Full wwPDB EM Validation Report (i)

Sep 19, 2026 – 11:40 AM JST

PDB ID	:	7Y7E / pdb_00007y7e
EMDB ID	:	EMD-33662
Title	:	Structure of the Bacterial Ribosome with human tRNA Asp(ManQ34) and mRNA(GAU)
Authors	:	Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.
Deposited on	:	2022-06-22
Resolution	:	2.41 Å(reported)
Based on initial model	:	7K00

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:

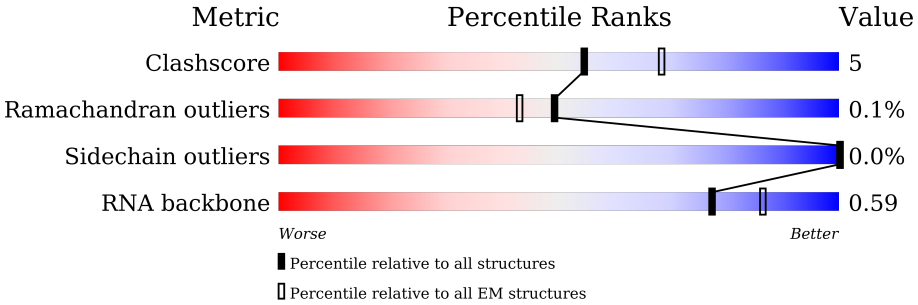
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

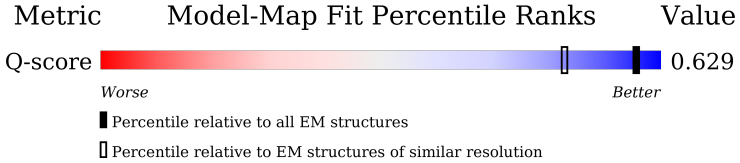
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.41 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	5662 (1.92 - 2.91)

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	A	1542	22% 65% 30% • •
2	B	241	93% 66% 27% 7%
3	C	233	42% 73% 16% 12%

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Mol	Chain	Length	Quality of chain
4	D	206	78% / 71% / 28%
5	E	167	22% / 82% / 11% / 7%
6	F	135	59% / 60% / 16% / 24%
7	G	179	59% / 68% / 17% / 15%
8	H	130	31% / 85% / 14%
9	I	130	58% / 72% / 25%
10	J	103	60% / 71% / 23% / 5%
11	K	129	39% / 71% / 20% / 9%
12	L	124	17% / 85% / 14%
13	M	118	60% / 69% / 26%
14	N	101	45% / 80% / 19%
15	O	89	45% / 75% / 24%
16	P	82	62% / 77% / 22%
17	Q	84	56% / 70% / 24% / 6%
18	R	75	41% / 69% / 19% / 12%
19	S	92	54% / 71% / 21% / 9%
20	T	87	68% / 79% / 20%
21	U	71	94% / 69% / 30%
22	a	2904	9% / 72% / 21% / 5%
23	b	120	10% / 80% / 19%
24	c	273	89% / 10%
25	d	209	10% / 92% / 8%
26	e	201	43% / 86% / 14%
27	f	179	58% / 80% / 19%
28	g	177	76% / 79% / 20%

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Mol	Chain	Length	Quality of chain
29	h	149	25% 22% 5% 72%
30	i	142	8% 87% 13%
31	j	123	11% 88% 12%
32	k	144	21% 92% 8%
33	l	136	6% 91% 9%
34	m	127	80% 13% 7%
35	n	117	35% 88% 10%
36	o	115	16% 90% 10%
37	p	118	5% 92% 8%
38	q	103	24% 94% 6%
39	r	110	11% 91% 9%
40	s	100	24% 78% 15% 7%
41	t	104	50% 79% 19%
42	u	94	34% 84% 16%
43	v	85	9% 89% 9%
44	w	78	15% 91% 8%
45	x	63	60% 79% 19%
46	y	59	14% 80% 19%
47	z	57	23% 81% 18%
48	0	55	18% 75% 18% 7%
49	1	46	91% 9%
50	2	65	5% 85% 12%
51	3	38	11% 89% 11%
52	4	70	81% 70% 16% 14%
53	X	35	11% 29% 6% 63%

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Mol	Chain	Length	Quality of chain
54	Z	77	39% 66% 25% 8%
55	V	75	33% 59% 28% 9%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 141918 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1520	32634	14562	5991	10561	1520	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	224	1753	1109	315	321	8	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	156	1152	717	217	212	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	103	839	530	151	151	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	153	1203	750	231	218	4	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	98	786	493	150	142	1	0	0

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	123	957	591	196	165	5	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	81	643	403	127	112	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	66	544	345	102	96	1	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	70	589	366	125	97	1	0	0

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	a	2753	59130	26384	10897	19096	2753	0	0

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	d	209	1566	980	288	294	4	0	0

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called 50S ribosomal protein L16.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 34 is a protein called 50S ribosomal protein L17.

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

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	t	102	779	492	146	141	0	0

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	84	628	388	126	113	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	x	62	501	308	98	94	1	0	0

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	0	51	417	269	76	72	0	0

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	1	46	377	228	90	57	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	2	64	504	323	105	74	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	3	38	302	185	65	48	4	0	0

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	4	60	480	299	90	85	6	0	0

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	X	13	279	125	52	89	13	0	0

- Molecule 54 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
54	Z	77	1645	734	297	536	77	1	0	0

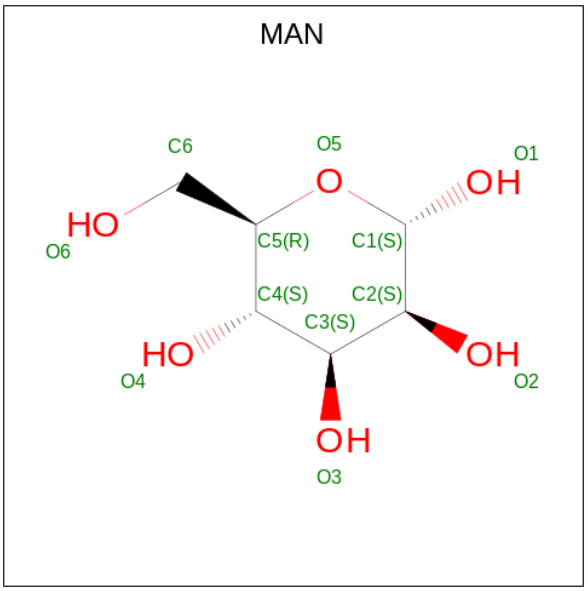
- Molecule 55 is a RNA chain called A-site tRNA-Asp.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	V	75	1612	726	283	529	74	0	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	A	56	56	56	0
56	a	181	181	181	0
56	b	3	3	3	0
56	c	1	1	1	0
56	d	1	1	1	0
56	z	1	1	1	0
56	Z	3	3	3	0
56	V	2	2	2	0

- Molecule 57 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



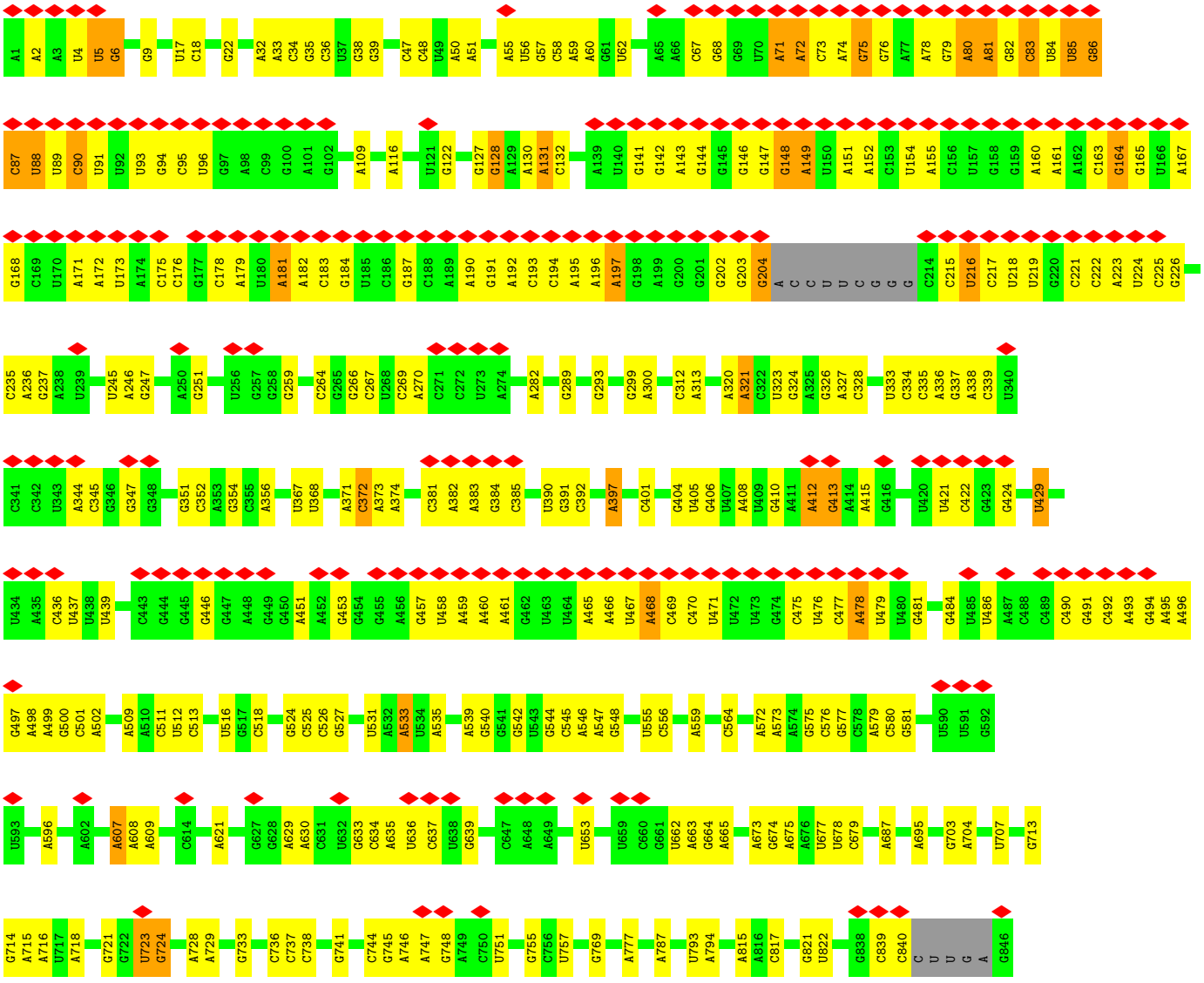
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
57	V	1	11	6	5	0

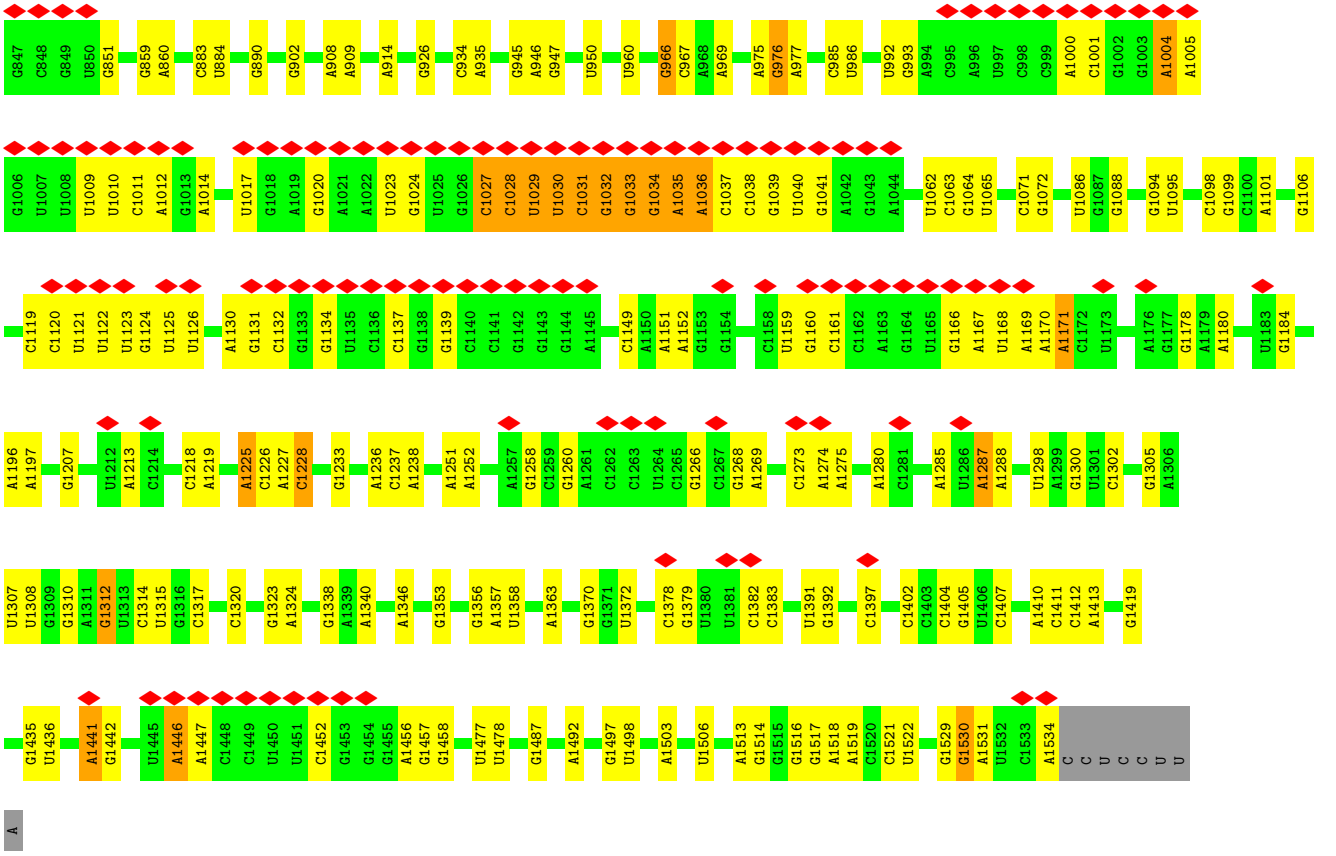
3 Residue-property plots (i)

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: 16S rRNA

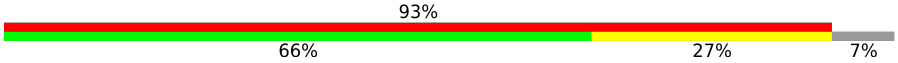
Chain A:

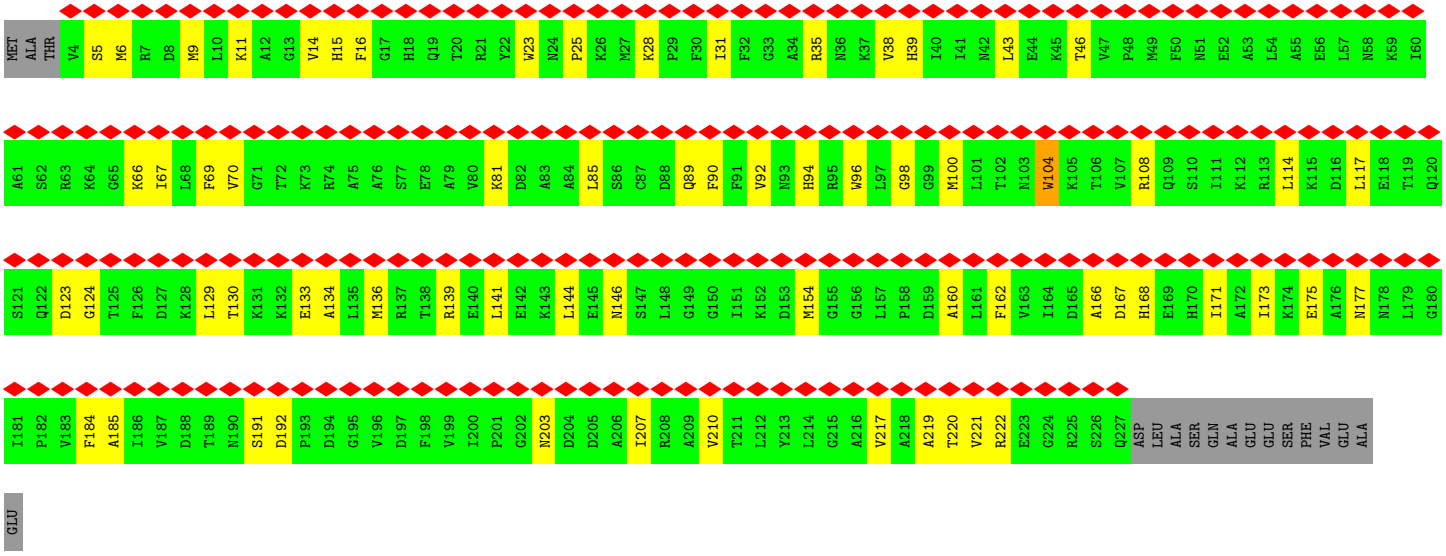




- Molecule 2: 30S ribosomal protein S2

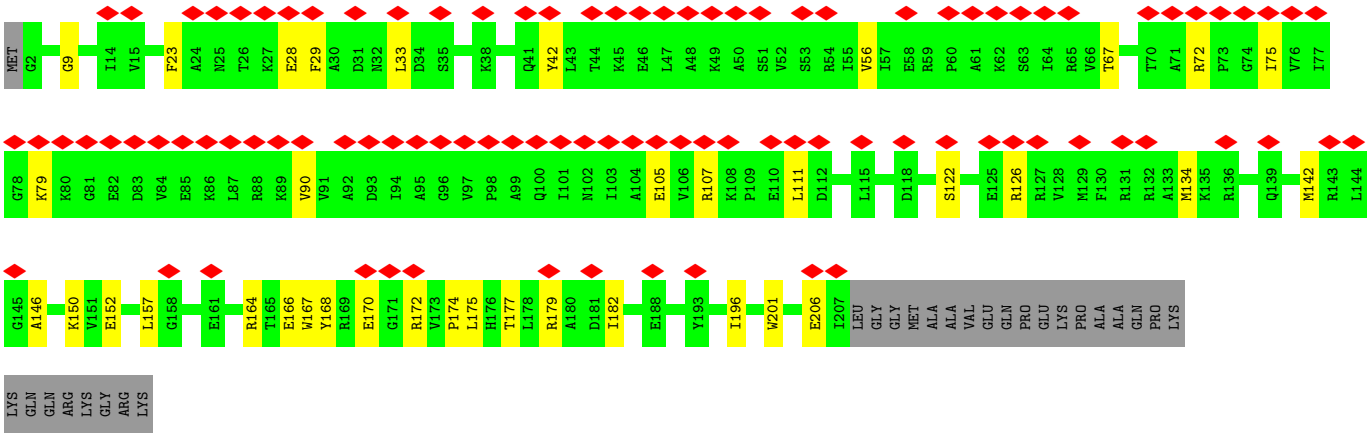
Chain B:





- Molecule 3: 30S ribosomal protein S3

Chain C:

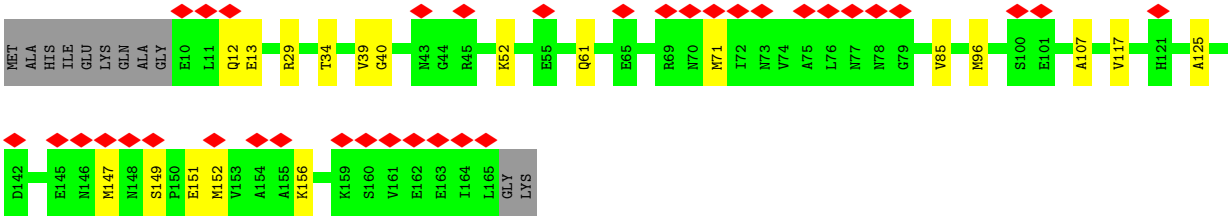


• Molecule 4: 30S ribosomal protein S4

Chain D:

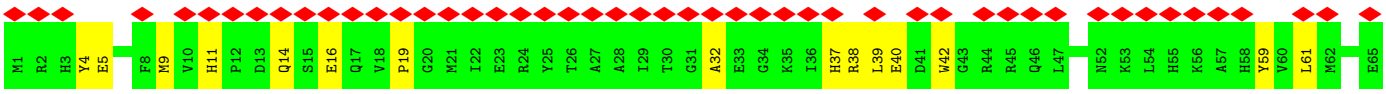
• Molecule 5: 30S ribosomal protein S5

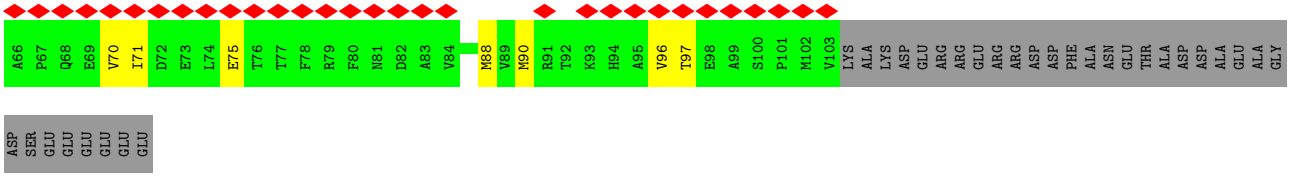
Chain E:



• Molecule 6: 30S ribosomal protein S6, fully modified isoform

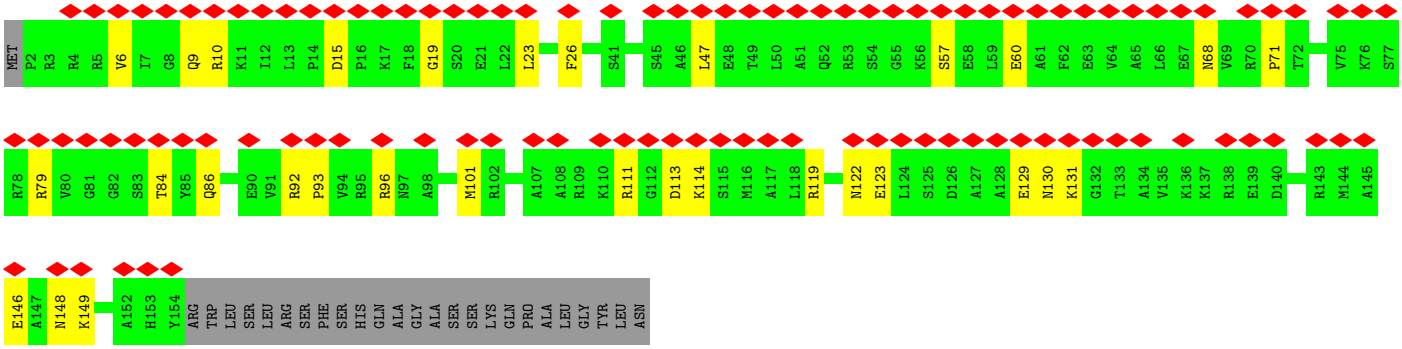
Chain F:





- Molecule 7: 30S ribosomal protein S7

Chain G:

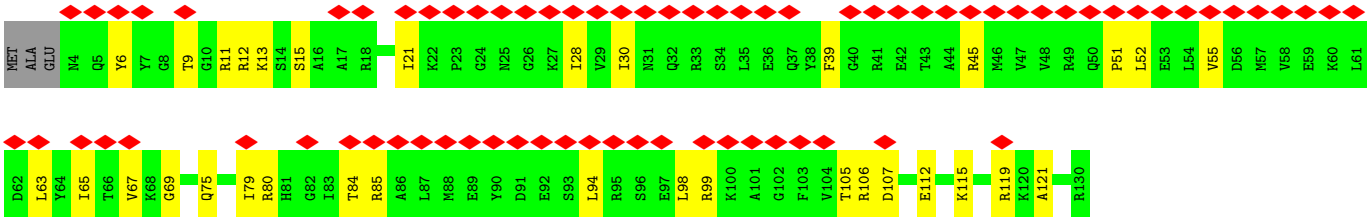


- Molecule 8: 30S ribosomal protein S8

Chain H:

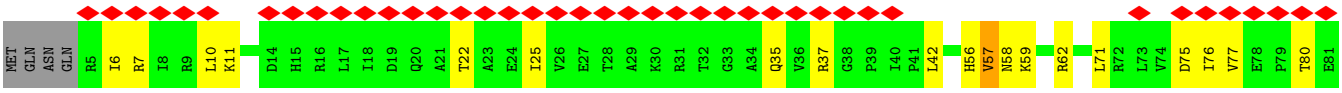
- Molecule 9: 30S ribosomal protein S9

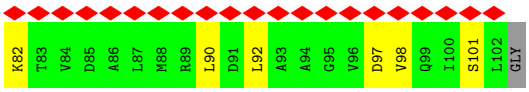
Chain I:



- Molecule 10: 30S ribosomal protein S10

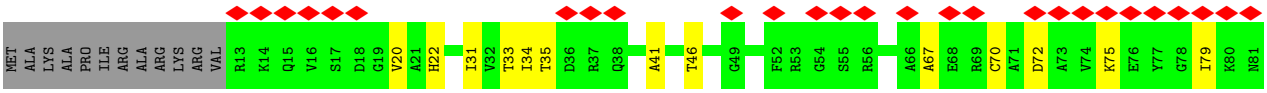
Chain J:

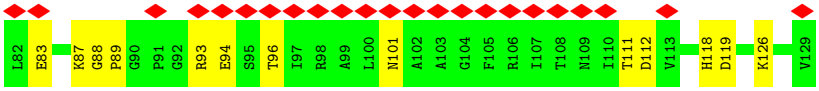




• Molecule 11: 30S ribosomal protein S11

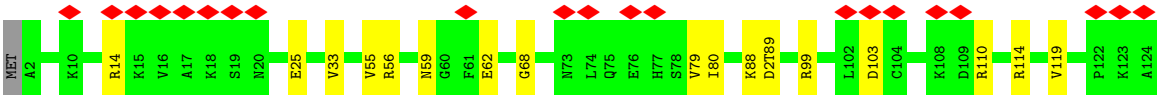
Chain K:





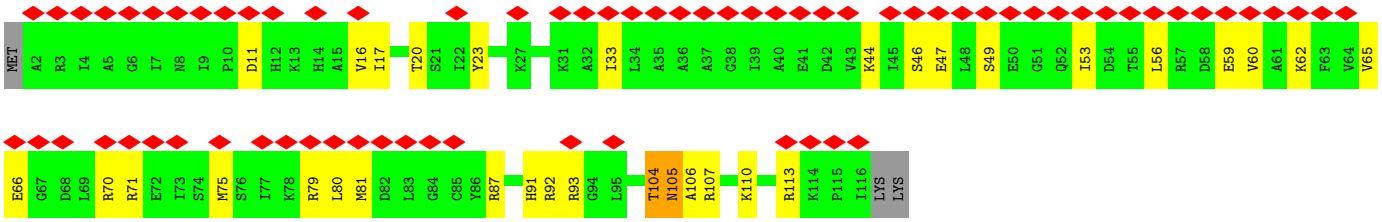
• Molecule 12: 30S ribosomal protein S12

Chain L:



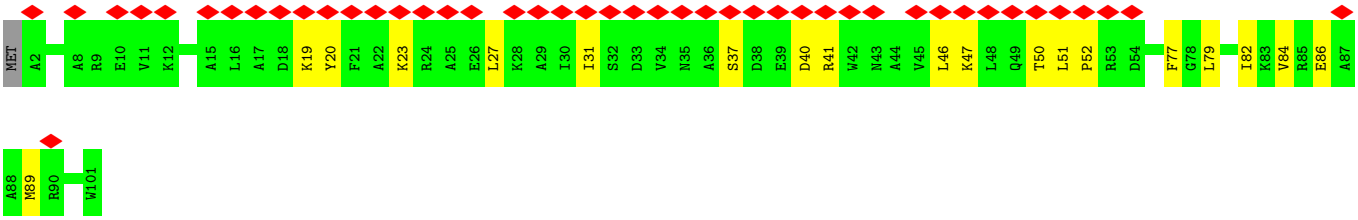
• Molecule 13: 30S ribosomal protein S13

Chain M:



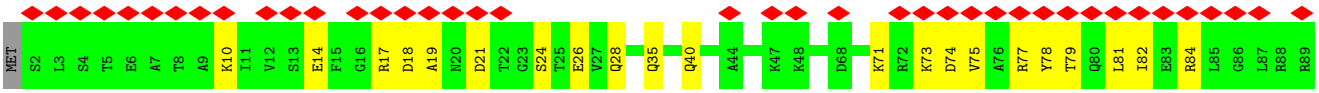
• Molecule 14: 30S ribosomal protein S14

Chain N:



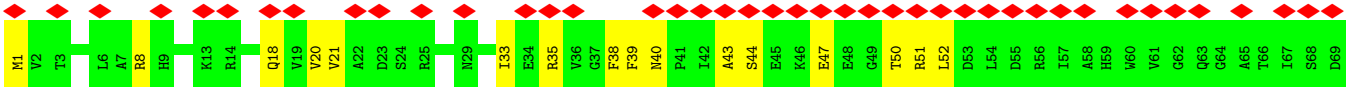
• Molecule 15: 30S ribosomal protein S15

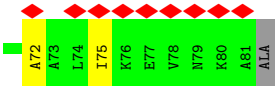
Chain O:



- Molecule 16: 30S ribosomal protein S16

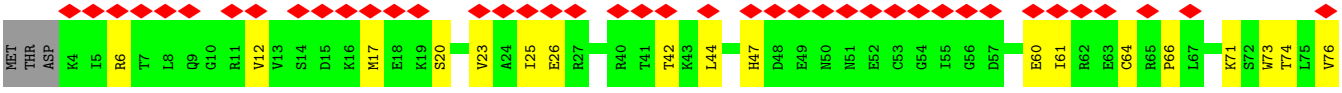
Chain P:

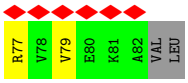




- Molecule 17: 30S ribosomal protein S17

Chain Q:



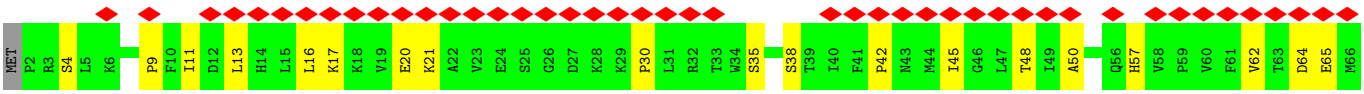


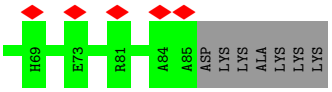
- Molecule 18: 30S ribosomal protein S18

Chain R:

- Molecule 19: 30S ribosomal protein S19

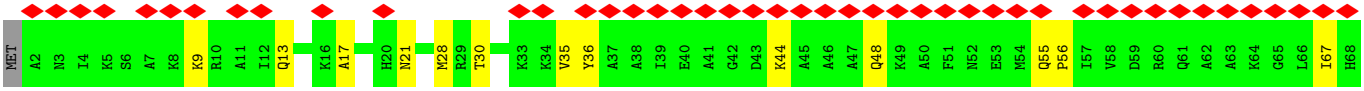
Chain S:

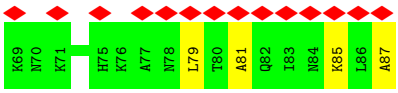




- Molecule 20: 30S ribosomal protein S20

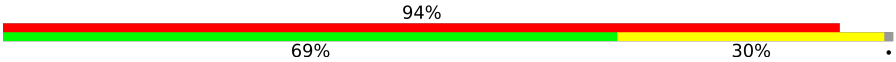
Chain T:

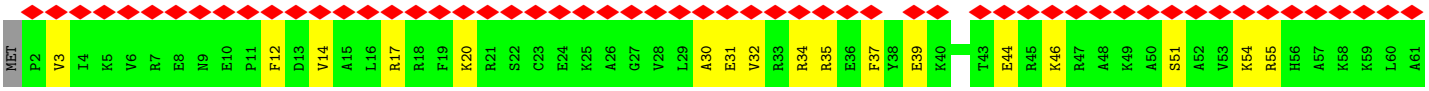


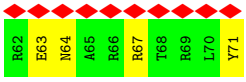


- Molecule 21: 30S ribosomal protein S21

Chain U:

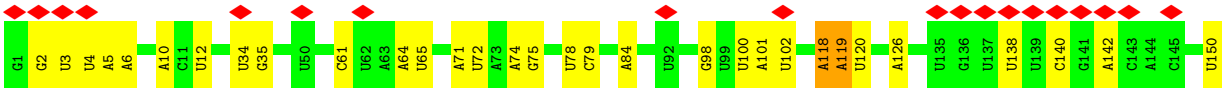


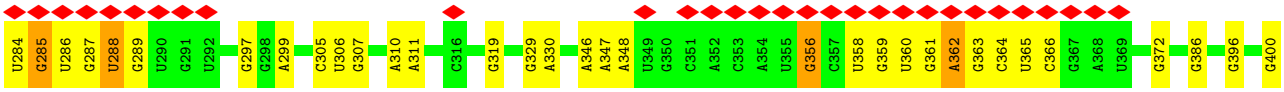


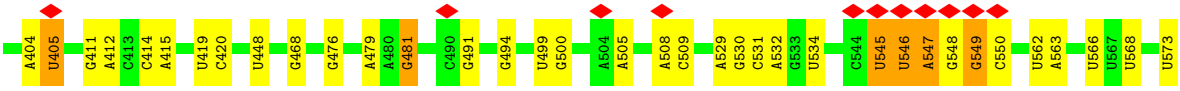


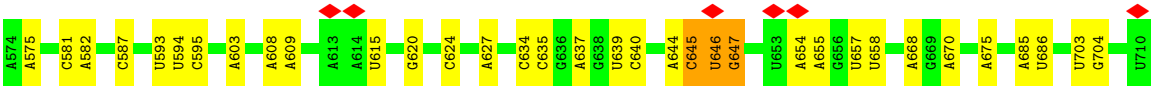
- Molecule 22: 23S rRNA

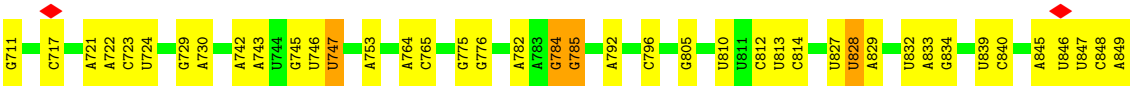
Chain a:

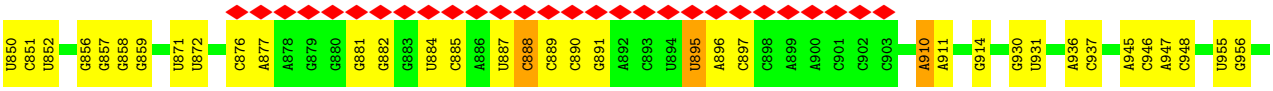


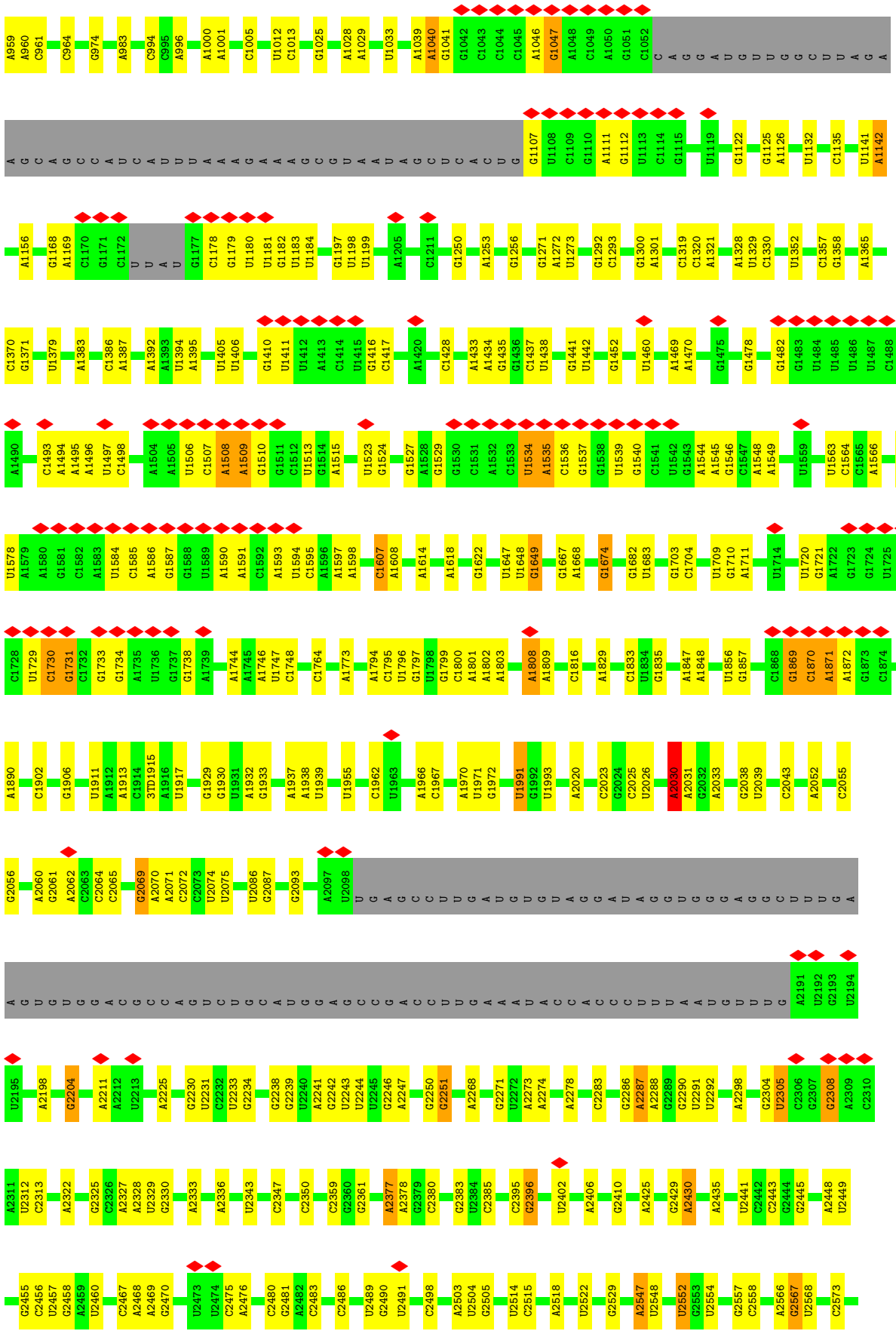








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A G G C A G G C C A U C A U U U A A A G A A A A G C G U A A A U A G C U C A C U G G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115 U1119 G1122 G1125 A1126 U1132 C1135 U1141 A1142
A1156 G1168 A1169 C1170 G1171 C1172 U U A U G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1197 U1198 U1199 A1205 C1211 G1250 A1253 G1256 G1271 A1272 U1273 G1292 C1293 G1300 A1301 C1319 C1320 A1321 A1328 U1329 C1330 U1352 C1357 G1358 A1365
C1370 G1371 U1379 A1383 C1386 A1387 A1392 A1393 U1394 A1395 U1405 U1406 G1410 U1411 U1412 A1413 C1414 U1415 G1416 C1417 A1420 C1428 A1433 A1434 G1435 G1436 C1437 U1438 G1441 U1442 G1452 U1460 A1469 A1470 G1475 G1478 G1482 G1483 U1484 U1485 U1486 U1487 C1488 C1489
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C1728 U1729 C1730 G1731 C1732 G1733 G1734 A1735 U1736 G1737 G1738 A1739 A1744 A1745 A1746 U1747 C1748 C1764 A1773 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 A1808 A1809 C1816 A1829 C1833 U1834 G1835 A1847 A1848 U1856 G1857 C1868 G1869 C1870 A1871 A1872 G1873 C1874 A1889
A1890 C1902 G1906 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 G1929 G1930 U1931 A1932 G1933 A1937 A1938 U1939 U1955 C1962 U1963 A1966 C1967 A1970 U1971 G1972 U1991 G1992 U1993 A2020 C2023 G2024 C2025 U2026 A2030 A2031 G2032 A2033 G2038 U2039 C2043 A2052 C2055
G2056 A2060 G2061 A2062 C2063 C2064 C2065 G2069 A2070 A2071 C2072 C2073 U2074 U2075 U2086 G2087 G2093 A2097 U2098 U G A G C C U U G G A U G U G U A G G A U A A G G C G G G U U G A A U G G G G A G G C C U U G A
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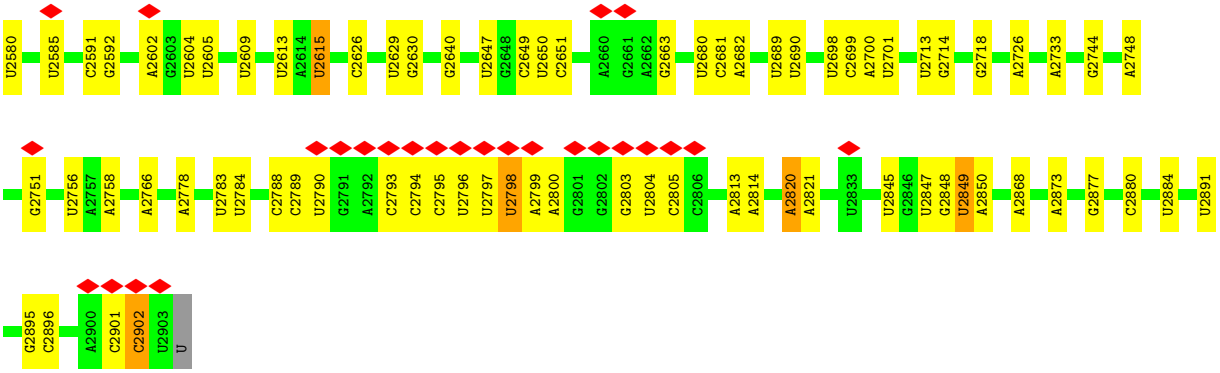
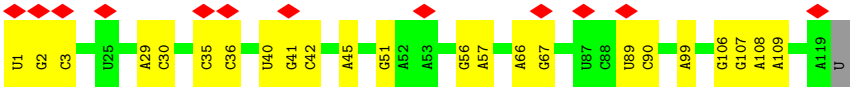


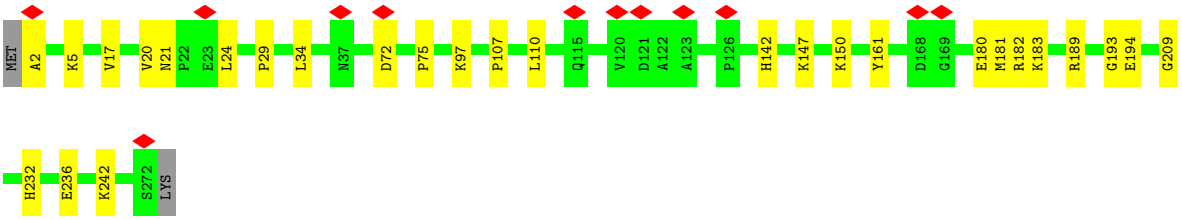
- Molecule 23: 5S rRNA

Chain b:



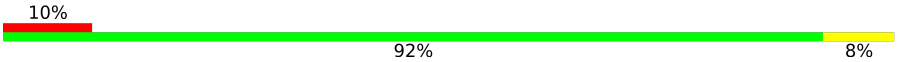
- Molecule 24: 50S ribosomal protein L2

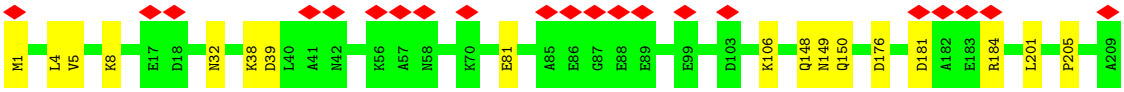
Chain c:



- Molecule 25: 50S ribosomal protein L3

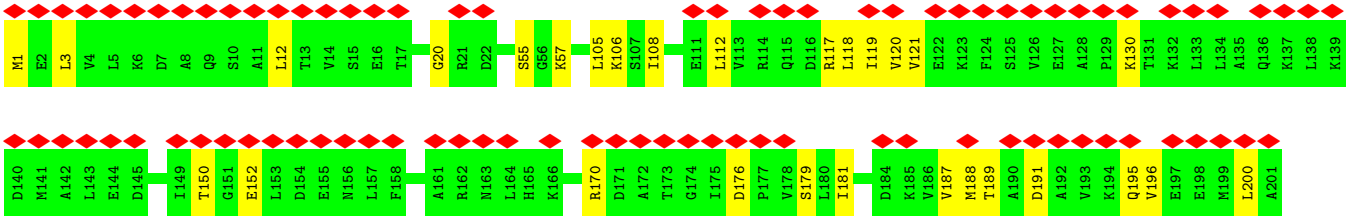
Chain d:





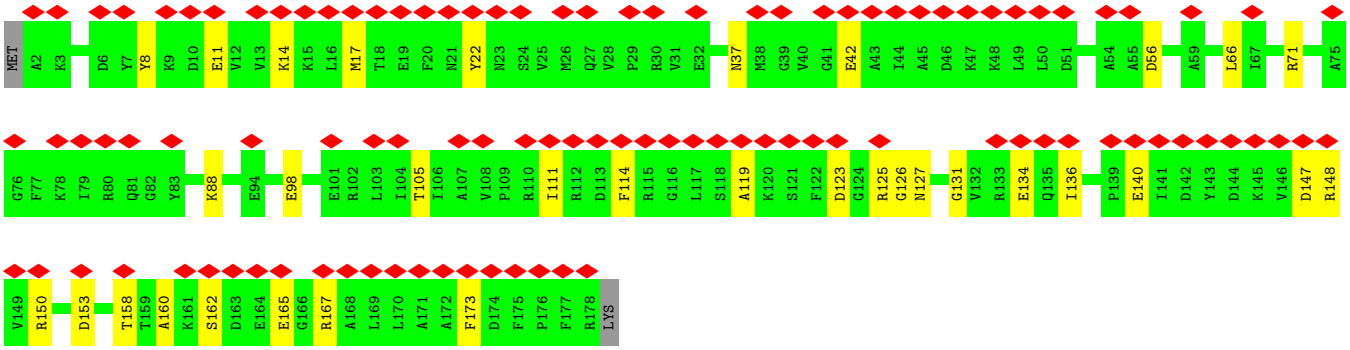
- Molecule 26: 50S ribosomal protein L4

Chain e:



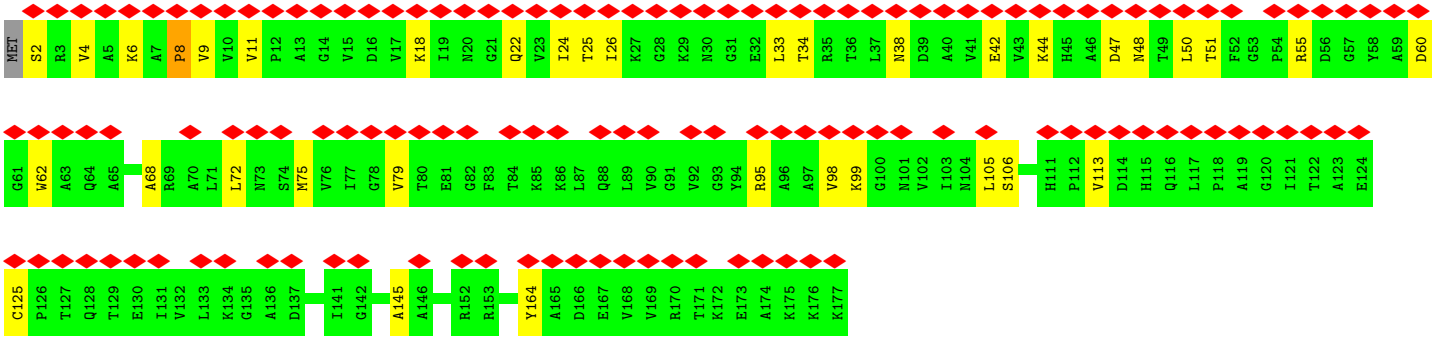
- Molecule 27: 50S ribosomal protein L5

Chain f:



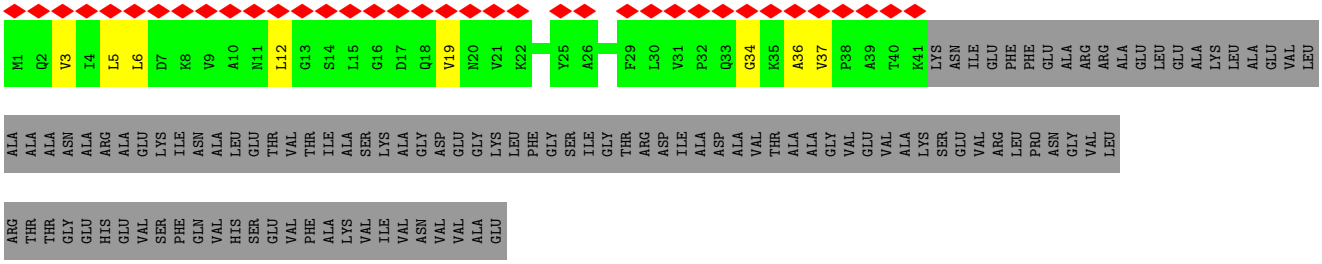
- Molecule 28: 50S ribosomal protein L6

Chain g:



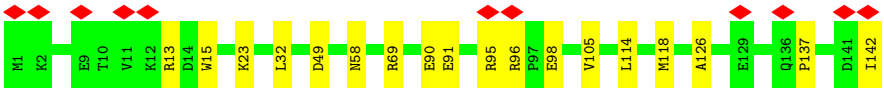
- Molecule 29: 50S ribosomal protein L9

Chain h:



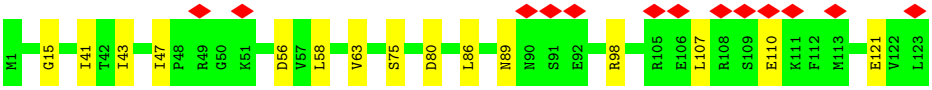
- Molecule 30: 50S ribosomal protein L13

Chain i:



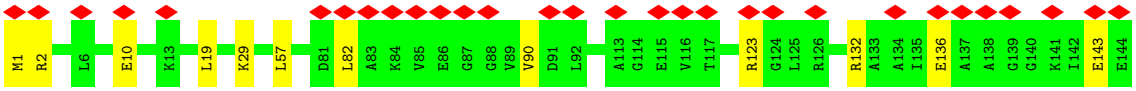
- Molecule 31: 50S ribosomal protein L14

Chain j: 11% 88% 12%



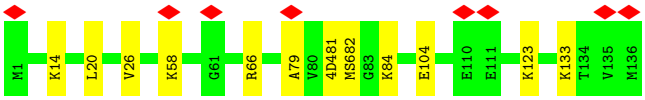
• Molecule 32: 50S ribosomal protein L15

Chain k: 21% 92% 8%



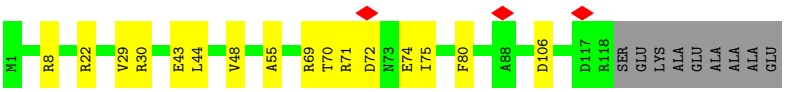
• Molecule 33: 50S ribosomal protein L16

Chain l: 6% 91% 9%



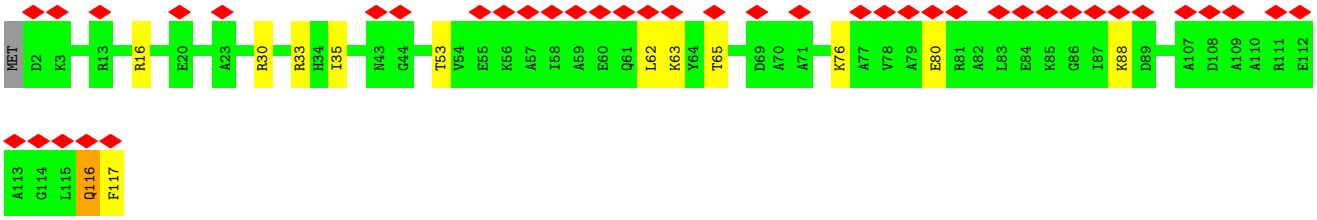
• Molecule 34: 50S ribosomal protein L17

Chain m: 80% 13% 7%



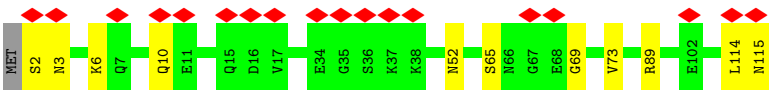
• Molecule 35: 50S ribosomal protein L18

Chain n: 35% 88% 10%



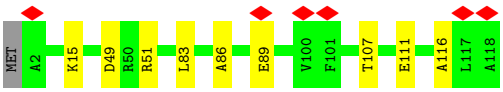
• Molecule 36: 50S ribosomal protein L19

Chain o: 16% 90% 10%



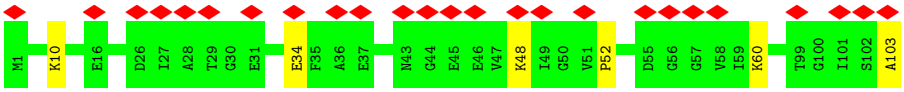
• Molecule 37: 50S ribosomal protein L20

Chain p: 5% 92% 8%



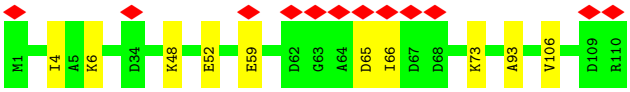
• Molecule 38: 50S ribosomal protein L21

Chain q: 24% 94% 6%



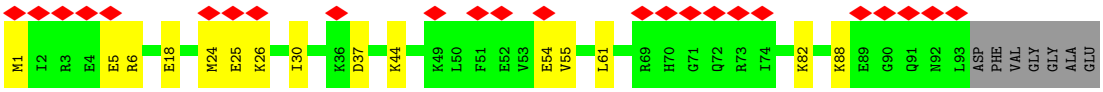
• Molecule 39: 50S ribosomal protein L22

Chain r: 11% 91% 9%



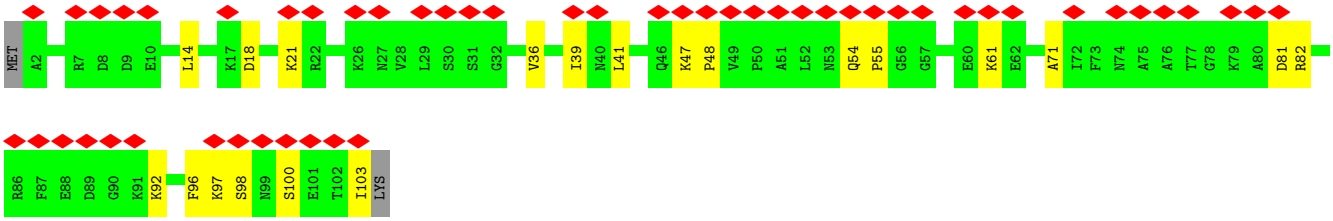
• Molecule 40: 50S ribosomal protein L23

Chain s: 24% 78% 15% 7%



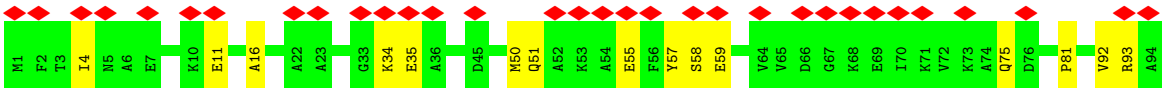
• Molecule 41: 50S ribosomal protein L24

Chain t: 50% 79% 19%



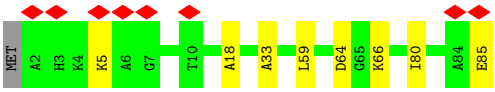
• Molecule 42: 50S ribosomal protein L25

Chain u: 34% 84% 16%



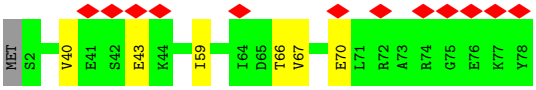
• Molecule 43: 50S ribosomal protein L27

Chain v: 9% 89% 9%



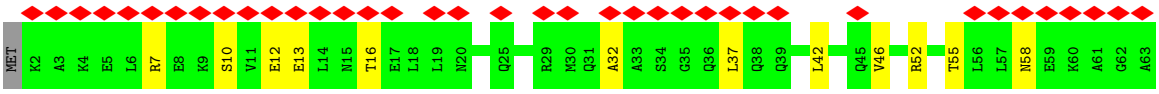
• Molecule 44: 50S ribosomal protein L28

Chain w: 15% 91% 8%



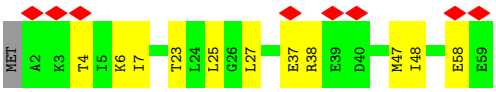
• Molecule 45: 50S ribosomal protein L29

Chain x: 60% 79% 19%



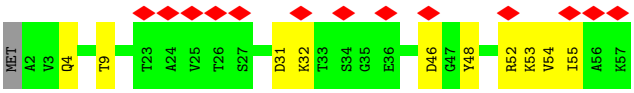
• Molecule 46: 50S ribosomal protein L30

Chain y: 14% 80% 19%



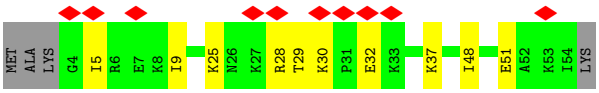
• Molecule 47: 50S ribosomal protein L32

Chain z: 23% 81% 18%



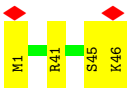
• Molecule 48: 50S ribosomal protein L33

Chain 0: 18% 75% 18% 7%



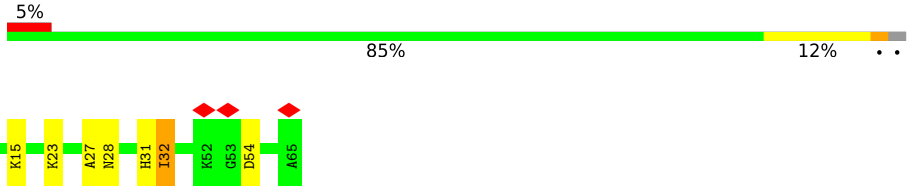
• Molecule 49: 50S ribosomal protein L34

Chain 1: 91% 9%



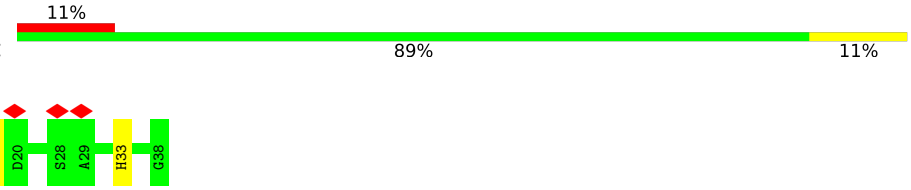
- Molecule 50: 50S ribosomal protein L35

Chain 2:



- Molecule 51: 50S ribosomal protein L36

Chain 3:

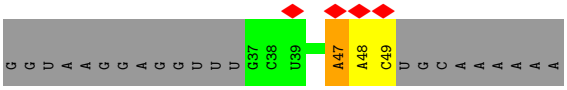


- Molecule 52: 50S ribosomal protein L31

Chain 4:

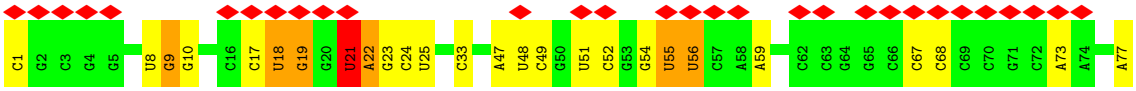
- Molecule 53: mRNA

Chain X:



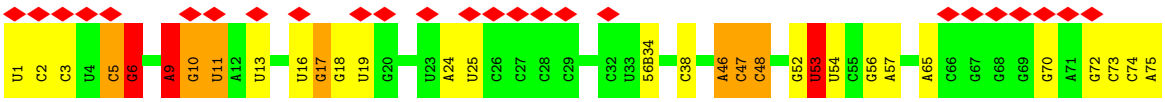
- Molecule 54: P-site tRNA-fMet

Chain Z:



- Molecule 55: A-site tRNA-Asp

Chain V:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	222985	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.316	Depositor
Minimum map value	-0.159	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	439.10498, 439.10498, 439.10498	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8285, 0.8285, 0.8285	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: OMU, H2U, 4D4, 1MA, 6MZ, G7M, 56B, MA6, 1MG, OMC, MG, D2T, 2MG, 5MC, MAN, PSU, UR3, 4SU, 2MA, OMG, 3TD, 4OC, MS6, 5MU, MEQ, IAS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.46	0/36261	0.33	0/56559
2	B	0.18	0/1784	0.45	1/2403 (0.0%)
3	C	0.38	0/1651	0.42	0/2225
4	D	0.30	0/1665	0.38	0/2227
5	E	0.40	0/1165	0.42	0/1568
6	F	0.32	0/858	0.40	0/1160
7	G	0.31	0/1219	0.44	0/1635
8	H	0.38	0/989	0.38	0/1326
9	I	0.38	0/1034	0.47	0/1375
10	J	0.34	0/796	0.48	0/1077
11	K	0.35	0/884	0.39	0/1191
12	L	0.40	0/960	0.42	0/1286
13	M	0.35	0/900	0.50	0/1204
14	N	0.38	0/817	0.46	0/1088
15	O	0.37	0/722	0.45	0/964
16	P	0.33	0/653	0.46	0/877
17	Q	0.37	0/650	0.40	0/871
18	R	0.37	0/553	0.43	0/742
19	S	0.32	0/685	0.41	0/922
20	T	0.32	0/676	0.41	0/895
21	U	0.24	0/597	0.50	0/792
22	a	0.56	0/65651	0.36	0/102413
23	b	0.45	0/2850	0.29	0/4444
24	c	0.49	0/2121	0.41	0/2852
25	d	0.48	0/1576	0.40	0/2119
26	e	0.40	0/1571	0.38	0/2113
27	f	0.35	0/1434	0.40	0/1926
28	g	0.31	0/1343	0.49	1/1816 (0.1%)
29	h	0.26	0/306	0.50	0/413
30	i	0.47	0/1152	0.45	0/1551
31	j	0.47	0/955	0.43	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	k	0.46	0/1062	0.43	0/1413
33	l	0.46	0/1073	0.40	0/1433
34	m	0.48	0/958	0.50	0/1281
35	n	0.38	0/902	0.46	0/1209
36	o	0.45	0/929	0.39	0/1242
37	p	0.52	0/960	0.42	0/1278
38	q	0.45	0/829	0.40	0/1107
39	r	0.44	0/864	0.41	0/1156
40	s	0.41	0/744	0.45	0/994
41	t	0.38	0/787	0.47	0/1051
42	u	0.39	0/766	0.41	0/1025
43	v	0.46	0/636	0.41	0/841
44	w	0.47	0/635	0.41	0/848
45	x	0.34	0/502	0.42	0/667
46	y	0.43	0/453	0.40	0/605
47	z	0.47	0/450	0.44	0/599
48	0	0.42	0/424	0.39	0/565
49	1	0.52	0/380	0.45	0/498
50	2	0.51	0/513	0.49	0/676
51	3	0.48	0/303	0.47	0/397
52	4	0.26	0/488	0.39	0/649
53	X	0.48	0/312	0.31	0/484
54	Z	0.41	0/1725	0.32	0/2687
55	V	0.39	0/1525	0.37	0/2375
All	All	0.49	0/152698	0.37	2/228393 (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
13	M	0	2
28	g	0	1
50	2	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	104	TRP	CA-CB-CG	5.48	124.01	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g	8	PRO	CA-N-CD	-5.31	104.56	112.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	2	31	HIS	Peptide
13	M	104	THR	Peptide
13	M	65	VAL	Peptide
28	g	47	ASP	Peptide

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	A	32634	0	16443	268	0
2	B	1753	0	1780	48	0
3	C	1624	0	1696	25	0
4	D	1643	0	1707	41	0
5	E	1152	0	1196	13	0
6	F	839	0	833	18	0
7	G	1203	0	1254	19	0
8	H	979	0	1031	11	0
9	I	1022	0	1070	26	0
10	J	786	0	828	21	0
11	K	877	0	883	19	0
12	L	957	0	1017	11	0
13	M	891	0	952	24	0
14	N	805	0	844	13	0
15	O	714	0	734	16	0
16	P	643	0	661	11	0
17	Q	641	0	682	17	0
18	R	544	0	565	11	0
19	S	668	0	693	17	0
20	T	670	0	719	13	0
21	U	589	0	629	16	0
22	a	59130	0	29768	315	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	b	2549	0	1291	11	0
24	c	2082	0	2154	19	0
25	d	1566	0	1618	10	0
26	e	1552	0	1619	20	0
27	f	1410	0	1444	25	0
28	g	1323	0	1371	22	0
29	h	303	0	327	5	0
30	i	1129	0	1162	13	0
31	j	946	0	1023	11	0
32	k	1053	0	1129	12	0
33	l	1075	0	1145	9	0
34	m	945	0	989	10	0
35	n	892	0	923	11	0
36	o	917	0	962	8	0
37	p	947	0	1019	7	0
38	q	816	0	839	4	0
39	r	857	0	922	7	0
40	s	738	0	807	11	0
41	t	779	0	831	13	0
42	u	753	0	780	9	0
43	v	628	0	642	5	0
44	w	625	0	652	3	0
45	x	501	0	531	10	0
46	y	449	0	488	7	0
47	z	444	0	458	7	0
48	0	417	0	451	8	0
49	1	377	0	418	4	0
50	2	504	0	572	7	0
51	3	302	0	343	4	0
52	4	480	0	482	10	0
53	X	279	0	141	2	0
54	Z	1645	0	842	12	0
55	V	1612	0	813	12	0
56	A	56	0	0	0	0
56	V	2	0	0	0	0
56	Z	3	0	0	0	0
56	a	181	0	0	0	0
56	b	3	0	0	0	0
56	c	1	0	0	0	0
56	d	1	0	0	0	0
56	z	1	0	0	0	0
57	V	11	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	141918	0	95183	1183	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 5.

All (1183) 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)
22:a:2304:G:H22	22:a:2312:U:H3	1.11	0.96
1:A:76:G:H1	1:A:93:U:H3	1.05	0.93
22:a:1607:C:N4	22:a:1622:G:OP2	2.08	0.85
7:G:68:ASN:ND2	7:G:130:ASN:OD1	2.10	0.85
6:F:5:GLU:OE2	18:R:24:LYS:NZ	2.11	0.83
22:a:881:G:O6	22:a:895:U:O4	1.96	0.82
13:M:93:ARG:NH2	22:a:888:C:OP1	2.14	0.81
22:a:276:U:O2'	22:a:278:A:N7	2.13	0.81
27:f:158:THR:HG22	27:f:160:ALA:H	1.46	0.81
27:f:22:TYR:OH	27:f:165:GLU:OE1	1.97	0.80
9:I:106:ARG:NH1	9:I:107:ASP:O	2.17	0.78
22:a:534:U:O2'	37:p:49:ASP:OD2	2.02	0.77
31:j:121:GLU:OE2	36:o:65:SER:OG	2.03	0.76
1:A:544:G:OP1	4:D:56:ARG:NH2	2.18	0.76
7:G:79:ARG:HG2	7:G:84:THR:HG22	1.68	0.75
10:J:37:ARG:HB2	10:J:75:ASP:HB2	1.67	0.74
23:b:51:G:OP1	35:n:63:LYS:NZ	2.21	0.74
10:J:7:ARG:HB2	10:J:101:SER:HB3	1.70	0.74
42:u:4:ILE:HG12	42:u:50:MET:HE1	1.68	0.74
1:A:337:G:H2'	1:A:338:A:C8	2.23	0.74
15:O:26:GLU:OE1	15:O:77:ARG:NH2	2.21	0.74
1:A:673:A:H2'	1:A:674:G:C8	2.23	0.73
4:D:144:SER:HB3	4:D:179:GLU:HG3	1.69	0.73
4:D:28:ILE:HG23	4:D:34:ILE:HD11	1.70	0.73
5:E:39:VAL:HG13	5:E:71:MET:HE3	1.71	0.73
14:N:37:SER:OG	14:N:40:ASP:OD1	2.08	0.72
22:a:286:U:H2'	22:a:287:G:H8	1.54	0.72
26:e:108:ILE:HG23	32:k:1:MET:HE1	1.72	0.72
1:A:147:G:H2'	1:A:148:G:C8	2.25	0.72
12:L:25:GLU:OE1	12:L:59:ASN:ND2	2.19	0.71
22:a:2204:G:OP2	24:c:147:LYS:NZ	2.23	0.71
1:A:82:G:O6	1:A:89:U:O4	2.08	0.71
22:a:2377:A:O2'	35:n:117:PHE:O	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1397:C:OP2	5:E:29:ARG:NH2	2.23	0.71
22:a:1802:A:H2'	22:a:1803:A:C8	2.26	0.71
4:D:174:ASP:OD2	4:D:177:LYS:NZ	2.22	0.71
1:A:80:A:N1	1:A:90:C:N4	2.38	0.71
9:I:28:ILE:HG12	9:I:63:LEU:HD12	1.73	0.70
24:c:161:TYR:HB3	24:c:194:GLU:HB3	1.73	0.70
22:a:956:G:N7	33:l:14:LYS:NZ	2.38	0.70
3:C:72:ARG:HB3	3:C:75:ILE:HD13	1.72	0.70
1:A:82:G:H1	1:A:89:U:H3	0.77	0.70
30:i:96:ARG:HA	30:i:96:ARG:HH11	1.57	0.70
1:A:339:C:OP2	31:j:98:ARG:NH1	2.23	0.69
13:M:79:ARG:NE	19:S:65:GLU:OE2	2.25	0.69
54:Z:48:U:H5"	54:Z:49:C:H5'	1.75	0.69
8:H:41:LYS:NZ	8:H:48:ASP:OD1	2.25	0.68
1:A:405:U:O4	4:D:2:ALA:N	2.26	0.68
13:M:23:TYR:HB3	13:M:66:GLU:HG2	1.75	0.68
22:a:2640:G:OP1	30:i:95:ARG:NH2	2.26	0.67
41:t:47:LYS:HG3	41:t:48:PRO:HD2	1.76	0.67
9:I:112:GLU:OE2	9:I:115:LYS:NZ	2.28	0.67
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.77	0.67
5:E:12:GLN:HG3	5:E:117:VAL:HG23	1.76	0.67
7:G:93:PRO:HA	7:G:96:ARG:HG3	1.77	0.67
7:G:113:ASP:OD2	7:G:122:ASN:ND2	2.28	0.67
24:c:142:HIS:ND1	24:c:193:GLY:O	2.24	0.67
4:D:102:VAL:HG13	4:D:114:ALA:HB1	1.77	0.66
28:g:22:GLN:OE1	28:g:55:ARG:NH2	2.28	0.66
10:J:6:ILE:HB	10:J:76:ILE:HB	1.78	0.66
1:A:1228:C:OP2	13:M:110:LYS:NZ	2.27	0.66
36:o:2:SER:OG	36:o:3:ASN:N	2.28	0.66
1:A:38:G:H22	1:A:397:A:H5'	1.61	0.65
22:a:2250:G:OP1	33:l:84:LYS:NZ	2.28	0.65
22:a:72:U:O4	45:x:58:ASN:ND2	2.29	0.65
15:O:14:GLU:OE2	15:O:84:ARG:NH2	2.27	0.65
1:A:1233:G:H5'	9:I:119:ARG:HH12	1.61	0.65
18:R:25:ASP:OD2	18:R:28:THR:OG1	2.07	0.65
25:d:4:LEU:HD22	25:d:32:ASN:HD22	1.60	0.65
31:j:43:ILE:HD12	31:j:56:ASP:HB2	1.77	0.65
22:a:848:C:H2'	22:a:849:A:H8	1.61	0.65
4:D:87:GLY:HA3	4:D:197:GLU:HG3	1.79	0.65
1:A:1040:U:H2'	1:A:1041:G:H8	1.63	0.64
2:B:94:HIS:ND1	2:B:146:ASN:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2483:C:N3	33:l:123:LYS:NZ	2.46	0.64
1:A:451:A:H61	1:A:481:G:H5'	1.61	0.64
1:A:477:C:H2'	1:A:478:A:C8	2.33	0.64
22:a:284:U:O2	22:a:356:G:O6	2.15	0.64
34:m:30:ARG:NH1	34:m:74:GLU:OE2	2.30	0.64
22:a:2328:A:H2'	22:a:2329:U:C6	2.33	0.64
35:n:76:LYS:NZ	35:n:80:GLU:OE2	2.30	0.64
1:A:946:A:H2'	1:A:947:G:C8	2.33	0.63
48:0:25:LYS:NZ	48:0:51:GLU:OE1	2.30	0.63
4:D:156:LYS:NZ	4:D:160:GLU:OE2	2.31	0.63
14:N:46:LEU:HD12	19:S:13:LEU:HD13	1.79	0.63
26:e:105:LEU:HD23	26:e:200:LEU:HD21	1.79	0.63
1:A:1086:U:H3	1:A:1099:G:H22	1.46	0.63
1:A:664:G:H22	1:A:741:G:H1	1.45	0.63
1:A:203:G:O2'	1:A:465:A:N1	2.30	0.63
30:i:114:LEU:HG	30:i:118:MET:HE3	1.81	0.63
9:I:12:ARG:HG3	9:I:13:LYS:H	1.63	0.62
26:e:1:MET:HE1	26:e:20:GLY:HA3	1.80	0.62
32:k:123:ARG:NH2	32:k:143:GLU:OE2	2.32	0.62
48:0:37:LYS:HG2	48:0:48:ILE:HD13	1.80	0.62
15:O:18:ASP:HB3	15:O:21:ASP:HB2	1.80	0.62
26:e:181:ILE:HG12	32:k:1:MET:HE3	1.81	0.62
48:0:5:ILE:O	48:0:28:ARG:NH2	2.29	0.62
28:g:105:LEU:HB2	28:g:113:VAL:HG23	1.80	0.62
1:A:723:U:O2'	1:A:724:G:OP2	2.17	0.62
12:L:55:VAL:HG11	12:L:80:ILE:HD11	1.81	0.62
55:V:16:U:O2'	55:V:17:G:O5'	2.16	0.62
1:A:1356:G:H2'	1:A:1357:A:C8	2.34	0.62
22:a:887:U:O2'	22:a:889:C:OP2	2.15	0.62
4:D:95:GLU:OE2	4:D:100:ASN:ND2	2.32	0.62
1:A:492:C:H2'	1:A:493:A:C8	2.34	0.62
2:B:16:PHE:O	2:B:203:ASN:ND2	2.32	0.62
19:S:17:LYS:HB3	19:S:21:LYS:HZ3	1.65	0.62
1:A:460:A:H2'	1:A:461:A:H8	1.65	0.61
7:G:57:SER:OG	7:G:60:GLU:OE1	2.18	0.61
2:B:114:LEU:HD12	2:B:144:LEU:HG	1.82	0.61
3:C:175:LEU:HD23	3:C:182:ILE:HD13	1.81	0.61
42:u:58:SER:OG	42:u:59:GLU:OE1	2.17	0.61
1:A:459:A:H2'	1:A:460:A:C8	2.35	0.61
23:b:1:U:H2'	23:b:2:G:H8	1.63	0.61
39:r:4:ILE:HG12	39:r:106:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:A:O2'	1:A:81:A:O5'	2.14	0.61
20:T:28:MET:HE1	20:T:67:ILE:HG21	1.82	0.61
11:K:35:THR:HG22	11:K:41:ALA:HA	1.82	0.61
22:a:286:U:H2'	22:a:287:G:C8	2.35	0.61
24:c:107:PRO:HD2	24:c:110:LEU:HD22	1.81	0.61
1:A:1166:G:N1	1:A:1169:A:OP2	2.33	0.61
24:c:232:HIS:HA	24:c:242:LYS:HE3	1.82	0.61
1:A:707:U:OP1	11:K:87:LYS:NZ	2.32	0.61
2:B:104:TRP:NE1	2:B:108:ARG:HH12	1.99	0.61
18:R:32:TYR:HE2	18:R:45:THR:HG21	1.65	0.61
1:A:337:G:H2'	1:A:338:A:H8	1.64	0.61
11:K:72:ASP:OD1	11:K:75:LYS:NZ	2.33	0.61
34:m:69:ARG:O	34:m:70:THR:OG1	2.18	0.60
5:E:151:GLU:N	5:E:151:GLU:OE1	2.34	0.60
22:a:856:G:H2'	22:a:857:G:C8	2.35	0.60
22:a:1046:A:H3'	22:a:1047:G:H5'	1.83	0.60
22:a:2547:A:H2'	22:a:2548:U:C6	2.35	0.60
19:S:35:SER:OG	19:S:38:SER:OG	2.14	0.60
2:B:43:LEU:HA	2:B:46:THR:HG22	1.82	0.60
17:Q:17:MET:HG3	17:Q:20:SER:OG	2.01	0.60
37:p:89:GLU:HG3	38:q:52:PRO:HB3	1.83	0.60
22:a:191:A:H2'	22:a:192:C:C6	2.37	0.60
1:A:1062:U:H2'	1:A:1063:C:C6	2.36	0.60
22:a:1478:G:H1	22:a:1513:U:H3	1.47	0.59
32:k:57:LEU:HD22	50:2:54:ASP:HB3	1.84	0.59
43:v:66:LYS:NZ	43:v:85:GLU:OE1	2.31	0.59
22:a:358:U:H2'	22:a:359:G:H8	1.67	0.59
40:s:6:ARG:NH2	40:s:37:ASP:OD1	2.33	0.59
1:A:131:A:H2'	1:A:132:C:C6	2.37	0.59
11:K:20:VAL:HG23	11:K:83:GLU:HB2	1.84	0.59
11:K:31:ILE:HG12	11:K:46:THR:HG22	1.84	0.59
16:P:18:GLN:OE1	16:P:35:ARG:NE	2.25	0.59
22:a:593:U:H2'	22:a:594:U:C6	2.38	0.59
22:a:1508:A:O2'	22:a:1509:A:O4'	2.15	0.59
31:j:63:VAL:HG12	31:j:107:LEU:HD11	1.85	0.59
1:A:187:G:N2	1:A:190:A:OP2	2.33	0.59
1:A:1130:A:H2'	1:A:1131:G:H8	1.67	0.59
1:A:475:C:H2'	1:A:476:U:H6	1.68	0.59
4:D:54:GLN:HB3	4:D:203:LEU:HD12	1.85	0.59
9:I:75:GLN:O	9:I:79:ILE:HG12	2.03	0.59
21:U:64:ASN:HA	21:U:67:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:C:H42	1:A:1035:A:H61	1.50	0.59
19:S:17:LYS:HB3	19:S:21:LYS:NZ	2.17	0.59
1:A:1038:C:H2'	1:A:1039:G:H8	1.67	0.59
32:k:132:ARG:O	32:k:136:GLU:HG2	2.03	0.59
7:G:129:GLU:O	7:G:131:LYS:NZ	2.35	0.59
22:a:639:U:H2'	22:a:640:C:C6	2.38	0.59
1:A:128:G:H5'	17:Q:6:ARG:NH2	2.17	0.58
22:a:84:A:N1	22:a:98:G:O2'	2.34	0.58
22:a:2291:U:H2'	22:a:2292:U:C6	2.38	0.58
1:A:142:G:H3'	1:A:143:A:H8	1.68	0.58
5:E:156:LYS:NZ	8:H:71:VAL:O	2.36	0.58
46:y:6:LYS:HB2	46:y:58:GLU:HB2	1.86	0.58
42:u:35:GLU:HG2	42:u:93:ARG:HH12	1.68	0.58
8:H:96:MET:HE3	8:H:99:LEU:HB2	1.83	0.58
28:g:11:VAL:HB	28:g:48:ASN:HB3	1.86	0.58
30:i:15:TRP:HB3	30:i:137:PRO:HB3	1.85	0.58
5:E:149:SER:H	5:E:152:MET:HE3	1.69	0.58
8:H:74:SER:HB3	8:H:130:ALA:HB3	1.86	0.58
9:I:112:GLU:HG2	9:I:121:ALA:HB1	1.85	0.58
22:a:476:G:N1	22:a:479:A:OP2	2.35	0.58
7:G:129:GLU:HG3	7:G:131:LYS:HG2	1.86	0.58
27:f:56:ASP:OD2	27:f:150:ARG:NH1	2.36	0.58
11:K:111:THR:HG23	21:U:3:VAL:HG22	1.85	0.57
22:a:2799:A:O2'	22:a:2800:A:H5"	2.04	0.57
1:A:408:A:OP2	4:D:8:LYS:NZ	2.37	0.57
8:H:13:ARG:NH1	8:H:26:THR:O	2.37	0.57
13:M:59:GLU:O	13:M:62:LYS:HG2	2.05	0.57
45:x:10:SER:OG	45:x:12:GLU:OE1	2.22	0.57
2:B:28:LYS:O	2:B:31:ILE:HG22	2.05	0.57
14:N:27:LEU:O	14:N:31:ILE:HG12	2.04	0.57
22:a:1386:C:H2'	22:a:1387:A:C8	2.39	0.57
28:g:42:GLU:OE2	28:g:55:ARG:NH1	2.38	0.57
22:a:2243:U:H2'	22:a:2244:U:C6	2.39	0.57
1:A:5:U:H4'	1:A:6:G:H5'	1.86	0.57
1:A:1034:G:O6	1:A:1035:A:N6	2.38	0.57
15:O:18:ASP:OD1	15:O:19:ALA:N	2.37	0.57
1:A:459:A:H2'	1:A:460:A:H8	1.69	0.57
22:a:191:A:H2'	22:a:192:C:H6	1.70	0.57
18:R:26:ILE:O	18:R:30:LYS:HG2	2.05	0.56
12:L:14:ARG:NH2	12:L:14:ARG:HB2	2.20	0.56
22:a:1746:A:H2'	22:a:1747:U:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:161:TYR:HB3	24:c:194:GLU:CB	2.36	0.56
47:z:31:ASP:OD1	47:z:32:LYS:N	2.38	0.56
1:A:56:U:H2'	1:A:57:G:H8	1.71	0.56
4:D:162:ALA:O	4:D:167:LYS:NZ	2.36	0.56
29:h:12:LEU:HD13	29:h:19:VAL:HG11	1.87	0.56
19:S:30:PRO:HB3	19:S:48:THR:HG23	1.88	0.56
22:a:849:A:H2'	22:a:850:U:C6	2.40	0.56
28:g:72:LEU:HD13	28:g:75:MET:HE2	1.87	0.56
1:A:1004:A:H2'	1:A:1005:A:O4'	2.05	0.56
4:D:12:SER:OG	4:D:17:THR:O	2.22	0.56
1:A:89:U:H2'	1:A:90:C:C2	2.41	0.56
1:A:1323:G:H2'	1:A:1324:A:C8	2.41	0.56
4:D:95:GLU:HA	4:D:100:ASN:ND2	2.20	0.56
52:4:58:ASP:OD1	52:4:59:ARG:N	2.38	0.56
1:A:475:C:H2'	1:A:476:U:C6	2.41	0.56
1:A:1151:A:HO2'	1:A:1152:A:H8	1.53	0.56
2:B:66:LYS:HZ1	2:B:154:MET:HE2	1.70	0.56
22:a:546:U:OP2	22:a:547:A:N6	2.37	0.56
46:y:27:LEU:O	46:y:38:ARG:NH1	2.38	0.56
22:a:284:U:H2'	22:a:285:G:H8	1.70	0.56
55:V:74:C:H2'	55:V:75:A:C8	2.41	0.56
2:B:219:ALA:HA	2:B:222:ARG:HH12	1.71	0.55
22:a:545:U:H4'	22:a:546:U:OP1	2.05	0.55
2:B:15:HIS:HB3	2:B:43:LEU:HD21	1.89	0.55
28:g:2:SER:O	28:g:6:LYS:N	2.34	0.55
6:F:37:HIS:HB3	6:F:97:THR:HG22	1.88	0.55
31:j:58:LEU:HA	31:j:89:ASN:ND2	2.22	0.55
3:C:134:MET:HE2	3:C:168:TYR:HD1	1.71	0.55
55:V:17:G:O2'	55:V:56:G:N2	2.26	0.55
7:G:71:PRO:O	7:G:96:ARG:HD2	2.06	0.55
22:a:2312:U:O2	27:f:37:ASN:ND2	2.31	0.55
22:a:2327:A:H2'	22:a:2328:A:C8	2.41	0.55
37:p:107:THR:O	37:p:111:GLU:HG2	2.06	0.55
48:0:9:ILE:HD12	48:0:51:GLU:HG3	1.88	0.55
1:A:191:G:H2'	1:A:192:A:H8	1.71	0.55
1:A:1178:G:N7	9:I:99:ARG:NH1	2.55	0.55
21:U:63:GLU:HB3	21:U:67:ARG:NH2	2.22	0.55
22:a:126:A:OP1	49:1:45:SER:OG	2.17	0.55
22:a:848:C:H2'	22:a:849:A:C8	2.41	0.55
1:A:401:C:O2'	1:A:621:A:N3	2.35	0.55
2:B:66:LYS:NZ	2:B:154:MET:HE2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:V:5:C:H2'	55:V:6:2MG:O4'	2.07	0.55
6:F:88:MET:SD	6:F:90:MET:HE2	2.46	0.55
17:Q:77:ARG:HH21	17:Q:79:VAL:HA	1.72	0.55
22:a:549:G:H2'	22:a:550:C:C6	2.41	0.55
28:g:24:ILE:O	28:g:34:THR:OG1	2.21	0.55
46:y:7:ILE:HD11	46:y:48:ILE:HD11	1.88	0.55
1:A:85:U:O2	1:A:87:C:N4	2.40	0.54
5:E:40:GLY:HA2	5:E:71:MET:HE1	1.89	0.54
6:F:38:ARG:HH11	6:F:61:LEU:HD21	1.71	0.54
16:P:44:SER:OG	16:P:47:GLU:OE2	2.23	0.54
26:e:106:LYS:HE3	26:e:200:LEU:HB3	1.88	0.54
1:A:202:G:H21	1:A:466:A:H61	1.54	0.54
9:I:15:SER:OG	9:I:69:GLY:O	2.23	0.54
15:O:71:LYS:HD2	15:O:78:TYR:CE2	2.42	0.54
22:a:548:G:H2'	22:a:549:G:H1'	1.88	0.54
22:a:1410:G:H2'	22:a:1411:U:C6	2.43	0.54
22:a:2718:G:O2'	22:a:2847:U:OP1	2.24	0.54
25:d:1:MET:HG3	25:d:205:PRO:HG2	1.89	0.54
44:w:59:ILE:HG12	44:w:67:VAL:HG21	1.88	0.54
1:A:460:A:H2'	1:A:461:A:C8	2.42	0.54
1:A:1149:C:OP2	9:I:11:ARG:NH2	2.36	0.54
2:B:66:LYS:HZ3	2:B:90:PHE:HB2	1.71	0.54
19:S:45:ILE:HG12	19:S:64:ASP:HA	1.87	0.54
1:A:171:A:H2'	1:A:172:A:C8	2.42	0.54
7:G:15:ASP:OD1	7:G:19:GLY:N	2.40	0.54
24:c:29:PRO:HG2	24:c:34:LEU:HD11	1.89	0.54
7:G:111:ARG:HD2	7:G:123:GLU:HG2	1.89	0.54
15:O:74:ASP:OD1	15:O:77:ARG:HG2	2.08	0.54
28:g:8:PRO:HB3	28:g:51:THR:HG22	1.90	0.54
1:A:56:U:H2'	1:A:57:G:C8	2.43	0.54
6:F:71:ILE:O	6:F:75:GLU:HG3	2.08	0.54
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.22	0.54
1:A:222:C:H2'	1:A:223:A:H8	1.73	0.54
3:C:152:GLU:HG3	3:C:167:TRP:HB3	1.90	0.54
13:M:107:ARG:HH12	13:M:113:ARG:HA	1.73	0.54
1:A:718:A:C8	11:K:118:HIS:HB3	2.43	0.54
2:B:136:MET:HA	2:B:139:ARG:HG2	1.89	0.54
22:a:1794:A:H2'	22:a:1795:C:C6	2.43	0.54
22:a:1796:U:H2'	22:a:1797:G:H8	1.73	0.54
5:E:34:THR:HG22	5:E:52:LYS:HG2	1.90	0.53
22:a:2469:A:N6	22:a:2481:G:O2'	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:r:65:ASP:OD2	39:r:65:ASP:N	2.41	0.53
2:B:9:MET:HE1	2:B:46:THR:HG23	1.90	0.53
25:d:5:VAL:H	25:d:32:ASN:HD21	1.57	0.53
3:C:142:MET:HG3	3:C:170:GLU:OE1	2.08	0.53
8:H:77:ARG:NH1	8:H:79:SER:O	2.41	0.53
20:T:44:LYS:HD3	20:T:87:ALA:HA	1.89	0.53
33:l:66:ARG:HD3	33:l:104:GLU:OE1	2.08	0.53
1:A:1273:C:H2'	1:A:1274:A:O4'	2.09	0.53
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.90	0.53
22:a:1590:A:H2'	22:a:1591:A:C8	2.44	0.53
22:a:2273:A:H2'	22:a:2274:A:C8	2.43	0.53
45:x:10:SER:OG	45:x:13:GLU:OE1	2.26	0.53
4:D:27:ALA:O	4:D:30:THR:OG1	2.25	0.53
22:a:2845:U:H5"	36:o:52:ASN:O	2.09	0.53
27:f:105:THR:HA	52:4:38:SER:HB3	1.91	0.53
52:4:8:LYS:NZ	52:4:10:GLU:OE2	2.42	0.53
1:A:323:U:H2'	1:A:324:G:O4'	2.08	0.53
1:A:1040:U:H2'	1:A:1041:G:C8	2.43	0.53
6:F:38:ARG:HH21	6:F:96:VAL:HG12	1.73	0.53
17:Q:25:ILE:HB	17:Q:42:THR:HG22	1.91	0.53
22:a:2329:U:H2'	22:a:2330:G:C8	2.43	0.53
29:h:6:LEU:HD11	29:h:37:VAL:HG13	1.91	0.53
22:a:581:C:H2'	22:a:582:A:C8	2.44	0.53
35:n:88:LYS:HD2	35:n:88:LYS:O	2.08	0.53
1:A:404:G:O2'	1:A:498:A:N1	2.40	0.53
1:A:714:G:H2'	1:A:715:A:C8	2.44	0.53
1:A:1314:C:H2'	1:A:1315:U:C6	2.43	0.53
13:M:107:ARG:HH21	13:M:110:LYS:HE3	1.73	0.53
36:o:89:ARG:NH1	36:o:115:ASN:O	2.42	0.53
13:M:17:ILE:O	13:M:20:THR:OG1	2.27	0.53
1:A:635:A:H2'	1:A:636:U:C6	2.43	0.53
1:A:1218:C:H2'	1:A:1219:A:C8	2.43	0.53
4:D:9:LEU:HD13	4:D:32:CYS:HB3	1.91	0.53
9:I:39:PHE:O	9:I:45:ARG:NH2	2.41	0.53
1:A:751:U:OP1	15:O:17:ARG:NH2	2.42	0.52
22:a:1141:U:H4'	22:a:1142:A:O4'	2.09	0.52
22:a:1871:A:H2'	22:a:1872:A:C8	2.44	0.52
1:A:677:U:H3	1:A:713:G:H22	1.56	0.52
1:A:744:C:H2'	1:A:745:G:H8	1.75	0.52
15:O:26:GLU:CD	15:O:26:GLU:H	2.18	0.52
22:a:994:C:O2	38:q:10:LYS:NZ	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:e:118:LEU:HD11	26:e:188:MET:HG3	1.90	0.52
22:a:1494:A:H2'	22:a:1495:A:C8	2.44	0.52
30:i:96:ARG:NH1	30:i:98:GLU:OE2	2.31	0.52
54:Z:54:G:H3'	54:Z:55:5MU:H73	1.91	0.52
22:a:1796:U:H2'	22:a:1797:G:C8	2.44	0.52
1:A:1169:A:H2'	1:A:1170:A:C8	2.45	0.52
13:M:104:THR:HG22	13:M:105:ASN:N	2.25	0.52
18:R:21:ILE:HG12	18:R:54:GLN:HB3	1.90	0.52
22:a:828:U:H2'	22:a:829:A:C8	2.45	0.52
1:A:429:U:H3'	4:D:9:LEU:HD12	1.92	0.52
1:A:713:G:H2'	1:A:714:G:C8	2.45	0.52
1:A:1412:C:H2'	1:A:1413:A:C8	2.44	0.52
4:D:95:GLU:HA	4:D:100:ASN:HD22	1.74	0.52
25:d:106:LYS:NZ	25:d:176:ASP:OD1	2.43	0.52
2:B:129:LEU:HD11	2:B:133:GLU:HB2	1.91	0.52
2:B:160:ALA:HB1	2:B:184:PHE:HE2	1.74	0.52
3:C:72:ARG:HG2	3:C:72:ARG:HH11	1.73	0.52
22:a:871:U:H2'	22:a:872:U:C6	2.45	0.52
1:A:1036:A:H2'	1:A:1037:C:O4'	2.10	0.52
1:A:1287:A:H2'	1:A:1288:A:C8	2.45	0.52
22:a:1469:A:H2'	22:a:1470:A:C8	2.45	0.52
26:e:170:ARG:NH2	26:e:176:ASP:OD1	2.41	0.52
1:A:1435:G:H2'	1:A:1436:U:C6	2.45	0.52
22:a:813:U:H2'	22:a:814:C:C6	2.45	0.52
32:k:82:LEU:HD22	32:k:90:VAL:HG21	1.92	0.52
45:x:12:GLU:O	45:x:16:THR:HG23	2.10	0.52
6:F:38:ARG:NH1	6:F:61:LEU:HD21	2.25	0.51
22:a:414:C:H2'	22:a:415:A:C8	2.45	0.51
22:a:568:U:H1'	22:a:2030:6MZ:H9C1	1.91	0.51
35:n:30:ARG:HB3	35:n:35:ILE:HG13	1.93	0.51
1:A:1098:C:O2'	21:U:71:TYR:O	2.24	0.51
9:I:52:LEU:HD11	9:I:63:LEU:HD11	1.92	0.51
22:a:1597:A:H5"	22:a:1598:A:H5'	1.92	0.51
38:q:34:GLU:OE1	38:q:60:LYS:HE3	2.09	0.51
48:0:25:LYS:NZ	48:0:32:GLU:O	2.40	0.51
1:A:728:A:H2'	1:A:729:A:C8	2.45	0.51
1:A:769:G:H4'	1:A:1513:A:H4'	1.93	0.51
1:A:1130:A:H2'	1:A:1131:G:C8	2.44	0.51
2:B:5:SER:OG	2:B:6:MET:N	2.42	0.51
22:a:594:U:H2'	22:a:595:C:C6	2.45	0.51
24:c:21:ASN:HB3	24:c:24:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:G:N7	21:U:46:LYS:HE2	2.25	0.51
54:Z:19:G:H1'	54:Z:59:A:C2	2.46	0.51
1:A:83:C:N3	1:A:86:G:N2	2.49	0.51
13:M:107:ARG:NH2	13:M:110:LYS:HE3	2.26	0.51
22:a:1870:C:O2'	22:a:1871:A:O4'	2.28	0.51
22:a:2469:A:H2'	22:a:2470:G:O4'	2.10	0.51
22:a:2901:C:N3	22:a:2902:C:N4	2.59	0.51
22:a:1392:A:N6	40:s:18:GLU:OE2	2.28	0.51
1:A:1312:G:P	52:4:63:ARG:HH12	2.33	0.51
22:a:2071:A:H2'	22:a:2072:C:C6	2.45	0.51
47:z:54:VAL:HG23	47:z:55:ILE:HG12	1.92	0.51
18:R:22:ASP:OD1	18:R:24:LYS:HE2	2.11	0.51
3:C:134:MET:HE2	3:C:168:TYR:CD1	2.46	0.51
18:R:41:PRO:HD2	18:R:44:ILE:HD12	1.93	0.51
27:f:8:TYR:HB2	27:f:173:PHE:HZ	1.76	0.51
41:t:97:LYS:O	41:t:98:SER:OG	2.28	0.51
8:H:64:LYS:HG3	8:H:71:VAL:HG21	1.93	0.51
22:a:1808:A:H3'	22:a:1809:A:C8	2.46	0.51
51:3:11:CYS:HB3	51:3:33:HIS:HE1	1.75	0.51
1:A:1031:C:H4'	1:A:1032:G:C6	2.47	0.50
22:a:172:A:H2'	22:a:173:A:H8	1.76	0.50
22:a:876:C:H2'	22:a:877:A:O4'	2.11	0.50
49:1:41:ARG:HG2	49:1:46:LYS:HD3	1.92	0.50
1:A:675:A:H1'	11:K:118:HIS:CD2	2.46	0.50
1:A:1391:U:H2'	1:A:1392:G:C8	2.46	0.50
2:B:31:ILE:HD11	2:B:39:HIS:CG	2.46	0.50
6:F:88:MET:HE3	18:R:64:TYR:CD2	2.47	0.50
19:S:45:ILE:HA	19:S:62:VAL:HG13	1.94	0.50
22:a:155:A:H2'	22:a:156:A:C8	2.47	0.50
22:a:645:C:H2'	22:a:647:G:C8	2.47	0.50
22:a:2298:A:OP1	27:f:71:ARG:NH2	2.40	0.50
22:a:494:G:H4'	39:r:6:LYS:HB2	1.93	0.50
22:a:608:A:H2'	22:a:609:A:C8	2.46	0.50
22:a:1405:U:H2'	22:a:1406:U:C6	2.46	0.50
22:a:2430:A:N3	22:a:2430:A:H2'	2.25	0.50
2:B:129:LEU:HD23	2:B:130:THR:N	2.26	0.50
10:J:10:LEU:HD22	10:J:98:VAL:HG22	1.92	0.50
15:O:79:THR:HA	15:O:82:ILE:HG12	1.93	0.50
21:U:30:ALA:O	21:U:34:ARG:HD3	2.11	0.50
22:a:219:A:N3	22:a:234:U:O2'	2.41	0.50
22:a:548:G:H2'	22:a:549:G:C1'	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:11:GLU:HA	27:f:14:LYS:HG2	1.94	0.50
1:A:635:A:H2'	1:A:636:U:H6	1.76	0.50
1:A:636:U:H2'	1:A:637:C:C6	2.47	0.50
12:L:110:ARG:HB2	12:L:119:VAL:HG21	1.92	0.50
2:B:129:LEU:HD21	2:B:133:GLU:HB2	1.93	0.50
9:I:21:ILE:HG22	9:I:63:LEU:HD23	1.93	0.50
19:S:9:PRO:HG3	52:4:64:PHE:CD2	2.47	0.50
22:a:307:G:N1	22:a:310:A:OP2	2.41	0.50
22:a:1179:G:H2'	22:a:1180:U:C6	2.47	0.50
22:a:1434:A:H2'	22:a:1435:G:C8	2.47	0.50
22:a:1870:C:O2'	22:a:1871:A:H8	1.93	0.50
22:a:2328:A:H2'	22:a:2329:U:H6	1.77	0.50
22:a:2850:A:N7	22:a:2868:A:O2'	2.40	0.50
27:f:111:ILE:HD11	27:f:114:PHE:CD1	2.46	0.50
30:i:69:ARG:HG2	30:i:90:GLU:HG2	1.92	0.50
32:k:10:GLU:CD	32:k:10:GLU:H	2.19	0.50
1:A:195:A:H2'	1:A:196:A:C8	2.47	0.50
1:A:1038:C:H2'	1:A:1039:G:C8	2.46	0.50
47:z:46:ASP:O	47:z:53:LYS:NZ	2.43	0.50
1:A:17:U:H2'	1:A:18:C:C6	2.47	0.50
1:A:324:G:N1	1:A:327:A:OP2	2.44	0.50
1:A:381:C:H2'	1:A:382:A:O4'	2.11	0.50
1:A:662:U:H2'	1:A:663:A:C8	2.46	0.50
22:a:3:U:H2'	22:a:4:U:C6	2.47	0.50
22:a:849:A:H2'	22:a:850:U:H6	1.77	0.50
22:a:2591:C:H2'	22:a:2592:G:C8	2.47	0.50
26:e:191:ASP:O	26:e:195:GLN:HG3	2.12	0.50
3:C:179:ARG:HB3	3:C:206:GLU:O	2.11	0.50
25:d:38:LYS:HE3	25:d:81:GLU:OE1	2.12	0.50
1:A:128:G:P	17:Q:6:ARG:HH22	2.35	0.49
1:A:945:G:C2	1:A:946:A:C8	3.00	0.49
10:J:56:HIS:CE1	10:J:57:VAL:HG13	2.47	0.49
14:N:51:LEU:HG	14:N:52:PRO:HD2	1.93	0.49
22:a:930:G:H1'	46:y:25:LEU:HD21	1.93	0.49
23:b:2:G:H2'	23:b:3:C:C6	2.47	0.49
1:A:356:A:N3	1:A:368:U:O2'	2.38	0.49
22:a:2514:U:H2'	22:a:2515:C:C6	2.47	0.49
2:B:100:MET:O	2:B:104:TRP:HE3	1.96	0.49
8:H:38:ASN:O	8:H:42:GLU:HG2	2.12	0.49
10:J:42:LEU:HB2	10:J:71:LEU:HB2	1.93	0.49
20:T:9:LYS:HE2	20:T:13:GLN:HE21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1028:A:H2'	22:a:1029:A:C8	2.47	0.49
23:b:66:A:H61	23:b:107:G:H2'	1.77	0.49
34:m:72:ASP:OD1	34:m:75:ILE:HB	2.12	0.49
2:B:171:ILE:O	2:B:175:GLU:HG3	2.13	0.49
1:A:62:U:OP1	1:A:385:C:O2'	2.30	0.49
4:D:3:ARG:HD2	4:D:115:ARG:HE	1.77	0.49
22:a:197:A:N6	22:a:2430:A:O2'	2.46	0.49
26:e:176:ASP:OD1	26:e:176:ASP:N	2.44	0.49
28:g:33:LEU:HD11	28:g:75:MET:HB2	1.94	0.49
30:i:13:ARG:NH1	30:i:49:ASP:O	2.39	0.49
44:w:40:VAL:HG13	44:w:43:GLU:HB2	1.93	0.49
1:A:674:G:H2'	1:A:675:A:H8	1.78	0.49
2:B:98:GLY:HA2	2:B:171:ILE:HD11	1.94	0.49
9:I:6:TYR:HB2	9:I:21:ILE:HG12	1.94	0.49
22:a:888:C:H2'	22:a:889:C:C6	2.48	0.49
27:f:111:ILE:HD11	27:f:114:PHE:HD1	1.78	0.49
44:w:66:THR:O	44:w:70:GLU:HG3	2.12	0.49
1:A:181:A:N6	1:A:195:A:N7	2.60	0.49
1:A:384:G:H2'	1:A:385:C:C6	2.48	0.49
13:M:33:ILE:HD13	13:M:60:VAL:HG22	1.95	0.49
13:M:92:ARG:HG2	22:a:888:C:C6	2.48	0.49
26:e:3:LEU:HD13	26:e:120:VAL:HG21	1.94	0.49
52:4:41:HIS:HB3	52:4:44:PHE:HD2	1.76	0.49
1:A:1029:U:H4'	1:A:1030:U:C5	2.47	0.49
3:C:79:LYS:HE3	3:C:79:LYS:HA	1.95	0.49
12:L:56:ARG:NH1	12:L:62:GLU:OE1	2.46	0.49
17:Q:64:CYS:SG	17:Q:74:THR:HG23	2.52	0.49
22:a:64:A:H2'	22:a:65:U:C6	2.46	0.49
22:a:1709:U:H2'	22:a:1710:G:H8	1.76	0.49
22:a:2756:U:OP2	51:3:19:ARG:NH2	2.42	0.49
24:c:5:LYS:HD2	24:c:17:VAL:HG22	1.94	0.49
54:Z:22:A:N6	54:Z:47:A:H2'	2.27	0.49
1:A:269:C:H2'	1:A:270:A:C8	2.48	0.49
1:A:405:U:OP2	4:D:3:ARG:NH1	2.46	0.49
1:A:539:A:H2'	1:A:540:G:C8	2.48	0.49
1:A:744:C:H2'	1:A:745:G:C8	2.48	0.49
22:a:1548:A:H2'	22:a:1549:A:C8	2.47	0.49
22:a:1614:A:C2	39:r:93:ALA:HB2	2.48	0.49
23:b:1:U:H2'	23:b:2:G:C8	2.44	0.49
33:l:26:VAL:HG13	33:l:104:GLU:HG2	1.94	0.49
1:A:1010:U:H2'	1:A:1011:C:C6	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:ARG:NE	3:C:166:GLU:OE2	2.45	0.48
12:L:33:VAL:HG22	12:L:79:VAL:HG22	1.95	0.48
28:g:60:ASP:OD1	28:g:60:ASP:N	2.45	0.48
1:A:127:G:O2'	17:Q:6:ARG:NH1	2.46	0.48
20:T:35:VAL:HG11	20:T:79:LEU:HD13	1.94	0.48
22:a:2246:G:H2'	22:a:2247:A:C8	2.48	0.48
22:a:284:U:H2'	22:a:285:G:C8	2.48	0.48
22:a:1563:U:H2'	22:a:1564:C:C6	2.47	0.48
22:a:2359:C:O2'	50:2:54:ASP:OD2	2.30	0.48
39:r:48:LYS:O	39:r:52:GLU:HG3	2.13	0.48
1:A:1251:A:H2'	1:A:1252:A:C8	2.48	0.48
2:B:167:ASP:OD1	2:B:168:HIS:N	2.45	0.48
17:Q:61:ILE:HG22	17:Q:73:TRP:HE3	1.79	0.48
22:a:796:C:OP1	26:e:57:LYS:HE2	2.13	0.48
25:d:39:ASP:N	25:d:39:ASP:OD1	2.43	0.48
7:G:23:LEU:HD11	7:G:47:LEU:HD11	1.94	0.48
9:I:55:VAL:HG21	9:I:94:LEU:HD13	1.95	0.48
10:J:11:LYS:HG2	10:J:71:LEU:HD23	1.96	0.48
22:a:278:A:N6	22:a:362:A:N7	2.62	0.48
22:a:634:C:H2'	22:a:635:C:C6	2.49	0.48
22:a:832:U:H2'	22:a:833:A:C8	2.49	0.48
23:b:2:G:H2'	23:b:3:C:H6	1.77	0.48
1:A:82:G:N2	1:A:89:U:O2	2.33	0.48
22:a:833:A:H2'	22:a:834:G:C8	2.49	0.48
22:a:1386:C:H2'	22:a:1387:A:H8	1.77	0.48
22:a:2064:C:H2'	22:a:2065:C:C6	2.49	0.48
41:t:18:ASP:HB3	41:t:21:LYS:HD2	1.94	0.48
1:A:821:G:H2'	1:A:822:U:C6	2.49	0.48
1:A:859:G:H2'	1:A:860:A:C8	2.48	0.48
1:A:1314:C:OP2	19:S:4:SER:OG	2.19	0.48
14:N:40:ASP:OD1	14:N:40:ASP:N	2.36	0.48
22:a:1703:G:H2'	22:a:1704:C:C6	2.49	0.48
34:m:8:ARG:HD2	34:m:43:GLU:HG2	1.96	0.48
3:C:157:LEU:HD23	3:C:196:ILE:HD13	1.96	0.48
22:a:2795:C:H2'	22:a:2796:U:H6	1.79	0.48
45:x:52:ARG:O	45:x:55:THR:HG22	2.14	0.48
1:A:501:C:OP1	12:L:114:ARG:NH2	2.36	0.48
10:J:7:ARG:HG3	10:J:7:ARG:HH11	1.79	0.48
10:J:22:THR:HA	10:J:25:ILE:HG22	1.96	0.48
13:M:49:SER:O	13:M:53:ILE:HG12	2.14	0.48
22:a:347:A:H2'	22:a:348:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2233:U:H2'	22:a:2234:G:C8	2.49	0.48
22:a:2820:A:N3	22:a:2820:A:H2'	2.29	0.48
51:3:12:ARG:HG2	51:3:12:ARG:HH11	1.79	0.48
1:A:412:A:O2'	1:A:413:G:H4'	2.13	0.47
1:A:1314:C:H2'	1:A:1315:U:H6	1.79	0.47
1:A:1513:A:H2'	1:A:1514:G:C8	2.49	0.47
22:a:1720:U:H2'	22:a:1721:G:O4'	2.14	0.47
27:f:42:GLU:OE1	27:f:42:GLU:N	2.47	0.47
27:f:98:GLU:OE1	52:4:9:TYR:OH	2.27	0.47
45:x:10:SER:H	45:x:13:GLU:CD	2.21	0.47
4:D:124:MET:HG3	4:D:146:ARG:HG2	1.95	0.47
22:a:644:A:H2'	22:a:645:C:O4'	2.14	0.47
22:a:2313:C:H5"	27:f:88:LYS:HD2	1.96	0.47
1:A:73:C:O2'	1:A:74:A:H8	1.97	0.47
1:A:218:U:H2'	1:A:219:U:O4'	2.15	0.47
3:C:42:TYR:OH	3:C:90:VAL:HG11	2.14	0.47
8:H:113:ASP:OD1	8:H:113:ASP:N	2.47	0.47
11:K:67:ALA:HB2	11:K:96:THR:HG23	1.95	0.47
22:a:1028:A:N6	22:a:1125:G:H2'	2.30	0.47
28:g:98:VAL:HG23	28:g:125:CYS:SG	2.54	0.47
5:E:85:VAL:HG11	5:E:147:MET:HB3	1.96	0.47
13:M:81:MET:HE3	13:M:91:HIS:HB3	1.97	0.47
50:2:32:ILE:O	50:2:32:ILE:HG13	2.13	0.47
18:R:32:TYR:CE2	18:R:45:THR:HG21	2.48	0.47
19:S:16:LEU:O	19:S:20:GLU:HG2	2.15	0.47
19:S:64:ASP:OD2	19:S:65:GLU:N	2.47	0.47
22:a:78:U:OP1	45:x:7:ARG:NH2	2.48	0.47
22:a:358:U:H2'	22:a:359:G:C8	2.48	0.47
22:a:2025:C:H2'	22:a:2026:U:C6	2.50	0.47
30:i:98:GLU:CD	30:i:98:GLU:H	2.22	0.47
40:s:5:GLU:OE1	40:s:5:GLU:N	2.42	0.47
40:s:54:GLU:HB3	40:s:88:LYS:HE3	1.96	0.47
12:L:68:GLY:O	12:L:99:ARG:NH1	2.46	0.47
15:O:35:GLN:HA	15:O:35:GLN:OE1	2.15	0.47
22:a:5:A:H2'	22:a:6:A:C8	2.50	0.47
41:t:96:PHE:O	41:t:100:SER:HA	2.14	0.47
1:A:1410:A:H2'	1:A:1411:C:C6	2.50	0.47
4:D:165:ARG:HG2	4:D:166:GLU:H	1.80	0.47
11:K:94:GLU:HG3	21:U:20:LYS:HE2	1.96	0.47
22:a:1183:U:H2'	22:a:1184:U:C6	2.49	0.47
22:a:1709:U:H2'	22:a:1710:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1730:C:O2'	22:a:1731:G:O5'	2.32	0.47
22:a:2020:A:H5'	47:z:9:THR:CG2	2.45	0.47
24:c:75:PRO:HG2	24:c:97:LYS:HG3	1.97	0.47
27:f:153:ASP:OD1	27:f:153:ASP:N	2.47	0.47
1:A:216:U:H2'	1:A:217:C:C6	2.50	0.47
1:A:437:U:O4'	4:D:154:ARG:NH2	2.48	0.47
3:C:9:GLY:HA3	14:N:89:MET:SD	2.54	0.47
22:a:172:A:H2'	22:a:173:A:C8	2.49	0.47
22:a:1594:U:H2'	22:a:1595:C:C6	2.49	0.47
34:m:22:ARG:HG3	34:m:70:THR:HA	1.97	0.47
55:V:9:1MA:O4'	55:V:46:A:H1'	2.15	0.47
1:A:745:G:H2'	1:A:746:A:C8	2.50	0.47
1:A:1063:C:OP2	1:A:1064:G:O2'	2.33	0.47
1:A:1225:A:H2'	1:A:1226:C:C5	2.50	0.47
1:A:1458:G:OP1	20:T:30:THR:OG1	2.31	0.47
9:I:84:THR:HG23	9:I:98:LEU:HD13	1.96	0.47
23:b:106:G:H2'	23:b:107:G:O4'	2.15	0.47
53:X:48:A:H2'	53:X:49:C:C6	2.50	0.47
1:A:221:C:H2'	1:A:222:C:H6	1.80	0.47
1:A:1029:U:O2'	1:A:1033:G:O6	2.32	0.47
7:G:6:VAL:HG12	7:G:6:VAL:O	2.14	0.47
9:I:65:ILE:HG21	9:I:79:ILE:HD12	1.95	0.47
11:K:22:HIS:HB2	11:K:33:THR:HG22	1.96	0.47
22:a:1182:G:H2'	22:a:1183:U:O4'	2.14	0.47
29:h:34:GLY:O	29:h:36:ALA:N	2.48	0.47
41:t:47:LYS:HE2	41:t:47:LYS:HB2	1.81	0.47
47:z:52:ARG:HB3	47:z:52:ARG:NH2	2.30	0.47
22:a:784:G:H5'	22:a:785:G:OP1	2.15	0.46
22:a:2038:G:H2'	22:a:2039:U:O4'	2.15	0.46
22:a:2895:G:H2'	22:a:2896:C:C6	2.50	0.46
1:A:575:G:O2'	1:A:821:G:OP2	2.31	0.46
1:A:976:G:OP2	1:A:1358:U:O2'	2.32	0.46
7:G:113:ASP:HB2	7:G:119:ARG:HG2	1.96	0.46
1:A:501:C:H2'	1:A:502:A:C8	2.50	0.46
11:K:88:GLY:O	11:K:93:ARG:NH1	2.45	0.46
26:e:188:MET:HE1	26:e:196:VAL:HG21	1.97	0.46
52:4:59:ARG:HH21	52:4:63:ARG:NH2	2.13	0.46
1:A:109:A:C6	1:A:326:G:C6	3.03	0.46
1:A:1513:A:H2'	1:A:1514:G:H8	1.80	0.46
6:F:38:ARG:NH2	6:F:96:VAL:HG12	2.30	0.46
7:G:92:ARG:NH1	7:G:92:ARG:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:76:VAL:HG12	17:Q:77:ARG:HG2	1.97	0.46
21:U:51:SER:O	21:U:54:LYS:HG2	2.16	0.46
22:a:620:G:N3	22:a:620:G:H5'	2.30	0.46
22:a:742:A:H2'	22:a:743:A:C8	2.50	0.46
10:J:92:LEU:HG	10:J:98:VAL:HG21	1.96	0.46
22:a:1178:C:H2'	22:a:1179:G:C8	2.50	0.46
22:a:1198:U:H2'	22:a:1199:U:C6	2.50	0.46
24:c:2:ALA:N	24:c:20:VAL:O	2.48	0.46
54:Z:55:5MU:H2'	54:Z:56:PSU:O4'	2.16	0.46
1:A:264:C:O2'	17:Q:66:PRO:O	2.33	0.46
2:B:31:ILE:HD11	2:B:39:HIS:ND1	2.30	0.46
7:G:9:GLN:OE1	7:G:10:ARG:N	2.47	0.46
10:J:59:LYS:HE2	10:J:62:ARG:HH22	1.80	0.46
17:Q:20:SER:HB3	17:Q:71:LYS:NZ	2.31	0.46
22:a:364:C:H2'	22:a:365:U:C6	2.51	0.46
22:a:468:G:H5"	26:e:55:SER:OG	2.16	0.46
22:a:549:G:H2'	22:a:550:C:H6	1.81	0.46
22:a:810:U:C4	32:k:29:LYS:O	2.69	0.46
22:a:1585:C:H2'	22:a:1586:A:O4'	2.15	0.46
22:a:2395:C:H2'	22:a:2396:G:O4'	2.16	0.46
26:e:119:ILE:HB	26:e:187:VAL:HG22	1.98	0.46
38:q:48:LYS:HE2	38:q:103:ALA:HB1	1.97	0.46
39:r:59:GLU:OE2	39:r:66:ILE:HB	2.16	0.46
1:A:392:C:OP1	16:P:8:ARG:NH2	2.49	0.46
22:a:2230:G:H2'	22:a:2231:U:C6	2.51	0.46
22:a:2788:C:H2'	22:a:2789:C:C6	2.50	0.46
54:Z:24:C:H2'	54:Z:25:U:C6	2.50	0.46
2:B:81:LYS:O	2:B:85:LEU:HD23	2.16	0.46
22:a:645:C:O2'	22:a:646:U:H5'	2.15	0.46
1:A:1120:C:H2'	1:A:1121:U:H6	1.81	0.46
22:a:703:U:H2'	22:a:704:G:O4'	2.16	0.46
46:y:4:THR:HB	46:y:37:GLU:OE2	2.15	0.46
55:V:10:G:O2'	55:V:11:U:OP1	2.31	0.46
55:V:24:A:H2'	55:V:25:U:C6	2.50	0.46
1:A:746:A:H2'	1:A:747:A:C8	2.50	0.46
1:A:1014:A:C2	1:A:1219:A:H1'	2.51	0.46
9:I:67:VAL:CG1	9:I:79:ILE:HD11	2.46	0.46
12:L:14:ARG:HB2	12:L:14:ARG:HH21	1.79	0.46
22:a:645:C:H2'	22:a:647:G:N7	2.31	0.46
22:a:1156:A:C8	37:p:51:ARG:HG2	2.51	0.46
26:e:176:ASP:OD1	26:e:179:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:n:33:ARG:O	35:n:65:THR:HG23	2.16	0.46
1:A:476:U:H2'	1:A:477:C:H6	1.82	0.45
2:B:66:LYS:NZ	2:B:90:PHE:HB2	2.31	0.45
4:D:35:GLU:HG2	4:D:36:GLN:N	2.32	0.45
15:O:10:LYS:HE2	15:O:10:LYS:HB2	1.75	0.45
27:f:123:ASP:OD2	27:f:127:ASN:ND2	2.47	0.45
32:k:1:MET:O	32:k:2:ARG:HD2	2.16	0.45
40:s:25:GLU:HG3	40:s:26:LYS:HG2	1.98	0.45
1:A:215:C:H2'	1:A:216:U:C6	2.51	0.45
1:A:476:U:H2'	1:A:477:C:C6	2.50	0.45
1:A:715:A:H2'	1:A:716:A:C8	2.50	0.45
1:A:1010:U:H2'	1:A:1011:C:H6	1.81	0.45
2:B:23:TRP:CZ3	2:B:25:PRO:HA	2.51	0.45
2:B:70:VAL:HG12	2:B:92:VAL:HB	1.96	0.45
22:a:2795:C:H2'	22:a:2796:U:C6	2.51	0.45
42:u:34:LYS:HE2	42:u:34:LYS:HA	1.97	0.45
1:A:1266:G:N2	1:A:1269:A:OP2	2.39	0.45
2:B:129:LEU:HD22	2:B:134:ALA:N	2.31	0.45
6:F:16:GLU:O	6:F:19:PRO:HD2	2.16	0.45
15:O:40:GLN:OE1	15:O:40:GLN:HA	2.16	0.45
22:a:274:C:H2'	22:a:275:C:O4'	2.17	0.45
35:n:116:GLN:HE21	35:n:116:GLN:N	2.14	0.45
1:A:1126:U:OP1	10:J:7:ARG:NH2	2.47	0.45
1:A:1170:A:H2'	1:A:1171:A:O4'	2.17	0.45
2:B:117:LEU:HG	2:B:141:LEU:HD12	1.98	0.45
4:D:41:HIS:HB3	4:D:44:ARG:HD3	1.99	0.45
13:M:80:LEU:HD23	13:M:80:LEU:HA	1.79	0.45
19:S:42:PRO:O	19:S:45:ILE:HD12	2.16	0.45
22:a:813:U:H2'	22:a:814:C:H6	1.81	0.45
22:a:851:C:H2'	22:a:852:U:H6	1.82	0.45
22:a:1570:A:H2'	22:a:1571:A:C8	2.52	0.45
22:a:1747:U:H2'	22:a:1748:C:C6	2.51	0.45
1:A:512:U:H2'	1:A:513:C:C6	2.52	0.45
1:A:839:C:H2'	1:A:840:C:C6	2.52	0.45
13:M:16:VAL:O	13:M:20:THR:HG23	2.17	0.45
22:a:2074:U:H2'	22:a:2075:U:C6	2.52	0.45
35:n:116:GLN:HE21	35:n:116:GLN:H	1.64	0.45
1:A:235:C:H2'	1:A:236:A:C8	2.51	0.45
1:A:259:G:OP1	20:T:36:TYR:OH	2.23	0.45
1:A:1122:U:H2'	1:A:1123:U:C6	2.51	0.45
3:C:29:PHE:HE2	14:N:77:PHE:CD1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:11:LYS:HB2	10:J:97:ASP:HB3	1.99	0.45
22:a:365:U:H2'	22:a:366:C:C6	2.52	0.45
22:a:851:C:H2'	22:a:852:U:C6	2.51	0.45
22:a:1000:A:H2'	22:a:1001:A:C8	2.51	0.45
22:a:1394:U:H2'	22:a:1395:A:O4'	2.16	0.45
23:b:42:C:C6	27:f:66:LEU:HB2	2.52	0.45
41:t:96:PHE:CE2	41:t:103:ILE:HG12	2.51	0.45
2:B:67:ILE:HG22	2:B:160:ALA:HB3	1.98	0.45
3:C:28:GLU:N	3:C:28:GLU:OE2	2.50	0.45
11:K:89:PRO:HB3	21:U:32:VAL:HG11	1.99	0.45
22:a:155:A:H2'	22:a:156:A:H8	1.82	0.45
22:a:947:A:H2'	22:a:948:C:C6	2.51	0.45
22:a:1889:A:H2'	22:a:1890:A:C8	2.52	0.45
22:a:2241:A:H2'	22:a:2242:G:C8	2.51	0.45
24:c:182:ARG:HG2	24:c:183:LYS:N	2.32	0.45
41:t:81:ASP:OD2	41:t:96:PHE:HB3	2.17	0.45
1:A:204:G:H1'	1:A:465:A:C2	2.52	0.45
1:A:555:U:H2'	1:A:556:C:C6	2.52	0.45
9:I:51:PRO:HG3	9:I:80:ARG:HG2	1.99	0.45
22:a:372:G:O2'	22:a:400:G:O6	2.24	0.45
22:a:1168:G:H2'	22:a:1169:A:C8	2.52	0.45
22:a:1433:A:H2'	22:a:1434:A:O4'	2.17	0.45
37:p:15:LYS:HB3	37:p:15:LYS:HE3	1.72	0.45
40:s:24:MET:HE2	40:s:30:ILE:HG22	1.98	0.45
21:U:14:VAL:HA	21:U:17:ARG:HE	1.82	0.45
22:a:414:C:H2'	22:a:415:A:H8	1.82	0.45
22:a:832:U:H2'	22:a:833:A:H8	1.82	0.45
22:a:1292:G:H2'	22:a:1293:C:C6	2.52	0.45
22:a:1799:G:O2'	24:c:180:GLU:OE1	2.31	0.45
1:A:320:A:H2'	1:A:321:A:O4'	2.17	0.45
1:A:908:A:H2'	1:A:909:A:C8	2.52	0.45
4:D:98:LEU:O	4:D:102:VAL:HG12	2.17	0.45
17:Q:47:HIS:HB3	17:Q:74:THR:HG22	1.99	0.45
37:p:86:ALA:HB2	37:p:116:ALA:HB2	1.98	0.45
41:t:54:GLN:N	41:t:55:PRO:HD2	2.32	0.45
1:A:533:A:O2'	1:A:535:A:OP2	2.28	0.44
2:B:67:ILE:HD13	2:B:221:VAL:HG21	1.99	0.44
2:B:104:TRP:NE1	2:B:108:ARG:NH1	2.65	0.44
17:Q:26:GLU:N	17:Q:26:GLU:OE2	2.49	0.44
22:a:1649:G:O2'	34:m:106:ASP:OD2	2.22	0.44
1:A:175:C:H2'	1:A:176:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:A:C2	1:A:374:A:C8	3.05	0.44
1:A:1023:U:C2	1:A:1024:G:C8	3.04	0.44
1:A:1029:U:H4'	1:A:1030:U:H5	1.82	0.44
1:A:1160:G:C2	1:A:1161:C:C6	3.05	0.44
2:B:166:ALA:HB2	2:B:185:ALA:HB1	1.98	0.44
9:I:12:ARG:O	9:I:13:LYS:C	2.59	0.44
10:J:37:ARG:HD2	10:J:37:ARG:HA	1.70	0.44
16:P:40:ASN:HB3	16:P:43:ALA:HB2	1.99	0.44
22:a:1682:G:H2'	22:a:1683:U:C6	2.51	0.44
22:a:1856:U:H2'	22:a:1857:G:O4'	2.18	0.44
22:a:2455:G:H2'	22:a:2456:C:C6	2.52	0.44
22:a:2557:G:H2'	22:a:2558:C:C6	2.51	0.44
1:A:494:G:O2'	1:A:496:A:H1'	2.18	0.44
14:N:79:LEU:HB2	14:N:84:VAL:HG23	1.99	0.44
22:a:288:U:H2'	22:a:289:G:H8	1.82	0.44
22:a:1506:U:H2'	22:a:1507:C:C6	2.53	0.44
22:a:2700:A:H2'	22:a:2701:U:C6	2.51	0.44
40:s:5:GLU:H	40:s:5:GLU:CD	2.22	0.44
1:A:33:A:H2'	1:A:34:C:C6	2.53	0.44
1:A:182:A:C4	1:A:184:G:C8	3.06	0.44
1:A:500:G:H2'	1:A:501:C:C6	2.52	0.44
1:A:1039:G:H2'	1:A:1040:U:C6	2.52	0.44
11:K:93:ARG:NH2	11:K:112:ASP:OD2	2.27	0.44
19:S:13:LEU:HD11	19:S:17:LYS:HE3	1.98	0.44
22:a:1357:C:H2'	22:a:1358:G:O4'	2.18	0.44
22:a:2291:U:OP1	22:a:2380:C:O2'	2.33	0.44
22:a:2615:U:C2	47:z:4:GLN:HA	2.52	0.44
34:m:71:ARG:HA	34:m:71:ARG:HD2	1.74	0.44
55:V:17:G:HO2'	55:V:56:G:H22	1.60	0.44
1:A:67:C:H2'	1:A:68:G:C8	2.52	0.44
1:A:154:U:H2'	1:A:155:A:C8	2.52	0.44
1:A:1071:C:H2'	1:A:1072:G:H8	1.83	0.44
1:A:1372:U:OP2	9:I:13:LYS:NZ	2.46	0.44
11:K:126:LYS:NZ	21:U:37:PHE:HB2	2.32	0.44
15:O:26:GLU:HG3	15:O:81:LEU:HD11	1.99	0.44
15:O:75:VAL:O	15:O:79:THR:HG23	2.17	0.44
22:a:1506:U:H2'	22:a:1507:C:H6	1.82	0.44
22:a:2467:C:H2'	22:a:2468:A:O4'	2.18	0.44
23:b:66:A:N6	23:b:107:G:H2'	2.31	0.44
45:x:42:LEU:O	45:x:46:VAL:HG23	2.17	0.44
1:A:78:A:H2'	1:A:79:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:G:H2'	1:A:148:G:H8	1.77	0.44
6:F:4:TYR:CD2	6:F:71:ILE:HG13	2.53	0.44
22:a:721:A:H2'	22:a:722:A:C8	2.53	0.44
22:a:1527:G:N1	22:a:1544:A:OP2	2.39	0.44
22:a:2680:U:O2'	22:a:2681:C:H5'	2.17	0.44
30:i:96:ARG:HA	30:i:96:ARG:NH1	2.28	0.44
1:A:839:C:H2'	1:A:840:C:H6	1.82	0.44
2:B:123:ASP:OD1	2:B:124:GLY:N	2.51	0.44
17:Q:25:ILE:HD11	17:Q:44:LEU:HD12	1.99	0.44
22:a:764:A:H5"	24:c:209:GLY:CA	2.48	0.44
22:a:1125:G:OP2	22:a:1126:A:O2'	2.27	0.44
22:a:2052:A:O2'	25:d:148:GLN:O	2.35	0.44
1:A:1098:C:P	2:B:139:ARG:HH22	2.41	0.44
3:C:111:LEU:HD22	3:C:146:ALA:HB2	1.98	0.44
22:a:1028:A:N3	22:a:2486:C:O2'	2.47	0.44
22:a:1039:A:H2'	22:a:1040:A:O4'	2.17	0.44
22:a:1869:G:H5'	22:a:1870:C:OP2	2.18	0.44
28:g:60:ASP:O	28:g:62:TRP:N	2.47	0.44
28:g:145:ALA:HB1	28:g:164:TYR:HE1	1.83	0.44
31:j:41:ILE:HD11	31:j:86:LEU:HD22	1.98	0.44
1:A:1027:C:N4	1:A:1035:A:H61	2.14	0.44
1:A:1106:G:H5"	3:C:172:ARG:HG2	1.99	0.44
1:A:1530:G:H2'	1:A:1531:A:C8	2.53	0.44
22:a:499:U:H2'	22:a:500:G:O4'	2.18	0.44
22:a:936:A:H2'	22:a:937:C:C6	2.53	0.44
22:a:1545:A:H2'	22:a:1546:G:O4'	2.18	0.44
22:a:1932:A:H2'	22:a:1933:G:O4'	2.18	0.44
1:A:167:A:N6	1:A:168:G:O6	2.51	0.43
1:A:1456:A:H2'	1:A:1457:G:O4'	2.18	0.43
1:A:1477:U:H2'	1:A:1478:U:C6	2.52	0.43
18:R:30:LYS:HB3	18:R:30:LYS:HE2	1.79	0.43
22:a:2847:U:H2'	22:a:2848:G:O4'	2.17	0.43
24:c:72:ASP:OD2	24:c:189:ARG:NH1	2.46	0.43
30:i:58:ASN:HA	30:i:126:ALA:O	2.18	0.43
35:n:53:THR:HB	35:n:65:THR:OG1	2.18	0.43
4:D:50:ASP:HA	4:D:53:VAL:HG22	2.00	0.43
21:U:55:ARG:HA	21:U:55:ARG:HD3	1.83	0.43
22:a:910:A:H2'	22:a:911:A:C8	2.52	0.43
22:a:2204:G:H4'	24:c:150:LYS:HG3	2.00	0.43
22:a:2713:U:H3'	22:a:2714:G:H5"	2.00	0.43
27:f:17:MET:SD	27:f:22:TYR:HB2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:29:LYS:O	32:k:29:LYS:HG2	2.17	0.43
43:v:33:ALA:N	43:v:64:ASP:OD1	2.51	0.43
1:A:1000:A:H2'	1:A:1001:C:C6	2.54	0.43
1:A:1180:A:OP1	9:I:105:THR:OG1	2.32	0.43
1:A:1441:A:N1	36:o:114:LEU:HD12	2.33	0.43
2:B:222:ARG:HB3	2:B:222:ARG:NH1	2.34	0.43
5:E:107:ALA:HB2	5:E:125:ALA:HB3	2.00	0.43
9:I:21:ILE:HG22	9:I:63:LEU:CD2	2.48	0.43
14:N:19:LYS:HD2	14:N:20:TYR:CE1	2.53	0.43
22:a:587:C:C2	32:k:19:LEU:HD12	2.53	0.43
22:a:1539:U:H2'	22:a:1540:G:H8	1.83	0.43
22:a:1667:G:O2'	22:a:1991:U:O4	2.35	0.43
53:X:47:A:O2'	53:X:48:A:N7	2.50	0.43
54:Z:51:U:H2'	54:Z:52:C:C6	2.53	0.43
1:A:946:A:H2'	1:A:947:G:H8	1.79	0.43
22:a:404:A:H1'	22:a:405:U:OP2	2.18	0.43
22:a:2849:U:H4'	22:a:2868:A:C2	2.54	0.43
33:l:133:LYS:HB3	33:l:133:LYS:HE2	1.58	0.43
1:A:634:C:H2'	1:A:635:A:H8	1.84	0.43
2:B:67:ILE:HD12	2:B:69:PHE:CE1	2.53	0.43
5:E:61:GLN:OE1	5:E:61:GLN:HA	2.18	0.43
22:a:150:U:H2'	22:a:151:C:C6	2.53	0.43
22:a:360:U:H2'	22:a:361:G:O4'	2.19	0.43
22:a:1107:G:N3	22:a:1107:G:H2'	2.33	0.43
22:a:2698:U:H2'	22:a:2699:C:C6	2.53	0.43
22:a:2751:G:H4'	28:g:4:VAL:HG23	2.01	0.43
22:a:2895:G:H2'	22:a:2896:C:H6	1.83	0.43
28:g:9:VAL:HG13	28:g:50:LEU:HB2	2.00	0.43
36:o:6:LYS:O	36:o:10:GLN:HG2	2.18	0.43
1:A:191:G:H2'	1:A:192:A:C8	2.51	0.43
1:A:193:C:H2'	1:A:194:C:C6	2.54	0.43
1:A:524:G:H2'	1:A:525:C:C6	2.53	0.43
4:D:156:LYS:HD2	4:D:156:LYS:HA	1.72	0.43
13:M:71:ARG:O	13:M:75:MET:HG2	2.19	0.43
16:P:72:ALA:O	16:P:75:ILE:HG22	2.19	0.43
22:a:78:U:H2'	22:a:79:C:C6	2.53	0.43
22:a:2552:OMU:HM23	22:a:2554:U:C6	2.53	0.43
26:e:112:LEU:HD22	26:e:117:ARG:HB2	2.01	0.43
26:e:150:THR:OG1	26:e:152:GLU:O	2.33	0.43
35:n:16:ARG:HD3	35:n:16:ARG:HA	1.85	0.43
45:x:12:GLU:HG2	45:x:13:GLU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:y:23:THR:HG23	46:y:47:MET:HG2	2.01	0.43
1:A:580:C:H2'	1:A:581:G:O4'	2.19	0.43
14:N:37:SER:O	14:N:41:ARG:HG3	2.18	0.43
22:a:207:A:H2'	22:a:208:C:O4'	2.19	0.43
22:a:857:G:H2'	22:a:858:G:O4'	2.19	0.43
22:a:1178:C:H2'	22:a:1179:G:H8	1.84	0.43
22:a:2649:C:H2'	22:a:2650:U:H6	1.83	0.43
31:j:110:GLU:CD	31:j:110:GLU:H	2.26	0.43
40:s:44:LYS:HG3	40:s:55:VAL:HG21	2.00	0.43
40:s:44:LYS:HE3	40:s:55:VAL:HG23	2.01	0.43
41:t:14:LEU:HD11	41:t:71:ALA:HB2	2.00	0.43
50:2:8:ARG:HA	50:2:8:ARG:HD2	1.91	0.43
1:A:1268:G:H2'	1:A:1269:A:C8	2.53	0.43
2:B:66:LYS:HD2	2:B:89:GLN:OE1	2.19	0.43
2:B:96:TRP:CZ2	2:B:100:MET:HB3	2.54	0.43
22:a:2243:U:H2'	22:a:2244:U:H6	1.84	0.43
22:a:2813:A:H2'	22:a:2814:A:H8	1.83	0.43
23:b:40:U:H2'	52:4:2:LYS:HE3	2.00	0.43
1:A:382:A:H2'	1:A:383:A:C8	2.54	0.43
1:A:1521:C:H2'	1:A:1522:U:C6	2.54	0.43
22:a:249:C:O2	50:2:12:LYS:NZ	2.47	0.43
22:a:675:A:N3	22:a:2443:C:O2'	2.48	0.43
22:a:1168:G:H2'	22:a:1169:A:H8	1.83	0.43
22:a:1181:U:H2'	22:a:1182:G:C8	2.54	0.43
22:a:1593:A:H2'	22:a:1594:U:C6	2.54	0.43
22:a:2271:G:OP1	43:v:18:ALA:HB1	2.19	0.43
25:d:8:LYS:HB2	25:d:201:LEU:HD11	2.00	0.43
31:j:107:LEU:HD23	31:j:107:LEU:HA	1.84	0.43
39:r:73:LYS:HB3	39:r:73:LYS:HE3	1.91	0.43
42:u:75:GLN:HB2	42:u:92:VAL:HG23	2.00	0.43
1:A:79:G:H1	1:A:80:A:N6	2.17	0.43
1:A:151:A:C5	1:A:171:A:N6	2.87	0.43
1:A:160:A:H2'	1:A:161:A:O4'	2.19	0.43
9:I:30:ILE:HA	9:I:65:ILE:HB	2.00	0.43
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.87	0.43
17:Q:60:GLU:C	17:Q:61:ILE:HD13	2.44	0.43
28:g:18:LYS:HB3	28:g:25:THR:HB	2.01	0.43
30:i:91:GLU:O	30:i:95:ARG:HG2	2.18	0.43
31:j:80:ASP:OD2	36:o:69:GLY:HA3	2.19	0.43
33:l:20:LEU:HD13	42:u:81:PRO:HG2	2.00	0.43
1:A:35:G:H2'	1:A:36:C:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1236:A:H2'	1:A:1237:C:C6	2.54	0.42
2:B:11:LYS:HD2	2:B:11:LYS:HA	1.91	0.42
5:E:96:MET:HE3	5:E:96:MET:HB2	1.90	0.42
6:F:90:MET:HE1	18:R:23:TYR:OH	2.19	0.42
10:J:35:GLN:HG2	10:J:77:VAL:HG23	2.01	0.42
13:M:11:ASP:HB3	13:M:46:SER:HB3	1.99	0.42
17:Q:12:VAL:HG12	17:Q:23:VAL:HG12	2.00	0.42
22:a:2803:G:H2'	22:a:2804:U:C6	2.54	0.42
40:s:61:LEU:HD11	40:s:82:LYS:HD3	2.00	0.42
48:0:29:THR:O	48:0:30:LYS:HD3	2.19	0.42
1:A:202:G:O2'	1:A:468:A:N3	2.47	0.42
1:A:371:A:H2'	1:A:372:C:O4'	2.19	0.42
1:A:950:U:O4	13:M:104:THR:HG21	2.19	0.42
3:C:105:GLU:OE2	3:C:107:ARG:NH2	2.52	0.42
4:D:105:MET:HG2	4:D:173:VAL:HG22	2.01	0.42
6:F:11:HIS:HB3	6:F:14:GLN:OE1	2.20	0.42
22:a:479:A:N3	22:a:481:G:H5"	2.34	0.42
22:a:1534:U:H4'	22:a:1535:A:H2'	2.00	0.42
27:f:126:GLY:O	27:f:158:THR:HB	2.20	0.42
55:V:52:G:H3'	55:V:53:5MU:H73	2.01	0.42
1:A:390:U:H2'	1:A:391:G:C8	2.54	0.42
6:F:9:MET:HE3	6:F:59:TYR:CZ	2.54	0.42
22:a:171:U:H2'	22:a:172:A:H8	1.85	0.42
22:a:1180:U:H2'	22:a:1181:U:O4'	2.19	0.42
22:a:2901:C:C4	22:a:2902:C:N4	2.83	0.42
28:g:44:LYS:HA	28:g:44:LYS:HD2	1.68	0.42
1:A:173:U:C2	1:A:197:A:N1	2.87	0.42
1:A:470:C:H2'	1:A:471:U:C6	2.53	0.42
1:A:608:A:H2'	1:A:609:A:O4'	2.18	0.42
16:P:20:VAL:HA	16:P:35:ARG:HA	2.02	0.42
20:T:9:LYS:CE	20:T:13:GLN:HE21	2.33	0.42
22:a:151:C:H2'	22:a:152:A:H8	1.83	0.42
22:a:1328:A:H2'	22:a:1330:C:C4	2.55	0.42
22:a:1496:A:H2'	22:a:1498:C:C5	2.54	0.42
22:a:2489:U:H2'	22:a:2490:G:O4'	2.19	0.42
34:m:55:ALA:HA	34:m:80:PHE:CE1	2.54	0.42
54:Z:1:C:H42	54:Z:73:A:H2	1.66	0.42
55:V:52:G:H2'	55:V:53:5MU:C6	2.54	0.42
6:F:32:ALA:CB	6:F:70:VAL:HG11	2.50	0.42
20:T:48:GLN:O	20:T:48:GLN:NE2	2.53	0.42
22:a:594:U:H2'	22:a:595:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1870:C:O2'	22:a:1871:A:C8	2.69	0.42
1:A:58:C:O2	1:A:58:C:H2'	2.19	0.42
1:A:74:A:H2'	1:A:75:G:O4'	2.19	0.42
1:A:410:G:P	4:D:26:ARG:HH11	2.43	0.42
1:A:1307:U:H2'	1:A:1308:U:C6	2.54	0.42
3:C:122:SER:O	3:C:126:ARG:HG3	2.20	0.42
4:D:58:LYS:HD3	4:D:203:LEU:HD22	2.01	0.42
20:T:55:GLN:HB2	20:T:56:PRO:HD3	2.00	0.42
21:U:39:GLU:OE2	21:U:44:GLU:HG2	2.20	0.42
22:a:2286:G:N3	22:a:2286:G:H2'	2.35	0.42
24:c:181:MET:HE3	24:c:181:MET:HB3	1.83	0.42
26:e:12:LEU:HD23	26:e:12:LEU:H	1.83	0.42
34:m:44:LEU:O	34:m:48:VAL:HG12	2.20	0.42
4:D:91:LEU:HD23	4:D:91:LEU:HA	1.84	0.42
4:D:126:ASN:ND2	4:D:141:ASP:OD1	2.53	0.42
7:G:146:GLU:OE1	7:G:149:LYS:HE3	2.19	0.42
11:K:34:ILE:HG13	11:K:70:CYS:SG	2.59	0.42
21:U:64:ASN:HA	21:U:67:ARG:HH12	1.82	0.42
31:j:75:SER:HB2	36:o:73:VAL:O	2.20	0.42
1:A:154:U:H2'	1:A:155:A:H8	1.85	0.42
1:A:678:U:H2'	1:A:679:C:C6	2.55	0.42
1:A:883:C:O2'	1:A:884:U:H5'	2.20	0.42
1:A:1032:G:H3'	1:A:1032:G:N3	2.35	0.42
1:A:1124:G:N2	1:A:1125:U:O4	2.45	0.42
6:F:42:TRP:HZ2	6:F:61:LEU:HD22	1.84	0.42
10:J:80:THR:HG22	10:J:82:LYS:H	1.85	0.42
16:P:1:MET:HE2	16:P:1:MET:HB3	1.86	0.42
22:a:419:U:H2'	22:a:420:C:C6	2.54	0.42
22:a:753:A:H5'	49:1:1:MET:SD	2.59	0.42
22:a:839:U:H2'	22:a:840:C:C6	2.55	0.42
22:a:1902:C:H4'	24:c:242:LYS:O	2.19	0.42
29:h:3:VAL:CG1	29:h:36:ALA:HB1	2.50	0.42
35:n:62:LEU:HD23	35:n:62:LEU:HA	1.85	0.42
41:t:81:ASP:OD1	41:t:82:ARG:N	2.53	0.42
47:z:31:ASP:OD2	47:z:48:TYR:HB3	2.20	0.42
49:1:1:MET:HE2	49:1:1:MET:HB2	1.91	0.42
1:A:1382:C:H2'	1:A:1383:C:H6	1.83	0.42
2:B:35:ARG:O	2:B:38:VAL:HG12	2.20	0.42
22:a:272:A:H2'	22:a:273:G:C8	2.55	0.42
22:a:288:U:H2'	22:a:289:G:C8	2.55	0.42
22:a:1437:C:H2'	22:a:1438:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2783:U:H2'	22:a:2784:U:C6	2.55	0.42
22:a:2804:U:H2'	22:a:2805:C:C6	2.55	0.42
28:g:26:ILE:HG22	28:g:79:VAL:HG21	2.02	0.42
31:j:15:GLY:O	31:j:47:ILE:HG12	2.20	0.42
54:Z:9:G:O2'	54:Z:10:G:N7	2.49	0.42
1:A:164:G:C2	1:A:165:G:C8	3.08	0.42
1:A:747:A:H2'	1:A:748:G:O4'	2.19	0.42
1:A:1119:C:H2'	1:A:1120:C:H6	1.84	0.42
1:A:1446:A:N7	1:A:1447:A:C6	2.88	0.42
2:B:191:SER:OG	2:B:192:ASP:N	2.53	0.42
3:C:56:VAL:HB	3:C:67:THR:CG2	2.50	0.42
4:D:118:VAL:HG22	4:D:123:ILE:HG13	2.00	0.42
17:Q:44:LEU:HD23	17:Q:44:LEU:HA	1.89	0.42
22:a:363:G:H2'	22:a:364:C:C6	2.55	0.42
22:a:1410:G:H2'	22:a:1411:U:H6	1.84	0.42
22:a:2567:G:H2'	22:a:2568:U:C6	2.54	0.42
24:c:236:GLU:OE2	24:c:236:GLU:HA	2.20	0.42
25:d:181:ASP:OD2	25:d:184:ARG:HD2	2.20	0.42
27:f:140:GLU:OE1	27:f:140:GLU:N	2.47	0.42
42:u:11:GLU:HG3	42:u:16:ALA:HB1	2.01	0.42
42:u:51:GLN:OE1	42:u:57:TYR:OH	2.27	0.42
51:3:11:CYS:HB3	51:3:33:HIS:CE1	2.54	0.42
1:A:178:C:H2'	1:A:179:A:H8	1.85	0.41
1:A:236:A:H2'	1:A:237:G:C8	2.55	0.41
1:A:439:U:H4'	4:D:121:LYS:HG3	2.01	0.41
1:A:468:A:H5'	1:A:469:C:OP2	2.19	0.41
1:A:723:U:HO2'	1:A:724:G:P	2.41	0.41
2:B:173:ILE:O	2:B:177:ASN:ND2	2.40	0.41
11:K:79:ILE:HD12	11:K:79:ILE:H	1.85	0.41
22:a:277:G:OP2	22:a:277:G:H8	2.02	0.41
22:a:1586:A:H2'	22:a:1587:G:O4'	2.20	0.41
23:b:29:A:H2'	23:b:30:C:C6	2.54	0.41
28:g:68:ALA:O	28:g:72:LEU:HD23	2.20	0.41
29:h:5:LEU:HD11	29:h:12:LEU:HD12	2.03	0.41
40:s:1:MET:HE2	40:s:1:MET:HB3	1.79	0.41
42:u:55:GLU:CD	42:u:55:GLU:H	2.28	0.41
1:A:72:A:N3	1:A:72:A:H2'	2.35	0.41
1:A:181:A:N6	1:A:195:A:C8	2.88	0.41
1:A:333:U:H2'	1:A:334:C:H6	1.85	0.41
1:A:490:C:H2'	1:A:491:G:H8	1.85	0.41
1:A:542:G:H5'	4:D:39:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:C:H2'	1:A:738:C:H6	1.85	0.41
2:B:9:MET:HE3	2:B:14:VAL:HG21	2.03	0.41
3:C:150:LYS:HE3	3:C:201:TRP:CE3	2.55	0.41
22:a:157:C:H2'	22:a:158:U:O4'	2.19	0.41
22:a:657:U:H2'	22:a:658:U:C6	2.56	0.41
22:a:1668:A:O2'	22:a:1674:G:N7	2.46	0.41
22:a:2377:A:H2'	22:a:2378:A:C8	2.55	0.41
27:f:134:GLU:HB3	27:f:136:ILE:HG12	2.01	0.41
33:l:79:ALA:O	43:v:5:LYS:HD3	2.21	0.41
1:A:88:U:H2'	1:A:89:U:C6	2.55	0.41
1:A:224:U:H2'	1:A:225:C:C6	2.55	0.41
1:A:1149:C:P	9:I:11:ARG:HH21	2.41	0.41
2:B:207:ILE:HA	2:B:210:VAL:HG12	2.02	0.41
2:B:217:VAL:HA	2:B:220:THR:HG22	2.01	0.41
3:C:23:PHE:CD1	10:J:97:ASP:HB2	2.56	0.41
4:D:168:PRO:HB3	4:D:170:TRP:CZ3	2.55	0.41
8:H:11:LEU:HD22	8:H:75:ILE:HD11	2.01	0.41
10:J:56:HIS:ND1	10:J:57:VAL:HG13	2.35	0.41
14:N:82:ILE:O	14:N:86:GLU:HG3	2.20	0.41
16:P:39:PHE:HD1	16:P:50:THR:OG1	2.03	0.41
16:P:51:ARG:HE	16:P:52:LEU:N	2.18	0.41
22:a:2:G:H2'	22:a:3:U:C6	2.56	0.41
22:a:1328:A:H2'	22:a:1330:C:C5	2.55	0.41
22:a:2522:U:O2'	22:a:2647:U:OP1	2.25	0.41
30:i:23:LYS:HE3	30:i:142:ILE:OXT	2.20	0.41
41:t:41:LEU:HA	41:t:61:LYS:O	2.20	0.41
50:2:27:ALA:O	50:2:28:ASN:HB2	2.19	0.41
55:V:1:U:H2'	55:V:2:C:C6	2.55	0.41
1:A:687:A:C2	1:A:704:A:C5	3.08	0.41
6:F:39:LEU:HD12	6:F:40:GLU:N	2.35	0.41
7:G:26:PHE:HD1	7:G:101:MET:HG2	1.86	0.41
13:M:106:ALA:O	13:M:110:LYS:HG3	2.20	0.41
15:O:24:SER:O	15:O:28:GLN:HG3	2.21	0.41
19:S:65:GLU:O	19:S:65:GLU:HG3	2.21	0.41
20:T:79:LEU:HD23	20:T:79:LEU:HA	1.85	0.41
22:a:959:A:H2'	22:a:960:A:C8	2.55	0.41
22:a:1319:C:O2'	22:a:1320:C:H5'	2.21	0.41
22:a:2246:G:H2'	22:a:2247:A:H8	1.86	0.41
22:a:2804:U:H2'	22:a:2805:C:H6	1.86	0.41
22:a:2813:A:H2'	22:a:2814:A:C8	2.55	0.41
26:e:121:VAL:O	26:e:189:THR:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:C:OP2	12:L:88:LYS:HE3	2.21	0.41
15:O:73:LYS:HD2	15:O:73:LYS:HA	1.75	0.41
20:T:9:LYS:O	20:T:13:GLN:HG3	2.21	0.41
22:a:297:G:OP1	41:t:92:LYS:NZ	2.41	0.41
22:a:2251:OMG:HM23	22:a:2251:OMG:H1'	1.86	0.41
26:e:130:LYS:HD2	26:e:130:LYS:HA	1.82	0.41
1:A:607:A:H2'	1:A:608:A:C8	2.56	0.41
1:A:1027:C:N3	1:A:1028:C:N4	2.66	0.41
22:a:306:U:H2'	22:a:307:G:O4'	2.21	0.41
22:a:581:C:H2'	22:a:582:A:H8	1.84	0.41
22:a:1871:A:H2'	22:a:1872:A:H8	1.86	0.41
22:a:2305:U:H5"	27:f:131:GLY:HA3	2.02	0.41
27:f:162:SER:OG	27:f:165:GLU:HG3	2.20	0.41
4:D:69:GLU:OE1	4:D:204:TYR:OH	2.30	0.41
21:U:31:GLU:O	21:U:35:ARG:HG2	2.20	0.41
22:a:2329:U:H2'	22:a:2330:G:H8	1.84	0.41
22:a:2766:A:H2'	22:a:2766:A:N3	2.35	0.41
45:x:32:ALA:HB2	45:x:37:LEU:HD23	2.02	0.41
1:A:73:C:C2	1:A:74:A:C8	3.09	0.41
1:A:674:G:H2'	1:A:675:A:C8	2.56	0.41
1:A:745:G:H2'	1:A:746:A:H8	1.86	0.41
10:J:59:LYS:HE2	10:J:62:ARG:NH2	2.35	0.41
22:a:151:C:H2'	22:a:152:A:C8	2.56	0.41
22:a:363:G:H2'	22:a:364:C:H6	1.86	0.41
22:a:884:U:H2'	22:a:885:C:C6	2.56	0.41
22:a:2480:C:H2'	22:a:2481:G:O4'	2.21	0.41
43:v:59:LEU:HD12	43:v:80:ILE:HD12	2.03	0.41
1:A:71:A:C4	1:A:72:A:C8	3.09	0.41
1:A:545:C:H5'	4:D:69:GLU:HB2	2.03	0.41
1:A:757:U:OP1	1:A:822:U:O2'	2.38	0.41
1:A:821:G:H2'	1:A:822:U:H6	1.86	0.41
1:A:1151:A:O2'	1:A:1152:A:H8	2.03	0.41
1:A:1298:U:OP2	7:G:114:LYS:NZ	2.54	0.41
11:K:126:LYS:HB2	11:K:126:LYS:HE2	1.88	0.41
12:L:79:VAL:O	12:L:103:ASP:HB2	2.21	0.41
13:M:66:GLU:O	13:M:70:ARG:HD3	2.21	0.41
19:S:11:ILE:HG13	19:S:38:SER:HB3	2.03	0.41
22:a:305:C:H2'	22:a:306:U:C6	2.56	0.41
22:a:566:U:OP1	32:k:29:LYS:HE2	2.20	0.41
22:a:634:C:H2'	22:a:635:C:H6	1.86	0.41
22:a:2287:A:OP1	48:0:30:LYS:NZ	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2793:C:H2'	22:a:2794:C:C6	2.56	0.41
25:d:5:VAL:H	25:d:32:ASN:ND2	2.19	0.41
30:i:32:LEU:HD23	30:i:105:VAL:HG21	2.03	0.41
34:m:29:VAL:HG11	34:m:75:ILE:HG23	2.03	0.41
37:p:83:LEU:HD23	37:p:83:LEU:HA	1.92	0.41
48:0:25:LYS:HE2	48:0:30:LYS:O	2.21	0.41
55:V:1:U:H2'	55:V:2:C:H6	1.85	0.41
1:A:223:A:H2'	1:A:224:U:C6	2.56	0.41
1:A:344:A:O5'	1:A:345:C:H5	2.04	0.41
1:A:544:G:OP1	4:D:59:GLN:NE2	2.35	0.41
10:J:25:ILE:HD12	10:J:90:LEU:HD22	2.02	0.41
16:P:21:VAL:O	16:P:33:ILE:HG22	2.21	0.41
22:a:286:U:C2	22:a:287:G:C8	3.09	0.41
22:a:964:C:O2'	22:a:2273:A:N3	2.49	0.41
22:a:1710:G:H2'	22:a:1711:A:C8	2.56	0.41
22:a:2649:C:H2'	22:a:2650:U:C6	2.56	0.41
22:a:2803:G:H2'	22:a:2804:U:H6	1.85	0.41
50:2:15:LYS:HB2	50:2:23:LYS:HE2	2.03	0.41
54:Z:21:H2U:H2'	54:Z:21:H2U:H61	1.62	0.41
54:Z:67:C:H2'	54:Z:68:C:C6	2.56	0.41
1:A:299:G:H2'	1:A:300:A:C8	2.56	0.40
1:A:312:C:H2'	1:A:313:A:C8	2.56	0.40
3:C:33:LEU:HD23	3:C:33:LEU:HA	1.89	0.40
22:a:12:U:O2	22:a:2626:C:H4'	2.21	0.40
22:a:299:A:N3	22:a:319:G:O2'	2.46	0.40
22:a:624:C:O2'	22:a:657:U:OP1	2.35	0.40
22:a:668:A:H2'	22:a:670:A:H62	1.86	0.40
22:a:1441:G:H2'	22:a:1442:U:C6	2.56	0.40
22:a:2290:G:H2'	22:a:2291:U:C6	2.57	0.40
22:a:2758:A:O2'	28:g:38:ASN:ND2	2.54	0.40
52:4:59:ARG:HH21	52:4:63:ARG:CZ	2.34	0.40
1:A:148:G:H2'	1:A:149:A:O4'	2.21	0.40
1:A:151:A:C2	1:A:152:A:H1'	2.57	0.40
1:A:512:U:H2'	1:A:513:C:H6	1.85	0.40
1:A:678:U:H2'	1:A:679:C:H6	1.87	0.40
1:A:1037:C:H2'	1:A:1038:C:H6	1.87	0.40
1:A:1310:G:OP2	13:M:87:ARG:NH2	2.54	0.40
3:C:142:MET:HE2	3:C:170:GLU:OE1	2.21	0.40
8:H:3:MET:HE2	8:H:3:MET:HB2	1.88	0.40
10:J:90:LEU:HD12	10:J:90:LEU:HA	1.89	0.40
14:N:47:LYS:O	14:N:50:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:38:PHE:CE2	16:P:51:ARG:HB3	2.57	0.40
20:T:81:ALA:O	20:T:85:LYS:HG2	2.21	0.40
22:a:118:A:OP2	22:a:119:A:H2'	2.22	0.40
22:a:1197:G:H2'	22:a:1198:U:H6	1.86	0.40
22:a:1370:C:H2'	22:a:1371:G:O4'	2.21	0.40
22:a:2070:A:H2'	22:a:2071:A:C8	2.57	0.40
27:f:125:ARG:HG3	27:f:125:ARG:HH11	1.86	0.40
41:t:36:VAL:HG13	41:t:39:ILE:HB	2.03	0.40
1:A:335:C:H2'	1:A:336:A:H8	1.86	0.40
1:A:629:A:H2'	1:A:630:A:O4'	2.22	0.40
2:B:162:PHE:HD1	2:B:184:PHE:HB2	1.86	0.40
6:F:96:VAL:HG12	6:F:96:VAL:O	2.20	0.40
22:a:723:C:H2'	22:a:724:U:O4'	2.22	0.40
22:a:1730:C:H1'	22:a:1731:G:C2	2.57	0.40
22:a:2086:U:H2'	22:a:2087:G:C8	2.56	0.40
22:a:2308:G:H2'	22:a:2308:G:N3	2.36	0.40
22:a:2793:C:H2'	22:a:2794:C:H6	1.86	0.40
22:a:2796:U:C4	22:a:2798:U:C4	3.10	0.40
27:f:119:ALA:O	27:f:167:ARG:NH1	2.55	0.40
27:f:147:ASP:OD1	27:f:148:ARG:N	2.54	0.40
28:g:95:ARG:HG2	28:g:106:SER:HB2	2.04	0.40
28:g:99:LYS:HB2	28:g:99:LYS:HE2	1.72	0.40
1:A:222:C:H2'	1:A:223:A:C8	2.54	0.40
1:A:539:A:H2'	1:A:540:G:H8	1.87	0.40
1:A:546:A:O2'	1:A:548:G:O2'	2.26	0.40
1:A:1404:C:H2'	1:A:1405:G:C8	2.56	0.40
4:D:116:GLN:HG2	4:D:154:ARG:HH12	1.86	0.40
5:E:13:GLU:HG2	5:E:39:VAL:HG23	2.04	0.40
11:K:101:ASN:ND2	21:U:12:PHE:CG	2.89	0.40
1:A:246:A:C2	1:A:282:A:C5	3.10	0.40
1:A:736:C:H2'	1:A:737:C:C6	2.57	0.40
1:A:985:C:H2'	1:A:986:U:C6	2.56	0.40
1:A:1011:C:H2'	1:A:1012:A:C8	2.57	0.40
9:I:9:THR:O	9:I:85:ARG:HD2	2.22	0.40
13:M:44:LYS:O	13:M:47:GLU:HG2	2.22	0.40
14:N:23:LYS:HB2	14:N:23:LYS:HE2	1.92	0.40
20:T:17:ALA:O	20:T:21:ASN:ND2	2.53	0.40
22:a:1733:G:H2'	22:a:1734:G:H8	1.87	0.40
22:a:2458:G:O2'	22:a:2460:U:O4	2.36	0.40
22:a:2650:U:H2'	22:a:2651:C:H6	1.87	0.40
33:l:58:LYS:HE2	33:l:58:LYS:HB2	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:y:4:THR:HA	46:y:38:ARG:O	2.20	0.40
54:Z:17:C:H2'	54:Z:18:U:C5	2.57	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	
2	B	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
3	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
4	D	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
5	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
6	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
7	G	151/179 (84%)	144 (95%)	7 (5%)	0	100	100
8	H	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
10	J	96/103 (93%)	91 (95%)	3 (3%)	2 (2%)	5	6
11	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
12	L	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
13	M	113/118 (96%)	108 (96%)	4 (4%)	1 (1%)	14	20
14	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	P	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
17	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
18	R	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
19	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
21	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
24	c	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
25	d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	35
26	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
27	f	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
28	g	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
29	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
30	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
31	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
32	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
33	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
34	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
35	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
36	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
37	p	115/118 (98%)	115 (100%)	0	0	100	100
38	q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
39	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
40	s	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
41	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
42	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
43	v	82/85 (96%)	80 (98%)	2 (2%)	0	100	100
44	w	75/78 (96%)	75 (100%)	0	0	100	100
45	x	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
48	0	49/55 (89%)	49 (100%)	0	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	7	10
51	3	36/38 (95%)	36 (100%)	0	0	100	100
52	4	56/70 (80%)	54 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5487/5913 (93%)	5288 (96%)	194 (4%)	5 (0%)	49 63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	57	VAL
25	d	149	ASN
50	2	32	ILE
10	J	58	ASN
13	M	105	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	186/199 (94%)	186 (100%)	0	100 100
3	C	170/190 (90%)	170 (100%)	0	100 100
4	D	172/173 (99%)	171 (99%)	1 (1%)	78 88
5	E	119/126 (94%)	119 (100%)	0	100 100
6	F	90/116 (78%)	90 (100%)	0	100 100
7	G	126/147 (86%)	126 (100%)	0	100 100
8	H	104/105 (99%)	104 (100%)	0	100 100
9	I	105/107 (98%)	105 (100%)	0	100 100
10	J	86/90 (96%)	86 (100%)	0	100 100
11	K	89/98 (91%)	89 (100%)	0	100 100
12	L	102/103 (99%)	102 (100%)	0	100 100
13	M	93/96 (97%)	93 (100%)	0	100 100
14	N	83/84 (99%)	83 (100%)	0	100 100
15	O	76/77 (99%)	76 (100%)	0	100 100
16	P	65/65 (100%)	65 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	60 (100%)	0	100	100
24	c	216/218 (99%)	216 (100%)	0	100	100
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	165 (100%)	0	100	100
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	137/138 (99%)	137 (100%)	0	100	100
29	h	32/114 (28%)	32 (100%)	0	100	100
30	i	116/116 (100%)	116 (100%)	0	100	100
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	107/107 (100%)	107 (100%)	0	100	100
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	85 (99%)	1 (1%)	63	79
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100
39	r	93/93 (100%)	93 (100%)	0	100	100
40	s	80/84 (95%)	80 (100%)	0	100	100
41	t	83/85 (98%)	83 (100%)	0	100	100
42	u	78/78 (100%)	78 (100%)	0	100	100
43	v	61/63 (97%)	61 (100%)	0	100	100
44	w	67/68 (98%)	67 (100%)	0	100	100
45	x	54/55 (98%)	54 (100%)	0	100	100
46	y	48/49 (98%)	48 (100%)	0	100	100
47	z	47/48 (98%)	47 (100%)	0	100	100
48	0	46/49 (94%)	46 (100%)	0	100	100
49	1	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	34 (100%)	0	100	100
52	4	55/62 (89%)	55 (100%)	0	100	100
All	All	4575/4825 (95%)	4573 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	116	GLN
35	n	116	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	24	ASN
3	C	8	ASN
3	C	123	GLN
4	D	116	GLN
4	D	140	ASN
4	D	152	GLN
5	E	132	ASN
7	G	68	ASN
9	I	126	GLN
11	K	24	HIS
11	K	38	GLN
11	K	40	ASN
19	S	14	HIS
20	T	13	GLN
20	T	21	ASN
20	T	75	HIS
21	U	9	ASN
24	c	53	HIS
24	c	134	ASN
25	d	32	ASN
25	d	42	ASN
25	d	148	GLN
25	d	185	ASN
26	e	9	GLN
33	l	13	HIS
34	m	73	ASN

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Mol	Chain	Res	Type
36	o	56	HIS
37	p	44	GLN
39	r	7	HIS
39	r	9	HIS
41	t	99	ASN
42	u	12	GLN
43	v	50	ASN
44	w	36	HIS
49	1	26	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1517/1542 (98%)	201 (13%)	5 (0%)
22	a	2749/2904 (94%)	283 (10%)	0
23	b	118/120 (98%)	12 (10%)	0
53	X	12/35 (34%)	1 (8%)	0
54	Z	76/77 (98%)	7 (9%)	0
55	V	74/75 (98%)	15 (20%)	2 (2%)
All	All	4546/4753 (95%)	519 (11%)	7 (0%)

All (519) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	4	U
1	A	5	U
1	A	6	G
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	55	A
1	A	59	A
1	A	60	A
1	A	71	A
1	A	72	A

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Mol	Chain	Res	Type
1	A	75	G
1	A	80	A
1	A	81	A
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	87	C
1	A	88	U
1	A	90	C
1	A	91	U
1	A	94	G
1	A	95	C
1	A	96	U
1	A	116	A
1	A	122	G
1	A	128	G
1	A	130	A
1	A	131	A
1	A	141	G
1	A	144	G
1	A	146	G
1	A	149	A
1	A	163	C
1	A	164	G
1	A	181	A
1	A	183	C
1	A	197	A
1	A	204	G
1	A	216	U
1	A	226	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	293	G
1	A	321	A
1	A	328	C
1	A	347	G
1	A	351	G

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Mol	Chain	Res	Type
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	397	A
1	A	406	G
1	A	412	A
1	A	413	G
1	A	415	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	436	C
1	A	446	G
1	A	453	G
1	A	457	G
1	A	458	U
1	A	467	U
1	A	468	A
1	A	478	A
1	A	479	U
1	A	484	G
1	A	486	U
1	A	495	A
1	A	497	G
1	A	499	A
1	A	509	A
1	A	511	C
1	A	518	C
1	A	531	U
1	A	533	A
1	A	547	A
1	A	559	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	596	A
1	A	607	A

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Mol	Chain	Res	Type
1	A	633	G
1	A	639	G
1	A	653	U
1	A	665	A
1	A	695	A
1	A	703	G
1	A	721	G
1	A	723	U
1	A	724	G
1	A	733	G
1	A	755	G
1	A	777	A
1	A	787	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	851	G
1	A	890	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1009	U
1	A	1017	U
1	A	1020	G
1	A	1027	C
1	A	1028	C
1	A	1029	U
1	A	1030	U
1	A	1031	C
1	A	1032	G

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Mol	Chain	Res	Type
1	A	1034	G
1	A	1035	A
1	A	1036	A
1	A	1065	U
1	A	1088	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1132	C
1	A	1134	G
1	A	1137	C
1	A	1139	G
1	A	1159	U
1	A	1167	A
1	A	1168	U
1	A	1171	A
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1258	G
1	A	1260	G
1	A	1275	A
1	A	1280	A
1	A	1285	A
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1320	C
1	A	1338	G
1	A	1340	A
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G

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Mol	Chain	Res	Type
1	A	1378	C
1	A	1379	G
1	A	1419	G
1	A	1441	A
1	A	1442	G
1	A	1446	A
1	A	1452	C
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1534	A
22	a	10	A
22	a	34	U
22	a	35	G
22	a	61	C
22	a	71	A
22	a	74	A
22	a	75	G
22	a	100	U
22	a	101	A
22	a	102	U
22	a	118	A
22	a	119	A
22	a	120	U
22	a	138	U
22	a	140	C
22	a	142	A
22	a	163	C
22	a	181	A
22	a	196	A
22	a	199	A
22	a	215	G
22	a	216	A
22	a	222	A
22	a	233	A
22	a	248	G
22	a	265	A

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Mol	Chain	Res	Type
22	a	272	A
22	a	277	G
22	a	278	A
22	a	279	A
22	a	281	C
22	a	282	A
22	a	285	G
22	a	288	U
22	a	311	A
22	a	329	G
22	a	330	A
22	a	346	A
22	a	356	G
22	a	362	A
22	a	386	G
22	a	396	G
22	a	405	U
22	a	411	G
22	a	412	A
22	a	448	U
22	a	481	G
22	a	491	G
22	a	505	A
22	a	508	A
22	a	509	C
22	a	529	A
22	a	530	G
22	a	531	C
22	a	532	A
22	a	545	U
22	a	546	U
22	a	547	A
22	a	549	G
22	a	562	U
22	a	563	A
22	a	573	U
22	a	575	A
22	a	603	A
22	a	615	U
22	a	627	A
22	a	637	A
22	a	645	C

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Mol	Chain	Res	Type
22	a	646	U
22	a	647	G
22	a	654	A
22	a	655	A
22	a	685	A
22	a	686	U
22	a	711	G
22	a	717	C
22	a	729	G
22	a	730	A
22	a	747	5MU
22	a	765	C
22	a	775	G
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	792	A
22	a	805	G
22	a	812	C
22	a	827	U
22	a	828	U
22	a	845	A
22	a	846	U
22	a	847	U
22	a	859	G
22	a	882	G
22	a	888	C
22	a	890	C
22	a	891	G
22	a	895	U
22	a	896	A
22	a	897	C
22	a	910	A
22	a	914	G
22	a	931	U
22	a	945	A
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	996	A

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Mol	Chain	Res	Type
22	a	1005	C
22	a	1012	U
22	a	1013	C
22	a	1025	G
22	a	1033	U
22	a	1040	A
22	a	1041	G
22	a	1047	G
22	a	1111	A
22	a	1112	G
22	a	1122	G
22	a	1132	U
22	a	1135	C
22	a	1142	A
22	a	1250	G
22	a	1253	A
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1273	U
22	a	1300	G
22	a	1301	A
22	a	1321	A
22	a	1329	U
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1416	G
22	a	1417	C
22	a	1428	C
22	a	1452	G
22	a	1460	U
22	a	1482	G
22	a	1493	C
22	a	1497	U
22	a	1508	A
22	a	1509	A
22	a	1510	G
22	a	1515	A
22	a	1523	U
22	a	1524	G

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Mol	Chain	Res	Type
22	a	1529	G
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1566	A
22	a	1569	A
22	a	1578	U
22	a	1584	U
22	a	1607	C
22	a	1608	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1674	G
22	a	1729	U
22	a	1730	C
22	a	1731	G
22	a	1738	G
22	a	1744	A
22	a	1764	C
22	a	1773	A
22	a	1800	C
22	a	1801	A
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1833	C
22	a	1847	A
22	a	1848	A
22	a	1869	G
22	a	1870	C
22	a	1871	A
22	a	1906	G
22	a	1913	A
22	a	1929	G
22	a	1930	G
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1966	A
22	a	1967	C

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Mol	Chain	Res	Type
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1993	U
22	a	2023	C
22	a	2030	6MZ
22	a	2031	A
22	a	2033	A
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2093	G
22	a	2198	A
22	a	2204	G
22	a	2211	A
22	a	2225	A
22	a	2238	G
22	a	2239	G
22	a	2268	A
22	a	2278	A
22	a	2283	C
22	a	2287	A
22	a	2288	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2336	A
22	a	2343	U
22	a	2347	C
22	a	2350	C
22	a	2361	G
22	a	2377	A
22	a	2383	G
22	a	2385	C
22	a	2396	G

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Mol	Chain	Res	Type
22	a	2402	U
22	a	2406	A
22	a	2410	G
22	a	2425	A
22	a	2429	G
22	a	2430	A
22	a	2435	A
22	a	2441	U
22	a	2448	A
22	a	2475	C
22	a	2476	A
22	a	2491	U
22	a	2505	G
22	a	2518	A
22	a	2529	G
22	a	2547	A
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2585	U
22	a	2602	A
22	a	2609	U
22	a	2613	U
22	a	2615	U
22	a	2629	U
22	a	2630	G
22	a	2663	G
22	a	2682	A
22	a	2689	U
22	a	2690	U
22	a	2726	A
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2778	A
22	a	2790	U
22	a	2797	U
22	a	2798	U
22	a	2820	A
22	a	2821	A
22	a	2849	U
22	a	2873	A

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Mol	Chain	Res	Type
22	a	2877	G
22	a	2880	C
22	a	2884	U
22	a	2891	U
22	a	2902	C
23	b	35	C
23	b	36	C
23	b	41	G
23	b	45	A
23	b	56	G
23	b	57	A
23	b	67	G
23	b	89	U
23	b	90	C
23	b	99	A
23	b	108	A
23	b	109	A
53	X	47	A
54	Z	9	G
54	Z	18	U
54	Z	19	G
54	Z	21	H2U
54	Z	22	A
54	Z	23	G
54	Z	77	A
55	V	3	C
55	V	5	C
55	V	6	2MG
55	V	9	1MA
55	V	11	U
55	V	17	G
55	V	18	G
55	V	46	A
55	V	47	5MC
55	V	48	5MC
55	V	53	5MU
55	V	65	A
55	V	70	G
55	V	72	G
55	V	73	C

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	148	G
1	A	723	U
1	A	1028	C
1	A	1033	G
1	A	1035	A
55	V	5	C
55	V	10	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	3TD	a	1915	22	18,22,23	3.89	7 (38%)	22,32,35	1.77	3 (13%)
22	2MG	a	2445	22	23,26,27	2.47	7 (30%)	32,38,41	2.16	10 (31%)
55	5MC	V	48	55	18,22,23	3.61	8 (44%)	26,32,35	1.05	2 (7%)
55	1MA	V	57	55	21,25,26	0.70	0	31,37,40	0.78	1 (3%)
22	6MZ	a	1618	22	22,25,26	2.61	5 (22%)	30,36,39	2.45	11 (36%)
1	G7M	A	527	1	23,26,27	2.74	8 (34%)	35,39,42	1.78	8 (22%)
22	PSU	a	1917	22	18,21,22	1.04	2 (11%)	22,30,33	1.92	5 (22%)
22	G7M	a	2069	22	23,26,27	2.68	8 (34%)	35,39,42	1.79	10 (28%)
55	5MC	V	38	55	18,22,23	3.53	8 (44%)	26,32,35	1.12	2 (7%)
54	5MU	Z	55	54	19,22,23	4.59	7 (36%)	28,32,35	3.77	9 (32%)
54	PSU	Z	56	54	18,21,22	1.03	1 (5%)	22,30,33	1.80	3 (13%)
22	2MG	a	1835	22	23,26,27	2.48	7 (30%)	32,38,41	2.30	10 (31%)
22	2MA	a	2503	56,22	22,25,26	3.72	10 (45%)	33,37,40	2.83	8 (24%)
22	OMU	a	2552	22	19,22,23	2.57	6 (31%)	26,31,34	1.93	5 (19%)
55	56B	V	34	55,57	29,35,36	2.92	11 (37%)	36,52,55	1.86	7 (19%)
55	5MU	V	53	55	19,22,23	4.49	7 (36%)	28,32,35	3.74	9 (32%)
22	5MU	a	1939	22	19,22,23	4.44	7 (36%)	28,32,35	3.85	10 (35%)
25	MEQ	d	150	25	8,9,10	1.20	0	5,10,12	1.41	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	1407	1	18,22,23	3.41	7 (38%)	26,32,35	1.01	1 (3%)
54	OMC	Z	33	54	19,22,23	2.74	7 (36%)	26,31,34	0.75	0
54	H2U	Z	21	54	18,21,22	1.09	3 (16%)	21,30,33	0.82	1 (4%)
55	1MA	V	9	55	21,25,26	0.74	1 (4%)	31,37,40	0.81	1 (3%)
12	D2T	L	89	12	7,9,10	1.32	0	6,11,13	2.25	3 (50%)
11	IAS	K	119	11	6,7,8	1.02	0	6,8,10	1.27	1 (16%)
1	5MC	A	967	1	18,22,23	3.55	7 (38%)	26,32,35	1.07	2 (7%)
22	6MZ	a	2030	22	22,25,26	2.69	6 (27%)	30,36,39	2.40	9 (30%)
22	5MC	a	1962	22	18,22,23	3.36	7 (38%)	26,32,35	1.13	2 (7%)
33	MS6	l	82	33	5,7,8	0.71	0	2,7,9	1.77	1 (50%)
55	5MC	V	47	55	18,22,23	3.58	7 (38%)	26,32,35	1.10	2 (7%)
22	PSU	a	746	56,22	18,21,22	1.07	2 (11%)	22,30,33	1.81	4 (18%)
22	1MG	a	745	22	22,26,27	2.53	7 (31%)	33,39,42	1.69	7 (21%)
1	2MG	A	1207	1	23,26,27	2.52	7 (30%)	32,38,41	2.20	9 (28%)
22	H2U	a	2449	22	18,21,22	1.45	3 (16%)	21,30,33	0.79	0
22	OMG	a	2251	22,54	23,26,27	2.51	8 (34%)	33,38,41	1.93	9 (27%)
22	PSU	a	2580	22	18,21,22	1.18	3 (16%)	22,30,33	2.09	6 (27%)
54	4SU	Z	8	54	18,21,22	3.99	8 (44%)	26,30,33	2.31	5 (19%)
55	2MG	V	6	55	23,26,27	2.57	8 (34%)	32,38,41	2.15	10 (31%)
1	4OC	A	1402	56,1	20,23,24	2.83	8 (40%)	26,32,35	0.99	3 (11%)
55	H2U	V	19	55	18,21,22	1.26	3 (16%)	21,30,33	0.89	1 (4%)
1	PSU	A	516	1	18,21,22	1.06	3 (16%)	22,30,33	1.79	4 (18%)
1	MA6	A	1519	1	23,26,27	1.49	5 (21%)	34,38,41	2.36	11 (32%)
33	4D4	l	81	33	9,11,12	1.78	2 (22%)	8,13,15	2.08	4 (50%)
1	UR3	A	1498	1	19,22,23	2.46	6 (31%)	26,32,35	1.34	1 (3%)
22	PSU	a	2605	22	18,21,22	1.10	2 (11%)	22,30,33	1.90	4 (18%)
55	PSU	V	54	55	18,21,22	1.05	2 (11%)	22,30,33	1.87	4 (18%)
22	5MU	a	747	22	19,22,23	4.42	7 (36%)	28,32,35	3.81	10 (35%)
22	PSU	a	1911	22	18,21,22	1.06	2 (11%)	22,30,33	2.00	5 (22%)
22	PSU	a	2504	22	18,21,22	1.07	1 (5%)	22,30,33	1.84	4 (18%)
22	PSU	a	2604	22	18,21,22	1.09	2 (11%)	22,30,33	2.02	5 (22%)
22	PSU	a	2457	22	18,21,22	1.14	3 (16%)	22,30,33	1.90	4 (18%)
55	PSU	V	13	55	18,21,22	1.01	1 (5%)	22,30,33	1.93	5 (22%)
1	2MG	A	1516	1	23,26,27	2.51	7 (30%)	32,38,41	2.24	11 (34%)
1	2MG	A	966	1	23,26,27	2.57	7 (30%)	32,38,41	2.29	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MA6	A	1518	1	23,26,27	1.48	5 (21%)	34,38,41	2.28	11 (32%)
22	OMC	a	2498	56,22	19,22,23	2.71	7 (36%)	26,31,34	0.96	1 (3%)
22	PSU	a	955	22	18,21,22	1.09	1 (5%)	22,30,33	1.94	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
22	2MG	a	2445	22	-	1/9/27/28	0/3/3/3
55	5MC	V	48	55	-	2/7/25/26	0/2/2/2
55	1MA	V	57	55	-	0/7/25/26	0/3/3/3
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
1	G7M	A	527	1	-	3/7/25/26	0/3/3/3
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
22	G7M	a	2069	22	-	1/7/25/26	0/3/3/3
55	5MC	V	38	55	-	0/7/25/26	0/2/2/2
54	5MU	Z	55	54	-	0/7/25/26	0/2/2/2
54	PSU	Z	56	54	-	0/7/25/26	0/2/2/2
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
22	2MA	a	2503	56,22	-	1/7/25/26	0/3/3/3
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
55	56B	V	34	55,57	-	0/12/43/44	0/4/4/4
55	5MU	V	53	55	-	0/7/25/26	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
25	MEQ	d	150	25	-	5/8/9/11	-
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
54	OMC	Z	33	54	-	0/9/27/28	0/2/2/2
54	H2U	Z	21	54	-	7/7/38/39	0/2/2/2
55	1MA	V	9	55	-	2/7/25/26	0/3/3/3
12	D2T	L	89	12	-	2/7/12/14	-
11	IAS	K	119	11	-	0/7/7/8	-
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
33	MS6	l	82	33	-	1/4/6/8	-
55	5MC	V	47	55	-	3/7/25/26	0/2/2/2
22	PSU	a	746	56,22	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
22	OMG	a	2251	22,54	-	0/9/27/28	0/3/3/3
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
54	4SU	Z	8	54	-	0/7/25/26	0/2/2/2
55	2MG	V	6	55	-	1/9/27/28	0/3/3/3
1	4OC	A	1402	56,1	-	2/9/29/30	0/2/2/2
55	H2U	V	19	55	-	3/7/38/39	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	2/11/29/30	0/3/3/3
33	4D4	l	81	33	-	5/11/12/14	-
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
55	PSU	V	54	55	-	2/7/25/26	0/2/2/2
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2504	22	-	2/7/25/26	0/2/2/2
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
55	PSU	V	13	55	-	0/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
1	2MG	A	966	1	-	1/9/27/28	0/3/3/3
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
22	OMC	a	2498	56,22	-	0/9/27/28	0/2/2/2
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2

All (274) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	C6-C5	11.60	1.48	1.35
22	a	2503	2MA	C4-N3	11.43	1.48	1.34
22	a	2030	6MZ	C6-N6	10.57	1.45	1.34
54	Z	55	5MU	C6-N1	10.55	1.56	1.38
22	a	1618	6MZ	C6-N6	10.54	1.45	1.34
54	Z	55	5MU	C2-N1	10.27	1.54	1.38
55	V	53	5MU	C6-N1	10.09	1.55	1.38
22	a	1939	5MU	C6-N1	10.02	1.55	1.38
22	a	747	5MU	C6-N1	9.96	1.55	1.38
55	V	53	5MU	C2-N1	9.68	1.54	1.38
22	a	747	5MU	C2-N1	9.54	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1939	5MU	C2-N1	9.29	1.53	1.38
55	V	48	5MC	C6-C5	9.17	1.49	1.34
55	V	47	5MC	C6-C5	9.09	1.49	1.34
54	Z	8	4SU	C4-N3	8.95	1.47	1.37
1	A	967	5MC	C6-C5	8.82	1.49	1.34
55	V	38	5MC	C6-C5	8.79	1.49	1.34
54	Z	55	5MU	C4-C5	8.73	1.59	1.44
1	A	1407	5MC	C6-C5	8.70	1.48	1.34
22	a	1962	5MC	C6-C5	8.52	1.48	1.34
55	V	53	5MU	C4-C5	8.42	1.58	1.44
22	a	747	5MU	C4-C5	8.32	1.58	1.44
22	a	1915	3TD	C2-N1	8.32	1.48	1.37
22	a	1939	5MU	C4-C5	8.23	1.58	1.44
22	a	1939	5MU	C4-N3	-8.12	1.23	1.38
55	V	53	5MU	C4-N3	-8.04	1.23	1.38
22	a	747	5MU	C4-N3	-7.84	1.24	1.38
54	Z	55	5MU	C4-N3	-7.56	1.24	1.38
1	A	966	2MG	C2-N3	7.47	1.46	1.31
55	V	6	2MG	C2-N3	7.38	1.46	1.31
54	Z	8	4SU	C2-N1	7.28	1.50	1.38
1	A	1207	2MG	C2-N3	7.17	1.45	1.31
22	a	1835	2MG	C2-N3	6.98	1.45	1.31
1	A	1516	2MG	C2-N3	6.96	1.45	1.31
55	V	34	56B	C14-C13	6.93	1.52	1.32
1	A	967	5MC	C4-N3	6.92	1.45	1.34
55	V	38	5MC	C4-N3	6.82	1.45	1.34
22	a	2251	OMG	C4-N3	6.81	1.50	1.34
55	V	47	5MC	C4-N3	6.79	1.45	1.34
55	V	48	5MC	C4-N3	6.76	1.45	1.34
22	a	2503	2MA	C2-N3	6.75	1.46	1.34
22	a	2445	2MG	C2-N3	6.72	1.44	1.31
22	a	1962	5MC	C4-N3	6.39	1.44	1.34
1	A	1407	5MC	C4-N3	6.33	1.44	1.34
55	V	6	2MG	C4-N3	6.29	1.49	1.34
1	A	1207	2MG	C4-N3	6.27	1.49	1.34
1	A	966	2MG	C4-N3	6.27	1.49	1.34
54	Z	8	4SU	C2-N3	6.25	1.49	1.38
54	Z	55	5MU	C6-C5	6.23	1.44	1.34
1	A	527	G7M	C2-N2	6.14	1.48	1.34
1	A	967	5MC	C2-N3	6.13	1.48	1.36
55	V	38	5MC	C2-N3	6.13	1.48	1.36
55	V	48	5MC	C2-N3	6.10	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	47	5MC	C2-N3	6.06	1.48	1.36
55	V	34	56B	O11-C11	-6.06	1.28	1.43
1	A	527	G7M	C4-N3	6.06	1.48	1.34
22	a	2069	G7M	C2-N2	6.05	1.48	1.34
22	a	1939	5MU	C6-C5	6.05	1.44	1.34
22	a	1835	2MG	C4-N3	6.01	1.48	1.34
55	V	53	5MU	C6-C5	5.99	1.44	1.34
22	a	2445	2MG	C4-N3	5.97	1.48	1.34
22	a	747	5MU	C6-C5	5.97	1.44	1.34
1	A	1402	4OC	C4-N3	5.94	1.43	1.32
1	A	1498	UR3	C2-N1	5.93	1.47	1.38
22	a	2503	2MA	C2-N1	5.92	1.44	1.34
22	a	2069	G7M	C4-N3	5.91	1.48	1.34
1	A	1516	2MG	C4-N3	5.90	1.48	1.34
1	A	1402	4OC	C6-C5	5.88	1.48	1.35
22	a	745	1MG	C4-N3	5.85	1.48	1.34
54	Z	8	4SU	C6-C5	5.83	1.48	1.35
55	V	34	56B	C4-N3	5.79	1.48	1.34
1	A	1407	5MC	C2-N3	5.76	1.48	1.36
22	a	1962	5MC	C2-N3	5.74	1.48	1.36
54	Z	8	4SU	C4-S4	-5.74	1.57	1.68
54	Z	33	OMC	C2-N3	5.70	1.47	1.36
22	a	2498	OMC	C2-N3	5.66	1.47	1.36
1	A	1498	UR3	C6-C5	5.62	1.48	1.35
22	a	2552	OMU	C2-N3	5.60	1.47	1.38
22	a	745	1MG	C2-N3	5.59	1.44	1.34
54	Z	33	OMC	C6-C5	5.58	1.48	1.35
22	a	2552	OMU	C2-N1	5.51	1.47	1.38
22	a	1915	3TD	C6-N1	5.49	1.45	1.36
22	a	745	1MG	C2-N2	5.48	1.44	1.34
22	a	2498	OMC	C6-C5	5.47	1.47	1.35
1	A	1402	4OC	C2-N3	5.34	1.47	1.36
1	A	527	G7M	C5-N7	-5.33	1.33	1.39
22	a	2069	G7M	C5-N7	-5.32	1.33	1.39
1	A	527	G7M	C2-N3	5.31	1.46	1.33
22	a	2552	OMU	C6-C5	5.28	1.47	1.35
22	a	2503	2MA	C6-N6	-5.12	1.21	1.34
55	V	34	56B	C11-C10	5.12	1.62	1.54
55	V	34	56B	C2-N3	5.08	1.45	1.33
54	Z	8	4SU	C5-C4	5.00	1.49	1.42
22	a	2503	2MA	C5-C6	4.95	1.54	1.41
22	a	2251	OMG	C2-N3	4.86	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2069	G7M	C2-N3	4.85	1.44	1.33
55	V	48	5MC	C6-N1	4.82	1.46	1.38
55	V	47	5MC	C6-N1	4.68	1.46	1.38
54	Z	33	OMC	C4-N4	4.68	1.44	1.33
55	V	6	2MG	C2-N1	4.64	1.44	1.36
1	A	967	5MC	C6-N1	4.64	1.46	1.38
22	a	2251	OMG	C2-N2	4.56	1.45	1.34
55	V	38	5MC	C6-N1	4.49	1.45	1.38
1	A	1516	2MG	C2-N1	4.48	1.43	1.36
1	A	1407	5MC	C6-N1	4.45	1.45	1.38
1	A	966	2MG	C2-N1	4.44	1.43	1.36
54	Z	33	OMC	C4-N3	4.42	1.43	1.34
22	a	2498	OMC	C4-N4	4.37	1.44	1.33
1	A	1207	2MG	C2-N1	4.30	1.43	1.36
1	A	1498	UR3	C2-N3	4.25	1.47	1.39
55	V	34	56B	C2-N2	4.24	1.44	1.34
22	a	1962	5MC	C6-N1	4.22	1.45	1.38
22	a	2445	2MG	C2-N1	4.12	1.43	1.36
55	V	48	5MC	C2-N1	4.11	1.48	1.40
22	a	2498	OMC	C4-N3	4.11	1.42	1.34
1	A	1402	4OC	C4-N4	4.03	1.44	1.35
22	a	2498	OMC	C2-N1	4.02	1.48	1.40
55	V	47	5MC	C4-N4	4.00	1.44	1.34
55	V	48	5MC	C4-N4	3.92	1.44	1.34
22	a	1915	3TD	C2-N3	3.92	1.47	1.38
1	A	967	5MC	C4-N4	3.92	1.44	1.34
22	a	1835	2MG	C2-N1	3.90	1.43	1.36
55	V	38	5MC	C4-N4	3.85	1.44	1.34
55	V	38	5MC	C2-N1	3.82	1.48	1.40
55	V	47	5MC	C2-N1	3.81	1.48	1.40
22	a	1962	5MC	C4-N4	3.80	1.44	1.34
22	a	2251	OMG	C5-N7	-3.73	1.31	1.39
1	A	1407	5MC	C4-N4	3.71	1.43	1.34
54	Z	33	OMC	C2-N1	3.71	1.48	1.40
1	A	967	5MC	C2-N1	3.70	1.48	1.40
22	a	2030	6MZ	C5-C4	-3.68	1.32	1.39
55	V	34	56B	C5-C6	3.66	1.52	1.44
22	a	1835	2MG	C5-N7	-3.61	1.32	1.39
22	a	745	1MG	C5-N7	-3.60	1.32	1.39
22	a	2552	OMU	O2-C2	-3.55	1.16	1.23
22	a	2503	2MA	C5-N7	-3.54	1.32	1.39
22	a	2445	2MG	C5-N7	-3.54	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Z	8	4SU	O2-C2	-3.51	1.16	1.23
1	A	1519	MA6	C5-C4	-3.50	1.32	1.39
1	A	966	2MG	C5-N7	-3.48	1.32	1.39
1	A	1402	4OC	C2-N1	3.47	1.47	1.40
22	a	2498	OMC	O2-C2	-3.47	1.17	1.23
1	A	1402	4OC	O2-C2	-3.47	1.17	1.23
1	A	527	G7M	C5-C6	3.47	1.53	1.43
1	A	1407	5MC	C2-N1	3.45	1.47	1.40
22	a	2449	H2U	C2-N3	-3.45	1.31	1.38
1	A	1518	MA6	C5-C4	-3.43	1.32	1.39
22	a	2251	OMG	O6-C6	-3.41	1.17	1.23
1	A	1402	4OC	C5-C4	3.39	1.48	1.40
22	a	1962	5MC	C2-N1	3.33	1.47	1.40
22	a	2449	H2U	C4-N3	-3.30	1.32	1.37
33	l	81	4D4	OB-CB	-3.29	1.36	1.43
1	A	1516	2MG	C5-N7	-3.29	1.32	1.39
22	a	2552	OMU	O4-C4	-3.28	1.18	1.24
55	V	6	2MG	C5-N7	-3.25	1.32	1.39
54	Z	33	OMC	O2-C2	-3.24	1.17	1.23
22	a	2069	G7M	O6-C6	-3.23	1.17	1.23
1	A	1207	2MG	C5-N7	-3.20	1.32	1.39
22	a	2449	H2U	C2-N1	-3.17	1.31	1.35
22	a	2069	G7M	C5-C6	3.16	1.52	1.43
22	a	2503	2MA	C6-N1	3.16	1.39	1.35
22	a	1618	6MZ	C5-C4	-3.12	1.33	1.39
55	V	19	H2U	C2-N3	-3.10	1.32	1.38
1	A	1518	MA6	C5-N7	-3.07	1.33	1.39
54	Z	56	PSU	C6-C5	3.04	1.38	1.35
1	A	1519	MA6	C5-N7	-3.04	1.33	1.39
55	V	19	H2U	C4-N3	-3.00	1.32	1.37
22	a	1835	2MG	O6-C6	-2.97	1.17	1.23
55	V	34	56B	O6-C6	-2.96	1.18	1.23
22	a	2030	6MZ	C5-N7	-2.96	1.33	1.39
1	A	1518	MA6	C8-N9	-2.95	1.32	1.37
1	A	1519	MA6	C8-N9	-2.94	1.32	1.37
22	a	1939	5MU	O2-C2	-2.94	1.17	1.23
1	A	1407	5MC	O2-C2	-2.93	1.18	1.23
1	A	527	G7M	O6-C6	-2.92	1.18	1.23
54	Z	8	4SU	C6-N1	2.90	1.45	1.38
22	a	2445	2MG	O6-C6	-2.88	1.18	1.23
22	a	2504	PSU	C6-C5	2.88	1.38	1.35
22	a	1962	5MC	O2-C2	-2.84	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2030	6MZ	C8-N9	-2.82	1.32	1.37
55	V	13	PSU	C6-C5	2.78	1.38	1.35
1	A	1498	UR3	O4-C4	-2.76	1.17	1.23
54	Z	21	H2U	C2-N3	-2.73	1.33	1.38
55	V	34	56B	C11-C12	2.73	1.58	1.53
22	a	745	1MG	C4-N9	-2.72	1.31	1.38
1	A	1519	MA6	C6-N6	2.71	1.44	1.36
22	a	1618	6MZ	C8-N9	-2.70	1.32	1.37
1	A	1498	UR3	O2-C2	-2.69	1.17	1.22
1	A	1516	2MG	O6-C6	-2.68	1.18	1.23
22	a	746	PSU	C6-C5	2.68	1.38	1.35
1	A	1207	2MG	O6-C6	-2.68	1.18	1.23
55	V	47	5MC	O2-C2	-2.67	1.18	1.23
1	A	1518	MA6	C6-N6	2.66	1.44	1.36
55	V	54	PSU	C6-C5	2.66	1.38	1.35
22	a	747	5MU	O2-C2	-2.65	1.18	1.23
1	A	1402	4OC	C6-N1	2.65	1.44	1.38
22	a	745	1MG	O6-C6	-2.65	1.17	1.23
22	a	1618	6MZ	C5-N7	-2.64	1.34	1.39
1	A	966	2MG	O6-C6	-2.64	1.18	1.23
22	a	745	1MG	C5-C6	2.64	1.52	1.45
1	A	967	5MC	O2-C2	-2.62	1.18	1.23
55	V	38	5MC	O2-C2	-2.58	1.18	1.23
55	V	53	5MU	O2-C2	-2.58	1.18	1.23
54	Z	33	OMC	C6-N1	2.56	1.44	1.38
22	a	1915	3TD	O4-C4	-2.56	1.17	1.23
1	A	1516	2MG	C4-N9	-2.54	1.31	1.38
22	a	2552	OMU	C4-N3	2.54	1.43	1.38
1	A	527	G7M	C2-N1	2.54	1.44	1.37
22	a	2445	2MG	C4-N9	-2.53	1.31	1.38
22	a	2580	PSU	O4'-C1'	-2.51	1.40	1.43
22	a	1911	PSU	C6-C5	2.48	1.38	1.35
22	a	1917	PSU	C6-C5	2.47	1.38	1.35
55	V	48	5MC	O2-C2	-2.46	1.19	1.23
54	Z	21	H2U	C4-N3	-2.45	1.33	1.37
55	V	6	2MG	O6-C6	-2.44	1.18	1.23
22	a	2498	OMC	C6-N1	2.42	1.43	1.38
1	A	1516	2MG	C5-C6	2.42	1.53	1.44
55	V	34	56B	C2-N1	2.41	1.43	1.37
22	a	1939	5MU	O4-C4	-2.40	1.19	1.23
55	V	6	2MG	C5-C6	2.38	1.53	1.44
22	a	2251	OMG	C8-N9	-2.38	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2251	OMG	C5-C6	2.38	1.53	1.44
1	A	1498	UR3	C6-N1	2.37	1.43	1.38
22	a	2457	PSU	C4-C5	-2.33	1.37	1.44
22	a	2580	PSU	C6-C5	2.33	1.38	1.35
1	A	516	PSU	C6-C5	2.32	1.38	1.35
22	a	2069	G7M	C2-N1	2.32	1.43	1.37
1	A	1207	2MG	C5-C6	2.31	1.53	1.44
22	a	2251	OMG	C4-N9	-2.31	1.32	1.38
55	V	34	56B	C5-C4	-2.31	1.36	1.44
55	V	53	5MU	O4-C4	-2.29	1.19	1.23
1	A	1519	MA6	C4-N9	-2.28	1.32	1.37
55	V	19	H2U	C2-N1	-2.27	1.32	1.35
1	A	966	2MG	C5-C6	2.27	1.52	1.44
22	a	955	PSU	C4-C5	-2.26	1.37	1.44
22	a	2605	PSU	C6-C5	2.26	1.38	1.35
22	a	2580	PSU	C4-C5	-2.25	1.37	1.44
22	a	2604	PSU	C6-C5	2.24	1.37	1.35
22	a	2605	PSU	C4-C5	-2.23	1.37	1.44
1	A	1518	MA6	C4-N9	-2.23	1.32	1.37
1	A	527	G7M	C6-N1	2.23	1.43	1.38
1	A	516	PSU	O4'-C1'	-2.23	1.40	1.43
22	a	747	5MU	O4-C4	-2.22	1.19	1.23
22	a	1835	2MG	C4-N9	-2.22	1.32	1.38
22	a	2503	2MA	C8-N9	-2.21	1.33	1.37
22	a	2069	G7M	C6-N1	2.19	1.42	1.38
54	Z	55	5MU	O2-C2	-2.18	1.19	1.23
1	A	516	PSU	C4-C5	-2.17	1.38	1.44
22	a	746	PSU	C4-C5	-2.17	1.38	1.44
55	V	9	1MA	C2-N1	2.16	1.39	1.35
22	a	2445	2MG	C5-C6	2.15	1.52	1.44
22	a	2604	PSU	C4-C5	-2.14	1.38	1.44
33	l	81	4D4	CZ-NE	2.14	1.37	1.33
22	a	1911	PSU	C4-C5	-2.12	1.38	1.44
22	a	1915	3TD	C4-N3	2.12	1.45	1.40
22	a	2457	PSU	O4'-C1'	-2.12	1.40	1.43
54	Z	55	5MU	O4-C4	-2.12	1.19	1.23
22	a	2503	2MA	CM2-C2	2.12	1.55	1.49
22	a	2457	PSU	C6-C5	2.11	1.37	1.35
1	A	1207	2MG	C4-N9	-2.10	1.32	1.38
54	Z	21	H2U	C2-N1	-2.10	1.32	1.35
22	a	1835	2MG	C5-C6	2.09	1.52	1.44
55	V	48	5MC	CM5-C5	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	O2-C2	-2.07	1.19	1.23
22	a	2030	6MZ	C4-N9	-2.06	1.33	1.37
55	V	6	2MG	C6-N1	2.06	1.42	1.38
1	A	966	2MG	C4-N9	-2.06	1.32	1.38
55	V	6	2MG	C4-N9	-2.05	1.32	1.38
22	a	2030	6MZ	C5-C6	-2.05	1.36	1.41
22	a	2503	2MA	C5-C4	-2.05	1.35	1.39
22	a	1618	6MZ	C6-N1	-2.04	1.31	1.35
55	V	38	5MC	CM5-C5	2.04	1.55	1.50
55	V	54	PSU	C4-C5	-2.04	1.38	1.44
22	a	1917	PSU	C4-C5	-2.01	1.38	1.44

All (290) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	Z	55	5MU	C5-C4-N3	12.94	126.36	115.31
22	a	1939	5MU	C5-C4-N3	12.58	126.05	115.31
55	V	53	5MU	C5-C4-N3	12.39	125.89	115.31
22	a	747	5MU	C5-C4-N3	12.39	125.88	115.31
22	a	1939	5MU	C5-C6-N1	-10.85	112.18	123.34
22	a	747	5MU	C5-C6-N1	-10.75	112.28	123.34
55	V	53	5MU	C5-C6-N1	-10.62	112.42	123.34
54	Z	55	5MU	C5-C6-N1	-10.42	112.62	123.34
22	a	2503	2MA	C5-C4-N3	-8.41	117.73	127.19
54	Z	8	4SU	C4-N3-C2	-8.13	119.44	127.34
22	a	2503	2MA	C4-N9-C1'	-6.77	110.47	126.59
22	a	1835	2MG	C2-N3-C4	6.65	120.28	112.04
1	A	966	2MG	C2-N3-C4	6.60	120.22	112.04
22	a	2503	2MA	C1'-N9-C8	6.57	141.97	127.14
1	A	1516	2MG	C2-N3-C4	6.49	120.09	112.04
22	a	2445	2MG	C2-N3-C4	6.48	120.07	112.04
1	A	1207	2MG	C2-N3-C4	6.38	119.95	112.04
55	V	6	2MG	C2-N3-C4	6.20	119.73	112.04
22	a	2552	OMU	C4-N3-C2	-6.14	118.47	126.58
1	A	1519	MA6	N1-C2-N3	-5.95	119.29	128.60
22	a	2030	6MZ	C9-N6-C6	-5.84	117.85	122.87
1	A	1518	MA6	N1-C2-N3	-5.81	119.52	128.60
55	V	34	56B	C5-C4-N3	-5.80	120.73	127.52
54	Z	55	5MU	O4-C4-C5	-5.76	118.22	124.90
22	a	1618	6MZ	C9-N6-C6	-5.74	117.93	122.87
1	A	966	2MG	C5-C4-N3	-5.70	119.22	128.46
22	a	747	5MU	O4-C4-C5	-5.70	118.30	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	2503	2MA	N3-C4-N9	5.69	134.89	126.99
22	a	2030	6MZ	N1-C2-N3	-5.60	119.85	128.60
22	a	1915	3TD	N1-C2-N3	5.59	120.55	116.14
22	a	1939	5MU	C4-N3-C2	-5.54	120.19	127.35
22	a	1835	2MG	C5-C4-N3	-5.52	119.51	128.46
22	a	2251	OMG	C5-C4-N3	-5.38	119.73	128.46
22	a	1939	5MU	O4-C4-C5	-5.38	118.67	124.90
22	a	747	5MU	C4-N3-C2	-5.36	120.41	127.35
22	a	1618	6MZ	C5-C4-N3	-5.33	119.80	126.75
54	Z	8	4SU	C5-C4-N3	5.32	119.62	114.69
22	a	2580	PSU	N1-C2-N3	5.29	121.12	115.13
22	a	2604	PSU	N1-C2-N3	5.26	121.08	115.13
55	V	6	2MG	C5-C4-N3	-5.23	119.98	128.46
22	a	2604	PSU	C4-N3-C2	-5.23	118.80	126.34
22	a	1911	PSU	N1-C2-N3	5.20	121.02	115.13
22	a	1618	6MZ	N1-C2-N3	-5.19	120.48	128.60
22	a	1939	5MU	N3-C2-N1	5.16	121.75	114.89
54	Z	55	5MU	C4-N3-C2	-5.16	120.68	127.35
1	A	1207	2MG	C5-C4-N3	-5.14	120.11	128.46
22	a	1835	2MG	C2-N1-C6	-5.13	118.57	124.48
22	a	1911	PSU	C4-N3-C2	-5.10	118.99	126.34
1	A	966	2MG	C2-N1-C6	-5.10	118.61	124.48
1	A	1498	UR3	C4-N3-C2	-5.06	119.80	124.56
22	a	2580	PSU	C4-N3-C2	-5.06	119.05	126.34
55	V	53	5MU	O4-C4-C5	-5.05	119.05	124.90
55	V	53	5MU	C4-N3-C2	-5.05	120.82	127.35
22	a	955	PSU	C4-N3-C2	-5.04	119.08	126.34
55	V	13	PSU	N1-C2-N3	5.02	120.82	115.13
22	a	955	PSU	N1-C2-N3	5.01	120.80	115.13
22	a	746	PSU	C4-N3-C2	-5.00	119.14	126.34
22	a	2457	PSU	C4-N3-C2	-5.00	119.14	126.34
22	a	1917	PSU	N1-C2-N3	4.98	120.77	115.13
22	a	2605	PSU	C4-N3-C2	-4.95	119.21	126.34
22	a	2030	6MZ	N9-C8-N7	-4.94	107.15	113.91
55	V	54	PSU	C4-N3-C2	-4.94	119.22	126.34
22	a	2457	PSU	N1-C2-N3	4.92	120.71	115.13
22	a	2605	PSU	N1-C2-N3	4.92	120.70	115.13
1	A	1519	MA6	C5-C4-N3	-4.88	120.38	126.75
22	a	2445	2MG	C5-C4-N3	-4.87	120.57	128.46
1	A	1516	2MG	C5-C4-N3	-4.86	120.57	128.46
22	a	2504	PSU	N1-C2-N3	4.84	120.62	115.13
55	V	54	PSU	N1-C2-N3	4.81	120.58	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	1917	PSU	C4-N3-C2	-4.77	119.46	126.34
1	A	516	PSU	C4-N3-C2	-4.77	119.47	126.34
54	Z	56	PSU	C4-N3-C2	-4.76	119.48	126.34
1	A	1516	2MG	C2-N1-C6	-4.74	119.03	124.48
22	a	747	5MU	N3-C2-N1	4.72	121.16	114.89
55	V	13	PSU	C4-N3-C2	-4.72	119.54	126.34
22	a	2504	PSU	C4-N3-C2	-4.71	119.55	126.34
22	a	746	PSU	N1-C2-N3	4.66	120.41	115.13
1	A	1207	2MG	C2-N1-C6	-4.65	119.12	124.48
1	A	1518	MA6	C5-C4-N3	-4.63	120.72	126.75
55	V	53	5MU	N3-C2-N1	4.59	120.99	114.89
22	a	1618	6MZ	N9-C8-N7	-4.56	107.68	113.91
22	a	745	1MG	C5-C4-N3	-4.55	121.07	128.46
55	V	6	2MG	C2-N1-C6	-4.55	119.25	124.48
1	A	1518	MA6	C2-N1-C6	4.54	122.48	111.75
1	A	1519	MA6	C2-N1-C6	4.52	122.44	111.75
54	Z	56	PSU	N1-C2-N3	4.47	120.20	115.13
22	a	2552	OMU	N3-C2-N1	4.46	120.81	114.89
22	a	2069	G7M	C2-N3-C4	4.45	120.23	112.30
1	A	1519	MA6	N9-C8-N7	-4.41	107.88	113.91
22	a	2445	2MG	C2-N1-C6	-4.39	119.43	124.48
22	a	2030	6MZ	C5-C4-N3	-4.39	121.02	126.75
1	A	516	PSU	N1-C2-N3	4.38	120.09	115.13
1	A	1518	MA6	C4-C5-C6	4.36	120.76	115.88
1	A	1518	MA6	N9-C8-N7	-4.36	107.95	113.91
1	A	527	G7M	C2-N3-C4	4.34	120.03	112.30
54	Z	55	5MU	N3-C2-N1	4.31	120.61	114.89
22	a	2251	OMG	C2-N3-C4	4.30	119.95	112.30
1	A	1519	MA6	C4-C5-C6	4.25	120.63	115.88
1	A	527	G7M	C5-C4-N3	-4.23	120.03	128.15
22	a	1915	3TD	C4-N3-C2	-4.20	120.05	124.61
54	Z	8	4SU	N3-C2-N1	4.18	120.44	114.89
22	a	2069	G7M	C5-C6-N1	4.17	120.50	111.79
55	V	34	56B	C7-C5-C4	-4.15	107.86	112.66
55	V	34	56B	C2-N3-C4	4.15	119.69	112.30
1	A	527	G7M	C5-C6-N1	4.05	120.25	111.79
1	A	966	2MG	N9-C4-N3	4.04	134.05	125.94
55	V	53	5MU	C5M-C5-C6	-3.99	117.52	122.85
22	a	747	5MU	C5M-C5-C6	-3.84	117.73	122.85
22	a	2552	OMU	C5-C4-N3	3.80	120.53	114.84
22	a	1835	2MG	N9-C4-N3	3.77	133.51	125.94
22	a	1939	5MU	C5M-C5-C6	-3.77	117.82	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	1962	5MC	C5-C6-N1	-3.71	119.52	123.34
22	a	2503	2MA	N9-C8-N7	-3.71	108.84	113.91
55	V	53	5MU	C5M-C5-C4	3.71	122.85	118.77
22	a	1618	6MZ	C4-C5-C6	3.70	119.67	116.81
22	a	2069	G7M	C5-C4-N3	-3.69	121.07	128.15
22	a	2251	OMG	N9-C4-N3	3.69	133.35	125.94
54	Z	8	4SU	C5-C4-S4	-3.63	119.80	124.47
22	a	2069	G7M	O6-C6-C5	-3.58	119.97	128.06
12	L	89	D2T	OD2-CG-CB	3.57	120.87	113.15
54	Z	55	5MU	C5M-C5-C6	-3.57	118.08	122.85
1	A	1519	MA6	C5-N7-C8	3.56	108.56	103.51
55	V	47	5MC	C5-C6-N1	-3.54	119.69	123.34
1	A	1518	MA6	C5-N7-C8	3.54	108.53	103.51
55	V	6	2MG	N9-C4-N3	3.53	133.04	125.94
22	a	1618	6MZ	C2-N3-C4	3.51	120.04	111.75
54	Z	55	5MU	C5M-C5-C4	3.51	122.63	118.77
55	V	38	5MC	C5-C6-N1	-3.49	119.75	123.34
1	A	1519	MA6	C2-N3-C4	3.44	119.88	111.75
12	L	89	D2T	OD1-CG-CB	-3.44	115.24	122.44
22	a	745	1MG	C2-N3-C4	3.42	119.67	111.98
1	A	1207	2MG	N9-C4-N3	3.41	132.79	125.94
22	a	2445	2MG	N9-C4-N3	3.40	132.78	125.94
1	A	1207	2MG	N9-C8-N7	-3.38	107.02	113.39
22	a	2251	OMG	N9-C8-N7	-3.36	107.06	113.39
22	a	2445	2MG	N9-C8-N7	-3.36	107.06	113.39
1	A	1516	2MG	N9-C8-N7	-3.35	107.07	113.39
1	A	527	G7M	C2-N1-C6	-3.35	119.00	125.10
1	A	527	G7M	N9-C4-N3	3.34	132.64	125.94
22	a	2030	6MZ	C2-N3-C4	3.31	119.58	111.75
1	A	967	5MC	C5-C6-N1	-3.29	119.95	123.34
22	a	745	1MG	N9-C8-N7	-3.29	107.19	113.39
22	a	747	5MU	C5M-C5-C4	3.29	122.39	118.77
22	a	1835	2MG	N9-C8-N7	-3.29	107.20	113.39
22	a	1939	5MU	C5M-C5-C4	3.28	122.38	118.77
33	l	81	4D4	NH1-CZ-NE	3.26	126.71	119.19
22	a	1939	5MU	O2-C2-N1	-3.24	118.48	122.79
22	a	2251	OMG	C2-N1-C6	-3.23	119.20	125.10
22	a	747	5MU	O2-C2-N1	-3.23	118.50	122.79
1	A	1518	MA6	C2-N3-C4	3.23	119.37	111.75
22	a	2580	PSU	O2-C2-N1	-3.22	119.24	122.79
1	A	1407	5MC	C5-C6-N1	-3.21	120.03	123.34
1	A	527	G7M	O6-C6-C5	-3.20	120.84	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	V	6	2MG	N9-C8-N7	-3.20	107.37	113.39
22	a	1618	6MZ	C5-N7-C8	3.18	108.03	103.51
22	a	2030	6MZ	C5-N7-C8	3.15	107.99	103.51
55	V	34	56B	C7-C8-N9	-3.15	107.97	111.06
1	A	966	2MG	N9-C8-N7	-3.14	107.48	113.39
55	V	48	5MC	C5-C6-N1	-3.12	120.13	123.34
22	a	1618	6MZ	N3-C4-N9	3.10	132.19	127.08
33	l	81	4D4	CB-CA-C	-3.08	106.86	111.77
22	a	2503	2MA	N3-C2-N1	-3.08	120.06	125.72
22	a	2030	6MZ	C4-C5-C6	3.07	119.19	116.81
55	V	34	56B	C2-N1-C6	-3.07	119.51	125.10
1	A	1519	MA6	C4-C5-N7	-3.06	106.89	110.62
22	a	1835	2MG	C5-C6-N1	3.05	120.93	113.19
22	a	2503	2MA	C6-C5-C4	3.03	121.26	117.18
22	a	2069	G7M	C2-N1-C6	-2.98	119.66	125.10
1	A	1518	MA6	C4-C5-N7	-2.98	106.99	110.62
22	a	2030	6MZ	C4-N9-C8	2.94	108.91	105.73
22	a	2503	2MA	C5-N7-C8	2.94	107.68	103.51
1	A	966	2MG	C5-C6-N1	2.94	120.65	113.19
1	A	1207	2MG	C5-C6-N1	2.92	120.62	113.19
22	a	1917	PSU	O2-C2-N1	-2.92	119.58	122.79
55	V	13	PSU	O2-C2-N1	-2.90	119.59	122.79
1	A	1519	MA6	N1-C6-N6	-2.90	113.92	117.08
22	a	2445	2MG	C5-C6-N1	2.90	120.55	113.19
22	a	2604	PSU	O2-C2-N1	-2.88	119.62	122.79
22	a	2251	OMG	C5-C6-N1	2.87	120.47	113.19
22	a	2069	G7M	CN7-N7-C5	2.86	130.32	126.77
1	A	1516	2MG	C5-C6-N1	2.86	120.45	113.19
22	a	2504	PSU	O2-C2-N1	-2.86	119.64	122.79
22	a	1835	2MG	CM2-N2-C2	-2.85	117.57	123.86
22	a	2069	G7M	N9-C4-N3	2.85	131.66	125.94
22	a	1911	PSU	O2-C2-N1	-2.83	119.67	122.79
22	a	2552	OMU	O4-C4-C5	-2.80	120.23	125.16
55	V	54	PSU	O2-C2-N1	-2.80	119.71	122.79
22	a	2445	2MG	O6-C6-C5	-2.79	119.19	126.60
22	a	955	PSU	O2-C2-N1	-2.79	119.72	122.79
22	a	746	PSU	O2-C2-N1	-2.77	119.74	122.79
22	a	1962	5MC	CM5-C5-C6	-2.73	119.20	122.85
22	a	2552	OMU	O2-C2-N1	-2.70	119.19	122.79
1	A	966	2MG	O6-C6-C5	-2.70	119.44	126.60
55	V	6	2MG	C5-C6-N1	2.69	120.02	113.19
1	A	1516	2MG	N9-C4-N3	2.68	131.32	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	745	1MG	C5-C6-N1	2.67	120.06	114.91
1	A	1519	MA6	C5-C4-N9	2.65	108.87	105.78
22	a	745	1MG	C1'-N9-C8	-2.64	119.17	126.70
55	V	53	5MU	O4-C4-N3	-2.64	115.06	120.12
55	V	13	PSU	C6-N1-C2	-2.64	119.98	122.68
22	a	745	1MG	N9-C4-N3	2.63	131.23	125.94
55	V	38	5MC	CM5-C5-C6	-2.63	119.33	122.85
22	a	1835	2MG	O6-C6-C5	-2.61	119.66	126.60
54	Z	56	PSU	O2-C2-N1	-2.60	119.93	122.79
1	A	1516	2MG	CM2-N2-C2	-2.60	118.12	123.86
22	a	2580	PSU	C6-N1-C2	-2.60	120.03	122.68
22	a	2445	2MG	N1-C2-N3	-2.59	119.95	123.95
55	V	34	56B	N9-C4-N3	2.57	131.11	125.94
1	A	1207	2MG	O6-C6-C5	-2.57	119.78	126.60
55	V	6	2MG	O6-C6-C5	-2.54	119.85	126.60
22	a	2504	PSU	C6-N1-C2	-2.54	120.08	122.68
22	a	1917	PSU	C6-N1-C2	-2.54	120.09	122.68
1	A	527	G7M	CN7-N7-C5	2.53	129.92	126.77
22	a	1939	5MU	O4-C4-N3	-2.52	115.28	120.12
1	A	1516	2MG	O6-C6-C5	-2.52	119.92	126.60
1	A	1518	MA6	C5-C4-N9	2.52	108.71	105.78
22	a	2030	6MZ	N3-C4-N9	2.51	131.22	127.08
22	a	1618	6MZ	C4-N9-C8	2.51	108.45	105.73
22	a	2580	PSU	C6-C5-C4	2.49	119.94	118.20
55	V	53	5MU	O2-C2-N1	-2.48	119.49	122.79
22	a	2457	PSU	O2-C2-N1	-2.48	120.06	122.79
33	l	81	4D4	NE-CZ-NH2	-2.48	116.34	120.70
33	l	82	MS6	CE-SD-CG	2.47	108.89	100.40
22	a	1911	PSU	C6-N1-C2	-2.46	120.17	122.68
54	Z	55	5MU	O4-C4-N3	-2.45	115.42	120.12
22	a	2580	PSU	O4'-C1'-C2'	2.45	108.59	105.14
1	A	1518	MA6	N1-C6-N6	-2.44	114.41	117.08
22	a	2251	OMG	O6-C6-C5	-2.42	120.17	126.60
33	l	81	4D4	O-C-CA	-2.39	118.51	124.78
1	A	1516	2MG	C1'-N9-C4	-2.37	119.46	126.50
22	a	1911	PSU	C6-C5-C4	2.37	119.86	118.20
22	a	2457	PSU	C6-N1-C2	-2.36	120.27	122.68
22	a	2498	OMC	O2-C2-N3	-2.36	118.50	122.33
54	Z	55	5MU	O2-C2-N1	-2.35	119.66	122.79
55	V	6	2MG	CM2-N2-C2	-2.35	118.67	123.86
22	a	955	PSU	C6-N1-C2	-2.35	120.28	122.68
55	V	13	PSU	C6-C5-C4	2.34	119.84	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1516	2MG	N1-C2-N3	-2.34	120.34	123.95
54	Z	21	H2U	C5-C6-N1	-2.33	103.94	111.61
12	L	89	D2T	O-C-CA	-2.33	118.67	124.78
1	A	1402	4OC	C6-C5-C4	2.33	119.81	116.96
55	V	34	56B	O12-C12-C11	-2.33	108.25	113.47
22	a	2251	OMG	C1'-N9-C4	-2.31	119.65	126.50
1	A	1207	2MG	N1-C2-N3	-2.31	120.39	123.95
22	a	2605	PSU	C6-N1-C2	-2.29	120.34	122.68
25	d	150	MEQ	OE1-CD-CG	2.29	126.20	122.02
22	a	1618	6MZ	C4-C5-N7	-2.29	107.83	110.62
55	V	57	1MA	C6-C5-N7	-2.25	128.11	132.20
22	a	747	5MU	O4-C4-N3	-2.24	115.82	120.12
22	a	1917	PSU	C6-C5-C4	2.24	119.76	118.20
1	A	516	PSU	O2-C2-N1	-2.23	120.34	122.79
1	A	516	PSU	O4'-C1'-C2'	2.23	108.29	105.14
1	A	1519	MA6	N3-C4-N9	2.22	130.74	127.08
22	a	1835	2MG	C8-N7-C5	2.22	108.26	104.24
1	A	1516	2MG	C8-N7-C5	2.22	108.26	104.24
22	a	747	5MU	C6-C5-C4	2.22	119.89	118.03
22	a	2251	OMG	C8-N7-C5	2.21	108.24	104.24
22	a	2604	PSU	C6-N1-C2	-2.21	120.42	122.68
55	V	9	1MA	C6-C5-N7	-2.21	128.18	132.20
22	a	2445	2MG	CM2-N2-C2	-2.21	118.99	123.86
22	a	1835	2MG	N1-C2-N3	-2.21	120.54	123.95
1	A	1207	2MG	C8-N7-C5	2.21	108.23	104.24
54	Z	8	4SU	O2-C2-N1	-2.18	119.89	122.79
55	V	54	PSU	C6-N1-C2	-2.17	120.46	122.68
55	V	19	H2U	C4-N3-C2	-2.15	124.01	125.79
22	a	1618	6MZ	C5-C6-N1	2.15	120.49	118.20
22	a	2604	PSU	C6-C5-C4	2.14	119.69	118.20
1	A	966	2MG	N1-C2-N3	-2.14	120.64	123.95
55	V	6	2MG	N1-C2-N3	-2.14	120.65	123.95
1	A	527	G7M	CN7-N7-C8	-2.14	121.54	124.84
1	A	967	5MC	CM5-C5-C6	-2.13	120.00	122.85
25	d	150	MEQ	CG-CD-NE2	-2.13	113.34	116.29
22	a	2069	G7M	CN7-N7-C8	-2.13	121.56	124.84
22	a	1939	5MU	C6-C5-C4	2.12	119.80	118.03
1	A	1518	MA6	N3-C4-N9	2.12	130.57	127.08
22	a	1915	3TD	C6-C5-C4	2.12	119.68	118.22
22	a	745	1MG	C8-N7-C5	2.11	108.06	104.24
55	V	6	2MG	C8-N7-C5	2.11	108.06	104.24
1	A	966	2MG	CM2-N2-C2	-2.11	119.20	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	119	IAS	OXT-C-CA	2.11	120.57	113.38
22	a	746	PSU	C6-N1-C2	-2.11	120.53	122.68
22	a	2069	G7M	N9-C8-N7	-2.10	107.00	112.21
55	V	48	5MC	CM5-C5-C6	-2.07	120.09	122.85
22	a	2605	PSU	O2-C2-N1	-2.06	120.52	122.79
1	A	966	2MG	C8-N7-C5	2.05	107.95	104.24
1	A	1402	4OC	O2-C2-N3	-2.04	119.01	122.33
22	a	2069	G7M	N1-C2-N3	-2.03	119.54	123.32
1	A	1402	4OC	CM4-N4-C4	-2.02	118.50	122.45
22	a	2445	2MG	C8-N7-C5	2.01	107.88	104.24
55	V	47	5MC	CM5-C5-C6	-2.01	120.17	122.85

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	O4'-C4'-C5'-O5'
12	L	89	D2T	CG-CB-SB-CB1
25	d	150	MEQ	C-CA-CB-CG
33	l	81	4D4	CA-CB-CG-CD
33	l	81	4D4	NE-CD-CG-CB
54	Z	21	H2U	O4'-C1'-N1-C6
54	Z	21	H2U	C2'-C1'-N1-C6
22	a	746	PSU	C2'-C1'-C5-C4
22	a	746	PSU	C2'-C1'-C5-C6
55	V	47	5MC	O4'-C4'-C5'-O5'
55	V	47	5MC	C3'-C4'-C5'-O5'
55	V	48	5MC	O4'-C4'-C5'-O5'
54	Z	21	H2U	C2'-C1'-N1-C2
1	A	1519	MA6	C3'-C4'-C5'-O5'
22	a	2030	6MZ	O4'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'
55	V	48	5MC	C3'-C4'-C5'-O5'
54	Z	21	H2U	O4'-C4'-C5'-O5'
54	Z	21	H2U	C3'-C4'-C5'-O5'
22	a	2504	PSU	O4'-C4'-C5'-O5'
25	d	150	MEQ	NE2-CD-CG-CB
25	d	150	MEQ	OE1-CD-CG-CB
33	l	81	4D4	OB-CB-CG-CD
1	A	527	G7M	C3'-C4'-C5'-O5'
22	a	2504	PSU	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	V	19	H2U	O4'-C4'-C5'-O5'
55	V	19	H2U	C3'-C4'-C5'-O5'
1	A	527	G7M	O4'-C4'-C5'-O5'
22	a	2445	2MG	C3'-C4'-C5'-O5'
33	l	82	MS6	CB-CG-SD-CE
25	d	150	MEQ	N-CA-CB-CG
1	A	527	G7M	C4'-C5'-O5'-P
55	V	9	1MA	C3'-C4'-C5'-O5'
54	Z	21	H2U	O4'-C1'-N1-C2
55	V	6	2MG	C3'-C4'-C5'-O5'
55	V	47	5MC	C4'-C5'-O5'-P
33	l	81	4D4	CG-CD-NE-CZ
22	a	746	PSU	O4'-C1'-C5-C4
55	V	54	PSU	O4'-C1'-C5-C4
1	A	1402	4OC	C3'-C4'-C5'-O5'
12	L	89	D2T	CA-CB-SB-CB1
55	V	9	1MA	O4'-C4'-C5'-O5'
25	d	150	MEQ	CA-CB-CG-CD
55	V	19	H2U	C2'-C1'-N1-C6
54	Z	21	H2U	C4'-C5'-O5'-P
22	a	746	PSU	O4'-C1'-C5-C6
55	V	54	PSU	O4'-C1'-C5-C6
22	a	2069	G7M	O4'-C4'-C5'-O5'
1	A	966	2MG	C3'-C4'-C5'-O5'
22	a	2503	2MA	O4'-C4'-C5'-O5'
33	l	81	4D4	O-C-CA-CB

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	Z	55	5MU	2	0
54	Z	56	PSU	1	0
22	a	2552	OMU	1	0
55	V	53	5MU	2	0
54	Z	21	H2U	1	0
55	V	9	1MA	1	0
22	a	2030	6MZ	1	0
22	a	2251	OMG	1	0
55	V	6	2MG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 249 ligands modelled in this entry, 248 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
57	MAN	V	103	55	11,11,12	1.94	5 (45%)	15,15,17	1.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MAN	V	103	55	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	V	103	MAN	O5-C1	-2.73	1.39	1.43
57	V	103	MAN	C4-C5	2.62	1.58	1.53
57	V	103	MAN	O2-C2	-2.60	1.37	1.43
57	V	103	MAN	O4-C4	-2.47	1.37	1.43
57	V	103	MAN	O3-C3	-2.35	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

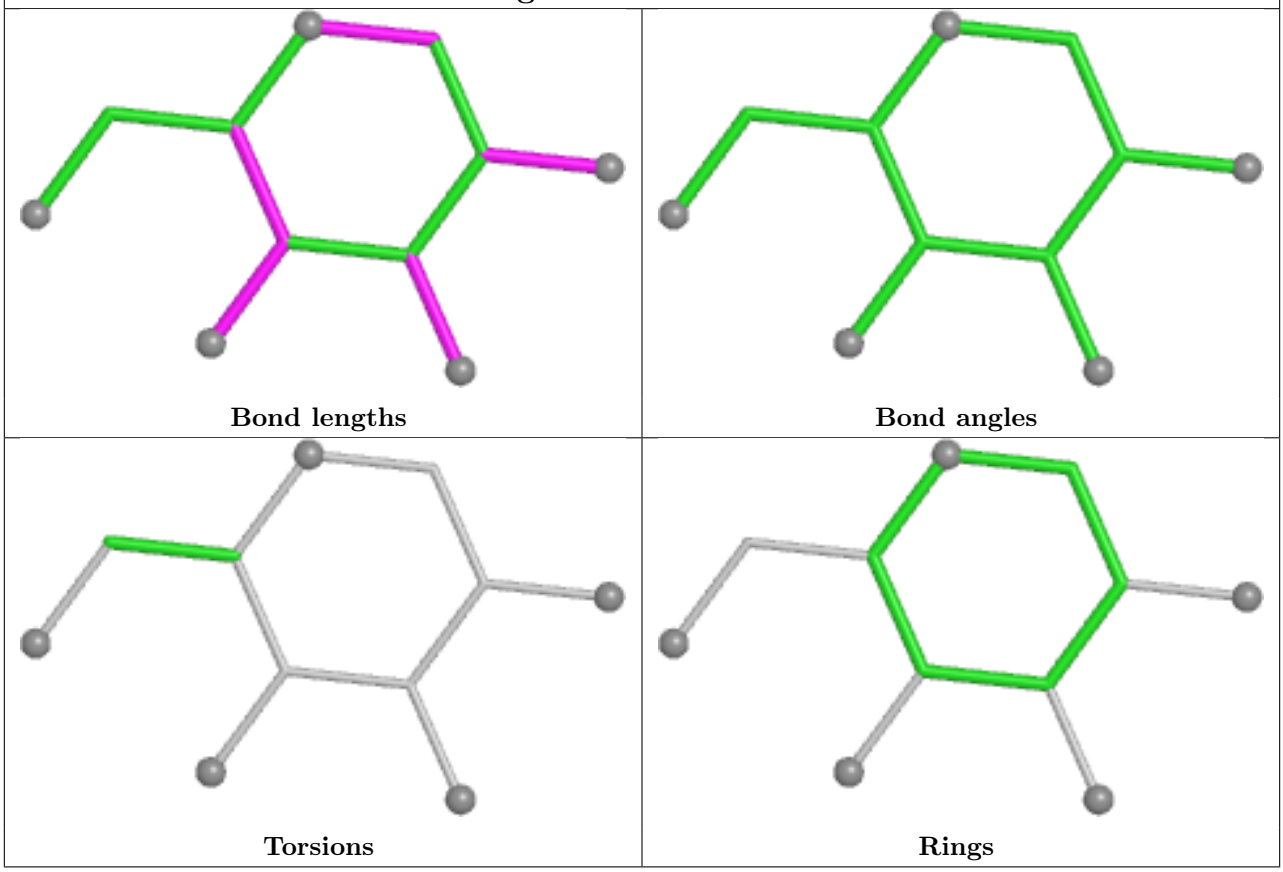
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand MAN V 103



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.

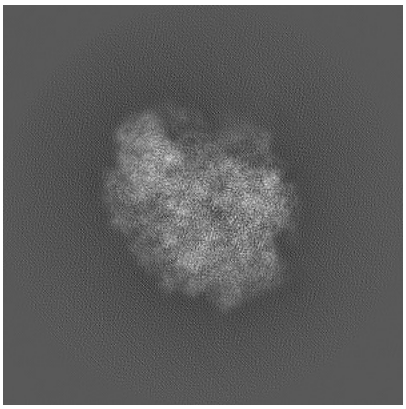
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-33662. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



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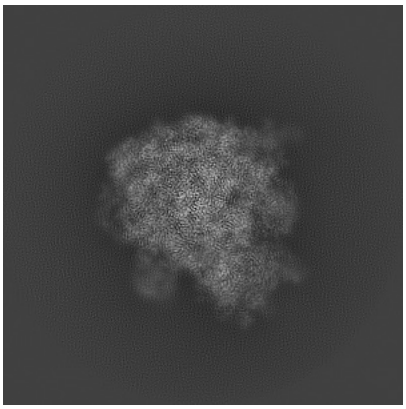

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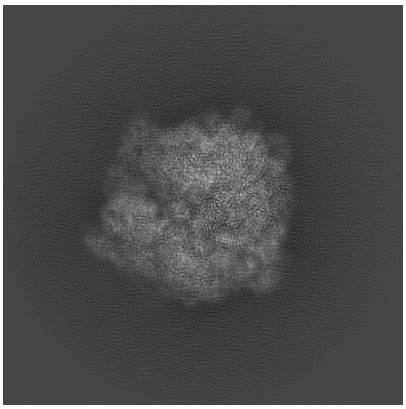
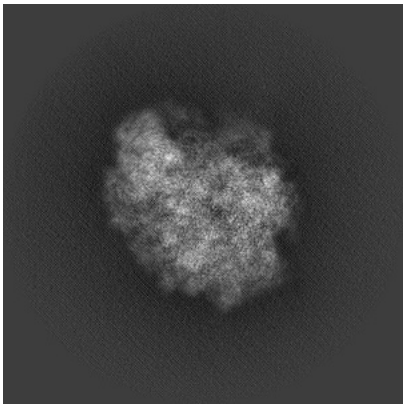


Z

6.1.2 Raw map



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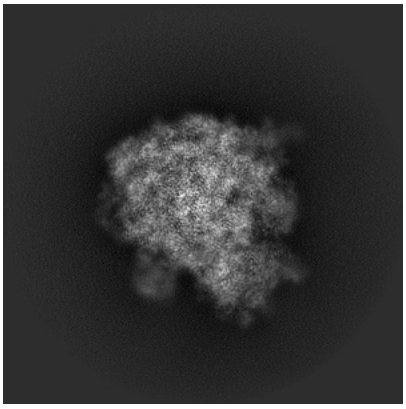
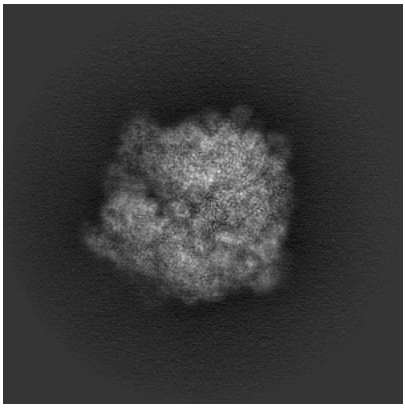


Y

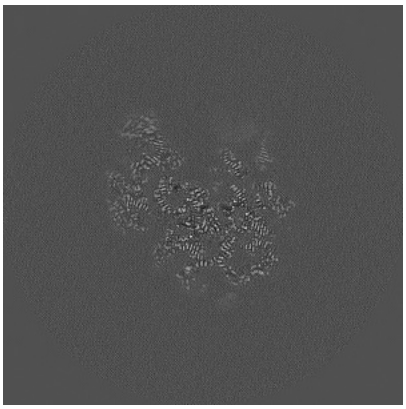


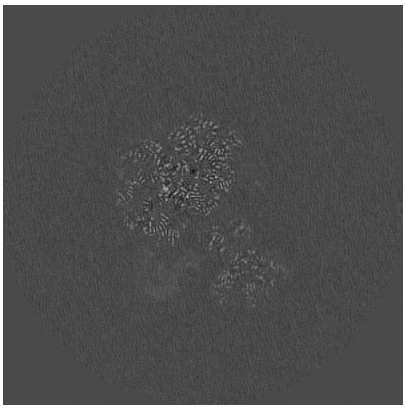
Z

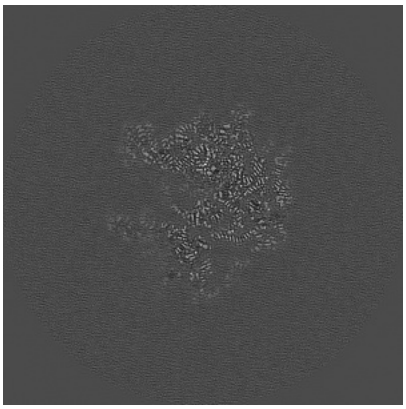
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

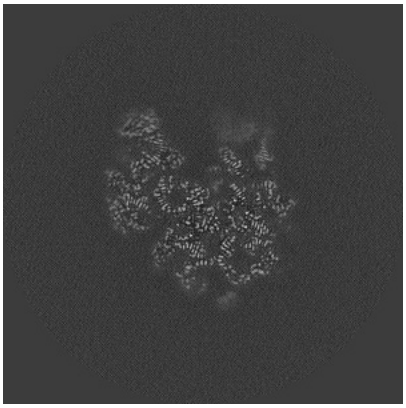
6.2.1 Primary map

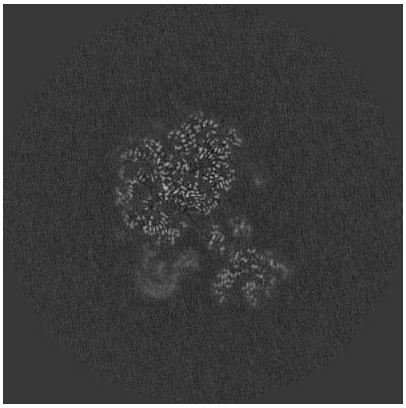

X Index: 265

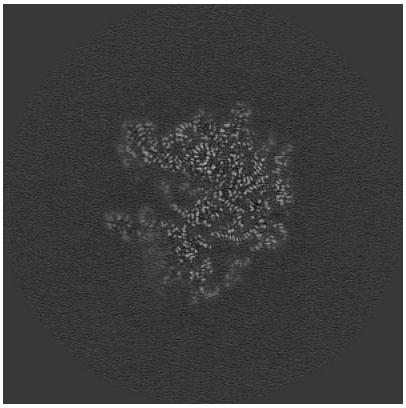

Y Index: 265


Z Index: 265

6.2.2 Raw map


X Index: 265

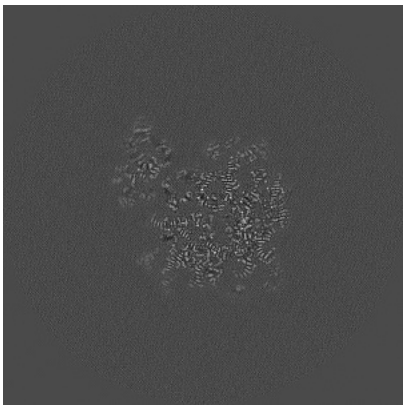

Y Index: 265


Z Index: 265

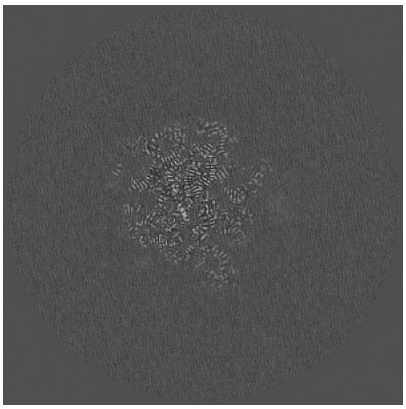
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

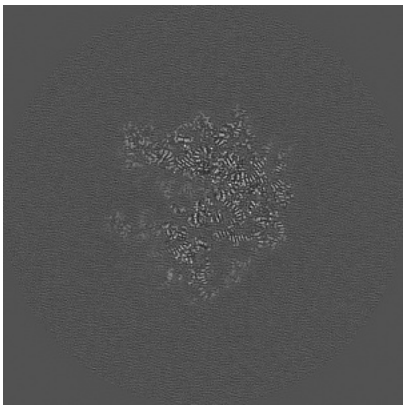
6.3.1 Primary map



X Index: 297

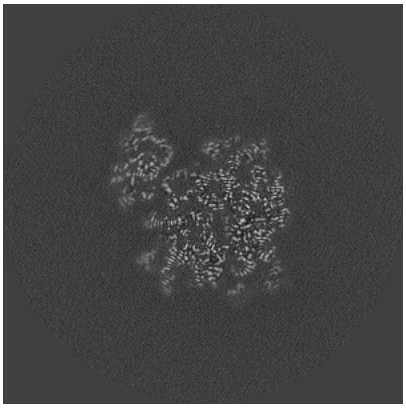


Y Index: 321

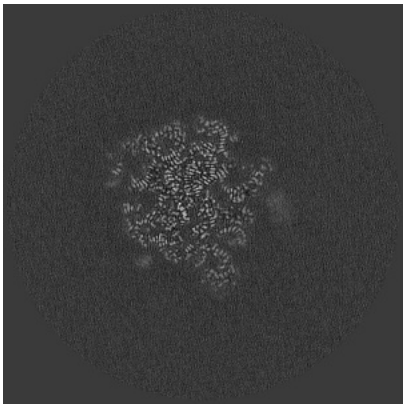


Z Index: 267

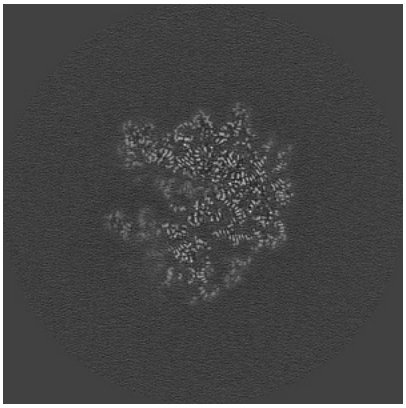
6.3.2 Raw map



X Index: 296



Y Index: 321

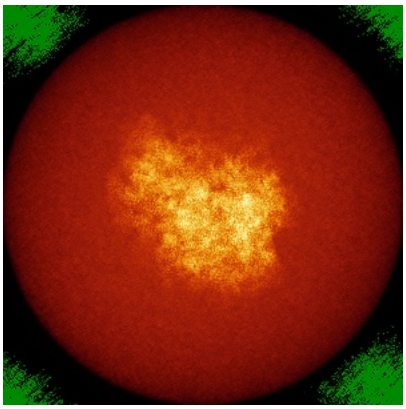


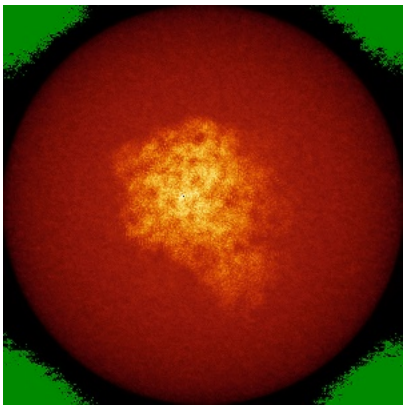
Z Index: 267

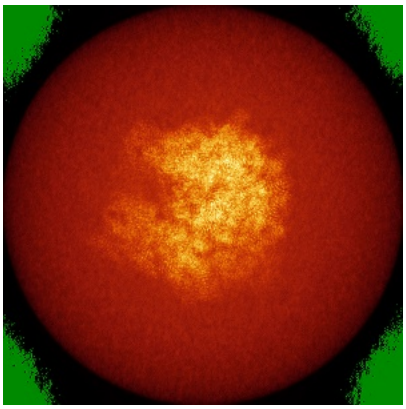
The images above show the largest variance slices of the map in three orthogonal directions.

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

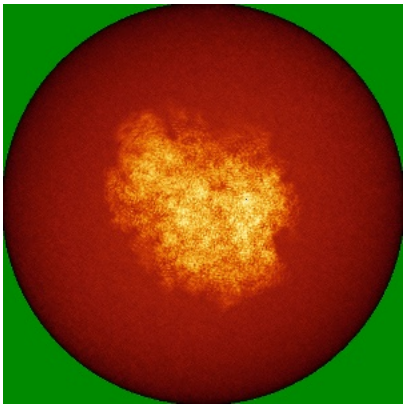
6.4.1 Primary map

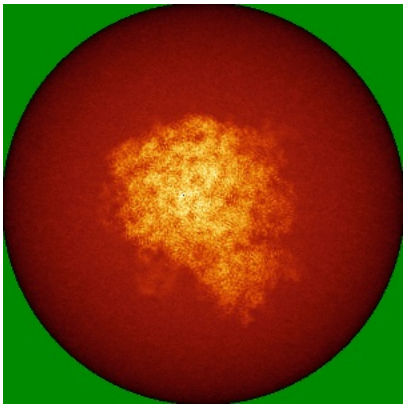

X

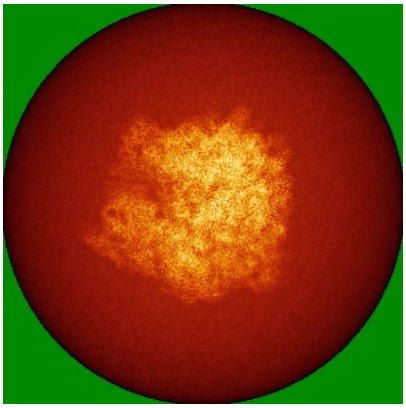

Y


Z

6.4.2 Raw map


X

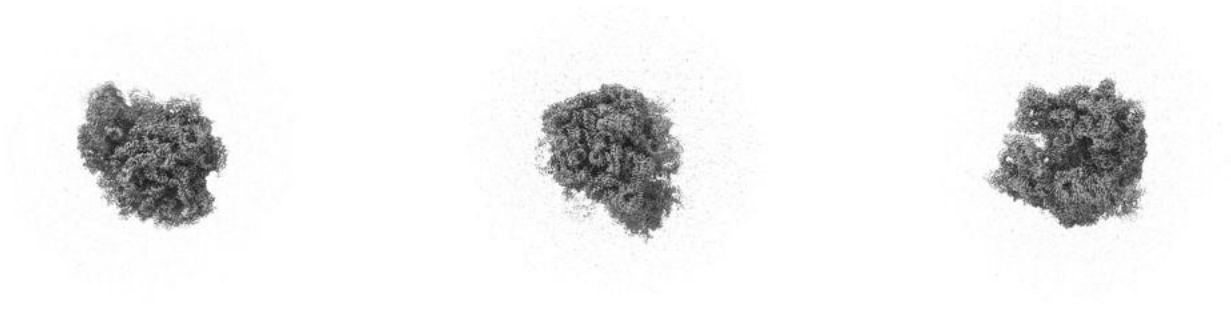

Y


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

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

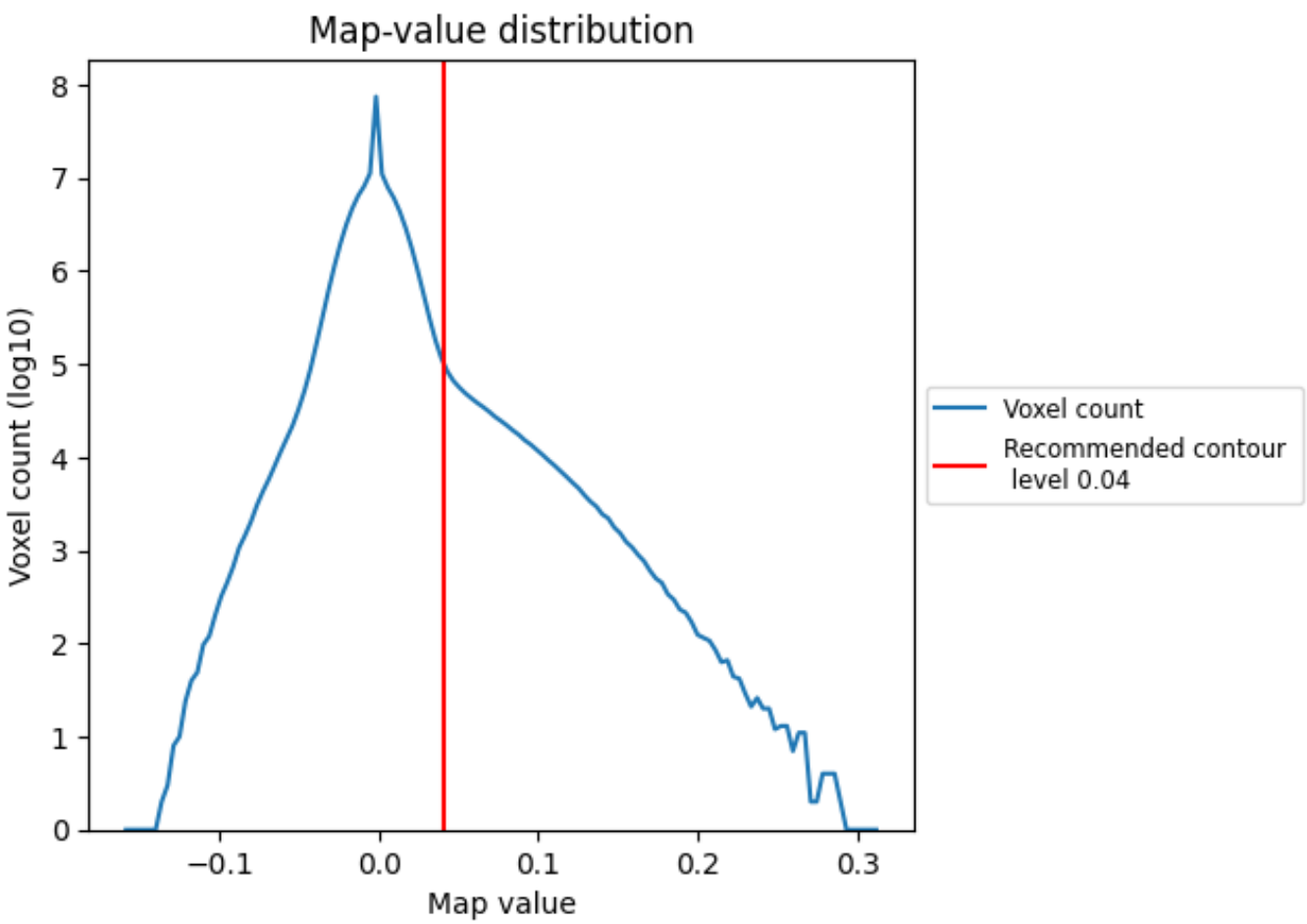
6.6 Mask visualisation (i)

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

7 Map analysis (i)

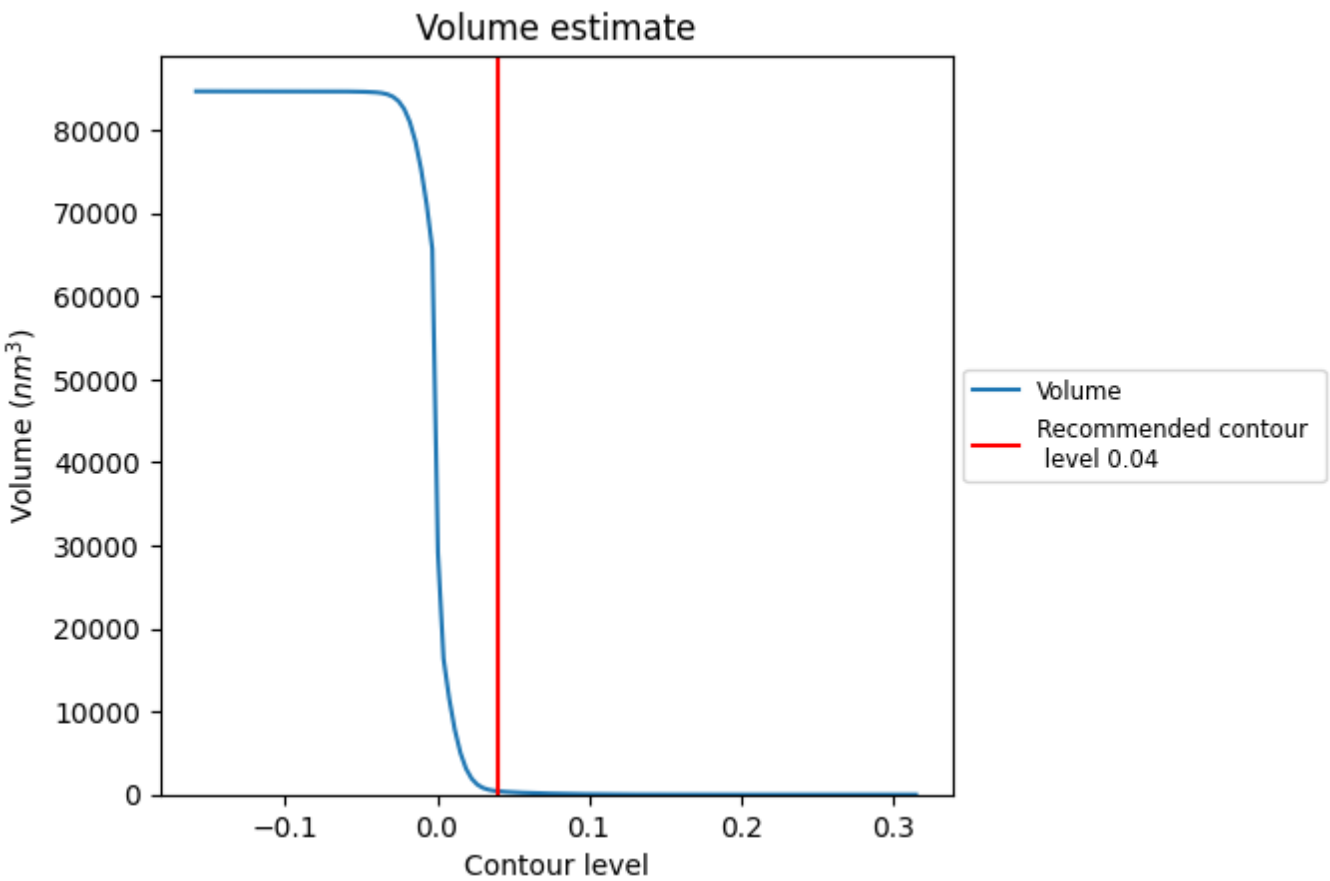
This section contains the results of statistical analysis of the map.

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.

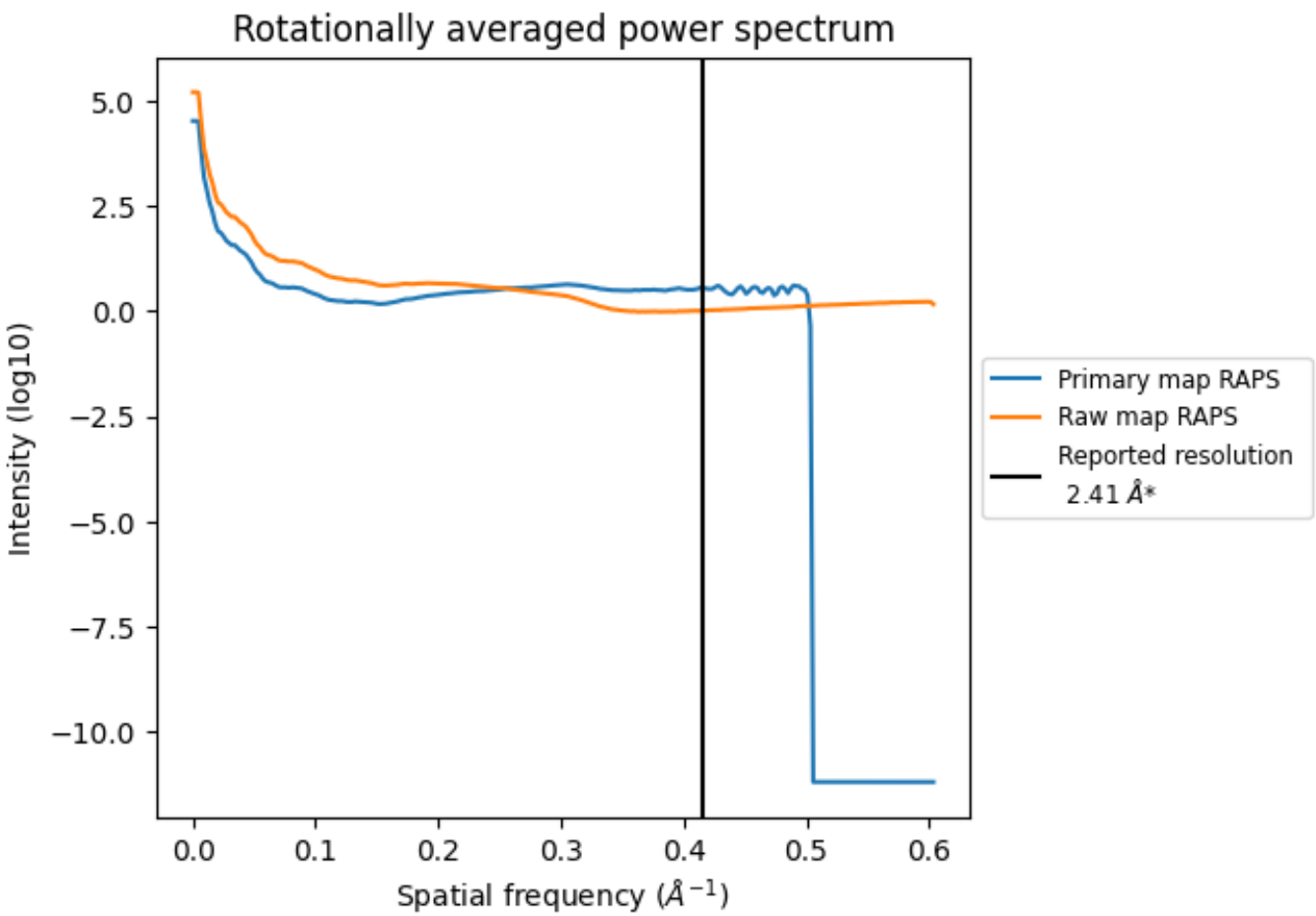
7.2 Volume estimate (i)



The volume at the recommended contour level is 410 nm^3; this corresponds to an approximate mass of 371 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)

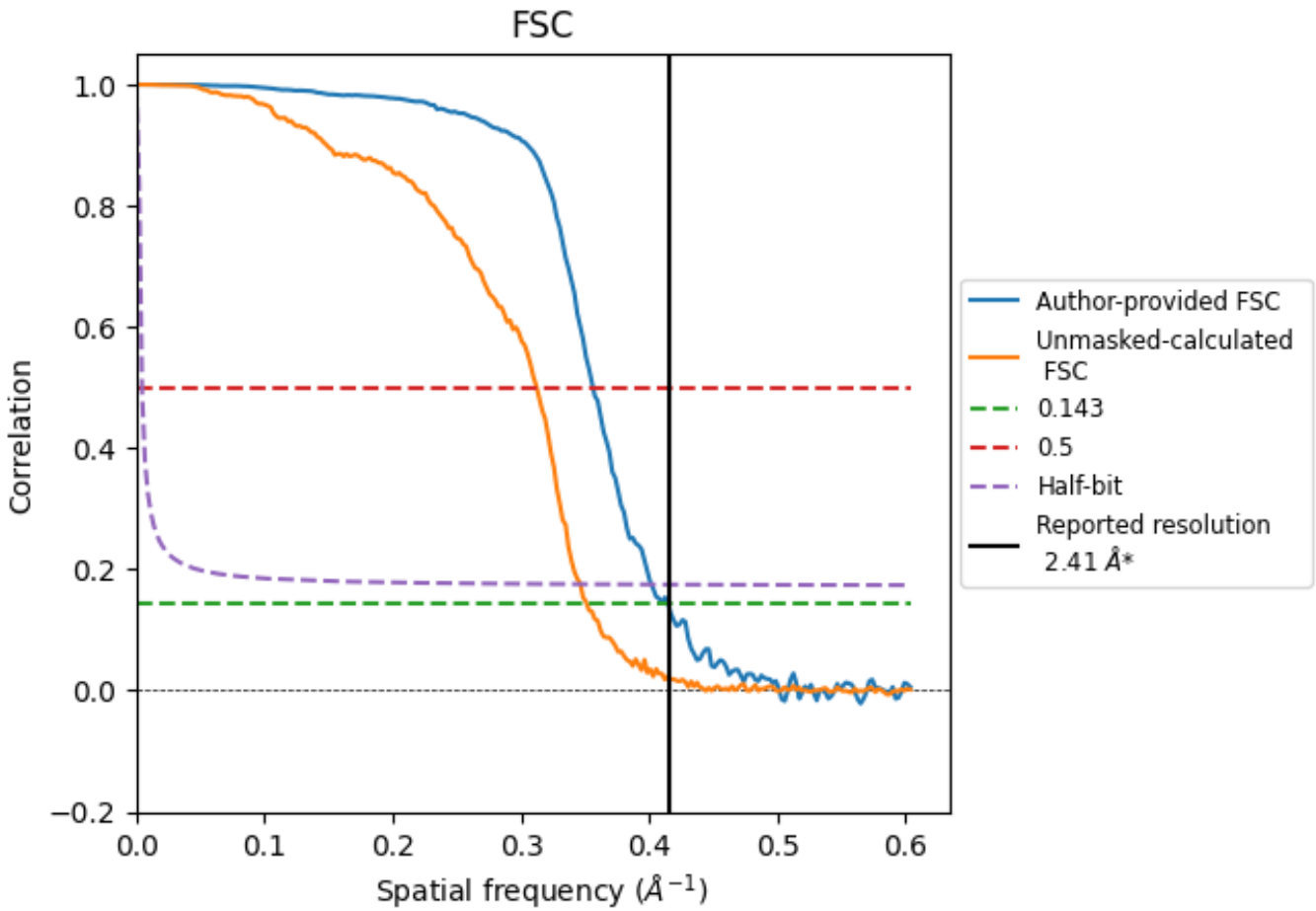


*Reported resolution corresponds to spatial frequency of 0.415 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.415 Å^{-1}

8.2 Resolution estimates (i)

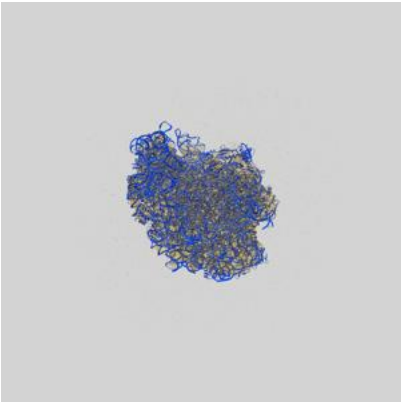
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.41	-	-
Author-provided FSC curve	2.41	2.81	2.49
Unmasked-calculated*	2.85	3.20	2.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.85 differs from the reported value 2.41 by more than 10 %

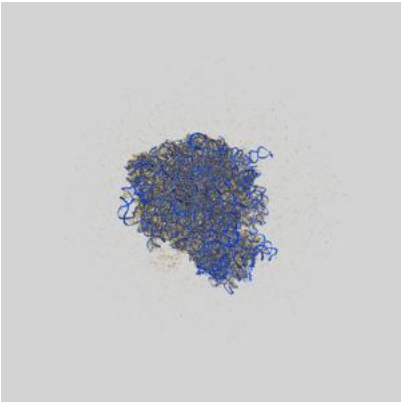
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-33662 and PDB model 7Y7E. Per-residue inclusion information can be found in section 3 on page 16.

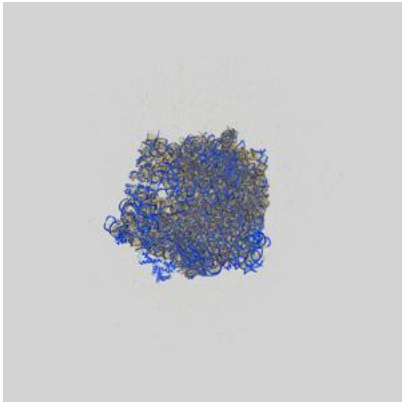
9.1 Map-model overlay (i)



X



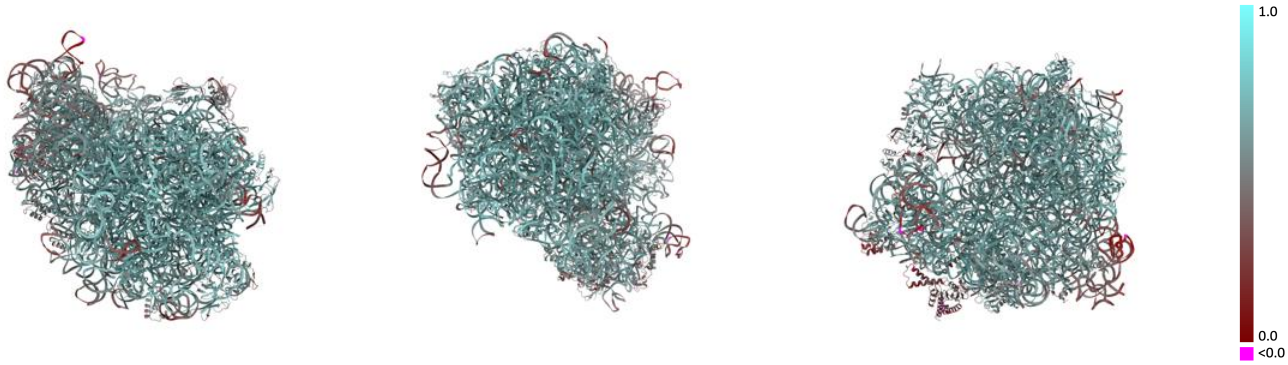
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

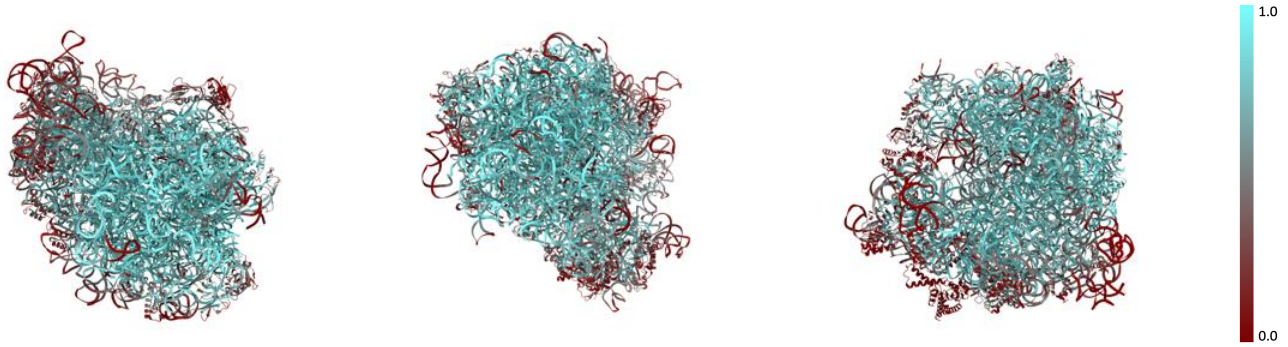
9.2 Q-score mapped to coordinate model (i)



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.

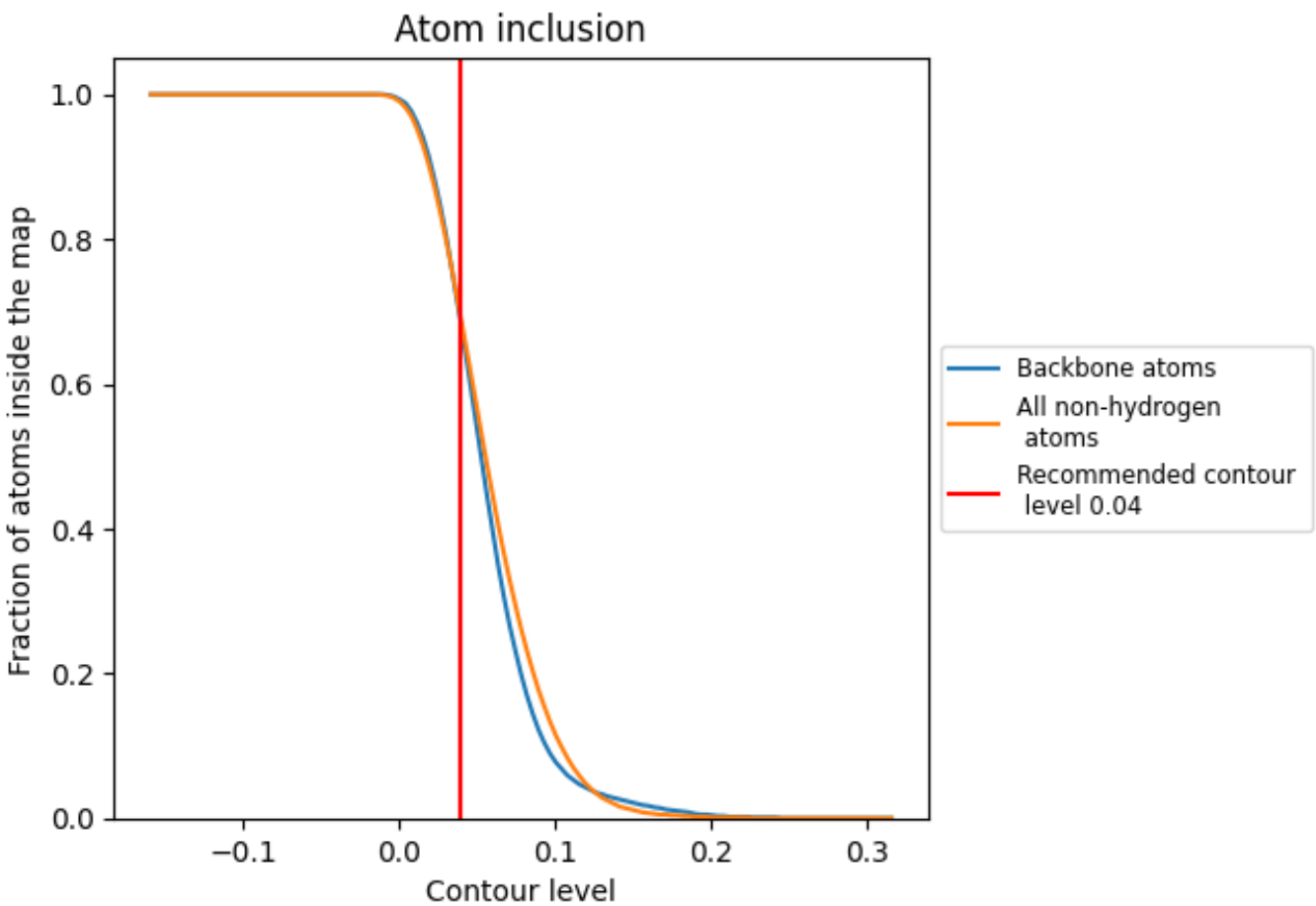
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 69% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.6290
0	0.6600	0.6400
1	0.9150	0.7150
2	0.8940	0.7070
3	0.7700	0.6640
4	0.1380	0.4510
A	0.6650	0.6100
B	0.0010	0.2980
C	0.4630	0.5940
D	0.2530	0.5320
E	0.6340	0.6400
F	0.2540	0.4900
G	0.2990	0.5270
H	0.5580	0.6170
I	0.3770	0.5580
J	0.3110	0.4710
K	0.4940	0.5860
L	0.6700	0.6510
M	0.3870	0.5750
N	0.4870	0.5910
O	0.5100	0.5800
P	0.3590	0.5220
Q	0.3790	0.5450
R	0.4470	0.5490
S	0.3560	0.5500
T	0.3150	0.5360
U	0.1160	0.4260
V	0.5290	0.5760
X	0.6200	0.6220
Z	0.5160	0.5690
a	0.8240	0.6670
b	0.6890	0.6230
c	0.8490	0.7070
d	0.7830	0.6850
e	0.5330	0.6210

Continued on next page...

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Chain	Atom inclusion	Q-score
f	0.3730	0.5630
g	0.2440	0.4900
h	0.1400	0.5100
i	0.7930	0.6780
j	0.7460	0.6820
k	0.6950	0.6520
l	0.8130	0.6920
m	0.8700	0.7000
n	0.5540	0.6090
o	0.6970	0.6610
p	0.8390	0.7080
q	0.6460	0.6390
r	0.7700	0.6760
s	0.5850	0.6180
t	0.4420	0.5690
u	0.5580	0.6050
v	0.7950	0.6750
w	0.7220	0.6590
x	0.3660	0.5380
y	0.7370	0.6540
z	0.7340	0.6600