Full wwPDB EM Validation Report (i)

Sep 17, 2026 – 05:00 AM EDT

PDB ID	:	7RYH / pdb_00007ryh
EMDB ID	:	EMD-24740
Title	:	A. baumannii Ribosome-TP-6076 complex: Empty 70S
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2021-08-25
Resolution	:	2.43 Å(reported)

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

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

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

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

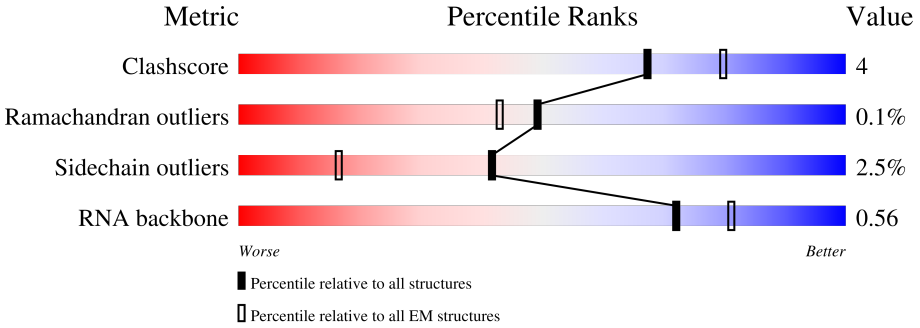
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

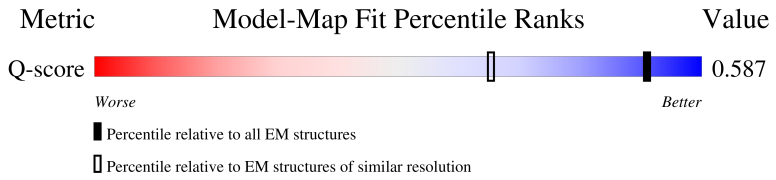
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.43 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	5787 (1.94 - 2.93)

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

Mol	Chain	Length	Quality of chain
1	0	51	• 82% 12% 6%
2	1	44	89% 11%
3	2	64	81% 17% •

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Mol	Chain	Length	Quality of chain
4	3	38	11% 74% 26%
5	A	2918	6% 70% 19% 8%
6	B	115	8% 72% 22% 6%
7	C	274	91% 8%
8	D	212	91% 9%
9	E	200	90% 10%
10	F	178	84% 56% 39%
11	G	177	27% 86% 12%
12	H	148	14% 39% 59%
13	I	142	93% 6%
14	J	122	89% 11%
15	K	146	90% 9%
16	L	137	87% 12%
17	M	125	94% 5%
18	N	116	8% 86% 12%
19	O	122	84% 10% 5%
20	P	119	94%
21	Q	103	96%
22	R	109	97%
23	S	106	75% 10% 14%
24	T	105	10% 83% 14%
25	U	98	87% 10%
26	V	85	87% 9%
27	W	78	90% 9%
28	X	65	6% 78% 14% 8%

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Mol	Chain	Length	Quality of chain
29	Y	58	84% 16%
30	Z	61	84% 5% 11%
31	a	1544	8% 73% 22%
32	b	250	53% 60% 30% 10%
33	c	250	74% 12% 14%
34	d	208	15% 75% 23%
35	e	165	78% 15% 6%
36	f	127	20% 63% 17% 18%
37	g	156	10% 70% 17% 13%
38	h	131	87% 12%
39	i	128	83% 14%
40	j	103	81% 16%
41	k	128	48% 83% 6% 9%
42	l	124	10% 85% 14%
43	m	118	78% 19%
44	n	101	86% 13%
45	o	89	85% 13%
46	p	101	77% 19%
47	q	85	81% 9% 8%
48	r	75	57% 11% 31%
49	s	91	75% 15% 10%
50	t	88	93% 5%
51	u	71	65% 77% 20%

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 135829 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	48	400	256	72	69	3	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	A	2685	57610	25715	10555	18655	2685	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	271	2104	1297	435	364	8	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	141	1117	713	199	202	3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	q	78	614	386	115	112	1	0	0

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

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

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

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

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

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

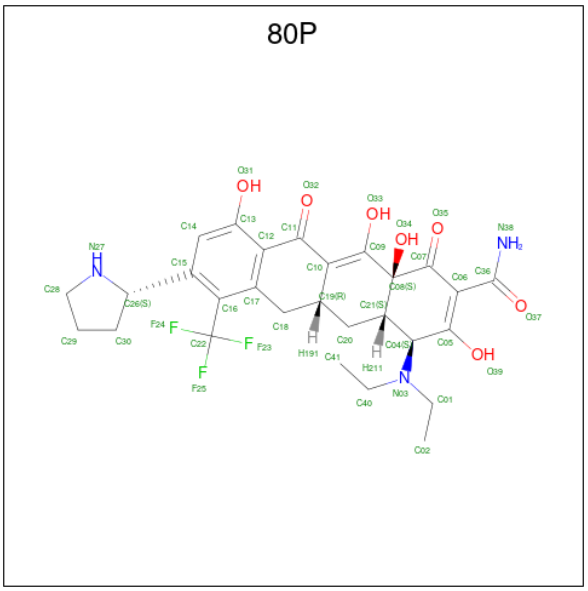
- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	u	57	473	294	96	82	1	0	0

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
52	3	1	1	1	0

- Molecule 53 is (4S,4aS,5aR,12aS)-4-(diethylamino)-3,10,12,12a-tetrahydroxy-1,11-dioxo-8-[(2S)-pyrrolidin-2-yl]-7-(trifluoromethyl)-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboxamide (CCD ID: 80P) (formula: $C_{28}H_{32}F_3N_3O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
53	a	1	Total	C	F	N	O	0
			41	28	3	3	7	
53	a	1	Total	C	F	N	O	0
			41	28	3	3	7	
53	a	1	Total	C	F	N	O	0
			41	28	3	3	7	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

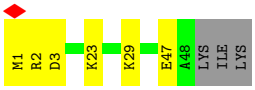
Mol	Chain	Residues	Atoms		AltConf
54	a	4	Total	Mg	0
			4	4	

3 Residue-property plots (i)

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

- Molecule 1: 50S ribosomal protein L33

Chain 0:

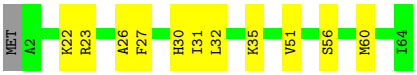


- Molecule 2: 50S ribosomal protein L34

Chain 1:

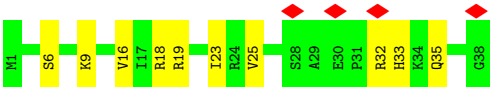
- Molecule 3: 50S ribosomal protein L35

Chain 2:



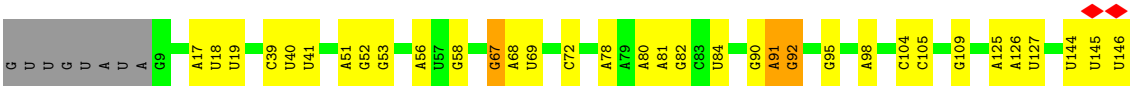
- Molecule 4: 50S ribosomal protein L36

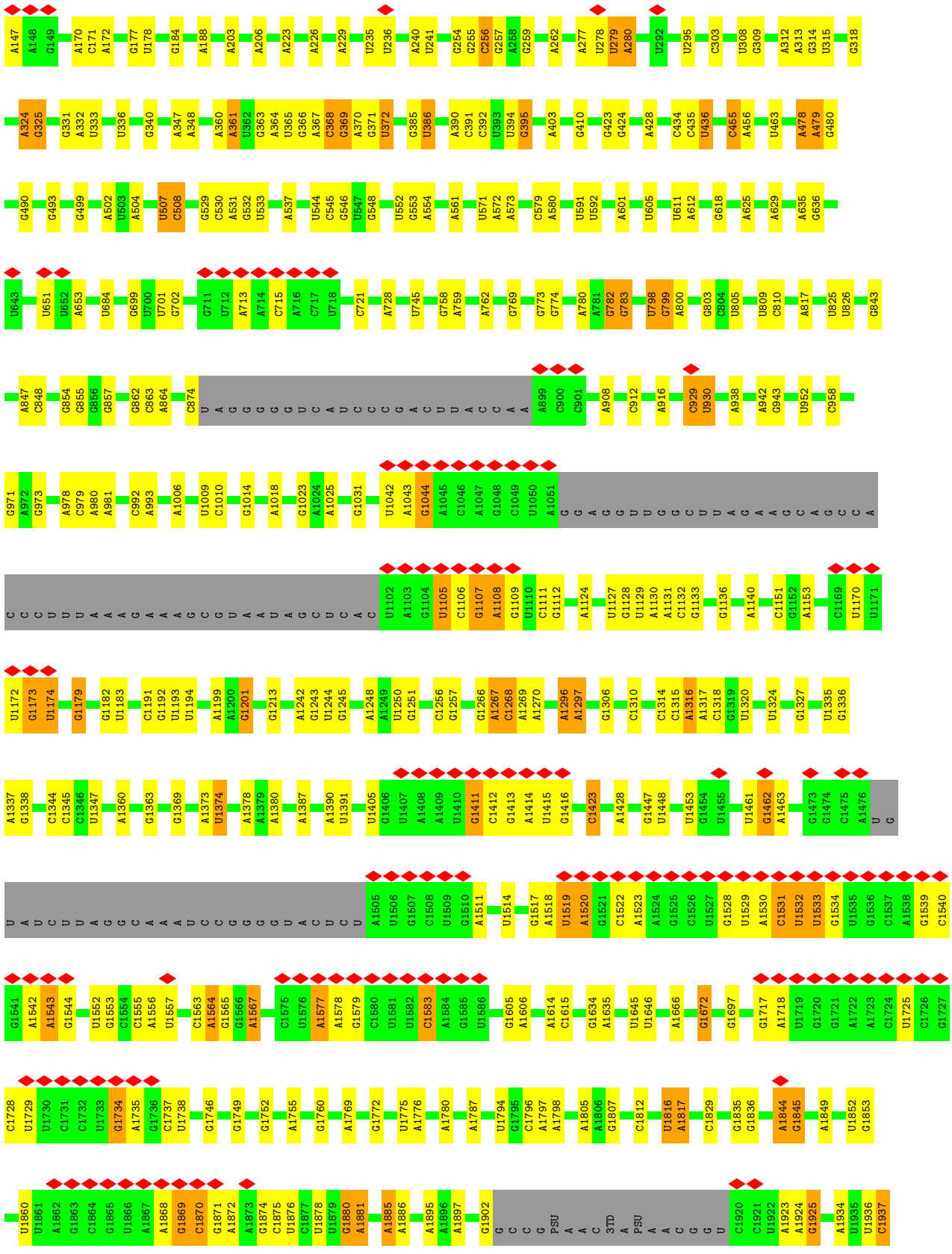
Chain 3:



- Molecule 5: 23S ribosomal RNA

Chain A:




A147 A148 G149 A170 C171 A172 G177 U178 G184 A188 A203 A206 A223 A226 A229 U235 U236 A240 U241 G254 G255 C256 G257 A258 C259 A262 A277 U278 U279 A280 U292 U295 C303 U308 G309 A312 A313 G314 U315 G318
A324 G325 G331 A332 U333 U336 G340 A347 A348 A360 A361 U362 G363 A364 U365 G366 A367 C368 G369 A370 G371 U372 G385 U386 A390 C391 C392 U393 U394 G395 A403 G410 G423 G424 A428 C434 C435 U436 C455 A456 U463 A478 A479 G480
G490 G493 G499 A502 U503 A504 U507 C508 G529 C530 A531 G532 U533 A537 U544 C545 G546 U547 G548 U552 G553 A554 A561 U571 A572 A573 C579 A580 U591 U592 A601 U605 U611 A612 G618 A625 A629 A635 G636
U643 U651 U652 A653 U684 G699 U700 U701 G702 G711 U712 A713 A714 C715 A716 C717 U718 C721 A728 U745 G758 A759 A762 G769 G773 G774 A780 A781 G782 G783 U798 G799 A800 G803 C804 U805 U809 C810 A817 U825 U826 G843
A847 C848 G854 C855 G856 G857 G862 C863 A864 C874 U A G G G G G U C A U C C C C G A C U U A C C C A A A899 C900 C901 A908 C912 A916 C929 U930 A938 A942 G943 U952 C958
G971 A972 G973 A978 C979 A980 A981 C992 A993 A1006 U1009 C1010 G1014 A1018 G1023 A1024 A1025 G1031 U1042 A1043 G1044 A1045 C1046 A1047 C1048 C1049 U1050 A1051 G G A G G U U G G C U U U A G A A G C A G C C C A
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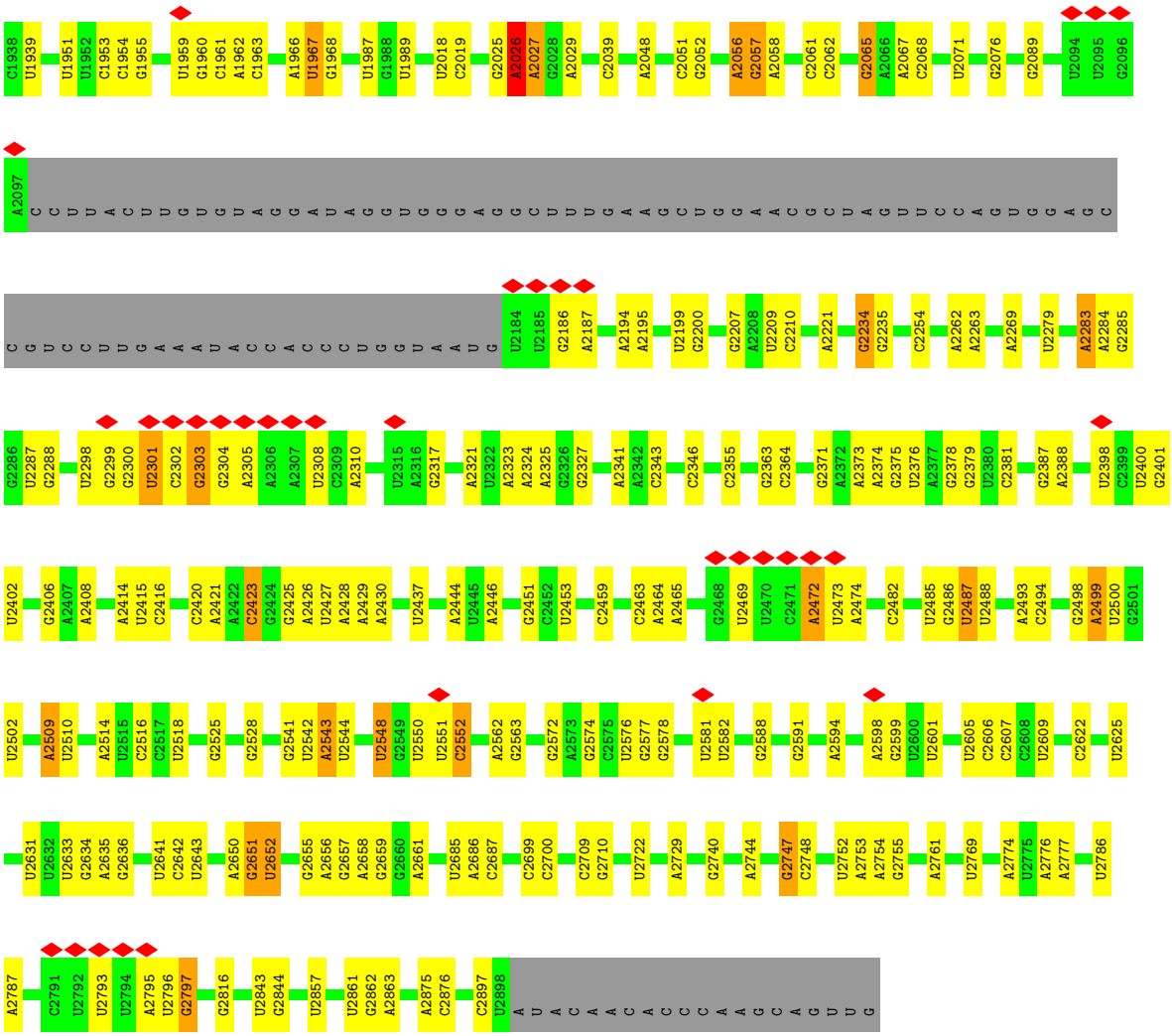
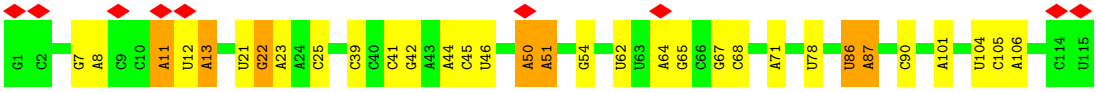
U1172 G1173 U1174 G1179 G1182 U1183 C1191 G1192 U1193 U1194 A1199 A1200 G1201 G1213 A1242 G1243 U1244 G1245 A1248 A1249 U1250 G1251 C1256 G1257 G1266 A1267 C1268 A1269 A1270 A1296 A1297 G1306 C1310 C1314 C1315 A1316 A1317 C1318 G1319 U1320 U1324 G1327 U1335 G1336
A1337 G1338 C1344 C1345 C1346 U1347 A1360 G1363 G1369 A1373 U1374 A1378 A1379 A1380 A1387 A1390 U1391 U1405 G1406 U1407 A1408 A1409 U1410 G1411 C1412 G1413 A1414 U1415 G1416 C1423 A1428 G1447 U1448 U1453 G1454 U1455 U1461 G1462 A1463 G1473 G1474 C1475 A1476 U G
U A U C U U A G G C A A U C C G G G U A C U C U A1505 U1506 G1507 C1508 U1509 G1510 A1511 U1514 G1517 A1518 U1519 A1520 G1521 C1522 A1523 A1524 G1525 C1526 U1527 G1528 U1529 A1530 C1531 U1532 U1533 G1534 U1535 G1536 C1537 A1538 G1539 C1540
G1541 A1542 A1543 G1544 U1552 G1553 C1554 C1555 A1556 U1557 C1563 A1564 G1565 G1566 A1567 C1575 U1576 A1577 A1578 G1579 C1580 U1581 U1582 C1583 A1584 G1585 U1586 G1605 A1606 A1614 C1615 G1634 A1635 U1645 U1646 A1666 G1672 G1697 G1717 A1718 U1719 G1720 G1721 A1722 A1723 C1724 U1725 C1726 G1727
C1728 U1729 U1730 C1731 C1732 U1733 G1734 A1735 G1736 C1737 U1738 G1746 G1749 G1752 A1755 G1760 A1769 G1772 U1775 A1776 A1780 A1787 U1794 G1795 C1796 A1797 A1798 A1805 A1806 G1807 C1812 U1816 A1817 C1829 G1835 G1836 A1844 G1845 A1849 U1852 G1853
U1860 U1861 A1862 G1863 C1864 G1865 U1866 A1867 A1868 G1869 C1870 G1871 A1872 A1873 G1874 C1875 U1876 C1877 U1878 U1879 G1880 A1881 A1885 A1886 A1895 A1896 A1897 G1902 G C C G PSU A A C 3TD A PSU A A C G G U C1920 C1921 U1922 A1923 A1924 G1925 A1934 U1935 U1936 C1937



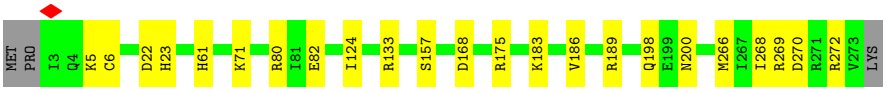
• Molecule 6: 5S ribosomal RNA

Chain B: 8% 72% 22% 6%



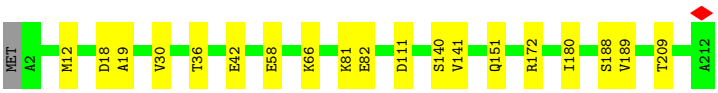
• Molecule 7: 50S ribosomal protein L2

Chain C: 91% 8%



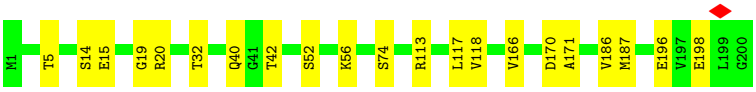
• Molecule 8: 50S ribosomal protein L3

Chain D: 91% 9%



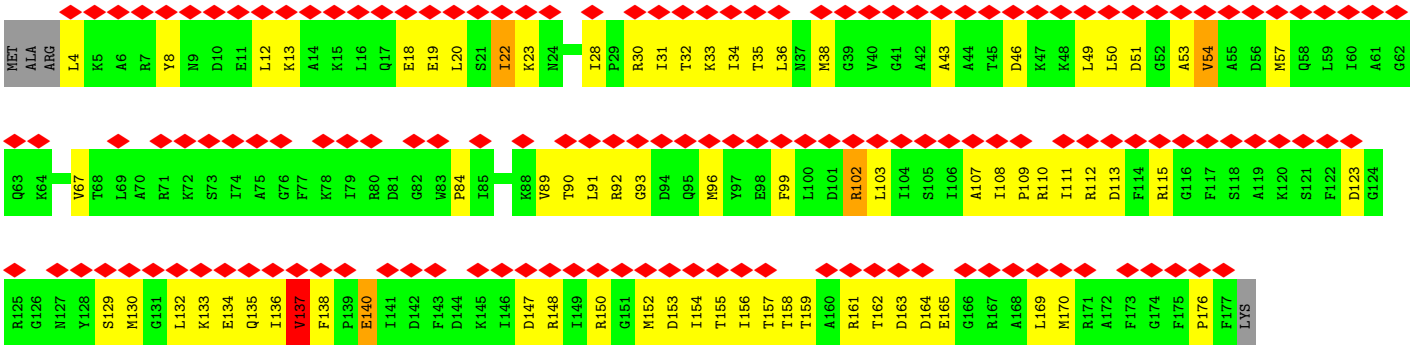
• Molecule 9: 50S ribosomal protein L4

Chain E:



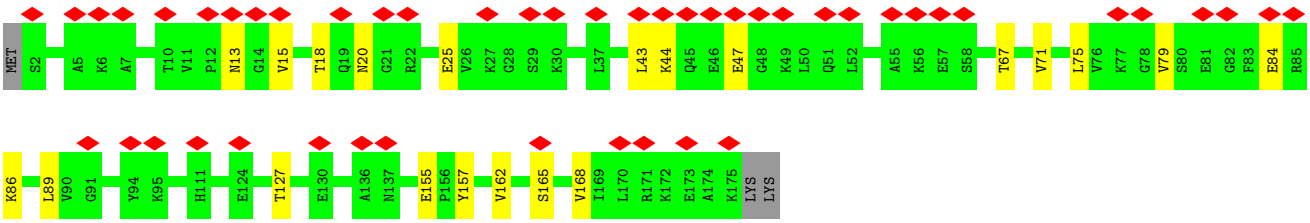
• Molecule 10: 50S ribosomal protein L5

Chain F:



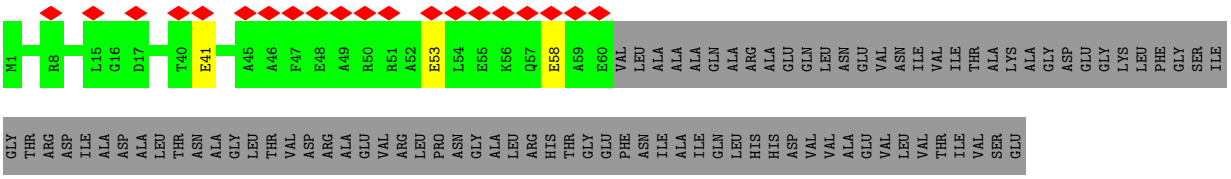
• Molecule 11: 50S ribosomal protein L6

Chain G:



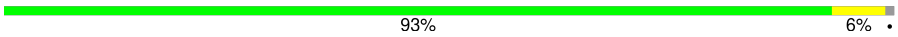
• Molecule 12: 50S ribosomal protein L9

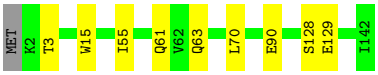
Chain H:



• Molecule 13: 50S ribosomal protein L13

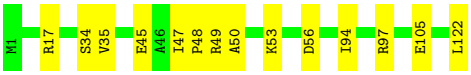
Chain I:





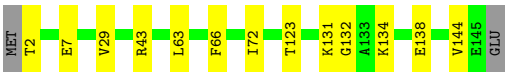
• Molecule 14: 50S ribosomal protein L14

Chain J:



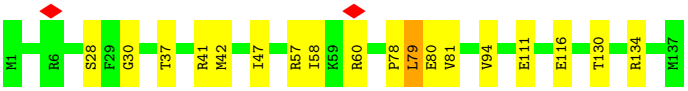
• Molecule 15: 50S ribosomal protein L15

Chain K:



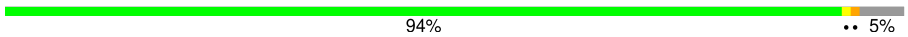
• Molecule 16: 50S ribosomal protein L16

Chain L:



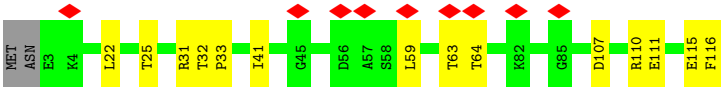
• Molecule 17: 50S ribosomal protein L17

Chain M:



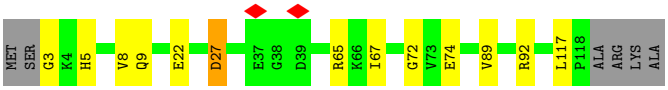
• Molecule 18: 50S ribosomal protein L18

Chain N:



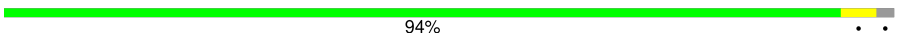
• Molecule 19: 50S ribosomal protein L19

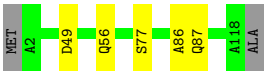
Chain O:



• Molecule 20: 50S ribosomal protein L20

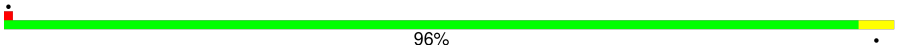
Chain P:





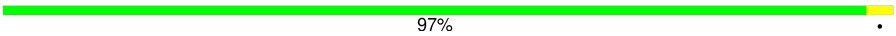
• Molecule 21: 50S ribosomal protein L21

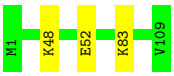
Chain Q:



• Molecule 22: 50S ribosomal protein L22

Chain R:



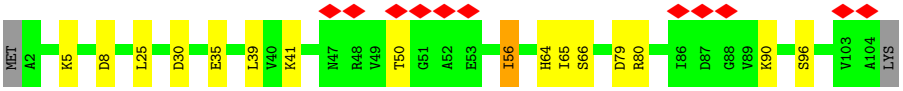


• Molecule 23: 50S ribosomal protein L23

Chain S:

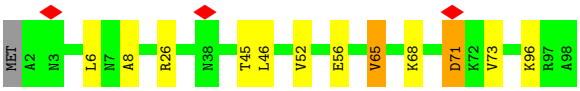
• Molecule 24: 50S ribosomal protein L24

Chain T:



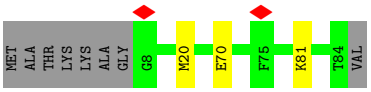
• Molecule 25: 50S ribosomal protein L25

Chain U:



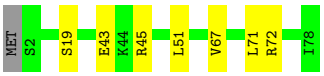
• Molecule 26: 50S ribosomal protein L27

Chain V:



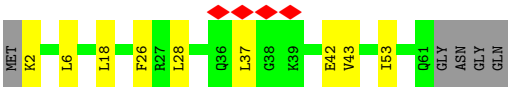
• Molecule 27: 50S ribosomal protein L28

Chain W:



• Molecule 28: 50S ribosomal protein L29

Chain X:

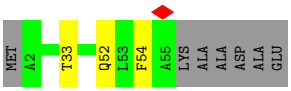


• Molecule 29: 50S ribosomal protein L30

Chain Y:

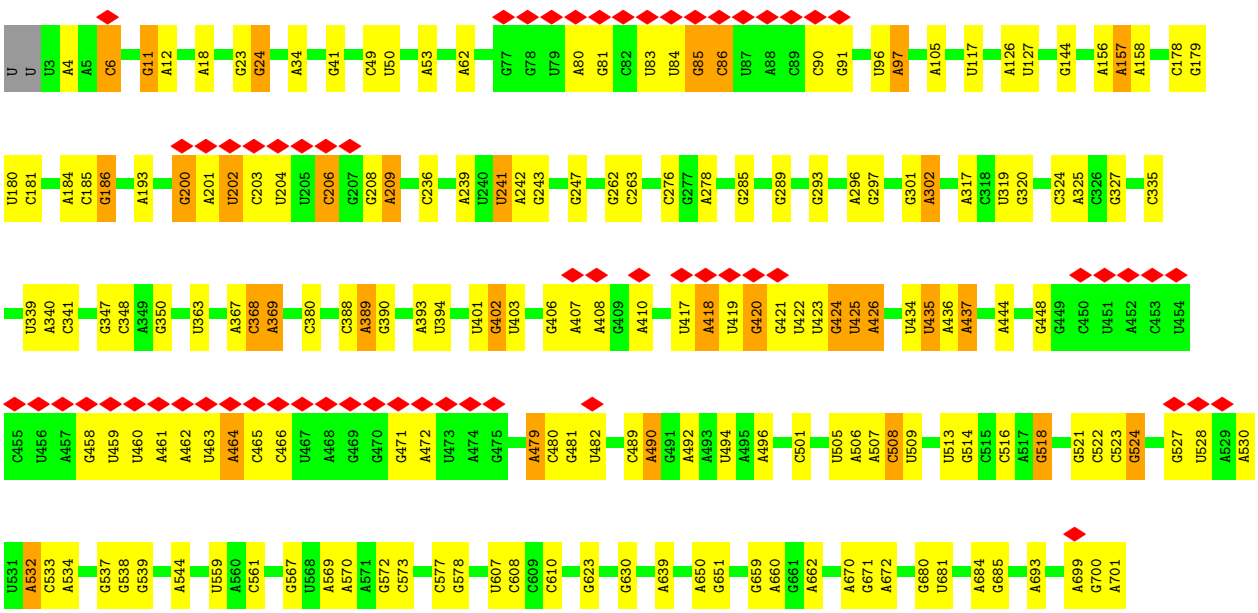
• Molecule 30: 50S ribosomal protein L32

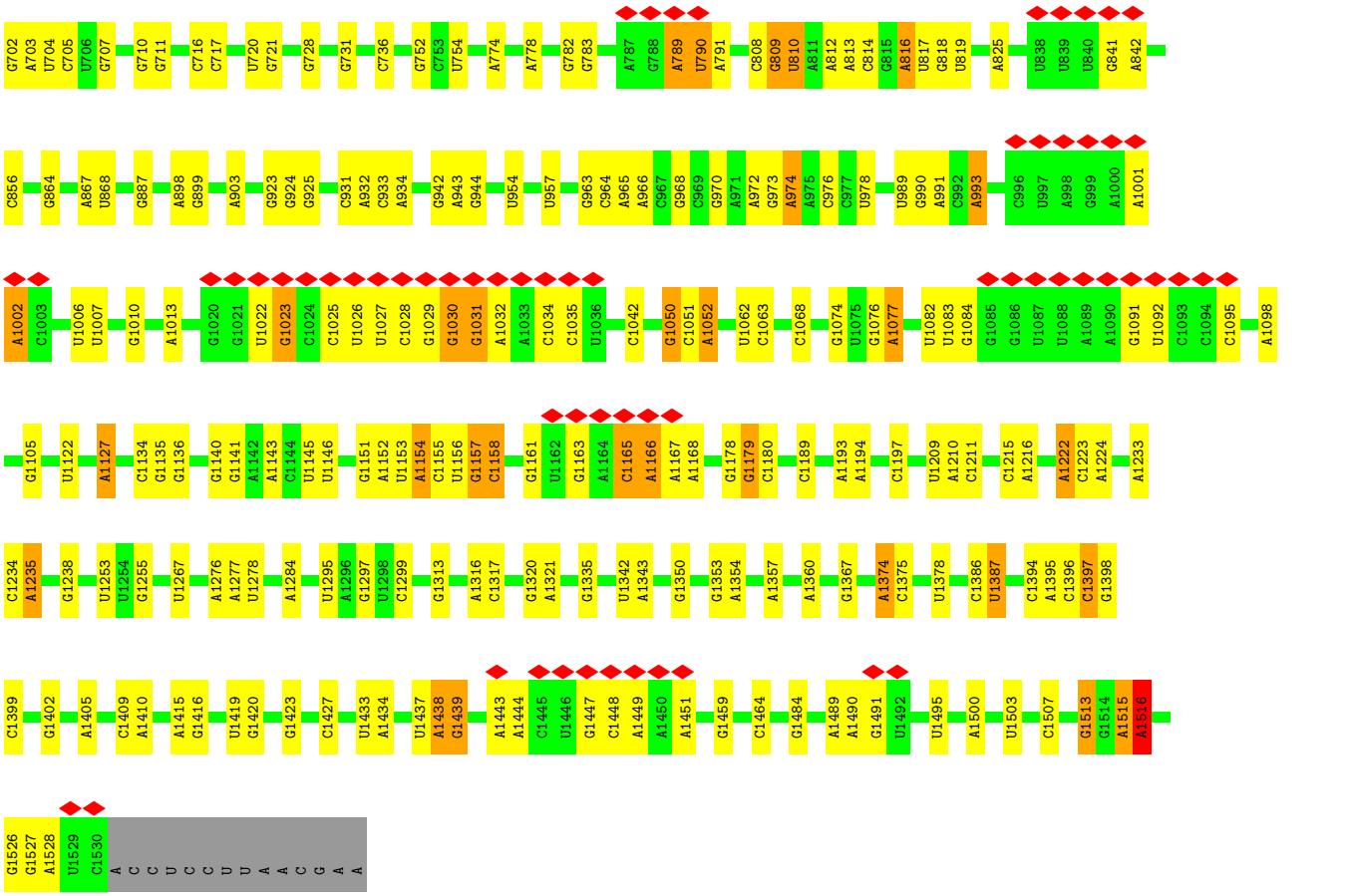
Chain Z:



• Molecule 31: 16S Ribosomal RNA

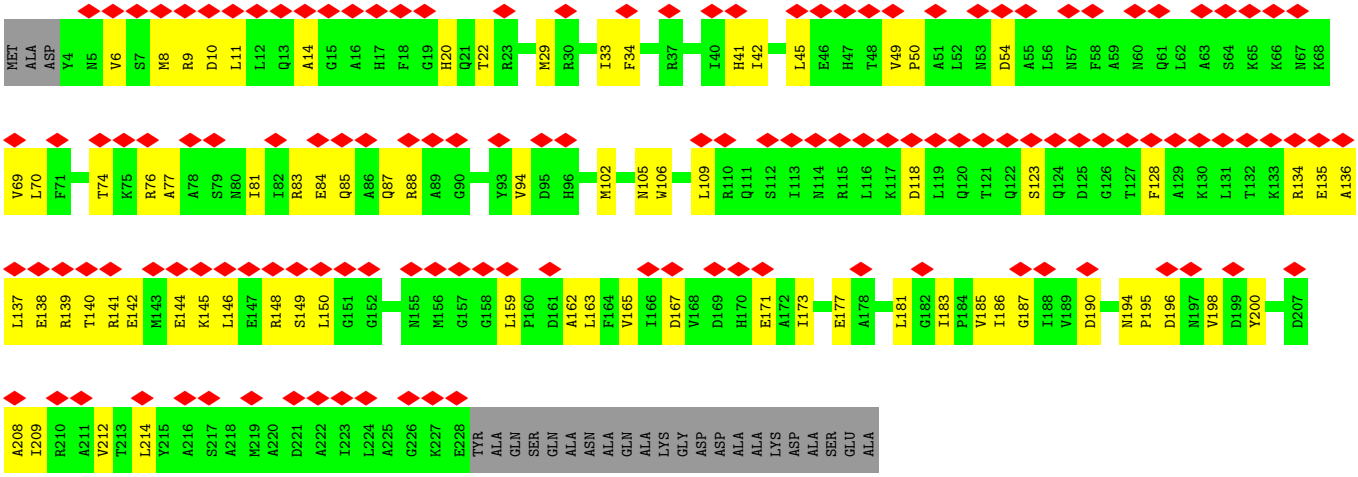
Chain a:





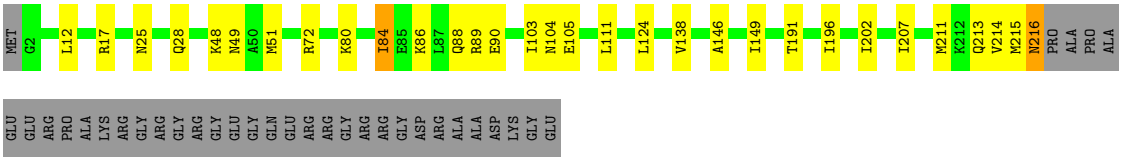
- Molecule 32: 30S ribosomal protein S2

Chain b:



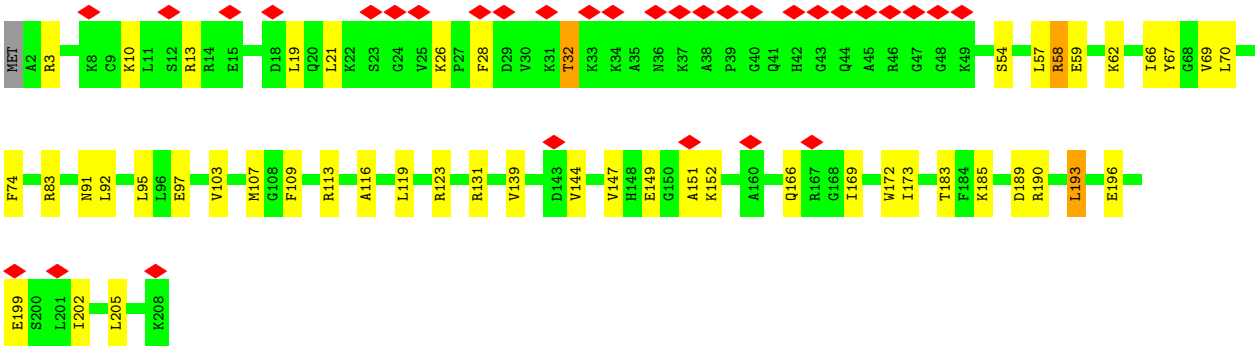
- Molecule 33: 30S ribosomal protein S3

Chain c:



- Molecule 34: 30S ribosomal protein S4

Chain d:

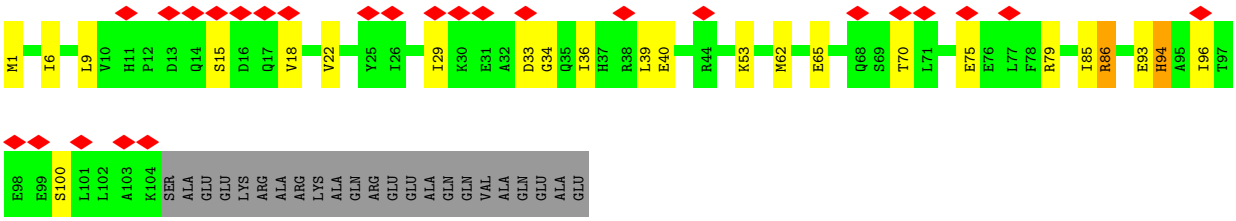


- Molecule 35: 30S ribosomal protein S5

Chain e:

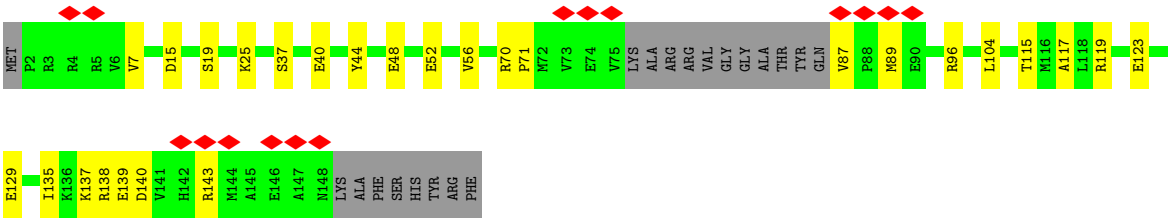
- Molecule 36: 30S ribosomal protein S6

Chain f:



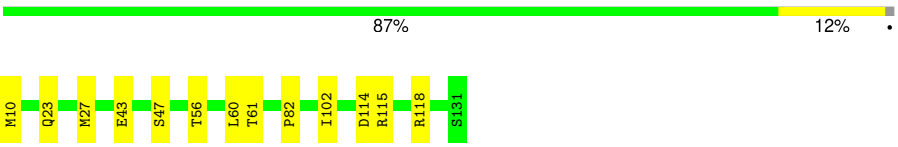
- Molecule 37: 30S ribosomal protein S7

Chain g:



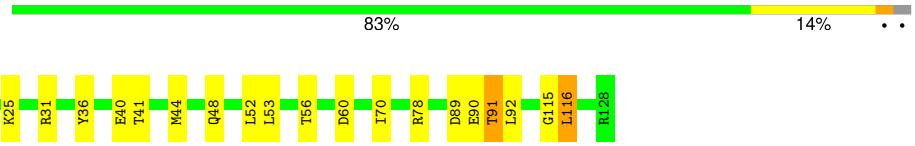
- Molecule 38: 30S ribosomal protein S8

Chain h:



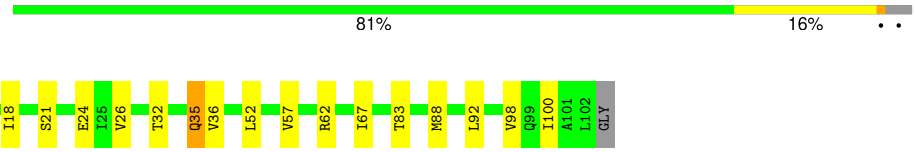
- Molecule 39: 30S ribosomal protein S9

Chain i:



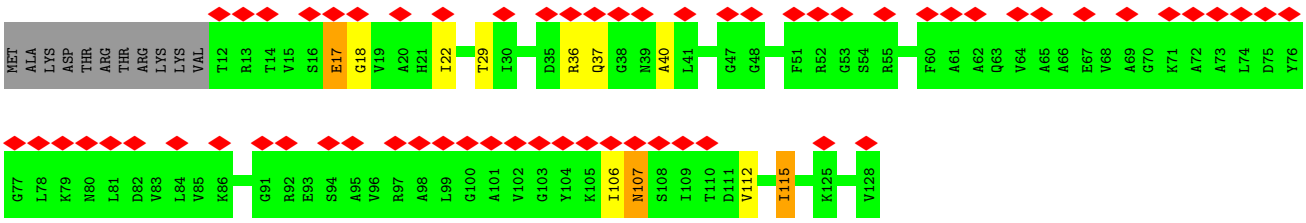
- Molecule 40: 30S ribosomal protein S10

Chain j:



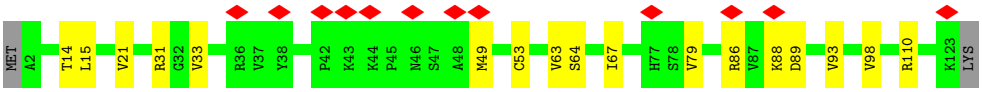
- Molecule 41: 30S ribosomal protein S11

Chain k:



- Molecule 42: 30S ribosomal protein S12

Chain l:

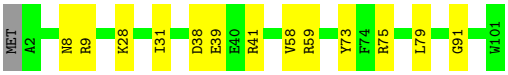


- Molecule 43: 30S ribosomal protein S13

Chain m:

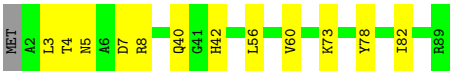
- Molecule 44: 30S ribosomal protein S14

Chain n:



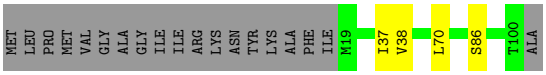
• Molecule 45: 30S ribosomal protein S15

Chain o:



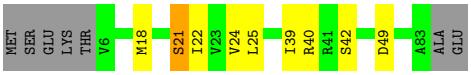
• Molecule 46: 30S ribosomal protein S16

Chain p:



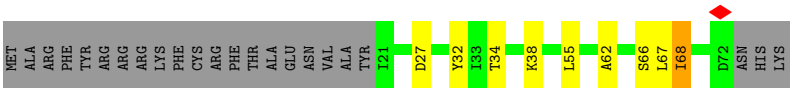
• Molecule 47: 30S ribosomal protein S17

Chain q:



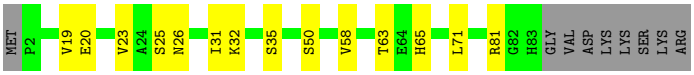
• Molecule 48: 30S ribosomal protein S18

Chain r:



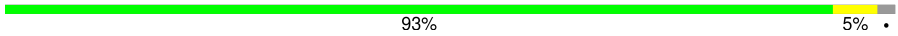
• Molecule 49: 30S ribosomal protein S19

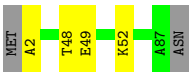
Chain s:



• Molecule 50: 30S ribosomal protein S20

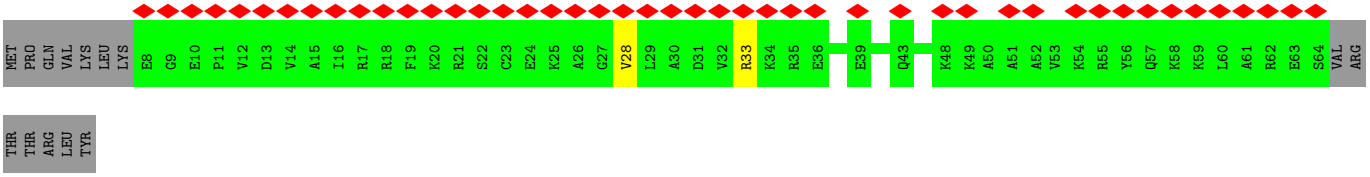
Chain t:





• Molecule 51: 30S ribosomal protein S21

Chain u:


MET
PRO
GLN
VAL
LYS
LEU
LYS
E8
G9
E10
P11
V12
D13
V14
A15
I16
R17
R18
F19
K20
R21
S22
C23
E24
K25
A26
G27
V28
L29
A30
D31
V32
R33
K34
R35
E36
E39
Q43
K48
K49
A50
A51
A52
V53
K54
R55
Y56
Q57
K58
K59
L60
A61
R62
E63
S64
VAL
ARG
THR
THR
ARG
LEU
TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127249	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.823	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	557.568, 557.568, 557.568	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.089, 1.089, 1.089	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: UR3, 7MG, ZN, MA6, 2MA, 5MU, 4OC, 5MC, OMU, PSU, OMG, MG, 80P, 2MG, 6MZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.15	0/407	0.37	0/540
2	1	0.15	0/367	0.29	0/481
3	2	0.13	0/515	0.39	0/678
4	3	0.16	0/296	0.34	0/389
5	A	0.10	0/64227	0.27	0/100172
6	B	0.08	0/2739	0.23	0/4266
7	C	0.13	0/2144	0.35	0/2880
8	D	0.13	0/1590	0.30	0/2142
9	E	0.13	0/1537	0.31	0/2073
10	F	0.22	0/1390	0.53	1/1863 (0.1%)
11	G	0.13	0/1337	0.32	0/1807
12	H	0.15	0/461	0.37	0/616
13	I	0.12	0/1143	0.31	0/1541
14	J	0.14	0/956	0.34	0/1286
15	K	0.12	0/1079	0.30	0/1439
16	L	0.13	0/1104	0.30	0/1475
17	M	0.15	0/956	0.33	0/1282
18	N	0.11	0/865	0.28	0/1156
19	O	0.13	0/925	0.33	0/1241
20	P	0.14	0/947	0.31	0/1262
21	Q	0.13	0/818	0.30	0/1094
22	R	0.14	0/831	0.31	0/1113
23	S	0.14	0/716	0.32	0/957
24	T	0.11	0/770	0.29	0/1034
25	U	0.12	0/770	0.31	0/1036
26	V	0.11	0/589	0.29	0/788
27	W	0.12	0/642	0.29	0/856
28	X	0.11	0/487	0.27	0/646
29	Y	0.16	0/468	0.34	0/624
30	Z	0.12	0/453	0.27	0/604
31	a	0.14	0/36476	0.29	0/56895
32	b	0.18	0/1799	0.50	0/2429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.18	0/1714	0.39	0/2304
34	d	0.17	0/1653	0.44	0/2213
35	e	0.14	0/1141	0.35	0/1537
36	f	0.14	0/882	0.32	0/1189
37	g	0.16	0/1087	0.39	0/1456
38	h	0.13	0/993	0.33	0/1331
39	i	0.18	0/1002	0.37	0/1339
40	j	0.17	0/811	0.38	0/1096
41	k	0.12	0/878	0.30	0/1189
42	l	0.15	0/958	0.36	0/1284
43	m	0.17	0/913	0.40	0/1226
44	n	0.18	0/803	0.40	0/1071
45	o	0.15	0/715	0.35	0/958
46	p	0.13	0/655	0.36	0/879
47	q	0.13	0/621	0.34	0/837
48	r	0.12	0/432	0.30	0/583
49	s	0.16	0/664	0.33	0/897
50	t	0.18	0/669	0.34	0/892
51	u	0.10	0/478	0.20	0/631
All	All	0.13	0/146873	0.30	1/219577 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
34	d	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	102	ARG	CB-CG-CD	5.93	124.94	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	d	58	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	400	0	425	2	0
2	1	363	0	401	3	0
3	2	509	0	566	7	0
4	3	295	0	326	6	0
5	A	57610	0	28970	201	0
6	B	2450	0	1241	17	0
7	C	2104	0	2168	15	0
8	D	1572	0	1610	9	0
9	E	1516	0	1569	11	0
10	F	1370	0	1420	76	0
11	G	1318	0	1373	10	0
12	H	458	0	480	0	0
13	I	1117	0	1136	5	0
14	J	946	0	1007	13	0
15	K	1071	0	1141	7	0
16	L	1087	0	1162	10	0
17	M	942	0	987	1	0
18	N	857	0	899	6	0
19	O	913	0	968	8	0
20	P	934	0	997	2	0
21	Q	807	0	842	2	0
22	R	826	0	894	2	0
23	S	710	0	768	6	0
24	T	766	0	816	10	0
25	U	760	0	783	7	0
26	V	581	0	583	2	0
27	W	632	0	667	4	0
28	X	486	0	528	6	0
29	Y	463	0	488	9	0
30	Z	447	0	435	1	0
31	a	32782	0	16508	156	0
32	b	1769	0	1787	66	0
33	c	1690	0	1774	23	0
34	d	1631	0	1691	41	0
35	e	1129	0	1174	19	0
36	f	867	0	868	17	0
37	g	1073	0	1118	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	985	0	1047	11	0
39	i	991	0	1048	13	0
40	j	801	0	832	8	0
41	k	862	0	877	8	0
42	l	945	0	998	12	0
43	m	903	0	962	13	0
44	n	792	0	833	11	0
45	o	705	0	712	7	0
46	p	644	0	655	1	0
47	q	614	0	658	5	0
48	r	426	0	447	8	0
49	s	646	0	663	5	0
50	t	663	0	715	4	0
51	u	473	0	503	1	0
52	3	1	0	0	0	0
53	a	123	0	0	1	0
54	a	4	0	0	0	0
All	All	135829	0	91520	841	0

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

All (841) 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)
11:G:86:LYS:NZ	11:G:165:SER:OG	1.91	1.01
5:A:67:G:O2'	5:A:69:U:OP2	1.89	0.91
5:A:1563:C:O2	5:A:1564:A:O2'	1.88	0.90
31:a:518:G:HO2'	31:a:533:C:HO2'	1.21	0.89
5:A:1880:G:O2'	5:A:1881:A:OP1	1.92	0.87
5:A:1519:U:O2'	5:A:1520:A:OP2	1.92	0.87
31:a:1402:G:O2'	31:a:1515:MA6:O2'	1.88	0.87
43:m:78:LYS:NZ	43:m:82:ASP:OD1	2.06	0.86
5:A:843:G:OP2	5:A:843:G:N2	2.09	0.86
31:a:1163:G:N2	31:a:1167:A:OP2	2.09	0.86
5:A:1962:A:N3	5:A:2588:G:O2'	2.06	0.85
31:a:1402:G:HO2'	31:a:1515:MA6:HO2'	1.16	0.84
32:b:11:LEU:HD13	32:b:45:LEU:HD12	1.56	0.84
5:A:2254:C:O2'	5:A:2423:C:OP2	1.95	0.84
5:A:1517:G:OP2	5:A:1518:A:O2'	1.96	0.84
10:F:31:ILE:HG21	10:F:96:MET:HE1	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1030:G:O2'	31:a:1031:G:O4'	1.97	0.82
37:g:70:ARG:O	37:g:138:ARG:NH1	2.12	0.82
10:F:147:ASP:OD2	10:F:150:ARG:NH2	2.13	0.80
7:C:266:MET:HE2	7:C:266:MET:HA	1.62	0.80
10:F:115:ARG:O	10:F:115:ARG:NH1	2.15	0.80
31:a:425:U:OP1	34:d:10:LYS:NZ	2.14	0.79
35:e:110:MET:HE2	35:e:126:CYS:SG	2.23	0.79
31:a:1157:G:O6	31:a:1179:G:O6	2.02	0.78
8:D:58:GLU:OE2	8:D:66:LYS:NZ	2.16	0.78
42:l:53:CYS:SG	42:l:67:ILE:HD11	2.24	0.78
31:a:1074:G:N2	31:a:1077:A:OP2	2.17	0.77
31:a:200:G:O6	31:a:209:A:N6	2.15	0.77
10:F:136:ILE:O	10:F:137:VAL:HG22	1.84	0.77
4:3:33:HIS:O	4:3:35:GLN:NE2	2.18	0.76
5:A:1749:G:N2	5:A:1752:G:OP2	2.17	0.76
5:A:1869:G:O2'	5:A:1870:C:O5'	2.04	0.76
1:0:1:MET:SD	1:0:2:ARG:N	2.60	0.75
6:B:11:A:N1	6:B:67:G:O2'	2.19	0.75
10:F:34:ILE:HG23	10:F:156:ILE:HD13	1.68	0.75
5:A:533:U:O2'	20:P:49:ASP:OD2	2.00	0.75
8:D:30:VAL:O	8:D:188:SER:OG	2.02	0.74
6:B:86:U:O2'	6:B:87:A:OP2	2.05	0.74
24:T:79:ASP:OD1	24:T:80:ARG:N	2.21	0.74
37:g:140:ASP:OD1	37:g:143:ARG:NH2	2.21	0.73
5:A:537:A:N6	5:A:553:G:O2'	2.21	0.73
6:B:22:G:O6	6:B:54:G:O2'	2.06	0.73
33:c:48:LYS:NZ	33:c:49:ASN:OD1	2.18	0.73
5:A:2301:U:O5'	10:F:133:LYS:NZ	2.21	0.72
31:a:693:A:N3	31:a:783:G:O2'	2.17	0.72
32:b:163:LEU:HD23	32:b:183:ILE:HD13	1.72	0.72
5:A:2373:A:O2'	18:N:116:PHE:OXT	2.01	0.72
9:E:20:ARG:O	9:E:113:ARG:NH2	2.23	0.72
31:a:567:G:O3'	31:a:816:A:O2'	2.08	0.71
35:e:31:SER:OG	35:e:52:ALA:O	2.06	0.71
39:i:48:GLN:OE1	39:i:78:ARG:NH1	2.24	0.71
10:F:8:TYR:HA	10:F:12:LEU:HD23	1.70	0.71
32:b:22:THR:HG22	32:b:41:HIS:CE1	2.26	0.71
35:e:98:ALA:HB3	35:e:102:THR:HG21	1.71	0.70
6:B:11:A:O2'	6:B:13:A:OP2	2.09	0.70
31:a:1025:C:O2	31:a:1031:G:N2	2.25	0.70
31:a:993:A:N1	31:a:1042:C:O2'	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1438:A:O2'	31:a:1439:G:O5'	2.10	0.69
32:b:49:VAL:HG13	32:b:50:PRO:HD3	1.74	0.69
10:F:162:THR:HG23	10:F:164:ASP:OD2	1.93	0.68
5:A:184:G:N2	5:A:184:G:OP2	2.25	0.68
10:F:50:LEU:O	10:F:54:VAL:HG12	1.93	0.68
34:d:147:VAL:HG12	34:d:151:ALA:HB3	1.75	0.68
31:a:1386:C:O2'	31:a:1387:U:OP1	2.10	0.68
32:b:194:ASN:ND2	32:b:196:ASP:OD1	2.22	0.68
45:o:3:LEU:O	45:o:8:ARG:NH2	2.26	0.67
33:c:51:MET:SD	33:c:72:ARG:NH1	2.68	0.67
4:3:19:ARG:NE	5:A:2752:U:OP2	2.26	0.67
10:F:31:ILE:CG2	10:F:96:MET:HE1	2.24	0.67
5:A:1937:C:N4	5:A:1961:C:O4'	2.28	0.67
29:Y:3:THR:OG1	29:Y:36:GLU:OE2	2.12	0.66
32:b:102:MET:HE2	32:b:102:MET:HA	1.77	0.66
5:A:2401:G:O2'	5:A:2408:A:N6	2.27	0.66
30:Z:52:GLN:NE2	30:Z:54:PHE:O	2.28	0.66
5:A:2591:G:N2	5:A:2594:A:OP2	2.26	0.66
10:F:22:ILE:HD12	10:F:22:ILE:O	1.95	0.66
32:b:135:GLU:N	32:b:135:GLU:OE1	2.29	0.66
33:c:25:ASN:ND2	33:c:28:GLN:OE1	2.29	0.66
10:F:140:GLU:N	10:F:140:GLU:OE2	2.28	0.66
37:g:40:GLU:OE2	39:i:41:THR:HG21	1.96	0.66
5:A:2795:A:O2'	5:A:2797:G:OP2	2.14	0.65
31:a:507:A:O2'	31:a:539:G:O2'	2.13	0.65
34:d:62:LYS:O	34:d:66:ILE:HG13	1.96	0.65
35:e:98:ALA:CB	35:e:102:THR:HG21	2.25	0.65
34:d:196:GLU:N	34:d:196:GLU:OE2	2.29	0.65
49:s:19:VAL:O	49:s:23:VAL:HG23	1.97	0.65
5:A:2027:A:N3	5:A:2451:G:O2'	2.30	0.65
23:S:17:GLU:O	23:S:21:VAL:HG23	1.97	0.65
35:e:130:THR:HG22	35:e:130:THR:O	1.96	0.65
5:A:978:A:OP2	5:A:979:C:N4	2.30	0.65
11:G:15:VAL:HG11	11:G:79:VAL:HG23	1.79	0.65
4:3:18:ARG:NH1	4:3:23:ILE:HD11	2.12	0.64
31:a:435:U:O4	31:a:436:A:N6	2.31	0.64
31:a:610:C:OP1	34:d:83:ARG:NH1	2.31	0.64
13:I:70:LEU:HD23	13:I:90:GLU:OE1	1.97	0.64
31:a:1513:G:N1	31:a:1516:MA6:OP2	2.29	0.64
5:A:1310:C:O2'	5:A:1387:A:N3	2.30	0.64
23:S:1:MET:HE1	23:S:41:GLU:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:138:GLU:O	32:b:142:GLU:OE2	2.16	0.63
36:f:1:MET:HE3	36:f:1:MET:N	2.13	0.63
7:C:5:LYS:NZ	7:C:6:CYS:O	2.24	0.63
7:C:175:ARG:HH11	7:C:175:ARG:HG2	1.64	0.63
31:a:1163:G:O2'	31:a:1167:A:N6	2.32	0.63
9:E:118:VAL:CG2	9:E:186:VAL:HG22	2.29	0.63
5:A:2631:U:O2'	8:D:82:GLU:OE2	2.16	0.63
5:A:2655:G:N2	5:A:2658:A:OP2	2.31	0.62
3:2:31:ILE:O	3:2:35:LYS:NZ	2.26	0.62
5:A:1411:G:N2	5:A:1583:C:H42	1.98	0.62
5:A:1531:C:O2'	5:A:1533:U:O4	2.17	0.62
34:d:123:ARG:O	34:d:131:ARG:NH1	2.32	0.62
10:F:34:ILE:HG23	10:F:156:ILE:CD1	2.29	0.62
32:b:29:MET:HE1	32:b:195:PRO:CG	2.28	0.62
32:b:77:ALA:HB1	32:b:209:ILE:CD1	2.30	0.62
31:a:347:G:OP1	50:t:2:ALA:HB2	2.00	0.62
31:a:991:A:N3	44:n:8:ASN:ND2	2.48	0.62
31:a:978:U:OP1	44:n:9:ARG:NH1	2.31	0.62
5:A:1605:G:N2	5:A:1605:G:OP2	2.32	0.62
5:A:2528:G:N2	5:A:2659:G:O2'	2.33	0.62
10:F:46:ASP:OD2	10:F:49:LEU:HD22	2.00	0.61
15:K:2:THR:N	15:K:7:GLU:OE2	2.33	0.61
16:L:57:ARG:NH1	16:L:116:GLU:OE2	2.33	0.61
10:F:152:MET:HE3	10:F:153:ASP:H	1.66	0.61
32:b:139:ARG:HA	32:b:142:GLU:OE2	2.00	0.61
31:a:524:7MG:O2'	31:a:532:A:N1	2.34	0.61
32:b:8:MET:HA	32:b:11:LEU:HD12	1.83	0.61
34:d:149:GLU:OE1	34:d:152:LYS:NZ	2.34	0.61
36:f:75:GLU:OE1	36:f:79:ARG:NH2	2.34	0.61
40:j:100:ILE:HD12	40:j:100:ILE:N	2.16	0.61
31:a:1002:A:N3	31:a:1034:C:O2'	2.33	0.61
16:L:58:ILE:HD12	16:L:60:ARG:H	1.65	0.60
16:L:79:LEU:HD12	16:L:80:GLU:N	2.17	0.60
36:f:1:MET:HE3	36:f:1:MET:H1	1.66	0.60
10:F:110:ARG:O	10:F:112:ARG:NH2	2.34	0.60
34:d:28:PHE:O	34:d:32:THR:HG22	2.01	0.60
17:M:86:ARG:NH1	17:M:117:ASP:O	2.34	0.60
31:a:954:U:OP1	49:s:81:ARG:NH1	2.34	0.60
6:B:41:C:O2	10:F:92:ARG:NH1	2.35	0.60
10:F:43:ALA:HA	10:F:49:LEU:HD21	1.83	0.60
34:d:169:ILE:HD12	34:d:169:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:30:HIS:NE2	5:A:2388:A:OP2	2.28	0.60
5:A:2301:U:N3	5:A:2303:G:O6	2.34	0.60
10:F:33:LYS:NZ	10:F:157:THR:OG1	2.17	0.60
5:A:1522:C:O2	5:A:1543:A:N6	2.35	0.60
29:Y:23:LEU:HD11	29:Y:53:MET:CE	2.32	0.60
5:A:1256:C:OP2	22:R:83:LYS:NZ	2.34	0.60
5:A:2518:U:O2'	5:A:2643:U:OP1	2.18	0.60
6:B:46:U:OP2	18:N:31:ARG:NH2	2.35	0.60
31:a:11:G:OP1	35:e:107:GLY:N	2.35	0.60
10:F:170:MET:SD	10:F:170:MET:N	2.76	0.59
10:F:38:MET:HE3	10:F:38:MET:N	2.18	0.59
26:V:70:GLU:OE1	26:V:81:LYS:NZ	2.35	0.59
41:k:115:ILE:HD11	51:u:28:VAL:HG13	1.85	0.59
5:A:2299:G:O2'	10:F:129:SER:OG	2.17	0.59
7:C:183:LYS:HG2	7:C:268:ILE:HD11	1.83	0.59
34:d:147:VAL:CG1	34:d:151:ALA:HB3	2.32	0.59
40:j:92:LEU:HD12	40:j:98:VAL:HG21	1.84	0.59
43:m:15:ALA:HA	43:m:45:ILE:HD11	1.85	0.59
5:A:1173:G:O2'	5:A:1174:U:O5'	2.20	0.59
5:A:2551:U:O2'	5:A:2552:C:O5'	2.21	0.59
6:B:12:U:OP2	6:B:68:C:O2'	2.20	0.59
7:C:183:LYS:CG	7:C:268:ILE:HD11	2.33	0.59
31:a:514:G:O2'	31:a:516:C:N3	2.32	0.59
31:a:523:C:OP2	42:l:88:LYS:NZ	2.36	0.59
10:F:67:VAL:HG12	10:F:84:PRO:HB3	1.85	0.58
25:U:52:VAL:O	25:U:56:GLU:OE1	2.19	0.58
10:F:132:LEU:HD21	10:F:137:VAL:CG2	2.33	0.58
14:J:49:ARG:NH2	31:a:1420:G:OP1	2.36	0.58
32:b:70:LEU:HD12	32:b:163:LEU:CD1	2.33	0.58
5:A:1718:A:N6	5:A:1734:G:O2'	2.35	0.58
5:A:2861:U:OP2	5:A:2862:G:O2'	2.12	0.58
31:a:808:C:O2'	31:a:898:A:N1	2.36	0.58
32:b:105:ASN:O	32:b:109:LEU:HD23	2.03	0.58
35:e:59:ILE:O	35:e:63:LEU:HD12	2.02	0.58
34:d:169:ILE:HD12	34:d:169:ILE:C	2.27	0.58
31:a:1077:A:H5"	35:e:20:VAL:HG11	1.86	0.58
31:a:507:A:HO2'	31:a:539:G:HO2'	1.47	0.58
43:m:3:ARG:O	43:m:57:ARG:NH1	2.37	0.58
5:A:2310:A:H4'	10:F:33:LYS:HZ1	1.68	0.58
10:F:93:GLY:O	10:F:96:MET:HG3	2.04	0.58
18:N:32:THR:HG22	18:N:33:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1489:A:H2'	31:a:1490:A:O4'	2.04	0.58
31:a:327:G:O2'	50:t:2:ALA:HB1	2.04	0.57
5:A:2371:G:N2	5:A:2374:A:OP2	2.35	0.57
35:e:12:GLU:HG2	35:e:38:VAL:HG12	1.85	0.57
23:S:5:ARG:O	23:S:9:VAL:HG23	2.03	0.57
45:o:4:THR:HG22	45:o:7:ASP:OD2	2.05	0.57
5:A:1111:C:N4	5:A:1112:G:O6	2.38	0.57
5:A:1413:G:H1'	5:A:1578:A:H61	1.68	0.57
35:e:130:THR:O	35:e:130:THR:CG2	2.52	0.57
5:A:2551:U:O2'	5:A:2552:C:O4'	2.21	0.57
10:F:136:ILE:C	10:F:137:VAL:HG13	2.30	0.57
39:i:52:LEU:HD23	39:i:53:LEU:HD12	1.87	0.57
16:L:58:ILE:HD12	16:L:60:ARG:N	2.20	0.57
31:a:572:G:O2'	31:a:818:G:OP2	2.11	0.57
31:a:964:5MC:OP2	31:a:965:A:O2'	2.20	0.57
32:b:33:ILE:HD11	32:b:41:HIS:ND1	2.20	0.57
5:A:1373:A:O2'	5:A:1374:U:OP2	2.20	0.56
31:a:1050:G:H4'	31:a:1051:C:H3'	1.86	0.56
31:a:710:G:H2'	31:a:711:G:C8	2.40	0.56
31:a:716:C:OP2	31:a:717:C:N4	2.38	0.56
31:a:1092:U:OP2	31:a:1105:G:N1	2.36	0.56
32:b:41:HIS:C	32:b:42:ILE:HD13	2.30	0.56
5:A:2026:6MZ:O2'	5:A:2027:A:OP2	2.20	0.56
31:a:670:A:H2'	31:a:671:G:C8	2.41	0.56
34:d:19:LEU:HB3	34:d:21:LEU:HD13	1.87	0.56
5:A:1860:U:OP1	5:A:2406:G:O2'	2.22	0.56
31:a:789:A:O2'	31:a:790:U:OP2	2.17	0.56
31:a:809:G:O2'	31:a:810:U:OP2	2.24	0.56
31:a:156:A:N6	31:a:339:U:O2'	2.39	0.56
34:d:107:MET:HG2	34:d:109:PHE:CD1	2.41	0.56
32:b:29:MET:HE1	32:b:195:PRO:HG3	1.88	0.55
24:T:79:ASP:OD2	24:T:96:SER:OG	2.12	0.55
44:n:38:ASP:OD2	44:n:39:GLU:N	2.39	0.55
48:r:67:LEU:C	48:r:68:ILE:HD13	2.32	0.55
31:a:242:A:C2	31:a:278:A:C5	2.95	0.55
32:b:83:ARG:NH1	32:b:87:GLN:HB2	2.22	0.55
35:e:55:VAL:O	35:e:59:ILE:HG13	2.07	0.55
48:r:27:ASP:N	48:r:27:ASP:OD1	2.37	0.55
13:I:61:GLN:O	13:I:63:GLN:NE2	2.40	0.55
31:a:85:G:O2'	31:a:86:C:OP2	2.16	0.55
31:a:1374:A:C6	37:g:7:VAL:HG11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:43:GLU:HG2	38:h:102:ILE:HG21	1.88	0.55
40:j:88:MET:N	40:j:88:MET:HE3	2.22	0.55
11:G:20:ASN:ND2	11:G:25:GLU:OE2	2.39	0.55
19:O:65:ARG:NH1	19:O:74:GLU:OE2	2.38	0.54
49:s:25:SER:OG	49:s:26:ASN:N	2.40	0.54
5:A:364:A:OP2	5:A:424:G:O2'	2.24	0.54
10:F:35:THR:HG22	10:F:155:THR:HB	1.89	0.54
37:g:135:ILE:O	37:g:139:GLU:HG3	2.08	0.54
38:h:10:MET:SD	38:h:27:MET:HE1	2.48	0.54
38:h:114:ASP:OD2	38:h:118:ARG:NH2	2.41	0.54
5:A:2753:A:N1	11:G:67:THR:HG21	2.22	0.54
31:a:1374:A:C5	37:g:7:VAL:HG11	2.43	0.54
5:A:929:C:O2'	5:A:930:U:O5'	2.23	0.54
5:A:1182:G:N2	5:A:1183:U:O4	2.40	0.54
14:J:50:ALA:O	14:J:53:LYS:NZ	2.40	0.54
31:a:6:C:H42	31:a:610:C:H5"	1.73	0.54
33:c:84:ILE:HD11	33:c:103:ILE:HD11	1.90	0.54
6:B:12:U:O3'	6:B:104:U:O2'	2.26	0.54
45:o:56:LEU:O	45:o:60:VAL:HG23	2.08	0.54
24:T:50:THR:O	24:T:50:THR:HG22	2.08	0.54
31:a:12:A:OP2	35:e:130:THR:HG21	2.08	0.54
31:a:458:G:N2	31:a:464:A:H61	2.06	0.54
5:A:308:U:H2'	5:A:309:G:O4'	2.09	0.53
31:a:1490:A:HO2'	31:a:1491:G:C5'	2.21	0.53
9:E:15:GLU:O	9:E:19:GLY:N	2.41	0.53
10:F:90:THR:C	10:F:91:LEU:HD12	2.33	0.53
16:L:78:PRO:O	16:L:79:LEU:CB	2.55	0.53
4:3:32:ARG:NH1	5:A:2472:A:N3	2.57	0.53
5:A:798:U:H4'	5:A:799:G:OP1	2.08	0.53
5:A:2071:U:OP2	5:A:2234:G:O2'	2.24	0.53
10:F:133:LYS:HE2	10:F:133:LYS:N	2.23	0.53
5:A:1462:G:OP2	5:A:1544:G:O2'	2.24	0.53
42:l:15:LEU:H	42:l:15:LEU:HD23	1.74	0.53
10:F:110:ARG:NH2	10:F:137:VAL:HB	2.23	0.53
16:L:30:GLY:O	16:L:134:ARG:NH2	2.42	0.53
32:b:163:LEU:HB2	32:b:185:VAL:HG22	1.90	0.53
5:A:782:G:H5'	5:A:783:G:OP1	2.09	0.53
5:A:1717:G:O2'	5:A:1735:A:N6	2.42	0.53
29:Y:23:LEU:HD11	29:Y:53:MET:HE2	1.90	0.53
32:b:33:ILE:HD11	32:b:41:HIS:CE1	2.44	0.53
31:a:185:C:H1'	31:a:186:G:OP2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:91:ASN:O	34:d:95:LEU:HG	2.09	0.52
31:a:887:G:O2'	31:a:903:A:N6	2.42	0.52
34:d:116:ALA:HA	34:d:119:LEU:HD12	1.91	0.52
5:A:1816:U:HO2'	7:C:157:SER:HG	1.54	0.52
31:a:1031:G:O2'	31:a:1032:A:O5'	2.19	0.52
5:A:854:G:H2'	5:A:855:G:C8	2.44	0.52
9:E:118:VAL:HG21	9:E:186:VAL:HG22	1.92	0.52
5:A:2485:U:O2'	5:A:2487:U:O4	2.25	0.52
25:U:71:ASP:OD1	25:U:71:ASP:N	2.40	0.52
31:a:204:U:O2'	31:a:206:C:OP1	2.27	0.52
32:b:50:PRO:O	32:b:54:ASP:OD1	2.28	0.52
32:b:74:THR:OG1	32:b:171:GLU:OE2	2.19	0.52
5:A:552:U:H2'	5:A:553:G:O4'	2.09	0.52
5:A:2298:U:O2'	10:F:123:ASP:O	2.22	0.52
10:F:34:ILE:CD1	10:F:96:MET:HB2	2.39	0.52
16:L:79:LEU:HD12	16:L:80:GLU:H	1.74	0.52
19:O:5:HIS:O	19:O:9:GLN:HG3	2.10	0.52
10:F:164:ASP:OD2	10:F:165:GLU:N	2.43	0.52
32:b:84:GLU:O	32:b:88:ARG:HD3	2.10	0.52
34:d:67:TYR:OH	34:d:97:GLU:OE2	2.28	0.52
28:X:18:LEU:HB2	28:X:53:ILE:HG21	1.91	0.52
31:a:1438:A:O2'	31:a:1439:G:C8	2.62	0.52
32:b:76:ARG:HB2	32:b:76:ARG:NH1	2.25	0.52
33:c:138:VAL:HG13	33:c:149:ILE:CG2	2.39	0.51
5:A:929:C:HO2'	5:A:930:U:P	2.33	0.51
19:O:27:ASP:OD1	19:O:27:ASP:N	2.43	0.51
24:T:64:HIS:ND1	24:T:66:SER:OG	2.43	0.51
31:a:707:G:OP1	36:f:53:LYS:NZ	2.43	0.51
32:b:20:HIS:ND1	32:b:190:ASP:OD1	2.43	0.51
5:A:254:G:OP2	5:A:256:C:N4	2.33	0.51
5:A:499:G:N1	5:A:502:A:OP2	2.43	0.51
5:A:1044:G:N1	5:A:1107:G:N7	2.58	0.51
34:d:92:LEU:C	34:d:92:LEU:HD23	2.35	0.51
44:n:28:LYS:HA	44:n:31:ILE:HD12	1.91	0.51
31:a:202:U:N3	31:a:208:G:O6	2.43	0.51
32:b:118:ASP:C	32:b:118:ASP:OD1	2.54	0.51
31:a:388:C:O3'	31:a:480:C:O2'	2.27	0.51
32:b:183:ILE:C	32:b:183:ILE:HD12	2.36	0.51
39:i:25:LYS:N	39:i:60:ASP:OD2	2.42	0.51
31:a:406:G:OP1	34:d:26:LYS:NZ	2.43	0.51
32:b:70:LEU:HD12	32:b:163:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:141:ARG:O	32:b:144:GLU:HG3	2.11	0.51
36:f:62:MET:SD	36:f:62:MET:N	2.84	0.51
50:t:48:THR:O	50:t:52:LYS:HG3	2.11	0.51
5:A:1044:G:H2'	5:A:1108:A:H61	1.76	0.51
42:l:49:MET:SD	42:l:49:MET:N	2.84	0.51
10:F:108:ILE:HG22	10:F:109:PRO:HD3	1.93	0.51
32:b:22:THR:HG22	32:b:41:HIS:NE2	2.25	0.51
5:A:1006:A:N3	5:A:1151:C:O2'	2.41	0.51
5:A:1816:U:H4'	5:A:1817:A:OP2	2.10	0.51
35:e:12:GLU:CG	35:e:38:VAL:HG12	2.40	0.51
5:A:1853:G:N2	5:A:1880:G:N3	2.60	0.50
10:F:158:THR:HG21	10:F:169:LEU:HD23	1.93	0.50
18:N:110:ARG:NH1	18:N:116:PHE:O	2.44	0.50
31:a:424:G:H3'	34:d:10:LYS:NZ	2.26	0.50
5:A:363:G:OP2	5:A:364:A:O2'	2.21	0.50
5:A:1380:A:O2'	5:A:1391:U:O2	2.27	0.50
5:A:1413:G:N1	5:A:1577:A:OP2	2.44	0.50
28:X:6:LEU:HD22	28:X:53:ILE:HD11	1.93	0.50
31:a:178:C:H3'	31:a:179:G:H21	1.76	0.50
14:J:17:ARG:HG3	14:J:17:ARG:HH11	1.77	0.50
31:a:933:C:C4	31:a:934:A:N7	2.80	0.50
31:a:424:G:H3'	34:d:10:LYS:HZ1	1.75	0.50
41:k:107:ASN:OD1	41:k:107:ASN:N	2.44	0.50
32:b:69:VAL:HG22	32:b:162:ALA:HB3	1.94	0.50
5:A:2363:G:C2	5:A:2364:C:C5	3.00	0.50
22:R:48:LYS:NZ	22:R:52:GLU:OE2	2.43	0.50
27:W:43:GLU:OE2	27:W:72:ARG:NH2	2.40	0.50
4:3:9:LYS:HG3	4:3:16:VAL:HG23	1.94	0.49
5:A:226:A:N3	5:A:241:U:O2'	2.40	0.49
5:A:309:G:N1	5:A:312:A:OP2	2.39	0.49
5:A:1423:C:O2'	5:A:1567:A:OP2	2.08	0.49
34:d:59:GLU:HG3	34:d:202:ILE:HD11	1.93	0.49
45:o:4:THR:OG1	45:o:5:ASN:N	2.45	0.49
5:A:2543:A:H2'	5:A:2544:U:C6	2.48	0.49
14:J:34:SER:OG	14:J:35:VAL:N	2.42	0.49
18:N:63:THR:O	18:N:64:THR:OG1	2.22	0.49
31:a:293:G:N2	31:a:296:A:OP2	2.45	0.49
31:a:1437:U:O2	31:a:1459:G:C2	2.65	0.49
33:c:138:VAL:HG13	33:c:149:ILE:HG23	1.93	0.49
36:f:6:ILE:HB	36:f:62:MET:HE2	1.93	0.49
38:h:43:GLU:OE1	38:h:115:ARG:NH2	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2577:G:OP2	5:A:2577:G:N2	2.39	0.49
31:a:1320:G:H2'	31:a:1321:A:C8	2.48	0.49
32:b:163:LEU:HD23	32:b:183:ILE:CD1	2.41	0.49
33:c:211:MET:HE2	33:c:216:ASN:C	2.37	0.49
11:G:89:LEU:HD23	11:G:162:VAL:HG22	1.95	0.49
47:q:18:MET:HE3	47:q:21:SER:HB2	1.95	0.49
10:F:30:ARG:O	10:F:159:THR:N	2.46	0.49
10:F:136:ILE:O	10:F:137:VAL:HG13	2.11	0.49
34:d:19:LEU:CB	34:d:21:LEU:HD13	2.43	0.49
5:A:713:A:O2'	45:o:40:GLN:OE1	2.25	0.49
34:d:189:ASP:O	34:d:193:LEU:HD22	2.13	0.49
37:g:89:MET:SD	37:g:89:MET:N	2.85	0.49
5:A:1794:U:O2'	5:A:1798:A:N3	2.37	0.48
31:a:479:A:H2'	31:a:480:C:O4'	2.13	0.48
31:a:1438:A:O2'	31:a:1439:G:P	2.71	0.48
32:b:6:VAL:HG22	32:b:10:ASP:OD1	2.13	0.48
43:m:97:VAL:HG12	43:m:97:VAL:O	2.12	0.48
10:F:136:ILE:O	10:F:137:VAL:CG2	2.60	0.48
42:l:21:VAL:HG23	42:l:21:VAL:O	2.12	0.48
31:a:1405:A:C6	31:a:1491:G:C6	3.01	0.48
5:A:1317:A:C5	5:A:1318:C:C5	3.01	0.48
16:L:42:MET:HE2	16:L:47:ILE:HG12	1.94	0.48
39:i:52:LEU:HD23	39:i:53:LEU:CD1	2.43	0.48
9:E:40:GLN:NE2	9:E:42:THR:OG1	2.42	0.48
31:a:736:C:O2'	45:o:42:HIS:ND1	2.39	0.48
40:j:52:LEU:HD23	40:j:62:ARG:HG2	1.96	0.48
31:a:419:U:H2'	31:a:420:G:O5'	2.13	0.48
31:a:1313:G:H4'	44:n:58:VAL:HG21	1.95	0.48
5:A:2324:A:H2'	5:A:2325:A:C8	2.49	0.48
31:a:974:A:O2'	31:a:976:C:OP2	2.27	0.48
43:m:2:ALA:HB3	43:m:9:ILE:CG1	2.44	0.48
14:J:105:GLU:N	14:J:105:GLU:OE2	2.46	0.48
16:L:37:THR:HG21	16:L:130:THR:HG23	1.96	0.48
19:O:67:ILE:HD13	19:O:72:GLY:HA2	1.96	0.48
31:a:508:C:O2'	31:a:509:U:OP2	2.24	0.48
9:E:117:LEU:HD21	9:E:187:MET:HE3	1.95	0.48
31:a:809:G:H1'	31:a:810:U:OP2	2.13	0.48
31:a:1222:A:H2'	31:a:1223:C:C5	2.49	0.48
31:a:1357:A:OP2	44:n:75:ARG:NH2	2.40	0.48
28:X:28:LEU:HD22	28:X:37:LEU:HD22	1.96	0.47
31:a:538:G:H2'	31:a:539:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:77:ALA:HB1	32:b:209:ILE:HD11	1.96	0.47
3:2:22:LYS:NZ	5:A:629:A:OP2	2.41	0.47
14:J:47:ILE:C	14:J:47:ILE:HD12	2.38	0.47
31:a:419:U:C2'	31:a:420:G:O5'	2.62	0.47
31:a:607:U:N3	31:a:608:C:C5	2.82	0.47
47:q:22:ILE:HG23	47:q:49:ASP:OD1	2.14	0.47
10:F:152:MET:HE3	10:F:152:MET:HA	1.95	0.47
14:J:94:ILE:HD12	14:J:94:ILE:C	2.38	0.47
27:W:43:GLU:OE1	27:W:45:ARG:NH1	2.45	0.47
31:a:1031:G:H2'	31:a:1032:A:O4'	2.15	0.47
44:n:38:ASP:OD2	44:n:39:GLU:OE1	2.33	0.47
47:q:39:ILE:HG22	47:q:40:ARG:N	2.30	0.47
10:F:46:ASP:CG	10:F:49:LEU:HD22	2.39	0.47
10:F:132:LEU:HD22	10:F:138:PHE:CE2	2.48	0.47
10:F:162:THR:OG1	10:F:163:ASP:N	2.47	0.47
34:d:103:VAL:HG21	34:d:139:VAL:HG21	1.97	0.47
39:i:90:GLU:CD	39:i:90:GLU:H	2.22	0.47
5:A:279:U:H4'	5:A:280:A:OP1	2.14	0.47
5:A:1317:A:C6	5:A:1318:C:C5	3.03	0.47
10:F:103:LEU:HD12	10:F:107:ALA:HB3	1.97	0.47
31:a:1386:C:HO2'	31:a:1387:U:P	2.36	0.47
33:c:207:ILE:O	33:c:207:ILE:HG22	2.14	0.47
33:c:215:MET:O	33:c:216:ASN:ND2	2.47	0.47
34:d:66:ILE:HG22	34:d:113:ARG:HH11	1.79	0.47
40:j:15:HIS:HA	40:j:18:ILE:HG22	1.96	0.47
5:A:360:A:H2'	5:A:361:A:O4'	2.15	0.47
5:A:394:U:O2'	5:A:395:G:N7	2.43	0.47
5:A:1044:G:C2'	5:A:1108:A:H61	2.28	0.47
5:A:2287:U:OP1	5:A:2376:U:O2'	2.32	0.47
5:A:2502:U:H2'	5:A:2572:G:O6	2.15	0.47
9:E:56:LYS:CD	9:E:56:LYS:H	2.28	0.47
10:F:32:THR:OG1	10:F:157:THR:O	2.20	0.47
10:F:159:THR:O	10:F:159:THR:HG22	2.15	0.47
25:U:6:LEU:HD12	25:U:65:VAL:HG21	1.96	0.47
31:a:367:A:H2'	31:a:368:C:O4'	2.15	0.47
32:b:167:ASP:OD1	32:b:167:ASP:C	2.57	0.47
39:i:115:GLY:C	39:i:116:LEU:HD23	2.40	0.47
41:k:17:GLU:OE1	41:k:18:GLY:N	2.48	0.47
43:m:49:ASP:OD1	43:m:50:ASP:N	2.48	0.47
5:A:90:G:OP1	24:T:90:LYS:NZ	2.45	0.47
38:h:10:MET:CG	38:h:27:MET:HE1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:34:THR:OG1	48:r:38:LYS:N	2.48	0.47
10:F:4:LEU:N	10:F:4:LEU:HD12	2.30	0.47
31:a:462:A:N1	31:a:464:A:O2'	2.47	0.47
5:A:434:C:O2	5:A:434:C:O4'	2.33	0.47
5:A:1870:C:H2'	5:A:1870:C:O2	2.14	0.47
31:a:1154:A:C2	31:a:1178:G:C4	3.02	0.47
31:a:1396:C:H4'	31:a:1397:C:C5'	2.45	0.47
31:a:1396:C:H4'	31:a:1397:C:H5"	1.97	0.47
32:b:145:LYS:HA	32:b:148:ARG:HG2	1.97	0.47
10:F:108:ILE:HD11	10:F:176:PRO:HG3	1.97	0.46
10:F:132:LEU:C	10:F:133:LYS:HE2	2.40	0.46
5:A:2387:G:O2'	5:A:2420:C:N4	2.48	0.46
32:b:186:ILE:HG22	32:b:200:TYR:HB2	1.96	0.46
42:l:63:VAL:HG22	42:l:64:SER:N	2.30	0.46
5:A:391:C:C2	5:A:392:C:C5	3.03	0.46
6:B:44:A:C5	6:B:45:C:C5	3.04	0.46
7:C:270:ASP:OD2	7:C:272:ARG:N	2.48	0.46
26:V:20:MET:SD	26:V:20:MET:N	2.89	0.46
28:X:28:LEU:HD11	28:X:42:GLU:HB3	1.96	0.46
31:a:1447:G:N1	31:a:1451:A:C6	2.84	0.46
32:b:85:GLN:HA	32:b:88:ARG:NH1	2.30	0.46
43:m:53:LEU:O	43:m:57:ARG:HG3	2.15	0.46
4:3:16:VAL:HG22	4:3:25:VAL:HG22	1.97	0.46
5:A:1953:C:C2	5:A:1954:C:C5	3.04	0.46
39:i:89:ASP:OD2	39:i:91:THR:HG22	2.15	0.46
7:C:133:ARG:HB3	7:C:186:VAL:HG22	1.98	0.46
31:a:1063:C:O2	31:a:1063:C:H2'	2.15	0.46
32:b:94:VAL:HG13	32:b:94:VAL:O	2.14	0.46
37:g:87:VAL:HG23	37:g:89:MET:SD	2.56	0.46
40:j:32:THR:HG21	40:j:83:THR:HA	1.97	0.46
5:A:91:A:H1'	5:A:92:G:OP2	2.15	0.46
31:a:202:U:H2'	31:a:202:U:O2	2.15	0.46
31:a:1051:C:H1'	31:a:1052:A:OP2	2.16	0.46
36:f:93:GLU:O	36:f:94:HIS:CG	2.69	0.46
9:E:14:SER:N	9:E:196:GLU:OE2	2.46	0.46
31:a:702:G:C4	31:a:703:A:C8	3.04	0.46
32:b:146:LEU:HD13	32:b:150:LEU:HD21	1.98	0.46
34:d:144:VAL:HG23	34:d:183:THR:HG22	1.96	0.46
3:2:32:LEU:HD13	5:A:2415:U:OP2	2.16	0.46
10:F:20:LEU:HD11	10:F:165:GLU:HG2	1.98	0.46
31:a:577:C:H2'	31:a:578:G:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:104:ASN:OD1	33:c:104:ASN:C	2.58	0.46
5:A:2843:U:H2'	5:A:2844:G:O4'	2.16	0.45
34:d:190:ARG:NH1	34:d:190:ARG:O	2.49	0.45
42:l:63:VAL:HG22	42:l:64:SER:H	1.81	0.45
43:m:2:ALA:HB3	43:m:9:ILE:HG12	1.97	0.45
5:A:435:C:O2	5:A:435:C:H2'	2.17	0.45
5:A:758:G:H2'	5:A:759:A:O4'	2.15	0.45
5:A:1737:C:H2'	5:A:1738:U:O4'	2.16	0.45
11:G:155:GLU:OE1	11:G:157:TYR:N	2.49	0.45
32:b:208:ALA:O	32:b:212:VAL:HG13	2.17	0.45
48:r:34:THR:HG1	48:r:38:LYS:C	2.17	0.45
19:O:89:VAL:HG11	19:O:92:ARG:CZ	2.46	0.45
31:a:420:G:H2'	31:a:421:G:C8	2.51	0.45
32:b:81:ILE:HG22	32:b:85:GLN:OE1	2.15	0.45
36:f:36:ILE:N	36:f:36:ILE:HD12	2.31	0.45
39:i:41:THR:HA	39:i:44:MET:HE3	1.98	0.45
5:A:2400:U:H2'	5:A:2401:G:O4'	2.17	0.45
31:a:1374:A:N6	37:g:7:VAL:HG21	2.32	0.45
5:A:177:G:H2'	5:A:178:U:C6	2.52	0.45
31:a:301:G:H5"	31:a:302:A:OP1	2.16	0.45
5:A:1412:C:H2'	5:A:1413:G:O4'	2.16	0.45
11:G:168:VAL:O	11:G:168:VAL:HG13	2.17	0.45
31:a:425:U:O2	31:a:426:A:C8	2.70	0.45
31:a:704:U:N3	31:a:705:C:C5	2.84	0.45
34:d:66:ILE:HG22	34:d:113:ARG:NH1	2.31	0.45
7:C:80:ARG:NE	7:C:82:GLU:OE1	2.50	0.45
31:a:4:A:H1'	31:a:610:C:HO2'	1.82	0.45
31:a:489:C:O2'	31:a:490:A:O5'	2.35	0.45
5:A:390:A:C5	5:A:391:C:C5	3.05	0.45
5:A:1105:U:H2'	5:A:1105:U:O2	2.15	0.45
5:A:2067:A:H2'	5:A:2068:C:C6	2.51	0.45
31:a:96:U:O2'	31:a:97:A:N7	2.44	0.45
31:a:402:G:C2	31:a:403:U:C5	3.05	0.45
32:b:136:ALA:O	32:b:140:THR:HG23	2.17	0.45
5:A:591:U:H2'	5:A:592:U:C6	2.52	0.45
10:F:31:ILE:HD11	10:F:156:ILE:HG23	1.98	0.45
31:a:401:U:OP2	34:d:3:ARG:NE	2.47	0.45
32:b:149:SER:HB2	32:b:150:LEU:HD23	1.99	0.45
38:h:56:THR:O	38:h:56:THR:HG22	2.17	0.45
6:B:101:A:H4'	25:U:96:LYS:HE2	1.97	0.45
10:F:93:GLY:N	10:F:96:MET:HG2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:107:ALA:O	10:F:111:ILE:HG23	2.17	0.45
10:F:113:ASP:OD2	10:F:113:ASP:C	2.60	0.45
31:a:681:U:O2	41:k:40:ALA:HB3	2.17	0.45
32:b:9:ARG:HG2	32:b:9:ARG:HH11	1.82	0.45
32:b:94:VAL:O	32:b:94:VAL:CG1	2.64	0.45
9:E:170:ASP:OD1	9:E:171:ALA:N	2.50	0.44
24:T:25:LEU:HD21	24:T:35:GLU:HB2	1.99	0.44
31:a:180:U:C2	31:a:181:C:C5	3.04	0.44
34:d:172:TRP:O	34:d:185:LYS:HD2	2.17	0.44
34:d:172:TRP:C	34:d:173:ILE:HD12	2.43	0.44
7:C:175:ARG:HG2	7:C:175:ARG:NH1	2.29	0.44
31:a:659:G:H2'	31:a:660:A:C8	2.52	0.44
5:A:277:A:O4'	5:A:279:U:N3	2.51	0.44
5:A:715:C:O4'	5:A:715:C:O2	2.34	0.44
5:A:1924:A:H2'	5:A:1925:G:O4'	2.16	0.44
7:C:268:ILE:HG22	7:C:269:ARG:HG3	1.99	0.44
10:F:49:LEU:HD23	10:F:50:LEU:H	1.82	0.44
32:b:142:GLU:HA	32:b:145:LYS:CD	2.47	0.44
33:c:12:LEU:HD11	44:n:91:GLY:HA2	1.99	0.44
34:d:123:ARG:O	34:d:131:ARG:CZ	2.65	0.44
39:i:31:ARG:HD3	39:i:36:TYR:HD1	1.83	0.44
5:A:279:U:H5'	5:A:280:A:OP1	2.17	0.44
5:A:372:U:C6	5:A:372:U:OP2	2.70	0.44
5:A:605:U:C5	5:A:618:G:C5	3.05	0.44
5:A:2747:G:N3	5:A:2747:G:H2'	2.32	0.44
11:G:43:LEU:HD22	11:G:44:LYS:N	2.32	0.44
31:a:1068:C:OP1	35:e:53:ARG:CZ	2.65	0.44
38:h:60:LEU:HD23	38:h:61:THR:N	2.33	0.44
39:i:40:GLU:HG3	39:i:44:MET:CE	2.47	0.44
44:n:31:ILE:O	44:n:41:ARG:NH2	2.46	0.44
5:A:17:A:H2'	5:A:18:U:O4'	2.17	0.44
5:A:1885:A:H2'	5:A:1886:A:O4'	2.18	0.44
5:A:1954:C:C2	5:A:1955:G:C8	3.05	0.44
5:A:2651:G:C2'	5:A:2652:U:OP2	2.65	0.44
21:Q:37:ASP:OD1	21:Q:37:ASP:N	2.51	0.44
31:a:976:C:O2	44:n:59:ARG:NH1	2.50	0.44
34:d:69:VAL:HG12	34:d:70:LEU:N	2.33	0.44
5:A:51:A:H2'	5:A:52:G:O4'	2.17	0.44
5:A:862:G:H2'	5:A:863:C:C6	2.52	0.44
5:A:1267:A:O2'	5:A:1268:C:H2'	2.18	0.44
5:A:1315:C:H2'	5:A:1324:U:OP1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1844:A:O2'	5:A:1845:G:P	2.75	0.44
13:I:15:TRP:CE3	13:I:55:ILE:HD11	2.52	0.44
14:J:45:GLU:HA	14:J:45:GLU:OE1	2.17	0.44
31:a:1145:U:H2'	31:a:1146:U:O4'	2.18	0.44
32:b:159:LEU:HD22	32:b:159:LEU:H	1.83	0.44
33:c:86:LYS:O	33:c:90:GLU:HG2	2.18	0.44
34:d:54:SER:O	34:d:58:ARG:HG2	2.16	0.44
35:e:14:LEU:HD12	35:e:36:THR:HG22	2.00	0.44
36:f:1:MET:N	36:f:1:MET:SD	2.88	0.44
38:h:10:MET:HG3	38:h:27:MET:HE1	2.00	0.44
33:c:149:ILE:HD12	33:c:202:ILE:HG12	1.98	0.44
38:h:3:MET:HE1	38:h:9:ASP:OD1	2.17	0.44
5:A:1193:U:C2	5:A:1194:U:C5	3.06	0.44
5:A:2651:G:O2'	5:A:2652:U:P	2.76	0.44
21:Q:51:ALA:HB3	21:Q:52:PRO:CD	2.47	0.44
33:c:104:ASN:OD1	33:c:105:GLU:N	2.51	0.44
40:j:35:GLN:N	40:j:35:GLN:CD	2.76	0.44
41:k:112:VAL:HG12	41:k:112:VAL:O	2.18	0.44
43:m:49:ASP:OD1	43:m:51:ALA:N	2.39	0.44
5:A:19:U:O2	5:A:2622:C:H4'	2.18	0.44
15:K:66:PHE:CD1	15:K:66:PHE:N	2.86	0.44
23:S:49:LEU:HD23	28:X:26:PHE:CZ	2.53	0.44
36:f:40:GLU:OE1	36:f:100:SER:OG	2.28	0.44
37:g:115:THR:HG22	37:g:117:ALA:H	1.83	0.44
5:A:1869:G:O2'	5:A:1870:C:O4'	2.28	0.43
10:F:53:ALA:O	10:F:57:MET:HE2	2.18	0.43
24:T:39:LEU:N	24:T:39:LEU:HD22	2.33	0.43
31:a:1023:G:N3	31:a:1023:G:H2'	2.33	0.43
32:b:77:ALA:HB1	32:b:209:ILE:HD12	1.99	0.43
31:a:701:A:C4	31:a:702:G:C8	3.06	0.43
38:h:5:ASP:OD1	38:h:82:PRO:HD3	2.18	0.43
10:F:161:ARG:HB2	10:F:161:ARG:CZ	2.47	0.43
13:I:128:SER:OG	13:I:129:GLU:OE2	2.36	0.43
35:e:99:SER:O	35:e:102:THR:HG22	2.18	0.43
47:q:39:ILE:HG22	47:q:40:ARG:H	1.83	0.43
50:t:49:GLU:OE2	50:t:49:GLU:HA	2.19	0.43
5:A:2262:A:H4'	5:A:2263:A:N3	2.34	0.43
31:a:1010:G:N2	31:a:1013:A:OP2	2.43	0.43
31:a:1353:G:H2'	31:a:1354:A:C8	2.52	0.43
46:p:37:ILE:HD13	46:p:70:LEU:HD13	2.00	0.43
31:a:489:C:H2'	31:a:490:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:f:85:ILE:O	36:f:86:ARG:CB	2.67	0.43
48:r:34:THR:OG1	48:r:38:LYS:O	2.19	0.43
5:A:435:C:C2	5:A:436:U:C5	3.06	0.43
10:F:115:ARG:O	10:F:115:ARG:HG2	2.18	0.43
31:a:534:A:OP1	42:l:110:ARG:NH2	2.52	0.43
31:a:1127:A:C8	31:a:1143:A:N1	2.86	0.43
34:d:173:ILE:HD12	34:d:173:ILE:N	2.33	0.43
5:A:1306:G:OP2	5:A:1306:G:N2	2.34	0.43
5:A:1634:G:H2'	5:A:1635:A:C8	2.54	0.43
5:A:1835:G:H1'	5:A:1923:A:C8	2.53	0.43
6:B:50:A:O2'	6:B:51:A:C8	2.71	0.43
10:F:137:VAL:O	10:F:137:VAL:HG23	2.18	0.43
31:a:23:G:H2'	31:a:24:G:C8	2.54	0.43
31:a:460:U:N3	31:a:463:U:OP2	2.48	0.43
31:a:537:G:H2'	31:a:538:G:O4'	2.19	0.43
32:b:14:ALA:HB2	32:b:214:LEU:HD22	2.00	0.43
10:F:133:LYS:HE2	10:F:133:LYS:CA	2.48	0.43
31:a:680:G:C2	31:a:681:U:C5	3.07	0.43
34:d:10:LYS:HE3	34:d:13:ARG:NH1	2.34	0.43
37:g:15:ASP:OD1	37:g:19:SER:N	2.52	0.43
49:s:20:GLU:OE1	49:s:20:GLU:HA	2.17	0.43
5:A:981:A:N3	5:A:981:A:H2'	2.34	0.43
25:U:8:ALA:HB2	25:U:46:LEU:HD23	2.01	0.43
32:b:142:GLU:HA	32:b:145:LYS:NZ	2.34	0.43
5:A:701:U:H2'	5:A:702:G:O4'	2.19	0.43
5:A:1267:A:C4'	5:A:1268:C:OP1	2.67	0.43
5:A:2633:U:H2'	5:A:2634:G:O4'	2.19	0.43
11:G:71:VAL:O	11:G:75:LEU:HG	2.18	0.43
14:J:56:ASP:OD2	14:J:56:ASP:N	2.52	0.43
15:K:134:LYS:O	15:K:138:GLU:HG2	2.19	0.43
31:a:516:C:O2	31:a:516:C:O4'	2.37	0.43
5:A:579:C:H2'	5:A:580:A:H8	1.84	0.42
5:A:1025:A:N3	5:A:2482:C:O2'	2.47	0.42
5:A:2509:A:H2'	5:A:2510:U:C6	2.54	0.42
14:J:17:ARG:HG3	14:J:17:ARG:NH1	2.34	0.42
23:S:34:ASP:OD1	23:S:35:ILE:N	2.51	0.42
31:a:418:A:O2'	31:a:419:U:C5	2.69	0.42
31:a:471:G:H2'	31:a:472:A:C8	2.54	0.42
32:b:42:ILE:HD13	32:b:42:ILE:N	2.34	0.42
33:c:17:ARG:HG2	33:c:17:ARG:HH11	1.84	0.42
33:c:191:THR:HG21	33:c:196:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:67:LEU:O	48:r:68:ILE:HD13	2.19	0.42
5:A:368:C:C4'	5:A:369:G:OP2	2.66	0.42
5:A:1199:A:O4'	5:A:1201:G:C8	2.72	0.42
10:F:135:GLN:N	10:F:150:ARG:O	2.51	0.42
15:K:131:LYS:HG2	15:K:132:GLY:N	2.33	0.42
18:N:25:THR:HG23	18:N:41:ILE:O	2.19	0.42
36:f:9:LEU:HB2	36:f:85:ILE:O	2.18	0.42
39:i:53:LEU:HG	39:i:92:LEU:HD22	2.01	0.42
41:k:22:ILE:HD12	41:k:22:ILE:N	2.34	0.42
47:q:25:LEU:HD21	47:q:42:SER:OG	2.19	0.42
31:a:789:A:H1'	31:a:790:U:OP2	2.19	0.42
36:f:22:VAL:HG21	36:f:39:LEU:HD21	2.01	0.42
44:n:73:TYR:O	44:n:79:LEU:O	2.36	0.42
3:2:56:SER:O	3:2:60:MET:HG3	2.19	0.42
14:J:47:ILE:HD12	14:J:48:PRO:O	2.19	0.42
27:W:67:VAL:O	27:W:71:LEU:HG	2.18	0.42
31:a:703:A:C4	31:a:704:U:C5	3.08	0.42
53:a:1602:80P:F24	53:a:1603:80P:F24	2.18	0.42
36:f:1:MET:H3	36:f:1:MET:CE	2.33	0.42
41:k:106:ILE:O	41:k:106:ILE:HG13	2.19	0.42
5:A:478:A:H4'	5:A:479:A:OP1	2.20	0.42
5:A:847:A:H2'	5:A:848:C:C6	2.54	0.42
5:A:2541:G:H2'	5:A:2542:U:O4'	2.20	0.42
24:T:41:LYS:HG2	24:T:56:ILE:HG22	2.02	0.42
29:Y:46:MET:O	29:Y:50:VAL:HG22	2.18	0.42
31:a:157:A:H2'	31:a:158:A:O4'	2.19	0.42
31:a:369:A:C2	31:a:479:A:C6	3.07	0.42
32:b:70:LEU:HB3	32:b:163:LEU:HD13	2.00	0.42
8:D:111:ASP:OD2	8:D:209:THR:HA	2.20	0.42
9:E:198:GLU:OE2	9:E:198:GLU:O	2.37	0.42
32:b:49:VAL:HG13	32:b:50:PRO:CD	2.45	0.42
33:c:48:LYS:O	33:c:48:LYS:HG2	2.18	0.42
5:A:369:G:OP2	5:A:369:G:C8	2.73	0.42
6:B:50:A:O2'	6:B:51:A:O5'	2.37	0.42
7:C:124:ILE:N	7:C:124:ILE:HD13	2.35	0.42
19:O:117:LEU:O	19:O:117:LEU:HD12	2.19	0.42
31:a:1409:C:H2'	31:a:1410:A:C8	2.55	0.42
33:c:111:LEU:HD22	33:c:146:ALA:HB2	2.02	0.42
39:i:70:ILE:N	39:i:70:ILE:HD12	2.34	0.42
45:o:78:TYR:O	45:o:82:ILE:HG23	2.20	0.42
5:A:2056:A:O2'	5:A:2057:G:OP2	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2283:A:C5	5:A:2285:G:C8	3.07	0.42
10:F:36:LEU:HD12	10:F:154:ILE:HG13	2.02	0.42
10:F:147:ASP:CG	10:F:148:ARG:N	2.77	0.42
11:G:84:GLU:OE1	11:G:84:GLU:C	2.63	0.42
31:a:489:C:C2'	31:a:490:A:O5'	2.68	0.42
31:a:942:G:C2	31:a:943:A:C8	3.07	0.42
31:a:1233:A:H2'	31:a:1234:C:C6	2.55	0.42
36:f:1:MET:N	36:f:65:GLU:OE2	2.48	0.42
37:g:71:PRO:HD2	37:g:96:ARG:HB2	2.02	0.42
5:A:324:A:H1'	5:A:325:G:OP1	2.20	0.42
5:A:805:U:OP2	15:K:43:ARG:NH2	2.51	0.42
5:A:1413:G:N2	5:A:1577:A:OP2	2.49	0.42
5:A:2641:U:H3'	5:A:2642:C:H5'	2.01	0.42
7:C:168:ASP:OD1	7:C:168:ASP:N	2.52	0.42
25:U:68:LYS:HG2	25:U:73:VAL:HG12	2.01	0.42
33:c:124:LEU:HD13	33:c:196:ILE:HG21	2.00	0.42
40:j:26:VAL:HG13	40:j:36:VAL:HG21	2.02	0.42
5:A:2699:C:C2	5:A:2700:C:C5	3.08	0.42
6:B:50:A:O2'	6:B:51:A:P	2.77	0.42
10:F:67:VAL:HG12	10:F:84:PRO:CB	2.48	0.42
32:b:83:ARG:HH11	32:b:87:GLN:CG	2.33	0.42
32:b:134:ARG:O	32:b:137:LEU:HG	2.20	0.42
34:d:173:ILE:N	34:d:173:ILE:CD1	2.83	0.42
37:g:37:SER:HA	37:g:40:GLU:OE1	2.20	0.42
5:A:2769:U:OP1	8:D:172:ARG:NE	2.48	0.41
14:J:122:LEU:HD12	14:J:122:LEU:OXT	2.19	0.41
32:b:123:SER:HA	32:b:128:PHE:CE2	2.54	0.41
34:d:10:LYS:HD2	34:d:13:ARG:HD3	2.02	0.41
34:d:107:MET:HG2	34:d:109:PHE:CG	2.55	0.41
5:A:1531:C:O2'	5:A:1532:U:O4'	2.37	0.41
5:A:1666:A:O2'	5:A:1672:G:N7	2.49	0.41
5:A:1844:A:C2'	5:A:1845:G:OP2	2.68	0.41
6:B:7:G:C2	6:B:8:A:C8	3.08	0.41
6:B:22:G:O2'	6:B:25:C:N4	2.53	0.41
10:F:32:THR:HG1	10:F:157:THR:C	2.23	0.41
10:F:36:LEU:HD23	10:F:89:VAL:HG23	2.02	0.41
10:F:134:GLU:HB3	10:F:136:ILE:HG22	2.02	0.41
42:l:89:ASP:OD1	42:l:89:ASP:C	2.62	0.41
43:m:106:ALA:O	43:m:110:LYS:HG3	2.20	0.41
5:A:973:G:O2'	5:A:1153:A:O2'	2.38	0.41
5:A:1316:A:C4	5:A:1317:A:C8	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1567:A:OP1	7:C:61:HIS:NE2	2.43	0.41
5:A:2048:A:H4'	8:D:151:GLN:O	2.19	0.41
5:A:2414:A:H2'	5:A:2415:U:O4'	2.20	0.41
5:A:2752:U:C4	5:A:2755:G:O6	2.74	0.41
10:F:23:LYS:HD2	10:F:23:LYS:N	2.35	0.41
23:S:1:MET:SD	23:S:6:ILE:HD11	2.60	0.41
31:a:1165:C:H5"	31:a:1166:A:OP2	2.20	0.41
36:f:15:SER:O	36:f:18:VAL:HG13	2.20	0.41
43:m:86:TYR:O	43:m:90:ARG:HG2	2.20	0.41
3:2:23:ARG:HD2	15:K:63:LEU:HD13	2.03	0.41
5:A:992:C:O2	13:I:3:THR:OG1	2.23	0.41
15:K:134:LYS:HD2	15:K:144:VAL:HG21	2.01	0.41
33:c:80:LYS:HD3	33:c:80:LYS:N	2.34	0.41
34:d:199:GLU:OE1	34:d:199:GLU:N	2.45	0.41
41:k:36:ARG:O	41:k:37:GLN:HB2	2.21	0.41
5:A:798:U:H4'	5:A:799:G:H3'	2.02	0.41
5:A:2752:U:H4'	5:A:2753:A:OP1	2.21	0.41
19:O:22:GLU:C	19:O:22:GLU:CD	2.88	0.41
24:T:5:LYS:N	24:T:8:ASP:OD2	2.43	0.41
29:Y:5:LYS:HD3	29:Y:36:GLU:HG2	2.02	0.41
29:Y:17:LYS:HE3	29:Y:17:LYS:HB3	1.90	0.41
31:a:1433:U:O4	31:a:1434:A:N6	2.54	0.41
36:f:29:ILE:HG22	36:f:34:GLY:HA2	2.02	0.41
42:l:53:CYS:SG	42:l:67:ILE:CD1	3.03	0.41
5:A:1519:U:C2'	5:A:1520:A:OP2	2.68	0.41
8:D:12:MET:HE2	8:D:12:MET:HB3	1.95	0.41
8:D:18:ASP:OD1	8:D:19:ALA:N	2.54	0.41
8:D:81:LYS:HG3	8:D:82:GLU:H	1.85	0.41
9:E:118:VAL:HG23	9:E:118:VAL:O	2.21	0.41
19:O:3:GLY:HA3	19:O:8:VAL:HG11	2.02	0.41
31:a:241:U:H2'	31:a:242:A:H5"	2.02	0.41
31:a:1157:G:C2	31:a:1158:C:C6	3.09	0.41
6:B:90:C:OP1	25:U:26:ARG:NH2	2.52	0.41
10:F:108:ILE:CG2	10:F:109:PRO:HD3	2.51	0.41
10:F:130:MET:HG2	10:F:154:ILE:HB	2.03	0.41
29:Y:5:LYS:CD	29:Y:36:GLU:HG2	2.51	0.41
31:a:319:U:H2'	31:a:320:G:O4'	2.21	0.41
31:a:701:A:C5	31:a:702:G:C8	3.09	0.41
31:a:704:U:C2	31:a:705:C:C5	3.08	0.41
31:a:1215:C:H2'	31:a:1216:A:C8	2.55	0.41
31:a:1313:G:N1	31:a:1316:A:OP2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:52:GLU:OE1	37:g:52:GLU:O	2.39	0.41
5:A:72:C:O2'	5:A:455:C:N3	2.50	0.41
5:A:314:G:C2	5:A:315:U:C6	3.09	0.41
5:A:1296:A:C4'	5:A:1297:A:OP1	2.69	0.41
5:A:1344:C:C2	5:A:1345:C:C5	3.09	0.41
5:A:1583:C:O2	5:A:1583:C:H2'	2.20	0.41
5:A:2287:U:H2'	5:A:2288:G:C8	2.56	0.41
10:F:133:LYS:O	10:F:134:GLU:HB2	2.20	0.41
16:L:41:ARG:HD2	16:L:94:VAL:HG21	2.02	0.41
20:P:86:ALA:O	20:P:87:GLN:HB2	2.21	0.41
31:a:389:A:C2	31:a:390:G:C8	3.08	0.41
31:a:1419:U:H2'	31:a:1420:G:C8	2.56	0.41
32:b:195:PRO:O	32:b:198:VAL:HG22	2.20	0.41
33:c:215:MET:HE2	33:c:215:MET:HB2	1.93	0.41
35:e:114:LEU:HD13	35:e:122:VAL:HG11	2.03	0.41
37:g:129:GLU:OE1	37:g:129:GLU:HA	2.20	0.41
38:h:23:GLN:OE1	38:h:23:GLN:HA	2.20	0.41
48:r:62:ALA:HB1	48:r:68:ILE:HG12	2.03	0.41
2:1:1:MET:HE2	2:1:1:MET:HB2	1.99	0.41
5:A:798:U:C4'	5:A:799:G:H3'	2.50	0.41
5:A:1124:A:N1	5:A:2459:C:O2'	2.53	0.41
5:A:1179:G:OP1	29:Y:29:ARG:NH1	2.53	0.41
5:A:1314:C:O2'	5:A:1315:C:H5'	2.21	0.41
5:A:1555:C:OP2	5:A:1556:A:O2'	2.28	0.41
5:A:1852:U:H2'	5:A:1853:G:O4'	2.21	0.41
5:A:1967:U:O2	5:A:1967:U:O4'	2.38	0.41
5:A:2463:C:H2'	5:A:2464:A:O4'	2.20	0.41
10:F:13:LYS:HD2	10:F:28:ILE:HD13	2.02	0.41
10:F:33:LYS:CD	10:F:33:LYS:C	2.94	0.41
10:F:110:ARG:O	10:F:110:ARG:HD2	2.20	0.41
10:F:132:LEU:HD22	10:F:138:PHE:CZ	2.56	0.41
31:a:185:C:H4'	31:a:186:G:O5'	2.21	0.41
32:b:102:MET:HE2	32:b:102:MET:CA	2.49	0.41
32:b:165:VAL:HG13	32:b:187:GLY:HA3	2.02	0.41
32:b:173:ILE:N	32:b:173:ILE:HD12	2.36	0.41
33:c:214:VAL:O	33:c:214:VAL:HG12	2.20	0.41
37:g:44:TYR:O	37:g:48:GLU:HG2	2.20	0.41
42:l:31:ARG:NH1	42:l:31:ARG:HG3	2.36	0.41
5:A:809:U:O2	5:A:1245:G:H5"	2.20	0.41
5:A:916:A:N3	6:B:78:U:O2'	2.49	0.41
5:A:1044:G:O6	5:A:1107:G:O6	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1191:C:C2	5:A:1192:G:C8	3.09	0.41
5:A:2026:6MZ:O2'	5:A:2027:A:P	2.79	0.41
7:C:22:ASP:OD1	7:C:23:HIS:N	2.54	0.41
10:F:99:PHE:O	10:F:102:ARG:HD3	2.21	0.41
28:X:2:LYS:HE3	28:X:6:LEU:HD21	2.01	0.41
31:a:436:A:C2'	31:a:437:A:O5'	2.68	0.41
31:a:754:U:OP1	31:a:819:U:O2'	2.32	0.41
32:b:106:TRP:HA	32:b:109:LEU:CD2	2.51	0.41
32:b:139:ARG:CA	32:b:142:GLU:OE2	2.68	0.41
5:A:434:C:C4	5:A:435:C:C6	3.09	0.40
5:A:2485:U:H2'	5:A:2486:G:O4'	2.21	0.40
31:a:671:G:H2'	31:a:672:A:H8	1.85	0.40
32:b:159:LEU:HD22	32:b:159:LEU:N	2.36	0.40
32:b:183:ILE:HD12	32:b:183:ILE:O	2.19	0.40
43:m:83:LEU:HD21	49:s:65:HIS:HB2	2.03	0.40
3:2:26:ALA:O	3:2:27:PHE:HB2	2.21	0.40
5:A:144:U:H2'	5:A:145:U:O4'	2.22	0.40
5:A:507:U:C4'	5:A:508:C:OP2	2.69	0.40
5:A:1018:A:H3'	5:A:1018:A:N3	2.37	0.40
5:A:1835:G:C2	5:A:1836:G:C8	3.09	0.40
5:A:2076:G:H5"	27:W:19:SER:HB2	2.04	0.40
14:J:97:ARG:NH1	31:a:335:C:OP2	2.54	0.40
32:b:177:GLU:O	32:b:181:LEU:HD23	2.20	0.40
34:d:57:LEU:HA	34:d:205:LEU:HD22	2.03	0.40
42:l:33:VAL:HG12	42:l:79:VAL:HG22	2.02	0.40
1:0:29:LYS:HA	1:0:47:GLU:OE1	2.21	0.40
2:1:30:VAL:HG22	2:1:33:ARG:NH2	2.36	0.40
5:A:386:U:O2	5:A:386:U:O4'	2.39	0.40
5:A:1775:U:OP2	5:A:1780:A:N6	2.45	0.40
29:Y:29:ARG:NH1	29:Y:29:ARG:HG2	2.36	0.40
31:a:434:U:H1'	31:a:435:U:P	2.61	0.40
31:a:1152:A:H2'	31:a:1153:U:O4'	2.21	0.40
43:m:68:ASP:OD1	43:m:68:ASP:N	2.52	0.40
2:1:10:LEU:HD11	2:1:14:ARG:NE	2.36	0.40
5:A:39:C:O2'	5:A:40:U:H5'	2.21	0.40
24:T:30:ASP:O	24:T:65:ILE:N	2.52	0.40
31:a:4:A:H1'	31:a:610:C:O2'	2.21	0.40
31:a:943:A:H2'	31:a:944:G:C8	2.57	0.40
31:a:1235:A:H2	31:a:1238:G:N3	2.19	0.40
31:a:1448:C:O2	31:a:1448:C:O5'	2.39	0.40
33:c:89:ARG:HG2	33:c:89:ARG:HH11	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:148:SER:OG	35:e:149:PRO:HD2	2.21	0.40
5:A:1875:C:H2'	5:A:1876:U:O4'	2.21	0.40
5:A:2061:C:N3	5:A:2062:C:C5	2.89	0.40
35:e:75:LEU:HD21	35:e:119:VAL:HG22	2.04	0.40
48:r:32:TYR:CD2	48:r:55:LEU:HD11	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	
1	0	46/51 (90%)	46 (100%)	0	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	C	269/274 (98%)	262 (97%)	7 (3%)	0	100	100
8	D	209/212 (99%)	201 (96%)	8 (4%)	0	100	100
9	E	198/200 (99%)	198 (100%)	0	0	100	100
10	F	172/178 (97%)	162 (94%)	9 (5%)	1 (1%)	21	25
11	G	172/177 (97%)	167 (97%)	4 (2%)	1 (1%)	21	25
12	H	58/148 (39%)	56 (97%)	2 (3%)	0	100	100
13	I	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
14	J	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
15	K	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
16	L	135/137 (98%)	131 (97%)	3 (2%)	1 (1%)	18	21
17	M	117/125 (94%)	117 (100%)	0	0	100	100
18	N	112/116 (97%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	O	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
20	P	115/119 (97%)	113 (98%)	2 (2%)	0	100	100
21	Q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
22	R	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
23	S	89/106 (84%)	88 (99%)	1 (1%)	0	100	100
24	T	101/105 (96%)	97 (96%)	4 (4%)	0	100	100
25	U	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
26	V	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
27	W	75/78 (96%)	75 (100%)	0	0	100	100
28	X	58/65 (89%)	58 (100%)	0	0	100	100
29	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	Z	52/61 (85%)	51 (98%)	1 (2%)	0	100	100
32	b	223/250 (89%)	212 (95%)	11 (5%)	0	100	100
33	c	213/250 (85%)	206 (97%)	7 (3%)	0	100	100
34	d	205/208 (99%)	199 (97%)	6 (3%)	0	100	100
35	e	153/165 (93%)	149 (97%)	4 (3%)	0	100	100
36	f	102/127 (80%)	98 (96%)	1 (1%)	3 (3%)	3	1
37	g	132/156 (85%)	129 (98%)	3 (2%)	0	100	100
38	h	128/131 (98%)	123 (96%)	5 (4%)	0	100	100
39	i	124/128 (97%)	121 (98%)	3 (2%)	0	100	100
40	j	98/103 (95%)	95 (97%)	3 (3%)	0	100	100
41	k	115/128 (90%)	113 (98%)	2 (2%)	0	100	100
42	l	120/124 (97%)	118 (98%)	2 (2%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
45	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	p	80/101 (79%)	80 (100%)	0	0	100	100
47	q	76/85 (89%)	76 (100%)	0	0	100	100
48	r	50/75 (67%)	50 (100%)	0	0	100	100
49	s	80/91 (88%)	80 (100%)	0	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	u	55/71 (78%)	55 (100%)	0	0	100	100
All	All	5401/5872 (92%)	5275 (98%)	120 (2%)	6 (0%)	49	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	137	VAL
16	L	79	LEU
11	G	13	ASN
36	f	33	ASP
36	f	94	HIS
36	f	86	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	44/47 (94%)	42 (96%)	2 (4%)	24	34
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	51 (98%)	1 (2%)	50	63
4	3	33/33 (100%)	32 (97%)	1 (3%)	36	48
7	C	217/220 (99%)	213 (98%)	4 (2%)	51	64
8	D	166/167 (99%)	160 (96%)	6 (4%)	31	42
9	E	155/155 (100%)	150 (97%)	5 (3%)	34	46
10	F	144/147 (98%)	137 (95%)	7 (5%)	22	31
11	G	139/142 (98%)	136 (98%)	3 (2%)	45	59
12	H	45/112 (40%)	42 (93%)	3 (7%)	15	19
13	I	117/118 (99%)	117 (100%)	0	100	100
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	106/108 (98%)	103 (97%)	3 (3%)	38	51
16	L	113/113 (100%)	110 (97%)	3 (3%)	39	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	M	96/101 (95%)	95 (99%)	1 (1%)	68	77
18	N	83/85 (98%)	78 (94%)	5 (6%)	17	23
19	O	98/102 (96%)	97 (99%)	1 (1%)	68	77
20	P	85/86 (99%)	83 (98%)	2 (2%)	43	56
21	Q	84/84 (100%)	83 (99%)	1 (1%)	63	74
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	77/87 (88%)	76 (99%)	1 (1%)	61	72
24	T	83/85 (98%)	82 (99%)	1 (1%)	63	74
25	U	79/80 (99%)	76 (96%)	3 (4%)	29	41
26	V	59/64 (92%)	59 (100%)	0	100	100
27	W	69/70 (99%)	68 (99%)	1 (1%)	59	70
28	X	53/56 (95%)	52 (98%)	1 (2%)	50	63
29	Y	54/54 (100%)	54 (100%)	0	100	100
30	Z	46/50 (92%)	45 (98%)	1 (2%)	45	59
32	b	185/200 (92%)	184 (100%)	1 (0%)	81	87
33	c	175/198 (88%)	171 (98%)	4 (2%)	44	57
34	d	170/171 (99%)	166 (98%)	4 (2%)	43	56
35	e	113/120 (94%)	110 (97%)	3 (3%)	39	52
36	f	94/111 (85%)	92 (98%)	2 (2%)	47	60
37	g	113/128 (88%)	107 (95%)	6 (5%)	20	28
38	h	108/109 (99%)	107 (99%)	1 (1%)	70	80
39	i	99/100 (99%)	95 (96%)	4 (4%)	28	39
40	j	89/91 (98%)	84 (94%)	5 (6%)	19	25
41	k	88/98 (90%)	84 (96%)	4 (4%)	24	34
42	l	104/106 (98%)	100 (96%)	4 (4%)	29	41
43	m	95/98 (97%)	91 (96%)	4 (4%)	26	37
44	n	81/82 (99%)	81 (100%)	0	100	100
45	o	71/72 (99%)	70 (99%)	1 (1%)	59	70
46	p	63/77 (82%)	61 (97%)	2 (3%)	34	46
47	q	70/76 (92%)	68 (97%)	2 (3%)	37	49
48	r	46/66 (70%)	44 (96%)	2 (4%)	26	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	s	70/78 (90%)	63 (90%)	7 (10%)	7	7
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	48/62 (77%)	47 (98%)	1 (2%)	47	60
All	All	4471/4756 (94%)	4358 (98%)	113 (2%)	42	54

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	3	ASP
1	0	23	LYS
3	2	51	VAL
4	3	6	SER
7	C	71	LYS
7	C	189	ARG
7	C	198	GLN
7	C	200	ASN
8	D	36	THR
8	D	42	GLU
8	D	140	SER
8	D	141	VAL
8	D	180	ILE
8	D	189	VAL
9	E	5	THR
9	E	32	THR
9	E	52	SER
9	E	74	SER
9	E	166	VAL
10	F	18	GLU
10	F	19	GLU
10	F	22	ILE
10	F	51	ASP
10	F	54	VAL
10	F	137	VAL
10	F	140	GLU
11	G	18	THR
11	G	47	GLU
11	G	127	THR
12	H	41	GLU
12	H	53	GLU
12	H	58	GLU
15	K	29	VAL

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Mol	Chain	Res	Type
15	K	72	ILE
15	K	123	THR
16	L	28	SER
16	L	81	VAL
16	L	111	GLU
17	M	86	ARG
18	N	22	LEU
18	N	59	LEU
18	N	107	ASP
18	N	111	GLU
18	N	115	GLU
19	O	27	ASP
20	P	56	GLN
20	P	77	SER
21	Q	41	VAL
23	S	72	THR
24	T	56	ILE
25	U	45	THR
25	U	65	VAL
25	U	71	ASP
27	W	51	LEU
28	X	43	VAL
30	Z	33	THR
32	b	34	PHE
33	c	84	ILE
33	c	88	GLN
33	c	213	GLN
33	c	216	ASN
34	d	32	THR
34	d	74	PHE
34	d	166	GLN
34	d	193	LEU
35	e	11	VAL
35	e	17	VAL
35	e	59	ILE
36	f	70	THR
36	f	96	ILE
37	g	25	LYS
37	g	56	VAL
37	g	104	LEU
37	g	119	ARG
37	g	123	GLU

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Mol	Chain	Res	Type
37	g	137	LYS
38	h	47	SER
39	i	20	SER
39	i	56	THR
39	i	91	THR
39	i	116	LEU
40	j	21	SER
40	j	24	GLU
40	j	35	GLN
40	j	57	VAL
40	j	67	ILE
41	k	17	GLU
41	k	29	THR
41	k	107	ASN
41	k	115	ILE
42	l	14	THR
42	l	86	ARG
42	l	93	VAL
42	l	98	VAL
43	m	63	VAL
43	m	74	SER
43	m	89	LEU
43	m	104	THR
45	o	73	LYS
46	p	38	VAL
46	p	86	SER
47	q	21	SER
47	q	24	VAL
48	r	66	SER
48	r	68	ILE
49	s	31	ILE
49	s	32	LYS
49	s	35	SER
49	s	50	SER
49	s	58	VAL
49	s	63	THR
49	s	71	LEU
51	u	33	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
7	C	23	HIS
7	C	48	HIS
7	C	185	HIS
8	D	108	GLN
8	D	133	GLN
10	F	58	GLN
11	G	38	HIS
11	G	104	ASN
11	G	139	GLN
12	H	43	ASN
13	I	47	HIS
13	I	136	GLN
13	I	138	GLN
18	N	35	HIS
20	P	101	HIS
21	Q	48	GLN
27	W	16	ASN
27	W	22	ASN
27	W	35	HIS
29	Y	24	GLN
29	Y	38	GLN
30	Z	6	ASN
33	c	18	HIS
33	c	25	ASN
33	c	28	GLN
33	c	100	GLN
34	d	50	GLN
40	j	15	HIS
42	l	112	GLN
46	p	64	GLN
49	s	56	ASN
49	s	57	HIS
50	t	6	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1527/1544 (98%)	254 (16%)	0
5	A	2679/2918 (91%)	402 (15%)	34 (1%)
6	B	114/115 (99%)	16 (14%)	2 (1%)
All	All	4320/4577 (94%)	672 (15%)	36 (0%)

All (672) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	41	U
5	A	53	G
5	A	56	A
5	A	58	G
5	A	67	G
5	A	68	A
5	A	78	A
5	A	80	A
5	A	81	A
5	A	82	G
5	A	92	G
5	A	95	G
5	A	98	A
5	A	104	C
5	A	105	C
5	A	109	G
5	A	125	A
5	A	126	A
5	A	127	U
5	A	146	U
5	A	147	A
5	A	170	A
5	A	171	C
5	A	172	A
5	A	188	A
5	A	203	A
5	A	206	A
5	A	223	A
5	A	229	A
5	A	235	U
5	A	236	U
5	A	240	A
5	A	255	G
5	A	257	G
5	A	259	G
5	A	262	A
5	A	278	U
5	A	279	U
5	A	280	A
5	A	295	U
5	A	303	C
5	A	313	A
5	A	318	G

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Mol	Chain	Res	Type
5	A	325	G
5	A	331	G
5	A	332	A
5	A	333	U
5	A	336	U
5	A	340	G
5	A	347	A
5	A	348	A
5	A	361	A
5	A	365	U
5	A	366	G
5	A	367	A
5	A	369	G
5	A	370	A
5	A	371	G
5	A	372	U
5	A	385	G
5	A	386	U
5	A	395	G
5	A	403	A
5	A	410	G
5	A	423	G
5	A	428	A
5	A	436	U
5	A	455	C
5	A	456	A
5	A	479	A
5	A	480	G
5	A	490	G
5	A	493	G
5	A	504	A
5	A	507	U
5	A	508	C
5	A	529	G
5	A	530	C
5	A	531	A
5	A	532	G
5	A	544	U
5	A	545	C
5	A	546	G
5	A	548	G
5	A	554	A

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Mol	Chain	Res	Type
5	A	561	A
5	A	571	U
5	A	572	A
5	A	573	A
5	A	601	A
5	A	611	U
5	A	612	A
5	A	625	A
5	A	635	A
5	A	636	G
5	A	651	U
5	A	653	A
5	A	684	U
5	A	699	G
5	A	721	C
5	A	728	A
5	A	745	U
5	A	762	A
5	A	769	G
5	A	773	G
5	A	774	G
5	A	780	A
5	A	782	G
5	A	783	G
5	A	799	G
5	A	800	A
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U
5	A	826	U
5	A	857	G
5	A	864	A
5	A	874	C
5	A	908	A
5	A	912	C
5	A	929	C
5	A	930	U
5	A	938	A
5	A	942	A
5	A	943	G
5	A	958	C

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Mol	Chain	Res	Type
5	A	971	G
5	A	980	A
5	A	993	A
5	A	1009	U
5	A	1010	C
5	A	1014	G
5	A	1023	G
5	A	1031	G
5	A	1042	U
5	A	1043	A
5	A	1044	G
5	A	1105	U
5	A	1106	C
5	A	1107	G
5	A	1108	A
5	A	1109	G
5	A	1128	G
5	A	1129	U
5	A	1130	A
5	A	1131	A
5	A	1132	C
5	A	1133	G
5	A	1136	G
5	A	1140	A
5	A	1170	U
5	A	1172	U
5	A	1173	G
5	A	1174	U
5	A	1201	G
5	A	1213	G
5	A	1242	A
5	A	1243	G
5	A	1244	U
5	A	1248	A
5	A	1250	U
5	A	1251	G
5	A	1257	G
5	A	1266	G
5	A	1267	A
5	A	1268	C
5	A	1269	A
5	A	1270	A

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Mol	Chain	Res	Type
5	A	1296	A
5	A	1297	A
5	A	1316	A
5	A	1320	U
5	A	1327	G
5	A	1336	G
5	A	1338	G
5	A	1347	U
5	A	1360	A
5	A	1363	G
5	A	1369	G
5	A	1374	U
5	A	1378	A
5	A	1390	A
5	A	1405	U
5	A	1411	G
5	A	1414	A
5	A	1415	U
5	A	1416	G
5	A	1423	C
5	A	1428	A
5	A	1447	G
5	A	1448	U
5	A	1453	U
5	A	1461	U
5	A	1462	G
5	A	1463	A
5	A	1511	A
5	A	1514	U
5	A	1519	U
5	A	1520	A
5	A	1523	A
5	A	1528	G
5	A	1529	U
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1534	G
5	A	1539	G
5	A	1540	C
5	A	1542	A

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Mol	Chain	Res	Type
5	A	1543	A
5	A	1552	U
5	A	1553	G
5	A	1557	U
5	A	1564	A
5	A	1565	G
5	A	1567	A
5	A	1577	A
5	A	1579	G
5	A	1583	C
5	A	1606	A
5	A	1614	A
5	A	1615	C
5	A	1645	U
5	A	1646	U
5	A	1672	G
5	A	1697	G
5	A	1725	U
5	A	1728	C
5	A	1729	U
5	A	1734	G
5	A	1746	G
5	A	1755	A
5	A	1760	G
5	A	1769	A
5	A	1772	G
5	A	1776	A
5	A	1787	A
5	A	1796	C
5	A	1797	A
5	A	1805	A
5	A	1807	G
5	A	1812	C
5	A	1817	A
5	A	1829	C
5	A	1845	G
5	A	1849	A
5	A	1868	A
5	A	1869	G
5	A	1870	C
5	A	1871	G
5	A	1872	A

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Mol	Chain	Res	Type
5	A	1874	G
5	A	1878	U
5	A	1881	A
5	A	1885	A
5	A	1895	A
5	A	1897	A
5	A	1902	G
5	A	1925	G
5	A	1934	A
5	A	1936	U
5	A	1937	C
5	A	1939	U
5	A	1951	U
5	A	1959	U
5	A	1960	G
5	A	1963	C
5	A	1966	A
5	A	1967	U
5	A	1968	G
5	A	1987	U
5	A	1989	U
5	A	2018	U
5	A	2019	C
5	A	2025	G
5	A	2026	6MZ
5	A	2027	A
5	A	2029	A
5	A	2039	C
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2058	A
5	A	2065	7MG
5	A	2089	G
5	A	2186	G
5	A	2187	A
5	A	2194	A
5	A	2195	A
5	A	2199	U
5	A	2200	G
5	A	2207	G

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Mol	Chain	Res	Type
5	A	2210	C
5	A	2221	A
5	A	2234	G
5	A	2235	G
5	A	2269	A
5	A	2279	U
5	A	2283	A
5	A	2284	A
5	A	2300	G
5	A	2301	U
5	A	2302	C
5	A	2303	G
5	A	2304	G
5	A	2305	A
5	A	2308	U
5	A	2317	G
5	A	2321	A
5	A	2323	A
5	A	2327	G
5	A	2341	A
5	A	2343	C
5	A	2346	C
5	A	2355	C
5	A	2375	G
5	A	2378	G
5	A	2379	G
5	A	2381	C
5	A	2398	U
5	A	2402	U
5	A	2416	C
5	A	2421	A
5	A	2423	C
5	A	2425	G
5	A	2426	A
5	A	2427	U
5	A	2428	A
5	A	2429	A
5	A	2430	A
5	A	2437	U
5	A	2444	A
5	A	2446	A
5	A	2465	A

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Mol	Chain	Res	Type
5	A	2469	U
5	A	2472	A
5	A	2473	U
5	A	2474	A
5	A	2487	U
5	A	2488	U
5	A	2493	A
5	A	2494	C
5	A	2498	G
5	A	2499	2MA
5	A	2509	A
5	A	2514	A
5	A	2516	C
5	A	2525	G
5	A	2543	A
5	A	2548	OMU
5	A	2550	U
5	A	2552	C
5	A	2562	A
5	A	2563	G
5	A	2574	G
5	A	2578	G
5	A	2581	U
5	A	2582	U
5	A	2598	A
5	A	2599	G
5	A	2605	U
5	A	2606	C
5	A	2607	C
5	A	2609	U
5	A	2625	U
5	A	2635	A
5	A	2636	G
5	A	2650	A
5	A	2651	G
5	A	2652	U
5	A	2656	A
5	A	2657	G
5	A	2661	A
5	A	2685	U
5	A	2686	A
5	A	2687	C

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Mol	Chain	Res	Type
5	A	2709	C
5	A	2710	G
5	A	2722	U
5	A	2729	A
5	A	2740	G
5	A	2744	A
5	A	2748	C
5	A	2754	A
5	A	2761	A
5	A	2774	A
5	A	2776	A
5	A	2777	A
5	A	2786	U
5	A	2787	A
5	A	2793	U
5	A	2796	U
5	A	2797	G
5	A	2816	G
5	A	2857	U
5	A	2863	A
5	A	2875	A
5	A	2876	C
5	A	2897	C
6	B	11	A
6	B	13	A
6	B	21	U
6	B	22	G
6	B	23	A
6	B	39	C
6	B	42	G
6	B	51	A
6	B	62	U
6	B	64	A
6	B	65	G
6	B	71	A
6	B	86	U
6	B	87	A
6	B	105	C
6	B	106	A
31	a	6	C
31	a	11	G
31	a	18	A

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Mol	Chain	Res	Type
31	a	24	G
31	a	34	A
31	a	41	G
31	a	49	C
31	a	50	U
31	a	53	A
31	a	62	A
31	a	80	A
31	a	81	G
31	a	83	U
31	a	84	U
31	a	85	G
31	a	86	C
31	a	90	C
31	a	91	G
31	a	97	A
31	a	105	A
31	a	117	U
31	a	126	A
31	a	127	U
31	a	144	G
31	a	157	A
31	a	184	A
31	a	186	G
31	a	193	A
31	a	200	G
31	a	201	A
31	a	202	U
31	a	203	C
31	a	206	C
31	a	209	A
31	a	236	C
31	a	239	A
31	a	241	U
31	a	243	G
31	a	247	G
31	a	262	G
31	a	263	C
31	a	276	C
31	a	285	G
31	a	289	G
31	a	297	G

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Mol	Chain	Res	Type
31	a	302	A
31	a	317	A
31	a	324	C
31	a	325	A
31	a	340	A
31	a	341	C
31	a	348	C
31	a	350	G
31	a	363	U
31	a	368	C
31	a	369	A
31	a	380	C
31	a	389	A
31	a	393	A
31	a	394	U
31	a	402	G
31	a	407	A
31	a	408	A
31	a	410	A
31	a	417	U
31	a	418	A
31	a	420	G
31	a	422	U
31	a	423	U
31	a	424	G
31	a	425	U
31	a	426	A
31	a	435	U
31	a	437	A
31	a	444	A
31	a	448	G
31	a	459	U
31	a	461	A
31	a	464	A
31	a	465	C
31	a	466	C
31	a	479	A
31	a	481	G
31	a	482	U
31	a	490	A
31	a	492	A
31	a	494	U

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Mol	Chain	Res	Type
31	a	496	A
31	a	501	C
31	a	505	U
31	a	506	A
31	a	508	C
31	a	518	G
31	a	521	G
31	a	522	C
31	a	527	G
31	a	528	U
31	a	530	A
31	a	532	A
31	a	544	A
31	a	559	U
31	a	561	C
31	a	569	A
31	a	570	A
31	a	573	C
31	a	623	G
31	a	630	G
31	a	639	A
31	a	650	A
31	a	651	G
31	a	662	A
31	a	684	A
31	a	685	G
31	a	699	A
31	a	700	G
31	a	720	U
31	a	721	G
31	a	728	G
31	a	731	G
31	a	752	G
31	a	774	A
31	a	778	A
31	a	782	G
31	a	789	A
31	a	790	U
31	a	791	A
31	a	809	G
31	a	810	U
31	a	812	A

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Mol	Chain	Res	Type
31	a	813	A
31	a	814	C
31	a	816	A
31	a	817	U
31	a	825	A
31	a	841	G
31	a	842	A
31	a	856	C
31	a	864	G
31	a	867	A
31	a	868	U
31	a	899	G
31	a	923	G
31	a	924	G
31	a	925	G
31	a	931	C
31	a	932	A
31	a	957	U
31	a	963	2MG
31	a	966	A
31	a	968	G
31	a	970	G
31	a	972	A
31	a	973	G
31	a	974	A
31	a	989	U
31	a	990	G
31	a	993	A
31	a	1001	A
31	a	1002	A
31	a	1006	U
31	a	1007	U
31	a	1022	U
31	a	1023	G
31	a	1026	U
31	a	1027	U
31	a	1028	C
31	a	1029	G
31	a	1030	G
31	a	1031	G
31	a	1035	C
31	a	1050	G

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Mol	Chain	Res	Type
31	a	1052	A
31	a	1062	U
31	a	1076	G
31	a	1077	A
31	a	1082	U
31	a	1083	U
31	a	1084	G
31	a	1091	G
31	a	1095	C
31	a	1098	A
31	a	1122	U
31	a	1127	A
31	a	1134	C
31	a	1135	G
31	a	1136	G
31	a	1140	G
31	a	1141	G
31	a	1151	G
31	a	1154	A
31	a	1155	C
31	a	1156	U
31	a	1157	G
31	a	1158	C
31	a	1161	G
31	a	1165	C
31	a	1166	A
31	a	1168	A
31	a	1179	G
31	a	1180	C
31	a	1189	C
31	a	1193	A
31	a	1194	A
31	a	1197	C
31	a	1209	U
31	a	1210	A
31	a	1211	C
31	a	1222	A
31	a	1224	A
31	a	1235	A
31	a	1253	U
31	a	1255	G
31	a	1267	U

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Mol	Chain	Res	Type
31	a	1276	A
31	a	1277	A
31	a	1278	U
31	a	1284	A
31	a	1295	U
31	a	1297	G
31	a	1299	C
31	a	1317	C
31	a	1335	G
31	a	1342	U
31	a	1343	A
31	a	1350	G
31	a	1360	A
31	a	1367	G
31	a	1374	A
31	a	1375	C
31	a	1378	U
31	a	1387	U
31	a	1394	C
31	a	1395	A
31	a	1397	C
31	a	1398	G
31	a	1415	A
31	a	1416	G
31	a	1423	G
31	a	1427	C
31	a	1438	A
31	a	1439	G
31	a	1443	A
31	a	1444	A
31	a	1449	A
31	a	1464	C
31	a	1484	G
31	a	1500	A
31	a	1503	U
31	a	1507	C
31	a	1513	G
31	a	1516	MA6
31	a	1526	G
31	a	1527	G
31	a	1528	A

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	84	U
5	A	91	A
5	A	256	C
5	A	279	U
5	A	324	A
5	A	365	U
5	A	368	C
5	A	371	G
5	A	463	U
5	A	478	A
5	A	507	U
5	A	782	G
5	A	798	U
5	A	799	G
5	A	929	C
5	A	1042	U
5	A	1106	C
5	A	1127	U
5	A	1173	G
5	A	1179	G
5	A	1267	A
5	A	1268	C
5	A	1296	A
5	A	1335	U
5	A	1337	A
5	A	1519	U
5	A	1564	A
5	A	1816	U
5	A	1844	A
5	A	1869	G
5	A	1880	G
5	A	2209	U
5	A	2651	G
5	A	2747	G
6	B	50	A
6	B	86	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	MA6	a	1516	31	23,26,27	1.38	4 (17%)	33,38,41	3.21	12 (36%)
31	7MG	a	524	31	23,26,27	1.11	1 (4%)	27,39,42	0.88	2 (7%)
31	UR3	a	1495	31	19,22,23	2.98	6 (31%)	26,32,35	1.59	3 (11%)
5	6MZ	A	2026	5	22,25,26	2.48	4 (18%)	29,36,39	3.31	10 (34%)
31	5MC	a	964	31	19,22,23	0.51	0	26,32,35	0.63	0
31	PSU	a	513	31	18,21,22	1.11	1 (5%)	21,30,33	1.86	4 (19%)
5	2MA	A	2499	5	22,25,26	3.97	9 (40%)	32,37,40	2.69	11 (34%)
5	PSU	A	2453	5	18,21,22	1.12	1 (5%)	21,30,33	1.99	6 (28%)
5	OMU	A	2548	5	19,22,23	3.13	8 (42%)	25,31,34	1.82	5 (20%)
31	MA6	a	1515	31	23,26,27	1.39	4 (17%)	33,38,41	3.19	12 (36%)
5	PSU	A	952	5	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
5	OMG	A	2247	5	23,26,27	0.44	0	32,38,41	0.50	0
31	2MG	a	1204	31	23,26,27	0.46	0	33,38,41	0.54	0
5	PSU	A	2500	5	18,21,22	1.12	1 (5%)	21,30,33	1.92	5 (23%)
5	PSU	A	2576	5	18,21,22	1.19	1 (5%)	21,30,33	2.02	6 (28%)
5	2MG	A	2441	5	23,26,27	0.45	0	33,38,41	0.49	0
31	4OC	a	1399	31	20,23,24	3.22	8 (40%)	25,32,35	0.90	1 (4%)
5	PSU	A	2601	5	18,21,22	1.11	1 (5%)	21,30,33	1.90	4 (19%)
5	7MG	A	2065	5	23,26,27	1.08	1 (4%)	27,39,42	0.89	2 (7%)
5	5MU	A	1935	5	19,22,23	0.37	0	27,32,35	0.55	0
31	2MG	a	963	31	23,26,27	0.48	0	33,38,41	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	MA6	a	1516	31	-	2/11/29/30	0/3/3/3
31	7MG	a	524	31	-	1/7/37/38	0/3/3/3
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
5	6MZ	A	2026	5	-	0/9/27/28	0/3/3/3
31	5MC	a	964	31	-	0/7/25/26	0/2/2/2
31	PSU	a	513	31	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	2MA	A	2499	5	-	4/7/25/26	0/3/3/3
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
5	OMU	A	2548	5	-	2/9/27/28	0/2/2/2
31	MA6	a	1515	31	-	0/11/29/30	0/3/3/3
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
5	OMG	A	2247	5	-	1/9/27/28	0/3/3/3
31	2MG	a	1204	31	-	0/9/27/28	0/3/3/3
5	PSU	A	2500	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
5	2MG	A	2441	5	-	0/9/27/28	0/3/3/3
31	4OC	a	1399	31	-	0/9/29/30	0/2/2/2
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
5	7MG	A	2065	5	-	0/7/37/38	0/3/3/3
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
31	2MG	a	963	31	-	2/9/27/28	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2499	2MA	C4-N3	12.11	1.49	1.34
5	A	2026	6MZ	C6-N6	10.16	1.45	1.34
5	A	2499	2MA	C2-N3	7.45	1.46	1.34
5	A	2548	OMU	C2-N1	7.41	1.50	1.38
31	a	1495	UR3	C2-N1	7.40	1.48	1.38
31	a	1399	4OC	C4-N3	7.24	1.45	1.32
5	A	2499	2MA	C6-N1	7.06	1.44	1.35
5	A	2548	OMU	C2-N3	6.96	1.50	1.38
31	a	1495	UR3	C6-C5	6.87	1.51	1.35
31	a	1399	4OC	C6-C5	6.28	1.49	1.35
31	a	1399	4OC	C2-N3	6.27	1.48	1.36
5	A	2499	2MA	C2-N1	6.10	1.44	1.34
31	a	1495	UR3	C2-N3	5.80	1.50	1.39
5	A	2548	OMU	C6-C5	5.79	1.48	1.35
31	a	1399	4OC	C4-N4	4.89	1.46	1.36
5	A	2499	2MA	C5-C6	4.74	1.54	1.41
31	a	524	7MG	C5-N7	4.58	1.41	1.35
5	A	2065	7MG	C5-N7	4.49	1.41	1.35
5	A	2548	OMU	C4-N3	4.43	1.46	1.38
31	a	1399	4OC	C2-N1	4.36	1.49	1.40
31	a	1515	MA6	C6-N6	4.06	1.48	1.36
31	a	1516	MA6	C6-N6	4.04	1.48	1.36
5	A	2576	PSU	C6-C5	3.87	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	513	PSU	C6-C5	3.81	1.39	1.35
5	A	952	PSU	C6-C5	3.74	1.39	1.35
5	A	2500	PSU	C6-C5	3.72	1.39	1.35
5	A	2601	PSU	C6-C5	3.69	1.39	1.35
5	A	2453	PSU	C6-C5	3.68	1.39	1.35
31	a	1399	4OC	C5-C4	3.65	1.49	1.41
31	a	1495	UR3	C6-N1	3.45	1.46	1.38
5	A	2499	2MA	C6-N6	-3.38	1.25	1.34
31	a	1399	4OC	C6-N1	3.37	1.46	1.38
5	A	2026	6MZ	C5-N7	-3.00	1.33	1.39
5	A	2548	OMU	C6-N1	2.93	1.45	1.38
5	A	2548	OMU	O4-C4	-2.88	1.18	1.24
31	a	1515	MA6	C5-C4	-2.85	1.34	1.39
31	a	1516	MA6	C5-C4	-2.78	1.34	1.39
31	a	1495	UR3	C4-N3	2.74	1.46	1.40
5	A	2026	6MZ	C5-C4	-2.63	1.34	1.39
31	a	1399	4OC	O2-C2	-2.63	1.18	1.23
5	A	2548	OMU	C5-C4	2.51	1.49	1.43
5	A	2548	OMU	O2-C2	-2.39	1.18	1.23
5	A	2499	2MA	C5-N7	-2.39	1.34	1.39
31	a	1495	UR3	C5-C4	2.36	1.49	1.43
31	a	1516	MA6	C5-N7	-2.30	1.34	1.39
5	A	2499	2MA	C4-N9	-2.25	1.33	1.37
31	a	1515	MA6	C5-N7	-2.25	1.35	1.39
5	A	2026	6MZ	C8-N9	-2.24	1.33	1.37
5	A	2499	2MA	C8-N7	2.15	1.35	1.31
31	a	1515	MA6	C8-N9	-2.15	1.33	1.37
31	a	1516	MA6	C8-N9	-2.04	1.34	1.37

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1516	MA6	N1-C6-N6	-11.47	102.88	116.86
31	a	1515	MA6	N1-C6-N6	-11.39	102.97	116.86
5	A	2026	6MZ	C4-N9-C1'	-8.42	106.94	126.63
5	A	2026	6MZ	C1'-N9-C8	8.40	145.75	127.09
31	a	1515	MA6	C5-C6-N6	7.75	137.59	125.33
31	a	1516	MA6	C5-C6-N6	7.72	137.55	125.33
5	A	2499	2MA	C1'-N9-C8	-7.24	111.03	127.09
5	A	2026	6MZ	C5-C4-N3	-6.43	117.87	126.72
5	A	2499	2MA	N9-C8-N7	-5.76	105.76	113.94
5	A	2026	6MZ	N1-C2-N3	-5.65	120.02	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1516	MA6	N1-C2-N3	-5.60	120.11	128.58
5	A	2548	OMU	C4-N3-C2	-5.57	119.69	126.61
5	A	2499	2MA	C5-C4-N3	-5.56	121.33	127.18
31	a	1515	MA6	N1-C2-N3	-5.55	120.18	128.58
31	a	1495	UR3	C4-N3-C2	-5.49	120.16	124.58
5	A	2499	2MA	C4-N9-C8	5.00	110.99	105.74
5	A	2026	6MZ	C4-C5-C6	4.91	120.86	116.78
5	A	2453	PSU	N1-C2-N3	4.90	120.34	115.17
5	A	952	PSU	C4-N3-C2	-4.90	119.63	126.37
5	A	2576	PSU	N1-C2-N3	4.89	120.32	115.17
5	A	2601	PSU	C4-N3-C2	-4.89	119.64	126.37
5	A	2453	PSU	C4-N3-C2	-4.87	119.67	126.37
5	A	2499	2MA	C4-N9-C1'	4.85	137.98	126.63
5	A	2576	PSU	C4-N3-C2	-4.83	119.72	126.37
5	A	2500	PSU	C4-N3-C2	-4.81	119.74	126.37
5	A	2500	PSU	N1-C2-N3	4.80	120.23	115.17
31	a	513	PSU	C4-N3-C2	-4.77	119.81	126.37
31	a	1516	MA6	C5-C4-N3	-4.76	120.17	126.72
31	a	513	PSU	N1-C2-N3	4.75	120.18	115.17
5	A	952	PSU	N1-C2-N3	4.75	120.18	115.17
5	A	2601	PSU	N1-C2-N3	4.75	120.17	115.17
31	a	1515	MA6	C5-C4-N3	-4.65	120.31	126.72
5	A	2026	6MZ	N3-C4-N9	4.48	134.78	127.17
31	a	1515	MA6	N9-C8-N7	-4.33	107.79	113.94
31	a	1516	MA6	N9-C8-N7	-4.30	107.83	113.94
5	A	2499	2MA	N3-C4-N9	4.12	132.22	126.99
31	a	1515	MA6	C4-C5-C6	4.04	120.09	115.91
31	a	1516	MA6	C4-C5-C6	4.04	120.08	115.91
5	A	2548	OMU	N3-C2-N1	3.96	120.05	114.89
5	A	2026	6MZ	C2-N3-C4	3.89	121.34	111.83
31	a	1495	UR3	C5-C4-N3	3.61	119.80	115.04
5	A	2548	OMU	C5-C4-N3	3.53	119.74	114.80
5	A	2026	6MZ	N9-C8-N7	-3.53	108.93	113.94
31	a	1515	MA6	C2-N1-C6	3.48	120.32	111.83
31	a	1516	MA6	C2-N1-C6	3.47	120.30	111.83
5	A	2499	2MA	C5-N7-C8	3.38	108.76	103.45
5	A	2499	2MA	N3-C2-N1	-3.30	119.95	125.77
31	a	1516	MA6	C2-N3-C4	3.25	119.77	111.83
31	a	1515	MA6	C2-N3-C4	3.21	119.67	111.83
31	a	1516	MA6	C5-N7-C8	2.96	108.10	103.45
5	A	2453	PSU	O2-C2-N1	-2.95	119.74	122.79
31	a	1515	MA6	C5-N7-C8	2.91	108.02	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2576	PSU	O2-C2-N1	-2.90	119.80	122.79
31	a	1516	MA6	N3-C4-N9	2.89	132.09	127.17
5	A	2548	OMU	O4-C4-C5	-2.87	120.20	125.16
5	A	2500	PSU	O2-C2-N1	-2.87	119.83	122.79
5	A	2026	6MZ	C5-N7-C8	2.85	107.93	103.45
5	A	952	PSU	O2-C2-N1	-2.85	119.85	122.79
31	a	513	PSU	O2-C2-N1	-2.82	119.88	122.79
31	a	1515	MA6	N3-C4-N9	2.81	131.95	127.17
5	A	2453	PSU	C6-C5-C4	2.62	119.94	118.17
5	A	2576	PSU	O4'-C1'-C2'	2.60	108.75	105.15
31	a	1515	MA6	C4-N9-C8	2.56	108.42	105.74
5	A	2601	PSU	O2-C2-N1	-2.52	120.19	122.79
5	A	2576	PSU	C6-N1-C2	-2.52	120.36	122.69
31	a	524	7MG	C4-C5-N7	2.51	108.34	105.38
5	A	2065	7MG	C4-C5-N7	2.50	108.33	105.38
31	a	1399	4OC	C6-C5-C4	2.45	119.95	117.00
31	a	1516	MA6	C4-N9-C8	2.43	108.29	105.74
5	A	2601	PSU	C6-N1-C2	-2.34	120.52	122.69
31	a	513	PSU	C6-N1-C2	-2.33	120.53	122.69
5	A	2026	6MZ	C5-C6-N1	2.32	120.64	118.15
5	A	2500	PSU	C6-C5-C4	2.29	119.72	118.17
5	A	2500	PSU	C6-N1-C2	-2.28	120.58	122.69
5	A	2453	PSU	C6-N1-C2	-2.27	120.58	122.69
31	a	1495	UR3	C6-N1-C2	-2.25	119.96	121.80
31	a	1515	MA6	C4-C5-N7	-2.24	108.02	110.58
5	A	2499	2MA	C4-C5-N7	-2.23	108.03	110.58
31	a	1516	MA6	C4-C5-N7	-2.22	108.04	110.58
5	A	2548	OMU	O2-C2-N1	-2.22	119.91	122.80
5	A	2499	2MA	CM2-C2-N1	2.21	120.44	117.13
5	A	2576	PSU	C6-C5-C4	2.21	119.66	118.17
5	A	2065	7MG	C5-C4-N9	2.19	109.14	106.33
5	A	952	PSU	C6-N1-C2	-2.17	120.67	122.69
31	a	524	7MG	C5-C4-N9	2.15	109.09	106.33
5	A	2499	2MA	N6-C6-N1	2.13	119.91	117.03
5	A	2453	PSU	O4'-C1'-C2'	2.09	108.05	105.15

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	a	963	2MG	O4'-C4'-C5'-O5'
31	a	1516	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	A	2247	OMG	C1'-C2'-O2'-CM2
5	A	2548	OMU	C3'-C4'-C5'-O5'
5	A	2548	OMU	O4'-C4'-C5'-O5'
31	a	513	PSU	C3'-C4'-C5'-O5'
31	a	513	PSU	O4'-C4'-C5'-O5'
31	a	963	2MG	C3'-C4'-C5'-O5'
31	a	1516	MA6	C3'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
5	A	2499	2MA	O4'-C4'-C5'-O5'
31	a	524	7MG	C3'-C4'-C5'-O5'
5	A	2499	2MA	C4'-C5'-O5'-P
5	A	2499	2MA	O4'-C1'-N9-C8

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	1516	MA6	1	0
31	a	524	7MG	1	0
5	A	2026	6MZ	2	0
31	a	964	5MC	1	0
31	a	1515	MA6	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
53	80P	a	1603	54	45,45,45	3.70	22 (48%)	51,72,72	2.48	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
53	80P	a	1602	54	45,45,45	3.90	22 (48%)	51,72,72	2.52	18 (35%)
53	80P	a	1601	54	45,45,45	3.68	20 (44%)	51,72,72	2.58	18 (35%)

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
53	80P	a	1603	54	-	5/22/87/87	0/5/5/5
53	80P	a	1602	54	-	11/22/87/87	0/5/5/5
53	80P	a	1601	54	-	10/22/87/87	0/5/5/5

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	a	1602	80P	C08-C09	12.22	1.62	1.52
53	a	1601	80P	C08-C09	12.12	1.62	1.52
53	a	1603	80P	C08-C09	11.82	1.62	1.52
53	a	1602	80P	C21-C04	10.57	1.64	1.54
53	a	1601	80P	C21-C04	9.80	1.63	1.54
53	a	1601	80P	C08-C21	9.40	1.61	1.53
53	a	1602	80P	C08-C21	8.32	1.60	1.53
53	a	1603	80P	C08-C21	7.78	1.60	1.53
53	a	1602	80P	C04-N03	7.50	1.54	1.47
53	a	1603	80P	C21-C04	7.16	1.61	1.54
53	a	1603	80P	C04-N03	6.73	1.54	1.47
53	a	1603	80P	C06-C36	6.71	1.61	1.47
53	a	1602	80P	C06-C36	6.70	1.61	1.47
53	a	1603	80P	C06-C07	6.53	1.64	1.46
53	a	1603	80P	C08-C07	6.34	1.63	1.55
53	a	1602	80P	C06-C07	5.75	1.61	1.46
53	a	1601	80P	C06-C36	5.73	1.59	1.47
53	a	1602	80P	C08-C07	5.72	1.62	1.55
53	a	1602	80P	C04-C05	5.64	1.62	1.51
53	a	1601	80P	C04-N03	5.48	1.52	1.47
53	a	1603	80P	C04-C05	5.21	1.62	1.51
53	a	1601	80P	C06-C07	5.18	1.60	1.46
53	a	1601	80P	C04-C05	5.17	1.61	1.51
53	a	1603	80P	C18-C17	5.04	1.59	1.51
53	a	1603	80P	C18-C19	4.56	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	a	1601	80P	C08-C07	4.44	1.60	1.55
53	a	1602	80P	C18-C17	4.41	1.58	1.51
53	a	1601	80P	C18-C19	4.34	1.64	1.52
53	a	1602	80P	C18-C19	4.19	1.63	1.52
53	a	1602	80P	C10-C11	3.79	1.55	1.46
53	a	1603	80P	C16-C17	3.74	1.46	1.40
53	a	1601	80P	C18-C17	3.70	1.57	1.51
53	a	1601	80P	C10-C11	3.58	1.54	1.46
53	a	1602	80P	C16-C17	3.56	1.46	1.40
53	a	1603	80P	C10-C11	3.51	1.54	1.46
53	a	1601	80P	C16-C17	3.47	1.46	1.40
53	a	1601	80P	C12-C11	3.47	1.55	1.46
53	a	1602	80P	C12-C11	3.36	1.55	1.46
53	a	1603	80P	C12-C11	3.13	1.54	1.46
53	a	1603	80P	C22-C16	3.10	1.58	1.51
53	a	1602	80P	C22-C16	3.05	1.58	1.51
53	a	1602	80P	C12-C13	2.88	1.46	1.41
53	a	1601	80P	C22-C16	2.83	1.58	1.51
53	a	1601	80P	C15-C26	2.74	1.56	1.52
53	a	1602	80P	C15-C26	2.72	1.56	1.52
53	a	1603	80P	C12-C13	2.72	1.45	1.41
53	a	1603	80P	C19-C10	2.71	1.54	1.51
53	a	1603	80P	C15-C26	2.60	1.55	1.52
53	a	1603	80P	C20-C19	2.53	1.59	1.53
53	a	1602	80P	C36-N38	2.50	1.40	1.33
53	a	1601	80P	C19-C10	2.48	1.54	1.51
53	a	1603	80P	C36-N38	2.47	1.40	1.33
53	a	1602	80P	C20-C19	2.46	1.58	1.53
53	a	1602	80P	C40-N03	2.45	1.54	1.47
53	a	1601	80P	C36-N38	2.41	1.40	1.33
53	a	1601	80P	C40-N03	2.32	1.54	1.47
53	a	1601	80P	C12-C13	2.27	1.45	1.41
53	a	1602	80P	C14-C15	2.25	1.43	1.39
53	a	1603	80P	C16-C15	2.24	1.43	1.40
53	a	1603	80P	C40-N03	2.24	1.53	1.47
53	a	1602	80P	C19-C10	2.23	1.53	1.51
53	a	1603	80P	C14-C15	2.20	1.43	1.39
53	a	1601	80P	C20-C19	2.06	1.58	1.53
53	a	1602	80P	C16-C15	2.05	1.43	1.40

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	a	1601	80P	C11-C10-C09	9.01	125.93	118.80
53	a	1602	80P	C11-C10-C09	8.86	125.81	118.80
53	a	1603	80P	C11-C10-C09	8.45	125.49	118.80
53	a	1601	80P	C08-C21-C04	5.38	119.00	111.64
53	a	1602	80P	C08-C21-C04	5.14	118.67	111.64
53	a	1603	80P	C12-C11-C10	4.84	127.35	118.28
53	a	1603	80P	C36-C06-C07	-4.73	115.37	120.97
53	a	1602	80P	C12-C11-C10	4.72	127.13	118.28
53	a	1601	80P	C18-C17-C16	4.67	127.19	119.75
53	a	1601	80P	O33-C09-C08	-4.61	106.69	113.37
53	a	1601	80P	C36-C06-C07	-4.56	115.57	120.97
53	a	1601	80P	C12-C11-C10	4.55	126.80	118.28
53	a	1602	80P	O33-C09-C08	-4.42	106.97	113.37
53	a	1603	80P	O33-C09-C08	-4.39	107.02	113.37
53	a	1603	80P	C13-C12-C17	4.28	123.62	119.03
53	a	1601	80P	C13-C12-C17	4.20	123.54	119.03
53	a	1602	80P	C18-C17-C16	4.19	126.43	119.75
53	a	1603	80P	C18-C17-C16	4.12	126.31	119.75
53	a	1602	80P	C13-C12-C17	4.09	123.42	119.03
53	a	1602	80P	C36-C06-C07	-3.97	116.28	120.97
53	a	1603	80P	C08-C21-C04	3.84	116.89	111.64
53	a	1601	80P	C20-C21-C04	-3.80	108.24	113.73
53	a	1601	80P	O33-C09-C10	3.56	130.44	123.52
53	a	1603	80P	C13-C12-C11	-3.56	116.18	121.45
53	a	1603	80P	C17-C18-C19	3.47	117.72	113.12
53	a	1603	80P	O33-C09-C10	3.44	130.20	123.52
53	a	1602	80P	O33-C09-C10	3.41	130.13	123.52
53	a	1602	80P	C20-C21-C04	-3.34	108.91	113.73
53	a	1601	80P	C13-C12-C11	-3.20	116.72	121.45
53	a	1602	80P	C17-C18-C19	3.20	117.36	113.12
53	a	1602	80P	F25-C22-C16	3.14	119.64	112.32
53	a	1602	80P	O32-C11-C10	-3.03	115.88	121.14
53	a	1602	80P	C13-C12-C11	-3.02	116.97	121.45
53	a	1601	80P	C17-C18-C19	2.99	117.08	113.12
53	a	1603	80P	O32-C11-C10	-2.99	115.94	121.14
53	a	1601	80P	O32-C11-C10	-2.96	115.99	121.14
53	a	1603	80P	O32-C11-C12	-2.96	116.71	122.06
53	a	1603	80P	C20-C21-C04	-2.89	109.56	113.73
53	a	1601	80P	F23-C22-C16	2.87	119.00	112.32
53	a	1603	80P	F25-C22-C16	2.85	118.97	112.32
53	a	1603	80P	O37-C36-N38	-2.82	116.56	122.89
53	a	1602	80P	O32-C11-C12	-2.80	116.99	122.06
53	a	1602	80P	O37-C36-N38	-2.78	116.67	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	a	1602	80P	C14-C13-C12	-2.74	117.85	120.92
53	a	1601	80P	O32-C11-C12	-2.68	117.21	122.06
53	a	1601	80P	O37-C36-N38	-2.63	116.99	122.89
53	a	1603	80P	C14-C13-C12	-2.59	118.01	120.92
53	a	1603	80P	C08-C07-C06	2.50	119.73	115.75
53	a	1601	80P	C14-C13-C12	-2.49	118.13	120.92
53	a	1603	80P	F23-C22-C16	2.26	117.60	112.32
53	a	1602	80P	C21-C08-C07	-2.21	108.51	111.05
53	a	1602	80P	F23-C22-C16	2.17	117.39	112.32
53	a	1601	80P	F25-C22-C16	2.12	117.27	112.32
53	a	1601	80P	C21-C08-C07	-2.06	108.69	111.05

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	a	1601	80P	C21-C04-N03-C01
53	a	1601	80P	C07-C06-C36-O37
53	a	1602	80P	C07-C06-C36-N38
53	a	1602	80P	C07-C06-C36-O37
53	a	1602	80P	C16-C15-C26-C30
53	a	1601	80P	C21-C04-N03-C40
53	a	1601	80P	C05-C06-C36-N38
53	a	1601	80P	C07-C06-C36-N38
53	a	1602	80P	C15-C16-C22-F25
53	a	1601	80P	C05-C04-N03-C01
53	a	1602	80P	C15-C16-C22-F24
53	a	1601	80P	C15-C16-C22-F23
53	a	1603	80P	C15-C16-C22-F25
53	a	1602	80P	C15-C16-C22-F23
53	a	1601	80P	C15-C16-C22-F24
53	a	1602	80P	C17-C16-C22-F25
53	a	1603	80P	C15-C16-C22-F24
53	a	1603	80P	C15-C16-C22-F23
53	a	1601	80P	C41-C40-N03-C04
53	a	1602	80P	C17-C16-C22-F23
53	a	1602	80P	C14-C15-C26-N27
53	a	1603	80P	C14-C15-C26-N27
53	a	1601	80P	C15-C16-C22-F25
53	a	1602	80P	C16-C15-C26-N27
53	a	1603	80P	C16-C15-C26-N27
53	a	1602	80P	C17-C16-C22-F24

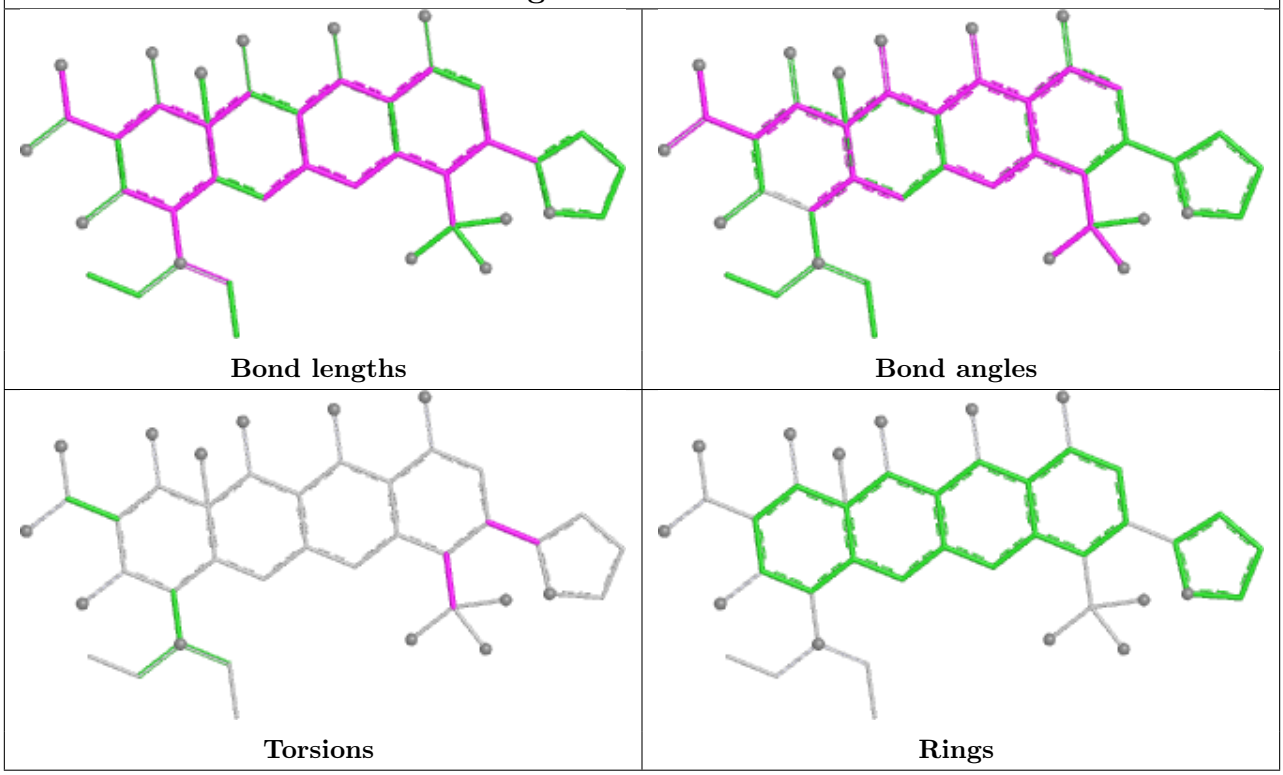
There are no ring outliers.

2 monomers are involved in 1 short contact:

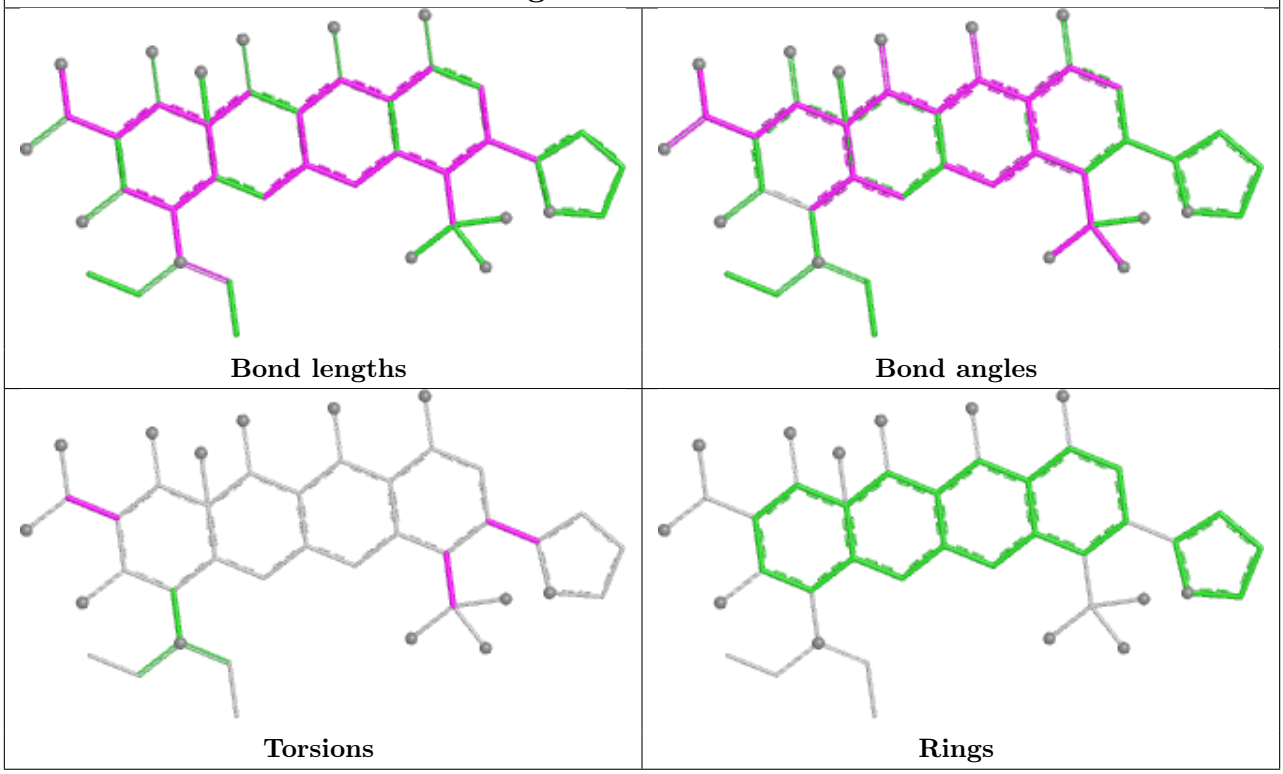
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	a	1603	80P	1	0
53	a	1602	80P	1	0

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

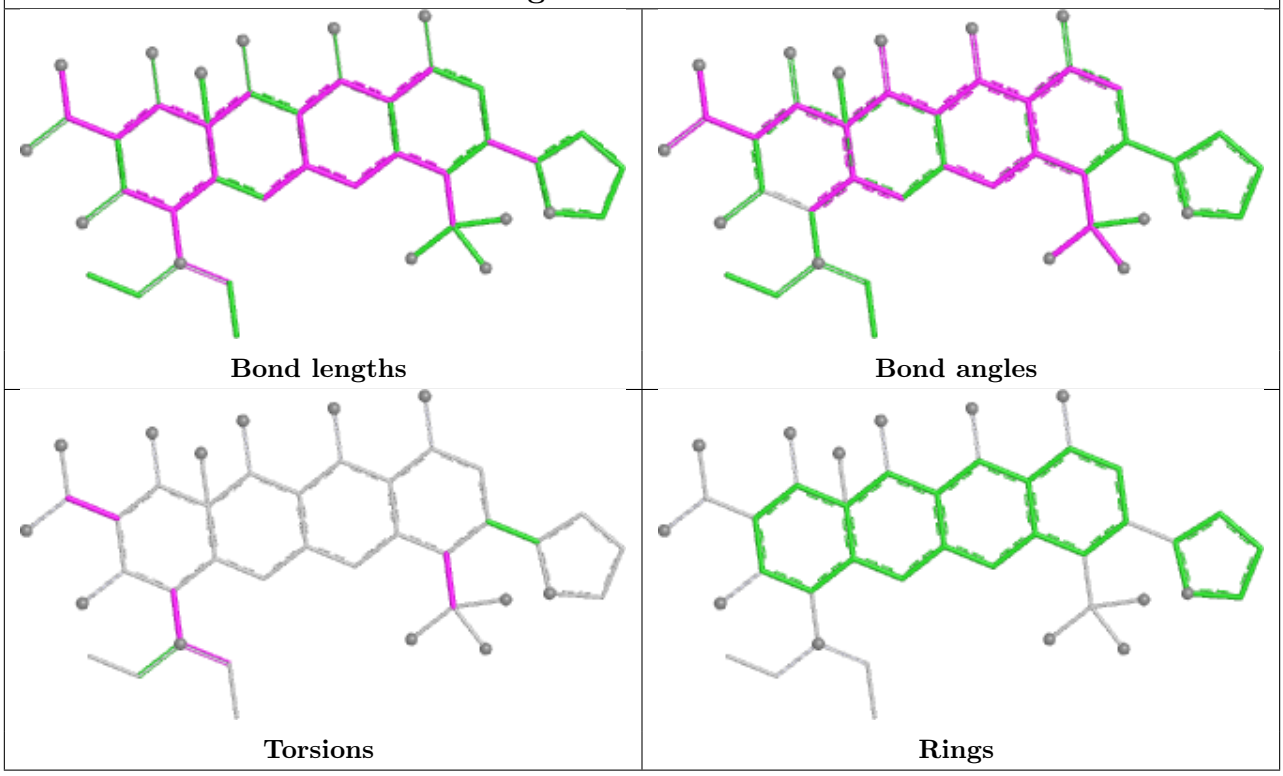
Ligand 80P a 1603



Ligand 80P a 1602



Ligand 80P a 1601



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.

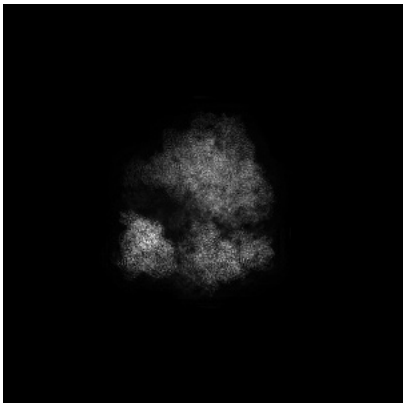
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24740. These allow visual inspection of the internal detail of the map and identification of artifacts.

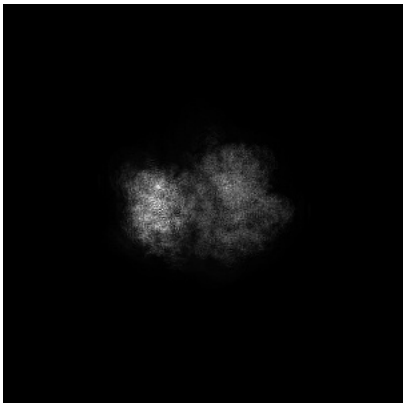
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

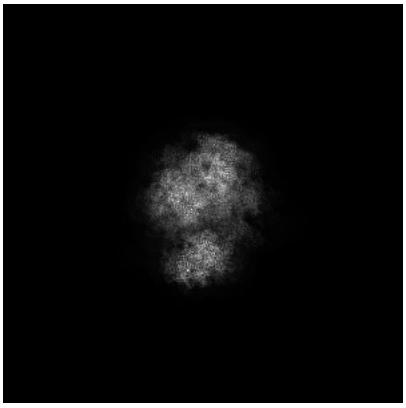
6.1.1 Primary map



X



Y



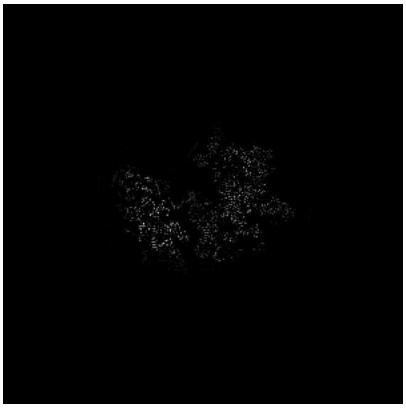
Z

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

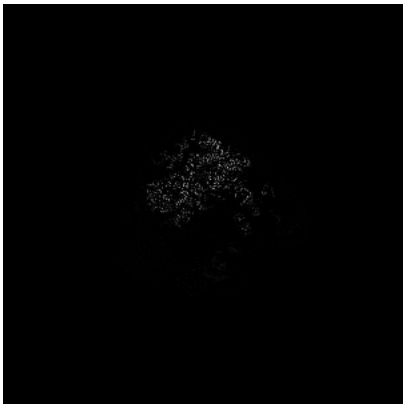
6.2 Central slices (i)

6.2.1 Primary map

X Index: 256



Y Index: 256

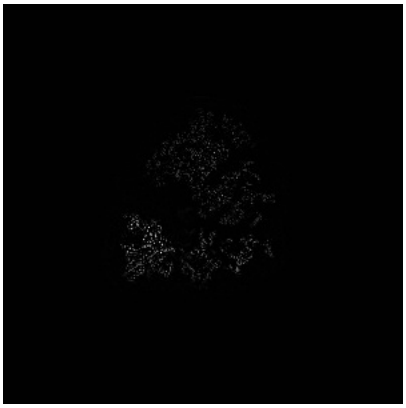


Z Index: 256

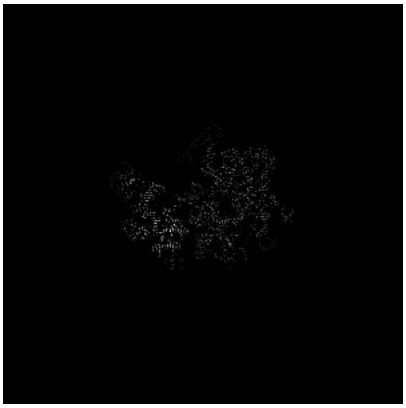
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

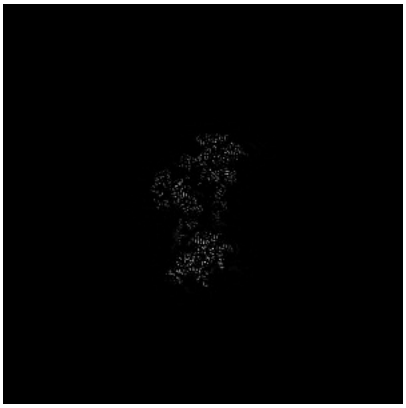
6.3.1 Primary map



X Index: 249



Y Index: 267

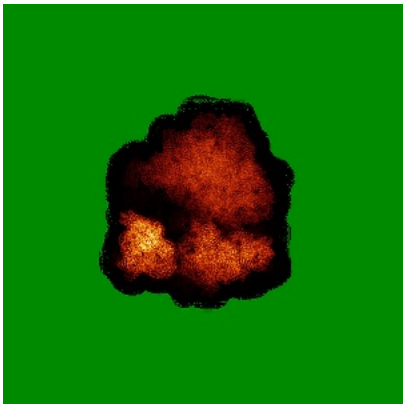


Z Index: 195

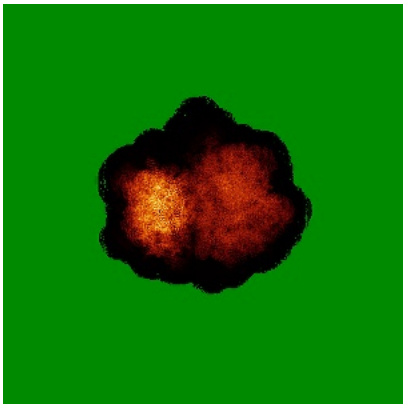
The images above show the largest variance slices of the map in three orthogonal directions.

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

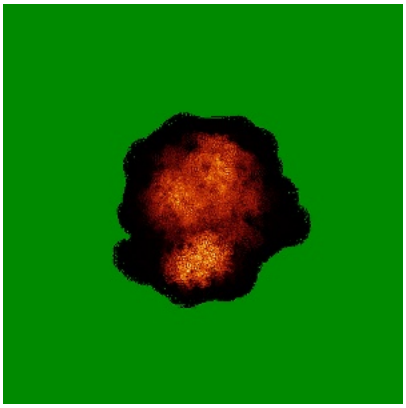
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

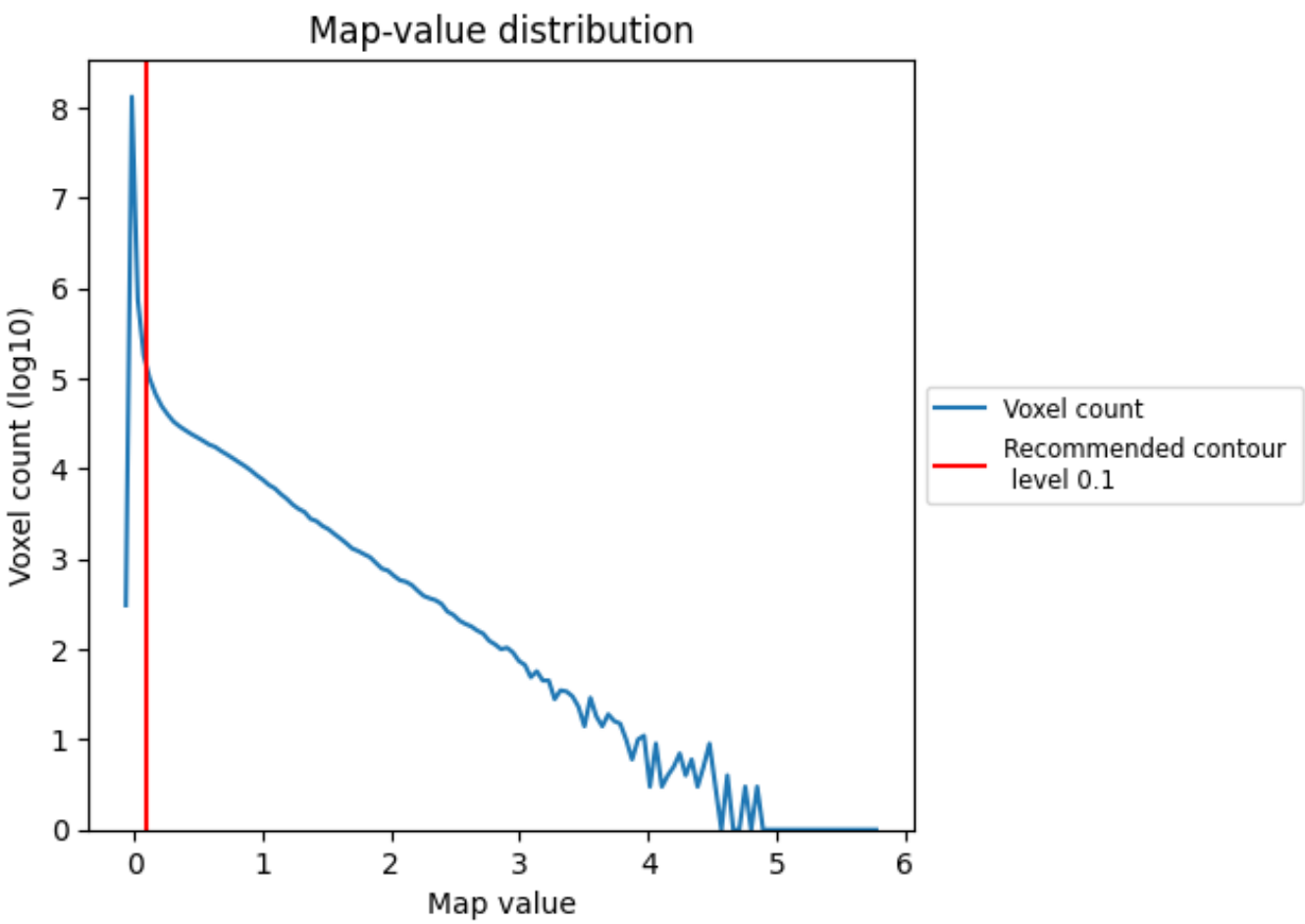
6.6 Mask visualisation (i)

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

7 Map analysis (i)

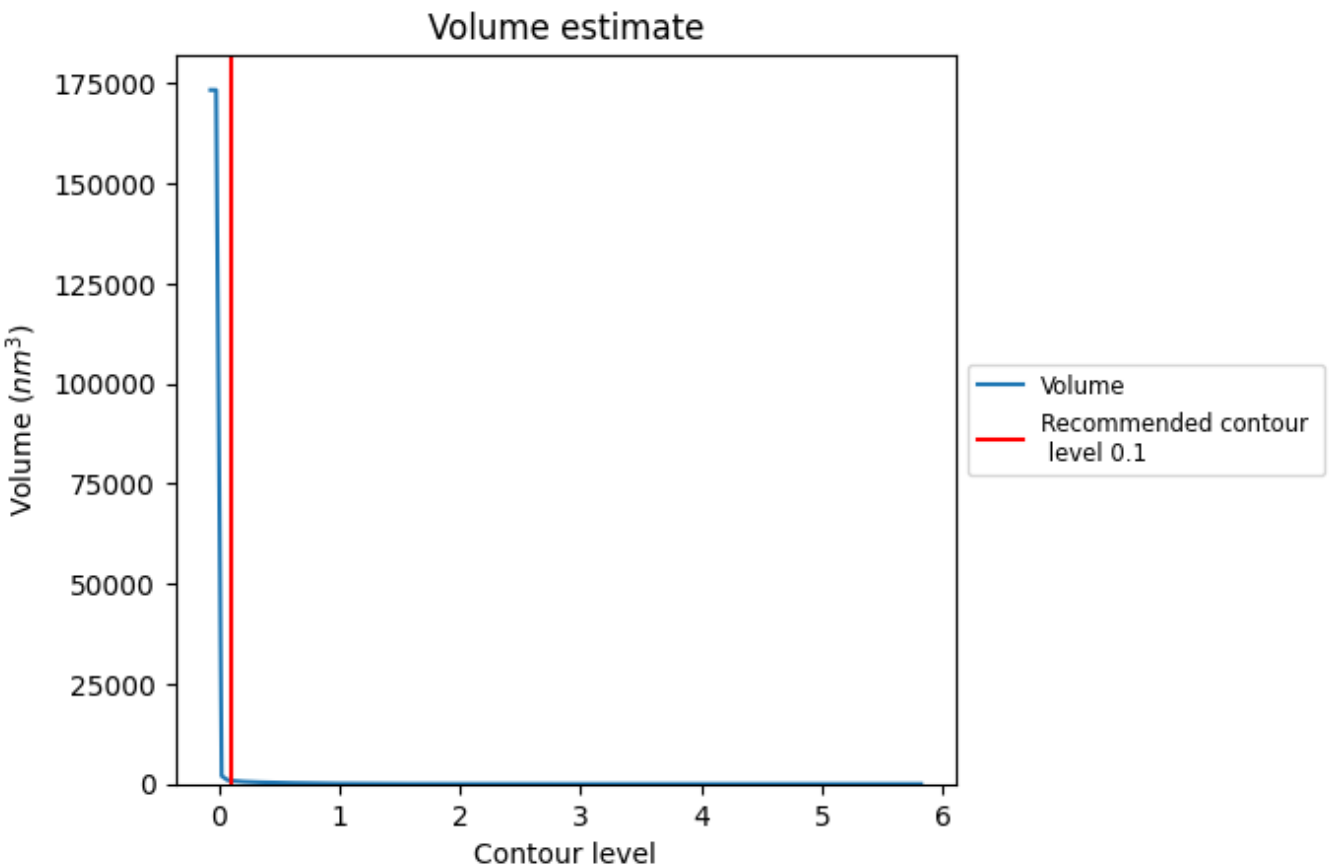
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

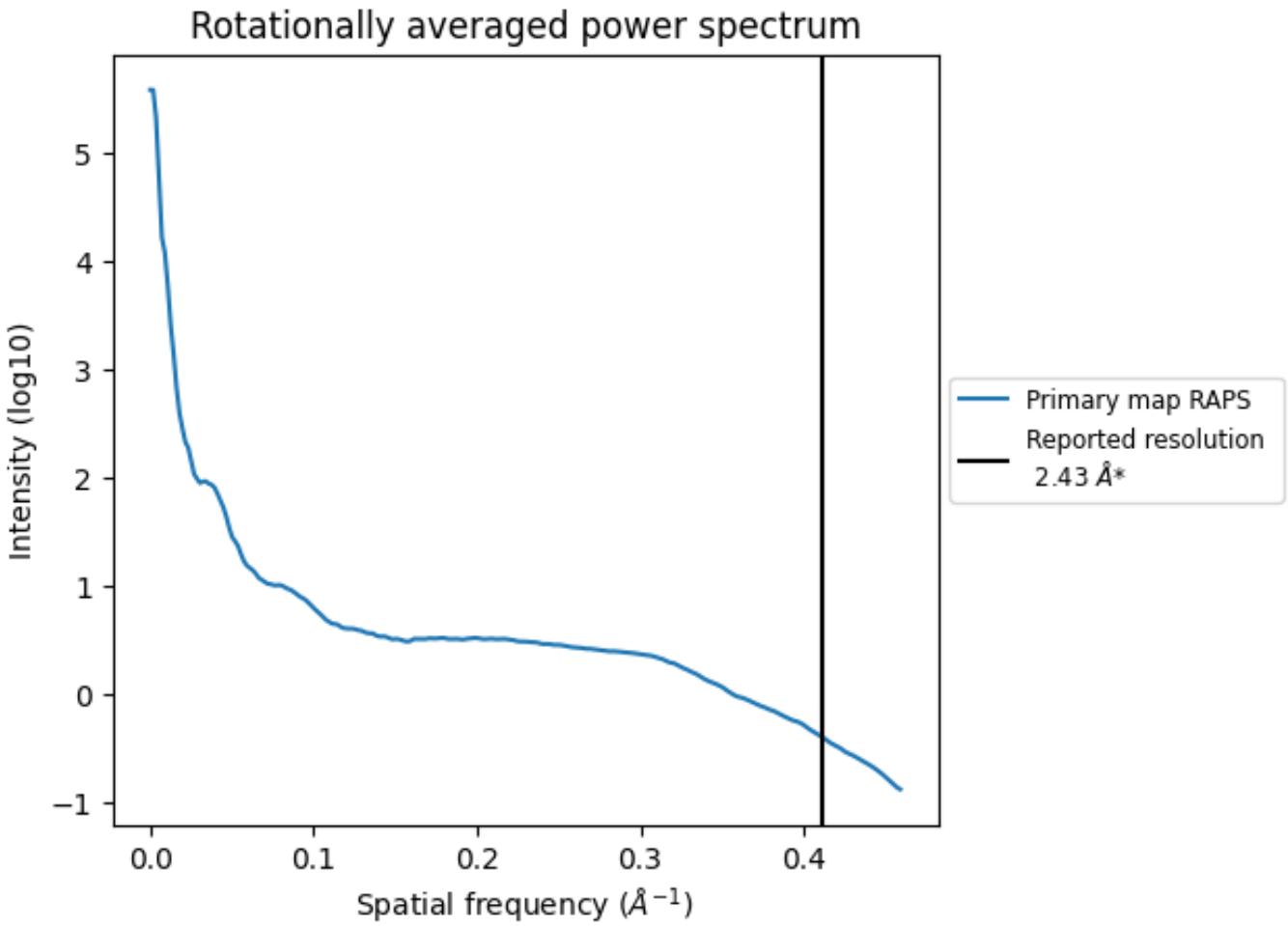
7.2 Volume estimate (i)



The volume at the recommended contour level is 876 nm^3; this corresponds to an approximate mass of 791 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 0.412 Å^{-1}

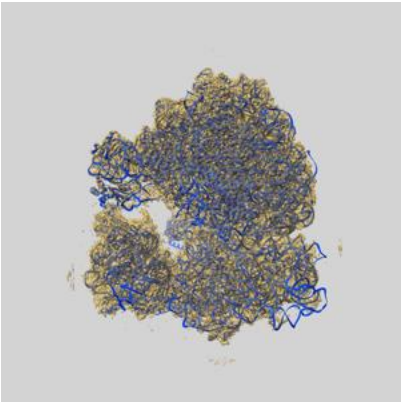
8 Fourier-Shell correlation (i)

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

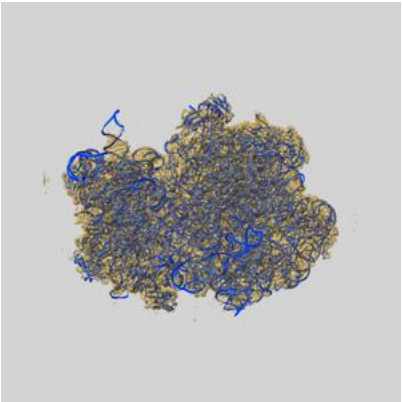
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24740 and PDB model 7RYH. Per-residue inclusion information can be found in section 3 on page 14.

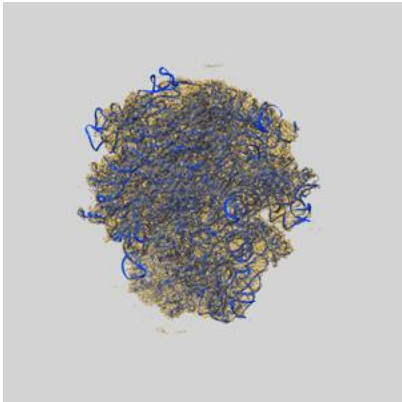
9.1 Map-model overlay (i)



X



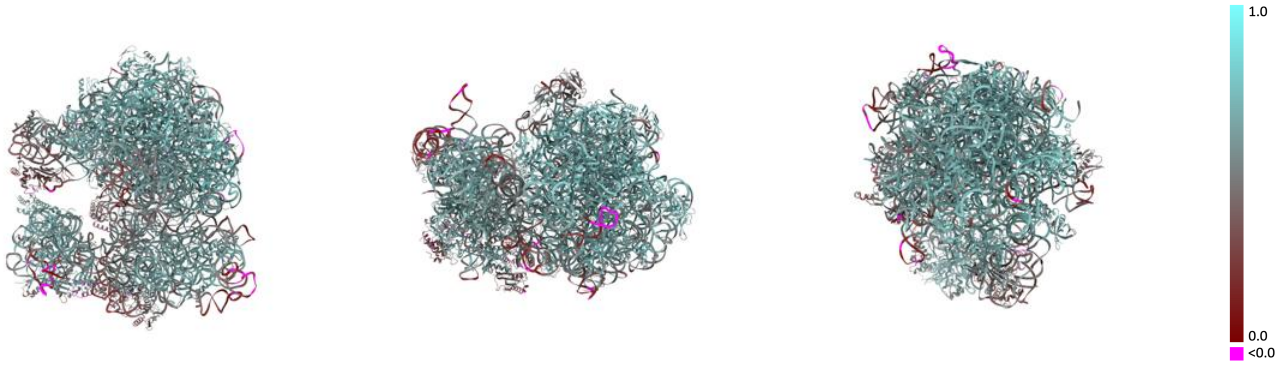
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

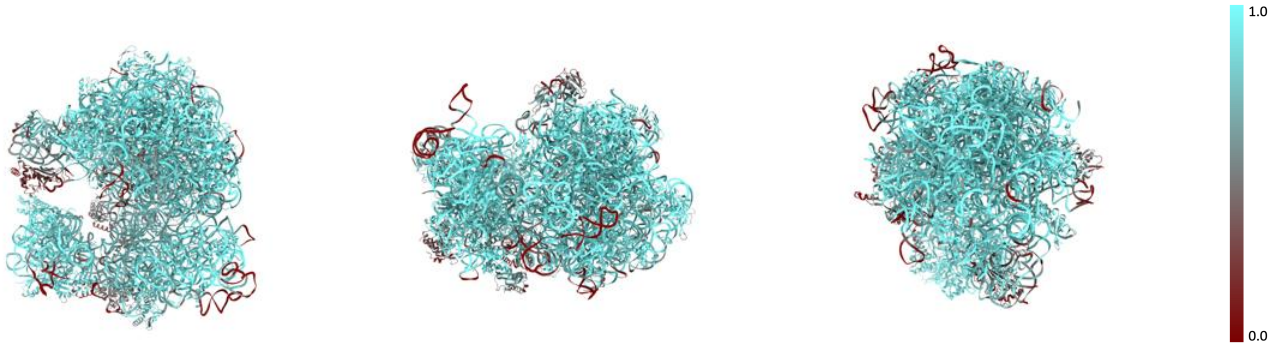
9.2 Q-score mapped to coordinate model (i)



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.

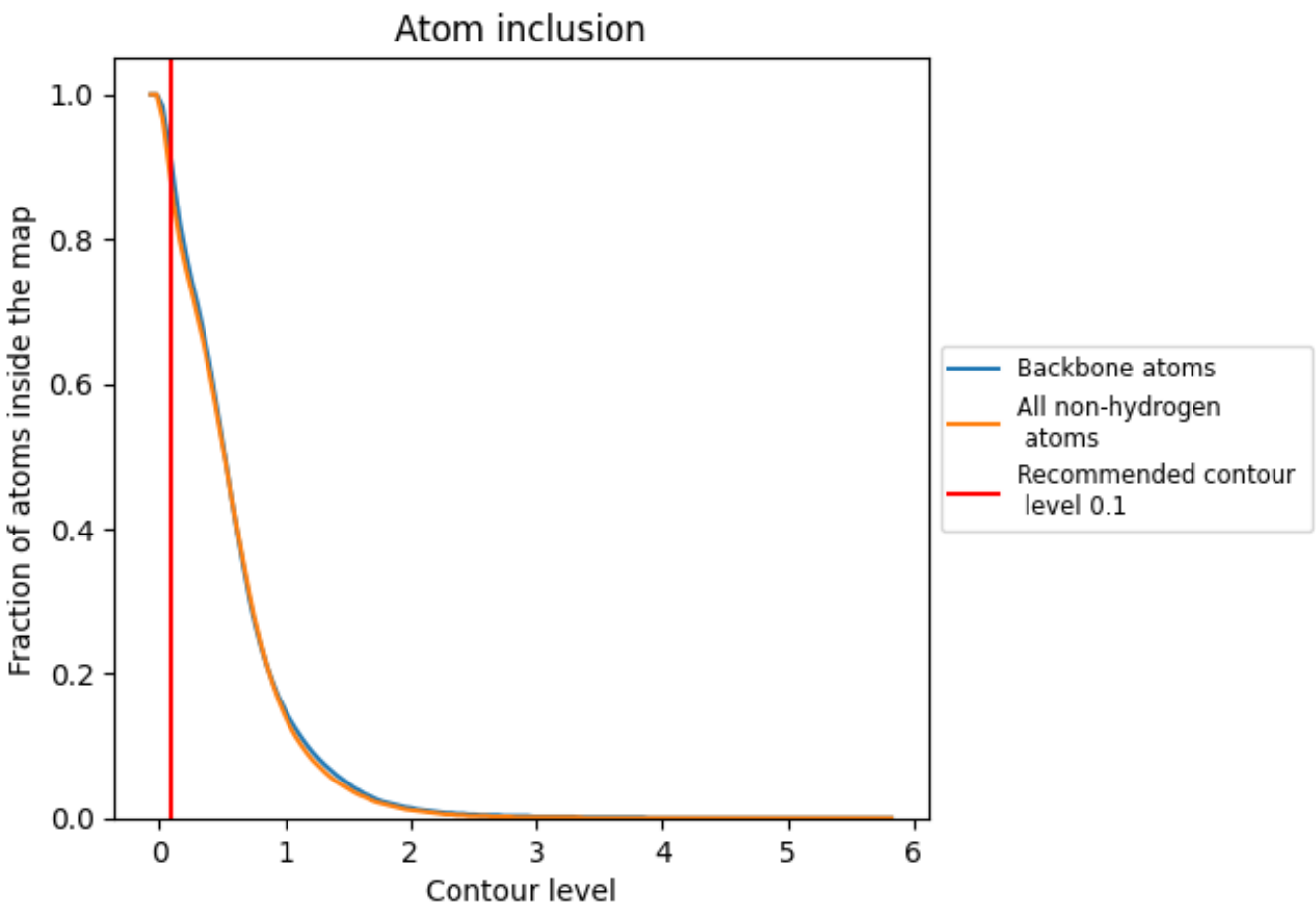
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8670	0.5870
0	0.8740	0.6210
1	0.9770	0.7290
2	0.9450	0.6720
3	0.7870	0.5740
A	0.9010	0.6170
B	0.7020	0.4820
C	0.9520	0.6820
D	0.9640	0.7110
E	0.9220	0.6780
F	0.1980	0.3040
G	0.5250	0.4620
H	0.5210	0.4420
I	0.9760	0.7100
J	0.9640	0.6850
K	0.9590	0.7060
L	0.9090	0.6550
M	0.9910	0.7290
N	0.7430	0.5140
O	0.9230	0.6710
P	0.9890	0.7300
Q	0.9590	0.7010
R	0.9640	0.7170
S	0.8550	0.6310
T	0.8190	0.6040
U	0.8630	0.6200
V	0.9330	0.6990
W	0.9300	0.6840
X	0.7540	0.5520
Y	0.9340	0.6800
Z	0.9220	0.6780
a	0.8700	0.5410
b	0.3580	0.2800
c	0.9510	0.6000
d	0.6680	0.4180

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Chain	Atom inclusion	Q-score
e	0.9340	0.6020
f	0.5810	0.3760
g	0.8170	0.4730
h	0.9670	0.6580
i	0.9740	0.6400
j	0.9370	0.6040
k	0.4070	0.3240
l	0.7500	0.5140
m	0.9760	0.6250
n	0.9670	0.6460
o	0.9410	0.5860
p	0.9650	0.6640
q	0.9470	0.6140
r	0.8010	0.4770
s	0.9790	0.6500
t	0.9810	0.6450
u	0.1850	0.2560