



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 06:33 AM UTC

PDB ID : 8C8X / pdb_00008c8x
EMDB ID : EMD-16494
Title : Cryo-EM captures early ribosome assembly in action
Authors : Lauer, S.; Nikolay, R.; Qin, B.
Deposited on : 2023-01-21
Resolution : 3.93 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

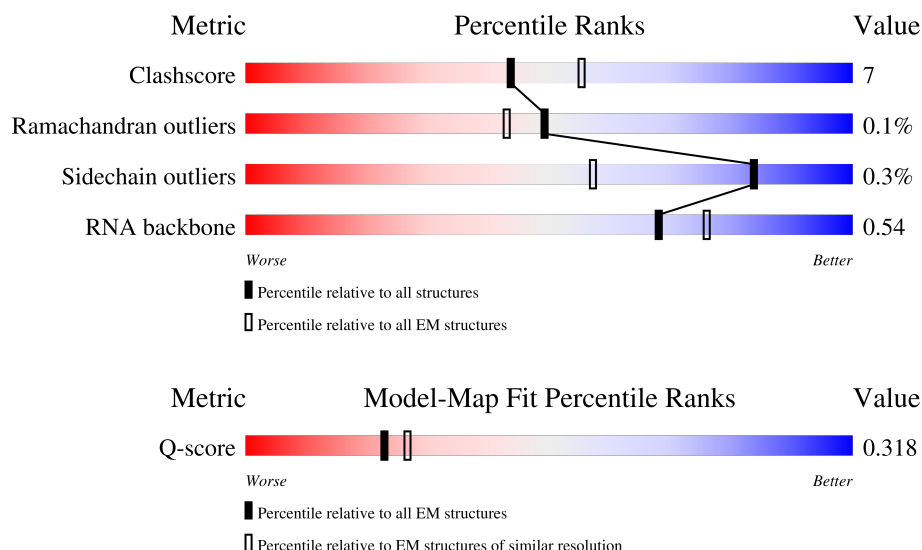
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.93 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	7811 (3.43 - 4.43)

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 $\leq 5\%$. 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	C	273	5% 70% 18% 12%
2	D	209	13% 73% 16% 11%
3	E	201	15% 82% 13% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	179	
5	H	149	
6	J	142	
7	K	123	
8	L	144	
9	N	127	
10	O	117	
11	P	115	
12	Q	118	
13	R	103	
14	S	110	
15	T	100	
16	U	104	
17	V	94	
18	W	85	
19	X	78	
20	Y	63	
21	Z	59	
22	0	57	
23	1	55	
24	2	46	
25	3	65	
26	M	136	
27	A	2904	
28	B	119	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 82776 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 L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	241	Total	C	N	O	S	0	0
			1858	1149	379	324	6		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	186	Total	C	N	O	S	0	0
			1393	880	250	259	4		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	190	Total	C	N	O	S	0	0
			1462	918	262	277	5		

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 6 is a protein called 50S ribosomal protein L13.

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

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 9 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 10 is a protein called 50S ribosomal protein L18.

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

- Molecule 11 is a protein called 50S ribosomal protein L19.

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

- Molecule 12 is a protein called 50S ribosomal protein L20.

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

- Molecule 13 is a protein called 50S ribosomal protein L21.

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

- Molecule 14 is a protein called 50S ribosomal protein L22.

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

- Molecule 15 is a protein called 50S ribosomal protein L23.

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

- Molecule 16 is a protein called 50S ribosomal protein L24.

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

- Molecule 17 is a protein called 50S ribosomal protein L25.

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

- Molecule 18 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 19 is a protein called 50S ribosomal protein L28.

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

- Molecule 20 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	61	Total	C	N	O	S	0	0
			499	308	97	92	2		

- Molecule 21 is a protein called 50S ribosomal protein L30.

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

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	124	Total	C	N	O	S	0	0
			984	629	187	163	5		

- Molecule 27 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A	2705	Total	C	N	O	P	0	0
			58086	25911	10706	18764	2705		

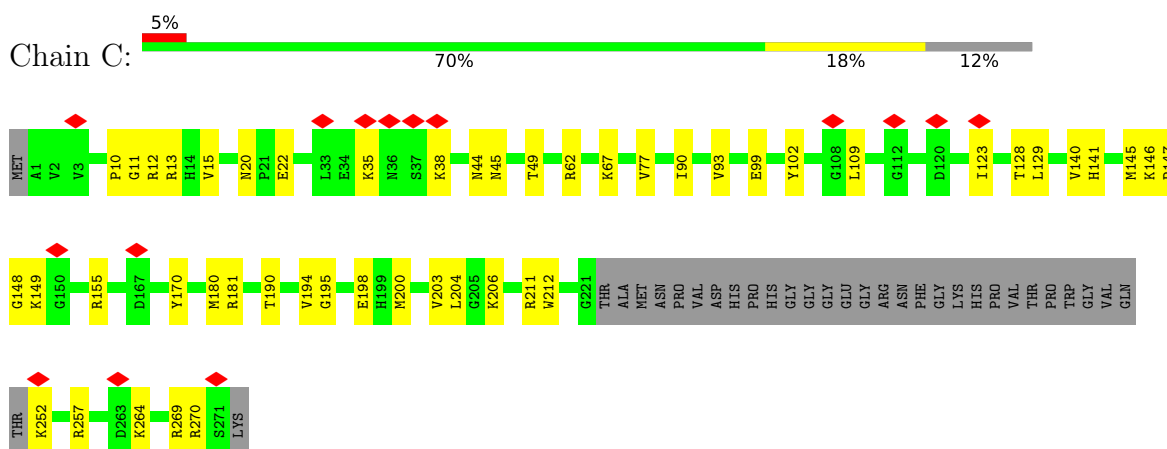
- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	B	119	2546	1135	466	827	118	0	0

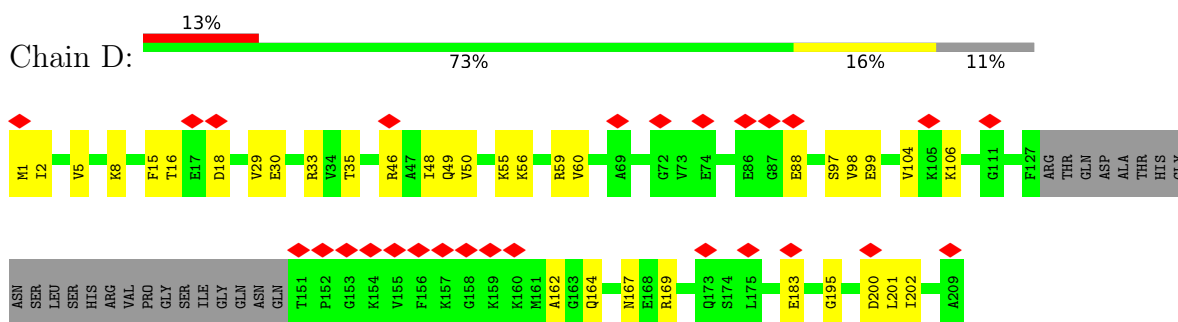
3 Residue-property plots

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.

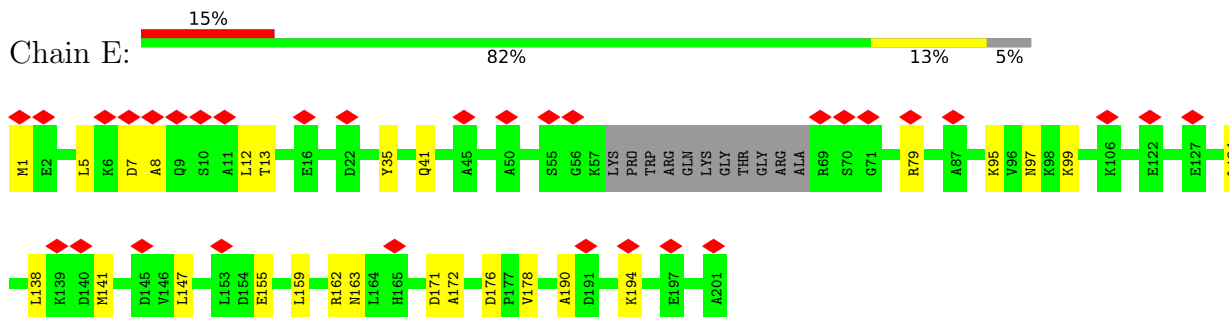
• Molecule 1: 50S ribosomal protein L2



• Molecule 2: 50S ribosomal protein L3



• Molecule 3: 50S ribosomal protein L4



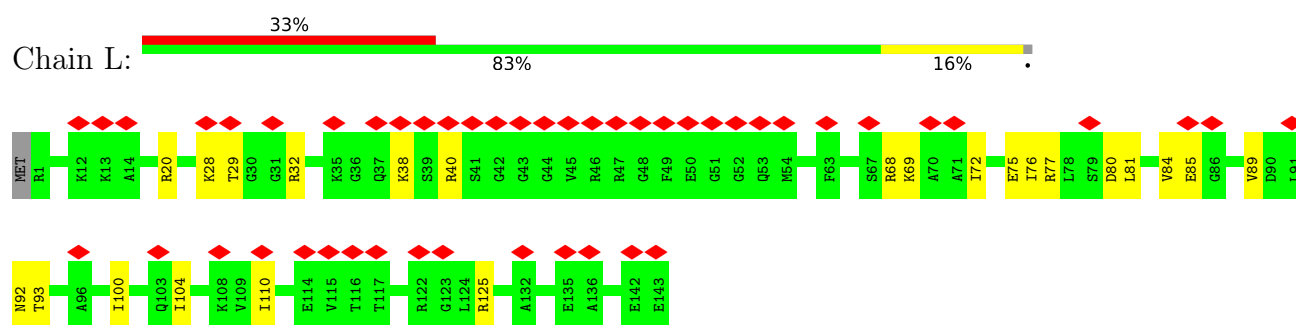
- Chain F:
-
- 77%
- 82%
- 17%
- Chain F:
- 66
- 67
- 68
- 69
- 70
- 71
- 72
- 73
- 74
- 75
- 76
- 77
- 78
- 79
- 80
- 81
- 82
- 83
- 84
- 85
- 86
- 87
- 88
- 89
- 90
- 91
- 92
- 93
- 94
- 95
- 96
- 97
- 98
- 99
- 100
- 101
- 102
- 103
- 104
- 105
- 106
- 107
- 108
- 109
- 110
- 111
- 112
- 113
- 114
- 115
- 116
- 117
- 118
- 119
- 120
- 121
- 122
- 123
- 124
- 125
- 126
- 127
- 128
- 129
- 130
- 131
- 132
- 133
- 134
- 135
- 136
- 137
- 138
- 139
- 140
- 141
- 142
- 143
- 144
- 145
- 146
- 147
- 148
- 149
- 150
- 151
- 152
- 153
- 154
- 155
- 156
- 157
- 158
- 159
- 160
- 161
- 162
- 163
- 164
- 165
- 166
- 167
- 168
- 169
- 170
- 171
- 172
- 173
- 174
- 175
- 176
- 177
- 178
- 179
- 180
- 181
- 182
- 183
- 184
- 185
- 186
- 187
- 188
- 189
- 190
- 191
- 192
- 193
- 194
- 195
- 196
- 197
- 198
- 199
- 200
- 201
- 202
- 203
- 204
- 205
- 206
- 207
- 208
- 209
- 210
- 211
- 212
- 213
- 214
- 215
- 216
- 217
- 218
- 219
- 220
- 221
- 222
- 223
- 224
- 225
- 226
- 227
- 228
- 229
- 230
- 231
- 232
- 233
- 234
- 235
- 236
- 237
- 238
- 239
- 240
- 241
- 242
- 243
- 244
- 245
- 246
- 247
- 248
- 249
- 250
- 251
- 252
- 253
- 254
- 255
- 256
- 257
- 258
- 259
- 260
- 261
- 262
- 263
- 264
- 265
- 266
- 267
- 268
- 269
- 270
- 271
- 272
- 273
- 274
- 275
- 276
- 277
- 278
- 279
- 280
- 281
- 282
- 283
- 284
- 285
- 286
- 287
- 288
- 289
- 290
- 291
- 292
- 293
- 294
- 295
- 296
- 297
- 298
- 299
- 300
- 301
- 302
- 303
- 304
- 305
- 306
- 307
- 308
- 309
- 310
- 311
- 312
- 313
- 314
- 315
- 316
- 317
- 318
- 319
- 320
- 321
- 322
- 323
- 324
- 325
- 326
- 327
- 328
- 329
- 330
- 331
- 332
- 333
- 334
- 335
- 336
- 337
- 338
- 339
- 340
- 341
- 342
- 343
- 344
- 345
- 346
- 347
- 348
- 349
- 350
- 351
- 352
- 353
- 354
- 355
- 356
- 357
- 358
- 359
- 360
- 361
- 362
- 363
- 364
- 365
- 366
- 367
- 368
- 369
- 370
- 371
- 372
- 373
- 374
- 375
- 376
- 377
- 378
- 379
- 380
- 381
- 382
- 383
- 384
- 385
- 386
- 387
- 388
- 389
- 390
- 391
- 392
- 393
- 394
- 395
- 396
- 397
- 398
- 399
- 400
- 401
- 402
- 403
- 404
- 405
- 406
- 407
- 408
- 409
- 410
- 411
- 412
- 413
- 414
- 415
- 416
- 417
- 418
- 419
- 420
- 421
- 422
- 423
- 424
- 425
- 426
- 427
- 428
- 429
- 430
- 431
- 432
- 433
- 434
- 435
- 436
- 437
- 438
- 439
- 440
- 441
- 442
- 443
- 444
- 445
- 446
- 447
- 448
- 449
- 450
- 451
- 452
- 453
- 454
- 455
- 456
- 457
- 458
- 459
- 460
- 461
- 462
- 463
- 464
- 465
- 466
- 467
- 468
- 469
- 470
- 471
- 472
- 473
- 474
- 475
- 476
- 477
- 478
- 479
- 480
- 481
- 482
- 483
- 484
- 485
- 486
- 487
- 488
- 489
- 490
- 491
- 492
- 493
- 494
- 495
- 496
- 497
- 498
- 499
- 500
- 501
- 502
- 503
- 504
- 505
- 506
- 507
- 508
- 509
- 510
- 511
- 512
- 513
- 514
- 515
- 516
- 517
- 518
- 519
- 520
- 521
- 522
- 523
- 524
- 525
- 526
- 527
- 528
- 529
- 530
- 531
- 532
- 533
- 534
- 535
- 5

- Chain H:
-
- | Position | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
|----------|
| ALA | 0.00 |
| GLU | 0.00 |
| VAL | 0.00 |
| SER | 0.00 |
| PHE | 0.00 |
| GLN | 0.00 |
| VAL | 0.00 |
| HIS | 0.00 |
| SER | 0.00 |
| GLU | 0.00 |
| THR | 0.00 |
| ARG | 0.00 |
| LEU | 0.00 |
| PRO | 0.00 |
| ASN | 0.00 |
| GLY | 0.00 |
| VAL | 0.00 |
| LEU | 0.00 |
| ARG | 0.00 |
| THR | 0.00 |
| GLY | 0.00 | 0.00 | 0.00 | 0.00 | | | | | | | | | | | | | | | | |

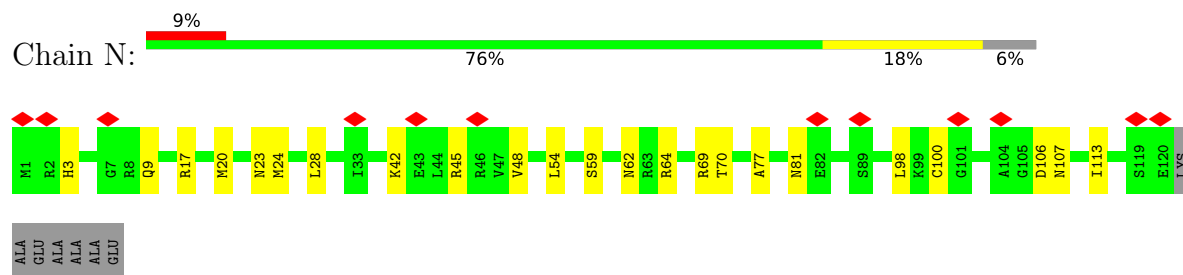
- Chain J:
-
- | Segment Color | Percentage |
|---------------|------------|
| Red | 13% |
| Green | 82% |
| Yellow | 18% |
- Chain J nodes (top to bottom): M1, K12, V17, V18, D19, A20, K23, A29, L32, L36, R37, H40, F43, V56, D60, A63, V64, T65, G66, K68, R69, T70, D71, T75, T81, G82, Q86, A94, R95, R96, P97, E98, R99, V100, I101, E102, R116, R120, K121, L122, K123, V124.
- Chain J nodes (bottom to top): Y125, A126, A134, Q135, Q136, P137, Q138, D141, I142.

- Chain K:
-
- 37% 79% 20% **
- M1 I2 Q3 T6 K7 L8 N9 V10 S14 G15 A16 V19 G26 G27 S28 H29 R30 R31 Y32 A33 G34 V35 G36 D37 I38 I43 K44 E45 A46 I47 P48 R49 G50 G51 G55 D56 R64 T65 K66 R70 D80 G81 N82 A83 L86 L87 N88 N89 N90 S91
- E92 Q93 P94 R98 I99 F100 G101 R105 E106 L107 R108 S109 E110 K111 F112 M113 I116 S117 L118 L119 P120 E121 V122 LEU

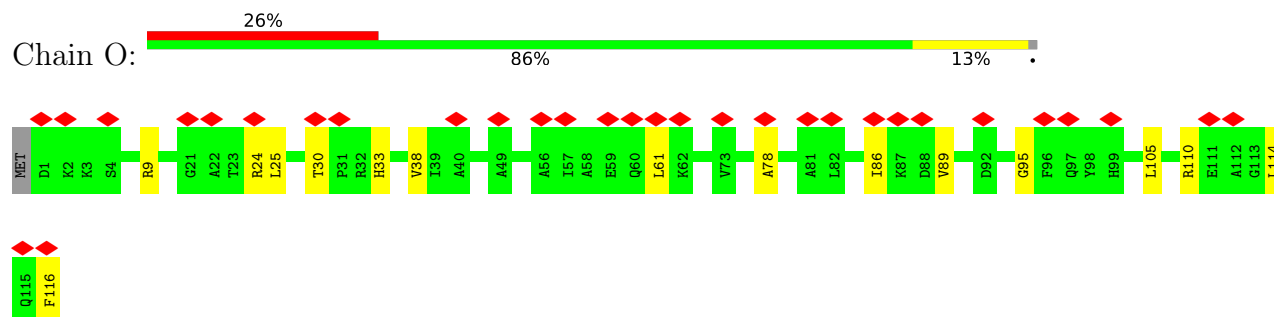
- 



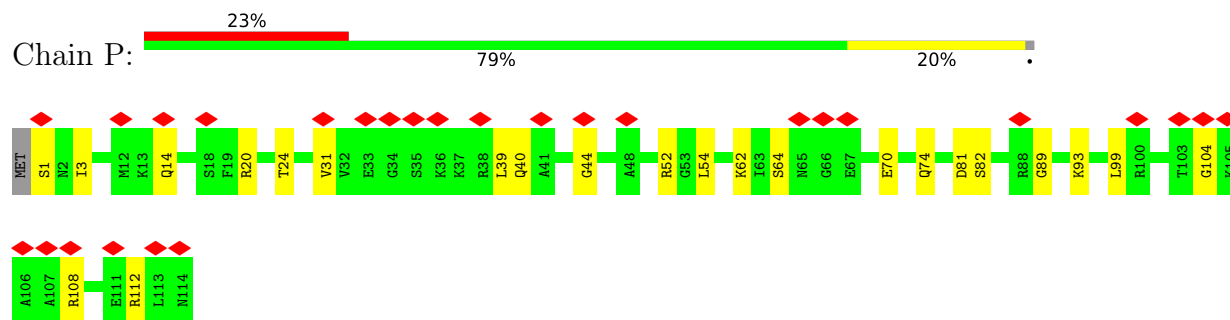
- Molecule 9: 50S ribosomal protein L17



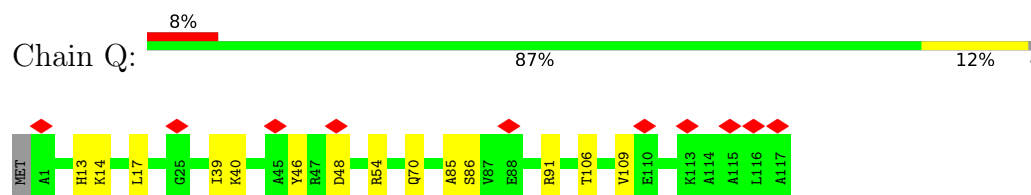
- Molecule 10: 50S ribosomal protein L18



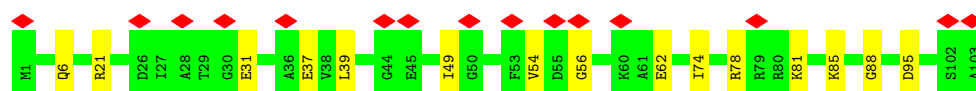
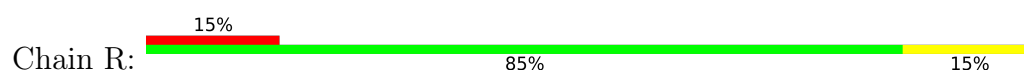
- Molecule 11: 50S ribosomal protein L19



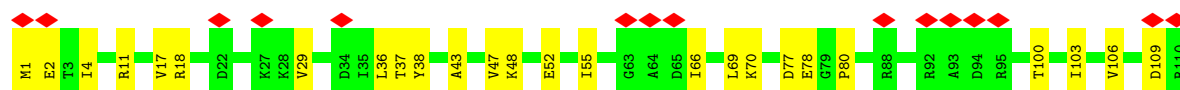
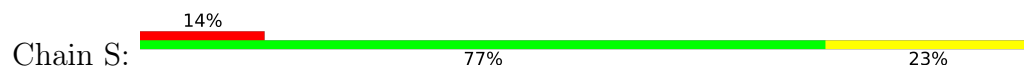
- Molecule 12: 50S ribosomal protein L20



- Molecule 13: 50S ribosomal protein L21



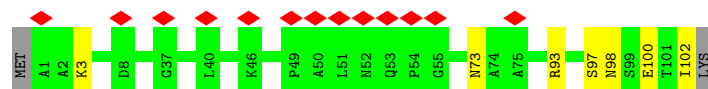
- Molecule 14: 50S ribosomal protein L22



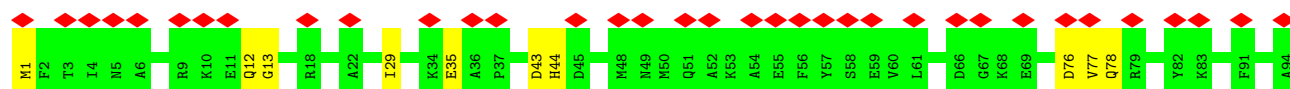
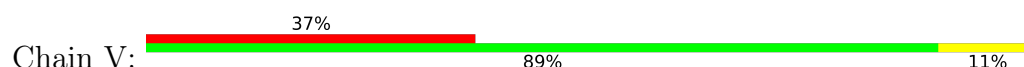
- Molecule 15: 50S ribosomal protein L23



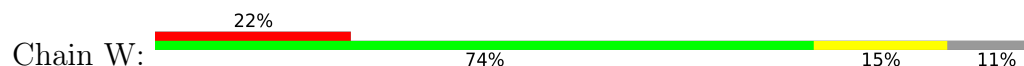
- Molecule 16: 50S ribosomal protein L24



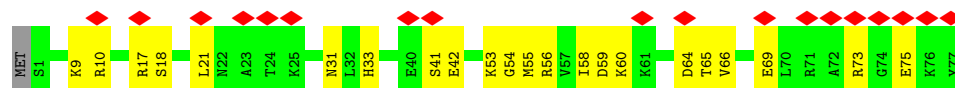
- Molecule 17: 50S ribosomal protein L25



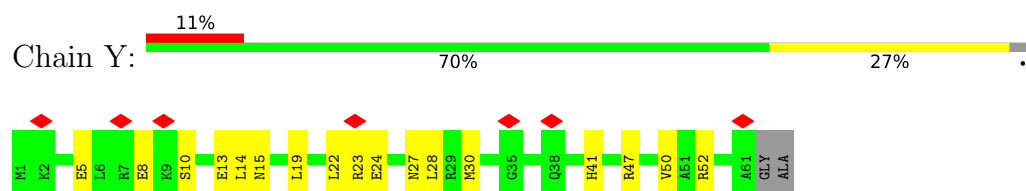
- Molecule 18: 50S ribosomal protein L27



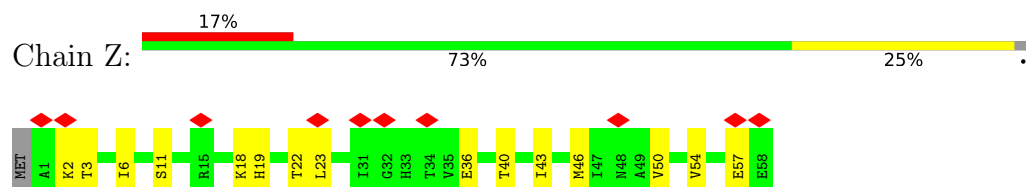
- Molecule 19: 50S ribosomal protein L28



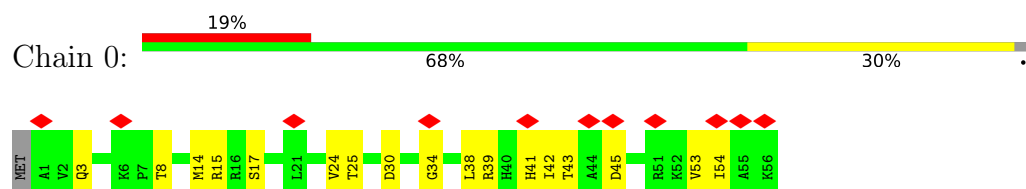
- Molecule 20: 50S ribosomal protein L29



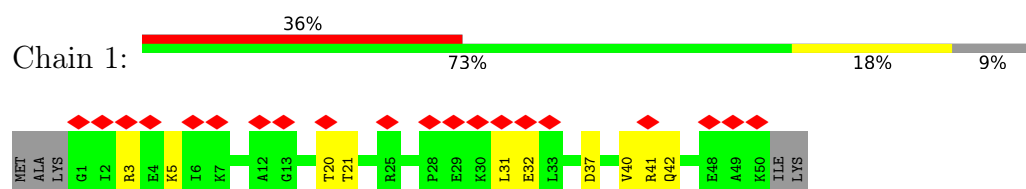
- Molecule 21: 50S ribosomal protein L30



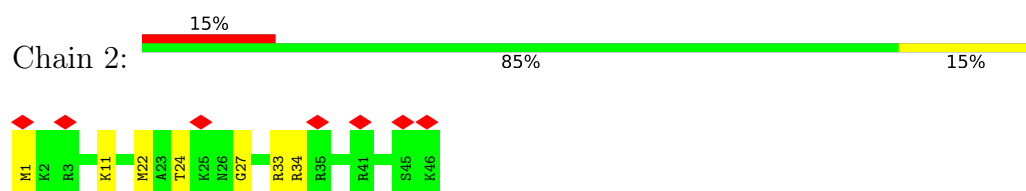
- Molecule 22: 50S ribosomal protein L32



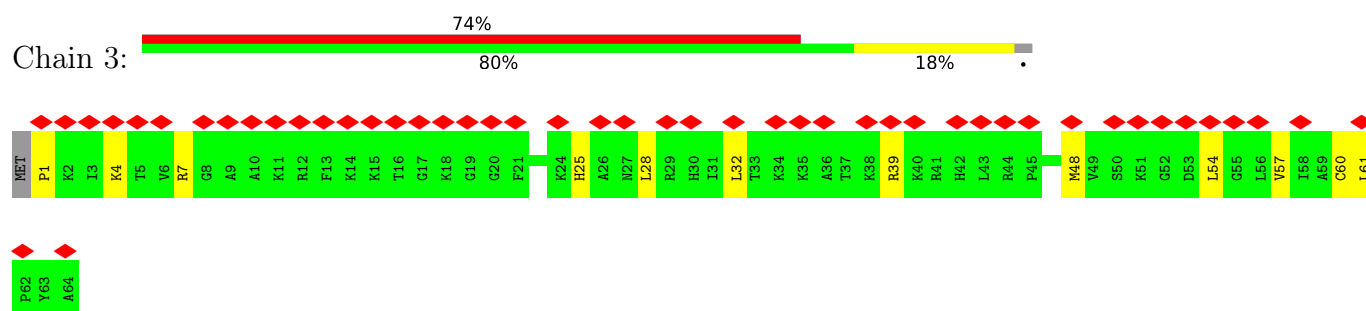
- Molecule 23: 50S ribosomal protein L33



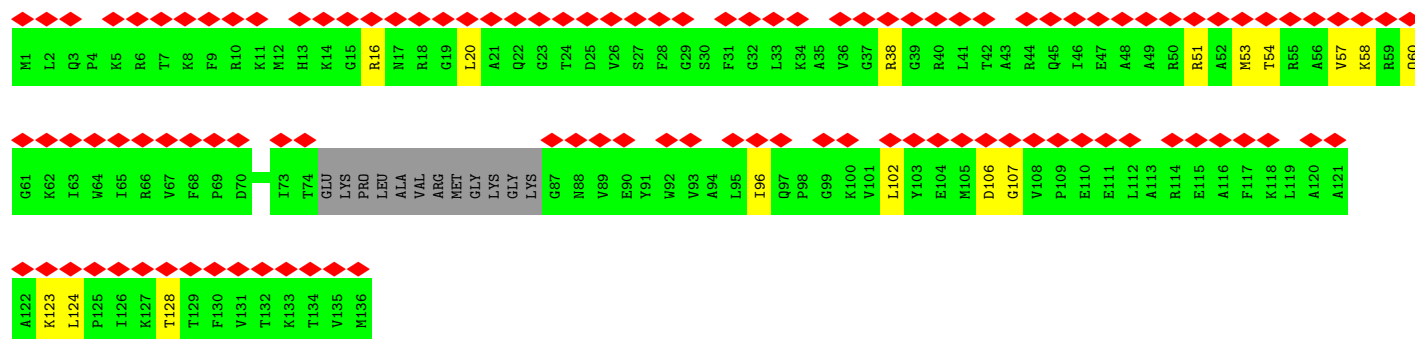
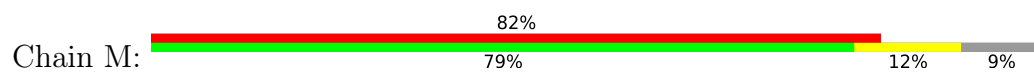
- Molecule 24: 50S ribosomal protein L34



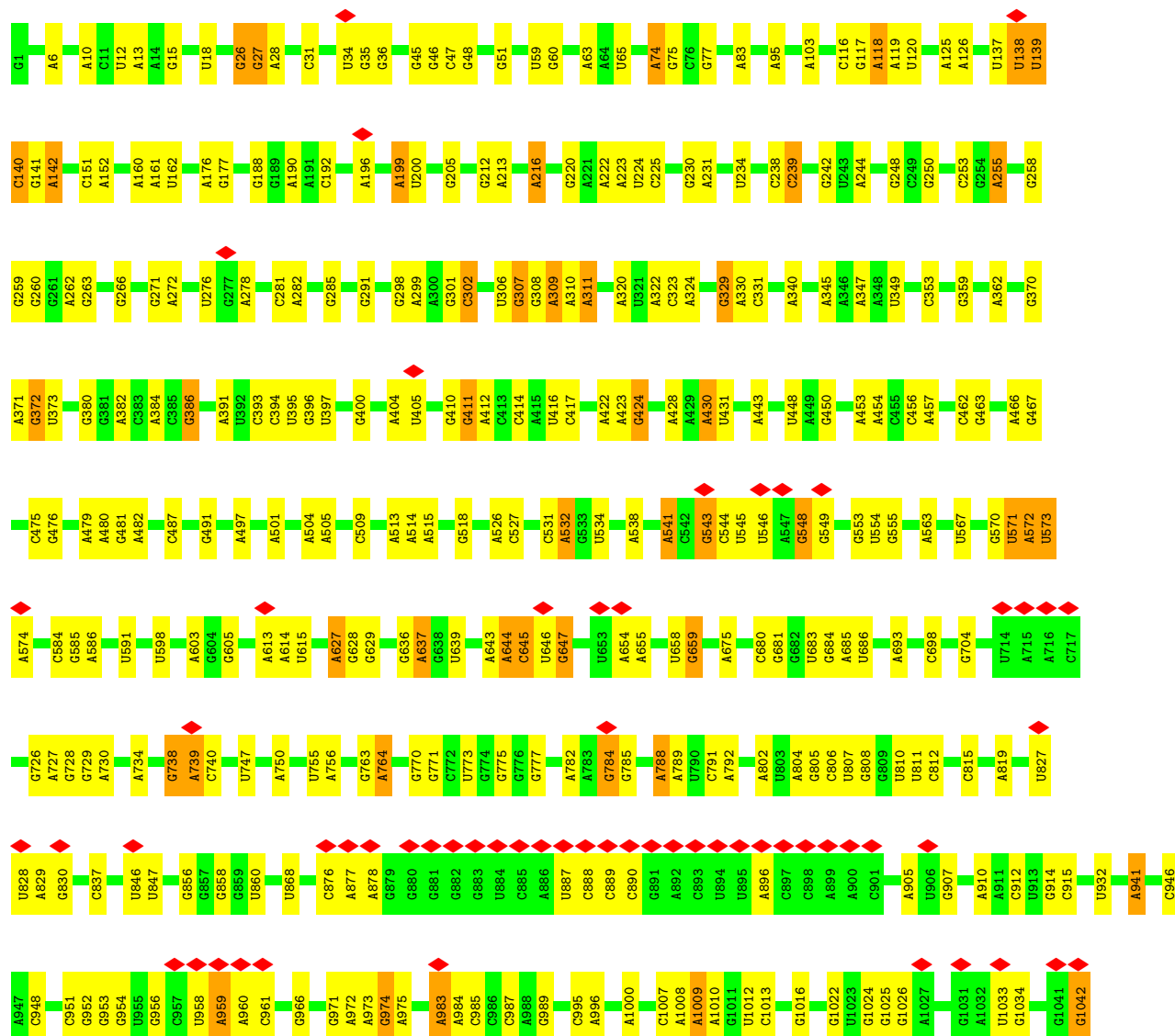
- Molecule 25: 50S ribosomal protein L35

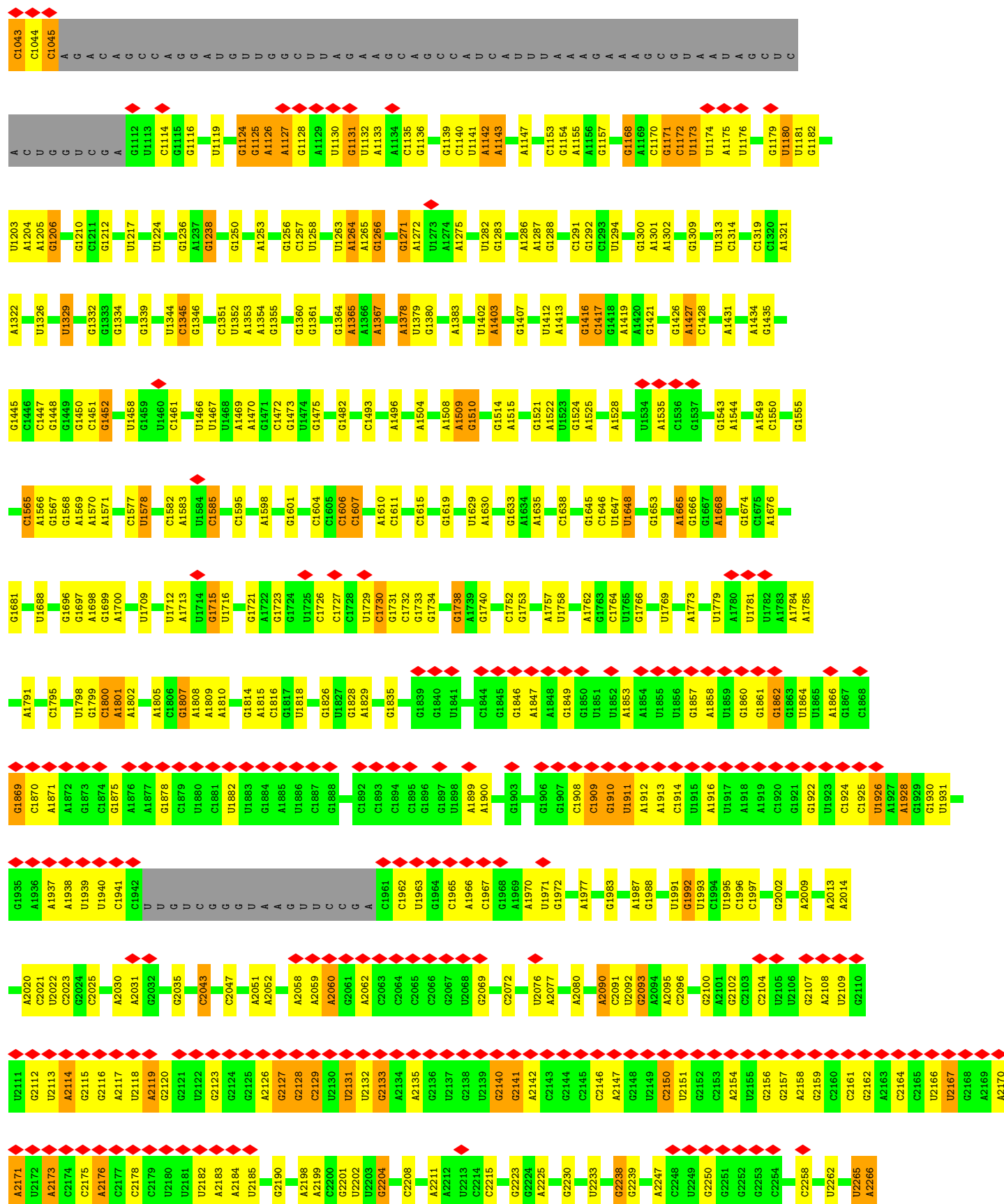


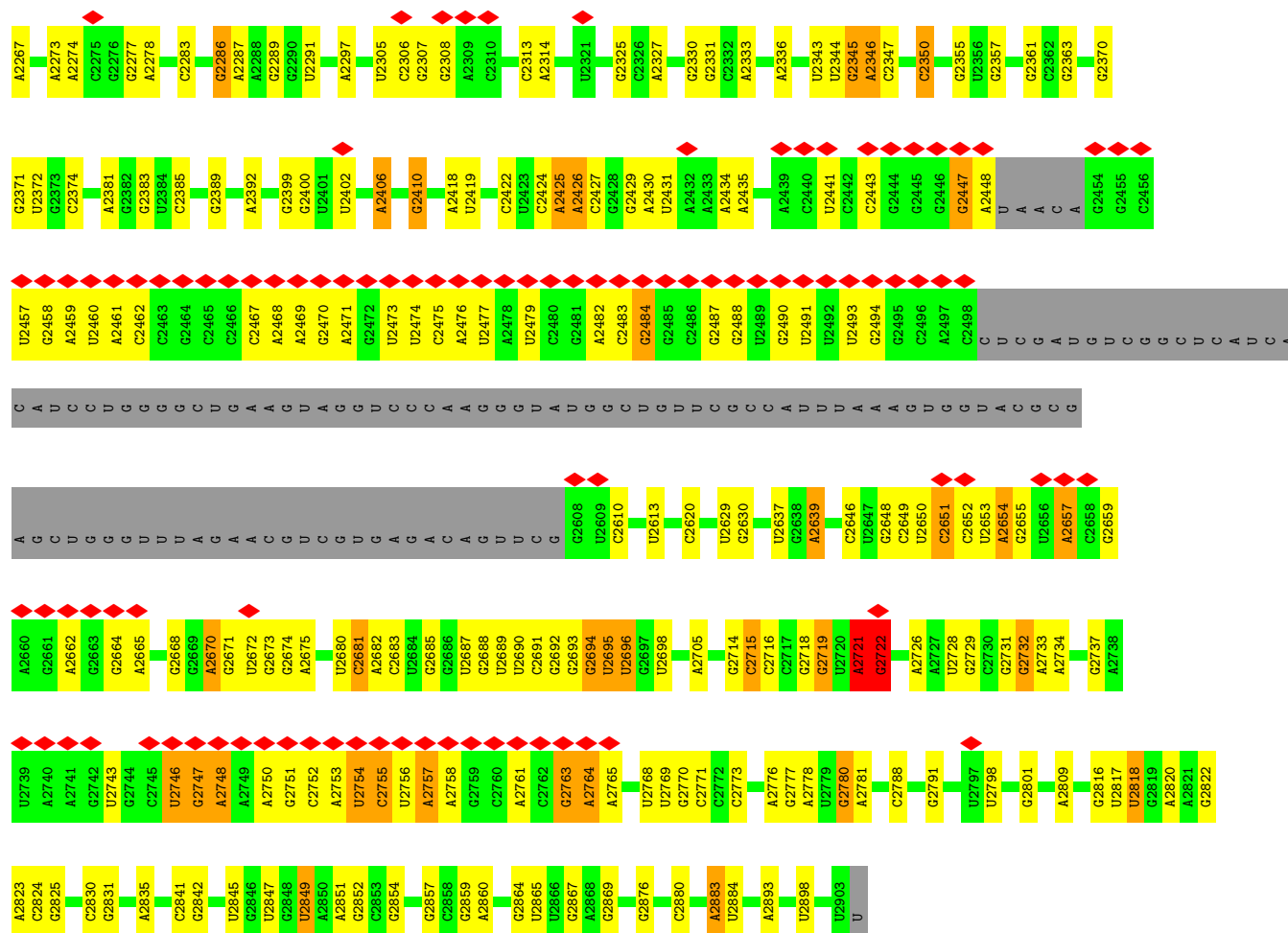
- Molecule 26: 50S ribosomal protein L16



• Molecule 27: 23S rRNA







• Molecule 28: 5S rRNA

Chain B: 5% 76% 21%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5772	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 ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.778	Depositor
Minimum map value	-0.642	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	375.0, 375.0, 375.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	C	0.09	0/1886	0.24	0/2528
2	D	0.08	0/1410	0.19	0/1894
3	E	0.09	0/1477	0.20	0/1986
4	F	0.09	0/1434	0.22	0/1926
5	H	0.34	0/389	0.41	0/523
6	J	0.09	0/1152	0.19	0/1551
7	K	0.09	0/947	0.22	0/1268
8	L	0.10	0/1054	0.26	0/1403
9	N	0.10	0/973	0.31	0/1301
10	O	0.09	0/902	0.19	0/1209
11	P	0.09	0/929	0.20	0/1242
12	Q	0.09	0/960	0.18	0/1278
13	R	0.09	0/829	0.22	0/1107
14	S	0.10	0/864	0.24	0/1156
15	T	0.22	0/744	0.36	0/994
16	U	0.10	0/787	0.26	0/1051
17	V	0.10	0/766	0.20	0/1025
18	W	0.10	0/582	0.20	0/769
19	X	0.10	0/635	0.21	0/848
20	Y	0.13	0/500	0.26	0/665
21	Z	0.11	0/453	0.22	0/605
22	0	0.11	0/450	0.19	0/599
23	1	0.14	0/416	0.20	0/554
24	2	0.13	0/380	0.23	0/498
25	3	0.07	0/513	0.19	0/676
26	M	0.10	0/1001	0.20	0/1338
27	A	0.25	9/65058 (0.0%)	0.19	6/101492 (0.0%)
28	B	0.05	0/2847	0.16	0/4440
All	All	0.22	9/90338 (0.0%)	0.20	6/135926 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	2722	G	C1'-N9	37.65	2.04	1.48
27	A	2721	A	C6-N1	23.13	1.81	1.35
27	A	2721	A	N1-C2	19.46	1.73	1.34
27	A	2721	A	N3-C4	18.47	1.71	1.34
27	A	2721	A	C2-N3	17.93	1.69	1.33
27	A	2721	A	C5-C6	14.15	1.69	1.41
27	A	2722	G	N9-C4	13.37	1.64	1.38
27	A	2721	A	C5-C4	12.74	1.64	1.38
27	A	2722	G	N9-C8	10.66	1.59	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	2722	G	N9-C1'-C2'	9.93	126.90	112.00
27	A	2722	G	C8-N9-C4	-9.87	76.80	106.40
27	A	2722	G	O4'-C1'-N9	6.88	118.82	108.50
27	A	2722	G	N7-C8-N9	6.52	132.67	113.10
27	A	2722	G	C4-N9-C1'	5.13	141.90	126.50
27	A	2721	A	N1-C2-N3	-5.01	114.26	129.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	C	1858	0	1952	38	0
2	D	1393	0	1454	24	0
3	E	1462	0	1523	19	0
4	F	1410	0	1447	24	0
5	H	384	0	405	31	0
6	J	1129	0	1162	19	0
7	K	938	0	1012	19	0
8	L	1045	0	1120	19	0
9	N	960	0	1000	20	0
10	O	892	0	926	12	0
11	P	917	0	965	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Q	947	0	1022	10	0
13	R	816	0	839	14	0
14	S	857	0	922	16	0
15	T	738	0	807	22	0
16	U	779	0	834	4	0
17	V	753	0	780	7	0
18	W	575	0	592	15	0
19	X	625	0	655	17	0
20	Y	499	0	535	11	0
21	Z	449	0	491	10	0
22	0	444	0	461	19	0
23	1	409	0	443	11	0
24	2	377	0	418	7	0
25	3	504	0	574	12	0
26	M	984	0	1051	12	0
27	A	58086	0	29218	503	0
28	B	2546	0	1292	17	0
All	All	82776	0	53900	830	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 7.

All (830) 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)
27:A:2721:A:C2	27:A:2722:G:H1'	1.28	1.68
27:A:2721:A:N3	27:A:2721:A:C4	1.71	1.58
27:A:2721:A:C2	27:A:2721:A:N3	1.69	1.55
27:A:2721:A:C2	27:A:2721:A:N1	1.73	1.55
27:A:2721:A:N1	27:A:2721:A:C6	1.81	1.48
27:A:2721:A:C2	27:A:2722:G:N9	1.81	1.46
27:A:2721:A:C6	27:A:2722:G:N9	1.88	1.40
27:A:2721:A:N1	27:A:2722:G:N9	1.69	1.40
27:A:2721:A:C2	27:A:2722:G:C1'	2.04	1.38
27:A:2721:A:N1	27:A:2722:G:C1'	1.92	1.30
27:A:2721:A:C6	27:A:2722:G:C1'	2.16	1.27
27:A:2721:A:C4	27:A:2722:G:N9	2.03	1.26
27:A:2721:A:C5	27:A:2722:G:N9	2.06	1.22
27:A:2721:A:C4	27:A:2722:G:C1'	2.23	1.22
27:A:2722:G:N9	27:A:2722:G:C1'	2.04	1.20
27:A:2721:A:N3	27:A:2722:G:N9	1.92	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2721:A:N3	27:A:2722:G:C1'	2.07	1.18
5:H:28:ASN:CA	5:H:32:PRO:HG2	1.76	1.16
27:A:2721:A:C4	27:A:2722:G:C8	2.36	1.13
27:A:2721:A:C4	27:A:2722:G:O4'	2.02	1.12
27:A:2721:A:C5	27:A:2722:G:C1'	2.31	1.12
27:A:2721:A:C6	27:A:2722:G:C4	2.40	1.08
27:A:2721:A:N1	27:A:2722:G:C4	2.21	1.07
27:A:2721:A:C6	27:A:2722:G:C2'	2.43	1.01
5:H:28:ASN:C	5:H:32:PRO:HG2	1.85	1.01
27:A:2721:A:N3	27:A:2722:G:C8	2.29	1.00
5:H:28:ASN:HA	5:H:32:PRO:HG2	1.42	0.98
5:H:3:VAL:HG21	5:H:30:LEU:HD22	1.45	0.98
27:A:2721:A:N1	27:A:2722:G:H1'	1.76	0.97
27:A:2721:A:N3	27:A:2722:G:H1'	1.85	0.92
27:A:1926:U:O2	27:A:1928:A:N7	2.03	0.90
27:A:2721:A:N1	27:A:2722:G:C2'	2.36	0.89
27:A:2671:G:O2'	27:A:2672:U:O4'	1.94	0.86
27:A:2857:G:N2	27:A:2860:A:OP2	2.09	0.86
27:A:395:U:O2'	27:A:396:G:N7	2.08	0.85
9:N:3:HIS:O	27:A:2722:G:O2'	1.93	0.85
27:A:1807:G:N2	27:A:1810:A:OP2	2.11	0.84
18:W:34:THR:HG1	27:A:2331:G:HO2'	0.87	0.84
27:A:948:C:O2	27:A:984:A:O2'	1.96	0.84
27:A:1124:G:O2'	27:A:1125:G:OP1	1.96	0.84
27:A:1378:A:O2'	27:A:1380:G:OP2	1.95	0.84
27:A:2127:G:O2'	27:A:2128:G:O5'	1.97	0.83
27:A:727:A:OP1	27:A:1431:A:O2'	1.96	0.82
9:N:107:ASN:ND2	27:A:2009:A:O4'	2.13	0.82
27:A:2746:U:O2'	27:A:2747:G:OP1	1.98	0.82
27:A:324:A:OP2	27:A:1205:A:N6	2.13	0.82
14:S:52:GLU:OE1	27:A:487:C:O2'	1.97	0.81
27:A:2721:A:C6	27:A:2722:G:H2'	2.15	0.81
13:R:85:LYS:NZ	27:A:815:C:OP2	2.11	0.81
27:A:2447:G:O2'	27:A:2448:A:O4'	1.98	0.81
5:H:28:ASN:HA	5:H:32:PRO:CG	2.11	0.80
5:H:26:ALA:O	5:H:30:LEU:HG	1.82	0.80
27:A:1007:C:OP2	27:A:1008:A:O2'	1.99	0.80
28:B:5:U:O2'	28:B:27:C:O2	2.00	0.80
27:A:1606:C:O2'	27:A:1607:C:OP2	1.99	0.80
27:A:1826:G:O2'	27:A:1971:U:OP2	1.99	0.80
26:M:51:ARG:O	26:M:54:THR:OG1	1.97	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1407:G:N2	27:A:1595:C:O2	2.12	0.80
16:U:97:SER:O	16:U:98:ASN:ND2	2.14	0.79
19:X:9:LYS:NZ	27:A:397:U:OP2	2.15	0.79
27:A:2695:U:O2'	27:A:2696:U:O5'	1.99	0.79
27:A:422:A:O2'	27:A:423:A:O4'	2.01	0.79
10:O:30:THR:OG1	10:O:33:HIS:O	1.99	0.79
27:A:2043:C:OP1	27:A:2777:G:O2'	1.99	0.79
5:H:31:VAL:HG13	5:H:32:PRO:HD3	1.64	0.79
27:A:514:A:O2'	27:A:515:A:O4'	1.98	0.79
27:A:1470:A:N6	27:A:1521:G:O2'	2.16	0.79
27:A:2150:C:O2'	27:A:2151:U:O4'	2.00	0.79
7:K:70:ARG:NH2	27:A:2683:C:O2	2.16	0.78
27:A:1798:U:O2'	27:A:1802:A:N3	2.16	0.78
27:A:1043:C:N4	27:A:1045:C:O4'	2.16	0.78
27:A:1126:A:O2'	27:A:1127:A:O5'	2.02	0.78
27:A:2345:G:O6	27:A:2371:G:O6	2.00	0.78
25:3:4:LYS:NZ	27:A:253:C:OP2	2.17	0.78
27:A:137:U:O2'	27:A:138:U:OP1	2.02	0.78
27:A:2258:C:O2'	27:A:2427:C:OP2	2.01	0.78
7:K:88:ASN:ND2	7:K:91:SER:OG	2.17	0.78
27:A:1528:A:OP2	27:A:1543:G:N2	2.17	0.78
4:F:91:ARG:NH1	28:B:43:C:O2	2.18	0.77
27:A:411:G:OP2	27:A:2406:A:O2'	2.01	0.77
27:A:1814:G:OP2	27:A:1815:A:O2'	2.02	0.77
15:T:73:ARG:NH2	27:A:65:U:O2'	2.16	0.77
6:J:98:GLU:OE2	6:J:126:ALA:N	2.18	0.77
27:A:291:G:O6	27:A:349:U:O2	2.03	0.77
9:N:42:LYS:NZ	27:A:2818:U:OP2	2.15	0.77
27:A:526:A:O2'	27:A:2043:C:O2	2.03	0.77
9:N:42:LYS:NZ	27:A:2817:U:OP1	2.15	0.77
15:T:4:GLU:O	15:T:6:ARG:N	2.18	0.76
27:A:234:U:O4	27:A:263:G:N2	2.18	0.76
2:D:169:ARG:NH1	27:A:2773:C:OP1	2.17	0.76
27:A:2721:A:C2	27:A:2722:G:C8	2.73	0.76
27:A:199:A:N6	27:A:2431:U:O2	2.19	0.76
27:A:200:U:O2	27:A:386:G:N2	2.18	0.76
15:T:37:ASP:O	15:T:81:LYS:NZ	2.16	0.76
20:Y:52:ARG:NH1	27:A:77:G:OP1	2.19	0.76
24:2:11:LYS:NZ	27:A:770:G:OP2	2.19	0.76
27:A:1860:G:O6	27:A:1882:U:O2	2.04	0.76
19:X:41:SER:OG	19:X:42:GLU:OE1	2.02	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:77:ARG:NH1	27:A:627:A:OP1	2.19	0.75
27:A:1309:G:O2'	27:A:1611:C:O2'	2.03	0.75
27:A:2107:G:O6	27:A:2182:U:O2	2.04	0.75
27:A:216:A:N7	27:A:431:U:O2	2.20	0.75
27:A:570:G:O2'	27:A:983:A:N1	2.18	0.75
27:A:704:G:N2	27:A:728:G:O6	2.20	0.75
1:C:170:TYR:OH	27:A:2223:G:OP1	2.01	0.74
27:A:391:A:O2'	27:A:410:G:OP1	2.03	0.74
27:A:382:A:N1	27:A:393:C:N4	2.35	0.74
27:A:2854:G:N1	27:A:2864:G:O6	2.20	0.74
1:C:270:ARG:NH1	27:A:1798:U:OP2	2.20	0.74
11:P:1:SER:N	27:A:2876:G:OP1	2.21	0.74
13:R:21:ARG:NE	13:R:95:ASP:OD1	2.21	0.74
27:A:1779:U:OP2	27:A:1784:A:N6	2.20	0.74
27:A:698:C:O2'	27:A:734:A:N6	2.21	0.74
27:A:1288:G:OP2	27:A:1288:G:N2	2.21	0.74
27:A:1696:G:N2	27:A:1977:A:O2'	2.21	0.74
28:B:14:U:OP2	28:B:70:C:O2'	2.05	0.74
20:Y:41:HIS:HD1	27:A:95:A:HO2'	1.36	0.74
2:D:35:THR:OG1	2:D:49:GLN:OE1	2.06	0.74
25:3:39:ARG:NE	27:A:2363:G:OP2	2.21	0.74
5:H:3:VAL:HG21	5:H:30:LEU:CD2	2.17	0.73
27:A:1142:A:O2'	27:A:1143:A:OP2	2.06	0.73
28:B:77:U:O2	28:B:99:A:N7	2.21	0.73
1:C:147:PRO:O	1:C:149:LYS:NZ	2.22	0.73
27:A:2721:A:N1	27:A:2722:G:N3	2.35	0.73
27:A:2289:G:O6	27:A:2343:U:O2	2.07	0.73
12:Q:91:ARG:NH2	27:A:1153:C:OP1	2.22	0.73
27:A:2651:C:H42	27:A:2670:A:H61	1.37	0.73
27:A:2721:A:C6	27:A:2722:G:N3	2.58	0.72
27:A:1475:G:O2'	27:A:1514:G:O6	2.08	0.72
27:A:463:G:N2	27:A:466:A:OP2	2.22	0.72
27:A:2140:G:O2'	27:A:2141:G:O5'	2.06	0.72
1:C:99:GLU:N	1:C:99:GLU:OE1	2.22	0.72
14:S:1:MET:SD	14:S:2:GLU:N	2.63	0.71
27:A:1992:G:N2	27:A:1996:C:O2'	2.24	0.71
27:A:2345:G:O2'	27:A:2381:A:N3	2.22	0.71
27:A:370:G:O2'	27:A:424:G:OP1	2.06	0.71
27:A:2816:G:N3	27:A:2883:A:O2'	2.21	0.71
1:C:264:LYS:NZ	27:A:2223:G:O2'	2.19	0.71
27:A:301:G:O2'	27:A:302:C:O5'	2.09	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:33:GLN:HE22	5:H:35:LYS:HB2	1.55	0.71
4:F:134:GLN:N	4:F:134:GLN:OE1	2.23	0.71
6:J:68:LYS:NZ	27:A:1140:C:OP2	2.23	0.71
27:A:1853:A:N3	27:A:2233:U:O2'	2.23	0.71
27:A:1629:U:O4	27:A:1630:A:N6	2.23	0.71
14:S:11:ARG:NH1	27:A:1322:A:OP1	2.24	0.70
8:L:125:ARG:NH2	27:A:636:G:OP2	2.23	0.70
18:W:31:GLN:OE1	18:W:31:GLN:N	2.24	0.70
20:Y:8:GLU:N	20:Y:8:GLU:OE1	2.24	0.70
21:Z:11:SER:OG	27:A:989:G:OP2	2.08	0.70
27:A:2694:G:O2'	27:A:2695:U:OP1	2.10	0.70
27:A:2748:A:N6	27:A:2757:A:N7	2.39	0.70
27:A:685:A:O2'	27:A:773:U:O4	2.06	0.70
27:A:2653:U:O2'	27:A:2668:G:N1	2.25	0.70
27:A:160:A:N3	27:A:2208:C:O2'	2.25	0.70
27:A:974:G:O2'	27:A:989:G:N2	2.25	0.70
27:A:1264:A:N6	27:A:2014:A:OP2	2.24	0.69
27:A:2291:U:O2	27:A:2374:C:O2'	2.09	0.69
15:T:4:GLU:O	15:T:5:GLU:HG2	1.91	0.69
3:E:99:LYS:NZ	27:A:605:G:OP1	2.24	0.69
18:W:30:ARG:NH2	27:A:2355:G:O2'	2.25	0.69
27:A:1205:A:O2'	27:A:1206:G:OP1	2.09	0.69
27:A:1426:G:OP2	27:A:1427:A:O2'	2.03	0.69
27:A:2047:C:O2'	27:A:2823:A:N1	2.25	0.69
1:C:67:LYS:NZ	1:C:148:GLY:O	2.25	0.69
27:A:1168:G:O6	27:A:1181:U:O2	2.10	0.69
21:Z:46:MET:O	21:Z:50:VAL:HG22	1.93	0.69
27:A:1668:A:N1	27:A:1676:A:N6	2.41	0.69
27:A:644:A:O2'	27:A:645:C:O5'	2.09	0.68
27:A:2171:A:O2'	27:A:2173:A:OP1	2.08	0.68
8:L:92:ASN:O	8:L:93:THR:OG1	2.10	0.68
23:1:5:LYS:NZ	27:A:2419:U:O2'	2.25	0.68
27:A:1697:G:OP2	27:A:1698:A:O2'	2.11	0.68
27:A:2788:C:O2'	27:A:2809:A:N3	2.27	0.68
27:A:541:A:N6	27:A:553:G:O6	2.27	0.68
27:A:1447:C:N4	27:A:1448:G:O6	2.25	0.68
27:A:1709:U:O2'	27:A:2859:G:N3	2.24	0.68
27:A:1170:C:N4	27:A:1171:G:O6	2.26	0.68
9:N:106:ASP:OD2	27:A:1287:A:N6	2.27	0.68
27:A:2659:G:N2	27:A:2662:A:OP2	2.25	0.68
26:M:38:ARG:NH2	28:B:90:C:O2'	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:ARG:NH1	27:A:2830:C:OP2	2.26	0.67
9:N:20:MET:HE3	9:N:24:MET:HE3	1.75	0.67
11:P:52:ARG:NH2	27:A:2845:U:O3'	2.27	0.67
9:N:77:ALA:O	9:N:81:ASN:ND2	2.27	0.67
27:A:2754:U:O2'	27:A:2755:C:O5'	2.09	0.67
27:A:2705:A:O2'	27:A:2852:G:OP1	2.12	0.67
27:A:1496:A:O2'	27:A:1577:C:O2'	2.13	0.67
7:K:31:ARG:NH2	27:A:2675:A:OP1	2.28	0.67
27:A:629:G:N3	27:A:639:U:O2'	2.27	0.67
25:3:32:LEU:HD21	27:A:2419:U:OP2	1.95	0.66
27:A:2399:G:O6	27:A:2418:A:N6	2.27	0.66
27:A:1445:G:O6	27:A:1466:U:O2	2.13	0.66
9:N:59:SER:OG	9:N:62:ASN:OD1	2.13	0.66
27:A:48:G:N2	27:A:177:G:OP1	2.17	0.66
27:A:956:G:O2'	27:A:959:A:N6	2.29	0.66
25:3:7:ARG:NH1	27:A:244:A:OP2	2.29	0.66
27:A:584:C:N4	27:A:585:G:O6	2.28	0.66
27:A:2651:C:N4	27:A:2670:A:H61	1.94	0.66
4:F:151:LEU:HD21	4:F:153:ILE:HD11	1.78	0.66
27:A:2721:A:C2	27:A:2722:G:C4	2.83	0.66
2:D:97:SER:OG	2:D:99:GLU:OE1	2.05	0.65
27:A:475:C:O2	27:A:479:A:N6	2.29	0.65
27:A:2721:A:C4	27:A:2722:G:H8	2.10	0.65
27:A:59:U:O2'	27:A:74:A:OP2	2.07	0.65
27:A:1287:A:O2'	27:A:1288:G:O4'	2.14	0.65
27:A:220:G:N1	27:A:428:A:OP2	2.30	0.65
27:A:675:A:N3	27:A:2443:C:O2'	2.30	0.65
27:A:2093:G:N3	27:A:2198:A:N6	2.45	0.65
13:R:31:GLU:N	13:R:31:GLU:OE1	2.30	0.64
27:A:2286:G:N2	27:A:2346:A:O2'	2.30	0.64
17:V:76:ASP:OD1	17:V:77:VAL:N	2.30	0.64
1:C:257:ARG:NH1	27:A:1799:G:OP1	2.29	0.64
26:M:16:ARG:NH1	27:A:954:G:OP2	2.30	0.64
27:A:2123:G:O6	27:A:2176:A:N6	2.31	0.64
1:C:269:ARG:NH2	27:A:1799:G:OP2	2.30	0.64
9:N:98:LEU:HG	22:0:42:ILE:HD11	1.79	0.64
13:R:81:LYS:NZ	27:A:972:A:OP1	2.31	0.64
2:D:49:GLN:NE2	2:D:50:VAL:O	2.31	0.63
2:D:46:ARG:NH2	2:D:88:GLU:O	2.32	0.63
6:J:96:ARG:NH1	27:A:2639:A:O3'	2.31	0.63
28:B:36:C:N4	28:B:49:C:O2	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:627:A:N6	27:A:637:A:O5'	2.31	0.63
23:1:41:ARG:NH1	27:A:643:A:N1	2.47	0.63
27:A:1016:G:O6	27:A:1147:A:N6	2.31	0.63
27:A:1416:G:O2'	27:A:1417:C:OP2	2.11	0.63
3:E:163:ASN:ND2	27:A:320:A:N3	2.47	0.62
19:X:17:ARG:NH2	19:X:21:LEU:O	2.32	0.62
6:J:116:ARG:NH2	27:A:527:C:O2'	2.32	0.62
20:Y:23:ARG:O	20:Y:27:ASN:ND2	2.32	0.62
27:A:2399:G:O2'	27:A:2400:G:O4'	2.14	0.62
15:T:54:GLU:OE1	15:T:54:GLU:N	2.31	0.62
27:A:276:U:O2'	27:A:278:A:N7	2.31	0.62
27:A:2721:A:N3	27:A:2722:G:O4'	2.33	0.62
19:X:53:LYS:NZ	27:A:372:G:O2'	2.32	0.62
1:C:62:ARG:NH2	27:A:1568:G:OP2	2.33	0.62
13:R:6:GLN:N	13:R:6:GLN:OE1	2.33	0.62
7:K:106:GLU:OE1	7:K:106:GLU:N	2.33	0.62
27:A:31:C:O2'	27:A:1238:G:OP1	2.18	0.62
8:L:40:ARG:NH2	27:A:806:C:OP2	2.32	0.61
10:O:9:ARG:NH1	10:O:95:GLY:O	2.33	0.61
11:P:89:GLY:O	11:P:112:ARG:NH1	2.34	0.61
15:T:4:GLU:C	15:T:6:ARG:H	2.08	0.61
27:A:2392:A:OP2	27:A:2422:C:N4	2.32	0.61
10:O:24:ARG:NH2	28:B:9:G:OP1	2.33	0.61
15:T:44:LYS:NZ	15:T:55:VAL:O	2.33	0.61
15:T:1:MET:HG3	27:A:142:A:H1'	1.81	0.61
27:A:18:U:O2'	27:A:554:U:OP1	2.18	0.61
11:P:74:GLN:N	11:P:74:GLN:OE1	2.34	0.61
1:C:77:VAL:HG21	1:C:109:LEU:HD11	1.83	0.61
27:A:2090:A:N6	27:A:2230:G:O6	2.33	0.61
4:F:15:LEU:HD12	4:F:27:VAL:HG13	1.83	0.60
27:A:2202:U:O2'	27:A:2204:G:OP1	2.18	0.60
16:U:73:ASN:ND2	16:U:100:GLU:OE2	2.35	0.60
27:A:2721:A:N1	27:A:2722:G:H2'	2.15	0.60
11:P:99:LEU:HD23	11:P:99:LEU:O	2.00	0.60
27:A:1283:G:N2	27:A:1286:A:OP2	2.35	0.60
2:D:164:GLN:NE2	2:D:167:ASN:OD1	2.34	0.60
27:A:1926:U:C2	27:A:1928:A:N7	2.70	0.60
23:1:3:ARG:NH2	23:1:21:THR:OG1	2.34	0.60
27:A:1604:C:O2'	27:A:1610:A:N1	2.28	0.60
5:H:3:VAL:CG2	5:H:30:LEU:HD13	2.32	0.60
27:A:2692:G:N3	27:A:2847:U:O2'	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:15:LEU:CD1	4:F:27:VAL:HG13	2.31	0.60
11:P:93:LYS:NZ	27:A:1753:G:O3'	2.31	0.60
21:Z:57:GLU:N	21:Z:57:GLU:OE1	2.35	0.60
1:C:77:VAL:HG22	1:C:93:VAL:HG12	1.84	0.60
6:J:134:ALA:O	27:A:2898:U:O2'	2.12	0.60
8:L:68:ARG:NH1	27:A:2406:A:O4'	2.33	0.60
27:A:1681:G:OP2	27:A:1757:A:N6	2.35	0.60
6:J:40:HIS:O	12:Q:70:GLN:NE2	2.34	0.59
9:N:69:ARG:O	9:N:70:THR:OG1	2.19	0.59
27:A:1869:G:N2	27:A:1871:A:O2'	2.35	0.59
5:H:26:ALA:HB1	5:H:30:LEU:CD1	2.33	0.59
27:A:116:C:O2'	27:A:126:A:N3	2.28	0.59
27:A:262:A:N3	27:A:430:A:O2'	2.25	0.59
27:A:784:G:O6	27:A:2072:C:O2'	2.21	0.59
27:A:2100:G:O6	27:A:2190:G:C6	2.55	0.59
27:A:2695:U:HO2'	27:A:2696:U:P	2.25	0.59
9:N:64:ARG:NH1	27:A:2851:A:O2'	2.36	0.59
27:A:1271:G:N2	27:A:1615:C:O2	2.35	0.59
13:R:37:GLU:OE1	13:R:37:GLU:N	2.36	0.59
27:A:1565:C:O2'	27:A:1566:A:O5'	2.18	0.59
27:A:192:C:O2'	27:A:802:A:N3	2.35	0.59
27:A:1139:G:O2'	27:A:1143:A:N1	2.34	0.59
2:D:59:ARG:NH2	27:A:2831:G:OP2	2.36	0.58
27:A:1681:G:O2'	27:A:1762:A:N3	2.32	0.58
27:A:2119:A:N6	27:A:2167:U:O2	2.22	0.58
7:K:30:ARG:NH1	7:K:37:ASP:OD2	2.37	0.58
27:A:538:A:H62	27:A:555:G:H21	1.49	0.58
1:C:62:ARG:NH2	27:A:1567:G:O2'	2.36	0.58
18:W:28:ILE:HG21	18:W:71:ILE:HG21	1.85	0.58
27:A:627:A:O4'	27:A:637:A:N6	2.36	0.58
10:O:25:LEU:CD2	10:O:38:VAL:HG22	2.34	0.58
5:H:28:ASN:C	5:H:32:PRO:CG	2.70	0.58
6:J:135:GLN:N	6:J:135:GLN:OE1	2.37	0.58
18:W:60:PHE:CD1	18:W:71:ILE:HD12	2.39	0.58
4:F:169:LEU:O	4:F:173:ASP:N	2.36	0.57
6:J:135:GLN:NE2	27:A:6:A:N3	2.52	0.57
14:S:37:THR:OG1	14:S:48:LYS:NZ	2.26	0.57
27:A:2128:G:O2'	27:A:2129:C:OP1	2.22	0.57
1:C:198:GLU:N	1:C:198:GLU:OE1	2.38	0.57
19:X:58:ILE:HD13	19:X:66:VAL:HG11	1.87	0.57
4:F:109:ARG:NH2	4:F:136:ILE:O	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:27:G:O2'	27:A:28:A:OP2	2.20	0.57
6:J:56:VAL:HB	6:J:124:VAL:HG23	1.85	0.57
27:A:750:A:OP1	27:A:1615:C:N4	2.36	0.57
6:J:43:GLU:N	6:J:43:GLU:OE1	2.38	0.57
19:X:56:ARG:NH2	27:A:400:G:OP2	2.38	0.57
27:A:345:A:N3	27:A:347:A:N6	2.52	0.57
27:A:414:C:O3'	27:A:1878:G:N2	2.38	0.56
16:U:3:LYS:O	16:U:93:ARG:NH1	2.37	0.56
4:F:38:GLY:O	27:A:2306:C:N4	2.37	0.56
5:H:26:ALA:HB1	5:H:30:LEU:HD11	1.87	0.56
12:Q:14:LYS:NZ	27:A:1217:U:OP1	2.38	0.56
13:R:78:ARG:NH2	27:A:975:A:OP1	2.38	0.56
27:A:1352:U:O2'	27:A:1570:A:N3	2.32	0.56
27:A:1723:G:N7	27:A:1738:G:N2	2.52	0.56
27:A:1715:G:O2'	27:A:1716:U:OP2	2.24	0.56
27:A:2306:C:OP2	27:A:2307:G:O2'	2.21	0.56
14:S:18:ARG:NH1	27:A:518:G:OP1	2.39	0.56
27:A:956:G:N2	27:A:960:A:H62	2.03	0.56
27:A:1000:A:OP2	27:A:1154:G:N1	2.34	0.56
15:T:6:ARG:NH2	15:T:37:ASP:OD2	2.38	0.56
13:R:88:GLY:O	27:A:1224:U:O2'	2.23	0.56
15:T:66:LYS:NZ	27:A:1339:G:O6	2.37	0.56
1:C:38:LYS:NZ	27:A:693:A:OP2	2.35	0.56
2:D:29:VAL:HG23	2:D:29:VAL:O	2.06	0.56
19:X:73:ARG:NH2	19:X:75:GLU:OE1	2.39	0.56
27:A:2721:A:C5	27:A:2722:G:C8	2.88	0.56
27:A:2140:G:O2'	27:A:2141:G:P	2.63	0.55
27:A:1809:A:O2'	27:A:1810:A:O4'	2.17	0.55
28:B:70:C:N3	28:B:107:G:N2	2.53	0.55
1:C:181:ARG:NH2	27:A:1800:C:OP2	2.39	0.55
27:A:1447:C:O2'	27:A:1544:A:N3	2.38	0.55
27:A:1726:C:H2'	27:A:1727:C:O4'	2.07	0.55
28:B:83:G:O6	28:B:94:A:N6	2.40	0.55
27:A:1024:G:OP2	27:A:1025:G:O2'	2.19	0.55
27:A:2469:A:N6	27:A:2482:A:N7	2.55	0.55
3:E:176:ASP:N	3:E:176:ASP:OD1	2.36	0.55
20:Y:5:GLU:OE1	20:Y:5:GLU:N	2.39	0.55
27:A:1861:G:O2'	27:A:1862:G:O5'	2.22	0.55
26:M:106:ASP:OD1	26:M:107:GLY:N	2.40	0.55
27:A:117:G:OP2	27:A:119:A:O2'	2.14	0.55
2:D:104:VAL:HG12	2:D:106:LYS:H	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:104:GLY:O	11:P:108:ARG:NH1	2.40	0.54
14:S:17:VAL:HG11	14:S:103:ILE:HD12	1.88	0.54
27:A:299:A:N1	27:A:322:A:O2'	2.32	0.54
27:A:1313:U:O2'	27:A:1332:G:O4'	2.25	0.54
27:A:2060:A:HO2'	27:A:2062:A:N6	2.06	0.54
8:L:28:LYS:NZ	27:A:810:U:OP2	2.40	0.54
27:A:161:A:OP2	27:A:162:U:O2'	2.22	0.54
27:A:956:G:H21	27:A:960:A:N6	2.04	0.54
20:Y:24:GLU:O	20:Y:28:LEU:HD23	2.08	0.54
6:J:122:LEU:HD23	6:J:123:LYS:N	2.22	0.54
10:O:25:LEU:HD22	10:O:38:VAL:HG22	1.89	0.54
12:Q:48:ASP:OD2	27:A:534:U:O2'	2.18	0.54
7:K:8:LEU:HB2	7:K:19:VAL:HG23	1.90	0.54
10:O:86:ILE:HG22	10:O:89:VAL:HG11	1.89	0.54
27:A:216:A:N7	27:A:431:U:C2	2.76	0.54
27:A:956:G:H21	27:A:960:A:H62	1.56	0.54
27:A:1864:U:OP1	27:A:2410:G:O2'	2.21	0.54
27:A:320:A:O2'	27:A:322:A:OP2	2.22	0.54
3:E:35:TYR:CD1	3:E:178:VAL:HG21	2.43	0.54
27:A:1172:C:O2'	27:A:1173:U:OP1	2.22	0.54
2:D:200:ASP:C	2:D:201:LEU:HD12	2.33	0.53
14:S:77:ASP:OD1	14:S:78:GLU:N	2.41	0.53
17:V:12:GLN:OE1	17:V:13:GLY:N	2.41	0.53
26:M:53:MET:O	26:M:57:VAL:HG22	2.07	0.53
27:A:2680:U:O2'	27:A:2681:C:O5'	2.26	0.53
1:C:44:ASN:OD1	1:C:45:ASN:N	2.41	0.53
27:A:308:G:O2'	27:A:329:G:N2	2.41	0.53
14:S:70:LYS:NZ	14:S:109:ASP:O	2.40	0.53
27:A:644:A:HO2'	27:A:645:C:P	2.31	0.53
27:A:2649:C:HO2'	27:A:2650:U:H6	1.53	0.53
14:S:80:PRO:O	14:S:100:THR:OG1	2.24	0.53
17:V:78:GLN:OE1	17:V:78:GLN:N	2.40	0.53
11:P:24:THR:OG1	11:P:44:GLY:O	2.25	0.53
18:W:7:SER:OG	27:A:2262:U:OP2	2.20	0.53
3:E:171:ASP:OD1	3:E:172:ALA:N	2.42	0.53
6:J:17:VAL:HG23	6:J:137:PRO:HB2	1.90	0.53
19:X:18:SER:OG	27:A:2080:A:OP1	2.24	0.53
27:A:647:G:N2	27:A:2350:C:O3'	2.41	0.53
2:D:15:PHE:CE2	11:P:54:LEU:HD21	2.43	0.53
27:A:2694:G:HO2'	27:A:2695:U:P	2.30	0.53
7:K:108:ARG:HA	7:K:116:ILE:HD11	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:35:GLU:N	17:V:35:GLU:OE1	2.41	0.53
26:M:58:LYS:O	26:M:60:GLN:N	2.41	0.53
4:F:33:ILE:CD1	4:F:95:MET:HE3	2.38	0.53
5:H:11:ASN:C	5:H:12:LEU:HD22	2.34	0.53
24:2:33:ARG:NH2	27:A:466:A:O2'	2.42	0.53
11:P:62:LYS:NZ	11:P:64:SER:OG	2.42	0.52
27:A:1908:C:H2'	27:A:1909:C:C1'	2.39	0.52
1:C:204:LEU:O	1:C:206:LYS:N	2.42	0.52
6:J:120:ARG:NE	27:A:2780:G:OP1	2.43	0.52
27:A:1866:A:N6	27:A:1875:G:O2'	2.42	0.52
27:A:2076:U:OP2	27:A:2238:G:N2	2.42	0.52
27:A:2721:A:C5	27:A:2722:G:O4'	2.54	0.52
1:C:49:THR:OG1	27:A:1805:A:N3	2.40	0.52
27:A:951:C:N4	27:A:952:G:O6	2.42	0.52
8:L:69:LYS:HA	8:L:72:ILE:HG22	1.91	0.52
27:A:2670:A:O2'	27:A:2671:G:O4'	2.25	0.52
27:A:2693:G:H2'	27:A:2694:G:C1'	2.39	0.52
2:D:183:GLU:OE1	2:D:183:GLU:N	2.39	0.52
27:A:788:A:OP1	27:A:791:C:N4	2.41	0.52
27:A:1688:U:O2'	27:A:1700:A:N7	2.37	0.52
27:A:532:A:N1	27:A:2035:G:N2	2.57	0.52
4:F:33:ILE:HD13	4:F:95:MET:HE3	1.91	0.52
7:K:37:ASP:OD1	7:K:38:ILE:N	2.43	0.52
8:L:32:ARG:NH2	8:L:38:LYS:O	2.43	0.52
27:A:571:U:O2'	27:A:573:U:OP2	2.27	0.52
27:A:2721:A:N3	27:A:2722:G:H8	2.02	0.52
5:H:31:VAL:CG1	5:H:32:PRO:HD3	2.39	0.52
21:Z:18:LYS:O	21:Z:22:THR:HG23	2.10	0.52
28:B:78:A:H62	28:B:98:G:H21	1.57	0.52
21:Z:36:GLU:N	21:Z:36:GLU:OE1	2.43	0.52
9:N:54:LEU:HD23	9:N:54:LEU:C	2.36	0.52
22:0:3:GLN:OE1	27:A:1263:U:O2'	2.22	0.52
27:A:83:A:O2'	27:A:103:A:N6	2.43	0.52
27:A:1428:C:N4	27:A:1570:A:OP2	2.38	0.52
28:B:78:A:H62	28:B:98:G:N2	2.07	0.52
3:E:95:LYS:O	27:A:659:G:O2'	2.28	0.51
24:2:34:ARG:NH1	27:A:467:G:OP2	2.41	0.51
25:3:1:PRO:N	27:A:591:U:O2'	2.43	0.51
27:A:310:A:O2'	27:A:311:A:OP2	2.21	0.51
27:A:2746:U:O4	27:A:2754:U:O2'	2.29	0.51
27:A:177:G:OP2	27:A:177:G:N2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1:MET:N	5:H:21:VAL:O	2.43	0.51
27:A:1987:A:C2	27:A:1988:G:N7	2.78	0.51
3:E:155:GLU:O	3:E:159:LEU:HD23	2.10	0.51
7:K:26:GLY:O	27:A:2673:G:O2'	2.29	0.51
12:Q:54:ARG:NH2	27:A:1155:A:O3'	2.42	0.51
27:A:27:G:H21	27:A:513:A:H62	1.58	0.51
27:A:1346:G:N1	27:A:1601:G:O6	2.44	0.51
20:Y:24:GLU:OE1	20:Y:24:GLU:N	2.41	0.51
27:A:2392:A:N6	27:A:2424:C:O2	2.43	0.51
7:K:92:GLU:OE1	7:K:92:GLU:N	2.42	0.51
18:W:60:PHE:CD1	18:W:71:ILE:HG23	2.45	0.51
9:N:23:ASN:OD1	27:A:1294:U:O2'	2.03	0.51
9:N:100:CYS:HB3	22:O:42:ILE:HD13	1.92	0.51
27:A:2467:C:N4	27:A:2468:A:N1	2.59	0.51
27:A:1266:G:N2	27:A:2013:A:OP2	2.35	0.51
27:A:1726:C:H2'	27:A:1727:C:C6	2.46	0.51
7:K:3:GLN:NE2	27:A:1666:G:N3	2.59	0.51
14:S:36:LEU:HD21	14:S:47:VAL:HG12	1.91	0.51
27:A:2100:G:O6	27:A:2190:G:C5	2.64	0.51
15:T:4:GLU:C	15:T:6:ARG:N	2.67	0.50
27:A:1653:G:OP1	27:A:2822:G:N1	2.44	0.50
11:P:70:GLU:OE1	11:P:70:GLU:N	2.44	0.50
23:1:41:ARG:NH1	27:A:2370:G:O2'	2.45	0.50
27:A:2135:A:N6	27:A:2156:G:O2'	2.44	0.50
27:A:2682:A:N1	27:A:2728:U:O2'	2.41	0.50
3:E:12:LEU:HD23	3:E:13:THR:O	2.11	0.50
9:N:20:MET:CE	9:N:24:MET:HE3	2.42	0.50
17:V:1:MET:SD	17:V:1:MET:N	2.82	0.50
27:A:258:G:H2'	27:A:259:G:C8	2.47	0.50
4:F:70:ARG:NH2	27:A:2313:C:OP2	2.44	0.50
27:A:2691:C:N3	27:A:2719:G:N2	2.59	0.50
2:D:56:LYS:O	2:D:60:VAL:HG23	2.12	0.49
5:H:9:VAL:HG22	5:H:10:ALA:H	1.77	0.49
24:2:22:MET:HE1	27:A:118:A:OP1	2.11	0.49
27:A:35:G:O2'	27:A:454:A:O4'	2.26	0.49
12:Q:85:ALA:O	12:Q:86:SER:OG	2.25	0.49
22:O:43:THR:OG1	22:O:45:ASP:OD1	2.24	0.49
26:M:124:LEU:HD23	26:M:128:THR:OG1	2.12	0.49
27:A:307:G:N1	27:A:309:A:O5'	2.45	0.49
1:C:155:ARG:NE	27:A:1818:U:OP2	2.44	0.49
9:N:28:LEU:C	9:N:28:LEU:HD23	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:476:G:N1	27:A:479:A:OP2	2.43	0.49
27:A:1801:A:N6	27:A:2201:G:O2'	2.43	0.49
27:A:2841:C:N4	27:A:2842:G:O6	2.45	0.49
5:H:3:VAL:HG21	5:H:30:LEU:HD13	1.94	0.49
27:A:2277:G:O6	27:A:2278:A:N6	2.45	0.49
2:D:98:VAL:HG22	2:D:98:VAL:O	2.13	0.49
8:L:28:LYS:O	8:L:29:THR:OG1	2.24	0.49
23:1:20:THR:HG22	23:1:21:THR:N	2.28	0.49
27:A:693:A:O2'	27:A:1353:A:N3	2.41	0.49
27:A:987:C:O2'	27:A:1000:A:N3	2.38	0.49
27:A:1860:G:O6	27:A:1882:U:C2	2.64	0.49
21:Z:2:LYS:NZ	21:Z:3:THR:O	2.41	0.49
1:C:35:LYS:NZ	27:A:1354:A:OP1	2.45	0.49
13:R:49:ILE:HG22	13:R:54:VAL:HG23	1.94	0.49
26:M:20:LEU:HD23	26:M:20:LEU:H	1.77	0.49
15:T:7:LEU:O	15:T:10:VAL:HG12	2.13	0.49
23:1:37:ASP:HB3	23:1:40:VAL:HG12	1.94	0.48
27:A:212:G:H2'	27:A:213:A:C8	2.47	0.48
27:A:2131:U:OP1	27:A:2133:G:O2'	2.24	0.48
27:A:2734:A:N6	27:A:2770:G:O2'	2.45	0.48
3:E:97:ASN:ND2	27:A:658:U:O2'	2.46	0.48
27:A:1752:C:N4	27:A:1753:G:O6	2.46	0.48
27:A:2650:U:O4	27:A:2671:G:N2	2.46	0.48
14:S:66:ILE:HA	14:S:69:LEU:HD23	1.95	0.48
27:A:966:G:O4'	27:A:2267:A:N6	2.46	0.48
19:X:31:ASN:OD1	19:X:33:HIS:NE2	2.46	0.48
19:X:64:ASP:OD1	19:X:65:THR:N	2.46	0.48
27:A:1319:C:N4	27:A:1334:G:O6	2.46	0.48
27:A:1995:U:OP2	27:A:1996:C:O2'	2.31	0.48
1:C:11:GLY:O	1:C:12:ARG:CB	2.61	0.48
4:F:157:THR:HG22	4:F:159:ALA:H	1.78	0.48
7:K:43:ILE:O	7:K:55:GLY:N	2.43	0.48
27:A:462:C:N4	27:A:463:G:O6	2.46	0.48
27:A:1606:C:O2'	27:A:1607:C:P	2.72	0.48
22:0:8:THR:HG21	27:A:2021:C:P	2.54	0.48
23:1:20:THR:HG22	23:1:21:THR:H	1.78	0.48
27:A:2128:G:HO2'	27:A:2129:C:P	2.35	0.48
27:A:2649:C:O2'	27:A:2650:U:O5'	2.32	0.48
27:A:2399:G:H2'	27:A:2400:G:C8	2.48	0.48
5:H:31:VAL:N	5:H:32:PRO:CD	2.77	0.48
23:1:3:ARG:NH2	23:1:21:THR:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:541:A:N6	27:A:553:G:C6	2.81	0.48
27:A:2077:A:N3	27:A:2434:A:O2'	2.45	0.47
2:D:162:ALA:O	27:A:2620:C:O2'	2.25	0.47
5:H:9:VAL:HG22	5:H:10:ALA:N	2.30	0.47
23:1:40:VAL:HG13	23:1:42:GLN:H	1.78	0.47
27:A:453:A:N3	27:A:457:A:O2'	2.46	0.47
9:N:9:GLN:OE1	27:A:1653:G:N1	2.47	0.47
15:T:2:ILE:HB	15:T:7:LEU:HD11	1.97	0.47
15:T:2:ILE:HG13	15:T:45:ALA:HB2	1.97	0.47
27:A:225:C:N3	27:A:231:A:N6	2.62	0.47
27:A:726:G:O2'	27:A:727:A:OP2	2.32	0.47
27:A:1291:C:N4	27:A:1292:G:O6	2.47	0.47
27:A:2127:G:H2'	27:A:2128:G:C8	2.49	0.47
7:K:30:ARG:NE	7:K:32:TYR:O	2.41	0.47
24:2:1:MET:N	27:A:1619:G:O2'	2.48	0.47
26:M:123:LYS:NZ	27:A:2467:C:O2'	2.48	0.47
27:A:571:U:O2'	27:A:572:A:O5'	2.27	0.47
27:A:1472:C:N4	27:A:1473:G:O6	2.47	0.47
27:A:1712:U:OP2	27:A:1713:A:O2'	2.23	0.47
2:D:55:LYS:HD2	2:D:60:VAL:HG22	1.97	0.47
3:E:5:LEU:N	3:E:5:LEU:HD12	2.30	0.47
7:K:3:GLN:O	7:K:6:THR:OG1	2.31	0.47
18:W:11:ARG:C	18:W:12:LEU:HD22	2.40	0.47
19:X:42:GLU:OE1	19:X:42:GLU:N	2.48	0.47
27:A:680:C:N4	27:A:681:G:O6	2.48	0.47
27:A:1419:A:N7	27:A:1578:U:N3	2.63	0.47
27:A:2637:U:O4	27:A:2776:A:N7	2.48	0.47
27:A:2674:G:H2'	27:A:2675:A:O4'	2.14	0.47
27:A:2737:G:N1	27:A:2768:U:C2	2.83	0.47
1:C:12:ARG:HG3	1:C:15:VAL:HG11	1.96	0.47
4:F:140:ILE:HD12	4:F:140:ILE:H	1.80	0.47
21:Z:19:HIS:O	21:Z:23:LEU:HD23	2.15	0.47
16:U:93:ARG:HB2	16:U:102:ILE:HD12	1.97	0.46
25:3:48:MET:SD	25:3:48:MET:N	2.85	0.46
27:A:554:U:H2'	27:A:555:G:O4'	2.15	0.46
27:A:1412:U:O4	27:A:1413:A:N6	2.48	0.46
28:B:29:A:H2	28:B:57:A:H62	1.63	0.46
4:F:47:LYS:C	4:F:48:LEU:HD12	2.40	0.46
9:N:45:ARG:HA	9:N:48:VAL:HG12	1.97	0.46
27:A:13:A:O2'	27:A:15:G:N7	2.48	0.46
1:C:145:MET:SD	1:C:146:LYS:N	2.88	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LYS:NZ	27:A:1795:C:O2	2.46	0.46
14:S:38:TYR:CD1	22:O:38:LEU:HD11	2.51	0.46
27:A:771:G:O2'	27:A:1355:G:O2'	2.00	0.46
27:A:2653:U:H5	27:A:2654:A:HO2'	1.63	0.46
2:D:2:ILE:HG21	2:D:48:ILE:HD11	1.98	0.46
6:J:138:GLN:N	6:J:138:GLN:OE1	2.48	0.46
27:A:416:U:H2'	27:A:417:C:O4'	2.15	0.46
27:A:1364:G:N2	27:A:1367:A:OP2	2.45	0.46
2:D:16:THR:OG1	2:D:18:ASP:OD1	2.27	0.46
2:D:15:PHE:HE2	11:P:54:LEU:HD21	1.80	0.46
14:S:43:ALA:O	14:S:47:VAL:HG23	2.16	0.46
17:V:29:ILE:HD12	28:B:75:G:H1'	1.98	0.46
19:X:10:ARG:HH21	27:A:1365:A:HO2'	1.60	0.46
23:1:32:GLU:OE1	23:1:32:GLU:N	2.48	0.46
24:2:24:THR:HG23	24:2:27:GLY:H	1.81	0.46
27:A:1524:G:C2	27:A:1525:A:C8	3.04	0.46
27:A:2127:G:O2'	27:A:2128:G:O4'	2.26	0.46
27:A:1131:G:N2	27:A:1132:U:O4	2.47	0.46
27:A:1582:C:O2'	27:A:1585:C:N3	2.41	0.46
3:E:79:ARG:NE	27:A:448:U:O4'	2.42	0.46
10:O:78:ALA:HB1	10:O:114:LEU:HD23	1.97	0.46
17:V:43:ASP:OD1	17:V:44:HIS:N	2.49	0.46
25:3:60:CYS:C	25:3:61:LEU:HD12	2.41	0.46
24:2:33:ARG:NH2	27:A:466:A:O3'	2.49	0.46
27:A:598:U:O2	27:A:659:G:O6	2.34	0.46
1:C:194:VAL:HG22	1:C:195:GLY:N	2.31	0.45
7:K:92:GLU:O	7:K:93:GLN:C	2.58	0.45
27:A:1275:A:O2'	27:A:1645:G:N3	2.50	0.45
27:A:2777:G:OP2	27:A:2781:A:O2'	2.31	0.45
3:E:41:GLN:N	27:A:443:A:OP1	2.44	0.45
27:A:2651:C:H2'	27:A:2652:C:C6	2.50	0.45
27:A:2728:U:N3	27:A:2729:G:N7	2.64	0.45
28:B:78:A:N6	28:B:98:G:H21	2.14	0.45
3:E:1:MET:SD	3:E:1:MET:N	2.81	0.45
15:T:13:ALA:HA	20:Y:30:MET:HE1	1.98	0.45
23:1:31:LEU:C	23:1:31:LEU:HD23	2.41	0.45
27:A:282:A:N6	27:A:359:G:O6	2.50	0.45
2:D:5:VAL:HG22	2:D:202:ILE:HD12	1.97	0.45
3:E:162:ARG:NH2	27:A:340:A:O2'	2.50	0.45
11:P:81:ASP:OD1	11:P:82:SER:N	2.50	0.45
20:Y:19:LEU:C	20:Y:19:LEU:HD23	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:729:G:O2'	27:A:763:G:H4'	2.17	0.45
1:C:123:ILE:HD12	1:C:123:ILE:N	2.31	0.45
18:W:28:ILE:N	18:W:28:ILE:HD12	2.32	0.45
27:A:137:U:HO2'	27:A:138:U:P	2.37	0.45
27:A:140:C:O2	27:A:140:C:O4'	2.34	0.45
27:A:238:C:H2'	27:A:239:C:C1'	2.46	0.45
27:A:755:U:O4	27:A:756:A:N6	2.49	0.45
27:A:1009:A:O2'	27:A:1010:A:O4'	2.29	0.45
27:A:1124:G:HO2'	27:A:1125:G:P	2.33	0.45
27:A:1351:C:O2'	27:A:1571:A:O2'	2.33	0.45
27:A:2128:G:H2'	27:A:2129:C:O4'	2.17	0.45
27:A:2114:A:H2'	27:A:2114:A:N3	2.32	0.45
3:E:134:LEU:O	3:E:138:LEU:HD23	2.16	0.45
5:H:11:ASN:O	5:H:12:LEU:HD22	2.16	0.45
27:A:291:G:O6	27:A:349:U:C2	2.69	0.45
27:A:1264:A:O5'	27:A:1265:A:H2'	2.16	0.45
3:E:141:MET:HE3	3:E:141:MET:HA	1.99	0.45
27:A:829:A:N7	27:A:2247:A:O2'	2.47	0.45
7:K:86:LEU:C	7:K:87:LEU:HD22	2.42	0.45
9:N:17:ARG:NH1	27:A:2002:G:OP1	2.42	0.45
11:P:14:GLN:OE1	11:P:14:GLN:N	2.49	0.45
27:A:804:A:H2'	27:A:806:C:C5	2.52	0.45
27:A:1361:G:O2'	27:A:2215:C:O2'	2.31	0.45
1:C:90:ILE:HD12	1:C:102:TYR:CD1	2.52	0.45
25:3:25:HIS:ND1	27:A:2361:G:OP1	2.50	0.45
27:A:1042:G:N1	27:A:1114:C:O2	2.49	0.45
27:A:1807:G:C2'	27:A:1809:A:H62	2.27	0.45
5:H:28:ASN:N	5:H:32:PRO:HG2	2.30	0.44
27:A:1791:A:N6	27:A:1828:G:O2'	2.50	0.44
27:A:1910:G:O2'	27:A:1911:U:O5'	2.27	0.44
27:A:2671:G:H2'	27:A:2672:U:C6	2.52	0.44
1:C:212:TRP:NE1	27:A:1566:A:O4'	2.50	0.44
27:A:1565:C:HO2'	27:A:1566:A:P	2.38	0.44
4:F:35:LEU:HD12	4:F:35:LEU:N	2.32	0.44
4:F:13:LYS:O	4:F:17:THR:HG23	2.17	0.44
6:J:100:VAL:HG13	6:J:101:ILE:N	2.32	0.44
11:P:39:LEU:HD12	11:P:39:LEU:N	2.32	0.44
27:A:1769:U:O2	27:A:1983:G:O6	2.35	0.44
27:A:2112:G:N3	27:A:2112:G:H2'	2.32	0.44
27:A:2649:C:O2'	27:A:2650:U:H6	2.01	0.44
22:0:8:THR:HG22	27:A:2020:A:C5'	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:3:32:LEU:H	25:3:32:LEU:HD23	1.83	0.44
27:A:242:G:N2	27:A:255:A:OP2	2.51	0.44
5:H:14:SER:OG	5:H:17:ASP:OD2	2.29	0.44
8:L:75:GLU:HB2	8:L:110:ILE:HD12	2.00	0.44
19:X:55:MET:HA	19:X:58:ILE:HG22	1.98	0.44
27:A:1421:G:N2	27:A:1578:U:O2	2.51	0.44
27:A:2330:G:H2'	27:A:2331:G:O4'	2.18	0.44
6:J:67:ASN:OD1	6:J:70:THR:OG1	2.35	0.44
7:K:38:ILE:N	7:K:38:ILE:HD12	2.32	0.44
27:A:738:G:H2'	27:A:739:A:O4'	2.18	0.44
27:A:1179:G:H3'	27:A:1180:U:C5'	2.48	0.44
27:A:1926:U:O2	27:A:1926:U:H2'	2.18	0.44
8:L:76:ILE:CG1	8:L:100:ILE:HD11	2.48	0.44
8:L:81:LEU:HD11	8:L:89:VAL:HG21	2.00	0.44
15:T:11:LEU:HD23	15:T:11:LEU:H	1.81	0.44
18:W:28:ILE:HD12	18:W:28:ILE:H	1.82	0.44
21:Z:6:ILE:HG23	21:Z:54:VAL:CG1	2.47	0.44
27:A:380:G:C2	27:A:395:U:O2	2.71	0.44
27:A:538:A:H62	27:A:555:G:N2	2.14	0.44
27:A:1203:U:OP2	27:A:1204:A:O2'	2.23	0.44
27:A:1638:C:O2	27:A:2698:U:O2'	2.35	0.44
27:A:2653:U:HO2'	27:A:2668:G:H1	1.61	0.44
1:C:200:MET:SD	1:C:200:MET:N	2.89	0.43
3:E:7:ASP:OD1	3:E:8:ALA:N	2.51	0.43
8:L:80:ASP:O	8:L:81:LEU:HB3	2.17	0.43
8:L:84:VAL:O	8:L:85:GLU:C	2.60	0.43
13:R:62:GLU:OE1	13:R:62:GLU:N	2.51	0.43
27:A:1434:A:N6	27:A:1435:G:O6	2.51	0.43
1:C:128:THR:HG22	1:C:190:THR:HG22	2.00	0.43
4:F:140:ILE:HD12	4:F:140:ILE:N	2.33	0.43
25:3:32:LEU:HD23	25:3:32:LEU:N	2.33	0.43
27:A:2091:C:OP2	27:A:2092:U:O2'	2.35	0.43
27:A:2150:C:H2'	27:A:2151:U:C6	2.53	0.43
2:D:1:MET:SD	2:D:1:MET:N	2.76	0.43
8:L:104:ILE:N	8:L:104:ILE:HD12	2.33	0.43
27:A:258:G:H2'	27:A:259:G:O4'	2.18	0.43
27:A:837:C:N3	27:A:941:A:N6	2.67	0.43
27:A:2657:A:N6	27:A:2664:G:H21	2.16	0.43
10:O:110:ARG:NH2	10:O:116:PHE:OXT	2.50	0.43
27:A:298:G:O2'	27:A:322:A:N1	2.42	0.43
27:A:306:U:O4	27:A:310:A:N7	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1360:G:C8	27:A:1361:G:C8	3.07	0.43
1:C:20:ASN:ND2	1:C:22:GLU:OE2	2.52	0.43
10:O:86:ILE:HG22	10:O:86:ILE:O	2.18	0.43
15:T:37:ASP:OD1	15:T:37:ASP:N	2.51	0.43
27:A:482:A:O2'	27:A:497:A:N1	2.52	0.43
28:B:73:A:N3	28:B:73:A:H2'	2.34	0.43
1:C:140:VAL:HG12	1:C:141:HIS:N	2.34	0.43
2:D:8:LYS:NZ	2:D:195:GLY:O	2.41	0.43
8:L:76:ILE:HG12	8:L:100:ILE:HD11	2.00	0.43
27:A:1521:G:OP2	27:A:1522:A:O2'	2.29	0.43
27:A:1549:A:O2'	27:A:1740:G:N2	2.49	0.43
5:H:29:PHE:O	5:H:30:LEU:C	2.61	0.43
5:H:33:GLN:NE2	5:H:35:LYS:HE2	2.34	0.43
12:Q:106:THR:HA	12:Q:109:VAL:HG12	2.01	0.43
19:X:58:ILE:HD13	19:X:66:VAL:CG1	2.47	0.43
22:O:53:VAL:HG12	22:O:54:ILE:N	2.33	0.43
26:M:54:THR:HA	26:M:57:VAL:HG22	1.99	0.43
27:A:2265:U:OP2	27:A:2266:A:O2'	2.37	0.43
27:A:2399:G:C2'	27:A:2400:G:O4'	2.66	0.43
18:W:60:PHE:HD1	18:W:71:ILE:HG23	1.83	0.43
26:M:96:ILE:HD13	26:M:102:LEU:HD21	2.00	0.43
27:A:1344:U:H3'	27:A:1345:C:H5'	2.01	0.43
27:A:1402:U:H3'	27:A:1403:A:H5''	2.00	0.43
15:T:4:GLU:HB3	15:T:5:GLU:OE1	2.18	0.43
27:A:959:A:O2'	27:A:960:A:O4'	2.27	0.43
14:S:4:ILE:CD1	14:S:106:VAL:HG22	2.49	0.42
27:A:373:U:O2'	27:A:423:A:N3	2.52	0.42
27:A:1042:G:O2'	27:A:1043:C:OP1	2.30	0.42
27:A:1766:G:C6	27:A:1987:A:N6	2.86	0.42
4:F:92:GLY:O	4:F:95:MET:HG2	2.19	0.42
5:H:10:ALA:O	5:H:12:LEU:N	2.44	0.42
5:H:34:GLY:O	5:H:35:LYS:HB2	2.19	0.42
7:K:64:ARG:HG2	7:K:83:ALA:HB3	2.01	0.42
12:Q:46:TYR:CD1	13:R:74:ILE:HG23	2.54	0.42
14:S:38:TYR:CG	22:O:38:LEU:HD11	2.54	0.42
27:A:545:U:O2'	27:A:548:G:N7	2.46	0.42
1:C:180:MET:N	1:C:180:MET:SD	2.92	0.42
6:J:122:LEU:HD23	6:J:122:LEU:C	2.44	0.42
22:O:53:VAL:HG12	22:O:54:ILE:H	1.84	0.42
27:A:281:C:N4	27:A:282:A:H62	2.18	0.42
27:A:1257:C:C2	27:A:1258:U:C5	3.08	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2266:A:N6	27:A:2273:A:OP2	2.53	0.42
27:A:2692:G:H4'	27:A:2869:G:H22	1.84	0.42
10:O:105:LEU:HD23	10:O:105:LEU:O	2.19	0.42
11:P:3:ILE:HD12	11:P:3:ILE:H	1.84	0.42
27:A:1550:C:H5'	27:A:1740:G:N2	2.35	0.42
27:A:514:A:HO2'	27:A:515:A:C4'	2.25	0.42
27:A:1326:U:N3	27:A:1648:U:O2'	2.50	0.42
4:F:126:ASN:ND2	27:A:2314:A:O2'	2.53	0.42
9:N:113:ILE:O	9:N:113:ILE:HG23	2.20	0.42
20:Y:10:SER:O	20:Y:14:LEU:HD23	2.19	0.42
27:A:684:G:O2'	27:A:788:A:N7	2.53	0.42
27:A:807:U:C2	27:A:808:G:C8	3.07	0.42
27:A:2692:G:O3'	27:A:2869:G:N2	2.52	0.42
28:B:40:U:O2'	28:B:43:C:OP2	2.37	0.42
2:D:30:GLU:OE2	2:D:33:ARG:NH2	2.51	0.42
3:E:147:LEU:C	3:E:147:LEU:HD23	2.45	0.42
27:A:36:G:N3	27:A:450:G:O2'	2.52	0.42
27:A:1924:C:H3'	27:A:1925:C:C5'	2.49	0.42
22:O:14:MET:SD	22:O:14:MET:C	3.03	0.42
26:M:53:MET:O	26:M:57:VAL:HG13	2.20	0.42
27:A:1730:C:O2	27:A:1731:G:N1	2.53	0.42
27:A:26:G:H1'	27:A:515:A:H61	1.85	0.42
27:A:2289:G:O6	27:A:2343:U:C2	2.72	0.42
1:C:129:LEU:N	1:C:129:LEU:HD23	2.35	0.42
4:F:59:ILE:CG1	4:F:140:ILE:HD11	2.50	0.42
27:A:1282:U:O4	27:A:1286:A:N7	2.53	0.42
27:A:2425:A:OP2	27:A:2426:A:O2'	2.36	0.42
5:H:29:PHE:HA	5:H:33:GLN:HG3	2.01	0.41
21:Z:40:THR:HG23	21:Z:43:ILE:H	1.84	0.41
22:O:39:ARG:O	22:O:41:HIS:ND1	2.40	0.41
25:3:28:LEU:C	25:3:28:LEU:HD12	2.45	0.41
4:F:37:MET:HG3	4:F:56:LEU:HD21	2.01	0.41
4:F:59:ILE:HG12	4:F:140:ILE:HD11	2.02	0.41
15:T:69:ARG:HG2	15:T:71:GLY:H	1.85	0.41
22:O:8:THR:HG21	27:A:2021:C:OP1	2.21	0.41
27:A:394:C:H2'	27:A:395:U:O4'	2.19	0.41
27:A:1205:A:HO2'	27:A:1206:G:P	2.38	0.41
1:C:10:PRO:HA	1:C:13:ARG:HB2	2.01	0.41
5:H:5:LEU:HD12	5:H:5:LEU:N	2.34	0.41
5:H:33:GLN:HE22	5:H:35:LYS:HE2	1.84	0.41
6:J:32:LEU:O	6:J:36:LEU:HD23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1509:A:O2'	27:A:1510:G:P	2.78	0.41
27:A:2714:G:C2	27:A:2715:C:C5	3.08	0.41
28:B:77:U:C2	28:B:99:A:N7	2.88	0.41
8:L:20:ARG:NH1	27:A:1250:G:OP2	2.54	0.41
27:A:47:C:N4	27:A:48:G:O6	2.53	0.41
27:A:176:A:H2'	27:A:177:G:N3	2.35	0.41
27:A:971:G:H2'	27:A:972:A:O4'	2.21	0.41
27:A:2127:G:O2'	27:A:2128:G:P	2.78	0.41
7:K:93:GLN:O	7:K:94:PRO:C	2.62	0.41
10:O:61:LEU:HD12	10:O:61:LEU:C	2.45	0.41
13:R:49:ILE:HG13	13:R:49:ILE:O	2.20	0.41
15:T:1:MET:SD	15:T:1:MET:N	2.90	0.41
18:W:27:ILE:HD12	18:W:27:ILE:N	2.36	0.41
18:W:28:ILE:HD11	18:W:52:ALA:HB2	2.02	0.41
22:O:15:ARG:HH22	27:A:1265:A:H3'	1.86	0.41
22:O:24:VAL:HG13	22:O:25:THR:N	2.35	0.41
27:A:2483:C:H3'	27:A:2484:G:H5''	2.03	0.41
1:C:203:VAL:O	1:C:204:LEU:HB2	2.20	0.41
3:E:190:ALA:O	3:E:194:LYS:NZ	2.53	0.41
15:T:87:LEU:O	15:T:88:LYS:HB3	2.20	0.41
27:A:188:G:O2'	27:A:1365:A:N6	2.53	0.41
22:O:15:ARG:NH1	27:A:1266:G:OP1	2.47	0.41
27:A:543:G:H2'	27:A:544:C:O4'	2.21	0.41
27:A:2651:C:H2'	27:A:2652:C:N1	2.36	0.41
27:A:2763:G:H1'	27:A:2764:A:P	2.60	0.41
21:Z:6:ILE:HG23	21:Z:54:VAL:HG13	2.03	0.41
27:A:301:G:HO2'	27:A:302:C:P	2.40	0.41
27:A:323:C:O2	27:A:323:C:O4'	2.38	0.41
27:A:393:C:H2'	27:A:394:C:C6	2.56	0.41
27:A:1665:A:N1	27:A:1996:C:N4	2.69	0.41
27:A:2107:G:O6	27:A:2182:U:C2	2.73	0.41
1:C:211:ARG:NH1	27:A:764:A:N3	2.69	0.41
4:F:174:PHE:O	4:F:175:PRO:C	2.63	0.41
5:H:3:VAL:HG21	5:H:30:LEU:CD1	2.51	0.41
10:O:105:LEU:HD23	10:O:105:LEU:C	2.45	0.41
14:S:29:VAL:HG13	14:S:55:ILE:HD11	2.03	0.41
18:W:23:LEU:H	18:W:23:LEU:HD23	1.86	0.41
22:O:14:MET:O	22:O:17:SER:OG	2.36	0.41
27:A:151:C:N4	27:A:152:A:N6	2.69	0.41
27:A:308:G:C6	27:A:501:A:C5	3.09	0.41
27:A:1124:G:O2'	27:A:1125:G:P	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1141:U:H4'	27:A:1142:A:O4'	2.21	0.41
27:A:1469:A:OP2	27:A:1522:A:N6	2.50	0.41
27:A:1566:A:O2'	27:A:1568:G:N2	2.54	0.41
27:A:2487:G:O2'	27:A:2488:G:O4'	2.30	0.41
27:A:2822:G:O2'	27:A:2824:C:OP2	2.28	0.41
13:R:54:VAL:HG12	13:R:56:GLY:H	1.86	0.41
27:A:2721:A:N6	27:A:2722:G:N3	2.69	0.41
8:L:81:LEU:O	8:L:84:VAL:HG12	2.21	0.40
13:R:39:LEU:HD13	13:R:49:ILE:HD13	2.03	0.40
19:X:54:GLY:O	19:X:58:ILE:HG22	2.21	0.40
20:Y:47:ARG:HA	20:Y:50:VAL:HG12	2.03	0.40
22:O:30:ASP:O	22:O:34:GLY:HA2	2.20	0.40
27:A:259:G:H2'	27:A:260:G:H8	1.87	0.40
27:A:1283:G:O2'	27:A:1329:U:N3	2.53	0.40
27:A:2183:A:H2'	27:A:2184:A:C8	2.56	0.40
18:W:62:VAL:HG13	18:W:62:VAL:O	2.20	0.40
22:O:38:LEU:H	22:O:38:LEU:HD12	1.87	0.40
27:A:2731:G:O2'	27:A:2732:G:O5'	2.39	0.40
1:C:194:VAL:HG22	1:C:195:GLY:H	1.87	0.40
4:F:30:VAL:O	4:F:30:VAL:HG23	2.21	0.40
6:J:19:ASP:OD1	6:J:20:ALA:N	2.54	0.40
19:X:59:ASP:OD1	19:X:60:LYS:N	2.55	0.40
19:X:66:VAL:O	19:X:69:GLU:HG3	2.21	0.40
25:3:54:LEU:HA	25:3:57:VAL:HG12	2.02	0.40
8:L:84:VAL:O	8:L:84:VAL:HG13	2.22	0.40
11:P:31:VAL:HG22	11:P:40:GLN:OE1	2.21	0.40
15:T:1:MET:N	27:A:139:U:O2	2.54	0.40
27:A:1282:U:H3	27:A:1286:A:H62	1.69	0.40
27:A:1846:G:O2'	27:A:1847:A:O4'	2.33	0.40
11:P:20:ARG:NH1	27:A:2849:U:O4	2.47	0.40
12:Q:13:HIS:O	12:Q:17:LEU:HD13	2.22	0.40
12:Q:39:ILE:HG23	12:Q:40:LYS:N	2.37	0.40
27:A:954:G:O2'	27:A:2274:A:N1	2.43	0.40
27:A:1450:G:N2	27:A:1452:G:O6	2.54	0.40
27:A:1633:G:O6	27:A:1635:A:N6	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	C	237/273 (87%)	223 (94%)	14 (6%)	0	100	100
2	D	182/209 (87%)	177 (97%)	5 (3%)	0	100	100
3	E	186/201 (92%)	183 (98%)	3 (2%)	0	100	100
4	F	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
5	H	48/149 (32%)	38 (79%)	9 (19%)	1 (2%)	5	32
6	J	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
7	K	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
8	L	141/144 (98%)	126 (89%)	15 (11%)	0	100	100
9	N	118/127 (93%)	112 (95%)	6 (5%)	0	100	100
10	O	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
11	P	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
12	Q	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
13	R	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
14	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
15	T	91/100 (91%)	82 (90%)	8 (9%)	1 (1%)	11	44
16	U	100/104 (96%)	86 (86%)	14 (14%)	0	100	100
17	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
18	W	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
19	X	75/78 (96%)	75 (100%)	0	0	100	100
20	Y	59/63 (94%)	53 (90%)	6 (10%)	0	100	100
21	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
22	0	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
23	1	48/55 (87%)	48 (100%)	0	0	100	100
24	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	3	62/65 (95%)	59 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	M	120/136 (88%)	113 (94%)	7 (6%)	0	100	100
All	All	2772/3052 (91%)	2636 (95%)	134 (5%)	2 (0%)	49	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	35	LYS
15	T	5	GLU

5.3.2 Protein sidechains ⓘ

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	C	193/218 (88%)	193 (100%)	0	100	100
2	D	145/164 (88%)	145 (100%)	0	100	100
3	E	157/165 (95%)	157 (100%)	0	100	100
4	F	148/150 (99%)	148 (100%)	0	100	100
5	H	40/114 (35%)	38 (95%)	2 (5%)	22	47
6	J	116/116 (100%)	116 (100%)	0	100	100
7	K	103/104 (99%)	102 (99%)	1 (1%)	68	76
8	L	102/103 (99%)	102 (100%)	0	100	100
9	N	100/103 (97%)	100 (100%)	0	100	100
10	O	86/87 (99%)	86 (100%)	0	100	100
11	P	99/100 (99%)	99 (100%)	0	100	100
12	Q	89/90 (99%)	89 (100%)	0	100	100
13	R	84/84 (100%)	84 (100%)	0	100	100
14	S	93/93 (100%)	93 (100%)	0	100	100
15	T	80/84 (95%)	79 (99%)	1 (1%)	61	72
16	U	83/85 (98%)	83 (100%)	0	100	100
17	V	78/78 (100%)	78 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	W	56/63 (89%)	56 (100%)	0	100	100
19	X	67/68 (98%)	67 (100%)	0	100	100
20	Y	55/55 (100%)	52 (94%)	3 (6%)	19	45
21	Z	48/49 (98%)	48 (100%)	0	100	100
22	0	47/48 (98%)	47 (100%)	0	100	100
23	1	45/49 (92%)	45 (100%)	0	100	100
24	2	38/38 (100%)	38 (100%)	0	100	100
25	3	51/52 (98%)	51 (100%)	0	100	100
26	M	100/109 (92%)	100 (100%)	0	100	100
All	All	2303/2469 (93%)	2296 (100%)	7 (0%)	84	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	H	31	VAL
5	H	33	GLN
7	K	93	GLN
15	T	1	MET
20	Y	13	GLU
20	Y	15	ASN
20	Y	22	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	52	HIS
2	D	32	ASN
2	D	164	GLN
2	D	167	ASN
3	E	97	ASN
5	H	18	GLN
5	H	28	ASN
5	H	33	GLN
7	K	9	ASN
7	K	88	ASN
8	L	34	HIS
11	P	65	ASN
11	P	76	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	S	60	HIS
15	T	15	HIS
16	U	44	HIS
17	V	49	ASN
17	V	87	GLN
19	X	15	ASN
20	Y	27	ASN
20	Y	38	GLN
20	Y	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	A	2701/2904 (93%)	468 (17%)	22 (0%)
28	B	118/119 (99%)	10 (8%)	0
All	All	2819/3023 (93%)	478 (16%)	22 (0%)

All (478) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	A	10	A
27	A	12	U
27	A	26	G
27	A	27	G
27	A	34	U
27	A	45	G
27	A	46	G
27	A	51	G
27	A	60	G
27	A	63	A
27	A	74	A
27	A	75	G
27	A	118	A
27	A	120	U
27	A	125	A
27	A	138	U
27	A	139	U
27	A	140	C
27	A	141	G
27	A	142	A
27	A	190	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	196	A
27	A	199	A
27	A	205	G
27	A	216	A
27	A	222	A
27	A	223	A
27	A	224	U
27	A	230	G
27	A	239	C
27	A	248	G
27	A	250	G
27	A	255	A
27	A	266	G
27	A	271	G
27	A	272	A
27	A	285	G
27	A	302	C
27	A	307	G
27	A	309	A
27	A	311	A
27	A	329	G
27	A	330	A
27	A	331	C
27	A	353	C
27	A	362	A
27	A	371	A
27	A	372	G
27	A	384	A
27	A	386	G
27	A	405	U
27	A	411	G
27	A	412	A
27	A	424	G
27	A	430	A
27	A	456	C
27	A	480	A
27	A	481	G
27	A	491	G
27	A	504	A
27	A	505	A
27	A	509	C
27	A	531	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	532	A
27	A	541	A
27	A	543	G
27	A	546	U
27	A	548	G
27	A	549	G
27	A	563	A
27	A	567	U
27	A	571	U
27	A	572	A
27	A	573	U
27	A	574	A
27	A	586	A
27	A	603	A
27	A	613	A
27	A	614	A
27	A	615	U
27	A	627	A
27	A	628	G
27	A	637	A
27	A	644	A
27	A	645	C
27	A	646	U
27	A	647	G
27	A	654	A
27	A	655	A
27	A	659	G
27	A	683	U
27	A	686	U
27	A	730	A
27	A	738	G
27	A	739	A
27	A	740	C
27	A	747	U
27	A	764	A
27	A	775	G
27	A	777	G
27	A	782	A
27	A	784	G
27	A	785	G
27	A	788	A
27	A	789	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	792	A
27	A	805	G
27	A	811	U
27	A	812	C
27	A	819	A
27	A	827	U
27	A	828	U
27	A	830	G
27	A	846	U
27	A	847	U
27	A	856	G
27	A	858	G
27	A	860	U
27	A	868	U
27	A	876	C
27	A	877	A
27	A	878	A
27	A	887	U
27	A	888	C
27	A	889	C
27	A	890	C
27	A	896	A
27	A	905	A
27	A	907	G
27	A	910	A
27	A	912	C
27	A	914	G
27	A	915	C
27	A	932	U
27	A	941	A
27	A	946	C
27	A	953	G
27	A	958	U
27	A	959	A
27	A	961	C
27	A	973	A
27	A	974	G
27	A	983	A
27	A	985	C
27	A	995	C
27	A	996	A
27	A	1009	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	1012	U
27	A	1013	C
27	A	1022	G
27	A	1026	G
27	A	1033	U
27	A	1034	G
27	A	1043	C
27	A	1044	C
27	A	1045	C
27	A	1116	G
27	A	1119	U
27	A	1125	G
27	A	1126	A
27	A	1127	A
27	A	1128	G
27	A	1130	U
27	A	1131	G
27	A	1133	A
27	A	1135	C
27	A	1136	G
27	A	1142	A
27	A	1143	A
27	A	1157	G
27	A	1168	G
27	A	1171	G
27	A	1172	C
27	A	1173	U
27	A	1174	U
27	A	1175	A
27	A	1176	U
27	A	1180	U
27	A	1182	G
27	A	1206	G
27	A	1210	G
27	A	1212	G
27	A	1236	G
27	A	1238	G
27	A	1253	A
27	A	1256	G
27	A	1264	A
27	A	1266	G
27	A	1271	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	1272	A
27	A	1300	G
27	A	1301	A
27	A	1302	A
27	A	1314	C
27	A	1321	A
27	A	1329	U
27	A	1345	C
27	A	1365	A
27	A	1367	A
27	A	1378	A
27	A	1379	U
27	A	1383	A
27	A	1403	A
27	A	1416	G
27	A	1417	C
27	A	1427	A
27	A	1451	C
27	A	1452	G
27	A	1458	U
27	A	1461	C
27	A	1467	U
27	A	1482	G
27	A	1493	C
27	A	1504	A
27	A	1508	A
27	A	1509	A
27	A	1510	G
27	A	1515	A
27	A	1535	A
27	A	1555	G
27	A	1565	C
27	A	1569	A
27	A	1578	U
27	A	1583	A
27	A	1585	C
27	A	1598	A
27	A	1607	C
27	A	1646	C
27	A	1647	U
27	A	1648	U
27	A	1665	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	1668	A
27	A	1674	G
27	A	1699	G
27	A	1715	G
27	A	1721	G
27	A	1729	U
27	A	1730	C
27	A	1732	C
27	A	1733	G
27	A	1734	G
27	A	1738	G
27	A	1758	U
27	A	1764	C
27	A	1773	A
27	A	1781	U
27	A	1785	A
27	A	1800	C
27	A	1801	A
27	A	1807	G
27	A	1808	A
27	A	1816	C
27	A	1829	A
27	A	1835	G
27	A	1849	G
27	A	1857	G
27	A	1858	A
27	A	1862	G
27	A	1869	G
27	A	1870	C
27	A	1899	A
27	A	1900	A
27	A	1909	C
27	A	1910	G
27	A	1911	U
27	A	1912	A
27	A	1913	A
27	A	1914	C
27	A	1916	A
27	A	1922	G
27	A	1926	U
27	A	1928	A
27	A	1930	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	1931	U
27	A	1937	A
27	A	1938	A
27	A	1939	U
27	A	1940	U
27	A	1941	C
27	A	1962	C
27	A	1963	U
27	A	1965	C
27	A	1966	A
27	A	1967	C
27	A	1970	A
27	A	1972	G
27	A	1991	U
27	A	1992	G
27	A	1993	U
27	A	1997	C
27	A	2022	U
27	A	2023	C
27	A	2025	C
27	A	2030	A
27	A	2031	A
27	A	2043	C
27	A	2051	A
27	A	2052	A
27	A	2058	A
27	A	2059	A
27	A	2060	A
27	A	2069	G
27	A	2090	A
27	A	2093	G
27	A	2095	A
27	A	2096	C
27	A	2102	G
27	A	2104	C
27	A	2108	A
27	A	2109	U
27	A	2113	U
27	A	2114	A
27	A	2115	G
27	A	2116	G
27	A	2118	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	2119	A
27	A	2120	G
27	A	2126	A
27	A	2127	G
27	A	2128	G
27	A	2129	C
27	A	2131	U
27	A	2132	U
27	A	2133	G
27	A	2140	G
27	A	2141	G
27	A	2142	A
27	A	2146	C
27	A	2147	A
27	A	2150	C
27	A	2154	A
27	A	2157	G
27	A	2158	A
27	A	2159	G
27	A	2161	C
27	A	2162	G
27	A	2164	C
27	A	2166	U
27	A	2167	U
27	A	2170	A
27	A	2171	A
27	A	2173	A
27	A	2175	C
27	A	2176	A
27	A	2178	C
27	A	2185	U
27	A	2199	A
27	A	2204	G
27	A	2211	A
27	A	2225	A
27	A	2238	G
27	A	2239	G
27	A	2250	G
27	A	2265	U
27	A	2266	A
27	A	2283	C
27	A	2286	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	2287	A
27	A	2297	A
27	A	2305	U
27	A	2308	G
27	A	2325	G
27	A	2327	A
27	A	2333	A
27	A	2336	A
27	A	2344	U
27	A	2345	G
27	A	2346	A
27	A	2347	C
27	A	2350	C
27	A	2357	G
27	A	2372	U
27	A	2383	G
27	A	2385	C
27	A	2389	G
27	A	2402	U
27	A	2406	A
27	A	2410	G
27	A	2425	A
27	A	2426	A
27	A	2429	G
27	A	2430	A
27	A	2435	A
27	A	2441	U
27	A	2447	G
27	A	2458	G
27	A	2459	A
27	A	2460	U
27	A	2461	A
27	A	2462	C
27	A	2471	A
27	A	2473	U
27	A	2474	U
27	A	2475	C
27	A	2476	A
27	A	2477	U
27	A	2479	U
27	A	2484	G
27	A	2490	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	2491	U
27	A	2493	U
27	A	2494	G
27	A	2610	C
27	A	2613	U
27	A	2629	U
27	A	2630	G
27	A	2639	A
27	A	2646	C
27	A	2648	G
27	A	2651	C
27	A	2654	A
27	A	2655	G
27	A	2657	A
27	A	2665	A
27	A	2670	A
27	A	2681	C
27	A	2685	G
27	A	2687	U
27	A	2688	G
27	A	2689	U
27	A	2690	U
27	A	2694	G
27	A	2695	U
27	A	2696	U
27	A	2715	C
27	A	2716	C
27	A	2718	G
27	A	2719	G
27	A	2721	A
27	A	2722	G
27	A	2726	A
27	A	2732	G
27	A	2733	A
27	A	2743	U
27	A	2746	U
27	A	2747	G
27	A	2748	A
27	A	2750	A
27	A	2751	G
27	A	2752	C
27	A	2753	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	2754	U
27	A	2755	C
27	A	2756	U
27	A	2757	A
27	A	2758	A
27	A	2761	A
27	A	2763	G
27	A	2764	A
27	A	2765	A
27	A	2769	U
27	A	2771	C
27	A	2778	A
27	A	2780	G
27	A	2791	G
27	A	2798	U
27	A	2801	G
27	A	2818	U
27	A	2820	A
27	A	2825	G
27	A	2835	A
27	A	2849	U
27	A	2865	U
27	A	2867	G
27	A	2880	C
27	A	2883	A
27	A	2884	U
27	A	2893	A
28	B	15	A
28	B	35	C
28	B	36	C
28	B	41	G
28	B	58	A
28	B	89	U
28	B	90	C
28	B	99	A
28	B	108	A
28	B	109	A

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	A	271	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	A	404	A
27	A	644	A
27	A	995	C
27	A	1042	G
27	A	1124	G
27	A	1126	A
27	A	1172	C
27	A	1606	C
27	A	1910	G
27	A	1938	A
27	A	2117	A
27	A	2127	G
27	A	2128	G
27	A	2140	G
27	A	2425	A
27	A	2457	U
27	A	2470	G
27	A	2694	G
27	A	2746	U
27	A	2754	U
27	A	2763	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

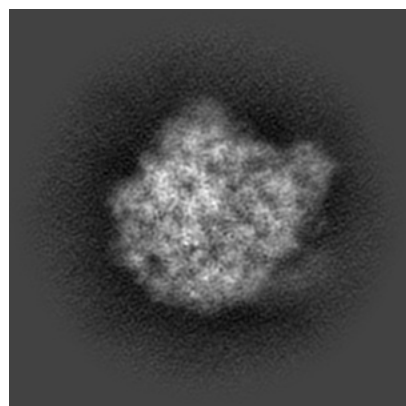
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16494. These allow visual inspection of the internal detail of the map and identification of artifacts.

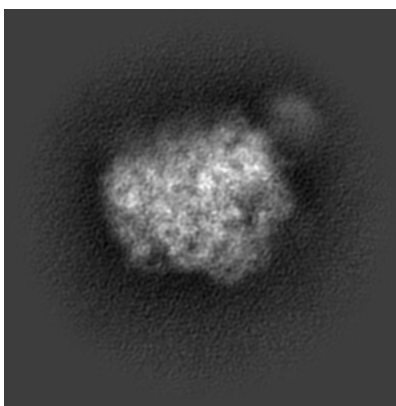
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

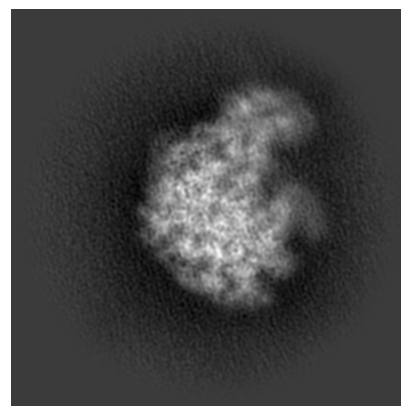
6.1.1 Primary map



X

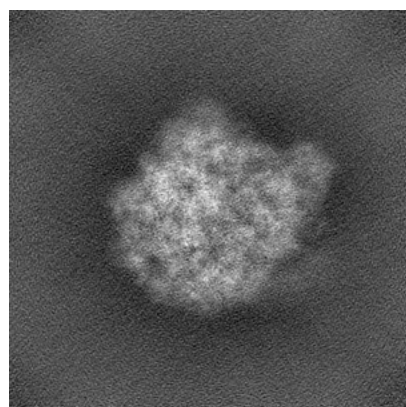


Y

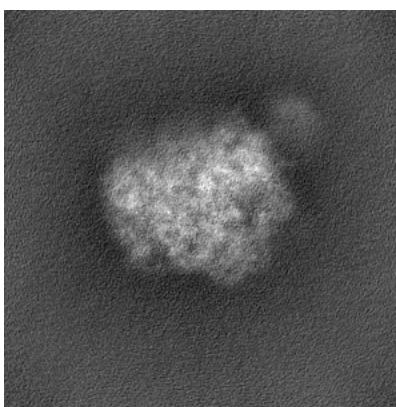


Z

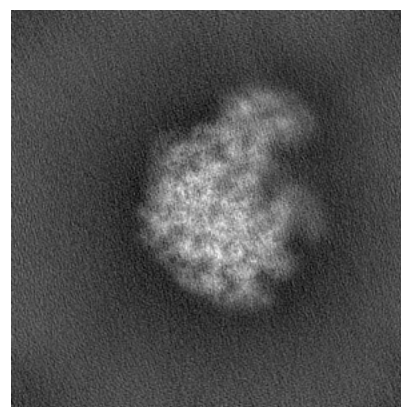
6.1.2 Raw map



X



Y

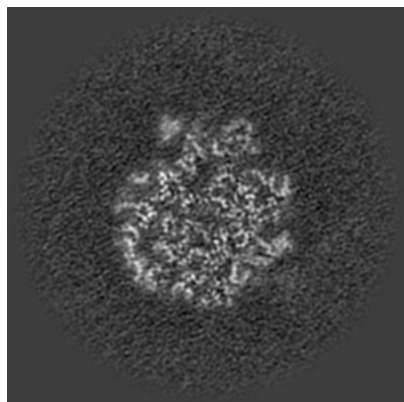


Z

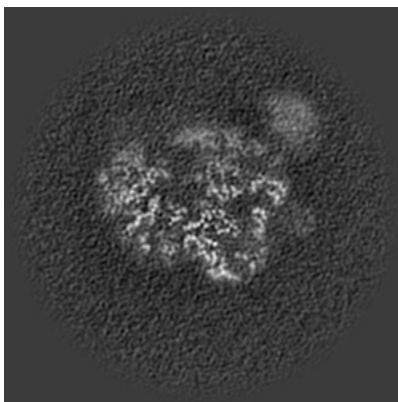
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

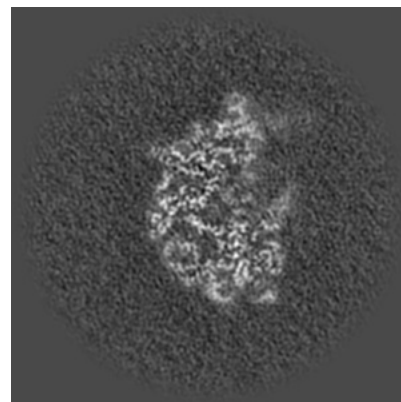
6.2.1 Primary map



X Index: 150

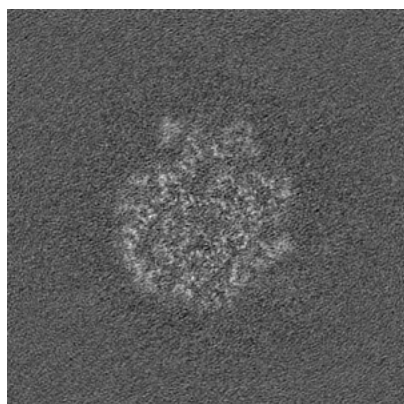


Y Index: 150

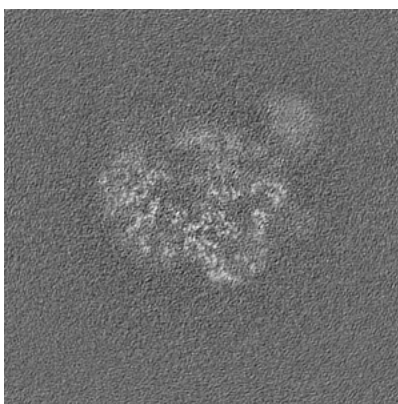


Z Index: 150

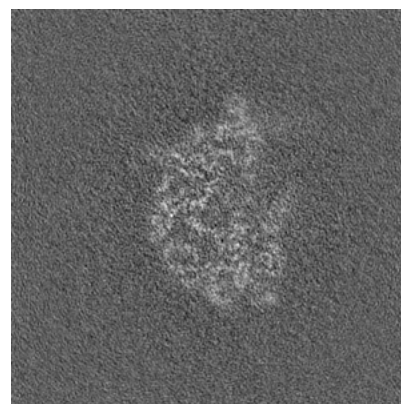
6.2.2 Raw map



X Index: 150



Y Index: 150

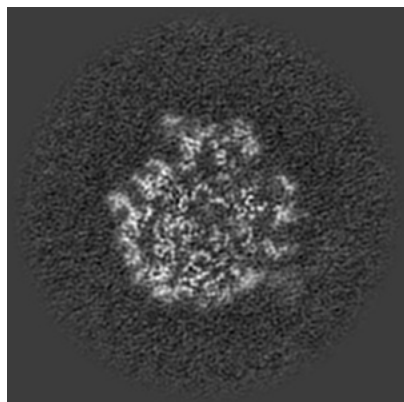


Z Index: 150

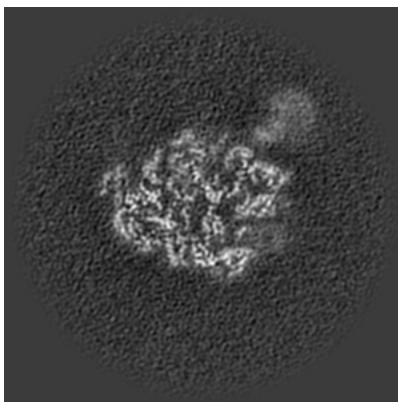
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

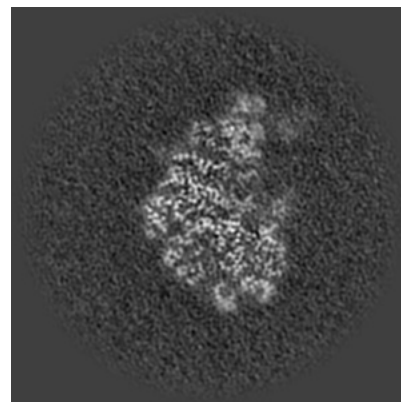
6.3.1 Primary map



X Index: 154

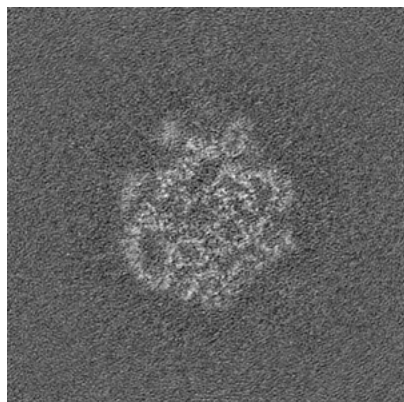


Y Index: 139

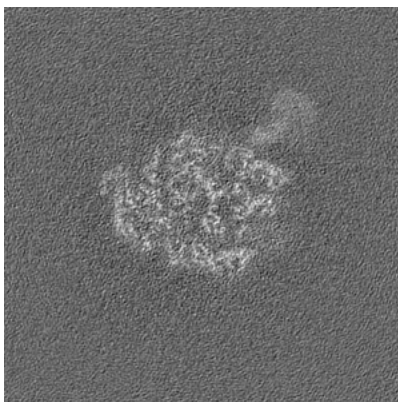


Z Index: 154

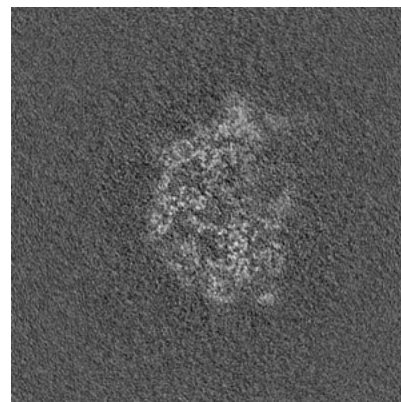
6.3.2 Raw map



X Index: 147



Y Index: 138

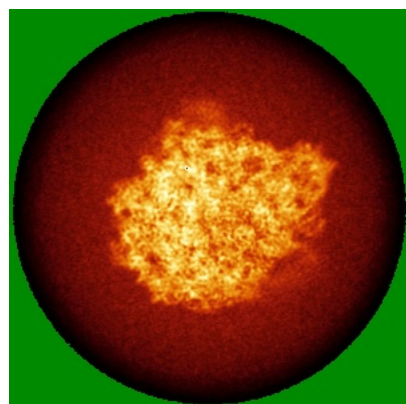


Z Index: 149

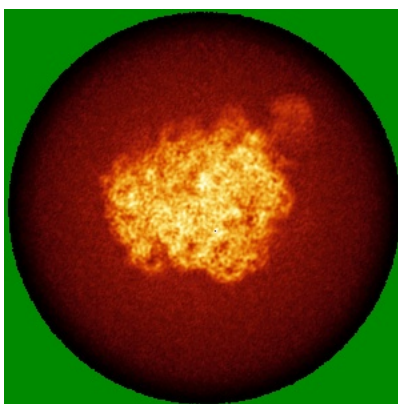
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

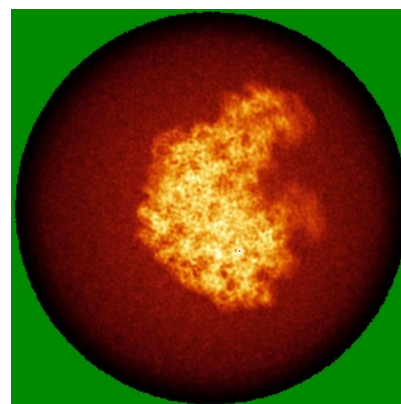
6.4.1 Primary map



X

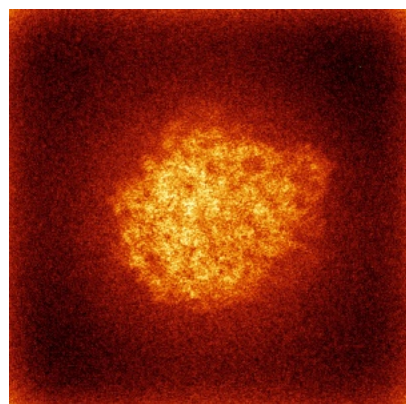


Y

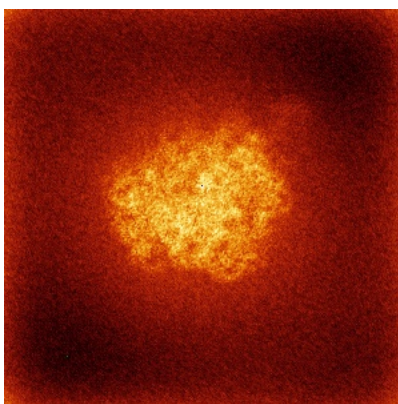


Z

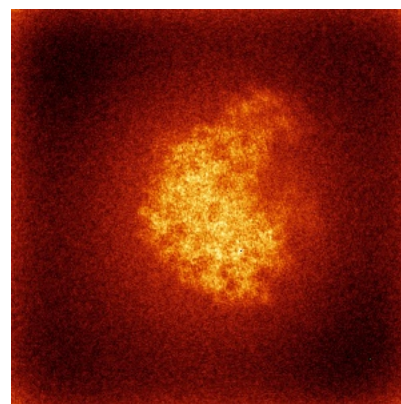
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

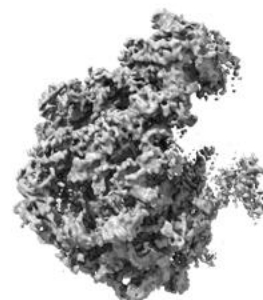
6.5.1 Primary map



X



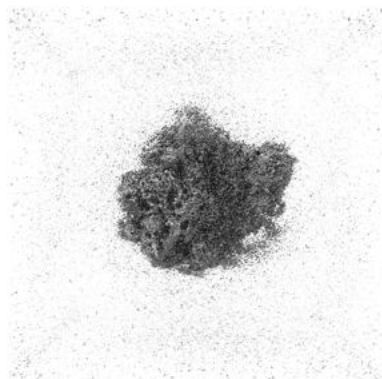
Y



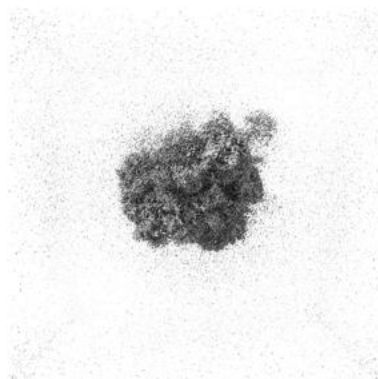
Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

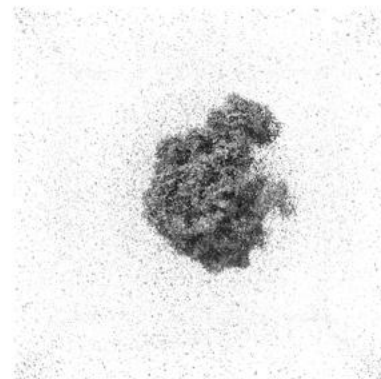
6.5.2 Raw map



X



Y



Z

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

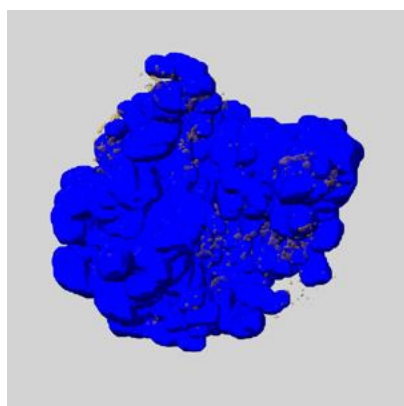
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

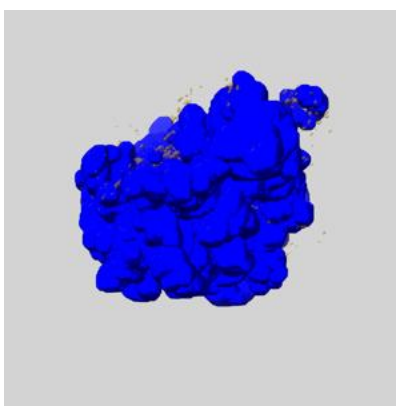
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

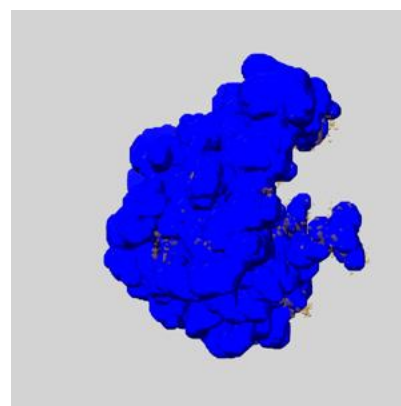
6.6.1 emd_16494_msk_1.map [i](#)



X



Y

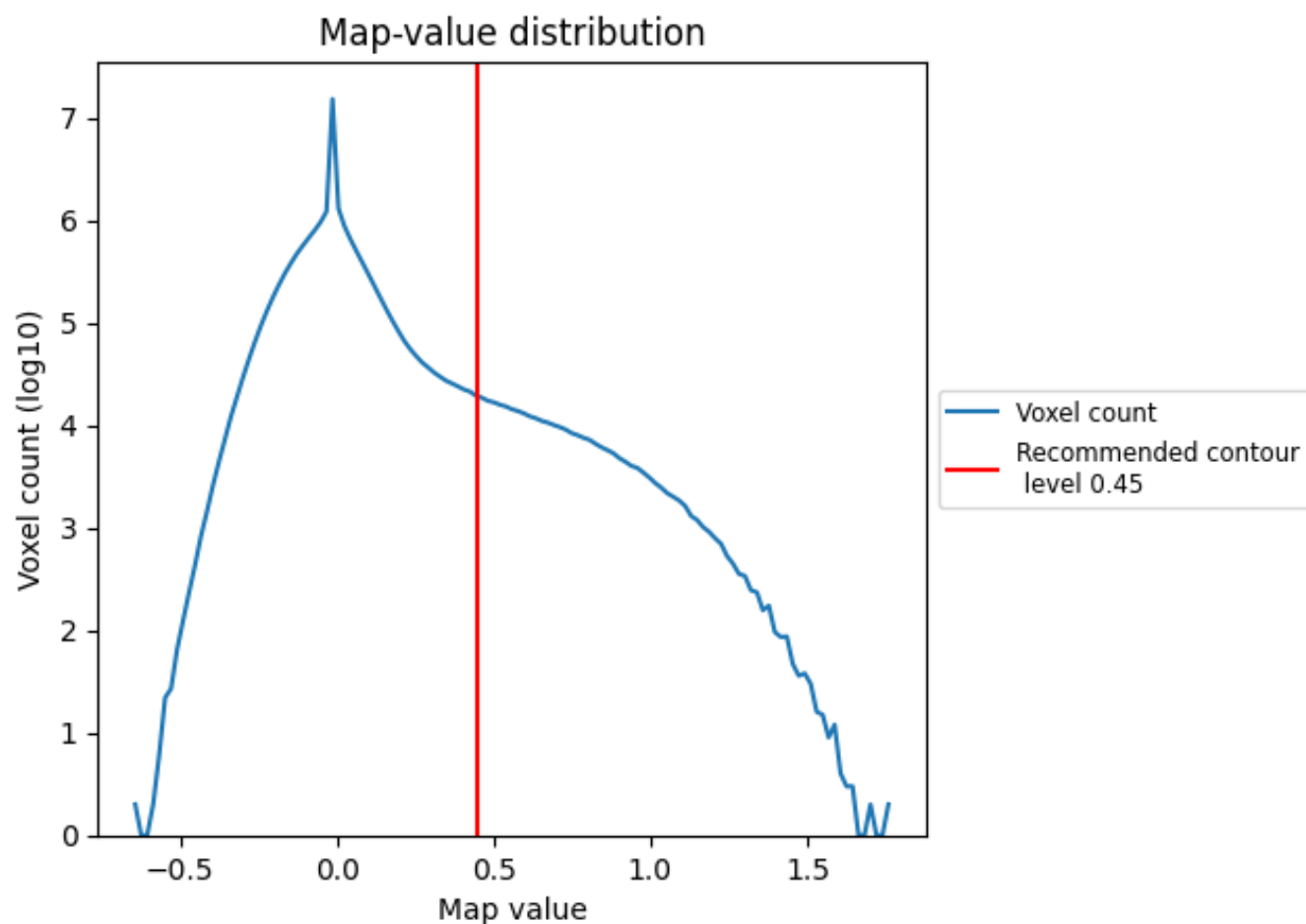


Z

7 Map analysis [i](#)

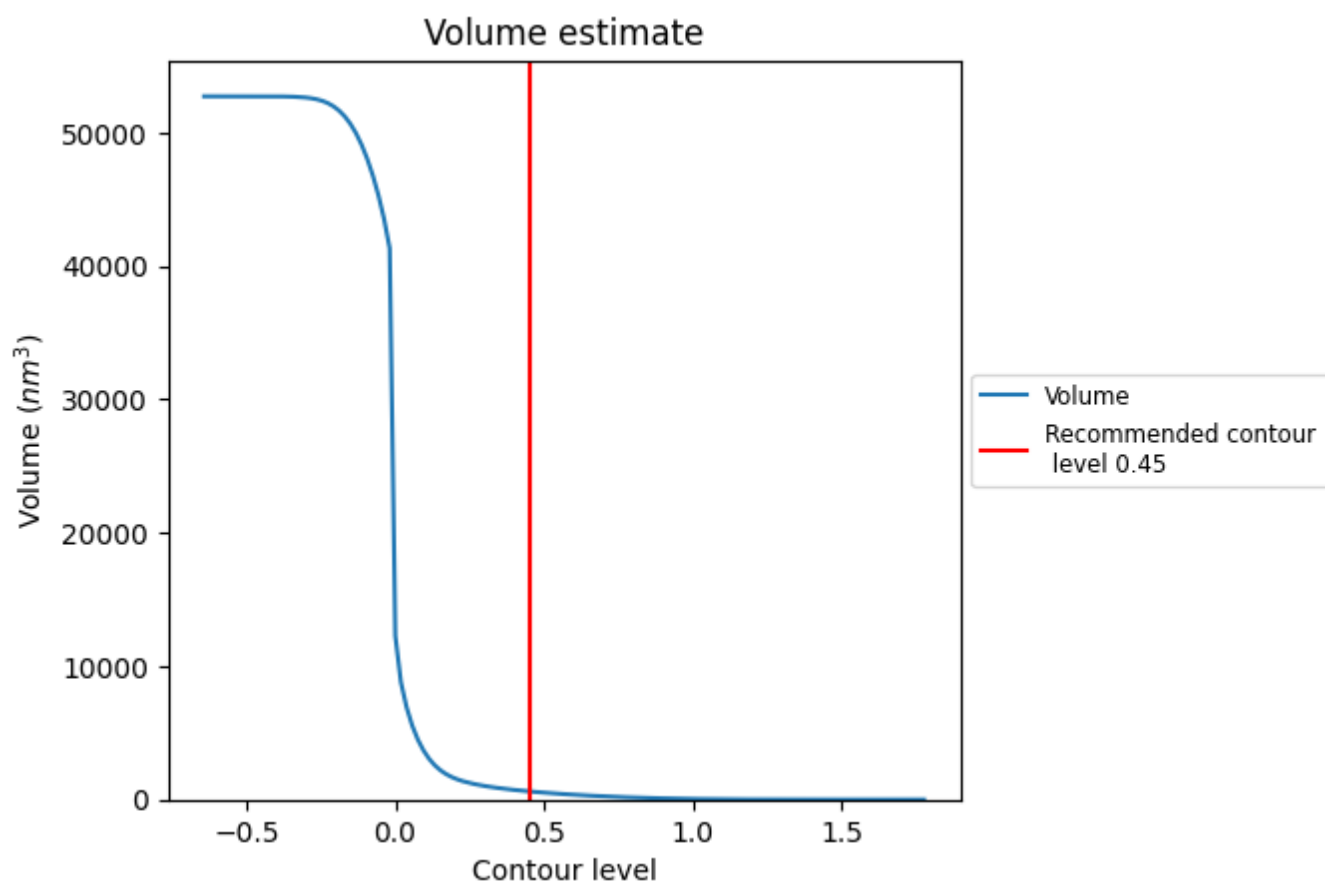
This section contains the results of statistical analysis of the map.

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.

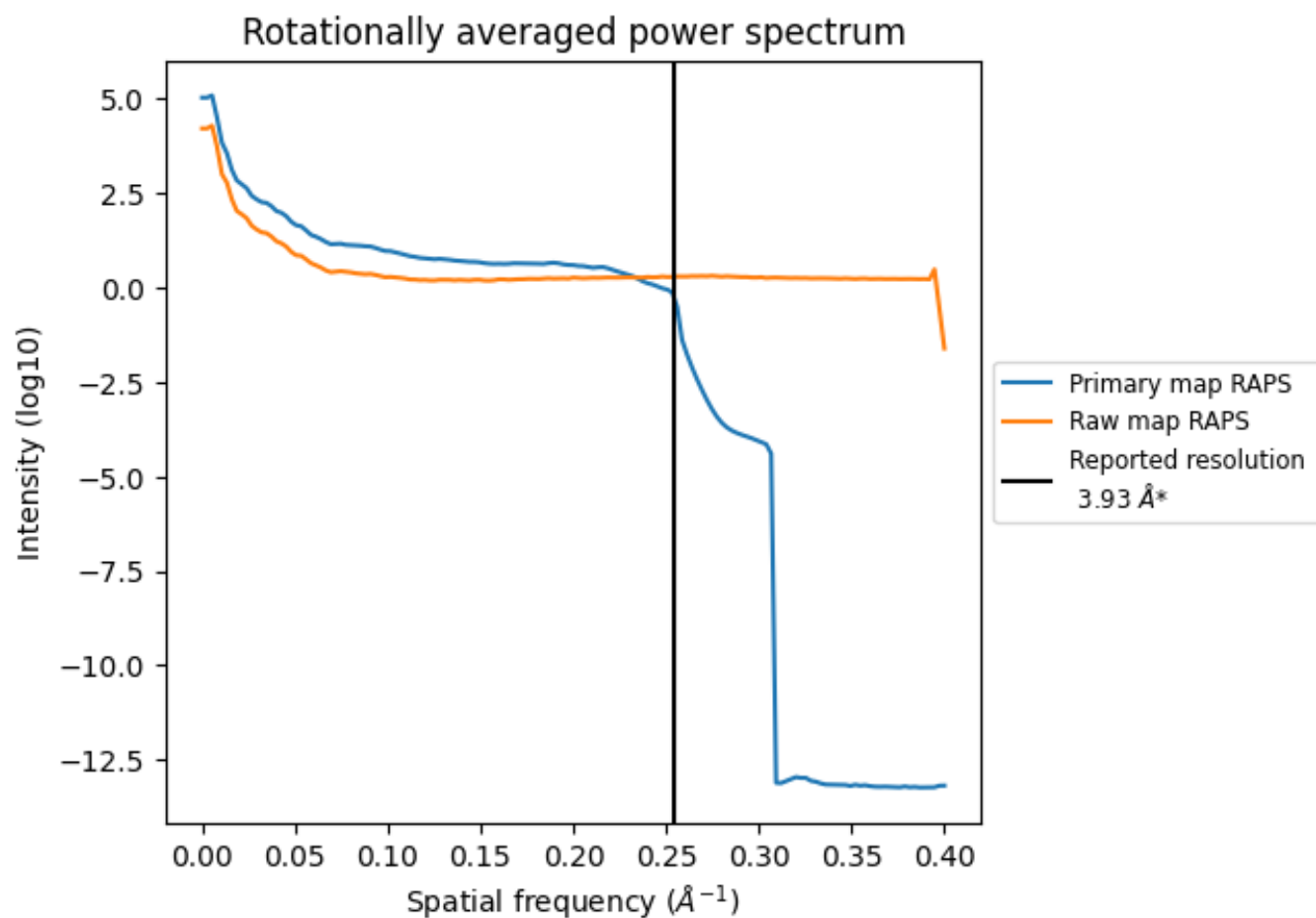
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 612 nm³; this corresponds to an approximate mass of 553 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 ⓘ

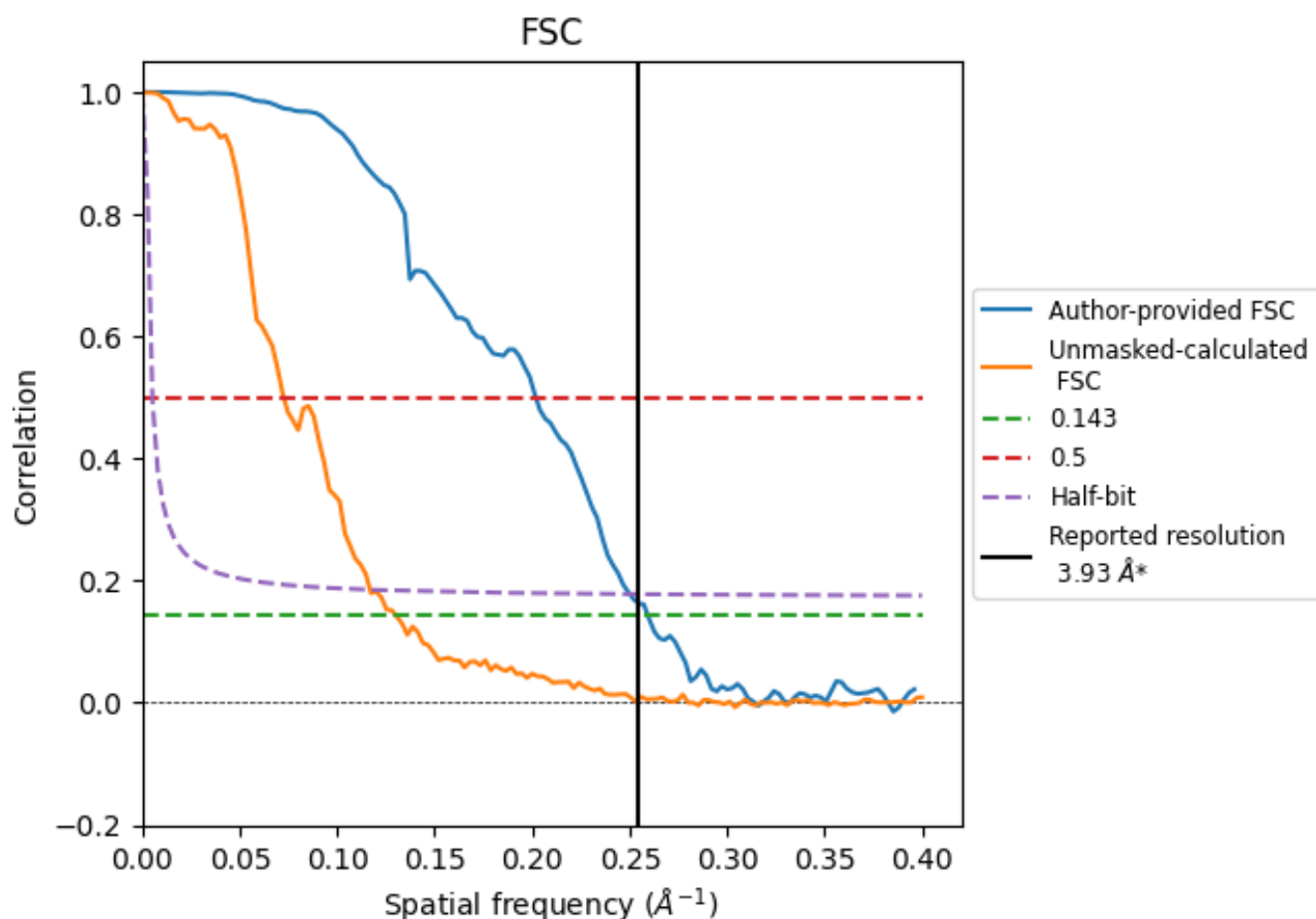


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.254 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

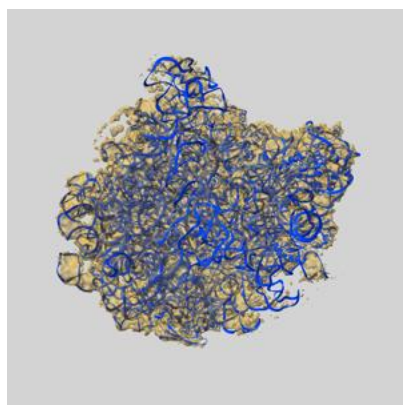
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	3.86	4.95	4.00
Unmasked-calculated*	7.70	13.77	8.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.70 differs from the reported value 3.93 by more than 10 %

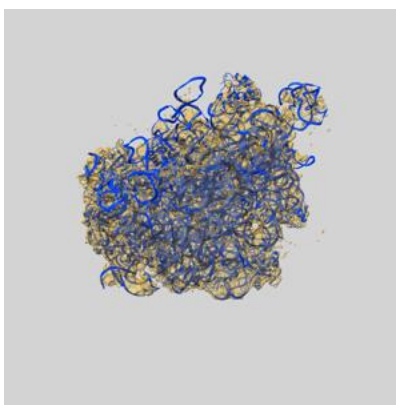
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16494 and PDB model 8C8X. Per-residue inclusion information can be found in section [3](#) on page [9](#).

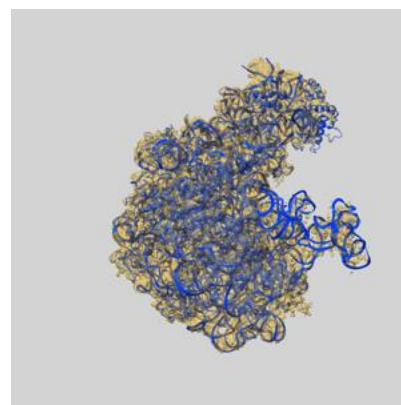
9.1 Map-model overlay [i](#)



X



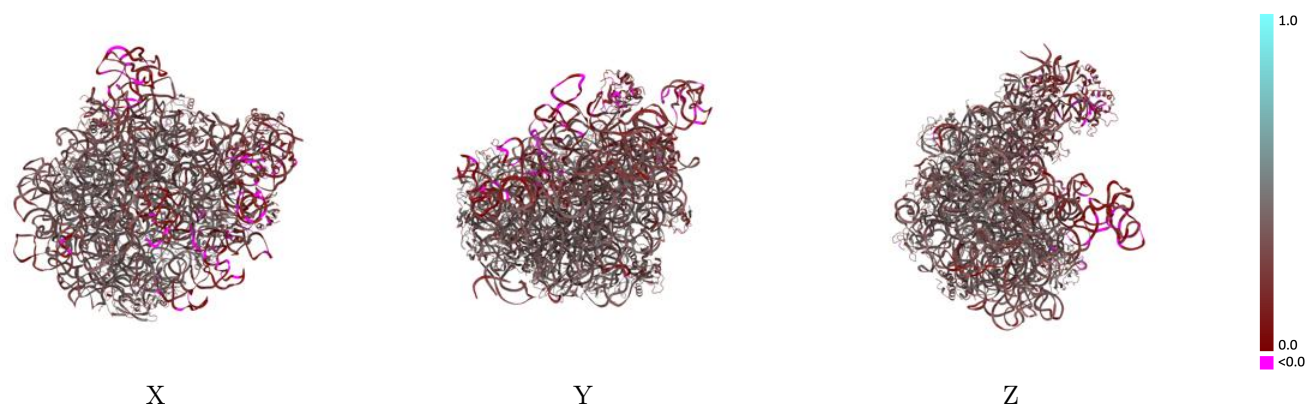
Y



Z

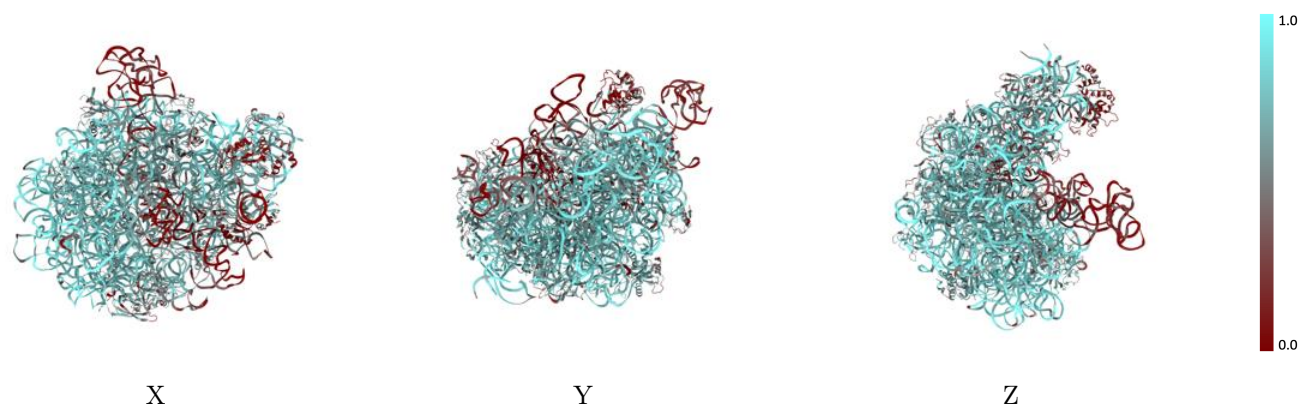
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



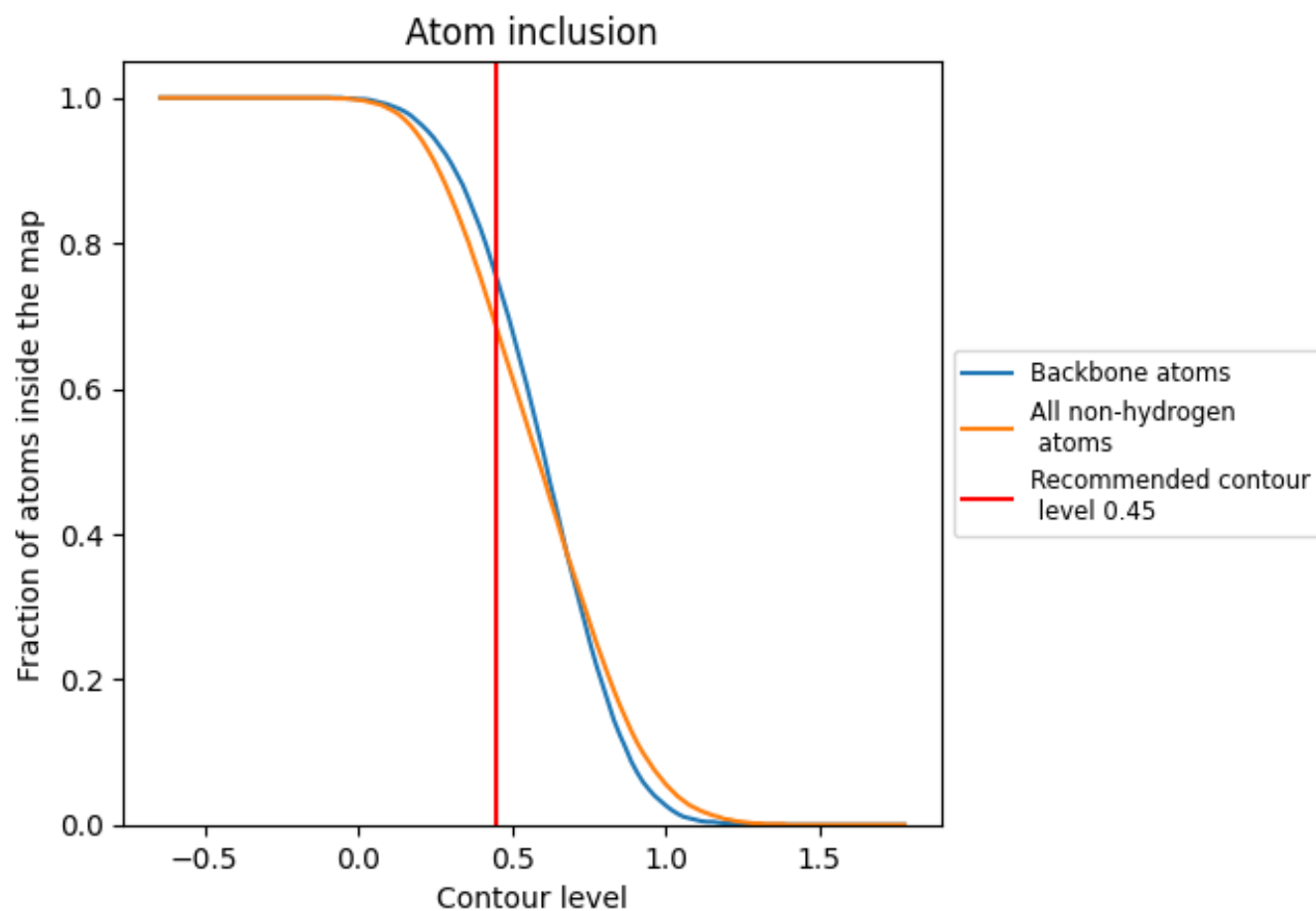
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6840	 0.3180
0	 0.6010	 0.3750
1	 0.4440	 0.3000
2	 0.6170	 0.4100
3	 0.2810	 0.3510
A	 0.7340	 0.3120
B	 0.7880	 0.2660
C	 0.6840	 0.3840
D	 0.6120	 0.3930
E	 0.6010	 0.3600
F	 0.2100	 0.1850
H	 0.5040	 0.2750
J	 0.6050	 0.3760
K	 0.4480	 0.3360
L	 0.5170	 0.3380
M	 0.1380	 0.2710
N	 0.6590	 0.3720
O	 0.5660	 0.2520
P	 0.5630	 0.3620
Q	 0.6790	 0.3820
R	 0.5830	 0.3690
S	 0.5990	 0.3980
T	 0.6140	 0.3620
U	 0.6310	 0.3460
V	 0.5160	 0.2910
W	 0.5210	 0.3400
X	 0.5820	 0.3750
Y	 0.6100	 0.3110
Z	 0.5930	 0.3800

