564	A
5	A	1565	G
5	A	1567	A
5	A	1576	U
5	A	1579	G
5	A	1581	U
5	A	1582	U
5	A	1605	G
5	A	1606	A
5	A	1609	C
5	A	1616	A
5	A	1617	G
5	A	1632	U
5	A	1633	A
5	A	1645	U
5	A	1646	U

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Mol	Chain	Res	Type
5	A	1662	A
5	A	1672	G
5	A	1675	A
5	A	1691	U
5	A	1697	G
5	A	1698	A
5	A	1705	G
5	A	1726	C
5	A	1728	C
5	A	1729	U
5	A	1733	U
5	A	1734	G
5	A	1760	G
5	A	1769	A
5	A	1776	A
5	A	1787	A
5	A	1796	C
5	A	1797	A
5	A	1805	A
5	A	1807	G
5	A	1812	C
5	A	1817	A
5	A	1825	A
5	A	1829	C
5	A	1830	U
5	A	1831	G
5	A	1849	A
5	A	1854	A
5	A	1862	A
5	A	1865	G
5	A	1871	G
5	A	1872	A
5	A	1885	A
5	A	1886	A
5	A	1895	A
5	A	1897	A
5	A	1905	C
5	A	1906	G
5	A	1908	A
5	A	1909	A
5	A	1910	C
5	A	1911	3TD

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Mol	Chain	Res	Type
5	A	1915	A
5	A	1917	G
5	A	1918	G
5	A	1919	U
5	A	1923	A
5	A	1926	G
5	A	1927	U
5	A	1933	A
5	A	1934	A
5	A	1936	U
5	A	1950	G
5	A	1951	U
5	A	1959	U
5	A	1960	G
5	A	1963	C
5	A	1966	A
5	A	1967	U
5	A	1968	G
5	A	1978	U
5	A	1987	U
5	A	1989	U
5	A	2018	U
5	A	2019	C
5	A	2025	G
5	A	2026	6MZ
5	A	2027	A
5	A	2029	A
5	A	2039	C
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2058	A
5	A	2065	7MG
5	A	2089	G
5	A	2194	A
5	A	2200	G
5	A	2203	C
5	A	2204	C
5	A	2207	G
5	A	2221	A
5	A	2222	C

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Mol	Chain	Res	Type
5	A	2234	G
5	A	2236	U
5	A	2261	U
5	A	2279	U
5	A	2283	A
5	A	2299	G
5	A	2301	U
5	A	2303	G
5	A	2304	G
5	A	2305	A
5	A	2308	U
5	A	2314	G
5	A	2317	G
5	A	2321	A
5	A	2323	A
5	A	2341	A
5	A	2343	C
5	A	2346	C
5	A	2353	C
5	A	2355	C
5	A	2378	G
5	A	2379	G
5	A	2380	U
5	A	2381	C
5	A	2398	U
5	A	2399	C
5	A	2402	U
5	A	2408	A
5	A	2420	C
5	A	2421	A
5	A	2423	C
5	A	2425	G
5	A	2426	A
5	A	2427	U
5	A	2430	A
5	A	2431	A
5	A	2437	U
5	A	2444	A
5	A	2446	A
5	A	2455	A
5	A	2465	A
5	A	2466	G

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Mol	Chain	Res	Type
5	A	2469	U
5	A	2470	U
5	A	2471	C
5	A	2472	A
5	A	2475	U
5	A	2476	C
5	A	2493	A
5	A	2498	G
5	A	2499	2MA
5	A	2503	C
5	A	2514	A
5	A	2516	C
5	A	2525	G
5	A	2543	A
5	A	2550	U
5	A	2562	A
5	A	2563	G
5	A	2568	A
5	A	2569	C
5	A	2581	U
5	A	2605	U
5	A	2606	C
5	A	2609	U
5	A	2625	U
5	A	2635	A
5	A	2636	G
5	A	2642	C
5	A	2650	A
5	A	2657	G
5	A	2661	A
5	A	2685	U
5	A	2686	A
5	A	2687	C
5	A	2709	C
5	A	2710	G
5	A	2722	U
5	A	2725	U
5	A	2729	A
5	A	2731	G
5	A	2732	G
5	A	2735	U
5	A	2740	G

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Mol	Chain	Res	Type
5	A	2744	A
5	A	2748	C
5	A	2754	A
5	A	2761	A
5	A	2762	G
5	A	2774	A
5	A	2777	A
5	A	2786	U
5	A	2787	A
5	A	2793	U
5	A	2796	U
5	A	2797	G
5	A	2804	A
5	A	2814	U
5	A	2816	G
5	A	2817	A
5	A	2830	G
5	A	2831	A
5	A	2845	G
5	A	2851	U
5	A	2853	G
5	A	2857	U
5	A	2863	A
5	A	2868	G
5	A	2875	A
5	A	2876	C
5	A	2880	U
6	B	2	C
6	B	13	A
6	B	14	G
6	B	22	G
6	B	23	A
6	B	39	C
6	B	40	C
6	B	42	G
6	B	43	A
6	B	44	A
6	B	50	A
6	B	51	A
6	B	64	A
6	B	65	G
6	B	71	A

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Mol	Chain	Res	Type
6	B	86	U
6	B	87	A
6	B	106	A
31	a	6	C
31	a	7	U
31	a	9	A
31	a	10	A
31	a	11	G
31	a	34	A
31	a	41	G
31	a	49	C
31	a	50	U
31	a	53	A
31	a	57	A
31	a	62	A
31	a	64	U
31	a	66	G
31	a	80	A
31	a	81	G
31	a	83	U
31	a	84	U
31	a	85	G
31	a	86	C
31	a	90	C
31	a	91	G
31	a	92	G
31	a	95	C
31	a	97	A
31	a	105	A
31	a	117	U
31	a	124	G
31	a	126	A
31	a	127	U
31	a	130	G
31	a	140	G
31	a	152	C
31	a	157	A
31	a	159	G
31	a	170	A
31	a	184	A
31	a	185	C
31	a	186	G

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Mol	Chain	Res	Type
31	a	193	A
31	a	200	G
31	a	205	U
31	a	206	C
31	a	208	G
31	a	241	U
31	a	243	G
31	a	247	G
31	a	262	G
31	a	263	C
31	a	276	C
31	a	285	G
31	a	289	G
31	a	324	C
31	a	337	C
31	a	340	A
31	a	341	C
31	a	342	G
31	a	343	G
31	a	348	C
31	a	350	G
31	a	359	A
31	a	363	U
31	a	368	C
31	a	388	C
31	a	393	A
31	a	402	G
31	a	407	A
31	a	409	G
31	a	410	A
31	a	418	A
31	a	419	U
31	a	420	G
31	a	425	U
31	a	426	A
31	a	434	U
31	a	442	G
31	a	447	A
31	a	460	U
31	a	461	A
31	a	462	A
31	a	463	U

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Mol	Chain	Res	Type
31	a	476	U
31	a	481	G
31	a	483	U
31	a	494	U
31	a	496	A
31	a	497	G
31	a	508	C
31	a	512	G
31	a	514	G
31	a	515	C
31	a	518	G
31	a	522	C
31	a	524	7MG
31	a	527	G
31	a	528	U
31	a	532	A
31	a	544	A
31	a	556	A
31	a	561	C
31	a	569	A
31	a	570	A
31	a	572	G
31	a	573	C
31	a	574	G
31	a	593	A
31	a	625	G
31	a	630	G
31	a	639	A
31	a	650	A
31	a	662	A
31	a	678	A
31	a	684	A
31	a	685	G
31	a	700	G
31	a	720	U
31	a	721	G
31	a	728	G
31	a	729	C
31	a	731	G
31	a	752	G
31	a	774	A
31	a	778	A

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Mol	Chain	Res	Type
31	a	790	U
31	a	791	A
31	a	810	U
31	a	812	A
31	a	814	C
31	a	816	A
31	a	839	U
31	a	841	G
31	a	846	U
31	a	887	G
31	a	888	U
31	a	911	A
31	a	923	G
31	a	924	G
31	a	926	G
31	a	931	C
31	a	932	A
31	a	951	G
31	a	957	U
31	a	963	2MG
31	a	966	A
31	a	968	G
31	a	972	A
31	a	973	G
31	a	974	A
31	a	980	A
31	a	989	U
31	a	990	G
31	a	994	U
31	a	1001	A
31	a	1006	U
31	a	1007	U
31	a	1019	U
31	a	1023	G
31	a	1027	U
31	a	1029	G
31	a	1030	G
31	a	1032	A
31	a	1033	A
31	a	1043	A
31	a	1051	C
31	a	1052	A

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Mol	Chain	Res	Type
31	a	1062	U
31	a	1063	C
31	a	1067	U
31	a	1068	C
31	a	1071	G
31	a	1085	G
31	a	1091	G
31	a	1092	U
31	a	1096	G
31	a	1098	A
31	a	1101	G
31	a	1122	U
31	a	1124	G
31	a	1130	A
31	a	1134	C
31	a	1136	G
31	a	1140	G
31	a	1156	U
31	a	1157	G
31	a	1163	G
31	a	1165	C
31	a	1166	A
31	a	1179	G
31	a	1180	C
31	a	1181	G
31	a	1182	G
31	a	1185	A
31	a	1188	A
31	a	1189	C
31	a	1193	A
31	a	1194	A
31	a	1198	A
31	a	1210	A
31	a	1224	A
31	a	1235	A
31	a	1238	G
31	a	1255	G
31	a	1276	A
31	a	1277	A
31	a	1284	A
31	a	1295	U
31	a	1297	G

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Mol	Chain	Res	Type
31	a	1299	C
31	a	1317	C
31	a	1335	G
31	a	1342	U
31	a	1343	A
31	a	1350	G
31	a	1360	A
31	a	1367	G
31	a	1378	U
31	a	1394	C
31	a	1395	A
31	a	1399	4OC
31	a	1407	A
31	a	1416	G
31	a	1423	G
31	a	1425	A
31	a	1426	C
31	a	1427	C
31	a	1436	C
31	a	1437	U
31	a	1438	A
31	a	1443	A
31	a	1445	C
31	a	1449	A
31	a	1469	U
31	a	1472	G
31	a	1491	G
31	a	1493	C
31	a	1496	A
31	a	1500	A
31	a	1503	U
31	a	1514	G
31	a	1516	MA6
31	a	1526	G
31	a	1527	G
31	a	1530	C
52	v	9	A
52	v	10	G
52	v	17	U
52	v	18	G
52	v	19	G
52	v	20	H2U

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Mol	Chain	Res	Type
52	v	21	U
52	v	22	A
52	v	23	G
52	v	34	U
52	v	37	U
52	v	48	U
52	v	49	C
52	v	50	A
52	v	62	C
52	v	65	G
52	v	75	C
53	w	2	U

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	91	A
5	A	249	G
5	A	256	C
5	A	272	A
5	A	324	A
5	A	334	A
5	A	365	U
5	A	368	C
5	A	371	G
5	A	406	G
5	A	424	G
5	A	478	A
5	A	496	A
5	A	507	U
5	A	782	G
5	A	799	G
5	A	957	A
5	A	1127	U
5	A	1173	G
5	A	1179	G
5	A	1187	G
5	A	1296	A
5	A	1337	A
5	A	1490	A
5	A	1519	U
5	A	1564	A

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Mol	Chain	Res	Type
5	A	1616	A
5	A	1632	U
5	A	1697	G
5	A	2379	G
5	A	2419	U
5	A	2443	G
5	A	2747	G
6	B	13	A
6	B	86	U

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

28 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	513	31	18,21,22	1.15	1 (5%)	21,30,33	1.96	6 (28%)
5	5MU	A	1935	5	19,22,23	0.38	0	27,32,35	0.51	0
5	7MG	A	2065	5	23,26,27	1.10	1 (4%)	27,39,42	0.90	2 (7%)
31	4OC	a	1399	31	20,23,24	3.21	8 (40%)	25,32,35	0.91	1 (4%)
31	2MG	a	963	56,31	23,26,27	0.46	0	33,38,41	0.54	0
31	UR3	a	1495	31	19,22,23	2.95	6 (31%)	26,32,35	1.64	4 (15%)
52	PSU	v	56	52	18,21,22	1.14	1 (5%)	21,30,33	1.82	4 (19%)
31	5MC	a	964	31	19,22,23	0.50	0	26,32,35	0.59	0
5	2MG	A	2441	5	23,26,27	0.45	0	33,38,41	0.47	0
5	2MA	A	2499	5,56	22,25,26	3.98	9 (40%)	32,37,40	2.70	11 (34%)
5	6MZ	A	2026	5	22,25,26	2.48	4 (18%)	29,36,39	3.35	11 (37%)
5	OMG	A	2247	5	23,26,27	0.45	0	32,38,41	0.50	0
52	4SU	v	8	52	18,21,22	4.46	8 (44%)	25,30,33	2.28	5 (20%)
5	PSU	A	2601	5	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
31	MA6	a	1516	31	23,26,27	1.39	4 (17%)	33,38,41	3.23	12 (36%)
5	PSU	A	2576	5	18,21,22	1.16	1 (5%)	21,30,33	1.99	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
52	H2U	v	20	52	18,21,22	0.48	0	19,30,33	1.40	3 (15%)
31	2MG	a	1204	31	23,26,27	0.48	0	33,38,41	0.47	0
5	PSU	A	952	5	18,21,22	1.09	1 (5%)	21,30,33	1.90	5 (23%)
31	7MG	a	524	31	23,26,27	1.12	1 (4%)	27,39,42	0.87	2 (7%)
5	OMU	A	2548	5	19,22,23	3.12	8 (42%)	25,31,34	1.82	5 (20%)
5	PSU	A	2453	5	18,21,22	1.17	1 (5%)	21,30,33	1.98	6 (28%)
5	PSU	A	1913	5	18,21,22	1.14	1 (5%)	21,30,33	1.89	5 (23%)
52	5MU	v	55	52	19,22,23	0.44	0	27,32,35	0.54	0
5	3TD	A	1911	5	19,22,23	4.47	6 (31%)	23,32,35	1.80	3 (13%)
31	MA6	a	1515	31	23,26,27	1.39	4 (17%)	33,38,41	3.13	11 (33%)
5	PSU	A	2500	5	18,21,22	1.12	1 (5%)	21,30,33	1.94	5 (23%)
5	PSU	A	1907	5	18,21,22	1.16	1 (5%)	21,30,33	1.96	5 (23%)

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	513	31	-	3/7/25/26	0/2/2/2
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
5	7MG	A	2065	5	-	1/7/37/38	0/3/3/3
31	4OC	a	1399	31	-	2/9/29/30	0/2/2/2
31	2MG	a	963	56,31	-	2/9/27/28	0/3/3/3
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
52	PSU	v	56	52	-	3/7/25/26	0/2/2/2
31	5MC	a	964	31	-	0/7/25/26	0/2/2/2
5	2MG	A	2441	5	-	1/9/27/28	0/3/3/3
5	2MA	A	2499	5,56	-	2/7/25/26	0/3/3/3
5	6MZ	A	2026	5	-	0/9/27/28	0/3/3/3
5	OMG	A	2247	5	-	1/9/27/28	0/3/3/3
52	4SU	v	8	52	-	3/7/25/26	0/2/2/2
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
31	MA6	a	1516	31	-	1/11/29/30	0/3/3/3
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
52	H2U	v	20	52	-	5/7/38/39	0/2/2/2
31	2MG	a	1204	31	-	0/9/27/28	0/3/3/3
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
31	7MG	a	524	31	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OMU	A	2548	5	-	0/9/27/28	0/2/2/2
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
5	PSU	A	1913	5	-	1/7/25/26	0/2/2/2
52	5MU	v	55	52	-	5/7/25/26	0/2/2/2
5	3TD	A	1911	5	-	2/7/25/26	0/2/2/2
31	MA6	a	1515	31	-	0/11/29/30	0/3/3/3
5	PSU	A	2500	5	-	0/7/25/26	0/2/2/2
5	PSU	A	1907	5	-	2/7/25/26	0/2/2/2

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1911	3TD	C6-C5	13.49	1.50	1.35
5	A	2499	2MA	C4-N3	12.16	1.50	1.34
5	A	1911	3TD	C2-N1	10.79	1.50	1.37
5	A	2026	6MZ	C6-N6	10.24	1.45	1.34
52	v	8	4SU	C2-N1	9.64	1.53	1.38
52	v	8	4SU	C4-N3	8.84	1.46	1.37
5	A	2499	2MA	C2-N3	7.48	1.46	1.34
31	a	1495	UR3	C2-N1	7.37	1.48	1.38
5	A	2548	OMU	C2-N1	7.35	1.50	1.38
52	v	8	4SU	C5-C4	7.31	1.51	1.42
52	v	8	4SU	C2-N3	7.23	1.50	1.38
31	a	1399	4OC	C4-N3	7.21	1.44	1.32
5	A	2499	2MA	C6-N1	7.10	1.44	1.35
5	A	2548	OMU	C2-N3	6.94	1.50	1.38
31	a	1495	UR3	C6-C5	6.75	1.50	1.35
52	v	8	4SU	C6-C5	6.49	1.50	1.35
31	a	1399	4OC	C2-N3	6.35	1.48	1.36
31	a	1399	4OC	C6-C5	6.27	1.49	1.35
5	A	2499	2MA	C2-N1	6.09	1.44	1.34
5	A	1911	3TD	C6-N1	5.82	1.45	1.36
5	A	2548	OMU	C6-C5	5.79	1.48	1.35
31	a	1495	UR3	C2-N3	5.72	1.50	1.39
5	A	1911	3TD	C2-N3	4.96	1.49	1.38
52	v	8	4SU	C4-S4	-4.85	1.60	1.68
31	a	1399	4OC	C4-N4	4.82	1.46	1.36
5	A	2499	2MA	C5-C6	4.80	1.54	1.41
5	A	2065	7MG	C5-N7	4.56	1.41	1.35
31	a	524	7MG	C5-N7	4.56	1.41	1.35
5	A	2548	OMU	C4-N3	4.42	1.46	1.38
31	a	1399	4OC	C2-N1	4.34	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1516	MA6	C6-N6	4.01	1.47	1.36
52	v	56	PSU	C6-C5	3.99	1.39	1.35
31	a	1515	MA6	C6-N6	3.99	1.47	1.36
5	A	2453	PSU	C6-C5	3.89	1.39	1.35
5	A	1913	PSU	C6-C5	3.83	1.39	1.35
31	a	513	PSU	C6-C5	3.83	1.39	1.35
5	A	1907	PSU	C6-C5	3.83	1.39	1.35
5	A	2576	PSU	C6-C5	3.80	1.39	1.35
5	A	2601	PSU	C6-C5	3.75	1.39	1.35
5	A	2500	PSU	C6-C5	3.71	1.39	1.35
5	A	952	PSU	C6-C5	3.64	1.39	1.35
31	a	1399	4OC	C5-C4	3.63	1.49	1.41
31	a	1495	UR3	C6-N1	3.47	1.46	1.38
31	a	1399	4OC	C6-N1	3.37	1.46	1.38
5	A	2499	2MA	C6-N6	-3.36	1.25	1.34
5	A	1911	3TD	C4-N3	3.16	1.47	1.40
5	A	2026	6MZ	C5-N7	-2.98	1.33	1.39
5	A	2548	OMU	O4-C4	-2.94	1.18	1.24
5	A	2548	OMU	C6-N1	2.93	1.45	1.38
31	a	1516	MA6	C5-C4	-2.86	1.34	1.39
31	a	1515	MA6	C5-C4	-2.80	1.34	1.39
31	a	1495	UR3	C4-N3	2.75	1.46	1.40
52	v	8	4SU	O2-C2	-2.73	1.18	1.23
52	v	8	4SU	C6-N1	2.67	1.44	1.38
31	a	1399	4OC	O2-C2	-2.66	1.18	1.23
5	A	2026	6MZ	C5-C4	-2.58	1.34	1.39
5	A	2548	OMU	C5-C4	2.48	1.49	1.43
5	A	2499	2MA	C5-N7	-2.46	1.34	1.39
5	A	2548	OMU	O2-C2	-2.43	1.18	1.23
31	a	1516	MA6	C5-N7	-2.37	1.34	1.39
31	a	1515	MA6	C5-N7	-2.36	1.34	1.39
31	a	1495	UR3	C5-C4	2.30	1.49	1.43
5	A	2499	2MA	C8-N7	2.23	1.36	1.31
5	A	1911	3TD	O2-C2	-2.22	1.19	1.23
5	A	2026	6MZ	C8-N9	-2.17	1.33	1.37
31	a	1516	MA6	C8-N9	-2.16	1.33	1.37
5	A	2499	2MA	C4-N9	-2.15	1.33	1.37
31	a	1515	MA6	C8-N9	-2.11	1.33	1.37

All (117) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1516	MA6	N1-C6-N6	-11.57	102.76	116.86
31	a	1515	MA6	N1-C6-N6	-11.08	103.36	116.86
5	A	2026	6MZ	C1'-N9-C8	8.58	146.15	127.09
5	A	2026	6MZ	C4-N9-C1'	-8.56	106.62	126.63
31	a	1516	MA6	C5-C6-N6	7.75	137.61	125.33
52	v	8	4SU	C4-N3-C2	-7.68	119.96	127.31
31	a	1515	MA6	C5-C6-N6	7.42	137.07	125.33
5	A	2499	2MA	C1'-N9-C8	-7.33	110.82	127.09
5	A	2026	6MZ	C5-C4-N3	-6.49	117.78	126.72
5	A	2499	2MA	C5-C4-N3	-5.73	121.15	127.18
31	a	1495	UR3	C4-N3-C2	-5.69	120.00	124.58
5	A	2548	OMU	C4-N3-C2	-5.62	119.63	126.61
5	A	1911	3TD	N1-C2-N3	5.61	120.21	116.13
5	A	2499	2MA	N9-C8-N7	-5.60	105.98	113.94
5	A	2026	6MZ	N1-C2-N3	-5.60	120.11	128.58
31	a	1515	MA6	N1-C2-N3	-5.51	120.24	128.58
31	a	1516	MA6	N1-C2-N3	-5.50	120.26	128.58
52	v	8	4SU	C5-C4-N3	5.21	119.59	114.75
5	A	2499	2MA	C4-N9-C1'	5.08	138.51	126.63
31	a	1516	MA6	C5-C4-N3	-5.00	119.83	126.72
5	A	2453	PSU	N1-C2-N3	4.91	120.34	115.17
5	A	2500	PSU	C4-N3-C2	-4.90	119.62	126.37
5	A	2453	PSU	C4-N3-C2	-4.88	119.65	126.37
5	A	1907	PSU	N1-C2-N3	4.88	120.31	115.17
5	A	1907	PSU	C4-N3-C2	-4.88	119.65	126.37
5	A	2576	PSU	N1-C2-N3	4.84	120.28	115.17
5	A	2601	PSU	C4-N3-C2	-4.84	119.70	126.37
31	a	513	PSU	N1-C2-N3	4.84	120.27	115.17
5	A	2576	PSU	C4-N3-C2	-4.82	119.73	126.37
5	A	952	PSU	C4-N3-C2	-4.82	119.73	126.37
5	A	2601	PSU	N1-C2-N3	4.80	120.23	115.17
5	A	2500	PSU	N1-C2-N3	4.80	120.23	115.17
31	a	1515	MA6	C5-C4-N3	-4.78	120.13	126.72
31	a	513	PSU	C4-N3-C2	-4.77	119.79	126.37
5	A	1913	PSU	C4-N3-C2	-4.76	119.82	126.37
5	A	952	PSU	N1-C2-N3	4.75	120.18	115.17
5	A	1913	PSU	N1-C2-N3	4.73	120.16	115.17
5	A	2499	2MA	C4-N9-C8	4.69	110.67	105.74
52	v	56	PSU	N1-C2-N3	4.64	120.06	115.17
5	A	2026	6MZ	C4-C5-C6	4.62	120.62	116.78
52	v	56	PSU	C4-N3-C2	-4.59	120.05	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2026	6MZ	N3-C4-N9	4.37	134.60	127.17
5	A	1911	3TD	C4-N3-C2	-4.35	120.01	124.61
31	a	1515	MA6	N9-C8-N7	-4.24	107.92	113.94
31	a	1516	MA6	N9-C8-N7	-4.22	107.94	113.94
31	a	1516	MA6	C4-C5-C6	4.21	120.26	115.91
5	A	2499	2MA	N3-C4-N9	4.14	132.24	126.99
31	a	1515	MA6	C4-C5-C6	4.13	120.18	115.91
5	A	2026	6MZ	C2-N3-C4	3.96	121.50	111.83
52	v	20	H2U	C5-C4-N3	-3.93	112.51	116.69
5	A	2548	OMU	N3-C2-N1	3.91	119.98	114.89
52	v	8	4SU	N3-C2-N1	3.89	119.96	114.89
31	a	1495	UR3	C5-C4-N3	3.68	119.89	115.04
5	A	2026	6MZ	N9-C8-N7	-3.63	108.79	113.94
52	v	8	4SU	C5-C4-S4	-3.62	120.18	124.31
5	A	2548	OMU	C5-C4-N3	3.57	119.80	114.80
31	a	1515	MA6	C2-N1-C6	3.41	120.16	111.83
31	a	1516	MA6	C2-N1-C6	3.39	120.12	111.83
5	A	2499	2MA	C5-N7-C8	3.36	108.72	103.45
5	A	2499	2MA	N3-C2-N1	-3.34	119.88	125.77
31	a	1516	MA6	C2-N3-C4	3.30	119.89	111.83
31	a	1515	MA6	C2-N3-C4	3.23	119.71	111.83
31	a	513	PSU	O2-C2-N1	-3.13	119.56	122.79
31	a	1516	MA6	N3-C4-N9	3.06	132.37	127.17
31	a	1515	MA6	N3-C4-N9	3.06	132.37	127.17
52	v	20	H2U	O2-C2-N1	3.05	126.77	123.10
5	A	2576	PSU	O2-C2-N1	-3.04	119.66	122.79
5	A	2026	6MZ	C5-N7-C8	3.01	108.17	103.45
31	a	1516	MA6	C5-N7-C8	2.94	108.07	103.45
5	A	1907	PSU	O2-C2-N1	-2.87	119.83	122.79
5	A	2500	PSU	O2-C2-N1	-2.87	119.83	122.79
5	A	2453	PSU	O2-C2-N1	-2.87	119.83	122.79
5	A	2548	OMU	O4-C4-C5	-2.83	120.29	125.16
31	a	1515	MA6	C5-N7-C8	2.81	107.86	103.45
52	v	56	PSU	O2-C2-N1	-2.78	119.92	122.79
5	A	952	PSU	O2-C2-N1	-2.78	119.92	122.79
5	A	1913	PSU	O2-C2-N1	-2.74	119.96	122.79
5	A	2601	PSU	O2-C2-N1	-2.58	120.12	122.79
31	a	1515	MA6	C4-N9-C8	2.54	108.41	105.74
31	a	524	7MG	C4-C5-N7	2.54	108.37	105.38
52	v	56	PSU	C6-N1-C2	-2.48	120.39	122.69
5	A	2576	PSU	O4'-C1'-C2'	2.47	108.56	105.15
5	A	2500	PSU	C6-C5-C4	2.45	119.83	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1907	PSU	C6-N1-C2	-2.45	120.42	122.69
5	A	2026	6MZ	C5-C6-N1	2.44	120.77	118.15
5	A	1913	PSU	C6-N1-C2	-2.44	120.43	122.69
5	A	2453	PSU	C6-C5-C4	2.42	119.81	118.17
5	A	2065	7MG	C4-C5-N7	2.41	108.23	105.38
52	v	8	4SU	C1'-N1-C2	2.41	121.92	117.59
31	a	1399	4OC	C6-C5-C4	2.40	119.89	117.00
5	A	2576	PSU	C6-N1-C2	-2.37	120.49	122.69
31	a	513	PSU	O4'-C1'-C2'	2.35	108.41	105.15
5	A	2453	PSU	C6-N1-C2	-2.35	120.51	122.69
5	A	2601	PSU	C6-N1-C2	-2.34	120.52	122.69
31	a	1516	MA6	C4-N9-C8	2.31	108.16	105.74
5	A	1907	PSU	C6-C5-C4	2.30	119.73	118.17
31	a	1495	UR3	C6-N1-C2	-2.29	119.92	121.80
5	A	2499	2MA	CM2-C2-N1	2.27	120.53	117.13
5	A	2576	PSU	C6-C5-C4	2.26	119.70	118.17
5	A	952	PSU	C6-N1-C2	-2.26	120.59	122.69
5	A	1911	3TD	C6-C5-C4	2.25	119.70	118.19
31	a	513	PSU	C6-N1-C2	-2.24	120.61	122.69
5	A	2499	2MA	C4-C5-N7	-2.24	108.02	110.58
31	a	1516	MA6	C4-C5-N7	-2.23	108.03	110.58
52	v	20	H2U	O2-C2-N3	-2.23	117.38	121.49
5	A	2065	7MG	C5-C4-N9	2.21	109.16	106.33
5	A	2548	OMU	O2-C2-N1	-2.20	119.93	122.80
5	A	2453	PSU	O4'-C1'-C2'	2.18	108.17	105.15
31	a	524	7MG	C5-C4-N9	2.17	109.12	106.33
31	a	513	PSU	C6-C5-C4	2.16	119.63	118.17
5	A	2026	6MZ	C4-C5-N7	-2.10	108.18	110.58
5	A	2601	PSU	C6-C5-C4	2.10	119.59	118.17
5	A	2500	PSU	C6-N1-C2	-2.10	120.75	122.69
5	A	2499	2MA	N6-C6-N1	2.09	119.85	117.03
5	A	1913	PSU	O4'-C1'-C2'	2.05	107.99	105.15
31	a	1495	UR3	C1'-N1-C2	2.05	120.40	117.04
5	A	952	PSU	C6-C5-C4	2.02	119.53	118.17

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	a	513	PSU	C2'-C1'-C5-C4
31	a	963	2MG	O4'-C4'-C5'-O5'
31	a	1399	4OC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
52	v	55	5MU	C2'-C1'-N1-C2
52	v	55	5MU	C2'-C1'-N1-C6
52	v	56	PSU	C2'-C1'-C5-C4
52	v	56	PSU	C2'-C1'-C5-C6
5	A	1911	3TD	C3'-C4'-C5'-O5'
5	A	1911	3TD	O4'-C4'-C5'-O5'
5	A	2247	OMG	C1'-C2'-O2'-CM2
52	v	20	H2U	C2'-C1'-N1-C2
31	a	524	7MG	C3'-C4'-C5'-O5'
31	a	1399	4OC	C3'-C4'-C5'-O5'
52	v	20	H2U	C3'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
31	a	524	7MG	O4'-C4'-C5'-O5'
52	v	20	H2U	O4'-C4'-C5'-O5'
5	A	2499	2MA	O4'-C4'-C5'-O5'
52	v	20	H2U	C2'-C1'-N1-C6
31	a	963	2MG	C3'-C4'-C5'-O5'
31	a	513	PSU	C3'-C4'-C5'-O5'
31	a	513	PSU	O4'-C4'-C5'-O5'
5	A	1907	PSU	C3'-C4'-C5'-O5'
31	a	1516	MA6	C4'-C5'-O5'-P
52	v	56	PSU	O4'-C1'-C5-C4
52	v	55	5MU	O4'-C1'-N1-C6
52	v	20	H2U	C4'-C5'-O5'-P
52	v	8	4SU	O4'-C1'-N1-C6
5	A	2065	7MG	C4'-C5'-O5'-P
5	A	1907	PSU	O4'-C4'-C5'-O5'
5	A	2441	2MG	C3'-C4'-C5'-O5'
5	A	1913	PSU	C3'-C4'-C5'-O5'
52	v	8	4SU	C2'-C1'-N1-C6
52	v	55	5MU	O4'-C1'-N1-C2
52	v	8	4SU	O4'-C1'-N1-C2
52	v	55	5MU	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1935	5MU	1	0
31	a	963	2MG	2	0
52	v	56	PSU	1	0
5	A	2026	6MZ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2247	OMG	1	0
52	v	8	4SU	1	0
52	v	20	H2U	5	0
52	v	55	5MU	2	0
31	a	1515	MA6	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 200 ligands modelled in this entry, 197 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	$\#\|Z\| > 2$
55	YQM	a	1601	56	43,44,44	3.44	22 (51%)	53,69,69	2.76	23 (43%)
55	YQM	A	3202	56	43,44,44	3.62	24 (55%)	53,69,69	2.79	23 (43%)
55	YQM	A	3201	56	43,44,44	3.78	23 (53%)	53,69,69	2.86	23 (43%)

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
55	YQM	a	1601	56	-	0/16/81/81	0/5/5/5
55	YQM	A	3202	56	-	3/16/81/81	0/5/5/5
55	YQM	A	3201	56	-	3/16/81/81	0/5/5/5

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	3201	YQM	C19-C20	14.67	1.64	1.52
55	A	3202	YQM	C19-C20	13.72	1.64	1.52
55	a	1601	YQM	C19-C20	12.52	1.63	1.52
55	A	3201	YQM	C19-C17	8.28	1.65	1.55
55	a	1601	YQM	C19-C17	8.05	1.65	1.55
55	A	3201	YQM	C05-C04	7.84	1.61	1.54
55	A	3202	YQM	C05-C04	7.74	1.61	1.54
55	A	3202	YQM	C19-C17	7.52	1.64	1.55
55	a	1601	YQM	C05-C04	7.25	1.61	1.54
55	A	3201	YQM	C21-C24	6.02	1.60	1.47
55	A	3202	YQM	C21-C24	5.83	1.59	1.47
55	a	1601	YQM	C21-C24	4.97	1.57	1.47
55	A	3202	YQM	C09-C10	4.67	1.45	1.38
55	a	1601	YQM	C19-C05	4.67	1.57	1.53
55	A	3202	YQM	C32-N31	4.59	1.45	1.35
55	A	3201	YQM	C32-N31	4.50	1.45	1.35
55	A	3201	YQM	C09-C10	4.47	1.45	1.38
55	A	3201	YQM	C19-C05	4.38	1.57	1.53
55	a	1601	YQM	C09-C10	4.34	1.45	1.38
55	A	3201	YQM	C14-C15	4.20	1.58	1.45
55	A	3201	YQM	C12-N31	4.06	1.49	1.41
55	A	3201	YQM	C14-C13	4.05	1.49	1.41
55	a	1601	YQM	C32-N31	4.05	1.44	1.35
55	A	3202	YQM	C14-C15	4.02	1.57	1.45
55	A	3202	YQM	C12-N31	3.93	1.49	1.41
55	a	1601	YQM	C17-C16	3.77	1.53	1.46
55	a	1601	YQM	C14-C15	3.74	1.56	1.45
55	A	3202	YQM	C14-C13	3.73	1.48	1.41
55	A	3201	YQM	C17-C16	3.72	1.53	1.46
55	A	3202	YQM	C19-C05	3.67	1.56	1.53
55	a	1601	YQM	C12-N31	3.59	1.48	1.41
55	A	3201	YQM	C15-C16	3.56	1.42	1.36
55	A	3202	YQM	C17-C16	3.41	1.53	1.46
55	A	3202	YQM	C15-C16	3.33	1.42	1.36
55	a	1601	YQM	C14-C13	3.31	1.47	1.41
55	A	3202	YQM	C34-C32	3.28	1.58	1.52
55	A	3201	YQM	C24-N26	3.25	1.42	1.33
55	A	3202	YQM	C24-N26	3.19	1.42	1.33
55	A	3202	YQM	C21-C22	3.18	1.54	1.44
55	A	3201	YQM	C34-C32	3.08	1.58	1.52
55	A	3201	YQM	C12-C13	3.06	1.44	1.40
55	A	3201	YQM	C21-C22	3.06	1.53	1.44
55	a	1601	YQM	C24-N26	3.05	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1601	YQM	C08-C09	3.01	1.55	1.51
55	A	3202	YQM	C36-N35	2.96	1.53	1.47
55	a	1601	YQM	C21-C22	2.95	1.53	1.44
55	A	3202	YQM	C08-C09	2.89	1.55	1.51
55	a	1601	YQM	C15-C16	2.85	1.41	1.36
55	A	3202	YQM	C12-C13	2.80	1.44	1.40
55	a	1601	YQM	C34-C32	2.76	1.57	1.52
55	a	1601	YQM	C11-C10	2.75	1.42	1.37
55	A	3201	YQM	C08-C09	2.75	1.55	1.51
55	A	3202	YQM	C08-C07	2.69	1.59	1.52
55	A	3201	YQM	C04-N02	2.68	1.53	1.47
55	a	1601	YQM	C12-C13	2.64	1.44	1.40
55	a	1601	YQM	C08-C07	2.61	1.59	1.52
55	A	3202	YQM	C11-C10	2.59	1.42	1.37
55	a	1601	YQM	C36-N35	2.58	1.52	1.47
55	A	3202	YQM	C06-C07	2.56	1.59	1.53
55	A	3201	YQM	C08-C07	2.55	1.59	1.52
55	a	1601	YQM	C04-N02	2.53	1.52	1.47
55	A	3201	YQM	C11-C10	2.40	1.41	1.37
55	A	3202	YQM	C04-N02	2.36	1.52	1.47
55	A	3201	YQM	C06-C07	2.34	1.58	1.53
55	A	3201	YQM	C07-C16	2.25	1.53	1.51
55	A	3201	YQM	C36-N35	2.22	1.52	1.47
55	A	3202	YQM	C07-C16	2.13	1.53	1.51
55	a	1601	YQM	C07-C16	2.05	1.53	1.51
55	A	3202	YQM	C11-C12	2.04	1.42	1.39

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	A	3201	YQM	C34-N35-C39	-7.48	103.64	113.34
55	A	3201	YQM	C34-C32-N31	7.08	127.33	114.23
55	a	1601	YQM	C34-N35-C39	-7.06	104.20	113.34
55	A	3202	YQM	C34-C32-N31	7.06	127.29	114.23
55	a	1601	YQM	C34-C32-N31	6.92	127.04	114.23
55	A	3202	YQM	C34-N35-C39	-6.11	105.42	113.34
55	A	3201	YQM	C11-C12-C13	-5.96	114.76	120.53
55	a	1601	YQM	C11-C12-C13	-5.95	114.77	120.53
55	A	3202	YQM	C11-C12-C13	-5.79	114.93	120.53
55	A	3202	YQM	C39-N35-C36	5.60	110.65	104.04
55	a	1601	YQM	O27-C20-C21	5.43	127.41	121.90
55	A	3201	YQM	O27-C20-C21	5.36	127.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	A	3202	YQM	O18-C17-C16	5.05	128.70	121.47
55	A	3201	YQM	O18-C17-C16	4.91	128.50	121.47
55	a	1601	YQM	O18-C17-C19	-4.87	109.84	119.11
55	A	3202	YQM	O27-C20-C21	4.86	126.83	121.90
55	A	3201	YQM	C07-C06-C05	4.66	118.33	110.38
55	A	3201	YQM	O33-C32-C34	-4.62	112.94	121.02
55	A	3202	YQM	O33-C32-C34	-4.60	112.97	121.02
55	a	1601	YQM	O33-C32-C34	-4.50	113.14	121.02
55	A	3201	YQM	O18-C17-C19	-4.43	110.67	119.11
55	A	3202	YQM	O18-C17-C19	-4.37	110.79	119.11
55	A	3202	YQM	C07-C06-C05	4.22	117.56	110.38
55	a	1601	YQM	O18-C17-C16	4.17	127.43	121.47
55	A	3201	YQM	C21-C24-N26	4.14	127.08	118.64
55	a	1601	YQM	C07-C16-C15	-4.12	115.43	121.44
55	A	3202	YQM	C21-C24-N26	4.10	127.00	118.64
55	a	1601	YQM	C07-C06-C05	4.02	117.23	110.38
55	a	1601	YQM	C21-C24-N26	3.96	126.72	118.64
55	A	3202	YQM	C19-C20-C21	-3.72	117.56	122.89
55	A	3201	YQM	O25-C24-N26	-3.69	114.62	122.89
55	A	3202	YQM	O25-C24-N26	-3.62	114.78	122.89
55	a	1601	YQM	O25-C24-N26	-3.51	115.02	122.89
55	A	3202	YQM	O27-C20-C19	-3.44	108.39	113.37
55	A	3202	YQM	C17-C19-C20	3.42	113.89	109.88
55	A	3201	YQM	C24-C21-C22	-3.42	116.79	120.87
55	A	3201	YQM	C17-C19-C20	3.38	113.84	109.88
55	A	3202	YQM	C07-C16-C15	-3.34	116.58	121.44
55	a	1601	YQM	C19-C20-C21	-3.31	118.15	122.89
55	a	1601	YQM	C14-C13-C12	3.30	124.70	118.98
55	A	3201	YQM	C07-C16-C15	-3.27	116.68	121.44
55	a	1601	YQM	O27-C20-C19	-3.23	108.69	113.37
55	A	3202	YQM	C14-C13-C12	3.23	124.58	118.98
55	a	1601	YQM	C39-N35-C36	3.19	107.81	104.04
55	A	3201	YQM	C14-C13-C12	3.18	124.48	118.98
55	A	3201	YQM	O27-C20-C19	-3.17	108.78	113.37
55	A	3201	YQM	C06-C05-C04	-3.13	109.21	113.73
55	A	3201	YQM	C19-C05-C04	3.10	115.88	111.64
55	a	1601	YQM	C19-C05-C04	3.05	115.81	111.64
55	A	3201	YQM	C39-N35-C36	3.05	107.64	104.04
55	a	1601	YQM	C06-C05-C04	-2.91	109.53	113.73
55	a	1601	YQM	C06-C07-C16	2.83	116.43	110.28
55	A	3202	YQM	C24-C21-C22	-2.80	117.53	120.87
55	a	1601	YQM	C17-C19-C20	2.78	113.14	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	A	3201	YQM	C19-C20-C21	-2.73	118.97	122.89
55	A	3202	YQM	C19-C05-C04	2.68	115.31	111.64
55	A	3201	YQM	C06-C07-C16	2.66	116.05	110.28
55	A	3202	YQM	C06-C05-C04	-2.51	110.11	113.73
55	A	3202	YQM	C06-C07-C16	2.50	115.70	110.28
55	a	1601	YQM	C24-C21-C22	-2.47	117.92	120.87
55	A	3201	YQM	O28-C19-C20	-2.36	106.37	110.14
55	a	1601	YQM	O28-C19-C20	-2.33	106.42	110.14
55	A	3201	YQM	O29-C15-C14	-2.23	113.53	118.45
55	A	3202	YQM	O28-C19-C20	-2.23	106.58	110.14
55	A	3201	YQM	O33-C32-N31	-2.18	119.73	123.64
55	A	3202	YQM	O33-C32-N31	-2.17	119.75	123.64
55	a	1601	YQM	O29-C15-C14	-2.15	113.71	118.45
55	a	1601	YQM	O33-C32-N31	-2.14	119.81	123.64
55	A	3202	YQM	O29-C15-C14	-2.13	113.75	118.45

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	3201	YQM	C11-C12-N31-C32
55	A	3201	YQM	C13-C12-N31-C32
55	A	3202	YQM	O33-C32-C34-N35
55	A	3202	YQM	N31-C32-C34-N35
55	A	3201	YQM	O33-C32-C34-N35
55	A	3202	YQM	C20-C21-C24-O25

There are no ring outliers.

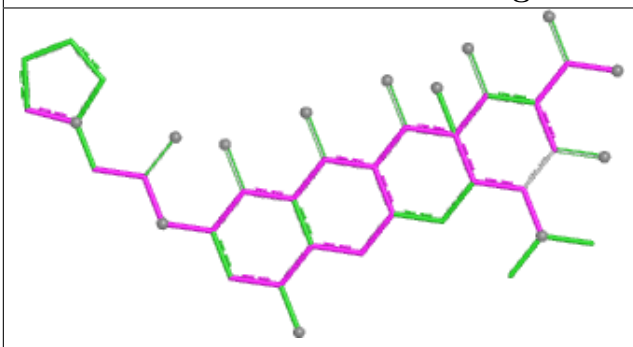
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	A	3201	YQM	1	0

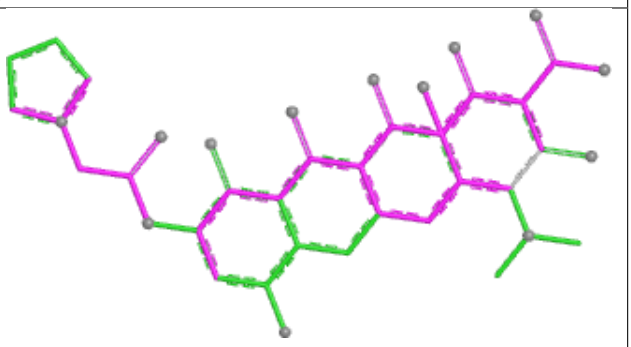
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

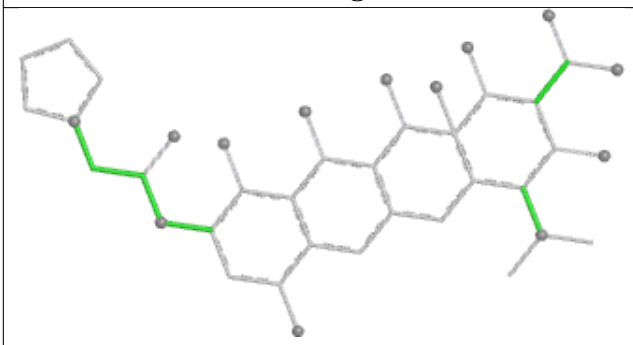
Ligand YQM a 1601



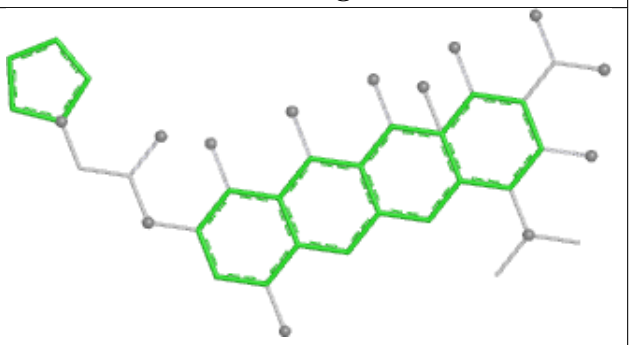
Bond lengths



Bond angles

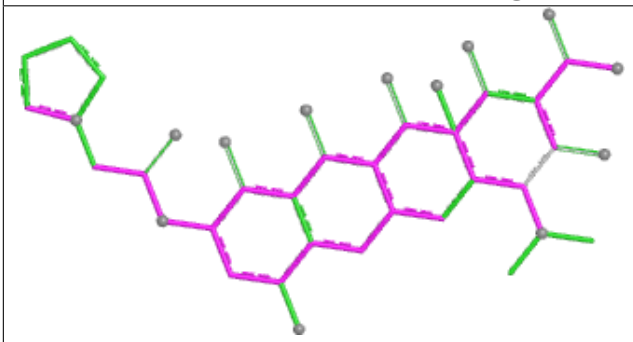


Torsions

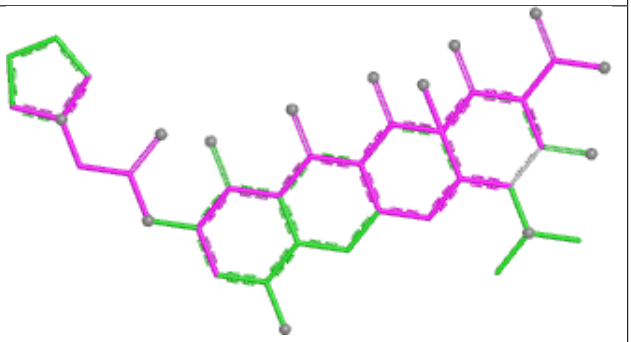


Rings

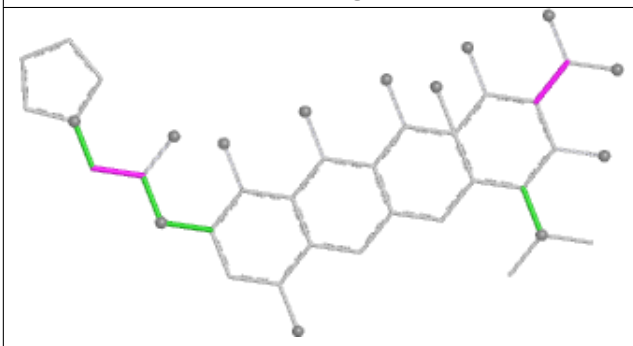
Ligand YQM A 3202



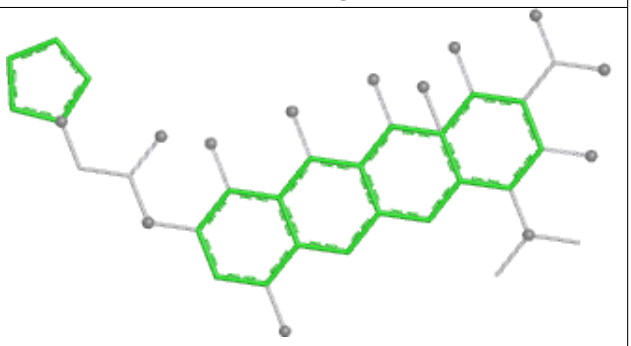
Bond lengths



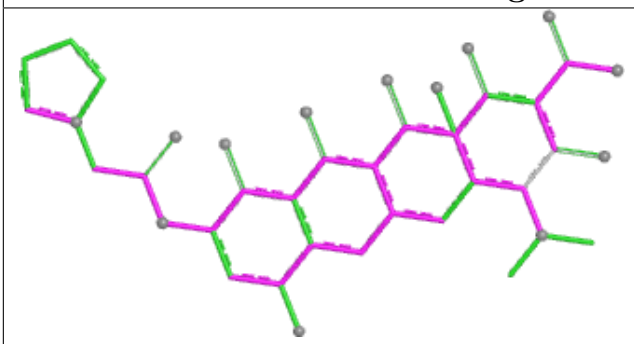
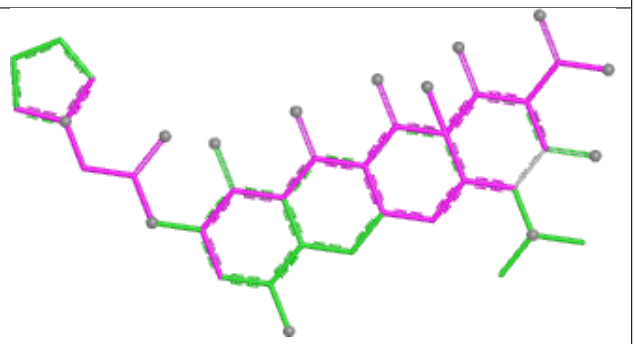
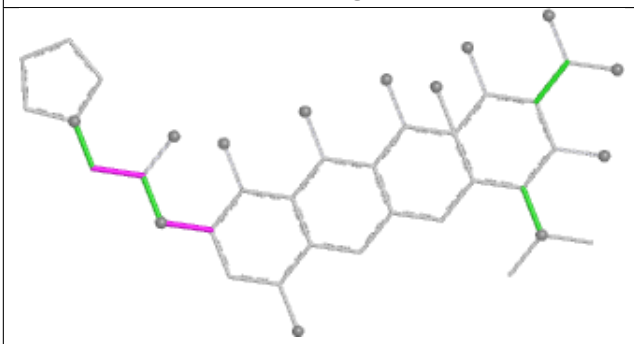
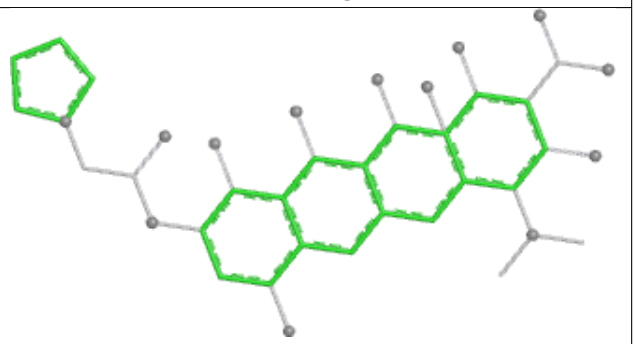
Bond angles



Torsions



Rings

Ligand YQM A 3201	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

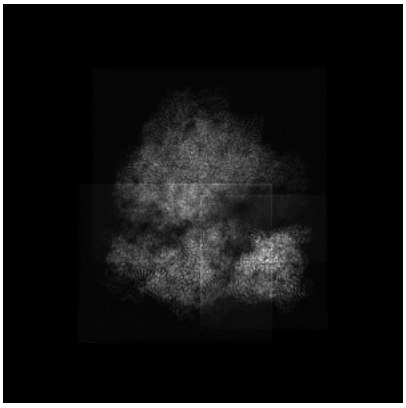
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23670. These allow visual inspection of the internal detail of the map and identification of artifacts.

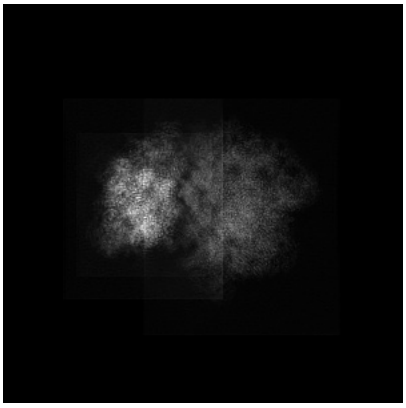
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

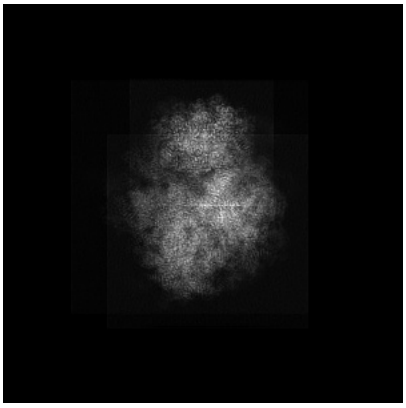
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 256

Y Index: 256

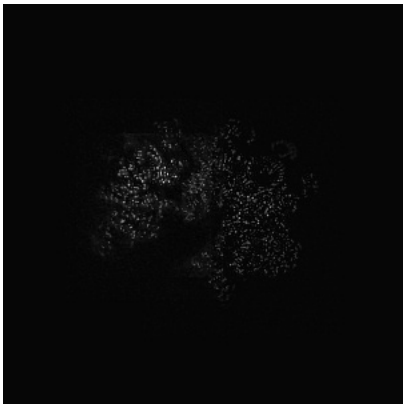
Z Index: 256

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

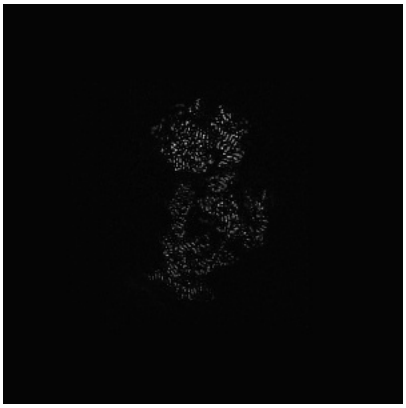
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 280



Y Index: 253

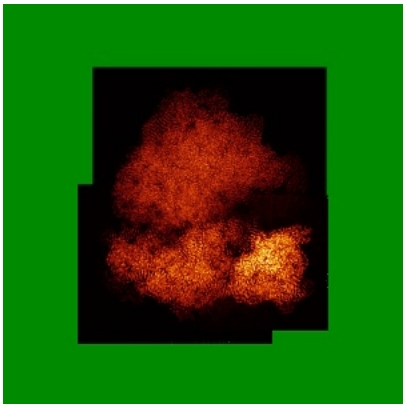


Z Index: 180

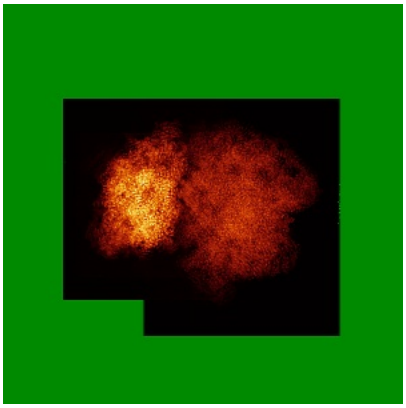
The images above show the largest variance slices of the map in three orthogonal directions.

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

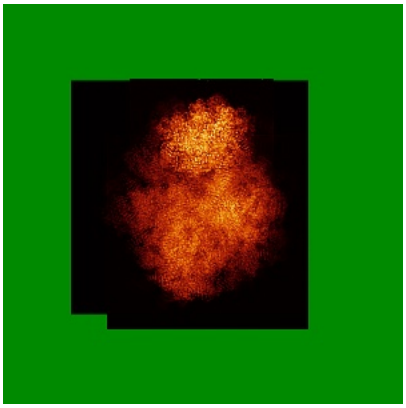
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

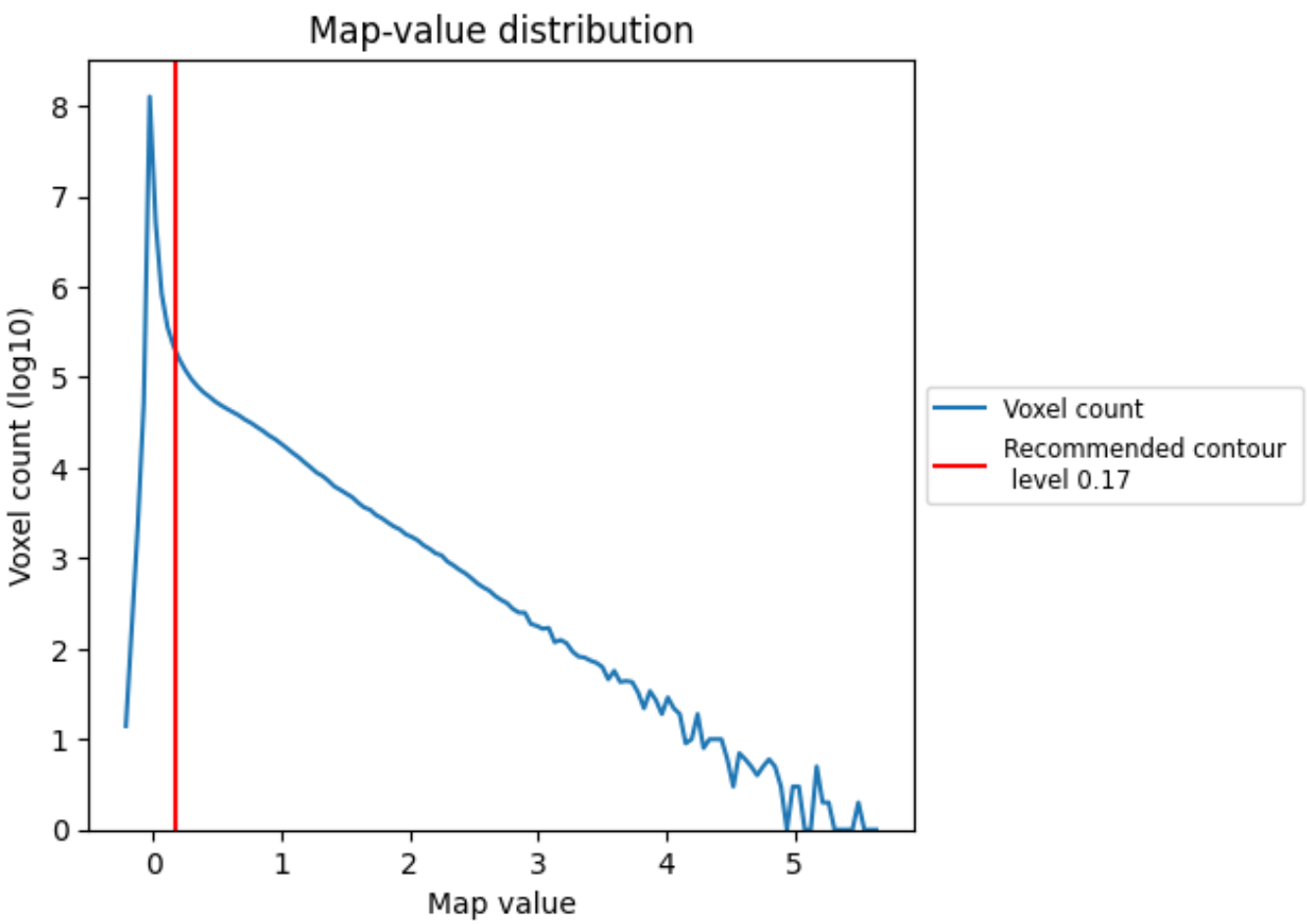
6.6 Mask visualisation (i)

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

7 Map analysis (i)

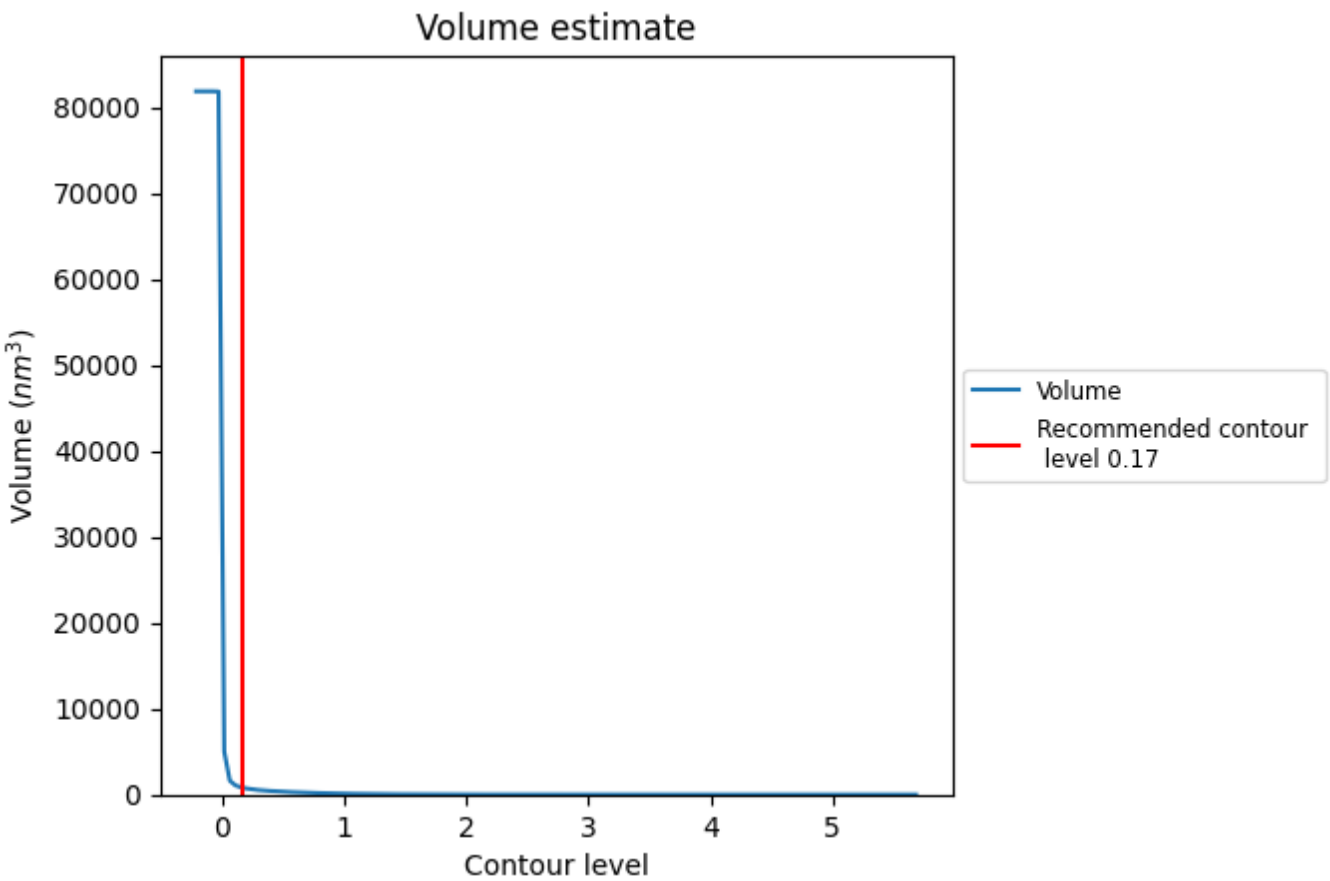
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

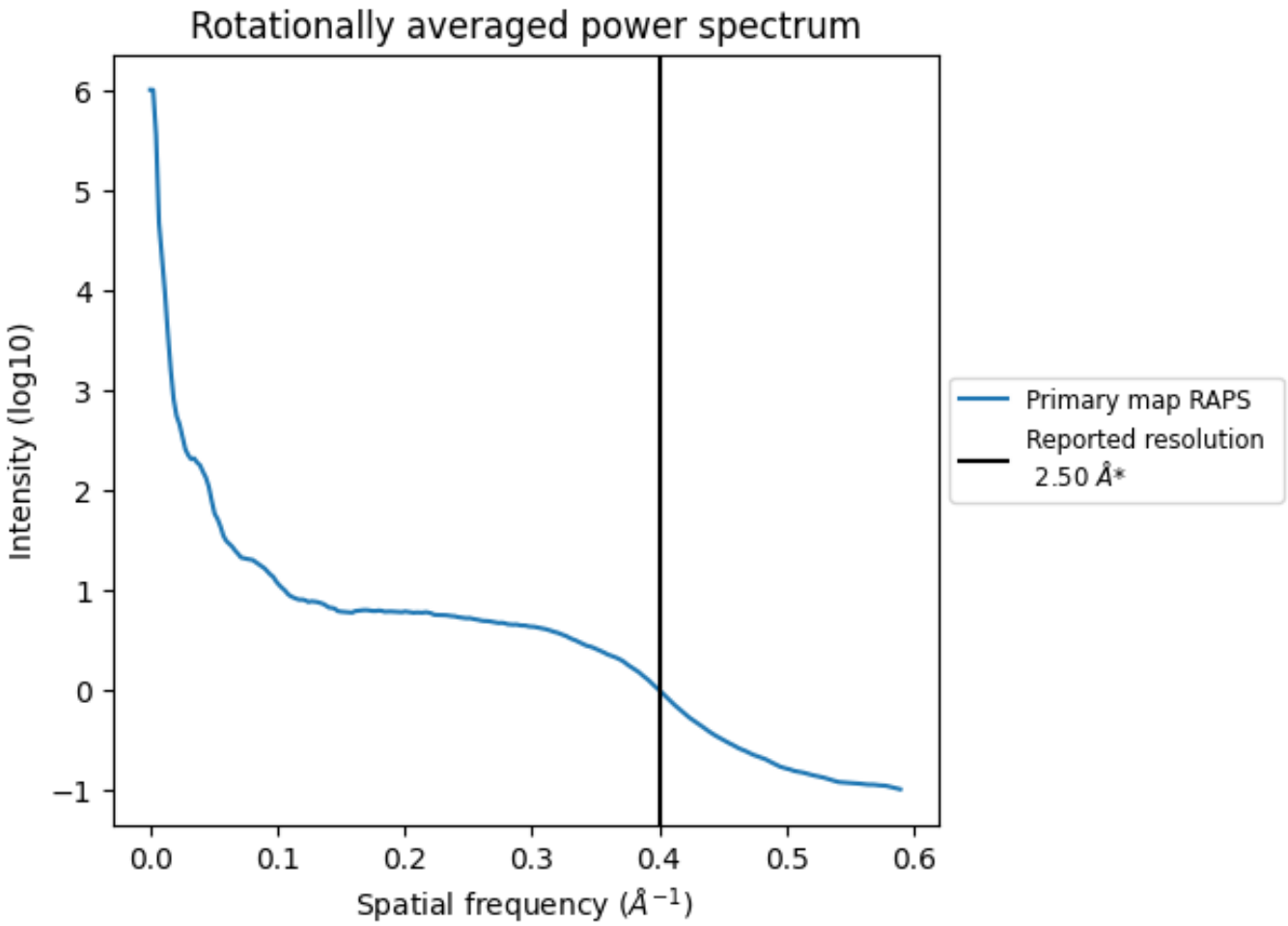
7.2 Volume estimate (i)



The volume at the recommended contour level is 812 nm^3; this corresponds to an approximate mass of 733 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

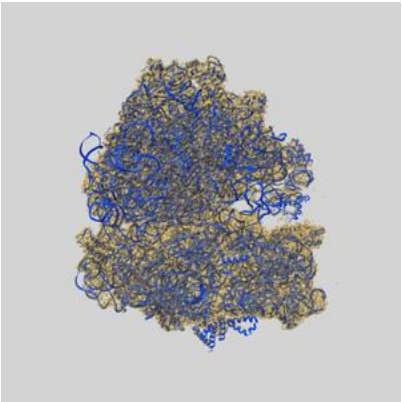
8 Fourier-Shell correlation (i)

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

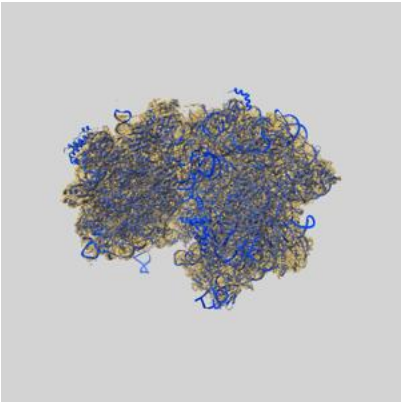
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23670 and PDB model 7M4Y. Per-residue inclusion information can be found in section 3 on page 15.

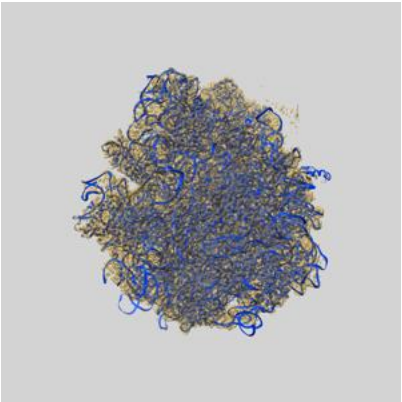
9.1 Map-model overlay (i)



X



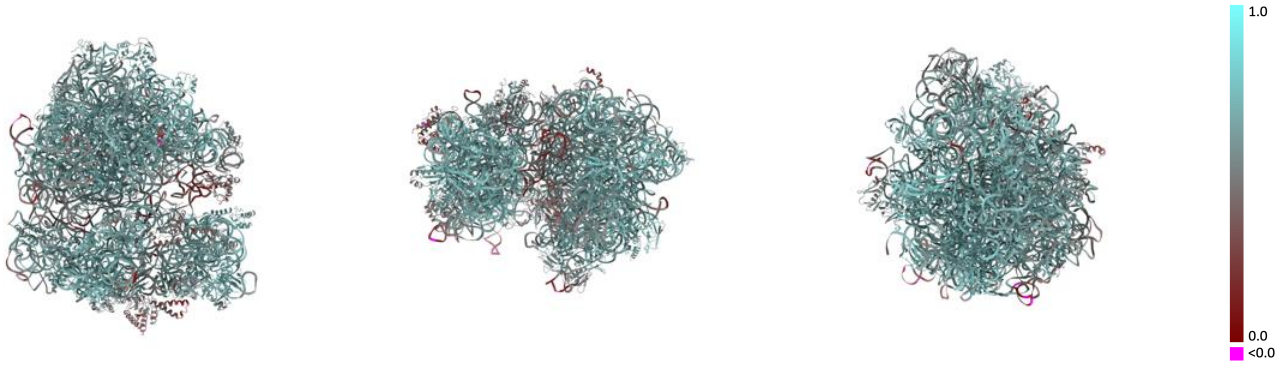
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

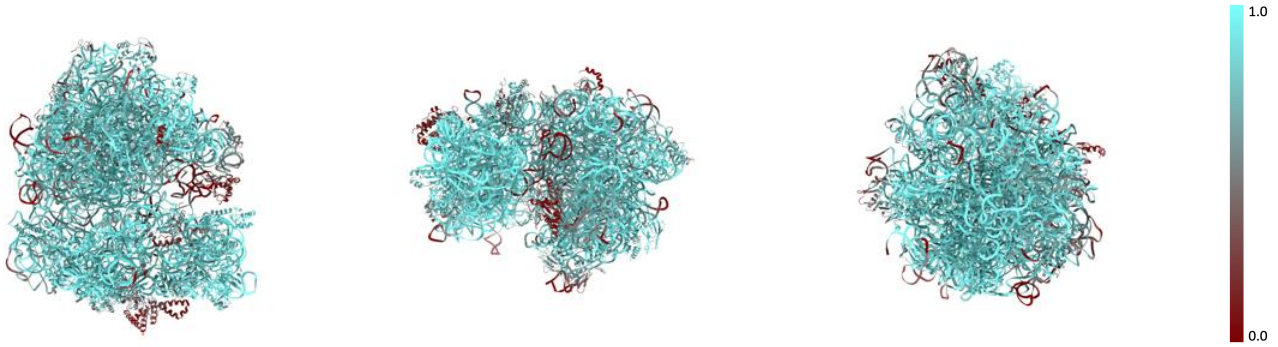
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

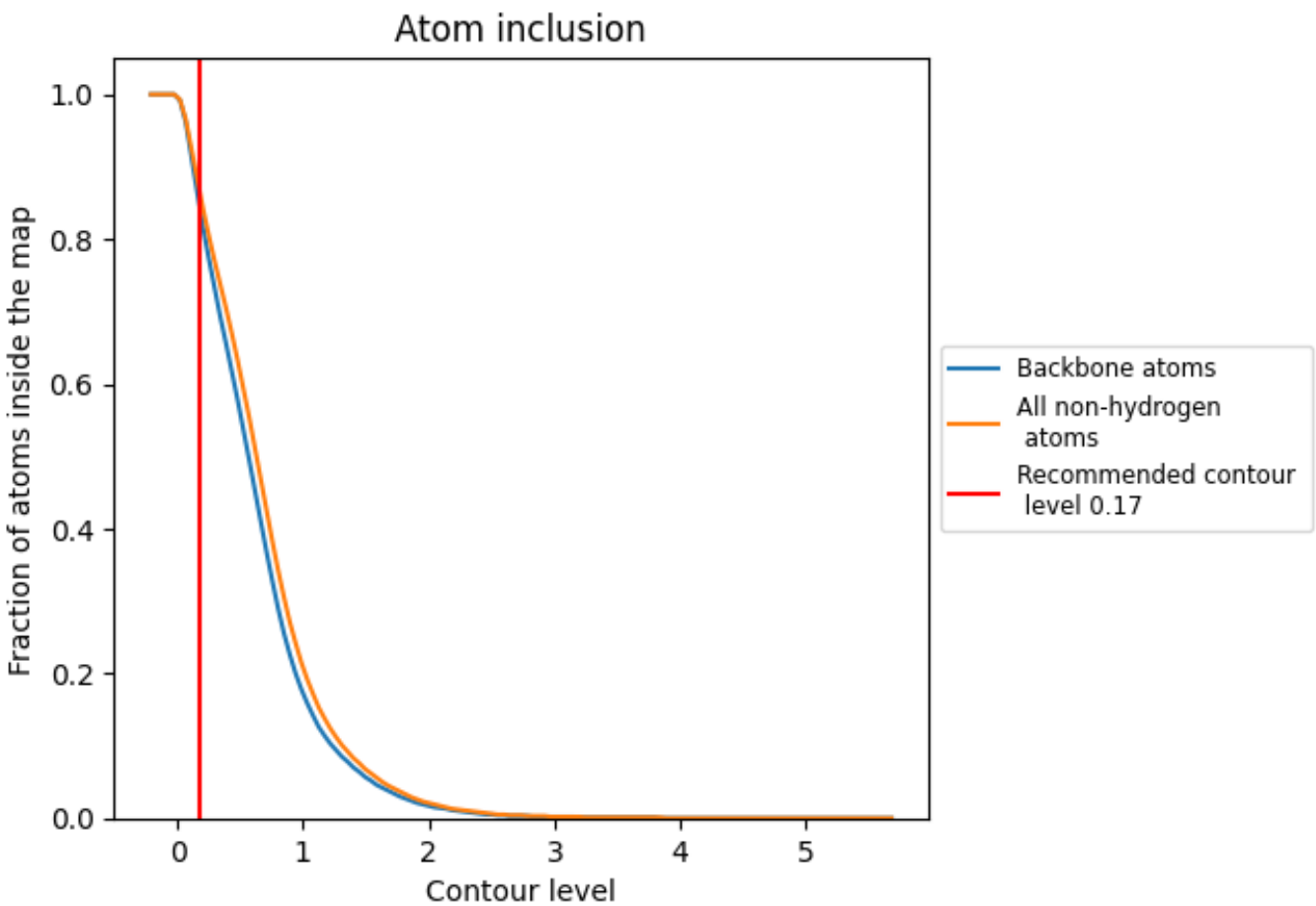
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.17).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.6260
0	0.8800	0.6910
1	0.9830	0.7470
2	0.9900	0.7440
3	0.9160	0.6750
A	0.8950	0.6340
B	0.7160	0.5560
C	0.9500	0.6880
D	0.9440	0.7150
E	0.8540	0.6780
F	0.1450	0.3840
G	0.6000	0.5470
H	0.2810	0.4320
I	0.9380	0.7190
J	0.9350	0.6670
K	0.9270	0.7130
L	0.8950	0.6790
M	0.9700	0.7350
N	0.6840	0.5890
O	0.8690	0.6580
P	0.9630	0.7290
Q	0.8970	0.6950
R	0.9370	0.7200
S	0.8010	0.6490
T	0.6630	0.5830
U	0.7830	0.6440
V	0.9330	0.7280
W	0.8910	0.7000
X	0.6320	0.5690
Y	0.8960	0.6960
Z	0.8850	0.6960
a	0.9320	0.6180
b	0.3180	0.3870
c	0.9420	0.6570
d	0.7890	0.5640

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Chain	Atom inclusion	Q-score
e	0.9310	0.6570
f	0.7750	0.5600
g	0.7720	0.5230
h	0.9550	0.6980
i	0.9640	0.6910
j	0.9010	0.6470
k	0.7050	0.5050
l	0.9130	0.6480
m	0.9720	0.6740
n	0.9610	0.6890
o	0.9460	0.6660
p	0.9360	0.6870
q	0.8670	0.5890
r	0.9220	0.6390
s	0.9750	0.7030
t	0.9580	0.6680
u	0.4120	0.4450
v	0.4760	0.3850
w	0.8460	0.4360