Full wwPDB EM Validation Report (i)

Nov 9, 2022 – 02:24 PM EST

PDB ID	:	6OT3
EMDB ID	:	EMD-20193
Title	:	RF2 accommodated state bound Release complex 70S at 24 ms
Authors	:	Fu, Z.; Indrisiunaite, G.; Kaledhonkar, S.; Shah, B.; Sun, M.; Chen, B.; Grassucci, R.A.; Ehrenberg, M.; Frank, J.
Deposited on	:	2019-05-02
Resolution	:	3.90 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:

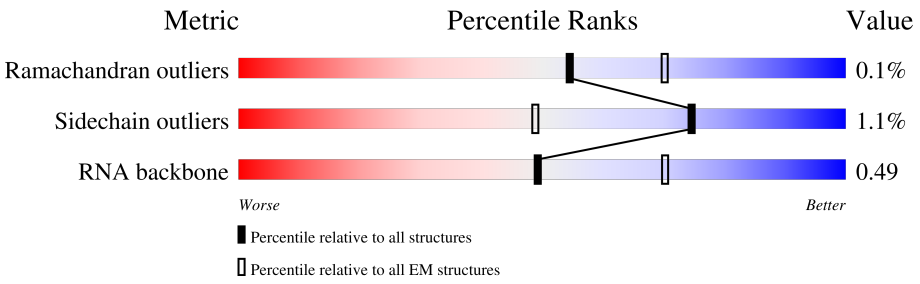
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	1	2903	73% 26%
2	2	1534	72% 27%
3	3	120	81% 19%
4	4	9	78% 22%
5	B	271	99% .
6	C	209	99% .
7	D	201	99% .
8	E	177	99% .

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Mol	Chain	Length	Quality of chain
9	F	175	99%
10	G	149	99%
11	J	142	99%
12	K	123	98%
13	L	144	100%
14	M	136	100%
15	N	119	99%
16	O	116	97%
17	P	114	99%
18	Q	117	99%
19	R	103	98%
20	S	110	100%
21	T	94	100%
22	U	103	100%
23	V	94	99%
24	W	76	100%
25	X	77	99%
26	Y	62	100%
27	Z	58	98%
28	a	66	97%
29	b	56	100%
30	c	52	98%
31	d	46	98%
32	e	64	98%
33	f	38	100%

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Mol	Chain	Length	Quality of chain
34	g	225	100%
35	h	208	98%
36	i	205	100%
37	j	156	99%
38	k	104	100%
39	l	151	99%
40	m	129	100%
41	n	127	98%
42	o	99	99%
43	p	117	100%
44	q	87	98%
45	r	116	100%
46	s	100	99%
47	t	88	91% 9%
48	u	82	98%
49	v	80	99%
50	w	66	98%
51	x	83	99%
52	y	86	100%
53	z	70	100%
54	5	76	72% 24%
55	A	357	100%
56	6	3	33% 100%

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 146899 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2903	62336	27816	11470	20147	2903	0	0

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1534	32929	14693	6041	10661	1534	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	120	2569	1144	468	837	120	0	0

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	9	184	83	26	66	9	0	0

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	175	1313	826	241	244	2	0	0

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	119	951	588	195	163	5	0	0

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	T	94	746	470	140	134	2	0	0

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	U	103	788	498	148	142	0	0

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W	76	582	360	117	104	1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	58	448	281	87	78	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	a	66	522	323	99	94	6	0	0

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	c	52	426	275	78	73	0	0

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	g	225	1760	1113	316	323	8	0	0

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	h	208	1636	1036	307	290	3	0	0

- Molecule 36 is a protein called 30S ribosomal protein S4.

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

- Molecule 37 is a protein called 30S ribosomal protein S5.

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

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	k	104	848	536	153	152	7	0	0

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	l	151	1181	735	227	215	4	0	0

- Molecule 40 is a protein called 30S ribosomal protein S8.

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

- Molecule 41 is a protein called 30S ribosomal protein S9.

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

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	o	99	790	495	151	143	1	0	0

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	p	117	877	540	174	160	3	0	0

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	q	87	673	417	137	116	3	0	0

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	r	116	900	558	181	158	3	0	0

- Molecule 46 is a protein called 30S ribosomal protein S14.

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

- Molecule 47 is a protein called 30S ribosomal protein S15.

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

- Molecule 48 is a protein called 30S ribosomal protein S16.

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

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	v	80	648	411	121	113	3	0	0

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	w	66	544	344	102	97	1	0	0

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	x	83	663	424	126	111	2	0	0

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	y	86	669	414	138	114	3	0	0

- Molecule 53 is a protein called 30S ribosomal protein S21.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
54	5	76	1627	727	296	527	76	1	0	0

- Molecule 55 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	A	357	2833	1742	498	583	10	0	0

- Molecule 56 is a protein called FME-PHE-PHE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	6	3	32	24	3	4	1	0	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	1	2	2	2	0
57	2	1	1	1	0
57	3	8	8	8	0
57	i	1	1	1	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

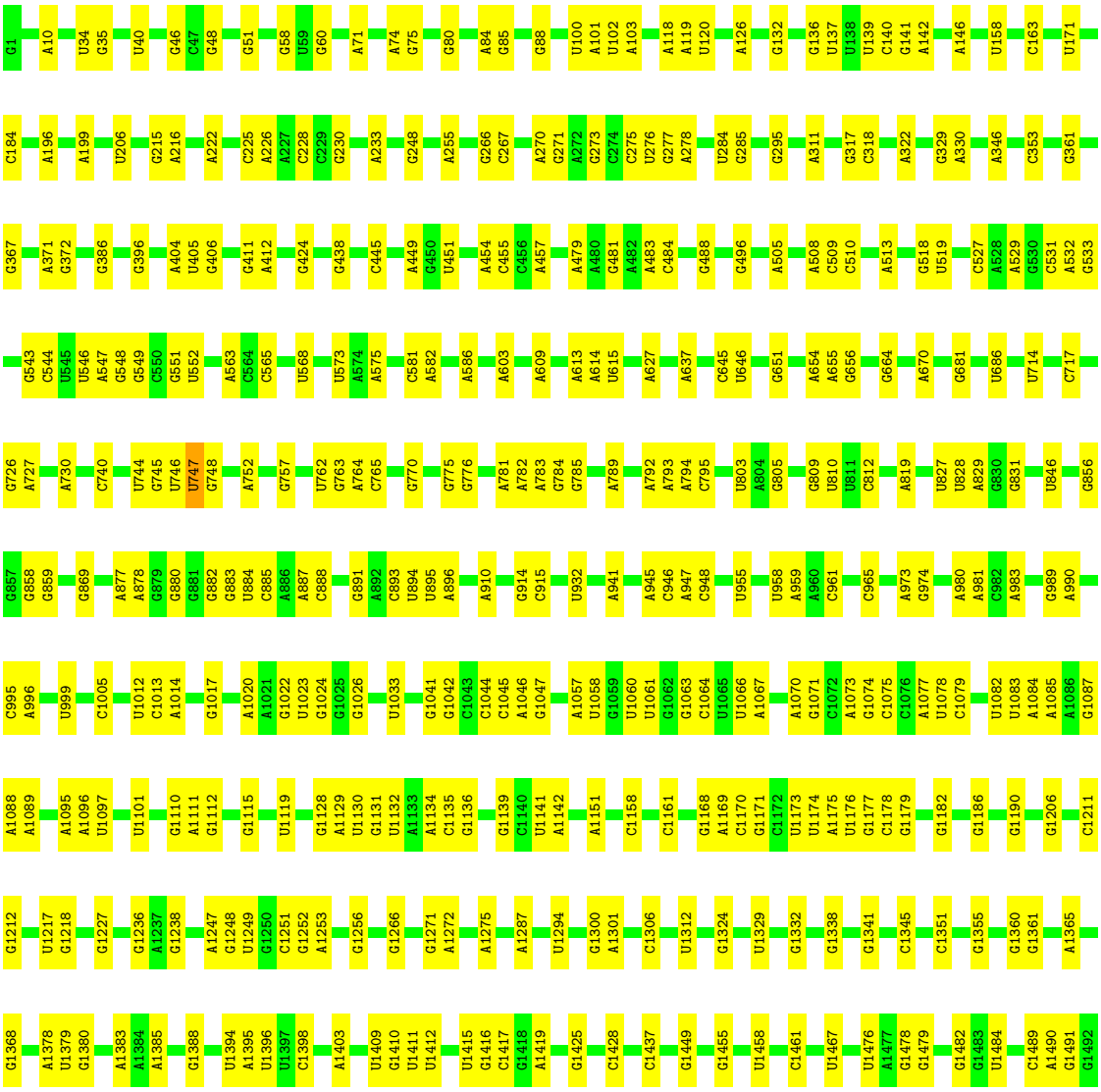
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
58	a	1	1	1	0
58	f	1	1	1	0

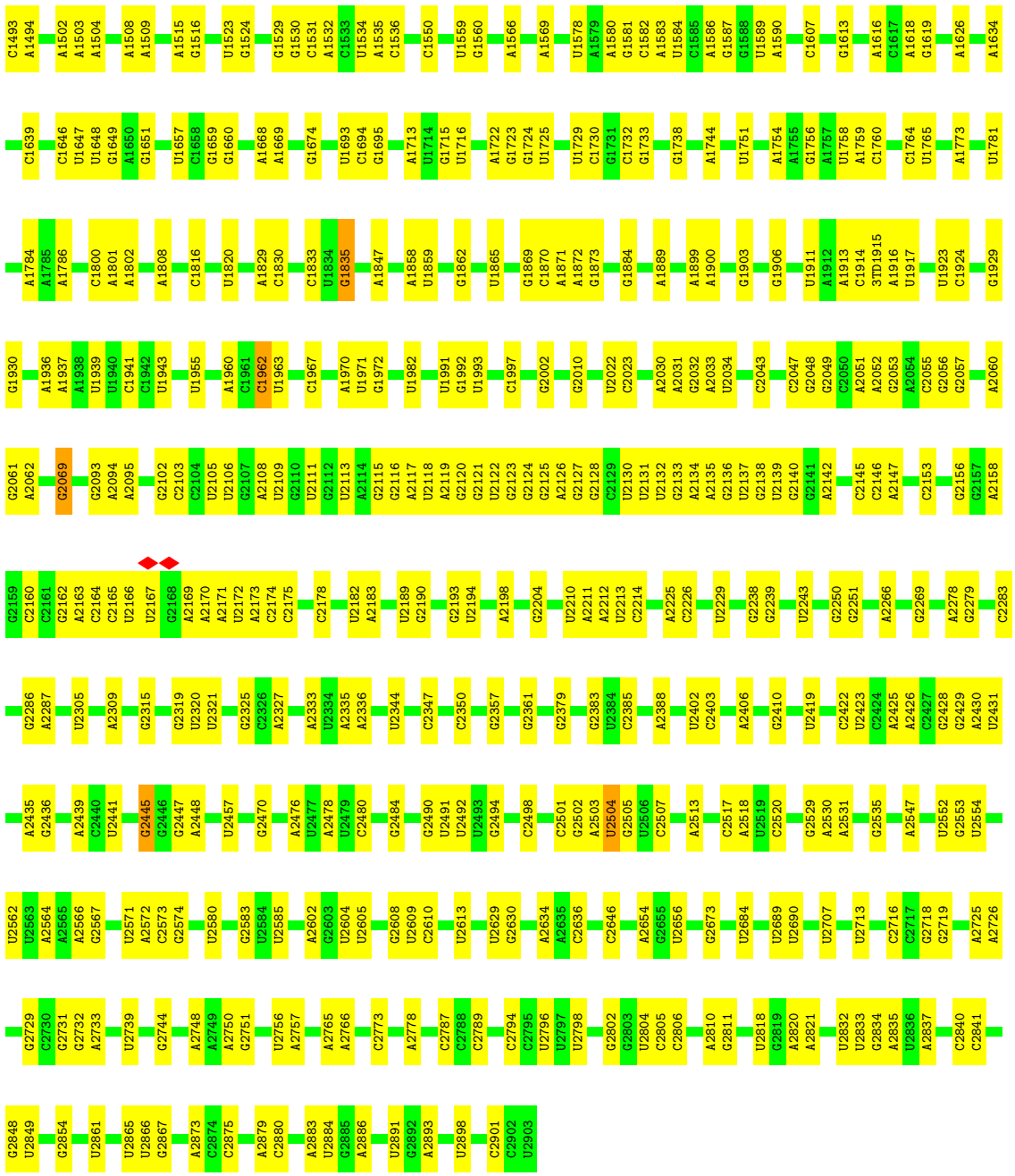
3 Residue-property plots (i)

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

- Molecule 1: 23S ribosomal RNA

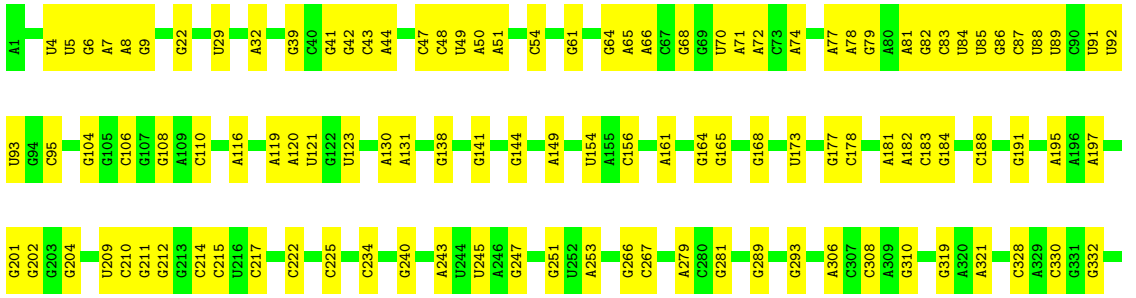
Chain 1: 73% 26%





• Molecule 2: 16S ribosomal RNA

Chain 2: 72% 27%



C345 G346 G347 G348 G351 C352 A353 G354 C355 A363 U367 U368 G369 C372 G376 C381 G384 G388 A389 U390 G391 U398 C401 G402 C403 G404 U405 G406 A411 A412 G413 A414 U421 C422 G423 G424 G428 U429 U438 U439 G444 A451 A452

A456 G457 U458 A459 U463 U464 A465 A466 U467 A468 U476 C477 A478 U479 U480 G481 A482 U486 A487 C488 C489 C490 A495 A496 G497 G505 C511 G515 U516 G517 C518 G521 G524 G527 U531 A532 A533 C545 A546 A547 A554 U562 G568 A572

A573 C576 G577 C578 G581 G587 G588 A596 U603 G615 C618 U632 G633 A640 U641 A648 A649 G650 U653 A665 G668 A673 U686 A687 A695 G700 G703 U717 A718 G721 G722 U723 G724 G731 G734 C744

A747 G748 G752 A753 C754 G755 G761 U772 G773 G774 A777 U793 A794 U798 G799 A814 A815 A816 C817 U820 G821 U822 C823 U828 G829 G832 C841 U842 U843 G844 A845 G846 G849 U850 G851 A864 C876 G877 A878 U884 G885 C893 G902

A913 A914 G926 C930 C934 A935 G942 A958 A959 U960 G966 C967 A968 A969 C970 G971 A975 G976 A977 G987 G988 U989 U992 G993 A994 C995 A996 G1003 A1004 U1008 U1009 U1010 C1011 U1017 G1018 A1019 G1020 U1023 G1026 C1027 C1028 U1029 U1030 C1031 G1032

G1033 G1034 A1035 A1036 C1037 C1038 G1043 G1050 G1053 C1054 A1055 U1056 U1065 C1066 A1067 U1085 U1086 G1089 A1092 A1093 G1094 U1095 A1101 A1102 C1103 G1104 G1108 C1109 G1124 U1125 U1126 C1132 G1133 G1134 U1135 C1136 G1139 C1140 C1141 A1145 A1151 A1152 C1158 U1159 G1160

A1167 U1168 A1169 A1170 A1171 A1176 G1177 G1184 G1193 A1196 A1197 C1200 A1201 G1206 G1207 U1212 A1213 C1214 A1227 C1228 G1231 A1238 A1239 U1240 G1241 A1254 G1255 A1256 A1257 G1258 C1259 G1260 A1261 A1275 G1279 A1280 U1286 A1287 G1297 U1298 A1299 G1300 U1301 C1302

G1305 C1317 C1320 G1331 C1336 G1337 G1338 A1339 A1340 A1363 A1368 C1369 G1370 G1379 U1380 C1384 C1397 A1398 G1401 C1402 C1403 C1404 C1407 G1419 G1422 A1429 G1432 A1441 A1446 U1451 C1452 G1453 G1458 G1475 G1487 G1488 G1489 U1490

G1491 A1492 G1497 U1498 A1499 A1503 A1507 C1510 G1511 U1512 G1516 G1517 A1518 A1519 G1529 G1530 A1531 U1532 C1533 A1534

- Molecule 3: 5S ribosomal RNA

Chain 3: 81% 19%

U1 G9 G13 U14 A15 G24 C31 U32 C35 C36 U40 G41 C42 C43 G44 A45 G56 A57 A58 A66 G67 C68 C88 U89 C90 A99 A109 A119 U120

- Molecule 4: mRNA

Chain 4: 78% 22%

U13 A20 A21

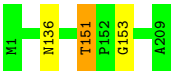
- Molecule 5: 50S ribosomal protein L2

Chain B: 99%

A2 R80 N260 S272

- Molecule 6: 50S ribosomal protein L3

Chain C: 99%



- Molecule 7: 50S ribosomal protein L4

Chain D: 99%

- Molecule 8: 50S ribosomal protein L5

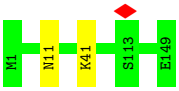
Chain E: 99%

- Molecule 9: 50S ribosomal protein L6

Chain F: 99%

- Molecule 10: 50S ribosomal protein L9

Chain G: 99%

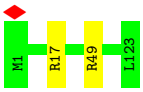


- Molecule 11: 50S ribosomal protein L13

Chain J: 99%

- Molecule 12: 50S ribosomal protein L14

Chain K: 98%



- Molecule 13: 50S ribosomal protein L15

Chain L: 100%

There are no outlier residues recorded for this chain.

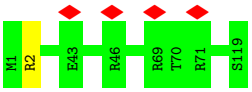
- Molecule 14: 50S ribosomal protein L16

Chain M: 100%

There are no outlier residues recorded for this chain.

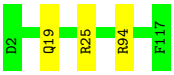
- Molecule 15: 50S ribosomal protein L17

Chain N: 99%



- Molecule 16: 50S ribosomal protein L18

Chain O: 97%



- Molecule 17: 50S ribosomal protein L19

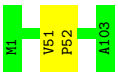
Chain P: 99%

- Molecule 18: 50S ribosomal protein L20

Chain Q: 99%

- Molecule 19: 50S ribosomal protein L21

Chain R: 98%



- Molecule 20: 50S ribosomal protein L22

Chain S: 100%

There are no outlier residues recorded for this chain.

• Molecule 21: 50S ribosomal protein L23

Chain T: 100%

There are no outlier residues recorded for this chain.

• Molecule 22: 50S ribosomal protein L24

Chain U: 100%

There are no outlier residues recorded for this chain.

• Molecule 23: 50S ribosomal protein L25

Chain V: 99%

M1 N24 A94

• Molecule 24: 50S ribosomal protein L27

Chain W: 100%

There are no outlier residues recorded for this chain.

• Molecule 25: 50S ribosomal protein L28

Chain X: 99%

S2 R27 Y78

• Molecule 26: 50S ribosomal protein L29

Chain Y: 100%

There are no outlier residues recorded for this chain.

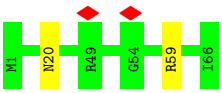
• Molecule 27: 50S ribosomal protein L30

Chain Z: 98%

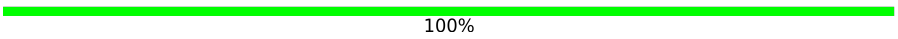
A2 R31 E59

• Molecule 28: 50S ribosomal protein L31

Chain a: 97%

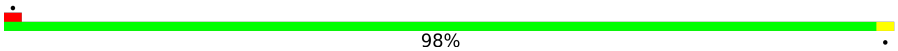


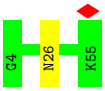
• Molecule 29: 50S ribosomal protein L32

Chain b: 

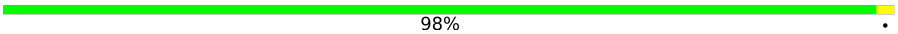
There are no outlier residues recorded for this chain.

• Molecule 30: 50S ribosomal protein L33

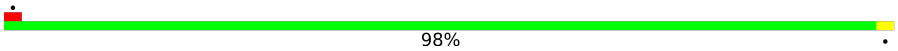
Chain c: 

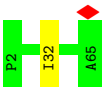


• Molecule 31: 50S ribosomal protein L34

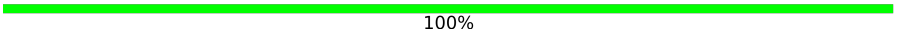
Chain d: 

• Molecule 32: 50S ribosomal protein L35

Chain e: 

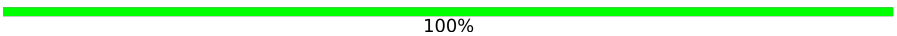


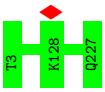
• Molecule 33: 50S ribosomal protein L36

Chain f: 

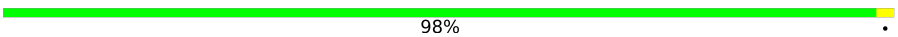
There are no outlier residues recorded for this chain.

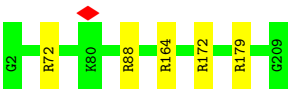
• Molecule 34: 30S ribosomal protein S2

Chain g: 



• Molecule 35: 30S ribosomal protein S3

Chain h: 



• Molecule 36: 30S ribosomal protein S4

Chain i: 100%

There are no outlier residues recorded for this chain.

• Molecule 37: 30S ribosomal protein S5

Chain j: 99%

• Molecule 38: 30S ribosomal protein S6

Chain k: 100%

There are no outlier residues recorded for this chain.

• Molecule 39: 30S ribosomal protein S7

Chain l: 99%

• Molecule 40: 30S ribosomal protein S8

Chain m: 100%

There are no outlier residues recorded for this chain.

• Molecule 41: 30S ribosomal protein S9

Chain n: 98%

• Molecule 42: 30S ribosomal protein S10

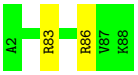
Chain o: 99%

• Molecule 43: 30S ribosomal protein S11

Chain p: 100%

• Molecule 44: 30S ribosomal protein S12

Chain q: 98%



• Molecule 45: 30S ribosomal protein S13

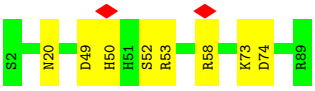
Chain r: 100%

• Molecule 46: 30S ribosomal protein S14

Chain s: 99%

• Molecule 47: 30S ribosomal protein S15

Chain t: 91% 9%



• Molecule 48: 30S ribosomal protein S16

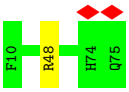
Chain u: 98%

• Molecule 49: 30S ribosomal protein S17

Chain v: 99%

• Molecule 50: 30S ribosomal protein S18

Chain w: 98%



• Molecule 51: 30S ribosomal protein S19

Chain x: 99%

• Molecule 52: 30S ribosomal protein S20

Chain y: 100%

There are no outlier residues recorded for this chain.

• Molecule 53: 30S ribosomal protein S21

Chain z: 100%

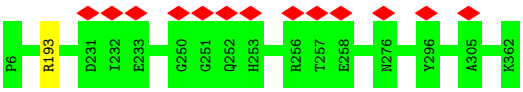
There are no outlier residues recorded for this chain.

• Molecule 54: P-tRNA

Chain 5: 72% 24%

• Molecule 55: Peptide chain release factor 2

Chain A: 100%



• Molecule 56: FME-PHE-PHE

Chain 6: 33% 100%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	41.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.66, 1.66, 1.66	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 2MG, G7M, OMG, MA6, OMU, 5MU, FME, 4OC, 1MG, 2MA, 6MZ, H2U, 4SU, OMC, 3TD, ZN, 5MC, UR3, MG

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	1	0.75	0/69286	0.99	0/108087
2	2	0.72	1/36590 (0.0%)	1.00	0/57074
3	3	0.67	0/2872	0.98	0/4478
4	4	0.56	0/203	1.03	0/312
5	B	0.39	0/2121	0.56	0/2852
6	C	0.40	0/1586	0.59	0/2134
7	D	0.37	0/1571	0.51	0/2113
8	E	0.39	0/1434	0.55	0/1926
9	F	0.38	0/1333	0.52	0/1805
10	G	0.33	0/1122	0.56	0/1515
11	J	0.40	0/1152	0.51	0/1551
12	K	0.37	0/955	0.57	0/1279
13	L	0.37	0/1062	0.58	0/1413
14	M	0.38	0/1093	0.55	0/1460
15	N	0.40	0/964	0.66	0/1289
16	O	0.34	0/902	0.52	0/1209
17	P	0.41	0/929	0.56	0/1242
18	Q	0.38	0/960	0.50	0/1278
19	R	0.45	0/829	0.60	0/1107
20	S	0.36	0/864	0.54	0/1156
21	T	0.36	0/752	0.52	0/1005
22	U	0.41	0/796	0.55	0/1062
23	V	0.37	0/766	0.49	0/1025
24	W	0.38	0/589	0.52	0/779
25	X	0.40	0/635	0.53	0/848
26	Y	0.33	0/502	0.47	0/667
27	Z	0.32	0/452	0.56	0/605
28	a	0.37	0/531	0.52	0/709
29	b	0.35	0/450	0.55	0/599
30	c	0.36	0/433	0.54	0/576
31	d	0.37	0/380	0.56	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	0.38	0/513	0.61	0/676
33	f	0.35	0/303	0.53	0/397
34	g	0.36	0/1791	0.54	0/2413
35	h	0.37	0/1663	0.53	0/2241
36	i	0.35	0/1665	0.50	0/2227
37	j	0.37	0/1165	0.57	0/1568
38	k	0.36	0/867	0.56	0/1171
39	l	0.33	0/1195	0.51	0/1602
40	m	0.37	0/989	0.54	0/1326
41	n	0.35	0/1034	0.55	0/1375
42	o	0.33	0/800	0.58	0/1082
43	p	0.34	0/893	0.49	0/1205
44	q	0.38	0/682	0.56	0/918
45	r	0.34	0/909	0.55	0/1215
46	s	0.33	0/817	0.50	0/1088
47	t	0.36	0/722	0.65	0/964
48	u	0.37	0/659	0.61	0/884
49	v	0.38	0/657	0.63	0/881
50	w	0.34	0/553	0.51	0/743
51	x	0.36	0/680	0.52	0/915
52	y	0.35	0/675	0.46	0/895
53	z	0.34	0/597	0.50	0/792
54	5	0.65	0/1704	1.00	0/2654
55	A	0.37	0/2873	0.57	0/3870
56	6	0.63	0/23	0.45	0/29
All	All	0.65	1/158543 (0.0%)	0.90	0/236784

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1158	C	O3'-P	-5.15	1.54	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	269/271 (99%)	254 (94%)	15 (6%)	0	100	100
6	C	207/209 (99%)	198 (96%)	7 (3%)	2 (1%)	15	52
7	D	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
8	E	175/177 (99%)	160 (91%)	14 (8%)	1 (1%)	25	63
9	F	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
10	G	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
11	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
12	K	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
13	L	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
15	N	117/119 (98%)	106 (91%)	11 (9%)	0	100	100
16	O	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
17	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
18	Q	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
19	R	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	15	52
20	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
21	T	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
22	U	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
23	V	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
24	W	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
25	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
26	Y	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
27	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
28	a	64/66 (97%)	56 (88%)	8 (12%)	0	100	100
29	b	54/56 (96%)	51 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	c	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
31	d	44/46 (96%)	44 (100%)	0	0	100	100
32	e	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	44
33	f	36/38 (95%)	36 (100%)	0	0	100	100
34	g	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
35	h	206/208 (99%)	189 (92%)	17 (8%)	0	100	100
36	i	203/205 (99%)	197 (97%)	6 (3%)	0	100	100
37	j	154/156 (99%)	142 (92%)	12 (8%)	0	100	100
38	k	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
39	l	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
40	m	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
41	n	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
42	o	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
43	p	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
44	q	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
45	r	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
46	s	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
47	t	86/88 (98%)	79 (92%)	5 (6%)	2 (2%)	6	38
48	u	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
49	v	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
50	w	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
51	x	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
52	y	84/86 (98%)	84 (100%)	0	0	100	100
53	z	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
55	A	355/357 (99%)	331 (93%)	24 (7%)	0	100	100
56	6	1/3 (33%)	1 (100%)	0	0	100	100
All	All	5929/6031 (98%)	5627 (95%)	295 (5%)	7 (0%)	54	84

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	C	151	THR
47	t	50	HIS

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Mol	Chain	Res	Type
47	t	74	ASP
19	R	52	PRO
32	e	32	ILE
8	E	124	GLY
6	C	153	GLY

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	
5	B	216/216 (100%)	214 (99%)	2 (1%)	78	87
6	C	164/164 (100%)	162 (99%)	2 (1%)	71	83
7	D	165/165 (100%)	162 (98%)	3 (2%)	59	77
8	E	148/148 (100%)	148 (100%)	0	100	100
9	F	136/136 (100%)	134 (98%)	2 (2%)	65	80
10	G	114/114 (100%)	112 (98%)	2 (2%)	59	77
11	J	116/116 (100%)	115 (99%)	1 (1%)	78	87
12	K	104/104 (100%)	102 (98%)	2 (2%)	57	75
13	L	103/103 (100%)	103 (100%)	0	100	100
14	M	109/109 (100%)	109 (100%)	0	100	100
15	N	99/99 (100%)	98 (99%)	1 (1%)	76	86
16	O	86/86 (100%)	83 (96%)	3 (4%)	36	62
17	P	99/99 (100%)	98 (99%)	1 (1%)	76	86
18	Q	89/89 (100%)	88 (99%)	1 (1%)	73	84
19	R	84/84 (100%)	83 (99%)	1 (1%)	71	83
20	S	93/93 (100%)	93 (100%)	0	100	100
21	T	81/81 (100%)	81 (100%)	0	100	100
22	U	84/84 (100%)	84 (100%)	0	100	100
23	V	78/78 (100%)	77 (99%)	1 (1%)	69	82
24	W	58/58 (100%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	X	67/67 (100%)	66 (98%)	1 (2%)	65	80
26	Y	54/54 (100%)	54 (100%)	0	100	100
27	Z	48/48 (100%)	47 (98%)	1 (2%)	53	73
28	a	59/59 (100%)	57 (97%)	2 (3%)	37	62
29	b	47/47 (100%)	47 (100%)	0	100	100
30	c	47/47 (100%)	46 (98%)	1 (2%)	53	73
31	d	38/38 (100%)	37 (97%)	1 (3%)	46	68
32	e	51/51 (100%)	51 (100%)	0	100	100
33	f	34/34 (100%)	34 (100%)	0	100	100
34	g	187/187 (100%)	187 (100%)	0	100	100
35	h	171/171 (100%)	166 (97%)	5 (3%)	42	65
36	i	172/172 (100%)	172 (100%)	0	100	100
37	j	119/119 (100%)	118 (99%)	1 (1%)	81	89
38	k	91/91 (100%)	91 (100%)	0	100	100
39	l	124/124 (100%)	123 (99%)	1 (1%)	81	89
40	m	104/104 (100%)	104 (100%)	0	100	100
41	n	105/105 (100%)	103 (98%)	2 (2%)	57	75
42	o	86/86 (100%)	85 (99%)	1 (1%)	71	83
43	p	90/90 (100%)	90 (100%)	0	100	100
44	q	74/74 (100%)	72 (97%)	2 (3%)	44	67
45	r	94/94 (100%)	94 (100%)	0	100	100
46	s	83/83 (100%)	82 (99%)	1 (1%)	71	83
47	t	76/76 (100%)	70 (92%)	6 (8%)	12	41
48	u	65/65 (100%)	63 (97%)	2 (3%)	40	64
49	v	74/74 (100%)	73 (99%)	1 (1%)	67	81
50	w	57/57 (100%)	56 (98%)	1 (2%)	59	77
51	x	72/72 (100%)	71 (99%)	1 (1%)	67	81
52	y	65/65 (100%)	65 (100%)	0	100	100
53	z	60/60 (100%)	60 (100%)	0	100	100
55	A	304/305 (100%)	303 (100%)	1 (0%)	92	95
56	6	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4946/4947 (100%)	4893 (99%)	53 (1%)	74 84

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	80	ARG
5	B	260	ASN
6	C	136	ASN
6	C	151	THR
7	D	40	ARG
7	D	44	ARG
7	D	163	ASN
9	F	73	ASN
9	F	176	LYS
10	G	11	ASN
10	G	41	LYS
11	J	96	ARG
12	K	17	ARG
12	K	49	ARG
15	N	2	ARG
16	O	19	GLN
16	O	25	ARG
16	O	94	ARG
17	P	51	ARG
18	Q	92	ARG
19	R	51	VAL
23	V	24	ASN
25	X	27	ARG
27	Z	31	ARG
28	a	20	ASN
28	a	59	ARG
30	c	26	ASN
31	d	41	ARG
35	h	72	ARG
35	h	88	ARG
35	h	164	ARG
35	h	172	ARG
35	h	179	ARG
37	j	132	ASN
39	l	130	ASN
41	n	106	ARG
41	n	113	ARG

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Mol	Chain	Res	Type
42	o	5	ARG
44	q	83	ARG
44	q	86	ARG
46	s	69	ARG
47	t	20	ASN
47	t	49	ASP
47	t	52	SER
47	t	53	ARG
47	t	58	ARG
47	t	73	LYS
48	u	1	MET
48	u	5	ARG
49	v	81	LYS
50	w	48	ARG
51	x	78	ARG
55	A	193	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
5	B	86	ASN
5	B	260	ASN
6	C	136	ASN
6	C	173	GLN
7	D	9	GLN
7	D	29	HIS
7	D	115	GLN
7	D	163	ASN
9	F	73	ASN
9	F	116	GLN
11	J	80	HIS
13	L	54	GLN
14	M	60	GLN
16	O	29	HIS
16	O	38	GLN
16	O	61	GLN
17	P	12	GLN
18	Q	44	GLN
18	Q	72	ASN
19	R	82	HIS
20	S	7	HIS
20	S	61	ASN

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Mol	Chain	Res	Type
21	T	70	HIS
22	U	46	GLN
22	U	54	GLN
23	V	24	ASN
25	X	34	HIS
26	Y	15	ASN
26	Y	20	ASN
27	Z	20	HIS
28	a	20	ASN
29	b	42	HIS
30	c	26	ASN
33	f	37	GLN
34	g	39	HIS
34	g	51	ASN
34	g	177	ASN
36	i	59	GLN
36	i	74	ASN
36	i	116	GLN
37	j	12	GLN
37	j	132	ASN
38	k	46	GLN
38	k	63	ASN
39	l	28	ASN
39	l	130	ASN
44	q	5	ASN
47	t	20	ASN
47	t	50	HIS
48	u	26	ASN
50	w	52	GLN
51	x	52	HIS
52	y	48	GLN
52	y	52	ASN
55	A	43	GLN
55	A	276	ASN
55	A	313	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2903 (99%)	755 (26%)	16 (0%)
2	2	1529/1534 (99%)	412 (26%)	5 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	3	119/120 (99%)	23 (19%)	0
4	4	8/9 (88%)	2 (25%)	0
54	5	74/76 (97%)	19 (25%)	0
All	All	4628/4642 (99%)	1211 (26%)	21 (0%)

All (1211) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	34	U
1	1	35	G
1	1	40	U
1	1	46	G
1	1	48	G
1	1	51	G
1	1	58	G
1	1	60	G
1	1	71	A
1	1	74	A
1	1	75	G
1	1	80	G
1	1	84	A
1	1	85	G
1	1	88	G
1	1	100	U
1	1	101	A
1	1	102	U
1	1	103	A
1	1	118	A
1	1	119	A
1	1	120	U
1	1	126	A
1	1	132	G
1	1	136	G
1	1	137	U
1	1	139	U
1	1	140	C
1	1	141	G
1	1	142	A
1	1	146	A
1	1	158	U
1	1	163	C

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Mol	Chain	Res	Type
1	1	171	U
1	1	184	C
1	1	196	A
1	1	199	A
1	1	206	U
1	1	215	G
1	1	216	A
1	1	222	A
1	1	225	C
1	1	226	A
1	1	228	C
1	1	230	G
1	1	233	A
1	1	248	G
1	1	255	A
1	1	266	G
1	1	267	C
1	1	270	A
1	1	271	G
1	1	273	G
1	1	275	C
1	1	276	U
1	1	277	G
1	1	278	A
1	1	284	U
1	1	285	G
1	1	295	G
1	1	311	A
1	1	317	G
1	1	318	C
1	1	322	A
1	1	329	G
1	1	330	A
1	1	346	A
1	1	353	C
1	1	361	G
1	1	367	G
1	1	371	A
1	1	372	G
1	1	386	G
1	1	396	G
1	1	405	U

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Mol	Chain	Res	Type
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
1	1	438	G
1	1	445	C
1	1	449	A
1	1	451	U
1	1	454	A
1	1	455	C
1	1	457	A
1	1	479	A
1	1	481	G
1	1	483	A
1	1	484	C
1	1	488	G
1	1	496	G
1	1	505	A
1	1	508	A
1	1	509	C
1	1	510	C
1	1	513	A
1	1	518	G
1	1	519	U
1	1	527	C
1	1	529	A
1	1	531	C
1	1	532	A
1	1	533	G
1	1	543	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	552	U
1	1	563	A
1	1	565	C
1	1	568	U
1	1	573	U
1	1	575	A

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Mol	Chain	Res	Type
1	1	581	C
1	1	582	A
1	1	586	A
1	1	603	A
1	1	609	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	627	A
1	1	637	A
1	1	645	C
1	1	646	U
1	1	651	G
1	1	654	A
1	1	655	A
1	1	656	G
1	1	664	G
1	1	670	A
1	1	681	G
1	1	686	U
1	1	714	U
1	1	717	C
1	1	726	G
1	1	727	A
1	1	730	A
1	1	740	C
1	1	744	U
1	1	747	5MU
1	1	748	G
1	1	752	A
1	1	757	G
1	1	762	U
1	1	763	G
1	1	764	A
1	1	765	C
1	1	770	G
1	1	775	G
1	1	776	G
1	1	781	A
1	1	782	A
1	1	783	A
1	1	784	G

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Mol	Chain	Res	Type
1	1	785	G
1	1	789	A
1	1	792	A
1	1	793	A
1	1	794	A
1	1	795	C
1	1	803	U
1	1	805	G
1	1	809	G
1	1	810	U
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	829	A
1	1	831	G
1	1	846	U
1	1	856	G
1	1	858	G
1	1	859	G
1	1	869	G
1	1	877	A
1	1	878	A
1	1	880	G
1	1	882	G
1	1	883	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	891	G
1	1	893	C
1	1	894	U
1	1	895	U
1	1	896	A
1	1	910	A
1	1	914	G
1	1	915	C
1	1	932	U
1	1	941	A
1	1	945	A
1	1	946	C

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Mol	Chain	Res	Type
1	1	947	A
1	1	948	C
1	1	958	U
1	1	959	A
1	1	961	C
1	1	965	C
1	1	973	A
1	1	974	G
1	1	980	A
1	1	981	A
1	1	983	A
1	1	989	G
1	1	990	A
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1014	A
1	1	1017	G
1	1	1020	A
1	1	1022	G
1	1	1023	U
1	1	1024	G
1	1	1026	G
1	1	1033	U
1	1	1041	G
1	1	1042	G
1	1	1044	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1057	A
1	1	1058	U
1	1	1060	U
1	1	1061	U
1	1	1063	G
1	1	1064	C
1	1	1066	U
1	1	1067	A
1	1	1070	A

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Mol	Chain	Res	Type
1	1	1071	G
1	1	1073	A
1	1	1074	G
1	1	1075	C
1	1	1077	A
1	1	1078	U
1	1	1079	C
1	1	1082	U
1	1	1083	U
1	1	1084	A
1	1	1085	A
1	1	1087	G
1	1	1088	A
1	1	1089	A
1	1	1095	A
1	1	1096	A
1	1	1097	U
1	1	1101	U
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1115	G
1	1	1119	U
1	1	1128	G
1	1	1129	A
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1134	A
1	1	1135	C
1	1	1136	G
1	1	1139	G
1	1	1141	U
1	1	1142	A
1	1	1151	A
1	1	1158	C
1	1	1161	C
1	1	1168	G
1	1	1169	A
1	1	1170	C
1	1	1171	G
1	1	1173	U

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Mol	Chain	Res	Type
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1182	G
1	1	1186	G
1	1	1190	G
1	1	1206	G
1	1	1211	C
1	1	1212	G
1	1	1217	U
1	1	1218	G
1	1	1227	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1248	G
1	1	1249	U
1	1	1251	C
1	1	1252	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1275	A
1	1	1287	A
1	1	1294	U
1	1	1300	G
1	1	1301	A
1	1	1306	C
1	1	1312	U
1	1	1324	G
1	1	1329	U
1	1	1332	G
1	1	1338	G
1	1	1341	G
1	1	1345	C
1	1	1351	C
1	1	1355	G

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Mol	Chain	Res	Type
1	1	1360	G
1	1	1361	G
1	1	1365	A
1	1	1368	G
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1385	A
1	1	1388	G
1	1	1394	U
1	1	1395	A
1	1	1396	U
1	1	1398	C
1	1	1403	A
1	1	1409	U
1	1	1410	G
1	1	1411	U
1	1	1412	U
1	1	1415	U
1	1	1416	G
1	1	1417	C
1	1	1419	A
1	1	1425	G
1	1	1428	C
1	1	1437	C
1	1	1449	G
1	1	1455	G
1	1	1458	U
1	1	1461	C
1	1	1467	U
1	1	1476	U
1	1	1478	G
1	1	1479	G
1	1	1482	G
1	1	1484	U
1	1	1489	C
1	1	1490	A
1	1	1491	G
1	1	1493	C
1	1	1494	A
1	1	1502	A

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Mol	Chain	Res	Type
1	1	1503	A
1	1	1504	A
1	1	1508	A
1	1	1509	A
1	1	1515	A
1	1	1516	G
1	1	1523	U
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1531	C
1	1	1532	A
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1550	C
1	1	1559	U
1	1	1560	G
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1581	G
1	1	1582	C
1	1	1583	A
1	1	1584	U
1	1	1586	A
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1607	C
1	1	1613	G
1	1	1616	A
1	1	1619	G
1	1	1626	A
1	1	1634	A
1	1	1639	C
1	1	1646	C
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G

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Mol	Chain	Res	Type
1	1	1657	U
1	1	1659	G
1	1	1660	G
1	1	1668	A
1	1	1669	A
1	1	1674	G
1	1	1693	U
1	1	1694	C
1	1	1695	G
1	1	1713	A
1	1	1715	G
1	1	1716	U
1	1	1722	A
1	1	1723	G
1	1	1724	G
1	1	1725	U
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1733	G
1	1	1738	G
1	1	1744	A
1	1	1751	U
1	1	1754	A
1	1	1756	G
1	1	1758	U
1	1	1759	A
1	1	1760	C
1	1	1764	C
1	1	1765	U
1	1	1773	A
1	1	1781	U
1	1	1784	A
1	1	1786	A
1	1	1800	C
1	1	1801	A
1	1	1802	A
1	1	1808	A
1	1	1816	C
1	1	1820	U
1	1	1829	A
1	1	1830	C

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Mol	Chain	Res	Type
1	1	1833	C
1	1	1835	2MG
1	1	1847	A
1	1	1858	A
1	1	1859	U
1	1	1862	G
1	1	1865	U
1	1	1869	G
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1873	G
1	1	1884	G
1	1	1889	A
1	1	1899	A
1	1	1900	A
1	1	1903	G
1	1	1906	G
1	1	1913	A
1	1	1914	C
1	1	1916	A
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1937	A
1	1	1941	C
1	1	1943	U
1	1	1955	U
1	1	1960	A
1	1	1962	5MC
1	1	1963	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1982	U
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C

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Mol	Chain	Res	Type
1	1	2002	G
1	1	2010	G
1	1	2022	U
1	1	2023	C
1	1	2031	A
1	1	2032	G
1	1	2033	A
1	1	2034	U
1	1	2043	C
1	1	2047	C
1	1	2048	G
1	1	2049	G
1	1	2051	A
1	1	2052	A
1	1	2053	G
1	1	2055	C
1	1	2056	G
1	1	2057	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2093	G
1	1	2094	A
1	1	2095	A
1	1	2102	G
1	1	2103	C
1	1	2105	U
1	1	2106	U
1	1	2108	A
1	1	2109	U
1	1	2111	U
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2120	G
1	1	2121	G
1	1	2122	U
1	1	2123	G

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Mol	Chain	Res	Type
1	1	2124	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2130	U
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2135	A
1	1	2136	G
1	1	2137	U
1	1	2138	G
1	1	2139	U
1	1	2140	G
1	1	2142	A
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2153	C
1	1	2156	G
1	1	2158	A
1	1	2160	C
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2166	U
1	1	2167	U
1	1	2169	A
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2174	C
1	1	2175	C
1	1	2178	C
1	1	2182	U
1	1	2183	A
1	1	2189	U
1	1	2190	G

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Mol	Chain	Res	Type
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2210	U
1	1	2211	A
1	1	2212	A
1	1	2213	U
1	1	2214	C
1	1	2225	A
1	1	2226	C
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2266	A
1	1	2269	G
1	1	2278	A
1	1	2279	G
1	1	2283	C
1	1	2287	A
1	1	2305	U
1	1	2309	A
1	1	2315	G
1	1	2319	G
1	1	2320	U
1	1	2321	U
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2335	A
1	1	2336	A
1	1	2344	U
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2361	G
1	1	2379	G
1	1	2383	G
1	1	2385	C
1	1	2388	A

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Mol	Chain	Res	Type
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2410	G
1	1	2419	U
1	1	2422	C
1	1	2423	U
1	1	2425	A
1	1	2426	A
1	1	2428	G
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2436	G
1	1	2439	A
1	1	2441	U
1	1	2445	2MG
1	1	2447	G
1	1	2448	A
1	1	2470	G
1	1	2476	A
1	1	2478	A
1	1	2480	C
1	1	2484	G
1	1	2490	G
1	1	2491	U
1	1	2492	U
1	1	2494	G
1	1	2501	C
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2507	C
1	1	2513	A
1	1	2517	C
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2530	A
1	1	2531	A
1	1	2535	G

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Mol	Chain	Res	Type
1	1	2547	A
1	1	2553	G
1	1	2554	U
1	1	2562	U
1	1	2564	A
1	1	2566	A
1	1	2567	G
1	1	2571	U
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2583	G
1	1	2585	U
1	1	2602	A
1	1	2604	U
1	1	2608	G
1	1	2609	U
1	1	2610	C
1	1	2613	U
1	1	2629	U
1	1	2630	G
1	1	2634	A
1	1	2636	C
1	1	2646	C
1	1	2654	A
1	1	2656	U
1	1	2673	G
1	1	2684	U
1	1	2689	U
1	1	2690	U
1	1	2707	U
1	1	2713	U
1	1	2716	C
1	1	2718	G
1	1	2719	G
1	1	2725	A
1	1	2726	A
1	1	2729	G
1	1	2731	G
1	1	2732	G
1	1	2733	A
1	1	2739	U

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Mol	Chain	Res	Type
1	1	2744	G
1	1	2748	A
1	1	2750	A
1	1	2751	G
1	1	2756	U
1	1	2757	A
1	1	2765	A
1	1	2766	A
1	1	2773	C
1	1	2778	A
1	1	2787	C
1	1	2789	C
1	1	2794	C
1	1	2796	U
1	1	2798	U
1	1	2802	G
1	1	2804	U
1	1	2805	C
1	1	2806	C
1	1	2810	A
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2821	A
1	1	2832	U
1	1	2833	U
1	1	2834	G
1	1	2835	A
1	1	2837	A
1	1	2840	C
1	1	2841	C
1	1	2848	G
1	1	2849	U
1	1	2854	G
1	1	2861	U
1	1	2865	U
1	1	2866	U
1	1	2867	G
1	1	2873	A
1	1	2875	C
1	1	2879	A
1	1	2880	C

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Mol	Chain	Res	Type
1	1	2883	A
1	1	2884	U
1	1	2886	A
1	1	2891	U
1	1	2893	A
1	1	2898	U
1	1	2901	C
2	2	4	U
2	2	5	U
2	2	6	G
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	29	U
2	2	32	A
2	2	39	G
2	2	41	G
2	2	42	G
2	2	43	C
2	2	44	A
2	2	47	C
2	2	48	C
2	2	49	U
2	2	50	A
2	2	51	A
2	2	54	C
2	2	61	G
2	2	64	G
2	2	65	A
2	2	66	A
2	2	68	G
2	2	70	U
2	2	71	A
2	2	72	A
2	2	74	A
2	2	77	A
2	2	78	A
2	2	79	G
2	2	81	A
2	2	82	G
2	2	83	C

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Mol	Chain	Res	Type
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	88	U
2	2	89	U
2	2	91	U
2	2	92	U
2	2	93	U
2	2	95	C
2	2	104	G
2	2	106	C
2	2	108	G
2	2	110	C
2	2	116	A
2	2	119	A
2	2	120	A
2	2	121	U
2	2	123	U
2	2	130	A
2	2	131	A
2	2	138	G
2	2	141	G
2	2	144	G
2	2	149	A
2	2	154	U
2	2	156	C
2	2	161	A
2	2	164	G
2	2	165	G
2	2	168	G
2	2	173	U
2	2	177	G
2	2	178	C
2	2	181	A
2	2	182	A
2	2	183	C
2	2	184	G
2	2	188	C
2	2	191	G
2	2	195	A
2	2	197	A

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Mol	Chain	Res	Type
2	2	201	G
2	2	202	G
2	2	204	G
2	2	209	U
2	2	210	C
2	2	211	G
2	2	212	G
2	2	214	C
2	2	215	C
2	2	217	C
2	2	222	C
2	2	225	C
2	2	234	C
2	2	240	G
2	2	243	A
2	2	245	U
2	2	247	G
2	2	251	G
2	2	253	A
2	2	266	G
2	2	267	C
2	2	279	A
2	2	281	G
2	2	289	G
2	2	293	G
2	2	306	A
2	2	308	C
2	2	310	G
2	2	319	G
2	2	321	A
2	2	328	C
2	2	330	C
2	2	332	G
2	2	345	C
2	2	347	G
2	2	348	G
2	2	351	G
2	2	352	C
2	2	353	A
2	2	354	G
2	2	355	C
2	2	363	A

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Mol	Chain	Res	Type
2	2	367	U
2	2	368	U
2	2	369	G
2	2	372	C
2	2	376	G
2	2	381	C
2	2	384	G
2	2	388	G
2	2	390	U
2	2	391	G
2	2	398	U
2	2	401	C
2	2	402	G
2	2	404	G
2	2	406	G
2	2	411	A
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	428	G
2	2	429	U
2	2	438	U
2	2	439	U
2	2	444	G
2	2	451	A
2	2	452	A
2	2	456	A
2	2	457	G
2	2	459	A
2	2	463	U
2	2	464	U
2	2	466	A
2	2	467	U
2	2	468	A
2	2	476	U
2	2	478	A
2	2	479	U
2	2	480	U
2	2	481	G

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Mol	Chain	Res	Type
2	2	482	A
2	2	486	U
2	2	488	C
2	2	490	C
2	2	495	A
2	2	496	A
2	2	497	G
2	2	505	G
2	2	511	C
2	2	515	G
2	2	517	G
2	2	518	C
2	2	521	G
2	2	524	G
2	2	527	G7M
2	2	531	U
2	2	532	A
2	2	533	A
2	2	545	C
2	2	547	A
2	2	554	A
2	2	562	U
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	578	C
2	2	581	G
2	2	587	G
2	2	588	G
2	2	596	A
2	2	603	U
2	2	615	G
2	2	618	C
2	2	632	U
2	2	633	G
2	2	640	A
2	2	641	U
2	2	648	A
2	2	649	A
2	2	650	G

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Mol	Chain	Res	Type
2	2	653	U
2	2	665	A
2	2	668	G
2	2	673	A
2	2	686	U
2	2	687	A
2	2	695	A
2	2	700	G
2	2	703	G
2	2	717	U
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	744	C
2	2	747	A
2	2	748	G
2	2	752	G
2	2	753	A
2	2	755	G
2	2	761	G
2	2	772	U
2	2	773	G
2	2	774	G
2	2	777	A
2	2	793	U
2	2	794	A
2	2	798	U
2	2	799	G
2	2	814	A
2	2	815	A
2	2	817	C
2	2	820	U
2	2	821	G
2	2	823	C
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	843	U

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Mol	Chain	Res	Type
2	2	844	G
2	2	845	A
2	2	846	G
2	2	849	G
2	2	851	G
2	2	864	A
2	2	876	C
2	2	877	G
2	2	878	A
2	2	884	U
2	2	885	G
2	2	893	C
2	2	902	G
2	2	913	A
2	2	914	A
2	2	926	G
2	2	930	C
2	2	934	C
2	2	935	A
2	2	942	G
2	2	958	A
2	2	960	U
2	2	966	2MG
2	2	969	A
2	2	971	G
2	2	975	A
2	2	976	G
2	2	977	A
2	2	987	G
2	2	989	U
2	2	992	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1003	G
2	2	1004	A
2	2	1008	U
2	2	1009	U
2	2	1011	C
2	2	1017	U
2	2	1018	G
2	2	1019	A

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Mol	Chain	Res	Type
2	2	1020	G
2	2	1023	U
2	2	1026	G
2	2	1028	C
2	2	1029	U
2	2	1030	U
2	2	1031	C
2	2	1033	G
2	2	1035	A
2	2	1036	A
2	2	1037	C
2	2	1038	C
2	2	1043	G
2	2	1050	G
2	2	1053	G
2	2	1054	C
2	2	1056	U
2	2	1065	U
2	2	1067	A
2	2	1085	U
2	2	1086	U
2	2	1089	G
2	2	1092	A
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1102	A
2	2	1104	G
2	2	1108	G
2	2	1124	G
2	2	1125	U
2	2	1126	U
2	2	1132	C
2	2	1133	G
2	2	1135	U
2	2	1136	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1145	A
2	2	1151	A
2	2	1152	A

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Mol	Chain	Res	Type
2	2	1160	G
2	2	1167	A
2	2	1169	A
2	2	1171	A
2	2	1176	A
2	2	1177	G
2	2	1184	G
2	2	1193	G
2	2	1196	A
2	2	1197	A
2	2	1200	C
2	2	1201	A
2	2	1206	G
2	2	1207	2MG
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1227	A
2	2	1228	C
2	2	1231	G
2	2	1238	A
2	2	1240	U
2	2	1241	G
2	2	1254	A
2	2	1256	A
2	2	1257	A
2	2	1258	G
2	2	1260	G
2	2	1261	A
2	2	1275	A
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1297	G
2	2	1299	A
2	2	1301	U
2	2	1302	C
2	2	1305	G
2	2	1317	C
2	2	1320	C
2	2	1331	G

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Mol	Chain	Res	Type
2	2	1336	C
2	2	1338	G
2	2	1340	A
2	2	1363	A
2	2	1368	A
2	2	1370	G
2	2	1379	G
2	2	1380	U
2	2	1384	C
2	2	1397	C
2	2	1398	A
2	2	1401	G
2	2	1404	C
2	2	1419	G
2	2	1422	G
2	2	1429	A
2	2	1432	G
2	2	1441	A
2	2	1446	A
2	2	1451	U
2	2	1452	C
2	2	1453	G
2	2	1458	G
2	2	1475	G
2	2	1487	G
2	2	1489	G
2	2	1491	G
2	2	1492	A
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1507	A
2	2	1510	C
2	2	1511	G
2	2	1512	U
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1531	A
2	2	1533	C
2	2	1534	A
3	3	9	G

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Mol	Chain	Res	Type
3	3	13	G
3	3	15	A
3	3	24	G
3	3	31	C
3	3	32	U
3	3	35	C
3	3	36	C
3	3	40	U
3	3	41	G
3	3	42	C
3	3	44	G
3	3	45	A
3	3	56	G
3	3	58	A
3	3	66	A
3	3	68	C
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
3	3	119	A
4	4	20	A
4	4	21	A
54	5	8	4SU
54	5	12	C
54	5	13	A
54	5	16	C
54	5	17	U
54	5	19	G
54	5	20	H2U
54	5	43	A
54	5	46	A
54	5	47	U
54	5	48	C
54	5	49	G
54	5	53	G
54	5	55	PSU
54	5	68	C
54	5	72	A
54	5	73	A
54	5	74	C

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Mol	Chain	Res	Type
54	5	76	A

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	404	A
1	1	613	A
1	1	784	G
1	1	894	U
1	1	947	A
1	1	1170	C
1	1	1175	A
1	1	1252	G
1	1	1379	U
1	1	1530	G
1	1	2146	C
1	1	2189	U
1	1	2193	G
1	1	2286	G
1	1	2425	A
1	1	2756	U
2	2	83	C
2	2	210	C
2	2	496	A
2	2	516	PSU
2	2	1109	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	1	1917	1	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PSU	2	516	2	18,21,22	1.00	1 (5%)	22,30,33	1.82	5 (22%)
2	UR3	2	1498	2	19,22,23	2.50	7 (36%)	26,32,35	1.26	2 (7%)
1	2MG	1	1835	1	18,26,27	2.48	7 (38%)	16,38,41	1.42	4 (25%)
1	2MG	1	2445	1	18,26,27	2.48	7 (38%)	16,38,41	1.43	3 (18%)
1	OMU	1	2552	1	19,22,23	2.84	8 (42%)	26,31,34	1.81	5 (19%)
1	6MZ	1	2030	1	18,25,26	2.15	3 (16%)	16,36,39	2.01	3 (18%)
54	5MU	5	54	54	19,22,23	4.76	7 (36%)	28,32,35	3.52	8 (28%)
1	2MA	1	2503	1	17,25,26	2.36	5 (29%)	17,37,40	1.34	2 (11%)
54	H2U	5	20	54	18,21,22	3.29	5 (27%)	21,30,33	1.86	5 (23%)
1	1MG	1	745	1	18,26,27	2.63	5 (27%)	19,39,42	1.40	3 (15%)
56	FME	6	77	56	8,9,10	0.88	0	7,9,11	0.59	0
2	G7M	2	527	2	20,26,27	3.92	10 (50%)	17,39,42	1.08	2 (11%)
1	3TD	1	1915	1	18,22,23	4.16	5 (27%)	22,32,35	1.58	3 (13%)
1	5MC	1	1962	1	18,22,23	3.55	7 (38%)	26,32,35	1.04	2 (7%)
1	6MZ	1	1618	1	18,25,26	2.08	3 (16%)	16,36,39	2.33	3 (18%)
1	PSU	1	955	1	18,21,22	1.01	1 (5%)	22,30,33	1.67	2 (9%)
2	MA6	2	1518	2	19,26,27	1.04	1 (5%)	18,38,41	2.75	2 (11%)
2	2MG	2	966	2	18,26,27	2.58	7 (38%)	16,38,41	1.43	3 (18%)
1	PSU	1	1911	1	18,21,22	1.10	1 (5%)	22,30,33	2.00	5 (22%)
2	2MG	2	1207	2	18,26,27	2.49	7 (38%)	16,38,41	1.45	4 (25%)
2	4OC	2	1402	2	20,23,24	2.97	8 (40%)	26,32,35	1.23	3 (11%)
54	4SU	5	8	54	18,21,22	3.57	7 (38%)	26,30,33	2.15	5 (19%)
1	PSU	1	746	1	18,21,22	1.04	1 (5%)	22,30,33	1.69	3 (13%)
54	4OC	5	32	54	20,23,24	2.98	8 (40%)	26,32,35	1.00	1 (3%)
1	5MU	1	747	1	19,22,23	4.76	7 (36%)	28,32,35	3.94	9 (32%)
1	PSU	1	2605	1	18,21,22	1.09	1 (5%)	22,30,33	1.95	5 (22%)
1	PSU	1	2580	1	18,21,22	1.08	2 (11%)	22,30,33	1.92	5 (22%)
1	5MU	1	1939	1	19,22,23	4.72	7 (36%)	28,32,35	3.84	10 (35%)
2	5MC	2	967	2	18,22,23	3.60	7 (38%)	26,32,35	1.01	1 (3%)
2	2MG	2	1516	2	18,26,27	2.56	7 (38%)	16,38,41	1.32	3 (18%)
1	G7M	1	2069	1	20,26,27	2.35	7 (35%)	17,39,42	1.33	2 (11%)
1	PSU	1	2504	1	18,21,22	1.18	1 (5%)	22,30,33	1.78	4 (18%)
1	OMG	1	2251	54,1	18,26,27	2.47	8 (44%)	19,38,41	1.58	4 (21%)
54	PSU	5	55	54	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
1	PSU	1	2457	1	18,21,22	1.14	3 (16%)	22,30,33	1.87	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5MC	2	1407	2	18,22,23	3.58	7 (38%)	26,32,35	1.11	2 (7%)
2	MA6	2	1519	2	19,26,27	1.02	1 (5%)	18,38,41	2.85	2 (11%)
1	OMC	1	2498	1	19,22,23	2.89	7 (36%)	26,31,34	0.89	1 (3%)

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
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
2	PSU	2	516	2	-	2/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
1	OMU	1	2552	1	-	1/9/27/28	0/2/2/2
1	6MZ	1	2030	1	-	3/5/27/28	0/3/3/3
54	5MU	5	54	54	-	0/7/25/26	0/2/2/2
1	2MA	1	2503	1	-	3/3/25/26	0/3/3/3
54	H2U	5	20	54	-	4/7/38/39	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
56	FME	6	77	56	-	3/7/9/11	-
2	G7M	2	527	2	-	2/3/25/26	0/3/3/3
1	3TD	1	1915	1	-	4/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	2/7/25/26	0/2/2/2
1	6MZ	1	1618	1	-	4/5/27/28	0/3/3/3
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
2	2MG	2	966	2	-	0/5/27/28	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	2/5/27/28	0/3/3/3
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
54	4SU	5	8	54	-	3/7/25/26	0/2/2/2
1	PSU	1	746	1	-	1/7/25/26	0/2/2/2
54	4OC	5	32	54	-	0/9/29/30	0/2/2/2
1	5MU	1	747	1	-	1/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	G7M	1	2069	1	-	1/3/25/26	0/3/3/3
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	OMG	1	2251	54,1	-	0/5/27/28	0/3/3/3
54	PSU	5	55	54	-	1/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	3/7/29/30	0/3/3/3
1	OMC	1	2498	1	-	0/9/27/28	0/2/2/2

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	12.48	1.49	1.35
1	1	747	5MU	C2-N1	11.02	1.56	1.38
54	5	20	H2U	C2-N1	10.80	1.51	1.35
54	5	54	5MU	C2-N1	10.70	1.55	1.38
1	1	1939	5MU	C2-N1	10.57	1.55	1.38
54	5	54	5MU	C6-N1	10.51	1.56	1.38
1	1	1939	5MU	C6-N1	10.14	1.55	1.38
2	2	527	G7M	C8-N7	10.04	1.51	1.33
1	1	747	5MU	C6-N1	9.98	1.55	1.38
1	1	747	5MU	C4-C5	9.62	1.60	1.44
1	1	1939	5MU	C4-C5	9.59	1.60	1.44
54	5	54	5MU	C4-C5	9.57	1.60	1.44
2	2	527	G7M	C8-N9	9.51	1.50	1.33
1	1	1915	3TD	C2-N1	9.27	1.49	1.37
1	1	1962	5MC	C6-C5	8.96	1.49	1.34
2	2	967	5MC	C6-C5	8.96	1.49	1.34
2	2	1407	5MC	C6-C5	8.89	1.49	1.34
1	1	747	5MU	C4-N3	-8.15	1.23	1.38
54	5	54	5MU	C4-N3	-8.12	1.23	1.38
1	1	1939	5MU	C4-N3	-8.04	1.23	1.38
54	5	8	4SU	C4-N3	7.73	1.45	1.37
54	5	8	4SU	C2-N1	7.53	1.50	1.38
1	1	2030	6MZ	C6-N6	7.39	1.47	1.35
1	1	745	1MG	C2-N2	7.25	1.47	1.34
1	1	1618	6MZ	C6-N6	7.17	1.46	1.35
1	1	2503	2MA	C2-N3	7.00	1.46	1.31
2	2	967	5MC	C4-N3	6.73	1.45	1.34
2	2	1402	4OC	C4-N3	6.69	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	5	32	4OC	C4-N3	6.64	1.44	1.32
1	1	1962	5MC	C4-N3	6.56	1.45	1.34
54	5	20	H2U	C2-N3	6.45	1.49	1.38
1	1	2552	OMU	C2-N3	6.44	1.49	1.38
2	2	1407	5MC	C4-N3	6.30	1.44	1.34
2	2	966	2MG	C2-N2	6.27	1.47	1.33
1	1	2498	OMC	C6-C5	6.27	1.49	1.35
2	2	1516	2MG	C2-N2	6.25	1.47	1.33
1	1	2552	OMU	C2-N1	6.22	1.48	1.38
2	2	967	5MC	C2-N3	6.06	1.48	1.36
1	1	2445	2MG	C2-N2	6.06	1.46	1.33
2	2	1498	UR3	C2-N1	6.01	1.47	1.38
1	1	1835	2MG	C2-N2	5.96	1.46	1.33
1	1	1962	5MC	C2-N3	5.95	1.48	1.36
1	1	2498	OMC	C2-N3	5.95	1.48	1.36
2	2	1407	5MC	C2-N3	5.94	1.48	1.36
2	2	1207	2MG	C2-N2	5.94	1.46	1.33
54	5	32	4OC	C6-C5	5.93	1.48	1.35
1	1	1939	5MU	C6-C5	5.86	1.44	1.34
54	5	8	4SU	C6-C5	5.85	1.48	1.35
2	2	1498	UR3	C6-C5	5.83	1.48	1.35
2	2	1402	4OC	C6-C5	5.72	1.48	1.35
2	2	1402	4OC	C2-N3	5.69	1.47	1.36
1	1	1915	3TD	C6-N1	5.69	1.45	1.36
54	5	32	4OC	C2-N3	5.64	1.47	1.36
2	2	527	G7M	C2-N3	5.62	1.46	1.33
1	1	747	5MU	C6-C5	5.61	1.43	1.34
54	5	54	5MU	C6-C5	5.59	1.43	1.34
1	1	2498	OMC	C4-N3	5.54	1.45	1.34
54	5	8	4SU	C2-N3	5.49	1.47	1.38
1	1	2552	OMU	C6-C5	5.39	1.47	1.35
1	1	745	1MG	C2-N3	5.28	1.44	1.34
1	1	2069	G7M	C2-N3	5.24	1.45	1.33
1	1	2251	OMG	C2-N3	5.21	1.45	1.33
54	5	8	4SU	C4-S4	-5.20	1.58	1.68
2	2	966	2MG	C4-N3	5.13	1.49	1.37
1	1	2445	2MG	C4-N3	4.98	1.49	1.37
1	1	2069	G7M	C4-N3	4.90	1.49	1.37
1	1	745	1MG	C4-N3	4.90	1.49	1.37
2	2	1207	2MG	C4-N3	4.88	1.49	1.37
1	1	2503	2MA	C4-N3	4.85	1.49	1.37
2	2	1516	2MG	C4-N3	4.84	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1835	2MG	C4-N3	4.76	1.48	1.37
2	2	967	5MC	C4-N4	4.74	1.46	1.34
1	1	1962	5MC	C4-N4	4.72	1.46	1.34
2	2	1407	5MC	C4-N4	4.72	1.46	1.34
54	5	20	H2U	C4-N3	4.69	1.45	1.37
2	2	527	G7M	C2-N2	4.67	1.45	1.34
1	1	2251	OMG	C2-N2	4.62	1.45	1.34
1	1	2251	OMG	C4-N3	4.59	1.48	1.37
2	2	1498	UR3	C2-N3	4.57	1.47	1.39
1	1	1915	3TD	C2-N3	4.52	1.48	1.38
2	2	1407	5MC	C6-N1	4.49	1.45	1.38
2	2	1402	4OC	C2-N1	4.42	1.49	1.40
2	2	967	5MC	C6-N1	4.39	1.45	1.38
2	2	1407	5MC	C2-N1	4.35	1.49	1.40
2	2	1516	2MG	C2-N1	4.23	1.43	1.36
1	1	2069	G7M	C2-N2	4.19	1.44	1.34
1	1	1962	5MC	C6-N1	4.18	1.45	1.38
2	2	966	2MG	C2-N1	4.13	1.43	1.36
54	5	32	4OC	C4-N4	4.10	1.44	1.35
2	2	1402	4OC	C4-N4	4.05	1.44	1.35
2	2	527	G7M	C6-N1	4.02	1.43	1.37
1	1	1835	2MG	C2-N1	4.00	1.43	1.36
2	2	967	5MC	C2-N1	3.98	1.48	1.40
2	2	1207	2MG	C2-N1	3.95	1.43	1.36
1	1	2504	PSU	C6-C5	3.90	1.39	1.35
54	5	32	4OC	C2-N1	3.86	1.48	1.40
2	2	527	G7M	C4-N3	3.84	1.46	1.37
54	5	32	4OC	C5-C4	3.80	1.48	1.40
1	1	2498	OMC	C4-N4	3.79	1.42	1.33
1	1	2445	2MG	C2-N1	3.75	1.42	1.36
1	1	2552	OMU	C4-N3	3.72	1.45	1.38
1	1	1962	5MC	C2-N1	3.70	1.48	1.40
1	1	2498	OMC	C2-N1	3.63	1.47	1.40
1	1	2498	OMC	C6-N1	3.59	1.46	1.38
2	2	1402	4OC	C5-C4	3.53	1.48	1.40
1	1	2069	G7M	C6-N1	3.49	1.43	1.37
1	1	2069	G7M	C5-C6	3.43	1.54	1.45
54	5	55	PSU	C6-C5	3.41	1.39	1.35
1	1	1962	5MC	O2-C2	-3.37	1.17	1.23
2	2	1407	5MC	O2-C2	-3.34	1.17	1.23
2	2	527	G7M	C2-N1	3.29	1.45	1.37
1	1	2445	2MG	O6-C6	-3.24	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2457	PSU	C6-C5	3.24	1.39	1.35
1	1	2605	PSU	C6-C5	3.21	1.39	1.35
2	2	967	5MC	O2-C2	-3.21	1.17	1.23
1	1	2030	6MZ	C5-C4	-3.17	1.32	1.40
1	1	1835	2MG	O6-C6	-3.16	1.16	1.23
1	1	2251	OMG	C6-N1	3.15	1.42	1.37
1	1	1911	PSU	C6-C5	3.15	1.39	1.35
2	2	966	2MG	O6-C6	-3.14	1.16	1.23
1	1	1618	6MZ	C5-C4	-3.14	1.32	1.40
1	1	1917	PSU	C6-C5	3.13	1.39	1.35
1	1	2552	OMU	O4-C4	-3.12	1.18	1.24
1	1	1835	2MG	C5-C4	-3.10	1.35	1.43
2	2	1516	2MG	C5-C4	-3.08	1.35	1.43
2	2	1516	2MG	O6-C6	-3.08	1.17	1.23
2	2	1516	2MG	C6-N1	3.08	1.42	1.37
1	1	2445	2MG	C5-C4	-3.06	1.35	1.43
2	2	1207	2MG	O6-C6	-3.05	1.17	1.23
54	5	8	4SU	C5-C4	3.05	1.46	1.42
1	1	745	1MG	C5-C4	-3.03	1.35	1.43
1	1	2030	6MZ	C2-N3	2.99	1.36	1.32
1	1	747	5MU	O4-C4	-2.98	1.17	1.23
1	1	746	PSU	C6-C5	2.98	1.38	1.35
2	2	966	2MG	C6-N1	2.98	1.42	1.37
54	5	32	4OC	O2-C2	-2.95	1.18	1.23
1	1	1939	5MU	O4-C4	-2.93	1.18	1.23
1	1	955	PSU	C6-C5	2.92	1.38	1.35
2	2	516	PSU	C6-C5	2.92	1.38	1.35
1	1	2251	OMG	C5-C4	-2.91	1.35	1.43
2	2	1207	2MG	C5-C4	-2.91	1.35	1.43
54	5	32	4OC	C6-N1	2.90	1.45	1.38
1	1	2498	OMC	O2-C2	-2.89	1.18	1.23
2	2	966	2MG	C5-C4	-2.89	1.35	1.43
54	5	54	5MU	O4-C4	-2.88	1.18	1.23
2	2	1207	2MG	C6-N1	2.86	1.42	1.37
2	2	1402	4OC	C6-N1	2.86	1.44	1.38
1	1	1915	3TD	C4-N3	2.85	1.46	1.40
1	1	1835	2MG	C6-N1	2.82	1.42	1.37
1	1	2503	2MA	C5-C4	-2.81	1.35	1.43
2	2	1207	2MG	C5-C6	2.79	1.53	1.47
1	1	747	5MU	O2-C2	-2.76	1.18	1.23
2	2	1518	MA6	C5-C4	-2.75	1.33	1.40
2	2	1402	4OC	O2-C2	-2.75	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2580	PSU	C6-C5	2.74	1.38	1.35
2	2	527	G7M	C5-C6	2.69	1.52	1.45
1	1	2445	2MG	C6-N1	2.63	1.41	1.37
1	1	2552	OMU	O2-C2	-2.61	1.18	1.23
54	5	8	4SU	O2-C2	-2.61	1.18	1.23
1	1	2251	OMG	C5-C6	2.60	1.52	1.47
2	2	1519	MA6	C5-C4	-2.59	1.34	1.40
2	2	966	2MG	C5-C6	2.59	1.52	1.47
1	1	1835	2MG	C5-C6	2.53	1.52	1.47
1	1	2251	OMG	O6-C6	-2.51	1.18	1.23
1	1	1939	5MU	O2-C2	-2.49	1.18	1.23
2	2	1498	UR3	C6-N1	2.48	1.44	1.38
1	1	2069	G7M	O6-C6	-2.48	1.18	1.23
1	1	2251	OMG	C2-N1	2.48	1.43	1.37
1	1	1618	6MZ	C2-N3	2.47	1.36	1.32
2	2	1516	2MG	C5-C6	2.46	1.52	1.47
1	1	2552	OMU	C6-N1	2.43	1.43	1.38
2	2	1498	UR3	O2-C2	-2.42	1.18	1.22
2	2	527	G7M	O6-C6	-2.41	1.18	1.23
1	1	2580	PSU	O4'-C1'	-2.38	1.40	1.43
54	5	54	5MU	O2-C2	-2.38	1.18	1.23
1	1	2069	G7M	C2-N1	2.35	1.43	1.37
2	2	1498	UR3	O4-C4	-2.34	1.18	1.23
1	1	2503	2MA	C2-N1	2.31	1.43	1.36
54	5	20	H2U	O4-C4	-2.29	1.18	1.23
54	5	20	H2U	O2-C2	-2.25	1.18	1.23
1	1	2445	2MG	C5-C6	2.21	1.51	1.47
1	1	2552	OMU	C5-C4	2.15	1.48	1.43
2	2	527	G7M	C5-C4	2.14	1.43	1.39
1	1	2503	2MA	C6-N1	2.05	1.42	1.38
1	1	2457	PSU	C4-C5	-2.05	1.38	1.44
2	2	1498	UR3	C5-C4	2.03	1.49	1.43
1	1	2457	PSU	O4'-C1'	-2.01	1.41	1.43
1	1	745	1MG	C6-N1	2.00	1.43	1.39

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	747	5MU	C5-C4-N3	13.13	126.52	115.31
1	1	1939	5MU	C5-C4-N3	12.75	126.19	115.31
54	5	54	5MU	C5-C4-N3	12.22	125.74	115.31
1	1	747	5MU	C5-C6-N1	-11.30	111.72	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1939	5MU	C5-C6-N1	-11.03	112.00	123.34
2	2	1519	MA6	N1-C6-N6	-10.12	106.41	117.06
54	5	54	5MU	C5-C6-N1	-9.75	113.31	123.34
2	2	1518	MA6	N1-C6-N6	-9.73	106.81	117.06
54	5	8	4SU	C4-N3-C2	-6.92	120.61	127.34
2	2	1519	MA6	N3-C2-N1	-6.06	119.21	128.68
1	1	1618	6MZ	C9-N6-C6	-6.01	117.70	122.87
2	2	1518	MA6	N3-C2-N1	-5.96	119.37	128.68
1	1	2552	OMU	C4-N3-C2	-5.68	119.08	126.58
1	1	747	5MU	C4-N3-C2	-5.68	120.00	127.35
1	1	1939	5MU	O4-C4-C5	-5.59	118.42	124.90
1	1	1939	5MU	C4-N3-C2	-5.48	120.25	127.35
1	1	747	5MU	O4-C4-C5	-5.46	118.57	124.90
1	1	2030	6MZ	N3-C2-N1	-5.46	120.15	128.68
54	5	20	H2U	C4-N3-C2	-5.46	121.26	125.79
1	1	1618	6MZ	N3-C2-N1	-5.42	120.20	128.68
1	1	1911	PSU	N1-C2-N3	5.18	121.00	115.13
54	5	8	4SU	C5-C4-N3	5.17	119.49	114.69
1	1	1911	PSU	C4-N3-C2	-5.14	118.94	126.34
1	1	2605	PSU	C4-N3-C2	-5.10	118.99	126.34
1	1	2605	PSU	N1-C2-N3	4.99	120.78	115.13
54	5	54	5MU	O4-C4-C5	-4.89	119.23	124.90
1	1	2580	PSU	N1-C2-N3	4.84	120.61	115.13
1	1	1915	3TD	N1-C2-N3	4.80	119.93	116.14
1	1	2457	PSU	N1-C2-N3	4.76	120.52	115.13
1	1	2030	6MZ	C9-N6-C6	-4.75	118.78	122.87
1	1	955	PSU	C4-N3-C2	-4.70	119.56	126.34
1	1	2457	PSU	C4-N3-C2	-4.68	119.60	126.34
54	5	55	PSU	N1-C2-N3	4.63	120.38	115.13
1	1	1917	PSU	C4-N3-C2	-4.61	119.69	126.34
1	1	1939	5MU	N3-C2-N1	4.60	121.00	114.89
1	1	746	PSU	C4-N3-C2	-4.60	119.71	126.34
1	1	2504	PSU	N1-C2-N3	4.56	120.30	115.13
2	2	516	PSU	N1-C2-N3	4.56	120.29	115.13
1	1	2504	PSU	C4-N3-C2	-4.55	119.78	126.34
2	2	1498	UR3	C4-N3-C2	-4.52	120.30	124.56
1	1	1917	PSU	N1-C2-N3	4.52	120.25	115.13
1	1	2580	PSU	C4-N3-C2	-4.51	119.85	126.34
1	1	747	5MU	N3-C2-N1	4.50	120.87	114.89
2	2	516	PSU	C4-N3-C2	-4.45	119.93	126.34
54	5	55	PSU	C4-N3-C2	-4.42	119.97	126.34
54	5	54	5MU	C4-N3-C2	-4.36	121.71	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	955	PSU	N1-C2-N3	4.20	119.88	115.13
1	1	746	PSU	N1-C2-N3	4.09	119.76	115.13
54	5	54	5MU	N3-C2-N1	4.04	120.25	114.89
1	1	2503	2MA	C5-C6-N1	3.90	120.75	114.02
1	1	2552	OMU	N3-C2-N1	3.87	120.02	114.89
1	1	1618	6MZ	C1'-N9-C4	-3.85	119.88	126.64
1	1	745	1MG	C5-C6-N1	3.85	119.68	113.90
54	5	54	5MU	C5M-C5-C4	3.81	122.95	118.77
2	2	966	2MG	C5-C6-N1	3.80	120.66	113.95
1	1	747	5MU	C5M-C5-C6	-3.79	117.79	122.85
1	1	2251	OMG	C5-C6-N1	3.74	120.56	113.95
1	1	2445	2MG	C5-C6-N1	3.74	120.56	113.95
1	1	1915	3TD	C4-N3-C2	-3.67	120.63	124.61
54	5	54	5MU	C5M-C5-C6	-3.61	118.03	122.85
1	1	1962	5MC	C5-C6-N1	-3.59	119.64	123.34
1	1	2552	OMU	C5-C4-N3	3.59	120.20	114.84
2	2	1207	2MG	C5-C6-N1	3.56	120.23	113.95
1	1	2069	G7M	C2-N1-C6	-3.55	118.56	125.10
1	1	1835	2MG	C5-C6-N1	3.54	120.19	113.95
1	1	1939	5MU	C5M-C5-C6	-3.52	118.15	122.85
54	5	8	4SU	C5-C4-S4	-3.44	120.03	124.47
2	2	1516	2MG	C5-C6-N1	3.42	119.99	113.95
2	2	967	5MC	C5-C6-N1	-3.40	119.84	123.34
1	1	2251	OMG	C2-N1-C6	-3.39	118.85	125.10
1	1	2580	PSU	O2-C2-N1	-3.36	119.09	122.79
54	5	8	4SU	C1'-N1-C2	3.32	123.57	117.57
54	5	20	H2U	O2-C2-N3	-3.31	115.33	121.50
54	5	8	4SU	N3-C2-N1	3.29	119.26	114.89
54	5	20	H2U	C5-C6-N1	3.25	122.33	111.61
54	5	20	H2U	N3-C2-N1	3.20	120.04	116.65
1	1	747	5MU	C5M-C5-C4	3.17	122.26	118.77
2	2	1402	4OC	O2-C2-N3	-3.14	117.22	122.33
1	1	1911	PSU	O2-C2-N1	-3.04	119.44	122.79
1	1	1939	5MU	C5M-C5-C4	2.96	122.03	118.77
1	1	2552	OMU	O4-C4-C5	-2.93	120.01	125.16
2	2	1407	5MC	C5-C6-N1	-2.92	120.34	123.34
1	1	2503	2MA	C8-N7-C5	2.88	108.48	102.99
1	1	2504	PSU	O2-C2-N1	-2.85	119.66	122.79
1	1	745	1MG	C8-N7-C5	2.83	108.38	102.99
1	1	2580	PSU	C6-N1-C2	-2.80	119.82	122.68
1	1	1939	5MU	O2-C2-N1	-2.74	119.14	122.79
1	1	747	5MU	O4-C4-N3	-2.72	114.91	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	5	54	5MU	O4-C4-N3	-2.66	115.03	120.12
54	5	55	PSU	O2-C2-N1	-2.65	119.87	122.79
1	1	2251	OMG	C8-N7-C5	2.64	108.01	102.99
1	1	746	PSU	O2-C2-N1	-2.61	119.91	122.79
2	2	527	G7M	O6-C6-N1	-2.61	117.57	120.65
1	1	2445	2MG	O6-C6-C5	-2.60	119.28	124.37
1	1	2030	6MZ	C1'-N9-C4	-2.59	122.08	126.64
2	2	527	G7M	C2-N1-C6	-2.59	120.32	125.10
1	1	2504	PSU	C6-N1-C2	-2.59	120.03	122.68
2	2	1207	2MG	CM2-N2-C2	-2.59	118.14	123.86
1	1	1917	PSU	O2-C2-N1	-2.58	119.95	122.79
1	1	2251	OMG	O6-C6-C5	-2.57	119.35	124.37
54	5	32	4OC	C6-C5-C4	2.57	120.10	116.96
2	2	1407	5MC	O2-C2-N3	-2.55	118.18	122.33
2	2	516	PSU	C6-N1-C2	-2.55	120.07	122.68
1	1	2457	PSU	C6-C5-C4	2.54	119.97	118.20
2	2	966	2MG	O6-C6-C5	-2.53	119.43	124.37
1	1	1835	2MG	C8-N7-C5	2.50	107.76	102.99
2	2	1516	2MG	O6-C6-C5	-2.49	119.50	124.37
54	5	55	PSU	C6-N1-C2	-2.49	120.13	122.68
1	1	1939	5MU	O4-C4-N3	-2.47	115.39	120.12
1	1	2552	OMU	O2-C2-N1	-2.46	119.52	122.79
2	2	1207	2MG	C8-N7-C5	2.45	107.66	102.99
1	1	2445	2MG	C8-N7-C5	2.45	107.65	102.99
2	2	966	2MG	C8-N7-C5	2.42	107.60	102.99
1	1	1835	2MG	CM2-N2-C2	-2.40	118.57	123.86
1	1	1911	PSU	C6-N1-C2	-2.39	120.23	122.68
1	1	745	1MG	O6-C6-C5	-2.38	119.98	124.19
1	1	2605	PSU	O2-C2-N1	-2.37	120.18	122.79
1	1	1917	PSU	C6-N1-C2	-2.35	120.28	122.68
2	2	1516	2MG	C8-N7-C5	2.34	107.45	102.99
1	1	2580	PSU	O4'-C1'-C2'	2.33	108.43	105.14
2	2	516	PSU	O3'-C3'-C4'	2.33	117.78	111.05
2	2	516	PSU	O2-C2-N1	-2.29	120.27	122.79
1	1	747	5MU	C6-C5-C4	2.29	119.95	118.03
1	1	2457	PSU	C6-N1-C2	-2.29	120.34	122.68
2	2	1402	4OC	C1'-N1-C2	2.26	123.47	118.42
1	1	1835	2MG	O6-C6-C5	-2.23	120.02	124.37
54	5	20	H2U	C5-C4-N3	2.21	119.13	116.65
1	1	2498	OMC	O2-C2-N3	-2.17	118.80	122.33
1	1	1915	3TD	O4-C4-N3	-2.16	116.33	120.30
2	2	1498	UR3	C1'-N1-C2	2.16	120.64	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2457	PSU	O2-C2-N1	-2.16	120.42	122.79
2	2	1402	4OC	C6-C5-C4	2.15	119.60	116.96
1	1	1939	5MU	C6-C5-C4	2.15	119.83	118.03
1	1	2605	PSU	C6-C5-C4	2.13	119.69	118.20
2	2	1207	2MG	O6-C6-C5	-2.12	120.23	124.37
1	1	2605	PSU	C6-N1-C2	-2.12	120.52	122.68
1	1	1911	PSU	C6-C5-C4	2.12	119.68	118.20
1	1	2069	G7M	N2-C2-N1	2.10	121.17	116.71
1	1	1962	5MC	CM5-C5-C6	-2.03	120.13	122.85
1	1	2457	PSU	O4'-C1'-C2'	2.01	107.98	105.14

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	C5-C6-N6-C9
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
1	1	2552	OMU	C1'-C2'-O2'-CM2
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	1207	2MG	O4'-C4'-C5'-O5'
2	2	1207	2MG	C3'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
54	5	20	H2U	O4'-C1'-N1-C2
54	5	20	H2U	O4'-C1'-N1-C6
56	6	77	FME	O1-CN-N-CA
56	6	77	FME	N-CA-CB-CG
1	1	1915	3TD	O4'-C4'-C5'-O5'
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	1835	2MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	1915	3TD	C3'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
2	2	1402	4OC	C3'-C4'-C5'-O5'
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
1	1	2503	2MA	C3'-C4'-C5'-O5'
54	5	20	H2U	O4'-C4'-C5'-O5'
54	5	20	H2U	C3'-C4'-C5'-O5'
54	5	8	4SU	O4'-C1'-N1-C6
54	5	8	4SU	O4'-C1'-N1-C2
1	1	2503	2MA	C4'-C5'-O5'-P
2	2	1519	MA6	C4'-C5'-O5'-P
1	1	2030	6MZ	C4'-C5'-O5'-P
56	6	77	FME	C-CA-CB-CG
1	1	747	5MU	C4'-C5'-O5'-P
54	5	8	4SU	C4'-C5'-O5'-P
1	1	1962	5MC	C2'-C1'-N1-C6
1	1	2069	G7M	O4'-C4'-C5'-O5'
1	1	1962	5MC	O4'-C1'-N1-C6
1	1	746	PSU	O4'-C1'-C5-C6
54	5	55	PSU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

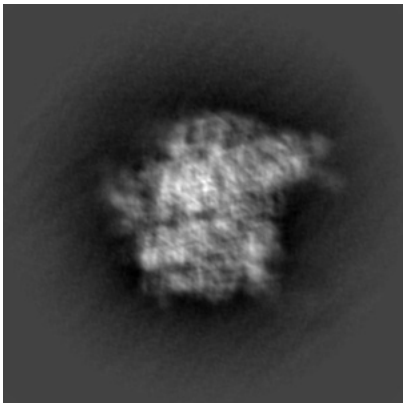
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20193. These allow visual inspection of the internal detail of the map and identification of artifacts.

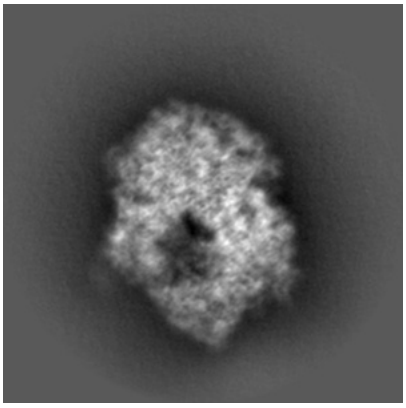
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

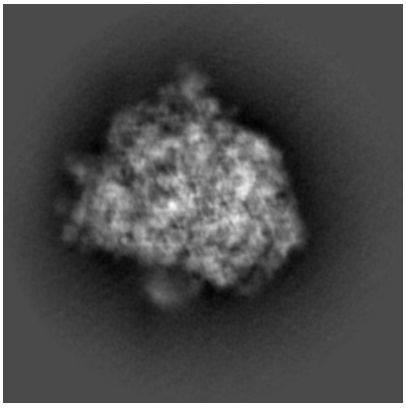
6.1.1 Primary map



X



Y

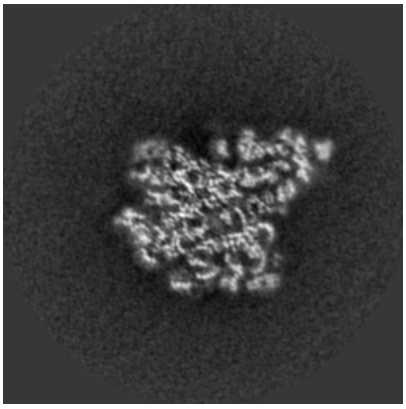


Z

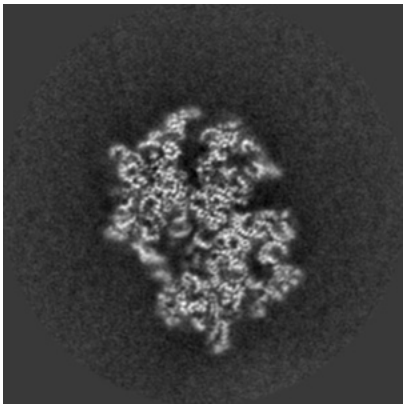
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

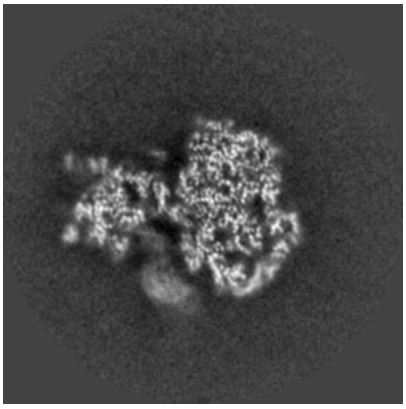
6.2.1 Primary map



X Index: 128



Y Index: 128

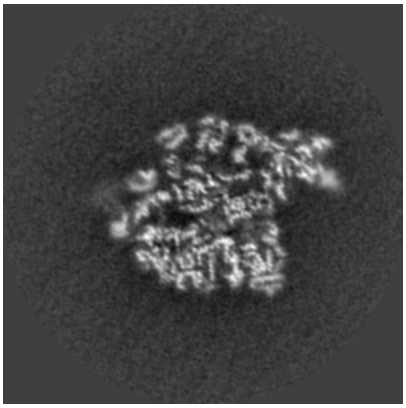


Z Index: 128

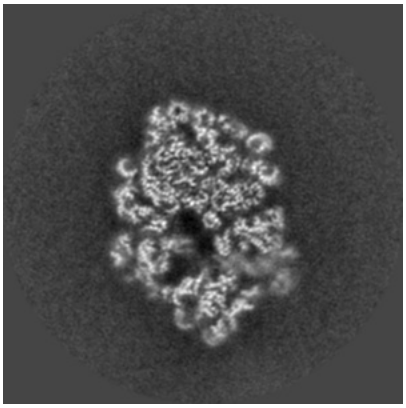
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

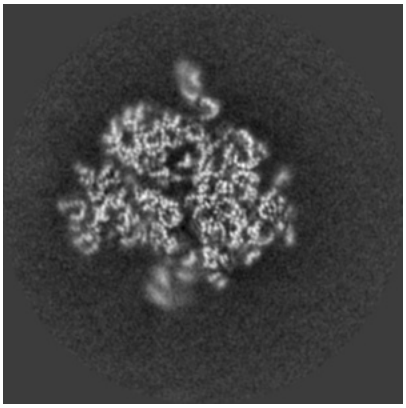
6.3.1 Primary map



X Index: 122



Y Index: 114

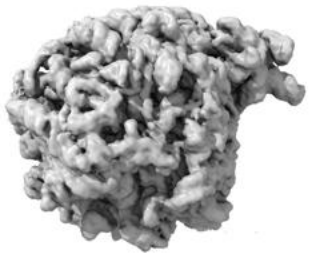


Z Index: 143

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

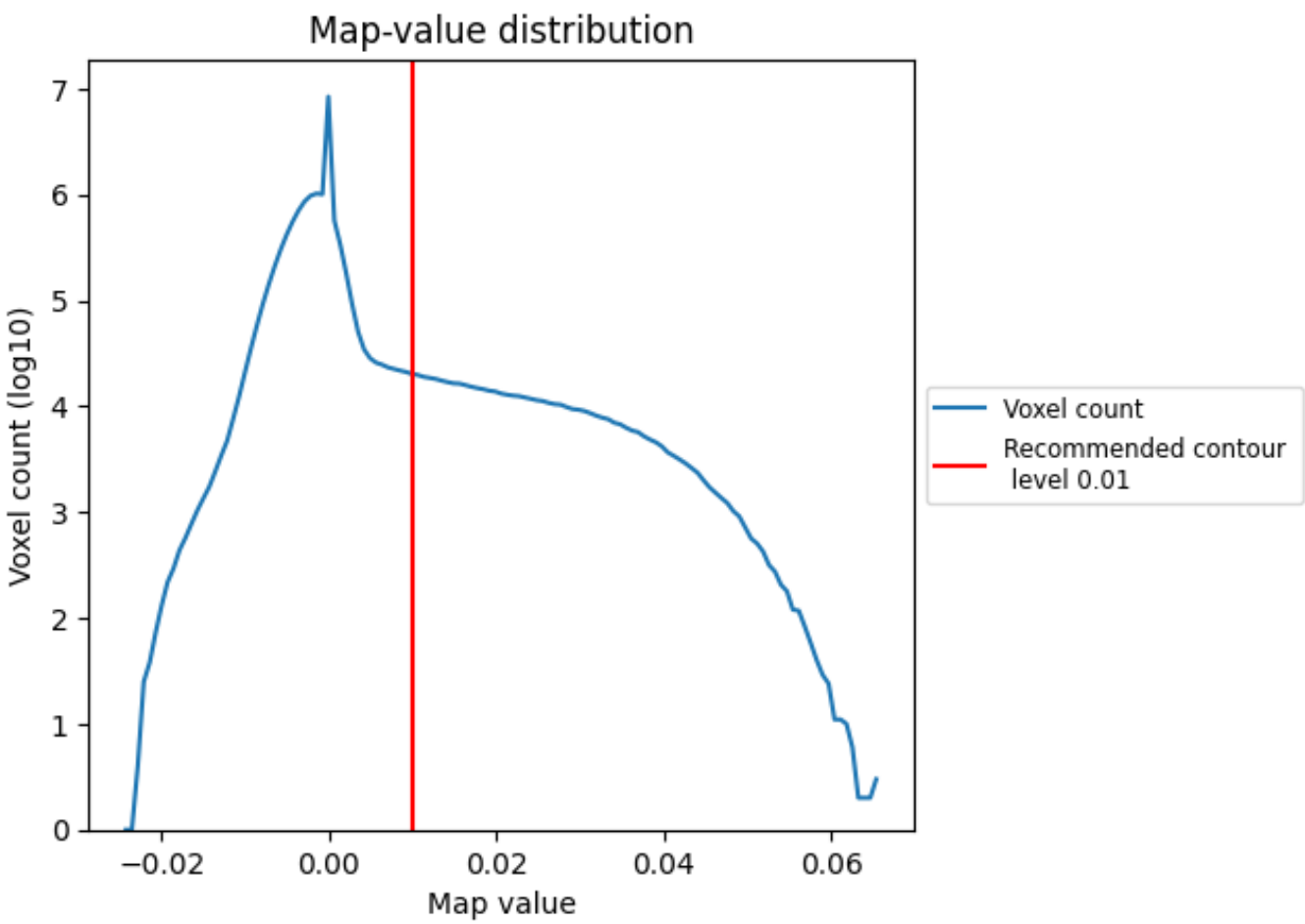
6.5 Mask visualisation (i)

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

7 Map analysis (i)

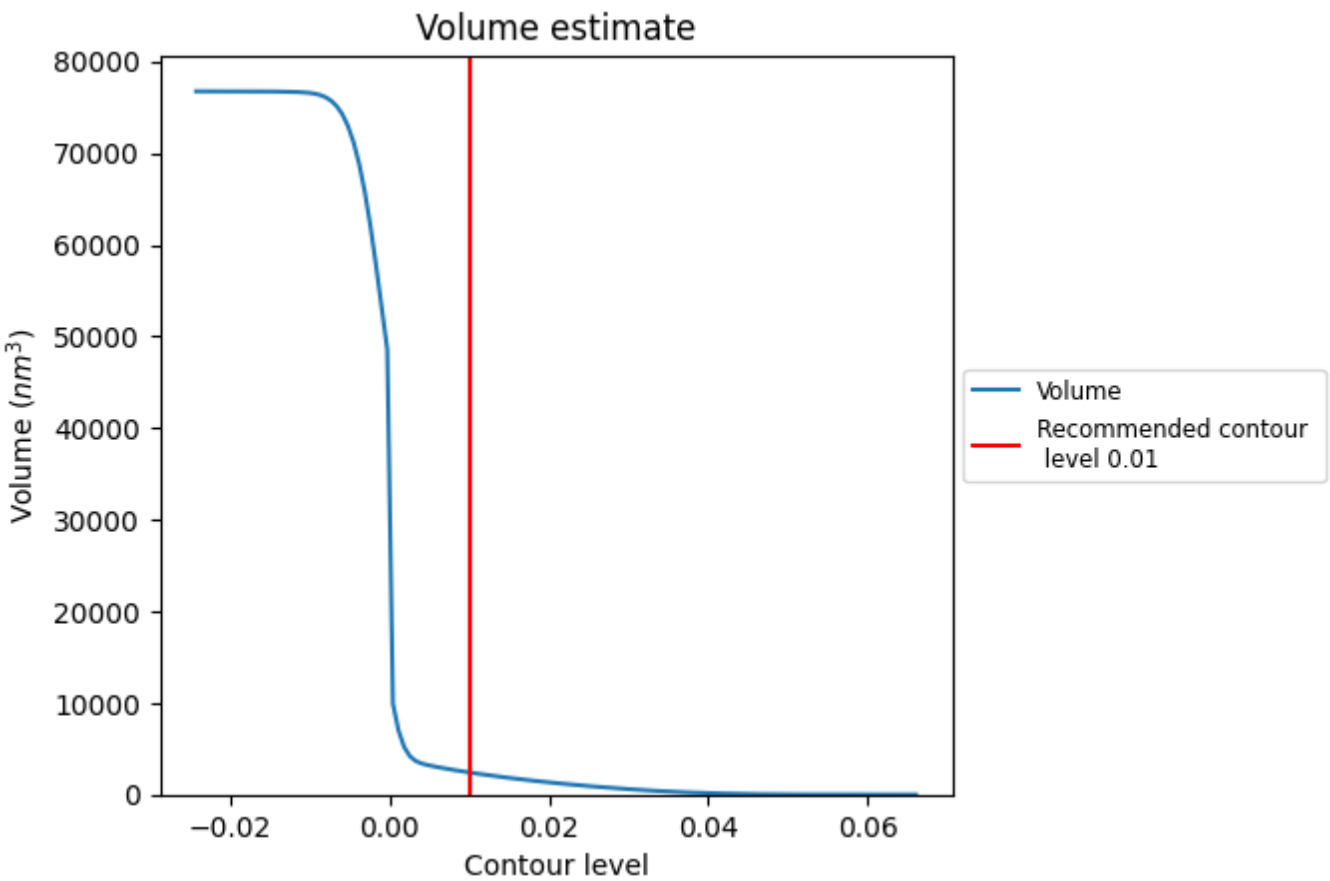
This section contains the results of statistical analysis of the map.

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.

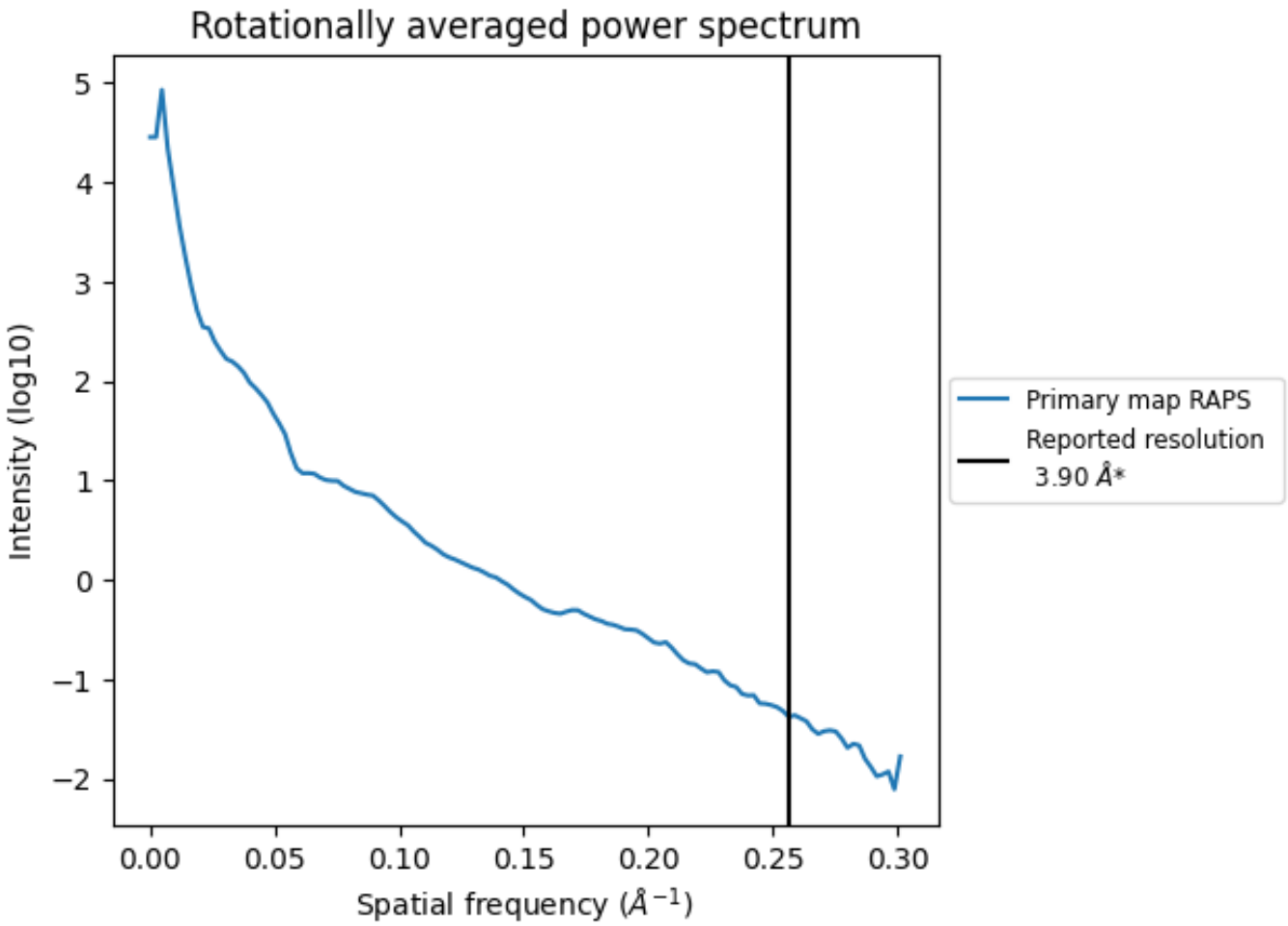
7.2 Volume estimate (i)



The volume at the recommended contour level is 2414 nm^3; this corresponds to an approximate mass of 2180 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 0.256 Å^{-1}

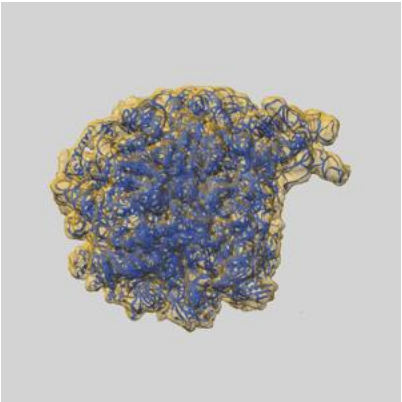
8 Fourier-Shell correlation (i)

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

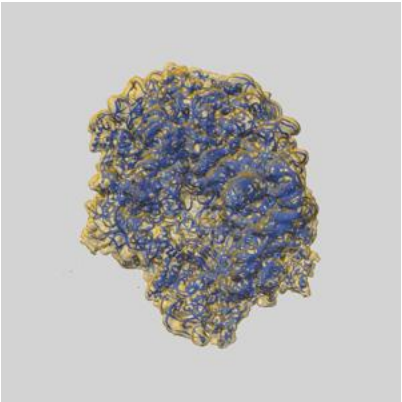
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20193 and PDB model 6OT3. Per-residue inclusion information can be found in section 3 on page 14.

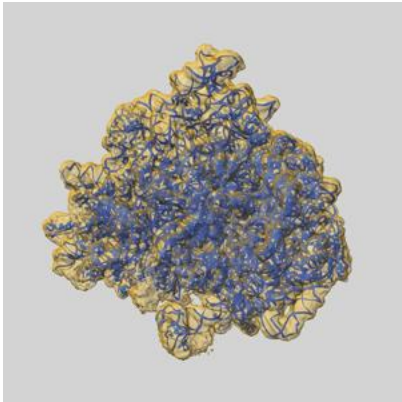
9.1 Map-model overlay (i)



X



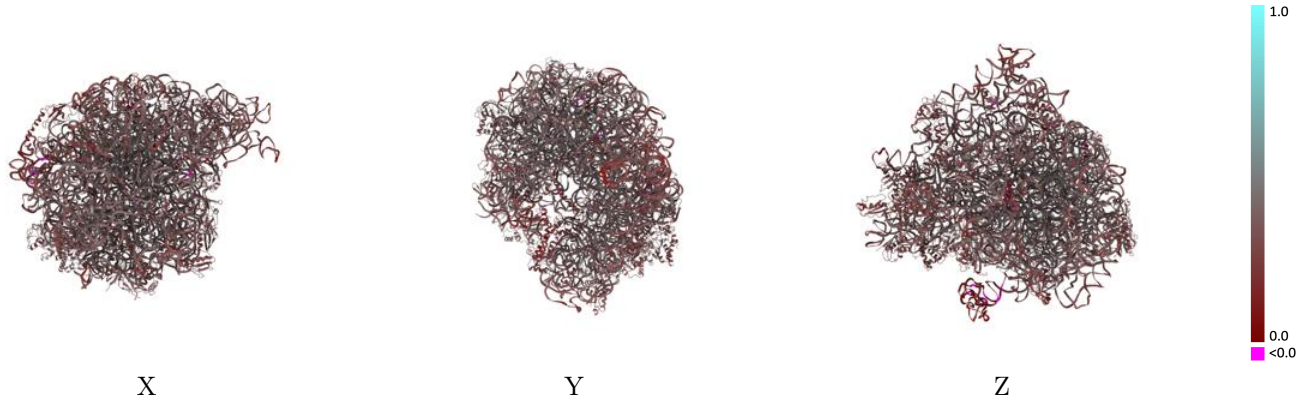
Y



Z

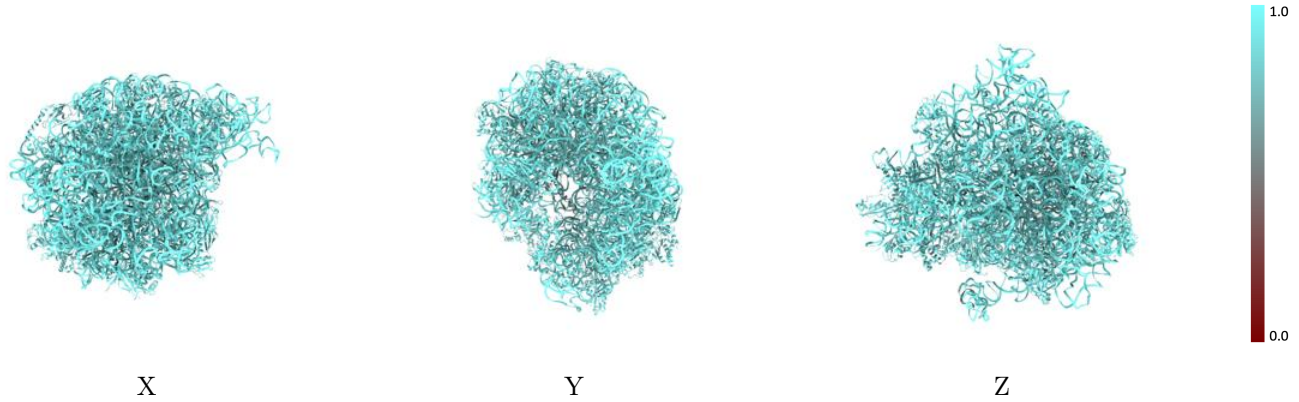
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



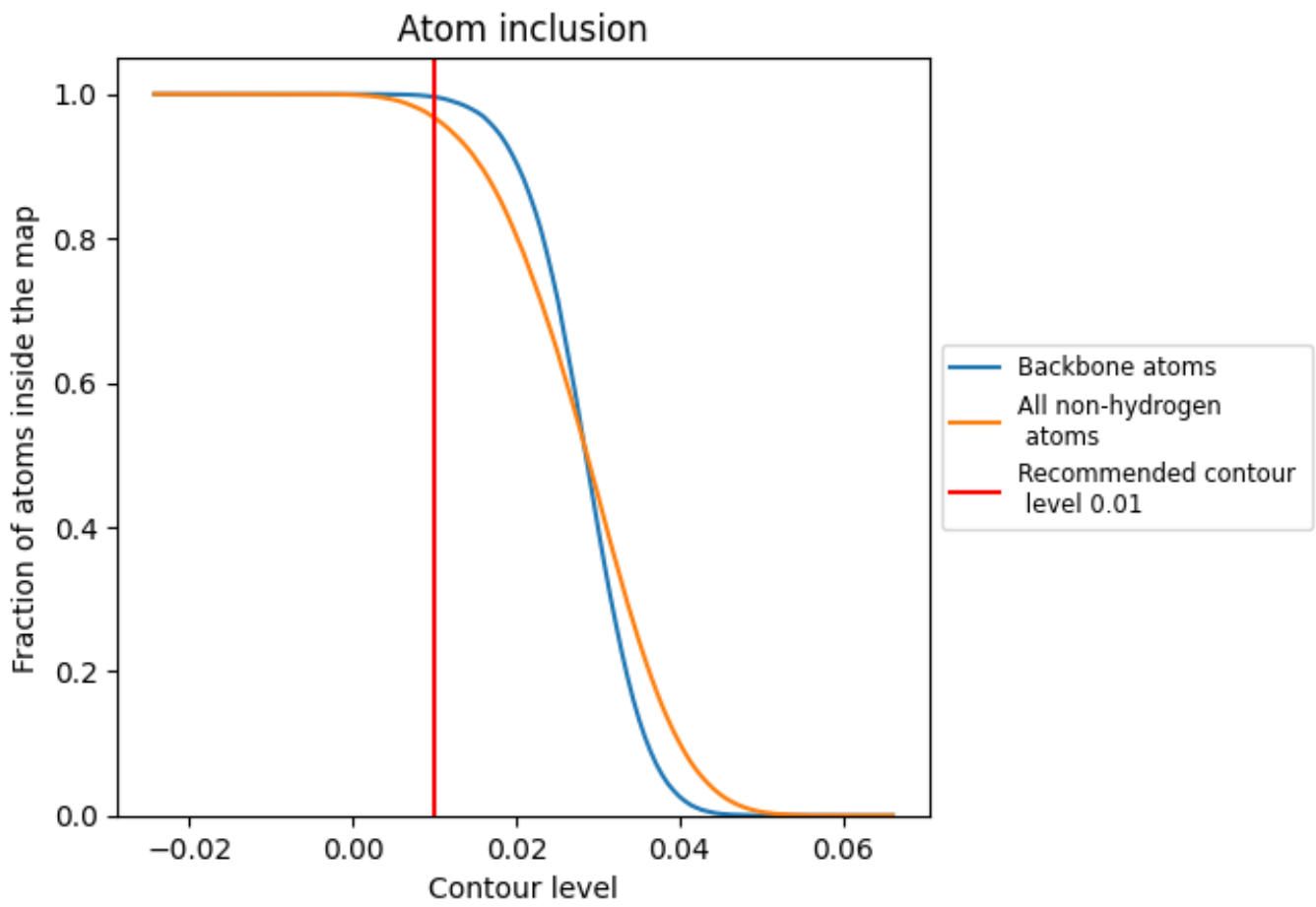
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 97% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9672	0.3480
1	0.9957	0.3640
2	0.9982	0.3560
3	0.9992	0.3490
4	0.9946	0.3690
5	0.9742	0.3360
6	0.7188	0.2220
A	0.8142	0.2480
B	0.8934	0.3790
C	0.9181	0.3550
D	0.9158	0.3480
E	0.9162	0.2980
F	0.9441	0.3200
G	0.8458	0.2660
J	0.9136	0.3540
K	0.8350	0.3410
L	0.9238	0.3660
M	0.8973	0.3630
N	0.9069	0.2820
O	0.9594	0.3270
P	0.8964	0.3220
Q	0.9218	0.3150
R	0.9285	0.3610
S	0.8744	0.3610
T	0.8986	0.3340
U	0.9497	0.3290
V	0.9553	0.3380
W	0.9134	0.3650
X	0.9002	0.3440
Y	0.9489	0.2730
Z	0.9128	0.3570
a	0.8984	0.2840
b	0.9252	0.3540
c	0.9282	0.3520
d	0.8930	0.3530

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Chain	Atom inclusion	Q-score
e	0.8839	0.3580
f	0.9249	0.3470
g	0.9023	0.2960
h	0.8912	0.3320
i	0.9353	0.3090
j	0.9204	0.3470
k	0.8984	0.3010
l	0.9082	0.2950
m	0.9271	0.3470
n	0.9346	0.3150
o	0.9046	0.3120
p	0.9074	0.3450
q	0.8618	0.3460
r	0.9171	0.2960
s	0.9328	0.3170
t	0.8971	0.2190
u	0.9522	0.3230
v	0.9288	0.3360
w	0.8719	0.3110
x	0.9304	0.3120
y	0.9251	0.2880
z	0.8301	0.2790