



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 01:34 pm BST

PDB ID : 9GHD / pdb_00009ghd
EMDB ID : EMD-51353
Title : Escherichia coli 70S ribosome in complex with Staphylococcus aureus FusB-EF-G (FusB-EF-G-70S*)
Authors : Gonzalez-Lopez, A.; Selmer, M.
Deposited on : 2024-08-15
Resolution : 2.41 Å (reported)
Based on initial models : 9GHE, 8P2H

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:

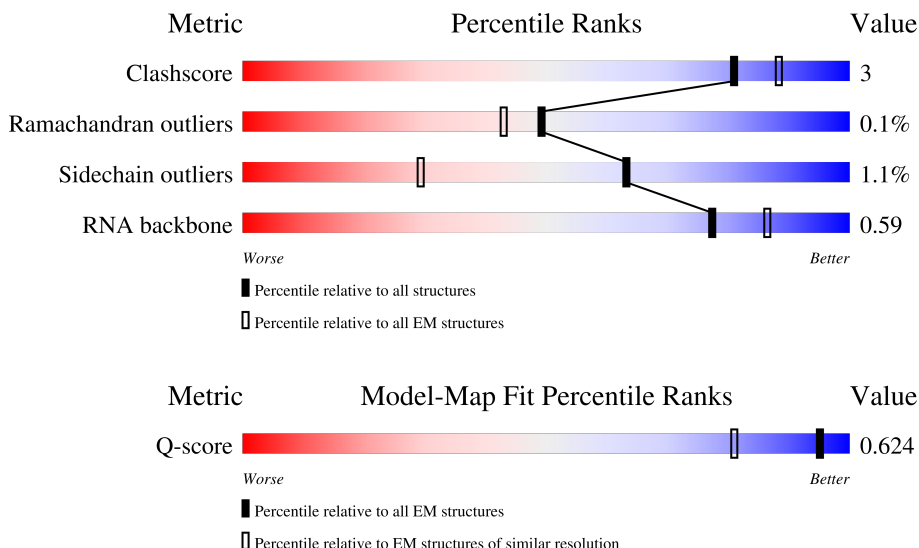
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 2.41 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5662 (1.92 - 2.91)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	0	55	
2	1	46	
3	2	65	

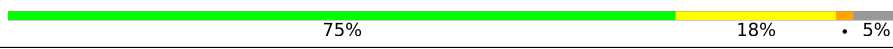
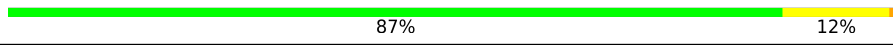
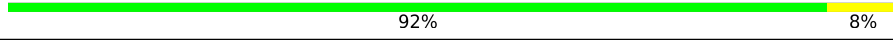
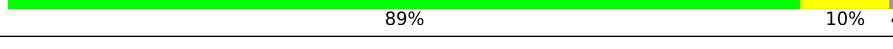
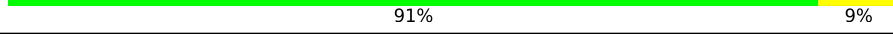
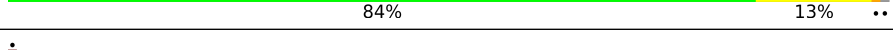
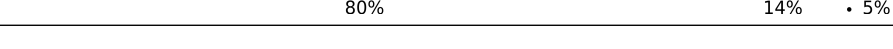
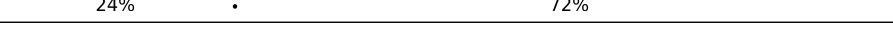
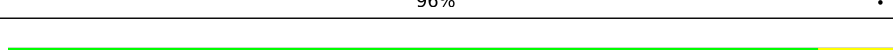
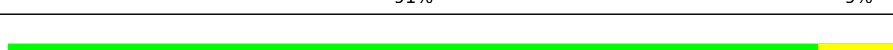
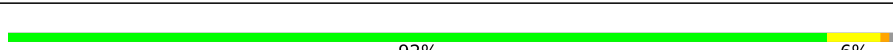
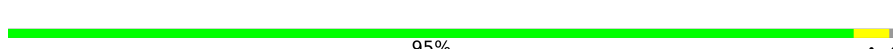
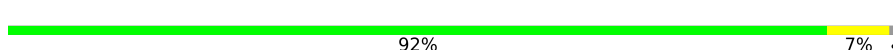
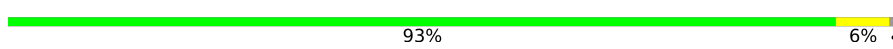
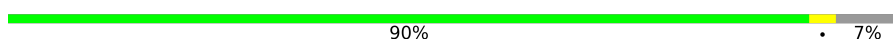
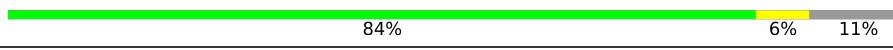
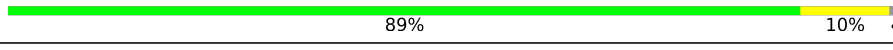
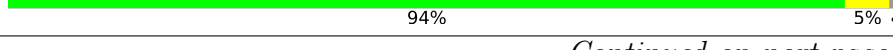
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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	9	24	
7	A	1554	
8	B	241	
9	C	233	
10	D	206	
11	E	167	
12	F	135	
13	G	179	
14	H	130	
15	I	130	
16	J	103	
17	K	129	
18	L	124	
19	M	118	
20	N	101	
21	O	89	
22	P	82	
23	Q	84	
24	R	75	
25	S	92	
26	T	87	
27	U	71	
28	V	213	

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Mol	Chain	Length	Quality of chain
29	W	693	
30	Z	77	
31	a	2930	
32	b	119	
33	c	273	
34	d	209	
35	e	201	
36	f	179	
37	g	177	
38	h	149	
39	i	142	
40	j	123	
41	k	144	
42	l	136	
43	m	127	
44	n	117	
45	o	115	
46	p	118	
47	q	103	
48	r	110	
49	s	100	
50	t	104	
51	u	94	
52	v	85	
53	w	78	

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Mol	Chain	Length	Quality of chain
54	x	63	89% 6%5%
55	y	59	93% 5%•
56	z	57	89% 5%5%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 143666 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 Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	50	Total	C	N	O	0	0
			413	267	75	71		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

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

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

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

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

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	7	Total	C	N	O	P	0	0
			154	69	32	46	7		

- Molecule 7 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1514	Total	C	N	O	P	0	0
			32500	14503	5963	10520	1514		

- Molecule 8 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	222	Total	C	N	O	S	0	0
			1737	1099	312	318	8		

- Molecule 9 is a protein called 30S ribosomal protein S3.

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

- Molecule 10 is a protein called 30S ribosomal protein S4.

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

- Molecule 11 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	154	Total	C	N	O	S	0	0
			1135	706	215	208	6		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	150	Total	C	N	O	S	0	0
			1176	732	226	214	4		

- Molecule 14 is a protein called 30S ribosomal protein S8.

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

- Molecule 15 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	125	Total	C	N	O	S	0	0
			1001	622	200	176	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	96	Total	C	N	O	S	0	0
			775	487	148	139	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 19 is a protein called 30S ribosomal protein S13.

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

- Molecule 20 is a protein called 30S ribosomal protein S14.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	79	Total	C	N	O	S	0	0
			629	394	124	110	1		

- Molecule 23 is a protein called 30S ribosomal protein S17.

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

- Molecule 24 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	64	Total	C	N	O	S	0	0
			524	330	99	94	1		

- Molecule 25 is a protein called 30S ribosomal protein S19.

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

- Molecule 26 is a protein called 30S ribosomal protein S20.

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

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 28 is a protein called Far1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	212	Total	C	N	O	S	0	0
			1765	1139	290	328	8		

- Molecule 29 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	214	Total	C	N	O	S	0	0
			1647	1035	277	323	12		

- Molecule 30 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	2782	Total	C	N	O	P	0	0
			59756	26665	11017	19292	2782		

- Molecule 32 is a RNA chain called 5S rRNA.

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

- Molecule 33 is a protein called 50S ribosomal protein L2.

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

- Molecule 34 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1552	972	286	291	3		

- Molecule 35 is a protein called 50S ribosomal protein L4.

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	168	Total	C	N	O	S	0	0
			1255	791	228	234	2		

- Molecule 38 is a protein called 50S ribosomal protein L9.

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

- Molecule 39 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	141	Total	C	N	O	S	0	0
			1121	709	211	198	3		

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL16.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

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

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	93	Total	C	N	O	S	0	0
			717	452	135	130			

- Molecule 51 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

- Molecule 52 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 53 is a protein called 50S ribosomal protein L28.

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

- Molecule 54 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 55 is a protein called 50S ribosomal protein L30.

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

- Molecule 56 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	A	31	Total	K	0
			31	31	
58	F	1	Total	K	0
			1	1	
58	M	1	Total	K	0
			1	1	
58	a	76	Total	K	0
			76	76	
58	c	2	Total	K	0
			2	2	
58	e	1	Total	K	0
			1	1	

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	A	55	Total 55	Mg 55	0
59	a	240	Total 240	Mg 240	0
59	b	3	Total 3	Mg 3	0
59	c	2	Total 2	Mg 2	0
59	d	1	Total 1	Mg 1	0
59	p	1	Total 1	Mg 1	0
59	z	1	Total 1	Mg 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: Large ribosomal subunit protein bL33

Chain 0:  84% 7% 9%



- Molecule 2: Large ribosomal subunit protein bL34

Chain 1:  93% . .



- Molecule 3: 50S ribosomal protein L35

Chain 2:  89% 9% .



- Molecule 4: 50S ribosomal protein L36

Chain 3:  92% 8%



- Molecule 5: 50S ribosomal protein L31

Chain 4:  71% 14% 14%



- Molecule 6: mRNA

Chain 9:  25% 71%

G
G
C
A
A
A
G
G
A
G
U
U
A
A
G
G
A
A
A
A
A
A

• Molecule 7: 16S rRNA

Chain A:  73% 22%

A
A2
A3
U4
U5
G6
A7
A8
G9
U12
U17
C18
G22
G31
A32
G39
C47
C48
U49
A50
A51
C52
U56
G57
G69
U70
A71
A72
C73
A74
G75
G76
A81
G82
C83
U84
U85
G86
C87
U88
G94
C95
U96
A119
A120
U121
G122
U123

G128
A129
A130
A131
G144
A151
A152
G158
G159
U17
C18
G164
C169
U170
A171
A172
A182
C183
C188
A189
A195
A196
A197
G198
A199
G202
G
A
C
C
U
C
C
G
G
C
C215
C225
G226
G240
U245
A246
G247
G251
C264
G265

G266
C267
U268
C269
A270
G289
U294
G299
A300
G305
C312
A320
A321
C328
A329
C330
G337
A338
G347
C352
A353
G354
G360
G361
G362
U367
C372
G376
C381
A382
A383
U398
G404
U405
G406
U407
A408
U409
G410
A411
A412
G413
A414

C417
U420
C422
G423
G424
U426
U429
A430
U438
U439
A451
A452
G457
U458
A459
A465
A466
A468
C469
G481
A482
C483
G484
U485
U486
A487
C488
C492
A493
G494
A499
G500
U508
A509
A510
C511
U516
G517
C518
G521
G527
G530

U531
A532
C536
G542
A547
C555
A559
U562
G567
G568
A572
A573
C576
A579
U590
U591
A595
A596
U610
U632
G633
U641
A642
G650
G654
U662
A663
G664
A665
U672
A673
G674
U677
G688
A702
G713

G714
A715
A718
U723
G724
A728
A729
G734
G741
G742
U751
G752
G755
G769
A777
A790
G791
A792
U793
A794
A815
A816
C817
C823
G832
C839
C
U
U
G
A
G
G847
C848
G849
A860
G861
G867
A873
G874
U884

G887
G890
A913
A914
U920
U921
G926
C934
A946
G947
U960
U961
A969
G975
G976
A977
C979
C984
U991
U992
G993
A994
C999
A1000
A1004
A1005
G1006
G1020
C1027
C1028
U1029
U1030
C1031
G1032
G1033
G1034
A1035
A1036
C1037
C1038
G1039
A1042

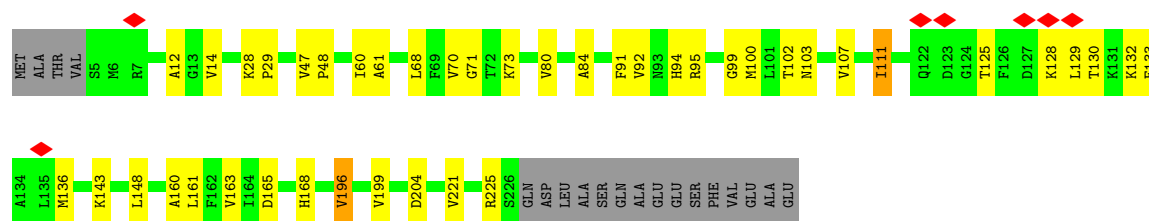
G1043
A1044
C1045
A1046
G1047
U1062
C1063
U1065
U1070
C1071
G1072
U1073
U1085
U1086
G1094
U1095
G1099
A1101
A1102
G1124
U1125
C1129
C1137
G1138
G1139
A1145
A1146
A1169
A1170
A1179
A1180
A1196
A1197
U1211
U1212
A1213
G1214
G1215
A1216
G1217
C1218
A1219
A1225
C1226

A1227
C1228
A1238
G1255
A1256
A1257
G1258
C1259
G1260
C1273
A1274
A1275
G1276
A1280
U1286
A1287
A1288
A1289
G1290
U1298
A1299
G1300
U1301
C1302
G1305
G1309
G1312
C1317
A1318
C1320
G1323
A1324
C1325
C1328
A1329
U1330
G1331
G1338
A1339
A1346
G1353
A1354
C
U

C
C
U
U
A
C
C
U
U
A
A
A
G
A
A
G
C

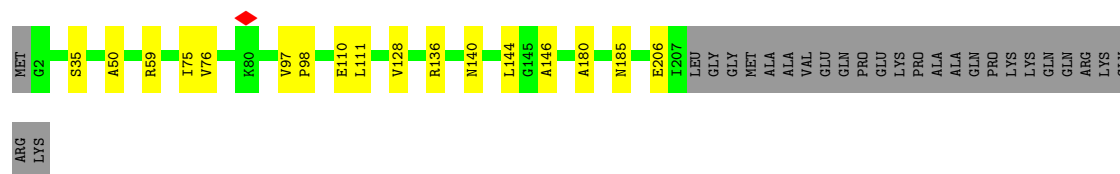
• Molecule 8: 30S ribosomal protein S2

Chain B:  74% 17% 8%



• Molecule 9: 30S ribosomal protein S3

Chain C: 81% 7% 12%



• Molecule 10: 30S ribosomal protein S4

Chain D: 86% 13%



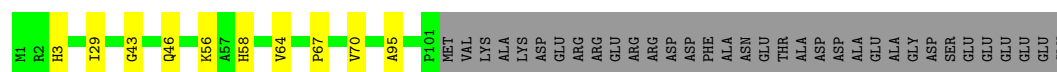
• Molecule 11: 30S ribosomal protein S5

Chain E: 78% 12% 8%



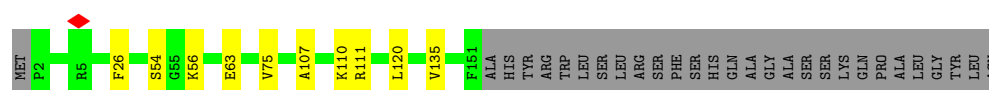
• Molecule 12: 30S ribosomal protein S6

Chain F: 67% 7% 25%



• Molecule 13: 30S ribosomal protein S7

Chain G: 78% 6% 16%

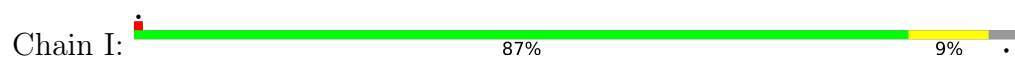


• Molecule 14: 30S ribosomal protein S8

Chain H: 97%



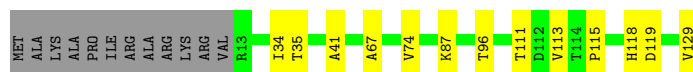
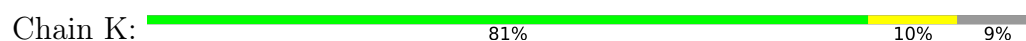
- Molecule 15: 30S ribosomal protein S9



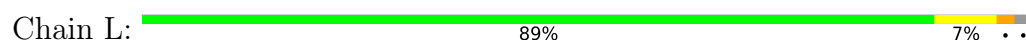
- Molecule 16: 30S ribosomal protein S10



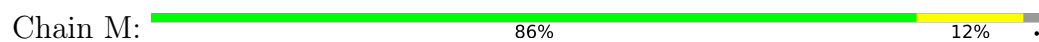
- Molecule 17: Small ribosomal subunit protein uS11



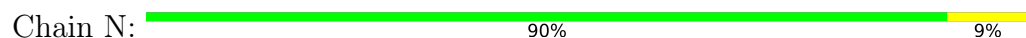
- Molecule 18: 30S ribosomal protein S12



- Molecule 19: 30S ribosomal protein S13



- Molecule 20: 30S ribosomal protein S14



- Molecule 21: Small ribosomal subunit protein uS15





- Molecule 22: 30S ribosomal protein S16

Chain P: 88% 9% .



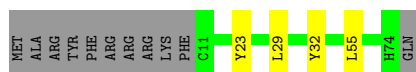
- Molecule 23: 30S ribosomal protein S17

Chain Q: 76% 17% . 6%



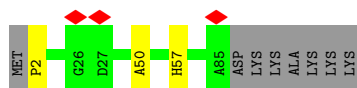
- Molecule 24: 30S ribosomal protein S18

Chain R: 80% 5% 15%



- Molecule 25: 30S ribosomal protein S19

Chain S: 88% . 9%



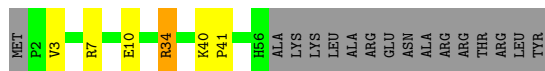
- Molecule 26: 30S ribosomal protein S20

Chain T: 91% 8% .



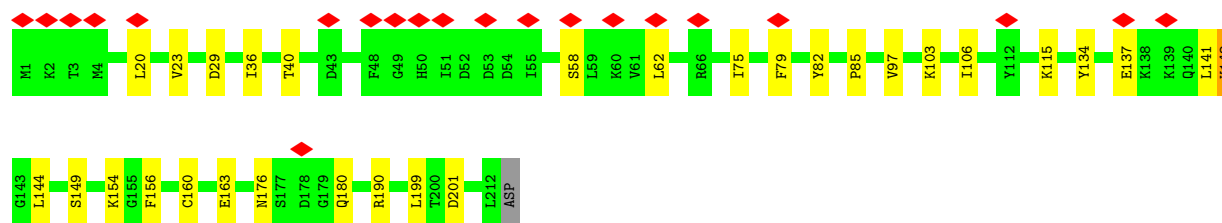
- Molecule 27: 30S ribosomal protein S21

Chain U: 69% 7% . 23%

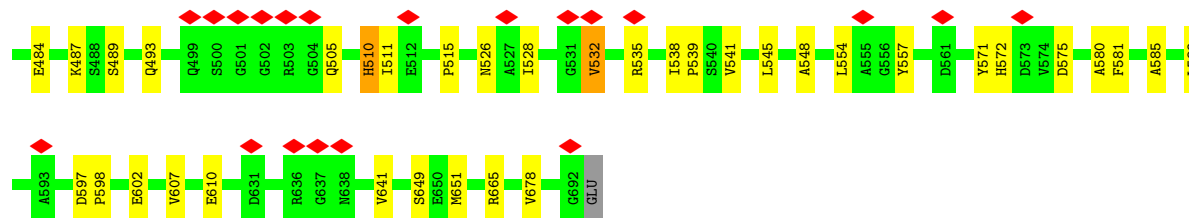
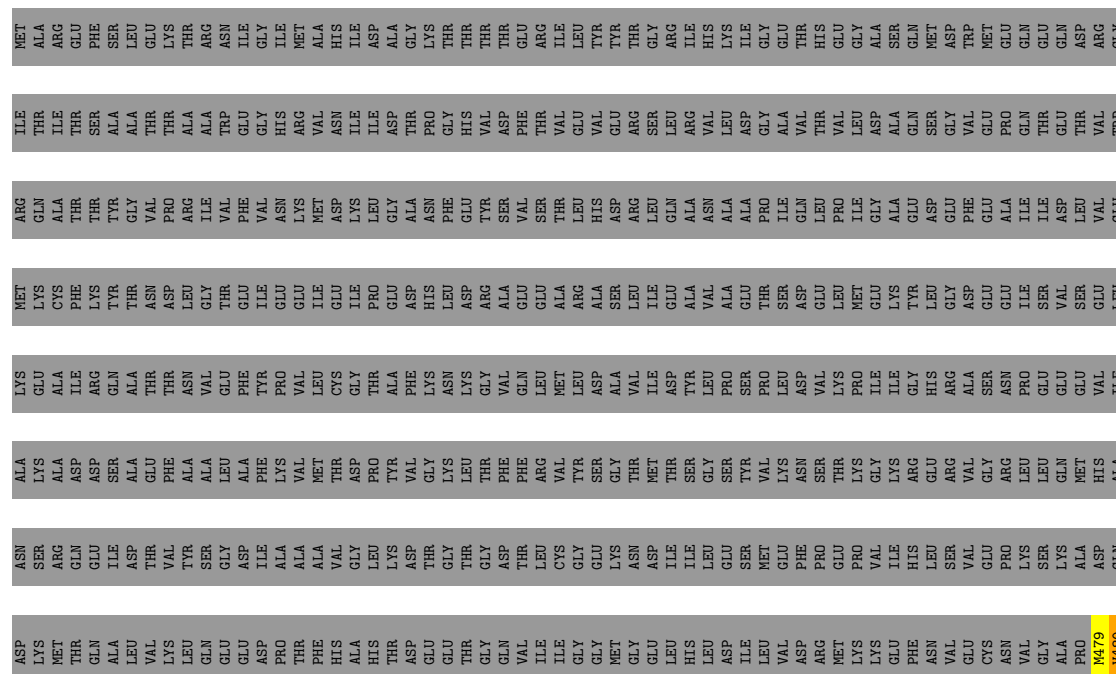


- Molecule 28: Far1

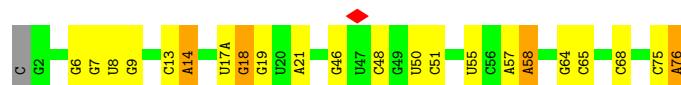
Chain V: 10% 85% 14%



• Molecule 29: Elongation factor G



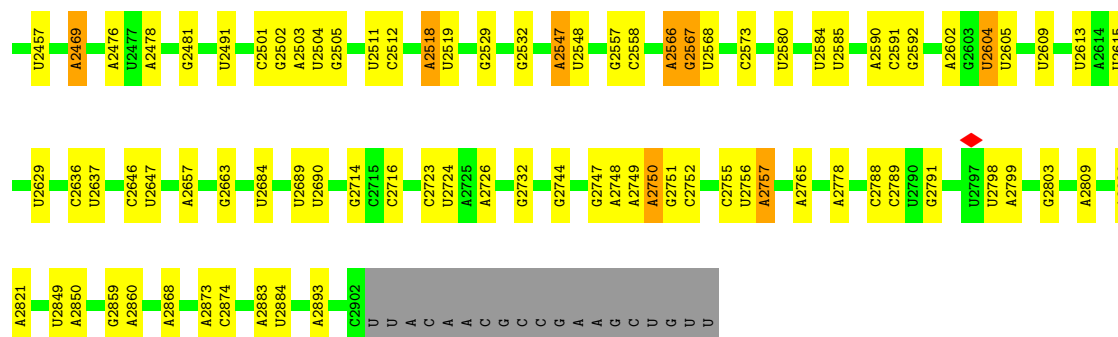
• Molecule 30: tRNA



• Molecule 31: 23S rRNA







• Molecule 32: 5S rRNA

Chain b: 87% 12% .



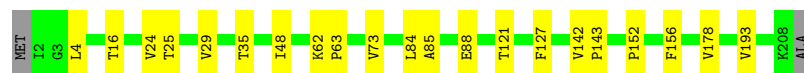
• Molecule 33: 50S ribosomal protein L2

Chain c: 92% 8% .



• Molecule 34: 50S ribosomal protein L3

Chain d: 89% 10% .



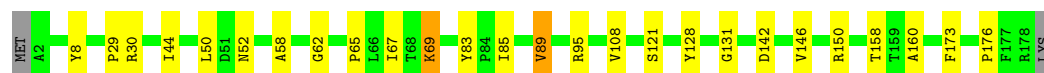
• Molecule 35: 50S ribosomal protein L4

Chain e: 91% 9%



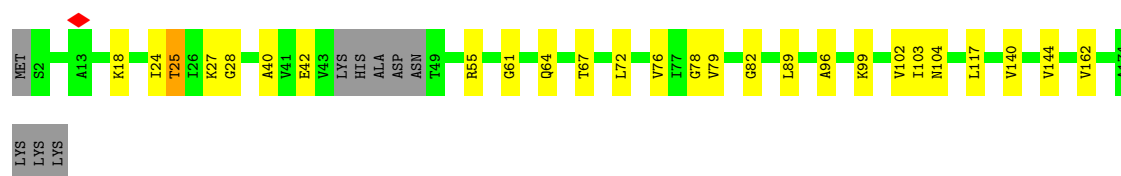
• Molecule 36: 50S ribosomal protein L5

Chain f: 84% 13% ..

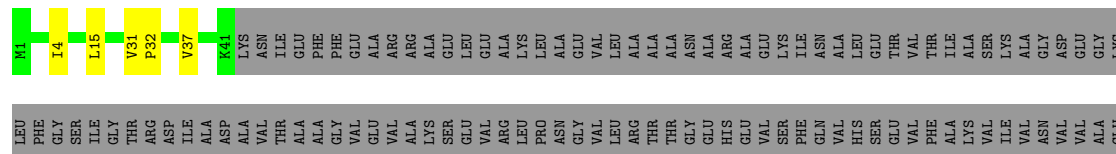


• Molecule 37: 50S ribosomal protein L6

Chain g: 80% 14% . 5%



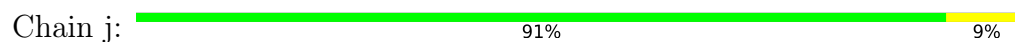
- Molecule 38: 50S ribosomal protein L9



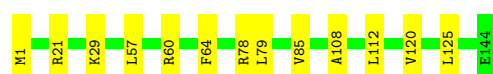
- Molecule 39: 50S ribosomal protein L13



- Molecule 40: 50S ribosomal protein L14



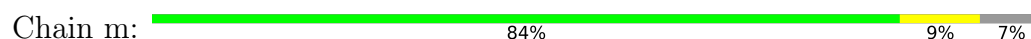
- Molecule 41: 50S ribosomal protein L15



- Molecule 42: Large ribosomal subunit protein uL16



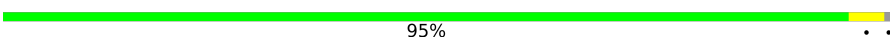
- Molecule 43: 50S ribosomal protein L17



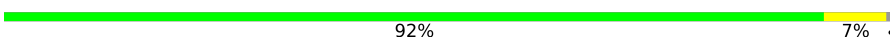
• Molecule 44: 50S ribosomal protein L18

Chain n:  92% 6% ..

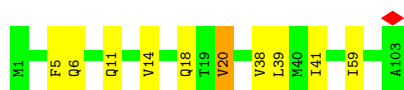
• Molecule 45: 50S ribosomal protein L19

Chain o:  95% ..

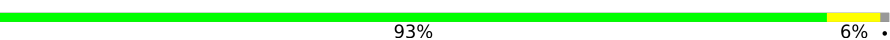
• Molecule 46: 50S ribosomal protein L20

Chain p:  92% 7% ..

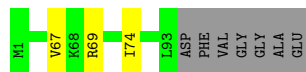
• Molecule 47: 50S ribosomal protein L21

Chain q:  90% 9% ..

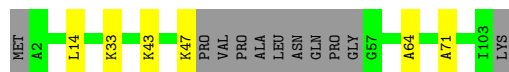
• Molecule 48: 50S ribosomal protein L22

Chain r:  93% 6% ..

• Molecule 49: 50S ribosomal protein L23

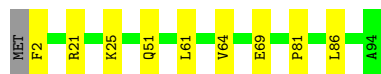
Chain s:  90% 7% ..

• Molecule 50: 50S ribosomal protein L24

Chain t:  84% 6% 11%

- Molecule 51: 50S ribosomal protein L25

Chain u:  89% 10%

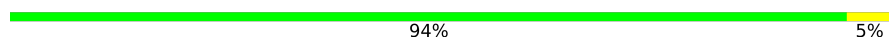


- Molecule 52: Large ribosomal subunit protein bL27

Chain v:  80% 8% 12%



- Molecule 53: 50S ribosomal protein L28

Chain w:  94% 5%

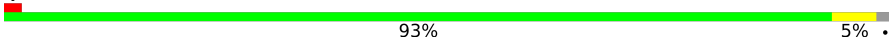


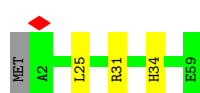
- Molecule 54: 50S ribosomal protein L29

Chain x:  89% 6% 5%



- Molecule 55: 50S ribosomal protein L30

Chain y:  93% 5%



- Molecule 56: 50S ribosomal protein L32

Chain z:  89% 5% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30847	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.47	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.843	Depositor
Minimum map value	-0.416	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	388.68002, 388.68002, 388.68002	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6478, 0.6478, 0.6478	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, 3TD, D2T, OMG, 4OC, 6MZ, 2MA, 1MG, OMU, OMC, MA6, 4D4, ZN, MG, IAS, 2MG, G7M, PSU, 5MU, K, MS6, 5MC, MEQ, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.46	0/420	0.84	0/560
2	1	0.48	0/370	0.87	0/487
3	2	0.49	0/513	0.86	0/676
4	3	0.48	0/303	0.74	0/397
5	4	0.48	0/488	0.87	0/649
6	9	0.55	0/173	0.74	0/268
7	A	0.52	1/36110 (0.0%)	0.77	1/56322 (0.0%)
8	B	0.46	0/1768	0.93	0/2381
9	C	0.46	0/1651	0.82	0/2225
10	D	0.44	0/1665	0.89	0/2227
11	E	0.48	0/1148	0.82	0/1545
12	F	0.45	0/843	0.79	0/1140
13	G	0.46	0/1190	0.89	0/1595
14	H	0.47	0/989	0.84	0/1326
15	I	0.45	0/1013	0.85	0/1350
16	J	0.47	0/784	0.84	0/1059
17	K	0.51	0/884	0.82	0/1191
18	L	0.47	0/945	0.80	0/1268
19	M	0.47	0/900	0.91	0/1204
20	N	0.47	0/817	0.88	0/1088
21	O	0.44	0/722	0.92	0/964
22	P	0.45	0/639	0.82	0/859
23	Q	0.46	0/650	0.77	0/871
24	R	0.45	0/532	0.93	0/715
25	S	0.49	0/685	0.86	0/922
26	T	0.46	0/676	0.93	0/895
27	U	0.47	0/467	0.91	0/620
28	V	0.43	0/1798	0.86	0/2415
29	W	0.47	0/1679	0.85	0/2261
30	Z	0.55	0/1813	0.75	0/2825
31	a	0.51	0/66355	0.78	4/103511 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.53	0/2850	0.77	1/4444 (0.0%)
33	c	0.48	0/2121	0.80	0/2852
34	d	0.46	0/1562	0.78	0/2102
35	e	0.45	0/1571	0.85	0/2113
36	f	0.45	0/1434	0.88	0/1926
37	g	0.47	0/1273	0.83	0/1725
38	h	0.47	0/306	0.81	0/413
39	i	0.45	0/1144	0.83	0/1541
40	j	0.45	0/955	0.79	0/1279
41	k	0.47	0/1062	0.83	0/1413
42	l	0.46	0/1073	0.81	0/1433
43	m	0.46	0/958	0.86	0/1281
44	n	0.46	0/902	0.87	0/1209
45	o	0.46	0/929	0.74	0/1242
46	p	0.45	0/960	0.89	0/1278
47	q	0.45	0/829	0.71	0/1107
48	r	0.46	0/852	0.83	0/1142
49	s	0.45	0/744	0.81	0/994
50	t	0.46	0/721	0.79	0/956
51	u	0.46	0/758	0.80	0/1015
52	v	0.47	0/576	0.74	0/762
53	w	0.46	0/635	0.81	0/848
54	x	0.41	0/492	0.90	0/655
55	y	0.46	0/453	0.83	0/605
56	z	0.47	0/435	0.85	0/581
All	All	0.50	1/154585 (0.0%)	0.80	6/230732 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	3	0	1
10	D	0	1
16	J	0	1
17	K	0	1
27	U	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	527	G7M	O3'-P	5.11	1.61	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	2501	C	O3'-P-O5'	-6.13	94.81	104.00
31	a	781	A	O3'-P-O5'	-5.86	95.21	104.00
31	a	2519	U	O3'-P-O5'	-5.30	96.05	104.00
31	a	1905	C	O3'-P-O5'	-5.20	96.20	104.00
32	b	66	A	O3'-P-O5'	-5.10	96.34	104.00
7	A	1035	A	C2'-C3'-O3'	5.07	117.10	109.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	36	ARG	Sidechain
10	D	184	ARG	Sidechain
16	J	38	GLY	Peptide
17	K	118	HIS	Peptide
27	U	34	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	413	0	448	3	0
2	1	367	0	405	2	0
3	2	504	0	572	4	0
4	3	302	0	340	1	0
5	4	480	0	478	6	0
6	9	154	0	77	0	0
7	A	32500	0	16367	131	0
8	B	1737	0	1763	21	0
9	C	1624	0	1696	9	0
10	D	1643	0	1707	18	0
11	E	1135	0	1179	15	0
12	F	824	0	815	5	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	G	1176	0	1233	4	0
14	H	979	0	1031	2	0
15	I	1001	0	1044	7	0
16	J	775	0	817	13	0
17	K	877	0	883	7	0
18	L	942	0	999	6	0
19	M	891	0	952	9	0
20	N	805	0	844	6	0
21	O	714	0	734	0	0
22	P	629	0	643	4	0
23	Q	641	0	682	9	0
24	R	524	0	543	2	0
25	S	668	0	693	2	0
26	T	670	0	719	5	0
27	U	460	0	486	4	0
28	V	1765	0	1803	17	0
29	W	1647	0	1608	24	0
30	Z	1623	0	825	4	0
31	a	59756	0	30054	177	0
32	b	2549	0	1291	7	0
33	c	2082	0	2153	12	0
34	d	1552	0	1601	11	0
35	e	1552	0	1619	10	0
36	f	1410	0	1444	16	0
37	g	1255	0	1296	12	0
38	h	303	0	327	1	0
39	i	1121	0	1150	2	0
40	j	946	0	1023	8	0
41	k	1053	0	1129	9	0
42	l	1075	0	1145	7	0
43	m	945	0	989	6	0
44	n	892	0	923	4	0
45	o	917	0	962	3	0
46	p	947	0	1019	6	0
47	q	816	0	839	5	0
48	r	845	0	909	4	0
49	s	738	0	807	3	0
50	t	717	0	766	4	0
51	u	745	0	768	5	0
52	v	569	0	581	4	0
53	w	625	0	652	2	0
54	x	491	0	523	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	y	449	0	488	2	0
56	z	429	0	440	2	0
57	3	1	0	0	0	0
57	4	1	0	0	0	0
58	A	31	0	0	0	0
58	F	1	0	0	0	0
58	M	1	0	0	0	0
58	a	76	0	0	0	0
58	c	2	0	0	0	0
58	e	1	0	0	0	0
59	A	55	0	0	0	0
59	a	240	0	0	0	0
59	b	3	0	0	0	0
59	c	2	0	0	0	0
59	d	1	0	0	0	0
59	p	1	0	0	0	0
59	z	1	0	0	0	0
All	All	143666	0	97284	605	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 3.

All (605) 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)
7:A:1035:A:O2'	7:A:1036:A:H5''	1.44	1.17
11:E:77:ASN:O	11:E:80:THR:HG22	1.83	0.78
36:f:108:VAL:HG11	36:f:176:PRO:HG3	1.66	0.76
47:q:6:GLN:HG2	47:q:11:GLN:HG2	1.68	0.76
28:V:85:PRO:HA	28:V:115:LYS:HA	1.70	0.73
36:f:52:ASN:HB2	36:f:150:ARG:HH22	1.52	0.72
7:A:1035:A:O2'	7:A:1036:A:C5'	2.34	0.70
7:A:158:G:H2'	7:A:159:G:H5''	1.73	0.70
47:q:6:GLN:HG3	47:q:39:LEU:HD11	1.73	0.70
7:A:1169:A:H2'	7:A:1170:A:C8	2.26	0.69
31:a:568:U:H1'	31:a:2030:6MZ:H9C1	1.73	0.69
33:c:29:PRO:HG2	33:c:34:LEU:HD11	1.72	0.69
26:T:42:GLY:HA2	26:T:86:LEU:HD11	1.74	0.69
7:A:429:U:H3'	10:D:9:LEU:HD12	1.73	0.69
7:A:158:G:C2'	7:A:159:G:H5''	2.24	0.68
16:J:21:ALA:HB1	16:J:92:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:12:U:H2'	31:a:12:U:O2	1.94	0.67
7:A:225:C:H2'	7:A:226:G:H5''	1.78	0.66
30:Z:76:A:H2'	31:a:2451:A:H1'	1.75	0.66
7:A:84:U:H2'	7:A:86:G:H21	1.59	0.66
7:A:158:G:H2'	7:A:159:G:C5'	2.28	0.65
7:A:1286:U:H2'	7:A:1287:A:H4'	1.79	0.64
49:s:67:VAL:HG12	49:s:74:ILE:HD11	1.80	0.64
7:A:1036:A:H2'	7:A:1037:C:O4'	1.97	0.63
32:b:36:C:N4	32:b:49:C:O2	2.32	0.63
3:2:62:LEU:HB3	3:2:65:ALA:HB2	1.81	0.62
7:A:518:C:H2'	7:A:530:G:C8	2.34	0.62
1:0:22:THR:HG21	31:a:2419:U:H4'	1.81	0.62
7:A:1005:A:H5''	7:A:1038:C:H1'	1.81	0.62
19:M:11:ASP:HA	19:M:45:ILE:HB	1.82	0.61
31:a:644:A:H2'	31:a:645:C:O4'	2.01	0.61
18:L:4:VAL:HG23	23:Q:34:TYR:HB3	1.83	0.61
7:A:823:C:HO2'	14:H:2:SER:N	1.98	0.60
15:I:116:VAL:HG11	16:J:62:ARG:HG3	1.82	0.60
7:A:664:G:H22	7:A:741:G:H1	1.49	0.60
31:a:1853:A:N1	31:a:2087:G:H1'	2.17	0.60
31:a:2193:G:H2'	31:a:2194:U:O4'	2.01	0.59
33:c:232:HIS:HA	33:c:242:LYS:HD2	1.84	0.59
7:A:542:G:H5'	10:D:39:GLY:HA3	1.85	0.59
7:A:417:C:H42	7:A:426:U:H3	1.50	0.59
31:a:1056:G:H4'	31:a:1086:A:C8	2.38	0.59
31:a:546:U:H3'	31:a:547:A:H8	1.67	0.59
31:a:547:A:H1'	31:a:548:G:C5	2.37	0.59
7:A:769:G:H4'	7:A:1513:A:H4'	1.85	0.58
8:B:100:MET:HA	8:B:107:VAL:HG21	1.84	0.58
28:V:149:SER:O	28:V:190:ARG:NH1	2.37	0.58
10:D:9:LEU:HD13	10:D:32:CYS:HB3	1.85	0.58
42:l:17:ASN:O	42:l:38:ARG:HD3	2.04	0.58
3:2:54:ASP:HB3	41:k:57:LEU:HD22	1.86	0.57
11:E:56:VAL:N	11:E:57:PRO:HD2	2.19	0.57
29:W:554:LEU:HD21	29:W:598:PRO:HG2	1.86	0.57
7:A:946:A:H2'	7:A:947:G:C8	2.40	0.57
31:a:2305:U:H5''	36:f:131:GLY:HA3	1.86	0.57
45:o:100:LEU:HD11	45:o:110:ILE:HD11	1.87	0.57
31:a:910:A:H2'	31:a:911:A:C8	2.40	0.56
5:4:18:CYS:HB3	5:4:40:CYS:HB3	1.87	0.56
7:A:867:G:O2'	7:A:873:A:N1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:156:PHE:HA	28:V:163:GLU:HA	1.87	0.56
37:g:89:LEU:HD11	37:g:96:ALA:HB2	1.87	0.56
9:C:111:LEU:HD22	9:C:146:ALA:HB2	1.87	0.56
28:V:29:ASP:HB2	29:W:665:ARG:HG3	1.87	0.56
8:B:125:THR:HA	8:B:128:LYS:HD3	1.88	0.56
37:g:24:ILE:HG21	37:g:72:LEU:HD21	1.88	0.56
7:A:509:A:H2'	7:A:510:A:C8	2.41	0.56
31:a:1079:C:H3'	31:a:1080:A:H8	1.70	0.56
15:I:118:LEU:HD22	15:I:124:ARG:HG2	1.89	0.55
54:x:9:LYS:O	54:x:60:LYS:NZ	2.39	0.55
5:4:42:PRO:HB2	5:4:48:GLN:HG3	1.88	0.55
47:q:5:PHE:HB3	47:q:59:ILE:HD12	1.89	0.55
7:A:1518:MA6:H103	7:A:1519:MA6:H102	1.88	0.55
28:V:29:ASP:CB	29:W:665:ARG:HG3	2.35	0.55
17:K:111:THR:HG23	27:U:3:VAL:HG22	1.87	0.55
5:4:11:GLU:HA	5:4:25:ARG:HA	1.88	0.55
31:a:494:G:H4'	48:r:6:LYS:HB2	1.89	0.55
7:A:673:A:H2'	7:A:674:G:C8	2.42	0.55
43:m:117:ASP:O	43:m:118:ARG:C	2.50	0.55
14:H:11:LEU:HD22	14:H:75:ILE:HD11	1.88	0.54
24:R:32:TYR:HB3	24:R:55:LEU:HD21	1.89	0.54
48:r:28:LYS:HB2	48:r:31:GLN:HG2	1.88	0.54
19:M:33:ILE:HG23	19:M:59:GLU:HB2	1.89	0.54
7:A:1273:C:H2'	7:A:1274:A:O4'	2.08	0.54
33:c:107:PRO:HD2	33:c:110:LEU:HD22	1.89	0.54
7:A:320:A:H2'	7:A:321:A:O4'	2.08	0.54
31:a:1778:U:H2'	31:a:1784:A:N6	2.23	0.54
11:E:115:LEU:HD13	11:E:123:VAL:HG11	1.89	0.54
18:L:110:ARG:HB3	18:L:119:VAL:HG21	1.90	0.54
50:t:33:LYS:HB3	50:t:64:ALA:HB1	1.90	0.54
31:a:2684:U:H4'	40:j:76:VAL:CG2	2.38	0.54
33:c:5:LYS:HD2	33:c:17:VAL:HG22	1.90	0.54
34:d:35:THR:HG22	34:d:73:VAL:HG21	1.90	0.54
29:W:528:ILE:HG23	29:W:532:VAL:HG23	1.88	0.53
18:L:43:LYS:HG2	18:L:89:D2T:H4	1.89	0.53
31:a:476:G:H4'	31:a:502:A:N1	2.24	0.53
16:J:92:LEU:HD12	16:J:98:VAL:HG22	1.91	0.52
31:a:1980:G:O2'	31:a:1982:U:OP2	2.26	0.52
16:J:37:ARG:HB2	16:J:75:ASP:HB2	1.91	0.52
1:0:10:LYS:HG3	1:0:54:ILE:HA	1.92	0.52
7:A:1287:A:H2'	7:A:1288:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:480:VAL:HG21	29:W:649:SER:HB3	1.92	0.52
7:A:159:G:H5'	7:A:159:G:H8	1.74	0.52
17:K:67:ALA:HB2	17:K:96:THR:HG23	1.90	0.52
31:a:811:U:H2'	41:k:21:ARG:HA	1.92	0.52
10:D:99:ASP:OD2	10:D:115:ARG:HA	2.10	0.52
31:a:930:G:H1'	55:y:25:LEU:HD11	1.91	0.52
7:A:299:G:H2'	7:A:300:A:C8	2.46	0.52
7:A:458:U:H2'	7:A:459:A:C8	2.44	0.52
31:a:1105:U:H2'	31:a:1106:G:C8	2.45	0.52
5:4:9:TYR:CE2	5:4:25:ARG:HB3	2.45	0.51
31:a:2859:G:H2'	31:a:2860:A:C8	2.45	0.51
37:g:89:LEU:HD22	37:g:162:VAL:HG22	1.90	0.51
10:D:172:GLU:HG3	10:D:183:LYS:HD2	1.92	0.51
31:a:1105:U:H2'	31:a:1106:G:H8	1.75	0.51
34:d:152:PRO:HG3	34:d:156:PHE:CZ	2.45	0.51
10:D:145:ILE:HG23	10:D:150:LYS:HG2	1.92	0.51
31:a:274:C:H2'	31:a:275:C:O4'	2.10	0.51
31:a:2038:G:H2'	31:a:2039:U:O4'	2.10	0.51
37:g:18:LYS:HB3	37:g:25:THR:HG23	1.92	0.51
13:G:54:SER:HB3	13:G:56:LYS:HE2	1.92	0.51
37:g:40:ALA:HB1	37:g:61:GLY:HA2	1.92	0.51
7:A:404:G:N7	10:D:2:ALA:HB3	2.25	0.51
11:E:38:VAL:HG11	11:E:114:VAL:HG22	1.93	0.51
26:T:86:LEU:O	26:T:87:ALA:C	2.53	0.51
31:a:1434:A:H2'	31:a:1435:G:C8	2.46	0.51
43:m:38:LEU:N	43:m:39:PRO:HD2	2.26	0.51
31:a:2328:A:H2'	31:a:2329:U:C6	2.46	0.51
31:a:2346:A:H3'	31:a:2347:C:H5''	1.93	0.51
10:D:102:VAL:HG13	10:D:107:PHE:HB2	1.94	0.50
26:T:39:ILE:HA	26:T:86:LEU:HD22	1.93	0.50
29:W:548:ALA:HB3	29:W:589:LEU:HD23	1.93	0.50
40:j:70:ARG:HD2	40:j:76:VAL:HG22	1.93	0.50
11:E:77:ASN:C	11:E:77:ASN:HD22	2.18	0.50
11:E:81:LEU:HB3	11:E:147:MET:SD	2.52	0.50
32:b:29:A:H2'	32:b:30:C:O4'	2.11	0.50
31:a:1881:C:H2'	31:a:1882:U:O4'	2.11	0.50
8:B:71:GLY:HA3	8:B:80:VAL:HG21	1.93	0.50
15:I:52:LEU:HD11	15:I:63:LEU:HD11	1.94	0.50
23:Q:21:ILE:HG13	23:Q:46:VAL:HB	1.94	0.50
29:W:487:LYS:HB2	29:W:597:ASP:O	2.12	0.50
30:Z:13:C:H2'	30:Z:14:A:H5''	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:2273:A:H2'	31:a:2274:A:C8	2.47	0.50
31:a:2312:U:H5'	36:f:85:ILE:HD11	1.94	0.50
7:A:195:A:H2'	7:A:196:A:C8	2.47	0.50
31:a:1720:U:H2'	31:a:1721:G:O4'	2.12	0.50
46:p:69:ALA:HB1	46:p:74:ILE:HG23	1.94	0.50
7:A:481:G:O2'	7:A:483:C:N4	2.41	0.50
7:A:977:A:O2'	7:A:979:C:OP2	2.29	0.49
31:a:191:A:H2'	31:a:192:C:C6	2.47	0.49
31:a:2327:A:H2'	31:a:2328:A:C8	2.47	0.49
7:A:1412:C:H2'	7:A:1413:A:C8	2.47	0.49
11:E:66:LYS:O	11:E:70:ASN:ND2	2.45	0.49
31:a:1028:A:N6	31:a:1125:G:H2'	2.28	0.49
7:A:1391:U:H2'	7:A:1392:G:C8	2.47	0.49
9:C:50:ALA:HA	9:C:75:ILE:HD11	1.95	0.49
31:a:2788:C:H2'	31:a:2789:C:C6	2.47	0.49
35:e:41:GLN:HG2	35:e:43:THR:HG23	1.95	0.49
7:A:50:A:O2'	7:A:360:G:N2	2.46	0.49
7:A:713:G:H2'	7:A:714:G:C8	2.47	0.49
28:V:79:PHE:HA	28:V:82:TYR:HD2	1.78	0.49
31:a:534:U:O2'	46:p:49:ASP:OD2	2.28	0.49
31:a:1028:A:H2'	31:a:1029:A:C8	2.47	0.49
7:A:382:A:H2'	7:A:383:A:C8	2.48	0.49
31:a:499:U:H5''	50:t:43:LYS:HE2	1.95	0.49
39:i:34:ARG:HG3	39:i:39:LYS:HB2	1.94	0.49
7:A:17:U:H2'	7:A:18:C:C6	2.48	0.49
7:A:381:C:H2'	7:A:382:A:O4'	2.13	0.49
31:a:2377:A:H2'	31:a:2378:A:C8	2.48	0.49
5:4:2:LYS:HE3	32:b:40:U:H2'	1.95	0.48
7:A:555:U:H2'	7:A:556:C:C6	2.48	0.48
28:V:20:LEU:HB2	28:V:40:THR:HG21	1.94	0.48
28:V:180:GLN:HA	29:W:526:ASN:HD22	1.78	0.48
31:a:849:A:H2'	31:a:850:U:C6	2.48	0.48
31:a:2684:U:H4'	40:j:76:VAL:HG21	1.94	0.48
34:d:62:LYS:N	34:d:63:PRO:HD2	2.28	0.48
43:m:28:LEU:HD23	43:m:48:VAL:HG21	1.93	0.48
7:A:1530:G:H2'	7:A:1531:A:C8	2.48	0.48
36:f:158:THR:HG22	36:f:160:ALA:H	1.78	0.48
25:S:50:ALA:HB1	25:S:57:HIS:HB3	1.94	0.48
24:R:23:TYR:HA	24:R:29:LEU:HD11	1.94	0.48
31:a:2469:A:H4'	42:l:55:ARG:CD	2.44	0.48
7:A:130:A:C8	23:Q:65:ARG:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:184:ARG:NH2	10:D:187:GLU:HG2	2.28	0.48
31:a:279:A:H2'	31:a:280:U:O4'	2.13	0.48
42:l:66:ARG:NH1	42:l:104:GLU:OE2	2.47	0.48
29:W:484:GLU:HG3	29:W:557:TYR:HB2	1.96	0.48
29:W:493:GLN:HA	29:W:510:HIS:HA	1.95	0.48
31:a:639:U:H2'	31:a:640:C:C6	2.49	0.48
31:a:1932:A:H2'	31:a:1933:G:O4'	2.13	0.48
31:a:2291:U:H2'	31:a:2292:U:C6	2.48	0.48
34:d:4:LEU:HD13	34:d:29:VAL:HG11	1.95	0.48
36:f:44:ILE:HA	36:f:83:TYR:CE2	2.49	0.48
7:A:1073:U:O2'	8:B:103:ASN:ND2	2.47	0.48
7:A:751:U:O2'	7:A:752:G:H5'	2.13	0.48
12:F:29:ILE:HD13	12:F:64:VAL:HG21	1.95	0.48
16:J:6:ILE:HG12	16:J:102:LEU:HG	1.96	0.48
13:G:107:ALA:O	13:G:111:ARG:HG3	2.14	0.47
16:J:86:ALA:HA	16:J:89:ARG:HE	1.79	0.47
39:i:110:PRO:O	39:i:115:GLY:HA3	2.14	0.47
42:l:20:LEU:HD13	51:u:81:PRO:HG2	1.96	0.47
9:C:35:SER:OG	9:C:59:ARG:NH2	2.47	0.47
31:a:1746:A:H2'	31:a:1747:U:C6	2.50	0.47
8:B:129:LEU:HB3	8:B:133:GLU:HB2	1.96	0.47
7:A:123:U:OP1	7:A:312:C:H5'	2.14	0.47
7:A:1323:G:H2'	7:A:1324:A:C8	2.49	0.47
35:e:48:THR:HG23	35:e:86:ALA:HB3	1.96	0.47
19:M:34:LEU:HD13	19:M:41:GLU:HA	1.97	0.47
29:W:610:GLU:HG3	29:W:641:VAL:HG22	1.96	0.47
31:a:207:A:H2'	31:a:208:C:O4'	2.14	0.47
31:a:1939:5MU:OP1	31:a:2604:PSU:O2'	2.32	0.47
51:u:64:VAL:HG22	51:u:69:GLU:HG2	1.96	0.47
5:4:28:VAL:HG21	5:4:32:LEU:HD21	1.97	0.47
8:B:130:THR:O	8:B:132:LYS:N	2.47	0.47
13:G:107:ALA:O	13:G:110:LYS:HG2	2.13	0.47
28:V:134:TYR:CE1	28:V:142:LYS:HB2	2.49	0.47
31:a:1418:G:H2'	31:a:1579:A:H62	1.80	0.47
37:g:64:GLN:O	37:g:67:THR:HG22	2.14	0.47
7:A:409:U:H5''	10:D:25:VAL:HG21	1.95	0.47
7:A:975:A:N1	7:A:1366:C:O2'	2.43	0.47
7:A:993:G:H2'	7:A:993:G:N3	2.29	0.47
7:A:1228:C:H1'	19:M:116:ILE:HD11	1.94	0.47
18:L:89:D2T:C	18:L:89:D2T:OD2	2.62	0.47
31:a:613:A:H2'	31:a:614:A:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:155:ALA:HB2	33:c:162:VAL:HG23	1.95	0.47
7:A:22:G:O2'	7:A:913:A:N1	2.45	0.47
31:a:609:A:H2'	31:a:610:C:O4'	2.14	0.47
11:E:77:ASN:C	11:E:77:ASN:ND2	2.73	0.47
19:M:40:ALA:HB3	19:M:43:VAL:HG23	1.96	0.47
29:W:602:GLU:HB3	29:W:678:VAL:HG22	1.97	0.47
31:a:221:A:N1	31:a:265:A:O2'	2.46	0.47
32:b:41:G:O6	36:f:69:LYS:HD2	2.15	0.47
29:W:489:SER:HB3	29:W:515:PRO:HD2	1.97	0.47
31:a:851:C:H2'	31:a:852:U:C6	2.50	0.47
7:A:632:U:H3'	7:A:633:G:H5'	1.96	0.46
7:A:1218:C:H2'	7:A:1219:A:C8	2.50	0.46
31:a:2584:U:H2'	31:a:2585:U:H2'	1.96	0.46
37:g:28:GLY:HA3	37:g:79:VAL:HB	1.97	0.46
7:A:492:C:H2'	7:A:493:A:C8	2.50	0.46
22:P:19:VAL:HG21	22:P:52:LEU:HD21	1.96	0.46
31:a:92:U:H2'	31:a:93:G:O4'	2.15	0.46
31:a:1094:U:H1'	31:a:1097:U:H5	1.80	0.46
31:a:1790:C:H2'	31:a:1791:A:C5	2.51	0.46
31:a:2747:G:O6	31:a:2755:C:H5''	2.14	0.46
43:m:24:MET:HE1	43:m:40:LYS:HD3	1.97	0.46
7:A:264:C:O2'	23:Q:66:PRO:O	2.31	0.46
15:I:41:ARG:HG2	15:I:41:ARG:HH11	1.81	0.46
17:K:87:LYS:HB2	17:K:113:VAL:HG23	1.98	0.46
31:a:547:A:H1'	31:a:548:G:C4	2.51	0.46
31:a:1469:A:H2'	31:a:1470:A:C8	2.50	0.46
31:a:1682:G:H2'	31:a:1683:U:C6	2.50	0.46
31:a:483:A:H5''	50:t:47:LYS:HD2	1.97	0.46
31:a:2646:C:H2'	31:a:2647:U:O4'	2.16	0.46
31:a:2850:A:N7	31:a:2868:A:O2'	2.43	0.46
36:f:50:LEU:HD11	36:f:67:ILE:HD12	1.97	0.46
38:h:31:VAL:N	38:h:32:PRO:HD2	2.31	0.46
31:a:1081:U:H2'	31:a:1082:U:C6	2.50	0.46
35:e:5:LEU:HD11	35:e:12:LEU:HB2	1.97	0.46
29:W:572:HIS:HB3	29:W:575:ASP:HB2	1.97	0.46
31:a:2395:C:H2'	31:a:2396:G:O4'	2.16	0.46
7:A:188:C:H2'	7:A:189:A:O4'	2.16	0.46
7:A:1005:A:C4	7:A:1006:G:H1'	2.51	0.46
31:a:353:C:C2'	31:a:354:A:H5'	2.46	0.46
32:b:90:C:H5'	42:l:17:ASN:O	2.16	0.46
7:A:1216:A:H5''	20:N:5:SER:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:124:MET:HE3	10:D:146:ARG:HG2	1.98	0.46
7:A:1275:A:H2'	7:A:1276:G:O4'	2.16	0.46
41:k:57:LEU:HA	41:k:60:ARG:HG2	1.97	0.46
7:A:151:A:OP2	7:A:169:C:N4	2.49	0.46
31:a:927:A:H2'	31:a:928:A:C8	2.51	0.46
37:g:78:GLY:HA2	37:g:82:GLY:HA2	1.98	0.46
8:B:196:VAL:HB	8:B:199:VAL:HG22	1.98	0.45
9:C:180:ALA:HA	9:C:206:GLU:HA	1.98	0.45
31:a:244:A:H2'	31:a:245:G:O4'	2.15	0.45
51:u:21:ARG:HA	51:u:25:LYS:O	2.16	0.45
7:A:790:A:H2'	7:A:791:G:C8	2.51	0.45
20:N:16:LEU:HD12	20:N:54:ASP:HB2	1.98	0.45
56:z:54:VAL:HG23	56:z:55:ILE:HG23	1.98	0.45
7:A:714:G:H2'	7:A:715:A:C8	2.51	0.45
37:g:103:ILE:HD11	37:g:117:LEU:HD21	1.98	0.45
47:q:14:VAL:HG11	47:q:20:VAL:HG21	1.99	0.45
51:u:51:GLN:HG2	51:u:86:LEU:HD11	1.98	0.45
55:y:31:ARG:HG2	55:y:34:HIS:HB2	1.98	0.45
16:J:66:GLU:HB3	20:N:99:ALA:HB2	1.98	0.45
31:a:813:U:H2'	31:a:814:C:C6	2.51	0.45
34:d:48:ILE:HG23	34:d:84:LEU:HD11	1.98	0.45
36:f:62:GLY:O	36:f:95:ARG:NH2	2.49	0.45
7:A:1289:A:H2'	7:A:1290:G:H5'	1.99	0.45
11:E:25:VAL:HG22	11:E:28:GLY:O	2.16	0.45
16:J:59:LYS:HE2	16:J:62:ARG:NH2	2.32	0.45
31:a:1808:A:H3'	31:a:1809:A:C8	2.51	0.45
31:a:819:A:C4	31:a:1189:A:C2	3.04	0.45
31:a:1248:G:OP1	35:e:44:ARG:NH2	2.49	0.45
7:A:920:U:H2'	7:A:921:U:C6	2.52	0.45
7:A:1101:A:H4'	7:A:1102:A:O5'	2.17	0.45
31:a:2014:A:H2'	31:a:2015:A:C8	2.52	0.45
43:m:67:PHE:O	43:m:71:ARG:N	2.48	0.45
7:A:1356:G:H2'	7:A:1357:A:C8	2.52	0.45
15:I:54:LEU:HD23	15:I:98:LEU:HD23	1.99	0.45
23:Q:25:ILE:HB	23:Q:42:THR:HG23	1.99	0.45
7:A:465:A:H2'	7:A:466:A:C8	2.52	0.45
7:A:1062:U:H2'	7:A:1063:C:C6	2.52	0.45
11:E:45:ARG:HG2	11:E:71:MET:HE2	1.99	0.45
29:W:538:ILE:HB	29:W:539:PRO:HD3	1.99	0.45
31:a:1079:C:H3'	31:a:1080:A:C8	2.51	0.45
7:A:860:A:H2'	7:A:861:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:18:G:H21	30:Z:58:A:H5'	1.82	0.44
3:2:47:LYS:HE3	41:k:64:PHE:CD1	2.53	0.44
9:C:110:GLU:HG2	9:C:140:ASN:HB3	1.98	0.44
31:a:1131:G:O2'	31:a:2026:U:H5'	2.15	0.44
31:a:1570:A:H2'	31:a:1571:A:C8	2.53	0.44
31:a:2547:A:H2'	31:a:2548:U:C6	2.53	0.44
10:D:129:VAL:HG21	10:D:146:ARG:HH21	1.81	0.44
28:V:176:ASN:OD1	28:V:180:GLN:N	2.49	0.44
31:a:478:A:N1	31:a:500:G:H4'	2.32	0.44
8:B:61:ALA:HB2	8:B:221:VAL:HG13	1.99	0.44
19:M:16:VAL:O	19:M:20:THR:HG23	2.17	0.44
31:a:784:G:H5'	31:a:785:G:OP1	2.17	0.44
31:a:1548:A:H2'	31:a:1549:A:C8	2.52	0.44
31:a:1827:U:OP2	33:c:221:ARG:HD2	2.18	0.44
7:A:56:U:H2'	7:A:57:G:C8	2.52	0.44
7:A:677:U:H3	7:A:713:G:H22	1.64	0.44
31:a:627:A:OP1	41:k:78:ARG:NH2	2.51	0.44
7:A:487:A:H2'	7:A:488:C:O4'	2.18	0.44
8:B:60:ILE:HD13	8:B:160:ALA:HB2	1.98	0.44
11:E:77:ASN:HD22	11:E:78:ASN:N	2.15	0.44
12:F:3:HIS:CD2	12:F:95:ALA:HB2	2.52	0.44
22:P:12:LYS:HG2	22:P:13:LYS:HG2	1.99	0.44
31:a:157:C:H2'	31:a:158:U:O4'	2.18	0.44
31:a:546:U:H3'	31:a:547:A:C8	2.51	0.44
31:a:723:C:H2'	31:a:724:U:O4'	2.18	0.44
31:a:1064:C:H2'	31:a:1065:U:O4'	2.18	0.44
31:a:2271:G:OP1	52:v:18:ALA:HB1	2.17	0.44
7:A:171:A:H2'	7:A:172:A:C8	2.52	0.44
8:B:111:ILE:HD13	8:B:148:LEU:HB3	1.98	0.44
15:I:115:LYS:HB2	15:I:118:LEU:HD12	1.99	0.44
28:V:160:CYS:HA	28:V:199:LEU:HD13	2.00	0.44
31:a:1853:A:H2'	31:a:1854:A:C8	2.53	0.44
31:a:2751:G:H2'	31:a:2751:G:N3	2.33	0.44
44:n:85:LYS:HB3	44:n:87:ILE:HD13	2.00	0.44
12:F:67:PRO:O	12:F:70:VAL:HG12	2.17	0.44
31:a:493:G:H2'	31:a:494:G:O4'	2.18	0.44
31:a:1386:C:H2'	31:a:1387:A:C8	2.53	0.44
31:a:2376:A:H2'	31:a:2377:A:O4'	2.18	0.44
31:a:2469:A:H61	31:a:2481:G:H1'	1.82	0.44
31:a:2723:C:H2'	31:a:2724:U:O4'	2.16	0.44
37:g:140:VAL:O	37:g:144:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:486:U:O2'	7:A:487:A:H5'	2.17	0.44
8:B:99:GLY:HA2	8:B:102:THR:OG1	2.18	0.44
10:D:36:GLN:HG3	10:D:43:ALA:HA	2.00	0.44
17:K:35:THR:HG22	17:K:41:ALA:HA	2.00	0.44
19:M:33:ILE:HD13	19:M:60:VAL:HG22	2.00	0.44
23:Q:10:GLY:HA3	23:Q:25:ILE:HD13	2.00	0.44
26:T:55:GLN:N	26:T:56:PRO:HD2	2.32	0.44
33:c:135:ILE:O	33:c:167:ARG:NH1	2.50	0.44
35:e:138:LEU:HD13	35:e:167:VAL:HG21	1.99	0.44
1:0:10:LYS:O	1:0:52:ALA:N	2.45	0.43
10:D:73:ARG:HG2	10:D:73:ARG:HH11	1.82	0.43
31:a:1088:A:N3	31:a:1088:A:H2'	2.33	0.43
31:a:2233:U:H2'	31:a:2234:G:C8	2.53	0.43
31:a:2590:A:H2'	31:a:2591:C:C6	2.52	0.43
50:t:14:LEU:HD11	50:t:71:ALA:HB2	1.99	0.43
7:A:1338:G:H2'	7:A:1339:A:C8	2.54	0.43
29:W:511:ILE:HD13	29:W:545:LEU:HD11	2.01	0.43
31:a:1179:G:H2'	31:a:1180:U:O4'	2.18	0.43
36:f:58:ALA:HB2	36:f:65:PRO:HD3	1.99	0.43
7:A:376:G:H5''	22:P:5:ARG:HB2	2.00	0.43
7:A:567:G:H2'	7:A:568:G:O4'	2.18	0.43
29:W:505:GLN:HA	29:W:575:ASP:O	2.17	0.43
42:l:66:ARG:HB2	42:l:101:VAL:O	2.19	0.43
52:v:37:ILE:HG21	52:v:80:ILE:HG21	1.99	0.43
53:w:13:VAL:HG23	53:w:29:PHE:HB2	1.99	0.43
7:A:8:A:H5'	11:E:125:ALA:O	2.18	0.43
7:A:1032:G:H2'	7:A:1033:G:H4'	2.00	0.43
7:A:1035:A:HO2'	7:A:1036:A:H5''	1.71	0.43
7:A:1328:C:H5''	19:M:28:THR:HG21	2.00	0.43
31:a:1869:G:H2'	31:a:1871:A:N7	2.33	0.43
31:a:2756:U:H1'	31:a:2757:A:H5''	2.01	0.43
36:f:8:TYR:OH	36:f:30:ARG:HG3	2.18	0.43
53:w:17:ASN:HB2	53:w:25:THR:OG1	2.17	0.43
54:x:6:LEU:HB3	54:x:56:LEU:HD13	1.99	0.43
7:A:1288:A:N1	7:A:1371:G:H1'	2.34	0.43
11:E:148:ASN:HA	11:E:152:MET:SD	2.58	0.43
31:a:720:U:H2'	31:a:721:A:C8	2.54	0.43
31:a:2750:A:H1'	31:a:2752:C:N4	2.33	0.43
34:d:25:THR:HG21	34:d:193:VAL:HG22	2.00	0.43
35:e:16:GLU:O	35:e:20:GLY:N	2.49	0.43
2:1:39:ARG:NH2	31:a:468:G:N7	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:70:U:H1'	7:A:71:A:N7	2.33	0.43
40:j:10:VAL:HG12	40:j:12:ASP:H	1.82	0.43
37:g:42:GLU:HB2	37:g:55:ARG:HG2	2.01	0.43
49:s:69:ARG:HH11	49:s:74:ILE:HD13	1.84	0.43
7:A:49:U:O2	7:A:362:G:H1'	2.19	0.43
7:A:579:A:H5'	7:A:728:A:H1'	2.01	0.43
8:B:84:ALA:CB	8:B:91:PHE:HB3	2.48	0.43
29:W:535:ARG:HD2	29:W:538:ILE:HD12	2.00	0.43
31:a:56:A:H2'	31:a:57:C:O4'	2.19	0.43
31:a:1405:U:H2'	31:a:1406:U:C6	2.54	0.43
31:a:1721:G:N2	31:a:1738:G:O2'	2.52	0.43
31:a:2646:C:OP2	31:a:2732:G:O2'	2.36	0.43
7:A:662:U:H2'	7:A:663:A:C8	2.54	0.43
31:a:1287:A:H5'	43:m:103:ARG:HD2	2.01	0.43
31:a:1747:U:H2'	31:a:1748:C:C6	2.54	0.43
31:a:2849:U:H4'	31:a:2868:A:C2	2.54	0.43
7:A:590:U:H2'	7:A:591:U:C6	2.54	0.42
16:J:25:ILE:HD11	16:J:92:LEU:HD11	2.01	0.42
7:A:269:C:H2'	7:A:270:A:C8	2.53	0.42
7:A:1032:G:H3'	7:A:1032:G:N3	2.35	0.42
18:L:76:GLU:O	18:L:77:HIS:HB2	2.19	0.42
28:V:199:LEU:HD11	28:V:201:ASP:O	2.19	0.42
29:W:571:TYR:HB3	29:W:581:PHE:HZ	1.83	0.42
31:a:247:G:H4'	31:a:386:G:C5	2.54	0.42
31:a:2636:C:H2'	31:a:2637:U:C6	2.53	0.42
35:e:149:ILE:HB	35:e:188:MET:HG2	2.00	0.42
7:A:31:G:O2'	7:A:48:C:N4	2.50	0.42
31:a:1183:U:H2'	31:a:1184:U:C6	2.55	0.42
31:a:2557:G:H2'	31:a:2558:C:C6	2.55	0.42
31:a:2615:U:C2	56:z:4:GLN:HA	2.54	0.42
49:s:69:ARG:NH1	49:s:74:ILE:HD13	2.34	0.42
2:1:12:ARG:NH1	31:a:465:G:OP1	2.50	0.42
7:A:486:U:H2'	7:A:487:A:H8	1.84	0.42
8:B:70:VAL:HB	8:B:163:VAL:HG22	2.02	0.42
16:J:6:ILE:HG13	16:J:79:PRO:HG3	2.01	0.42
23:Q:27:ARG:HG3	23:Q:40:ARG:HB2	2.01	0.42
27:U:34:ARG:HH11	27:U:34:ARG:HG2	1.84	0.42
28:V:58:SER:HB3	28:V:75:ILE:HG23	2.00	0.42
28:V:97:VAL:HG21	28:V:141:LEU:HD23	2.01	0.42
31:a:580:U:H2'	31:a:581:C:C6	2.54	0.42
36:f:142:ASP:O	36:f:146:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:420:U:H2'	7:A:421:U:H5''	2.02	0.42
31:a:64:A:H2'	31:a:65:U:C6	2.55	0.42
31:a:372:G:O2'	31:a:400:G:O6	2.35	0.42
31:a:1046:A:H3'	31:a:1047:G:C5'	2.49	0.42
31:a:1179:G:C6	31:a:1180:U:C2	3.06	0.42
31:a:1564:C:H2'	31:a:1565:C:C6	2.55	0.42
33:c:165:VAL:HG11	33:c:181:MET:HE1	2.01	0.42
7:A:672:U:H2'	7:A:673:A:C8	2.54	0.42
9:C:128:VAL:HG11	9:C:136:ARG:HH22	1.85	0.42
12:F:46:GLN:HA	12:F:56:LYS:HG2	2.01	0.42
16:J:77:VAL:HG12	16:J:78:GLU:HG2	2.00	0.42
31:a:634:C:H2'	31:a:635:C:C6	2.55	0.42
31:a:756:A:H2'	31:a:757:G:O4'	2.19	0.42
31:a:1021:A:H3'	31:a:1021:A:N3	2.35	0.42
31:a:1141:U:H4'	31:a:1142:A:O4'	2.19	0.42
31:a:1226:A:OP1	46:p:16:LYS:NZ	2.45	0.42
31:a:2532:G:O2'	31:a:2657:A:N1	2.45	0.42
34:d:142:VAL:HB	34:d:143:PRO:HD2	2.01	0.42
46:p:49:ASP:HA	46:p:52:GLN:HB2	2.01	0.42
7:A:294:U:OP1	7:A:610:U:O2'	2.34	0.42
31:a:1179:G:C5	31:a:1180:U:C2	3.08	0.42
31:a:1728:C:H2'	31:a:1730:C:O2	2.20	0.42
31:a:2251:OMG:HM23	31:a:2251:OMG:H1'	1.88	0.42
32:b:48:U:H2'	32:b:49:C:C6	2.55	0.42
44:n:53:THR:HB	44:n:65:THR:HB	2.00	0.42
7:A:1492:A:O2'	31:a:1913:A:N6	2.53	0.42
8:B:94:HIS:O	8:B:95:ARG:C	2.63	0.42
16:J:51:VAL:HB	20:N:81:ARG:HB2	2.02	0.42
31:a:698:C:O2'	31:a:734:A:N6	2.52	0.42
31:a:1528:A:H2'	31:a:1529:G:O4'	2.19	0.42
32:b:39:A:H2'	32:b:40:U:C6	2.54	0.42
41:k:108:ALA:HB3	41:k:125:LEU:HD22	2.01	0.42
52:v:47:ALA:HB2	52:v:59:LEU:HD22	2.02	0.42
7:A:1070:U:H2'	7:A:1071:C:C6	2.55	0.42
28:V:23:VAL:HG21	28:V:36:ILE:HG21	2.02	0.42
29:W:554:LEU:HD11	29:W:598:PRO:HB2	2.01	0.42
31:a:1070:A:N7	31:a:1096:A:O2'	2.50	0.42
31:a:1906:G:H2'	31:a:1907:G:H5''	2.02	0.42
7:A:75:G:O2'	7:A:76:G:H5'	2.19	0.42
7:A:1309:G:N7	19:M:98:ARG:NH2	2.68	0.42
8:B:28:LYS:N	8:B:29:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:145:ILE:CG2	10:D:150:LYS:HG2	2.50	0.42
17:K:34:ILE:HB	17:K:74:VAL:HG11	2.01	0.42
28:V:154:LYS:HE2	28:V:163:GLU:HG2	2.01	0.42
29:W:479:MET:SD	29:W:479:MET:N	2.93	0.42
29:W:541:VAL:HG13	29:W:585:ALA:HB2	2.01	0.42
31:a:365:U:H2'	31:a:366:C:C6	2.55	0.42
31:a:2567:G:H2'	31:a:2568:U:C6	2.54	0.42
36:f:121:SER:HB2	36:f:128:TYR:CE1	2.55	0.42
7:A:451:A:H4'	7:A:452:A:O5'	2.20	0.41
9:C:50:ALA:HB1	9:C:76:VAL:HG22	2.01	0.41
12:F:43:GLY:HA2	12:F:58:HIS:CE1	2.54	0.41
18:L:66:TYR:CB	18:L:87:VAL:HG21	2.50	0.41
31:a:280:U:H2'	31:a:281:C:C6	2.55	0.41
31:a:1065:U:H2'	31:a:1066:U:O4'	2.19	0.41
31:a:1805:A:N3	33:c:50:THR:HB	2.34	0.41
31:a:2749:A:H3'	31:a:2750:A:H2'	2.01	0.41
31:a:2789:C:H2'	31:a:2893:A:N7	2.35	0.41
34:d:121:THR:HB	34:d:127:PHE:CD2	2.54	0.41
7:A:999:C:H2'	7:A:1000:A:C8	2.55	0.41
7:A:1004:A:H2'	7:A:1005:A:O4'	2.20	0.41
8:B:133:GLU:HA	8:B:136:MET:HE2	2.03	0.41
11:E:101:GLU:N	11:E:101:GLU:OE1	2.53	0.41
29:W:607:VAL:HG21	29:W:651:MET:SD	2.61	0.41
31:a:479:A:N3	31:a:481:G:H5''	2.35	0.41
31:a:1090:A:C2	31:a:1102:C:H1'	2.55	0.41
31:a:2511:U:H2'	31:a:2512:C:O4'	2.20	0.41
36:f:65:PRO:HA	36:f:89:VAL:HG13	2.02	0.41
41:k:79:LEU:HD11	41:k:112:LEU:HD12	2.01	0.41
7:A:87:C:H2'	7:A:88:U:C6	2.55	0.41
7:A:457:G:N3	7:A:457:G:H2'	2.35	0.41
7:A:1255:G:O2'	7:A:1258:G:N3	2.47	0.41
7:A:1504:G:H4'	7:A:1505:G:C4	2.54	0.41
10:D:145:ILE:HD12	10:D:155:VAL:HG11	2.02	0.41
17:K:87:LYS:HG3	17:K:115:PRO:HD3	2.02	0.41
31:a:722:A:H2'	31:a:723:C:O4'	2.21	0.41
31:a:975:A:H1'	31:a:990:A:C2	2.54	0.41
31:a:2070:A:H2'	31:a:2071:A:O4'	2.20	0.41
34:d:85:ALA:HB3	34:d:88:GLU:HG3	2.01	0.41
20:N:10:GLU:HG3	20:N:63:ARG:HD2	2.02	0.41
22:P:40:ASN:HB3	22:P:43:ALA:HB2	2.01	0.41
31:a:84:A:N1	31:a:98:G:O2'	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:565:C:H2'	31:a:566:U:O4'	2.21	0.41
7:A:741:G:H2'	7:A:742:G:O4'	2.20	0.41
9:C:97:VAL:HB	9:C:98:PRO:HD2	2.01	0.41
10:D:61:VAL:HG21	10:D:200:ILE:HD11	2.03	0.41
27:U:7:ARG:HG3	27:U:10:GLU:HB2	2.01	0.41
35:e:12:LEU:HD11	35:e:194:LYS:HD3	2.03	0.41
40:j:88:ASN:HB3	40:j:91:SER:OG	2.20	0.41
42:l:33:LEU:HD13	42:l:117:PHE:HB3	2.02	0.41
44:n:2:ASP:OD1	44:n:2:ASP:N	2.54	0.41
48:r:4:ILE:HG22	48:r:106:VAL:HG22	2.01	0.41
51:u:2:PHE:HB2	51:u:61:LEU:HD22	2.02	0.41
3:2:45:ARG:N	3:2:46:PRO:HD2	2.36	0.41
7:A:128:G:H2'	7:A:129:A:C8	2.56	0.41
7:A:151:A:H2'	7:A:152:A:O4'	2.20	0.41
7:A:225:C:C2'	7:A:226:G:H5''	2.48	0.41
7:A:493:A:H2'	7:A:494:G:C8	2.56	0.41
7:A:718:A:H5'	17:K:119:IAS:C	2.50	0.41
7:A:1072:G:H2'	7:A:1073:U:C6	2.56	0.41
8:B:221:VAL:O	8:B:225:ARG:HG3	2.20	0.41
31:a:121:G:H4'	31:a:149:A:H5'	2.02	0.41
31:a:1927:A:H2'	31:a:1928:A:C8	2.56	0.41
35:e:153:LEU:HD21	35:e:158:PHE:HB2	2.03	0.41
45:o:8:LEU:O	45:o:11:GLU:HG2	2.20	0.41
7:A:1086:U:H3	7:A:1099:G:H22	1.68	0.41
7:A:1179:A:H2'	7:A:1180:A:O4'	2.20	0.41
7:A:1324:A:H2'	7:A:1325:C:O4'	2.21	0.41
23:Q:59:VAL:HB	23:Q:75:LEU:HD21	2.02	0.41
28:V:62:LEU:HG	28:V:75:ILE:HD13	2.02	0.41
31:a:460:A:H2'	31:a:461:C:O4'	2.20	0.41
44:n:39:VAL:HB	44:n:49:VAL:HG23	2.01	0.41
7:A:266:G:H3'	23:Q:69:LYS:HB2	2.01	0.41
8:B:73:LYS:HG3	8:B:168:HIS:CD2	2.56	0.41
31:a:127:A:H5''	31:a:128:C:O4'	2.21	0.41
31:a:632:A:H2'	31:a:633:A:C8	2.55	0.41
31:a:1562:U:H2'	31:a:1563:U:O4'	2.21	0.41
36:f:29:PRO:HB3	36:f:160:ALA:HB2	2.02	0.41
7:A:499:A:H4'	7:A:500:G:H5'	2.02	0.41
7:A:1301:U:O2'	7:A:1302:C:H3'	2.21	0.41
9:C:50:ALA:HA	9:C:75:ILE:CD1	2.51	0.41
10:D:145:ILE:CD1	10:D:155:VAL:HG21	2.51	0.41
26:T:44:LYS:HD2	26:T:87:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:55:U:O2'	30:Z:57:A:N7	2.51	0.41
31:a:90:U:H3'	31:a:91:A:H2'	2.02	0.41
31:a:181:A:H2'	31:a:182:A:C8	2.55	0.41
31:a:2518:A:N3	31:a:2518:A:H2'	2.36	0.41
31:a:2591:C:H2'	31:a:2592:G:C8	2.56	0.41
46:p:58:ARG:HA	46:p:61:TRP:CE3	2.56	0.41
48:r:20:VAL:HG11	48:r:44:ALA:HA	2.03	0.41
7:A:1305:G:N2	7:A:1331:G:H1'	2.35	0.41
7:A:1435:G:H2'	7:A:1436:U:C6	2.56	0.41
11:E:149:SER:OG	11:E:152:MET:HG2	2.20	0.41
20:N:46:LEU:O	20:N:50:THR:HG23	2.21	0.41
27:U:40:LYS:HG2	27:U:41:PRO:HD2	2.03	0.41
31:a:608:A:H2'	31:a:609:A:C8	2.55	0.41
31:a:1085:A:H2'	31:a:1086:A:N3	2.36	0.41
31:a:1182:G:H2'	31:a:1183:U:O4'	2.21	0.41
31:a:1199:U:H1'	46:p:4:VAL:HG22	2.02	0.41
31:a:1607:C:H4'	31:a:1608:A:O5'	2.21	0.41
35:e:145:ASP:HA	35:e:166:LYS:HB3	2.04	0.41
41:k:1:MET:HE2	41:k:1:MET:HB3	1.98	0.41
7:A:1328:C:H2'	7:A:1329:A:O4'	2.20	0.40
7:A:1496:C:H2'	7:A:1497:G:O4'	2.21	0.40
8:B:12:ALA:HB3	8:B:14:VAL:HG23	2.03	0.40
31:a:1061:U:H3'	31:a:1062:G:H5''	2.03	0.40
33:c:31:ALA:N	33:c:32:PRO:CD	2.84	0.40
15:I:19:VAL:HG22	15:I:65:ILE:HG23	2.02	0.40
31:a:308:G:H2'	31:a:309:A:C8	2.56	0.40
31:a:987:C:H2'	31:a:988:A:O4'	2.21	0.40
31:a:1434:A:H2'	31:a:1435:G:H8	1.87	0.40
31:a:1816:C:H3'	33:c:62:TYR:CE1	2.55	0.40
31:a:2202:U:O2'	31:a:2204:G:OP1	2.38	0.40
37:g:99:LYS:O	37:g:102:VAL:HG22	2.21	0.40
52:v:50:ASN:HB2	52:v:82:ILE:HB	2.03	0.40
7:A:95:C:H2'	7:A:96:U:C6	2.55	0.40
7:A:337:G:H2'	7:A:338:A:C8	2.57	0.40
7:A:407:U:H2'	7:A:408:A:C8	2.57	0.40
7:A:728:A:H2'	7:A:729:A:C8	2.56	0.40
8:B:47:VAL:N	8:B:48:PRO:HD2	2.35	0.40
8:B:68:LEU:HD11	8:B:92:VAL:HG23	2.02	0.40
31:a:655:A:H4'	31:a:656:G:H5'	2.02	0.40
34:d:16:THR:O	45:o:79:PRO:HG2	2.20	0.40
34:d:24:VAL:HG12	34:d:178:VAL:HG21	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:107:LEU:HB2	40:j:116:ILE:HD11	2.04	0.40
7:A:51:A:H4'	7:A:52:C:C5'	2.51	0.40
7:A:158:G:C2'	7:A:159:G:C5'	2.91	0.40
7:A:429:U:O4'	7:A:430:A:H8	2.03	0.40
7:A:1312:G:N7	25:S:2:PRO:HD2	2.36	0.40
16:J:8:ILE:HA	16:J:99:GLN:O	2.22	0.40
31:a:2566:A:N1	40:j:28:SER:OG	2.51	0.40
33:c:271:ARG:O	33:c:272:SER:C	2.65	0.40
36:f:8:TYR:HB2	36:f:173:PHE:CZ	2.56	0.40
40:j:40:LYS:HE3	40:j:57:VAL:HG12	2.04	0.40
4:3:16:ILE:HD13	4:3:25:VAL:HG22	2.04	0.40
13:G:26:PHE:HZ	13:G:120:LEU:HD11	1.87	0.40
29:W:505:GLN:HB3	29:W:580:ALA:HB2	2.03	0.40
41:k:79:LEU:CD1	41:k:112:LEU:HD12	2.52	0.40
47:q:38:VAL:HG11	47:q:41:ILE:CG1	2.52	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	0	48/55 (87%)	48 (100%)	0	0	100	100
2	1	43/46 (94%)	43 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	55 (98%)	1 (2%)	0	100	100
8	B	220/241 (91%)	214 (97%)	5 (2%)	1 (0%)	24	35
9	C	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
10	D	203/206 (98%)	202 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	E	152/167 (91%)	150 (99%)	2 (1%)	0	100	100
12	F	99/135 (73%)	98 (99%)	1 (1%)	0	100	100
13	G	148/179 (83%)	147 (99%)	1 (1%)	0	100	100
14	H	127/130 (98%)	127 (100%)	0	0	100	100
15	I	123/130 (95%)	120 (98%)	3 (2%)	0	100	100
16	J	92/103 (89%)	87 (95%)	4 (4%)	1 (1%)	11	16
17	K	113/129 (88%)	111 (98%)	2 (2%)	0	100	100
18	L	118/124 (95%)	114 (97%)	4 (3%)	0	100	100
19	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
20	N	98/101 (97%)	98 (100%)	0	0	100	100
21	O	86/89 (97%)	86 (100%)	0	0	100	100
22	P	77/82 (94%)	75 (97%)	2 (3%)	0	100	100
23	Q	77/84 (92%)	77 (100%)	0	0	100	100
24	R	62/75 (83%)	62 (100%)	0	0	100	100
25	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
26	T	84/87 (97%)	84 (100%)	0	0	100	100
27	U	53/71 (75%)	53 (100%)	0	0	100	100
28	V	210/213 (99%)	208 (99%)	2 (1%)	0	100	100
29	W	212/693 (31%)	209 (99%)	3 (1%)	0	100	100
33	c	269/273 (98%)	265 (98%)	4 (2%)	0	100	100
34	d	204/209 (98%)	200 (98%)	4 (2%)	0	100	100
35	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
36	f	175/179 (98%)	174 (99%)	1 (1%)	0	100	100
37	g	164/177 (93%)	162 (99%)	2 (1%)	0	100	100
38	h	39/149 (26%)	38 (97%)	1 (3%)	0	100	100
39	i	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
40	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
41	k	142/144 (99%)	139 (98%)	2 (1%)	1 (1%)	18	27
42	l	132/136 (97%)	131 (99%)	1 (1%)	0	100	100
43	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
44	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
46	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
47	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
48	r	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
49	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
50	t	89/104 (86%)	89 (100%)	0	0	100	100
51	u	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
52	v	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
53	w	75/78 (96%)	75 (100%)	0	0	100	100
54	x	58/63 (92%)	58 (100%)	0	0	100	100
55	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
56	z	52/57 (91%)	52 (100%)	0	0	100	100
All	All	5832/6819 (86%)	5752 (99%)	77 (1%)	3 (0%)	49	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	J	57	VAL
41	k	29	LYS
8	B	165	ASP

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	0	46/49 (94%)	46 (100%)	0	100	100
2	1	37/38 (97%)	37 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	B	184/199 (92%)	179 (97%)	5 (3%)	39	60
9	C	170/190 (90%)	168 (99%)	2 (1%)	63	79
10	D	172/173 (99%)	167 (97%)	5 (3%)	37	57
11	E	117/126 (93%)	113 (97%)	4 (3%)	32	52
12	F	88/116 (76%)	88 (100%)	0	100	100
13	G	124/147 (84%)	121 (98%)	3 (2%)	43	63
14	H	104/105 (99%)	104 (100%)	0	100	100
15	I	103/107 (96%)	102 (99%)	1 (1%)	68	82
16	J	85/90 (94%)	84 (99%)	1 (1%)	63	79
17	K	89/98 (91%)	88 (99%)	1 (1%)	65	81
18	L	101/103 (98%)	98 (97%)	3 (3%)	36	56
19	M	93/96 (97%)	93 (100%)	0	100	100
20	N	83/84 (99%)	83 (100%)	0	100	100
21	O	76/77 (99%)	76 (100%)	0	100	100
22	P	64/65 (98%)	64 (100%)	0	100	100
23	Q	73/78 (94%)	70 (96%)	3 (4%)	27	44
24	R	55/65 (85%)	55 (100%)	0	100	100
25	S	72/79 (91%)	72 (100%)	0	100	100
26	T	65/66 (98%)	65 (100%)	0	100	100
27	U	48/61 (79%)	48 (100%)	0	100	100
28	V	203/204 (100%)	198 (98%)	5 (2%)	42	62
29	W	174/579 (30%)	171 (98%)	3 (2%)	53	73
33	c	216/218 (99%)	216 (100%)	0	100	100
34	d	162/163 (99%)	162 (100%)	0	100	100
35	e	165/165 (100%)	165 (100%)	0	100	100
36	f	148/150 (99%)	146 (99%)	2 (1%)	59	77
37	g	130/138 (94%)	126 (97%)	4 (3%)	35	55
38	h	32/114 (28%)	29 (91%)	3 (9%)	8	12
39	i	115/116 (99%)	114 (99%)	1 (1%)	70	84
40	j	104/104 (100%)	104 (100%)	0	100	100
41	k	103/103 (100%)	101 (98%)	2 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	l	107/107 (100%)	106 (99%)	1 (1%)	70	84
43	m	98/103 (95%)	98 (100%)	0	100	100
44	n	86/87 (99%)	84 (98%)	2 (2%)	44	64
45	o	99/100 (99%)	99 (100%)	0	100	100
46	p	89/90 (99%)	89 (100%)	0	100	100
47	q	84/84 (100%)	82 (98%)	2 (2%)	43	63
48	r	92/93 (99%)	92 (100%)	0	100	100
49	s	80/84 (95%)	80 (100%)	0	100	100
50	t	76/85 (89%)	76 (100%)	0	100	100
51	u	77/78 (99%)	77 (100%)	0	100	100
52	v	56/63 (89%)	56 (100%)	0	100	100
53	w	67/68 (98%)	67 (100%)	0	100	100
54	x	54/55 (98%)	54 (100%)	0	100	100
55	y	48/49 (98%)	48 (100%)	0	100	100
56	z	46/48 (96%)	46 (100%)	0	100	100
All	All	4900/5608 (87%)	4847 (99%)	53 (1%)	63	81

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

Mol	Chain	Res	Type
8	B	111	ILE
8	B	143	LYS
8	B	161	LEU
8	B	196	VAL
8	B	204	ASP
9	C	144	LEU
9	C	185	ASN
10	D	35	GLU
10	D	44	ARG
10	D	45	LYS
10	D	99	ASP
10	D	147	GLU
11	E	26	LYS
11	E	77	ASN
11	E	101	GLU
11	E	148	ASN
13	G	63	GLU

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Mol	Chain	Res	Type
13	G	75	VAL
13	G	135	VAL
15	I	42	GLU
16	J	36	VAL
17	K	129	VAL
18	L	4	VAL
18	L	52	VAL
18	L	55	VAL
23	Q	28	PHE
23	Q	33	ILE
23	Q	42	THR
28	V	103	LYS
28	V	106	ILE
28	V	137	GLU
28	V	142	LYS
28	V	144	LEU
29	W	480	VAL
29	W	510	HIS
29	W	532	VAL
36	f	69	LYS
36	f	89	VAL
37	g	25	THR
37	g	27	LYS
37	g	76	VAL
37	g	104	ASN
38	h	4	ILE
38	h	15	LEU
38	h	37	VAL
39	i	9	GLU
41	k	85	VAL
41	k	120	VAL
42	l	6	ARG
44	n	49	VAL
44	n	56	LYS
47	q	18	GLN
47	q	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	20	ASN
5	4	41	HIS

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Mol	Chain	Res	Type
5	4	61	ASN
5	4	65	ASN
8	B	18	HIS
8	B	42	ASN
8	B	58	ASN
8	B	89	GLN
8	B	103	ASN
9	C	8	ASN
9	C	139	GLN
9	C	140	ASN
10	D	136	GLN
11	E	70	ASN
11	E	77	ASN
11	E	82	GLN
12	F	3	HIS
12	F	17	GLN
12	F	68	GLN
12	F	94	HIS
13	G	68	ASN
14	H	4	GLN
14	H	18	GLN
16	J	15	HIS
16	J	58	ASN
16	J	99	GLN
17	K	40	ASN
17	K	118	HIS
18	L	77	HIS
18	L	112	GLN
20	N	66	GLN
21	O	35	GLN
21	O	80	GLN
22	P	59	HIS
25	S	14	HIS
26	T	84	ASN
28	V	150	ASN
28	V	161	ASN
28	V	198	GLN
28	V	204	GLN
29	W	505	GLN
29	W	510	HIS
29	W	526	ASN
29	W	551	ASN

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Mol	Chain	Res	Type
29	W	640	GLN
33	c	25	HIS
33	c	37	ASN
34	d	94	GLN
35	e	90	GLN
35	e	115	GLN
35	e	195	GLN
36	f	23	ASN
36	f	27	GLN
37	g	22	GLN
39	i	136	GLN
40	j	93	GLN
41	k	104	GLN
43	m	9	GLN
43	m	31	HIS
44	n	29	HIS
44	n	100	HIS
45	o	66	ASN
46	p	81	ASN
47	q	12	HIS
47	q	43	ASN
51	u	12	GLN
51	u	49	ASN
54	x	15	ASN
55	y	9	GLN
55	y	20	HIS
56	z	6	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	Z	75/77 (97%)	19 (25%)	3 (4%)
31	a	2778/2930 (94%)	327 (11%)	0
32	b	118/119 (99%)	8 (6%)	0
6	9	6/24 (25%)	1 (16%)	0
7	A	1511/1554 (97%)	185 (12%)	37 (2%)
All	All	4488/4704 (95%)	540 (12%)	40 (0%)

All (540) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	9	19	G
7	A	4	U
7	A	5	U
7	A	8	A
7	A	9	G
7	A	32	A
7	A	39	G
7	A	47	C
7	A	48	C
7	A	51	A
7	A	69	G
7	A	70	U
7	A	71	A
7	A	72	A
7	A	73	C
7	A	74	A
7	A	75	G
7	A	81	A
7	A	82	G
7	A	83	C
7	A	84	U
7	A	85	U
7	A	86	G
7	A	87	C
7	A	94	G
7	A	95	C
7	A	120	A
7	A	122	G
7	A	131	A
7	A	144	G
7	A	159	G
7	A	164	G
7	A	182	A
7	A	183	C
7	A	197	A
7	A	226	G
7	A	240	G
7	A	245	U
7	A	247	G
7	A	251	G
7	A	266	G
7	A	267	C
7	A	289	G

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Mol	Chain	Res	Type
7	A	321	A
7	A	328	C
7	A	329	A
7	A	330	C
7	A	347	G
7	A	352	C
7	A	354	G
7	A	367	U
7	A	372	C
7	A	398	U
7	A	406	G
7	A	411	A
7	A	412	A
7	A	413	G
7	A	414	A
7	A	421	U
7	A	422	C
7	A	423	G
7	A	424	G
7	A	429	U
7	A	438	U
7	A	439	U
7	A	457	G
7	A	467	U
7	A	468	A
7	A	469	C
7	A	484	G
7	A	486	U
7	A	508	U
7	A	511	C
7	A	518	C
7	A	521	G
7	A	531	U
7	A	532	A
7	A	536	C
7	A	547	A
7	A	559	A
7	A	562	U
7	A	572	A
7	A	573	A
7	A	576	C
7	A	596	A

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Mol	Chain	Res	Type
7	A	633	G
7	A	641	U
7	A	642	A
7	A	650	G
7	A	654	G
7	A	665	A
7	A	688	G
7	A	723	U
7	A	724	G
7	A	734	G
7	A	755	G
7	A	777	A
7	A	793	U
7	A	794	A
7	A	815	A
7	A	817	C
7	A	832	G
7	A	849	G
7	A	874	G
7	A	887	G
7	A	890	G
7	A	914	A
7	A	926	G
7	A	934	C
7	A	960	U
7	A	961	U
7	A	969	A
7	A	975	A
7	A	976	G
7	A	977	A
7	A	984	C
7	A	992	U
7	A	993	G
7	A	994	A
7	A	1004	A
7	A	1020	G
7	A	1027	C
7	A	1029	U
7	A	1030	U
7	A	1031	C
7	A	1033	G
7	A	1034	G

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Mol	Chain	Res	Type
7	A	1035	A
7	A	1036	A
7	A	1039	G
7	A	1042	A
7	A	1043	G
7	A	1044	A
7	A	1046	A
7	A	1065	U
7	A	1085	U
7	A	1094	G
7	A	1095	U
7	A	1101	A
7	A	1124	G
7	A	1125	U
7	A	1137	C
7	A	1139	G
7	A	1145	A
7	A	1146	A
7	A	1196	A
7	A	1197	A
7	A	1211	U
7	A	1212	U
7	A	1213	A
7	A	1214	C
7	A	1225	A
7	A	1226	C
7	A	1227	A
7	A	1238	A
7	A	1256	A
7	A	1260	G
7	A	1275	A
7	A	1280	A
7	A	1287	A
7	A	1300	G
7	A	1317	C
7	A	1319	A
7	A	1320	C
7	A	1338	G
7	A	1346	A
7	A	1353	G
7	A	1363	A
7	A	1378	C

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Mol	Chain	Res	Type
7	A	1379	G
7	A	1398	A
7	A	1419	G
7	A	1433	A
7	A	1447	A
7	A	1453	G
7	A	1492	A
7	A	1494	G
7	A	1497	G
7	A	1503	A
7	A	1505	G
7	A	1506	U
7	A	1517	G
7	A	1529	G
7	A	1530	G
7	A	1533	C
7	A	1534	A
30	Z	6	G
30	Z	7	G
30	Z	8	U
30	Z	9	G
30	Z	14	A
30	Z	17(A)	U
30	Z	18	G
30	Z	19	G
30	Z	21	A
30	Z	46	G
30	Z	48	C
30	Z	50	U
30	Z	51	C
30	Z	58	A
30	Z	64	G
30	Z	65	C
30	Z	68	C
30	Z	75	C
30	Z	76	A
31	a	10	A
31	a	12	U
31	a	13	A
31	a	15	G
31	a	34	U
31	a	63	A

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Mol	Chain	Res	Type
31	a	71	A
31	a	74	A
31	a	75	G
31	a	101	A
31	a	103	A
31	a	118	A
31	a	119	A
31	a	120	U
31	a	131	A
31	a	135	U
31	a	139	U
31	a	142	A
31	a	162	U
31	a	181	A
31	a	196	A
31	a	199	A
31	a	200	U
31	a	215	G
31	a	216	A
31	a	221	A
31	a	222	A
31	a	228	C
31	a	248	G
31	a	272	A
31	a	276	U
31	a	277	G
31	a	278	A
31	a	279	A
31	a	281	C
31	a	285	G
31	a	289	G
31	a	310	A
31	a	311	A
31	a	330	A
31	a	345	A
31	a	346	A
31	a	353	C
31	a	354	A
31	a	361	G
31	a	362	A
31	a	386	G
31	a	411	G

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Mol	Chain	Res	Type
31	a	412	A
31	a	451	U
31	a	481	G
31	a	491	G
31	a	503	A
31	a	504	A
31	a	505	A
31	a	509	C
31	a	513	A
31	a	531	C
31	a	532	A
31	a	533	G
31	a	544	C
31	a	545	U
31	a	547	A
31	a	548	G
31	a	549	G
31	a	555	G
31	a	556	A
31	a	563	A
31	a	573	U
31	a	574	A
31	a	575	A
31	a	586	A
31	a	603	A
31	a	613	A
31	a	614	A
31	a	615	U
31	a	627	A
31	a	637	A
31	a	645	C
31	a	646	U
31	a	647	G
31	a	653	U
31	a	654	A
31	a	655	A
31	a	686	U
31	a	716	A
31	a	717	C
31	a	730	A
31	a	747	5MU
31	a	764	A

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Mol	Chain	Res	Type
31	a	765	C
31	a	775	G
31	a	776	G
31	a	782	A
31	a	784	G
31	a	785	G
31	a	805	G
31	a	812	C
31	a	827	U
31	a	828	U
31	a	845	A
31	a	846	U
31	a	858	G
31	a	859	G
31	a	910	A
31	a	914	G
31	a	915	C
31	a	931	U
31	a	934	U
31	a	946	C
31	a	961	C
31	a	962	G
31	a	974	G
31	a	983	A
31	a	984	A
31	a	985	C
31	a	996	A
31	a	1012	U
31	a	1013	C
31	a	1022	G
31	a	1026	G
31	a	1033	U
31	a	1041	G
31	a	1047	G
31	a	1054	A
31	a	1059	G
31	a	1060	U
31	a	1061	U
31	a	1069	A
31	a	1070	A
31	a	1077	A
31	a	1080	A

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Mol	Chain	Res	Type
31	a	1083	U
31	a	1087	G
31	a	1088	A
31	a	1091	G
31	a	1101	U
31	a	1112	G
31	a	1116	G
31	a	1128	G
31	a	1129	A
31	a	1130	U
31	a	1132	U
31	a	1133	A
31	a	1134	A
31	a	1135	C
31	a	1142	A
31	a	1169	A
31	a	1170	C
31	a	1171	G
31	a	1179	G
31	a	1253	A
31	a	1256	G
31	a	1271	G
31	a	1272	A
31	a	1273	U
31	a	1300	G
31	a	1301	A
31	a	1302	A
31	a	1303	G
31	a	1320	C
31	a	1321	A
31	a	1352	U
31	a	1365	A
31	a	1379	U
31	a	1383	A
31	a	1409	U
31	a	1411	U
31	a	1416	G
31	a	1419	A
31	a	1428	C
31	a	1451	C
31	a	1452	G
31	a	1453	A

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Mol	Chain	Res	Type
31	a	1455	G
31	a	1458	U
31	a	1459	G
31	a	1460	U
31	a	1482	G
31	a	1490	A
31	a	1493	C
31	a	1494	A
31	a	1508	A
31	a	1509	A
31	a	1510	G
31	a	1515	A
31	a	1534	U
31	a	1535	A
31	a	1536	C
31	a	1537	G
31	a	1538	G
31	a	1569	A
31	a	1578	U
31	a	1585	C
31	a	1608	A
31	a	1647	U
31	a	1648	U
31	a	1649	G
31	a	1674	G
31	a	1715	G
31	a	1729	U
31	a	1730	C
31	a	1734	G
31	a	1737	G
31	a	1738	G
31	a	1744	A
31	a	1764	C
31	a	1773	A
31	a	1782	U
31	a	1791	A
31	a	1800	C
31	a	1801	A
31	a	1808	A
31	a	1809	A
31	a	1816	C
31	a	1847	A

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Mol	Chain	Res	Type
31	a	1848	A
31	a	1858	A
31	a	1870	C
31	a	1871	A
31	a	1872	A
31	a	1873	G
31	a	1906	G
31	a	1907	G
31	a	1913	A
31	a	1914	C
31	a	1915	3TD
31	a	1929	G
31	a	1930	G
31	a	1931	U
31	a	1937	A
31	a	1938	A
31	a	1955	U
31	a	1967	C
31	a	1970	A
31	a	1971	U
31	a	1972	G
31	a	1991	U
31	a	1993	U
31	a	2020	A
31	a	2023	C
31	a	2031	A
31	a	2033	A
31	a	2043	C
31	a	2055	C
31	a	2056	G
31	a	2060	A
31	a	2061	G
31	a	2062	A
31	a	2069	G7M
31	a	2093	G
31	a	2096	C
31	a	2193	G
31	a	2198	A
31	a	2204	G
31	a	2211	A
31	a	2225	A
31	a	2238	G

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Mol	Chain	Res	Type
31	a	2268	A
31	a	2278	A
31	a	2282	G
31	a	2283	C
31	a	2287	A
31	a	2288	A
31	a	2305	U
31	a	2308	G
31	a	2312	U
31	a	2322	A
31	a	2324	U
31	a	2325	G
31	a	2333	A
31	a	2335	A
31	a	2336	A
31	a	2347	C
31	a	2350	C
31	a	2366	A
31	a	2383	G
31	a	2385	C
31	a	2402	U
31	a	2406	A
31	a	2425	A
31	a	2428	G
31	a	2429	G
31	a	2430	A
31	a	2431	U
31	a	2435	A
31	a	2441	U
31	a	2448	A
31	a	2469	A
31	a	2476	A
31	a	2478	A
31	a	2491	U
31	a	2502	G
31	a	2505	G
31	a	2518	A
31	a	2529	G
31	a	2547	A
31	a	2566	A
31	a	2567	G
31	a	2573	C

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Mol	Chain	Res	Type
31	a	2602	A
31	a	2609	U
31	a	2613	U
31	a	2629	U
31	a	2663	G
31	a	2689	U
31	a	2690	U
31	a	2714	G
31	a	2716	C
31	a	2726	A
31	a	2744	G
31	a	2748	A
31	a	2750	A
31	a	2757	A
31	a	2765	A
31	a	2778	A
31	a	2791	G
31	a	2798	U
31	a	2799	A
31	a	2803	G
31	a	2809	A
31	a	2820	A
31	a	2821	A
31	a	2873	A
31	a	2874	C
31	a	2883	A
31	a	2884	U
32	b	35	C
32	b	36	C
32	b	37	C
32	b	44	G
32	b	56	G
32	b	89	U
32	b	90	C
32	b	109	A

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	7	A
7	A	12	U
7	A	70	U

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Mol	Chain	Res	Type
7	A	73	C
7	A	119	A
7	A	121	U
7	A	199	A
7	A	305	G
7	A	412	A
7	A	438	U
7	A	531	U
7	A	595	A
7	A	641	U
7	A	702	A
7	A	884	U
7	A	991	U
7	A	992	U
7	A	993	G
7	A	1034	G
7	A	1035	A
7	A	1042	A
7	A	1047	G
7	A	1094	G
7	A	1124	G
7	A	1129	C
7	A	1145	A
7	A	1196	A
7	A	1211	U
7	A	1225	A
7	A	1298	U
7	A	1319	A
7	A	1320	C
7	A	1397	C
7	A	1447	A
7	A	1452	C
7	A	1459	G
7	A	1505	G
30	Z	7	G
30	Z	17(A)	U
30	Z	18	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
31	H2U	a	2449	31	18,21,22	0.61	0	21,30,33	0.85	2 (9%)
31	PSU	a	746	59,31	18,21,22	0.91	1 (5%)	22,30,33	0.62	0
18	D2T	L	89	18	7,9,10	0.95	0	6,11,13	2.24	4 (66%)
31	PSU	a	2604	31	18,21,22	0.91	1 (5%)	22,30,33	0.69	0
31	OMG	a	2251	30,58,31	23,26,27	0.33	0	33,38,41	0.39	0
31	5MU	a	1939	58,31	19,22,23	0.28	0	28,32,35	0.35	0
31	5MU	a	747	31	19,22,23	0.27	0	28,32,35	0.37	0
7	5MC	A	967	7	18,22,23	0.32	0	26,32,35	0.49	0
7	2MG	A	966	7	23,26,27	0.38	0	32,38,41	0.40	0
31	PSU	a	2605	31	18,21,22	0.93	1 (5%)	22,30,33	0.74	0
7	4OC	A	1402	7	20,23,24	0.37	0	26,32,35	0.49	0
17	IAS	K	119	17	6,7,8	0.92	0	6,8,10	1.01	0
31	PSU	a	1911	31	18,21,22	0.89	1 (5%)	22,30,33	0.65	0
7	MA6	A	1518	7	23,26,27	0.25	0	34,38,41	0.65	1 (2%)
31	6MZ	a	1618	31	22,25,26	0.31	0	30,36,39	0.52	0
7	MA6	A	1519	7	23,26,27	0.25	0	34,38,41	0.71	1 (2%)
31	3TD	a	1915	31	18,22,23	0.96	1 (5%)	22,32,35	0.63	0
31	2MG	a	2445	31	23,26,27	0.38	0	32,38,41	0.38	0
7	PSU	A	516	7,59	18,21,22	0.90	1 (5%)	22,30,33	0.64	0
31	G7M	a	2069	31	23,26,27	0.74	1 (4%)	35,39,42	0.61	0
31	PSU	a	2580	58,31	18,21,22	0.94	1 (5%)	22,30,33	0.78	1 (4%)
42	MS6	l	82	42	5,7,8	0.24	0	2,7,9	0.04	0
42	4D4	l	81	42	9,11,12	0.50	0	8,13,15	0.60	0
7	2MG	A	1207	7,58	23,26,27	0.39	0	32,38,41	0.42	0
31	PSU	a	2504	58,31	18,21,22	0.89	1 (5%)	22,30,33	0.69	0
31	OMC	a	2498	59,31	19,22,23	0.27	0	26,31,34	0.48	0
31	5MC	a	1962	31	18,22,23	0.33	0	26,32,35	0.48	0
31	2MG	a	1835	31	23,26,27	0.38	0	32,38,41	0.34	0
31	6MZ	a	2030	31	22,25,26	0.31	0	30,36,39	0.59	0
7	G7M	A	527	7	23,26,27	0.72	1 (4%)	35,39,42	0.60	0
31	PSU	a	2457	31	18,21,22	0.91	1 (5%)	22,30,33	0.60	0
31	2MA	a	2503	58,59,31	22,25,26	0.96	1 (4%)	33,37,40	1.08	4 (12%)
31	OMU	a	2552	31	19,22,23	0.20	0	26,31,34	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	MEQ	d	150	34	8,9,10	0.42	0	5,10,12	0.54	0
7	5MC	A	1407	7	18,22,23	0.33	0	26,32,35	0.58	0
7	UR3	A	1498	7	19,22,23	0.28	0	26,32,35	0.68	0
31	1MG	a	745	31	22,26,27	0.49	0	33,39,42	0.47	0
31	PSU	a	1917	31	18,21,22	0.90	1 (5%)	22,30,33	0.54	0
31	PSU	a	955	31	18,21,22	0.92	1 (5%)	22,30,33	0.58	0
7	2MG	A	1516	7	23,26,27	0.37	0	32,38,41	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	H2U	a	2449	31	-	0/7/38/39	0/2/2/2
31	PSU	a	746	59,31	-	3/7/25/26	0/2/2/2
18	D2T	L	89	18	-	2/7/12/14	-
31	PSU	a	2604	31	-	0/7/25/26	0/2/2/2
31	OMG	a	2251	30,58,31	-	1/9/27/28	0/3/3/3
31	5MU	a	1939	58,31	-	0/7/25/26	0/2/2/2
31	5MU	a	747	31	-	0/7/25/26	0/2/2/2
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
7	2MG	A	966	7	-	0/9/27/28	0/3/3/3
31	PSU	a	2605	31	-	0/7/25/26	0/2/2/2
7	4OC	A	1402	7	-	0/9/29/30	0/2/2/2
17	IAS	K	119	17	-	2/7/7/8	-
31	PSU	a	1911	31	-	2/7/25/26	0/2/2/2
7	MA6	A	1518	7	-	0/11/29/30	0/3/3/3
31	6MZ	a	1618	31	-	0/9/27/28	0/3/3/3
7	MA6	A	1519	7	-	0/11/29/30	0/3/3/3
31	3TD	a	1915	31	-	2/7/25/26	0/2/2/2
31	2MG	a	2445	31	-	0/9/27/28	0/3/3/3
7	PSU	A	516	7,59	-	0/7/25/26	0/2/2/2
31	G7M	a	2069	31	-	2/7/25/26	0/3/3/3
31	PSU	a	2580	58,31	-	0/7/25/26	0/2/2/2
42	MS6	l	82	42	-	1/4/6/8	-
42	4D4	l	81	42	-	1/11/12/14	-
7	2MG	A	1207	7,58	-	0/9/27/28	0/3/3/3
31	PSU	a	2504	58,31	-	0/7/25/26	0/2/2/2
31	OMC	a	2498	59,31	-	0/9/27/28	0/2/2/2
31	5MC	a	1962	31	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	2MG	a	1835	31	-	0/9/27/28	0/3/3/3
31	6MZ	a	2030	31	-	2/9/27/28	0/3/3/3
7	G7M	A	527	7	-	1/7/25/26	0/3/3/3
31	PSU	a	2457	31	-	0/7/25/26	0/2/2/2
31	2MA	a	2503	58,59,31	-	3/7/25/26	0/3/3/3
31	OMU	a	2552	31	-	0/9/27/28	0/2/2/2
34	MEQ	d	150	34	-	2/8/9/11	-
7	5MC	A	1407	7	-	0/7/25/26	0/2/2/2
7	UR3	A	1498	7	-	0/7/25/26	0/2/2/2
31	1MG	a	745	31	-	0/7/25/26	0/3/3/3
31	PSU	a	1917	31	-	0/7/25/26	0/2/2/2
31	PSU	a	955	31	-	0/7/25/26	0/2/2/2
7	2MG	A	1516	7	-	0/9/27/28	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	2580	PSU	C6-C5	3.74	1.39	1.35
31	a	2605	PSU	C6-C5	3.66	1.39	1.35
31	a	1915	3TD	C6-C5	3.64	1.39	1.35
31	a	746	PSU	C6-C5	3.62	1.39	1.35
31	a	2457	PSU	C6-C5	3.59	1.39	1.35
31	a	955	PSU	C6-C5	3.58	1.39	1.35
7	A	516	PSU	C6-C5	3.55	1.39	1.35
31	a	1917	PSU	C6-C5	3.53	1.39	1.35
31	a	2504	PSU	C6-C5	3.53	1.39	1.35
31	a	2604	PSU	C6-C5	3.53	1.39	1.35
31	a	1911	PSU	C6-C5	3.51	1.39	1.35
31	a	2069	G7M	C8-N7	2.74	1.38	1.33
7	A	527	G7M	C8-N7	2.60	1.37	1.33
31	a	2503	2MA	C6-N6	-2.34	1.28	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	89	D2T	CB-CA-N	3.81	117.23	109.10
7	A	1518	MA6	C2-N1-C6	2.92	118.65	111.75
31	a	2503	2MA	C5-C4-N3	-2.90	123.93	127.19
7	A	1519	MA6	C2-N1-C6	2.90	118.61	111.75
31	a	2503	2MA	CM2-C2-N1	2.85	121.61	117.15
18	L	89	D2T	OD1-CG-CB	-2.53	117.15	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	2449	H2U	O2-C2-N1	-2.31	120.20	123.11
31	a	2580	PSU	C3'-C2'-C1'	2.30	104.32	101.64
31	a	2449	H2U	N3-C2-N1	2.17	118.95	116.65
31	a	2503	2MA	C2-N1-C6	2.17	121.46	118.08
18	L	89	D2T	OD2-CG-CB	2.16	117.83	113.15
31	a	2503	2MA	N3-C2-N1	-2.13	121.80	125.72
18	L	89	D2T	O-C-CA	-2.07	119.34	124.78

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	a	746	PSU	C2'-C1'-C5-C4
31	a	1911	PSU	O4'-C1'-C5-C4
31	a	1911	PSU	O4'-C1'-C5-C6
31	a	1915	3TD	C3'-C4'-C5'-O5'
31	a	1915	3TD	O4'-C4'-C5'-O5'
31	a	2030	6MZ	O4'-C4'-C5'-O5'
31	a	2251	OMG	C1'-C2'-O2'-CM2
31	a	2030	6MZ	C3'-C4'-C5'-O5'
34	d	150	MEQ	NE2-CD-CG-CB
34	d	150	MEQ	OE1-CD-CG-CB
18	L	89	D2T	CG-CB-SB-CB1
42	l	82	MS6	CB-CG-SD-CE
31	a	2069	G7M	C4'-C5'-O5'-P
31	a	2503	2MA	C4'-C5'-O5'-P
31	a	746	PSU	O4'-C1'-C5-C4
31	a	1962	5MC	O4'-C1'-N1-C6
31	a	1962	5MC	C2'-C1'-N1-C6
17	K	119	IAS	O-C-CA-N
18	L	89	D2T	SB-CB-CG-OD2
7	A	527	G7M	C3'-C4'-C5'-O5'
31	a	2503	2MA	O4'-C4'-C5'-O5'
31	a	746	PSU	O4'-C1'-C5-C6
31	a	2503	2MA	O4'-C1'-N9-C8
17	K	119	IAS	CA-CB-CG-OD1
31	a	2069	G7M	O4'-C4'-C5'-O5'
31	a	1962	5MC	O4'-C1'-N1-C2
42	l	81	4D4	O-C-CA-CB
31	a	1962	5MC	C2'-C1'-N1-C2

There are no ring outliers.

8 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	89	D2T	2	0
31	a	2604	PSU	1	0
31	a	2251	OMG	1	0
31	a	1939	5MU	1	0
17	K	119	IAS	1	0
7	A	1518	MA6	1	0
7	A	1519	MA6	1	0
31	a	2030	6MZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 417 ligands modelled in this entry, 417 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.

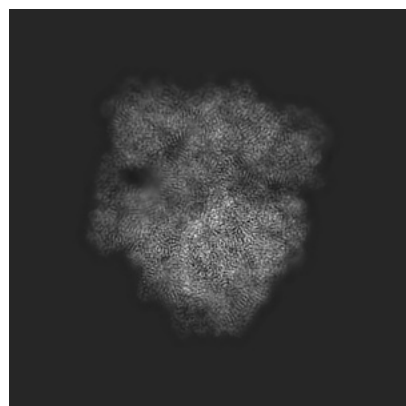
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51353. These allow visual inspection of the internal detail of the map and identification of artifacts.

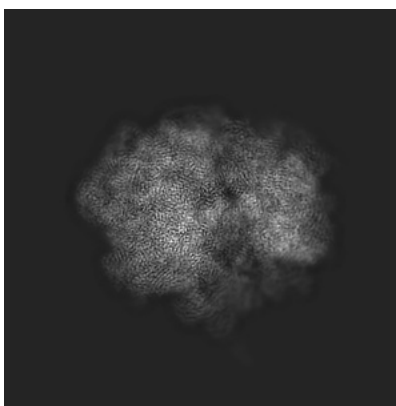
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

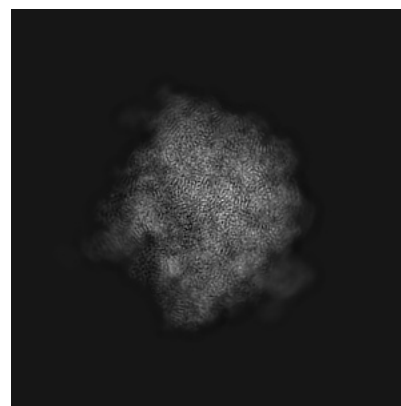
6.1.1 Primary map



X

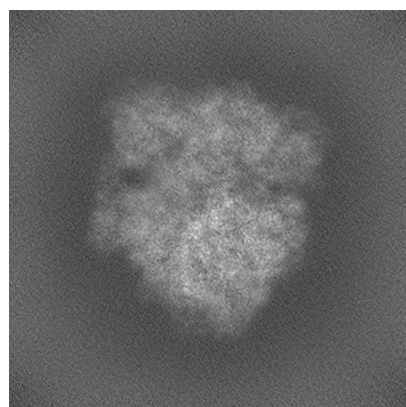


Y

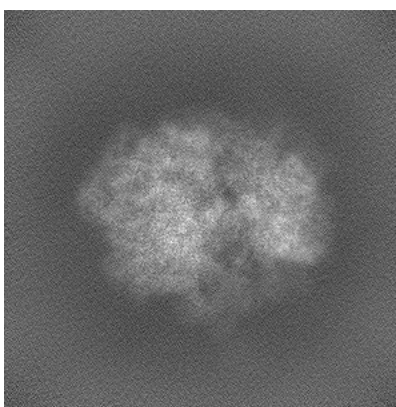


Z

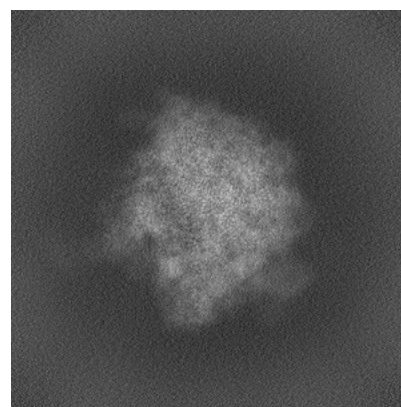
6.1.2 Raw map



X



Y

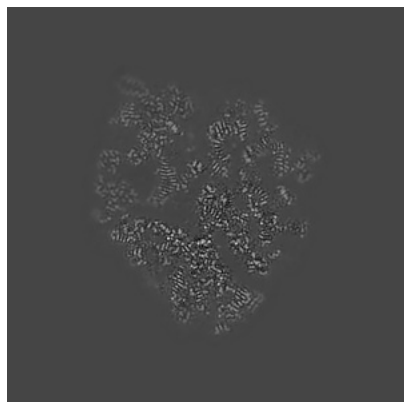


Z

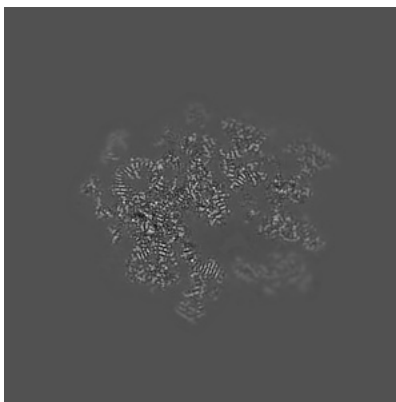
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

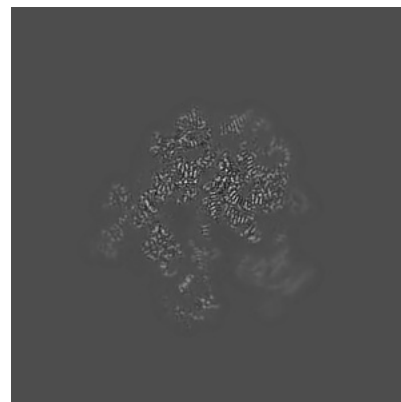
6.2.1 Primary map



X Index: 300

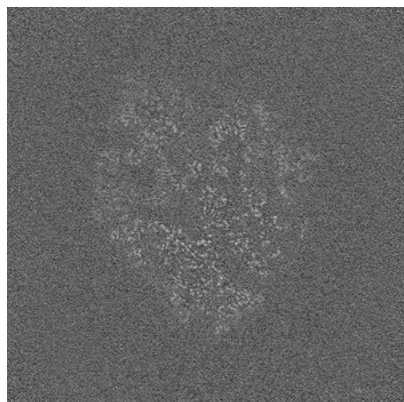


Y Index: 300

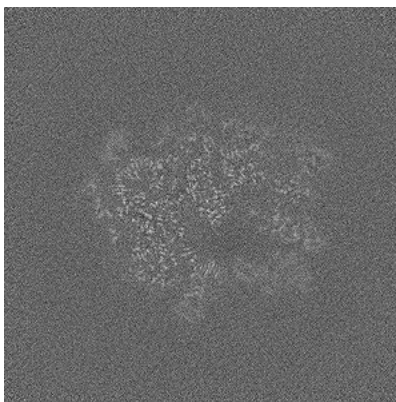


Z Index: 300

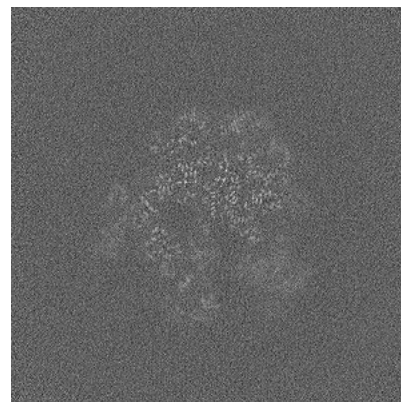
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

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

6.3 Largest variance slices [i](#)

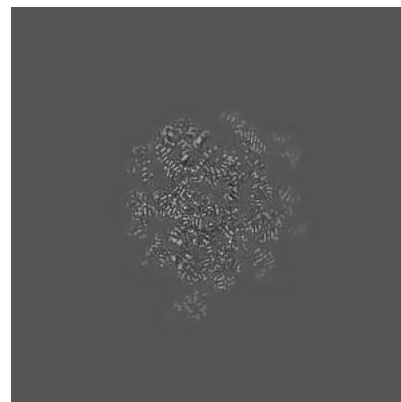
6.3.1 Primary map



X Index: 286

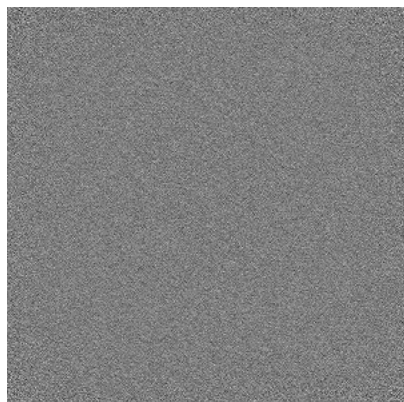


Y Index: 319

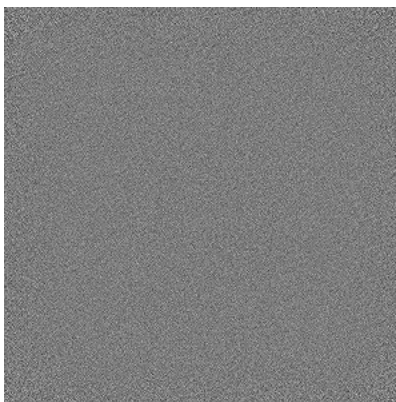


Z Index: 241

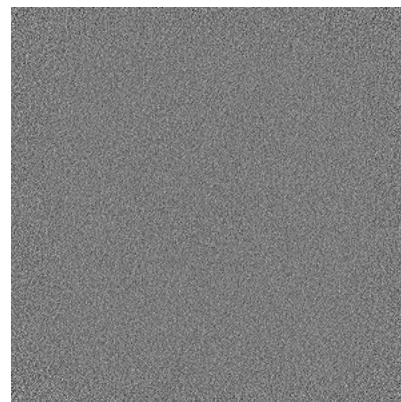
6.3.2 Raw map



X Index: 0



Y Index: 0

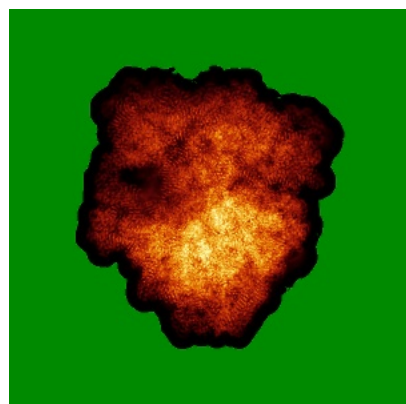


Z Index: 0

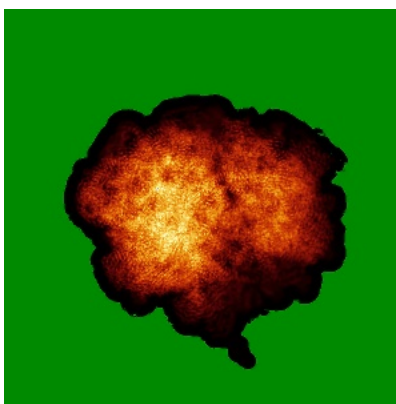
The images above show the largest variance slices of the map in three orthogonal directions.

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

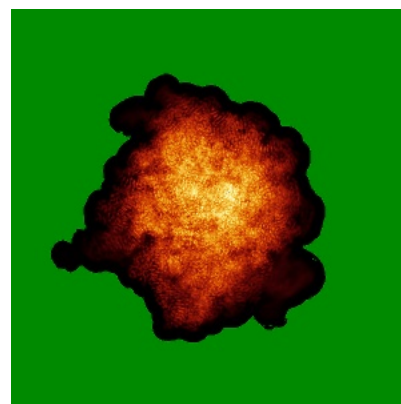
6.4.1 Primary map



X

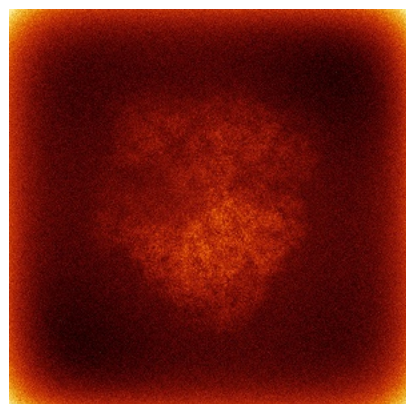


Y

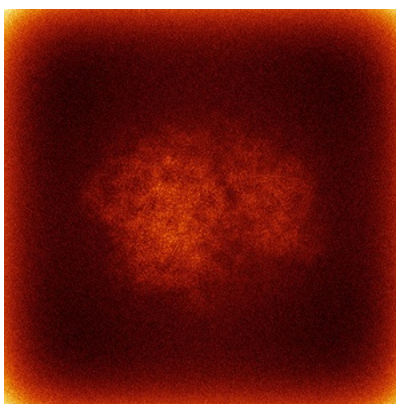


Z

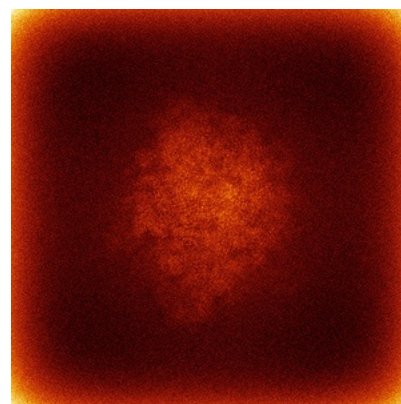
6.4.2 Raw map



X



Y

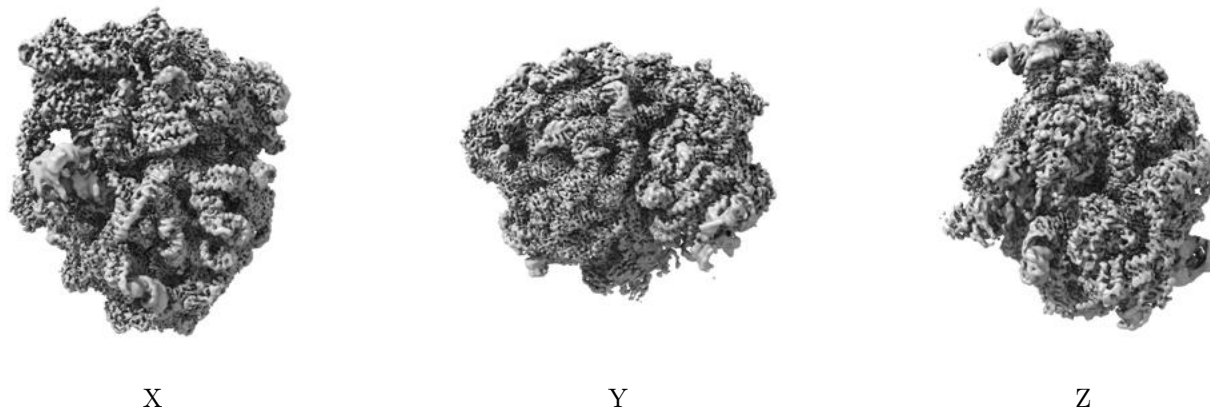


Z

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.

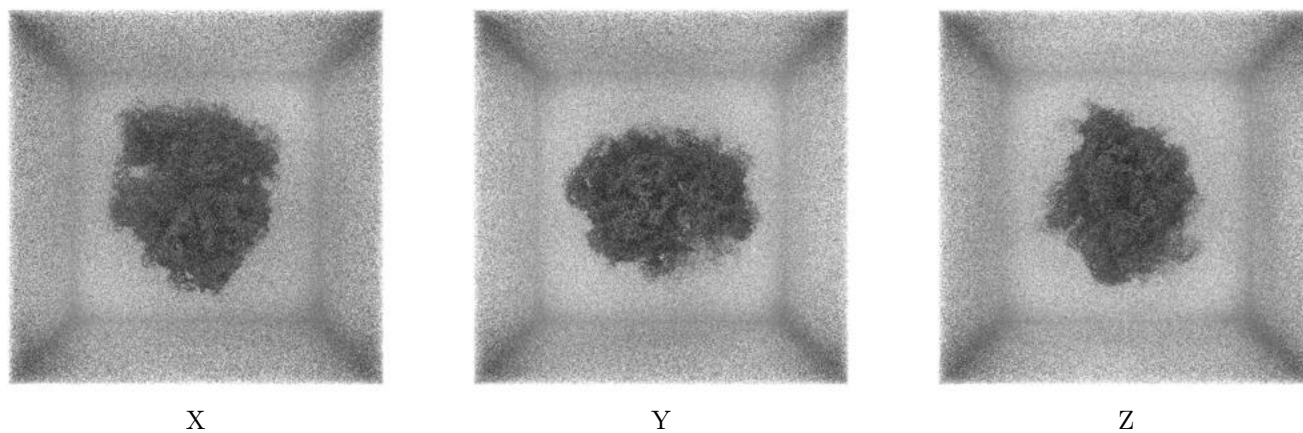
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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



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.

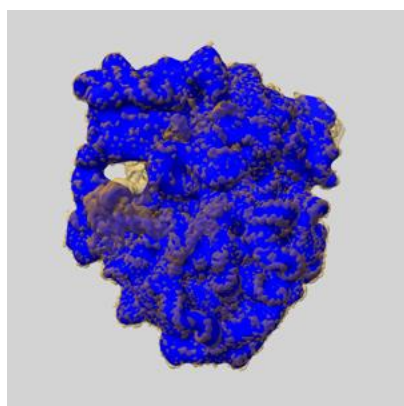
6.6 Mask visualisation [i](#)

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

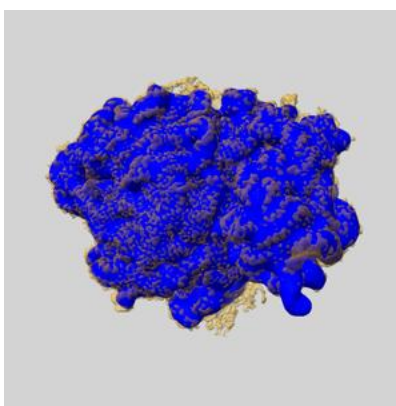
A mask typically either:

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

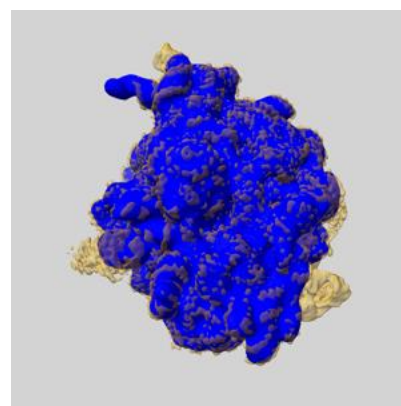
6.6.1 emd_51353_msk_1.map [i](#)



X



Y

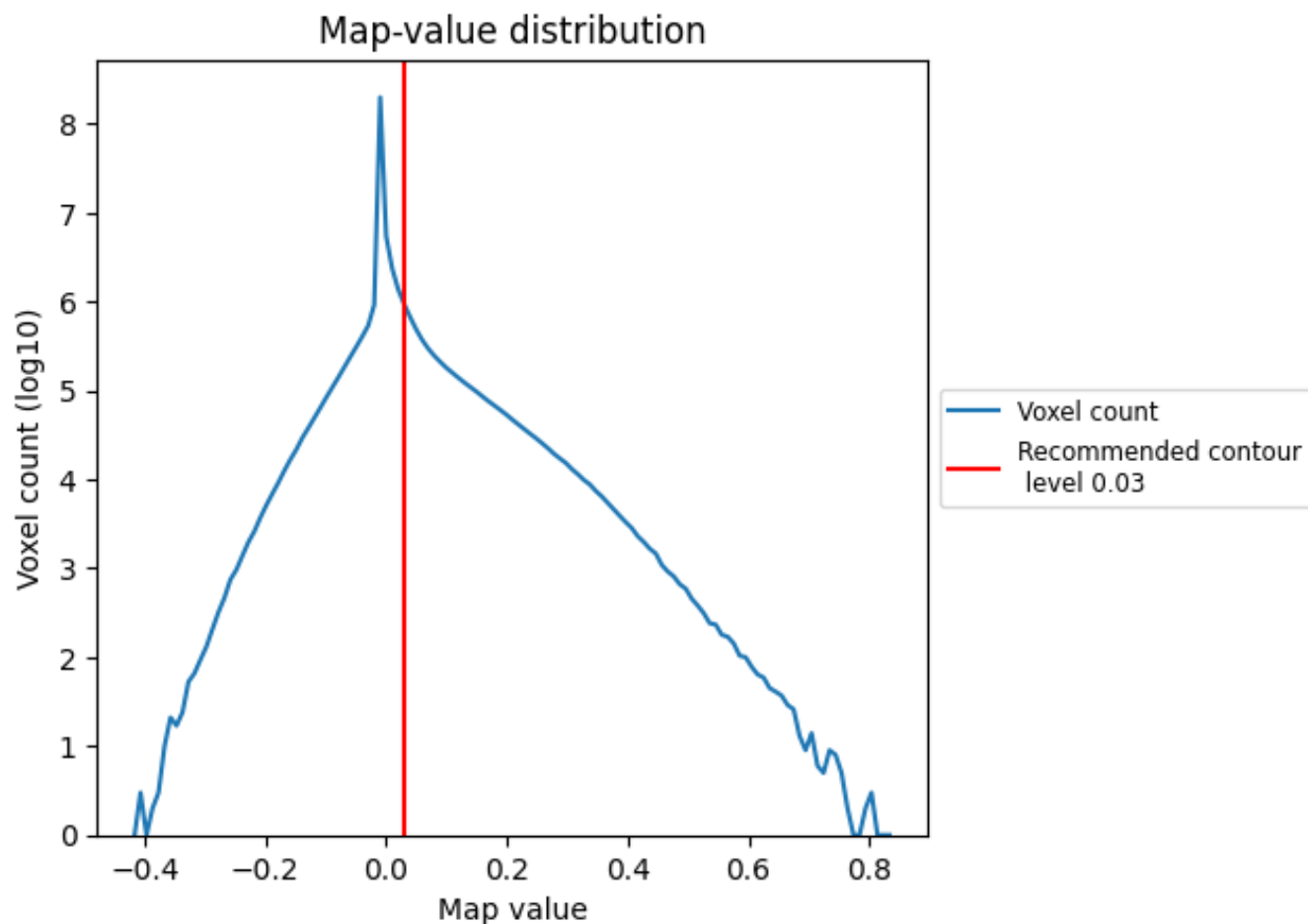


Z

7 Map analysis [i](#)

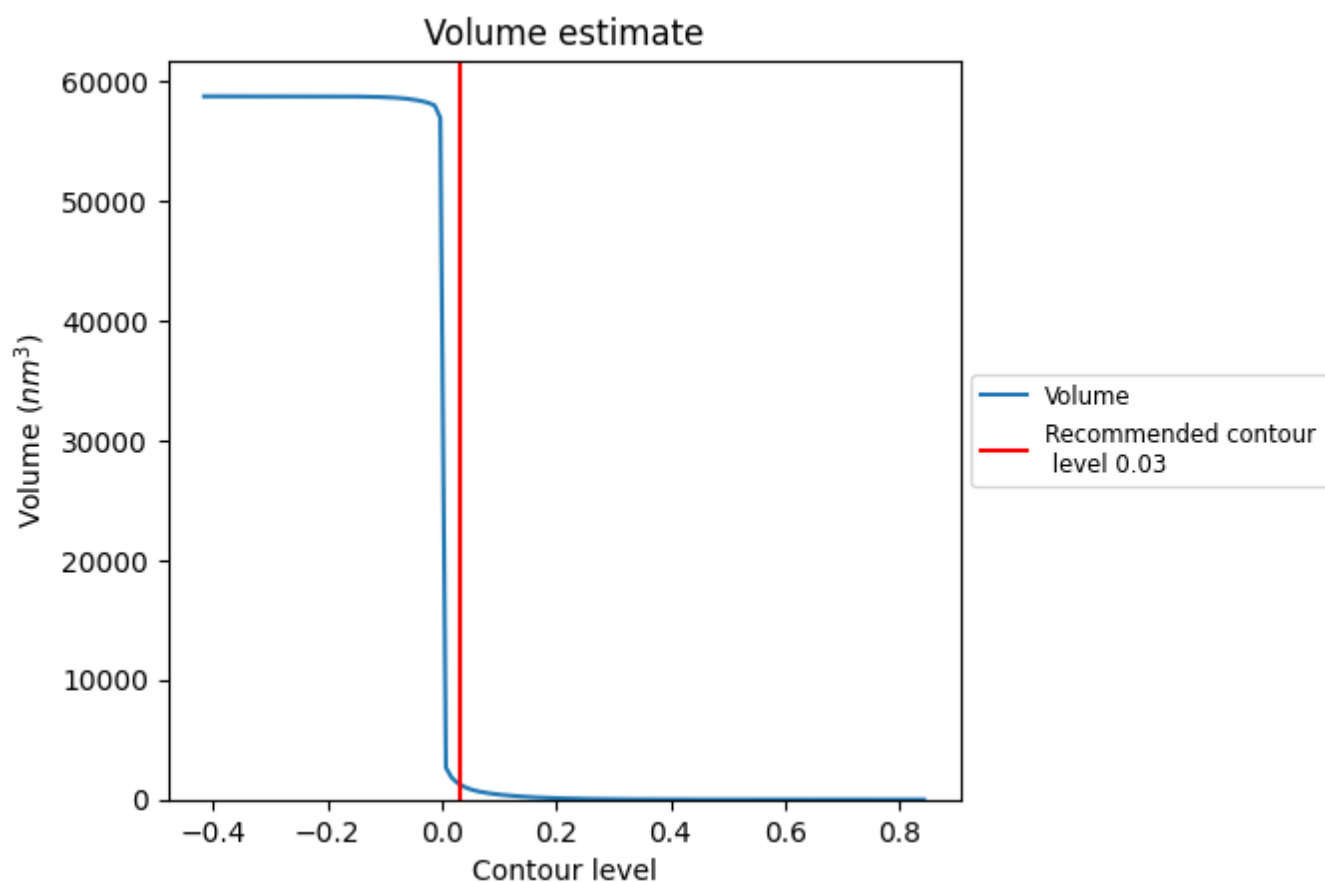
This section contains the results of statistical analysis of the map.

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.

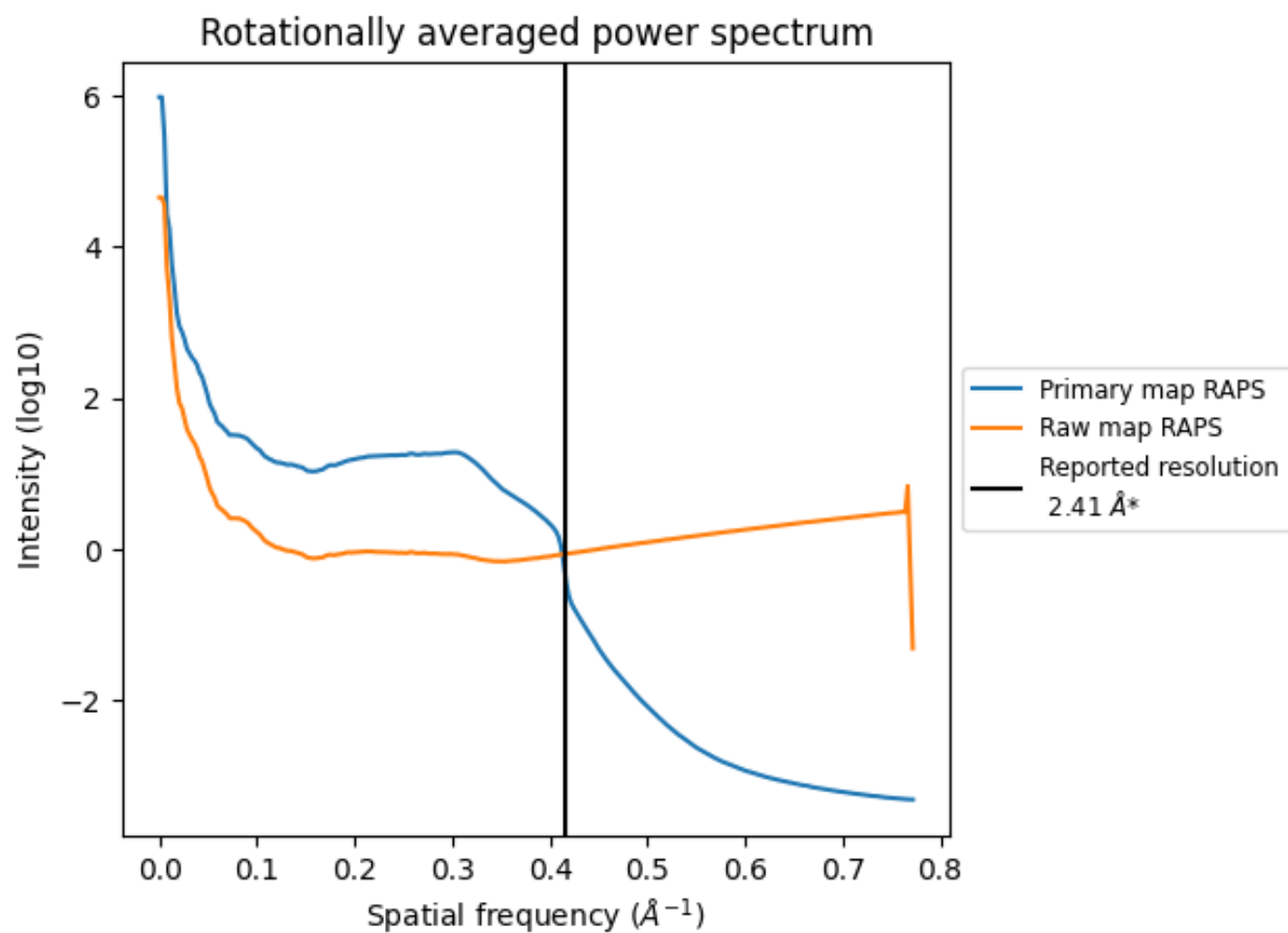
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1309 nm^3 ; this corresponds to an approximate mass of 1183 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 ⓘ

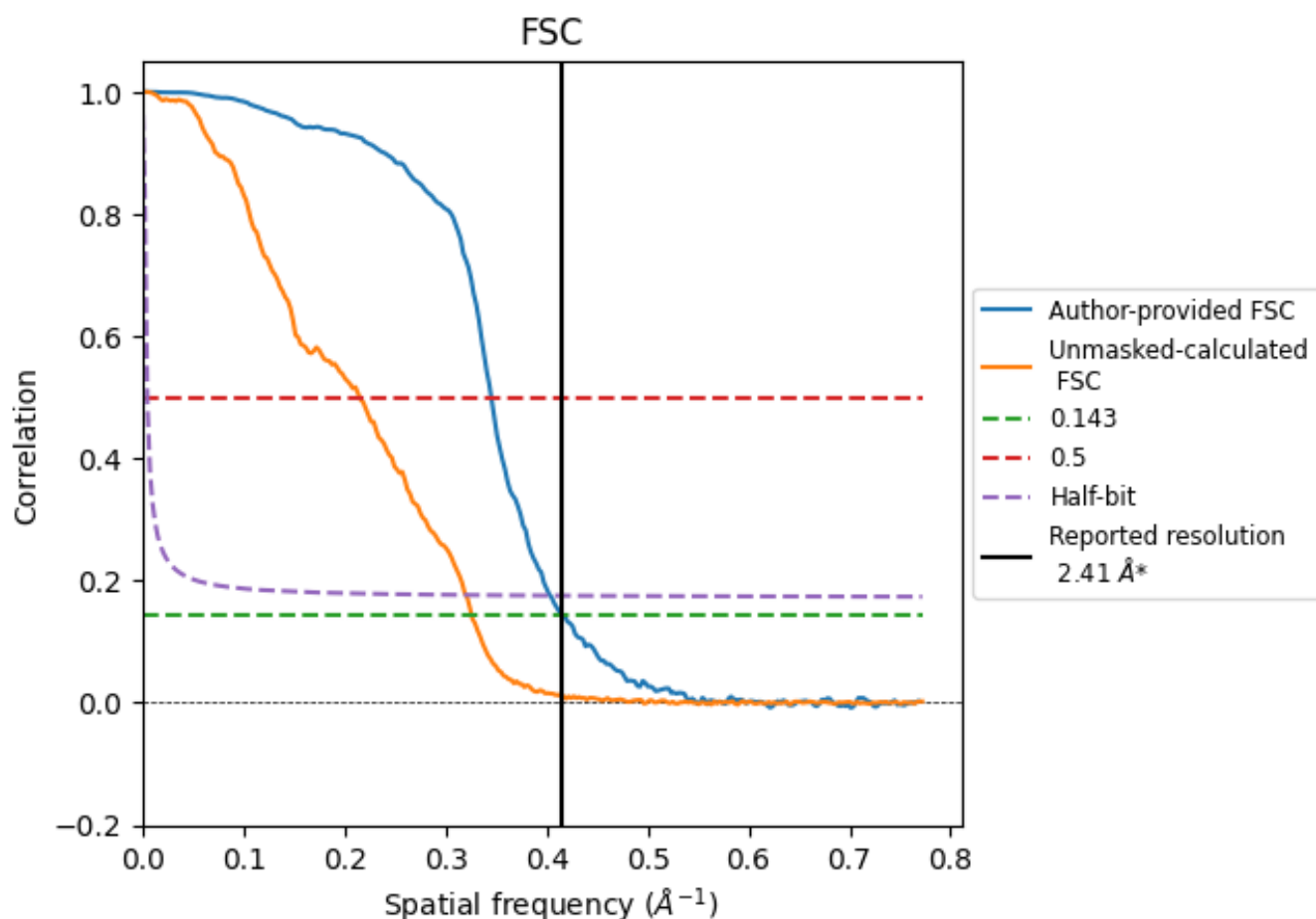


*Reported resolution corresponds to spatial frequency of 0.415 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.415 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

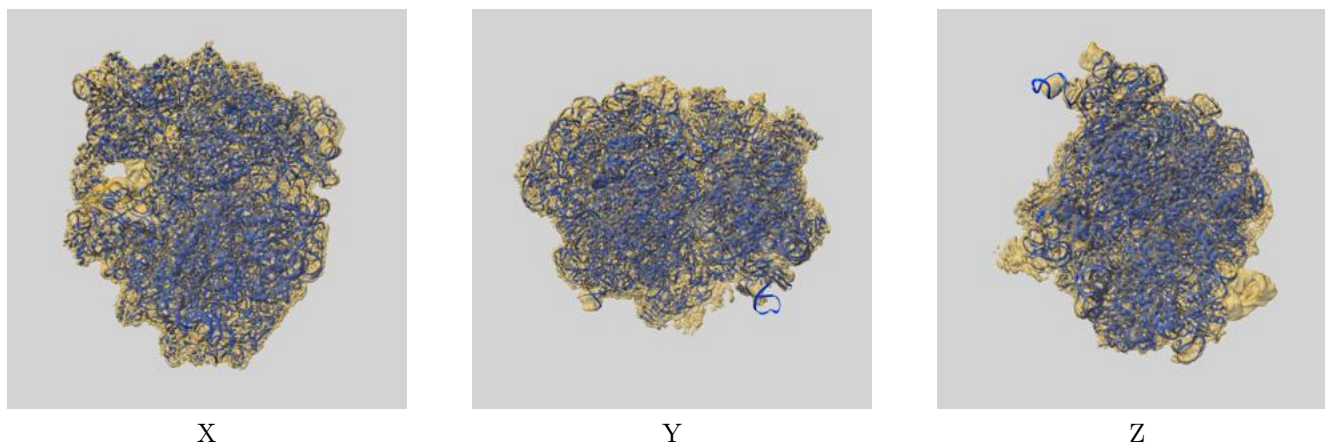
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.41	-	-
Author-provided FSC curve	2.41	2.90	2.48
Unmasked-calculated*	3.07	4.65	3.12

*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 3.07 differs from the reported value 2.41 by more than 10 %

9 Map-model fit [i](#)

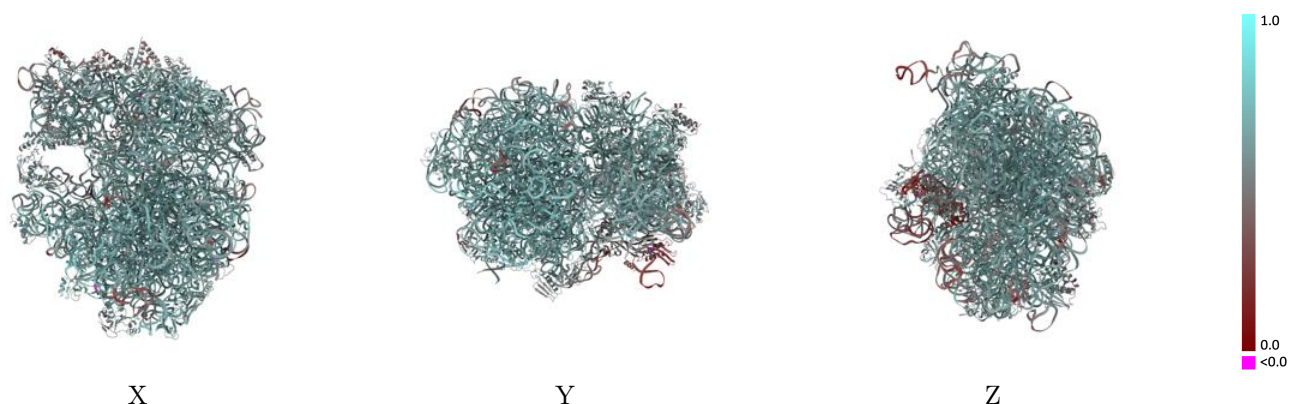
This section contains information regarding the fit between EMDB map EMD-51353 and PDB model 9GHD. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



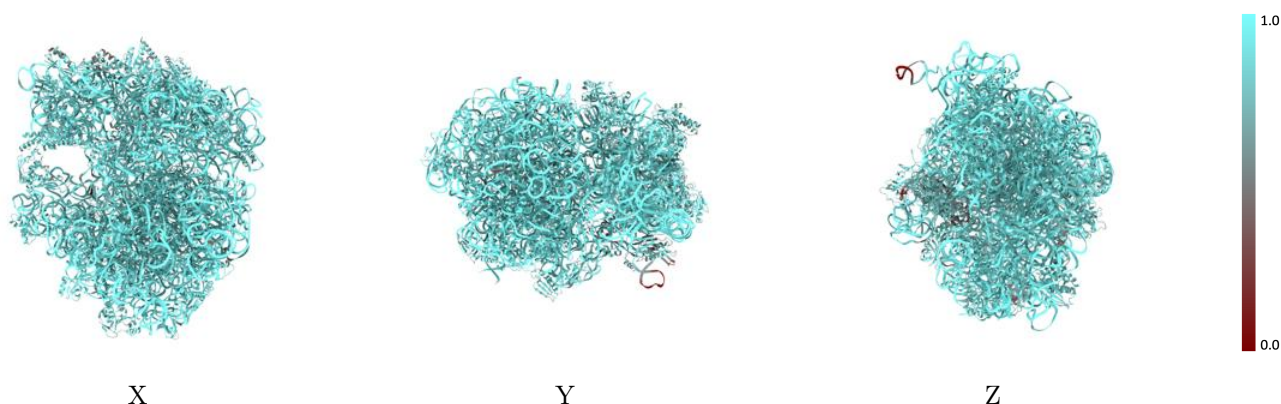
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



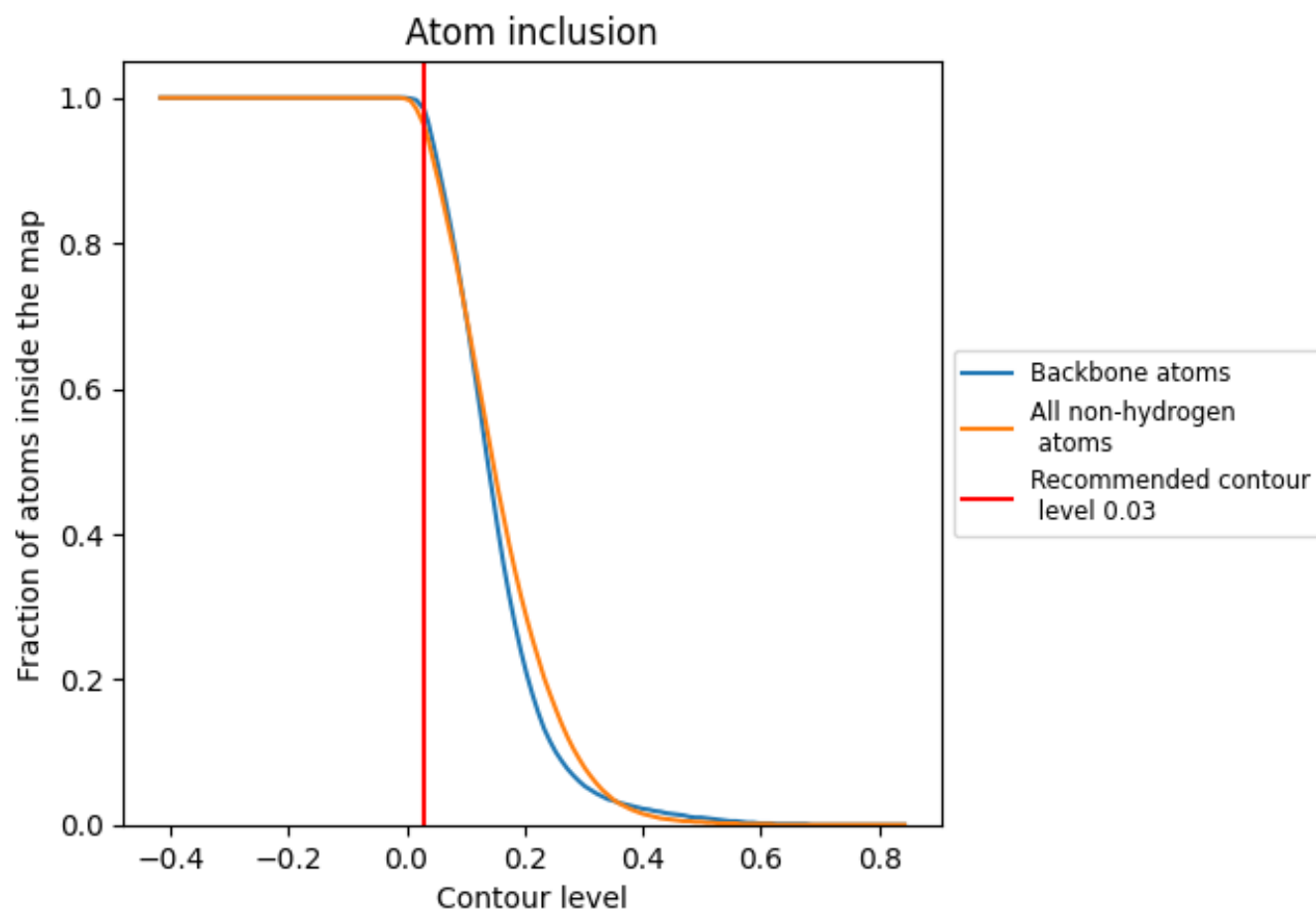
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9620	 0.6240
0	 0.9330	 0.6220
1	 0.9970	 0.7090
2	 0.9980	 0.6990
3	 0.9630	 0.6300
4	 0.8370	 0.4940
9	 0.9870	 0.6180
A	 0.9820	 0.6220
B	 0.8210	 0.5000
C	 0.8980	 0.5630
D	 0.9090	 0.5680
E	 0.9430	 0.6170
F	 0.9130	 0.5560
G	 0.8640	 0.5350
H	 0.9530	 0.6170
I	 0.9020	 0.5510
J	 0.8200	 0.4980
K	 0.9240	 0.5970
L	 0.9430	 0.6120
M	 0.9050	 0.5690
N	 0.9260	 0.5700
O	 0.9360	 0.6030
P	 0.9360	 0.6020
Q	 0.9250	 0.5740
R	 0.9280	 0.5850
S	 0.8940	 0.5490
T	 0.9440	 0.5970
U	 0.8570	 0.5340
V	 0.6450	 0.3290
W	 0.6640	 0.3060
Z	 0.9530	 0.5880
a	 0.9900	 0.6550
b	 0.9910	 0.6330
c	 0.9800	 0.6800
d	 0.9700	 0.6680



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Chain	Atom inclusion	Q-score
e	 0.9360	 0.6270
f	 0.8890	 0.5440
g	 0.8770	 0.5400
h	 0.8970	 0.5560
i	 0.9750	 0.6620
j	 0.9510	 0.6490
k	 0.9660	 0.6570
l	 0.9650	 0.6520
m	 0.9930	 0.6870
n	 0.9320	 0.6000
o	 0.9480	 0.6450
p	 0.9870	 0.6920
q	 0.9400	 0.6290
r	 0.9650	 0.6590
s	 0.9350	 0.6080
t	 0.9480	 0.6070
u	 0.9120	 0.6000
v	 0.9730	 0.6690
w	 0.9680	 0.6590
x	 0.9210	 0.5830
y	 0.9540	 0.6570
z	 0.9780	 0.6680