



Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 11:26 PM EDT

PDB ID : 4V73 / pdb_00004v73
EMDB ID : EMD-2473
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in hybrid pre-translocation state (pre5a)
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on : 2013-10-14
Resolution : 15.00 Å(reported)
Based on initial models : 2HGP, 2K4C, 2WRI, 3I1O

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:

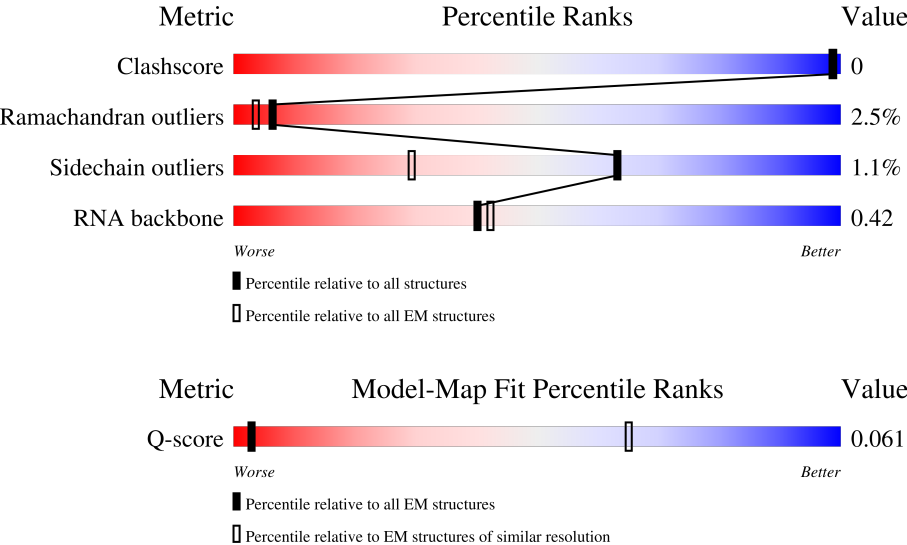
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 15.00 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	37 (14.50 - 15.50)

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	AB	220	42% 97%
2	AC	208	41% 97%
3	AD	206	43% 95%

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Mol	Chain	Length	Quality of chain
4	AE	152	29% 94% 6%
5	AF	101	32% 91% 8%
6	AG	152	27% 97%
7	AH	130	37% 95%
8	AI	128	23% 95% 5%
9	AJ	100	32% 94% 6%
10	AK	118	40% 97%
11	AL	124	38% 90% 9%
12	AM	115	30% 95%
13	AN	101	30% 95%
14	AO	89	35% 94%
15	AP	81	43% 98%
16	AQ	82	39% 95%
17	AR	57	33% 95% 5%
18	AS	81	12% 98%
19	AT	86	19% 100%
20	AU	53	53% 81% 15%
21	AA	1533	8% 60% 32% 7%
22	A1	76	12% 54% 36% 9%
23	A2	15	47% 33% 47% 20%
24	A3	77	21% 65% 27% 5%
25	BC	273	48% 97%
26	BD	209	48% 95% 5%
27	BE	201	35% 96%
28	BF	179	26% 97%

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Mol	Chain	Length	Quality of chain
29	BG	177	
30	BH	149	
31	BI	142	
32	BJ	142	
33	BK	123	
34	BL	144	
35	BM	136	
36	BN	121	
37	BO	117	
38	BP	115	
39	BQ	118	
40	BR	103	
41	BS	110	
42	BT	94	
43	BU	104	
44	BV	94	
45	BW	80	
46	BX	79	
47	BY	63	
48	BZ	59	
49	B0	57	
50	B1	52	
51	B2	46	
52	B3	65	
53	B4	38	

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Mol	Chain	Length	Quality of chain
54	BA	2903	11% 60% 33% 6%
55	BB	118	19% 67% 30%
56	B5	234	38% 94% 5%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147653 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 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	220	Total	C	N	O	S	0	1
			1708	1083	306	312	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	7	ACE	-	acetylation	UNP P0A7V0
AB	226	NH2	-	amidation	UNP P0A7V0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	207	Total	C	N	O	S	0	1
			1625	1028	306	288	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	207	NH2	-	amidation	UNP P0A7V3

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	152	Total	C	N	O	S	0	1
			1109	689	212	202	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	acetylation	UNP P0A7W1
AE	159	NH2	-	amidation	UNP P0A7W1

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	101	Total	C	N	O	S	0	1
			818	515	149	148	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	101	NH2	-	amidation	UNP P02358

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	152	Total	C	N	O	S	0	1
			1178	732	227	215	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	acetylation	UNP P02359
AG	152	NH2	-	amidation	UNP P02359

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AI	128	Total	C	N	O	S	0	0
			1025	636	206	180	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	2	ACE	-	acetylation	UNP P0A7X3

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AJ	100	Total	C	N	O	S	0	1
			790	495	151	143	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	acetylation	UNP P0A7R5
AJ	103	NH2	-	amidation	UNP P0A7R5

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	118	Total	C	N	O	S	0	0
			880	542	174	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	11	ACE	-	acetylation	UNP P0A7R9

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AM	114	Total	C	N	O	S	0	1
			877	541	178	155	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AM	114	NH2	-	amidation	UNP P0A7S9

- Molecule 13 is a protein called 30S ribosomal protein S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	81	Total	C	N	O	S	0	1
			639	400	127	111	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	81	NH2	-	amidation	UNP P0A7T3

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	82	Total	C	N	O	S	0	1
			652	413	122	114	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	acetylation	UNP P0AG63
AQ	83	NH2	-	amidation	UNP P0AG63

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AR	57	Total	C	N	O		0	1
			459	290	87	82			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	18	ACE	-	acetylation	UNP P0A7T7

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Chain	Residue	Modelled	Actual	Comment	Reference
AR	74	NH2	-	amidation	UNP P0A7T7

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AS	81	Total	C	N	O	S	0	1
			641	410	121	108	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	acetylation	UNP P0A7U3
AS	81	NH2	-	amidation	UNP P0A7U3

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AT	86	Total	C	N	O	S	0	0
			668	413	137	115	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	1	ACE	-	acetylation	UNP P0A7U7

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AU	53	Total	C	N	O	S	0	1
			429	267	87	74	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	acetylation	UNP P68679
AU	54	NH2	-	amidation	UNP P68679

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0
			32828	14642	6024	10633	1529		

- Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A1	76	Total	C	N	O	P	S	0	0
			1627	728	292	531	75	1		

- Molecule 23 is a RNA chain called 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	15	Total	C	N	O	P	0	0
			309	140	46	109	14		

- Molecule 24 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A3	77	Total	C	N	O	P	S	0	0
			1642	734	297	534	76	1		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BC	272	Total	C	N	O	S	0	1
			2083	1288	424	364	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	272	NH2	-	amidation	UNP P60422

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

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

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	123	Total	C	N	O	S	0	1
			939	587	181	165	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	123	NH2	-	amidation	UNP P0ADY3

- Molecule 34 is a protein called 50S ribosomal protein L15.

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

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BN	121	Total	C	N	O	S	0	1
			961	593	197	166	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	121	NH2	-	amidation	UNP P0AG44

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BT	94	Total	C	N	O	S	0	1
			739	466	140	131	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	94	NH2	-	amidation	UNP P0ADZ0

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	BU	103	Total	C	N	O	0	1
			780	492	147	141		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	103	NH2	-	amidation	UNP P60624

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BW	80	Total	C	N	O	S	0	0
			599	369	120	109	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	5	ACE	-	acetylation	UNP P0A7L8

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BX	-1	ACE	-	acetylation	UNP P0A7M2

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	B1	52	Total	C	N	O	0	1
			413	265	76	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	2	ACE	-	acetylation	UNP P0A7N9
B1	53	NH2	-	amidation	UNP P0A7N9

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BA	2903	Total	C	N	O	P	0	0
			62317	27801	11467	20147	2902		

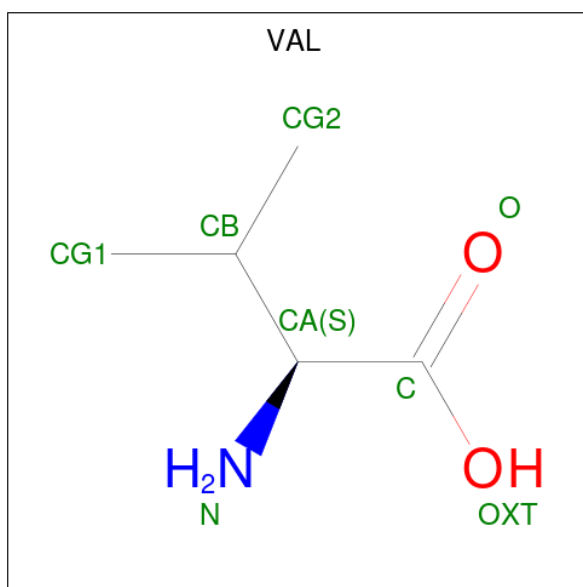
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BB	117	Total	C	N	O	P	0	0
			2504	1116	459	813	116		

- Molecule 56 is a protein called 50S ribosomal protein L1.

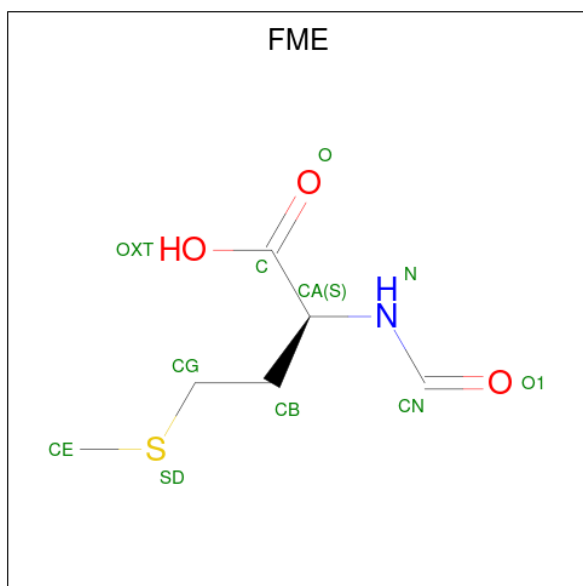
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (CCD ID: VAL) (formula: C₅H₁₁NO₂).



Mol	Chain	Residues	Atoms				AltConf
57	A1	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 58 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).

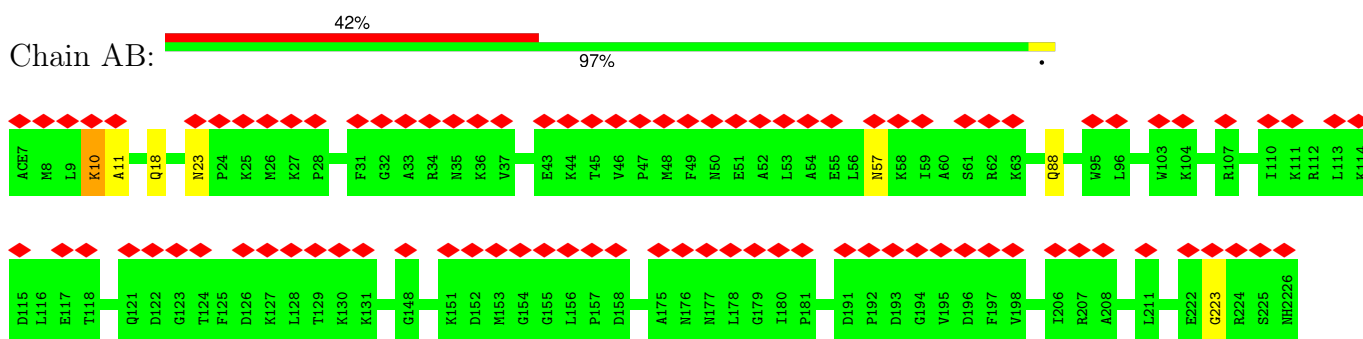


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

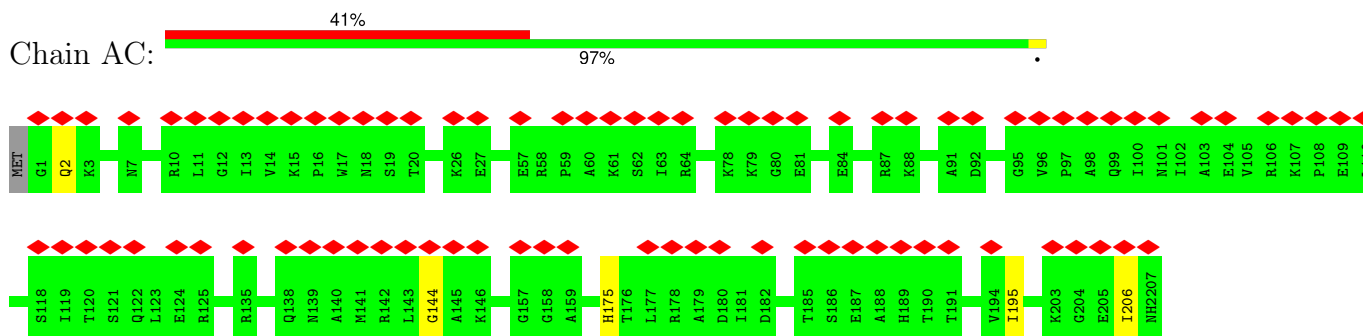
3 Residue-property plots

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

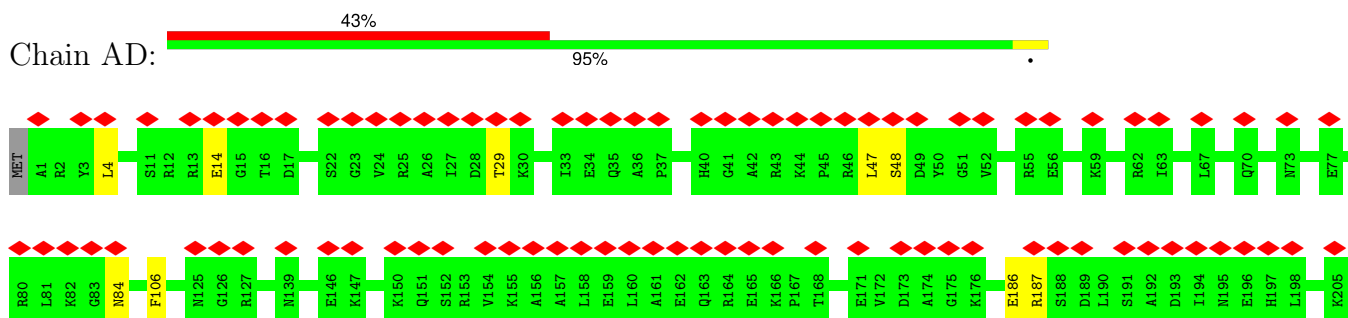
- Molecule 1: 30S ribosomal protein S2



- Molecule 2: 30S ribosomal protein S3

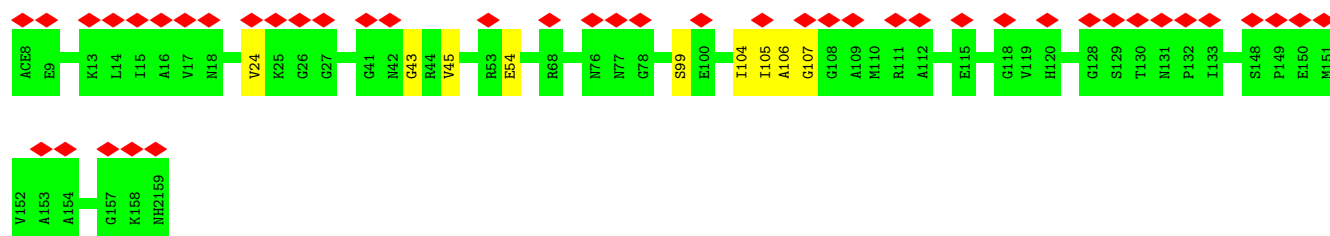


- Molecule 3: 30S ribosomal protein S4

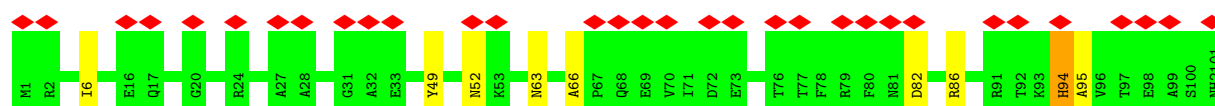
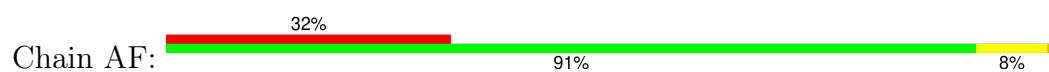


- Molecule 4: 30S ribosomal protein S5

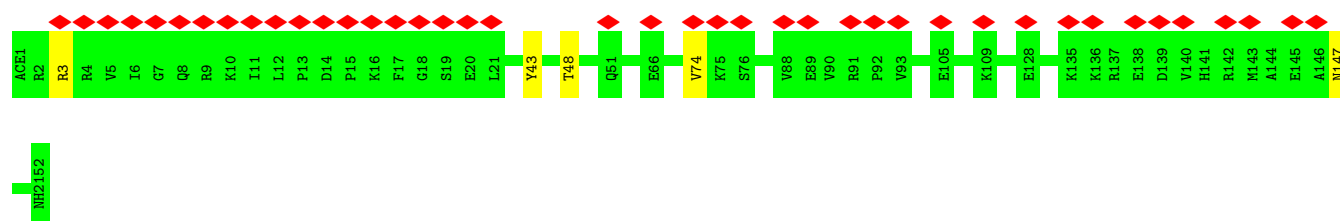




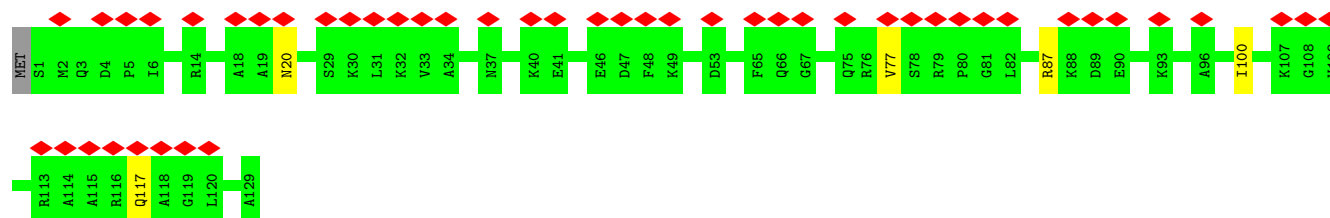
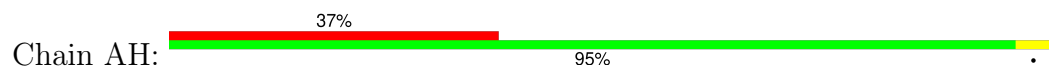
• Molecule 5: 30S ribosomal protein S6



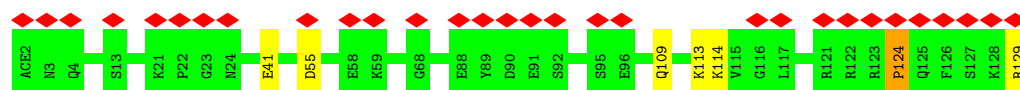
• Molecule 6: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S8

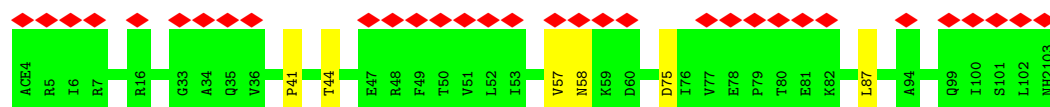


• Molecule 8: 30S ribosomal protein S9

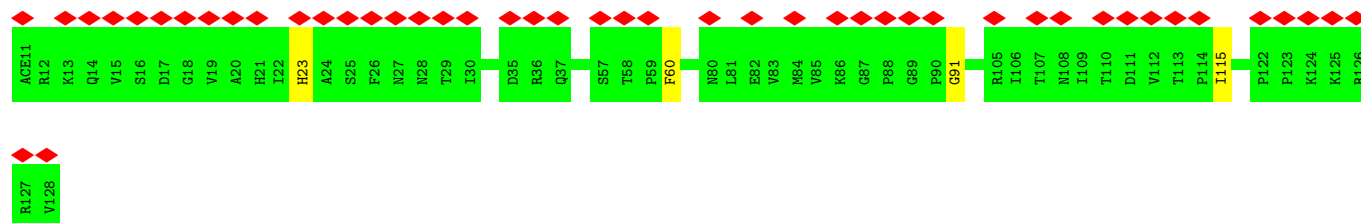
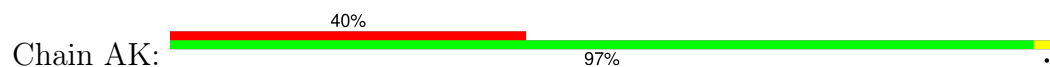


• Molecule 9: 30S ribosomal protein S10

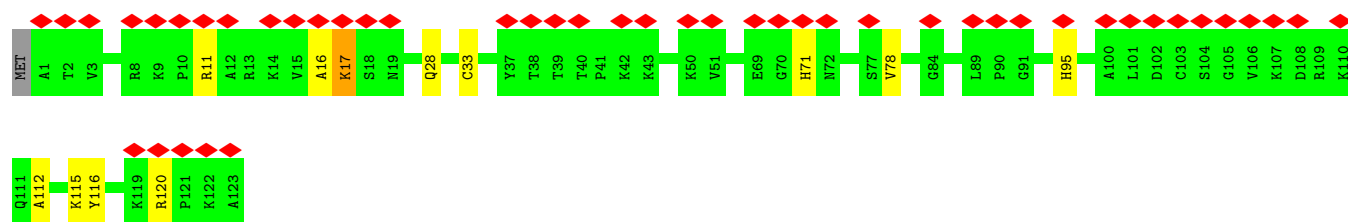
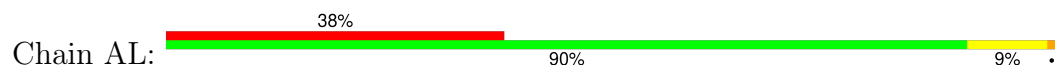




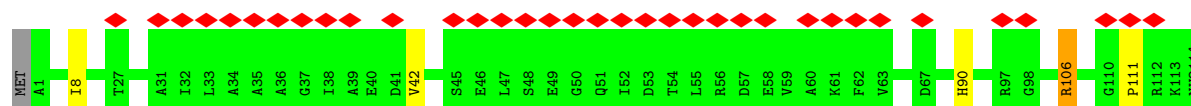
- Molecule 10: 30S ribosomal protein S11



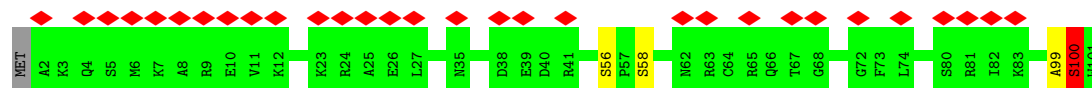
- Molecule 11: 30S ribosomal protein S12



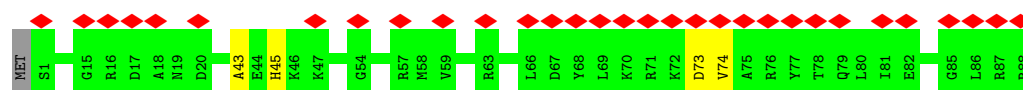
- Molecule 12: 30S ribosomal protein S13



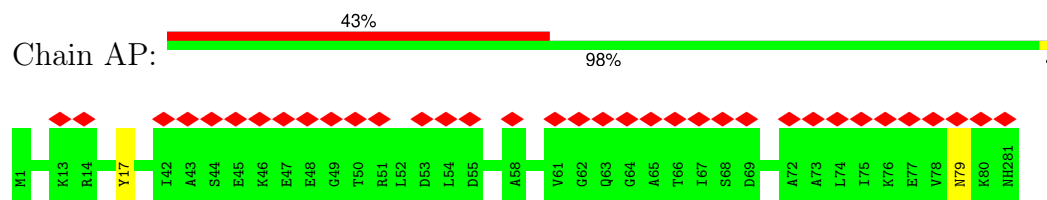
- Molecule 13: 30S ribosomal protein S14



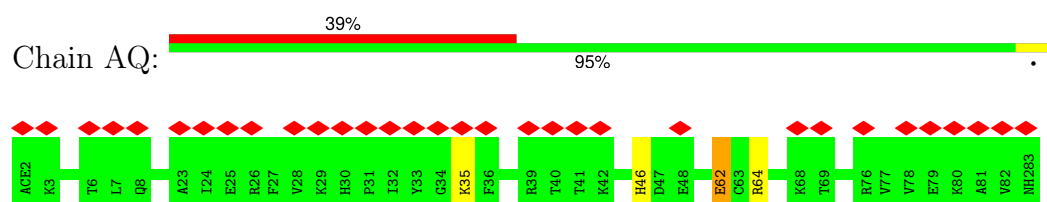
- Molecule 14: 30S ribosomal protein S15



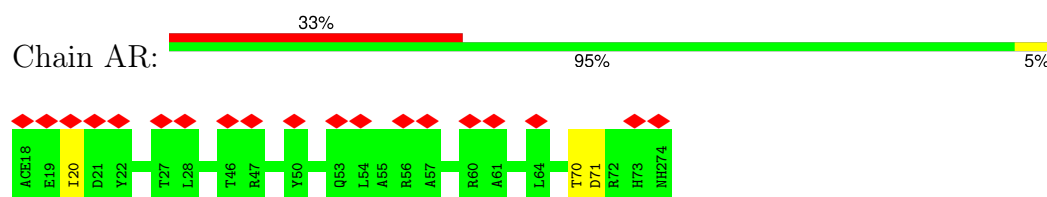
- Molecule 15: 30S ribosomal protein S16



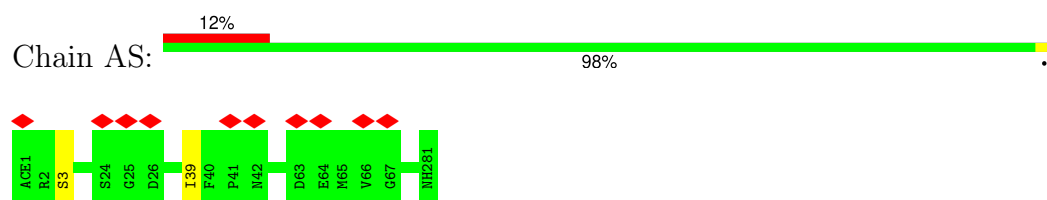
- Molecule 16: 30S ribosomal protein S17



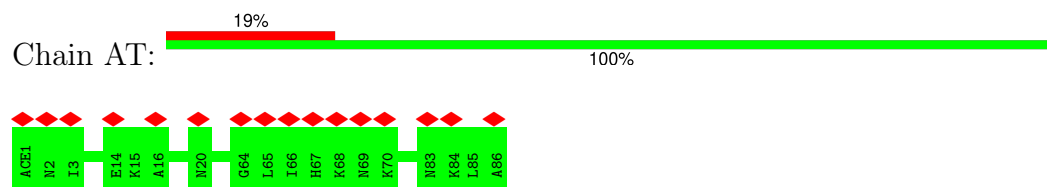
- Molecule 17: 30S ribosomal protein S18



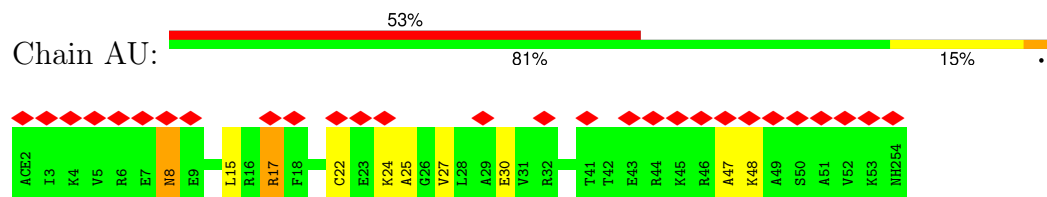
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20

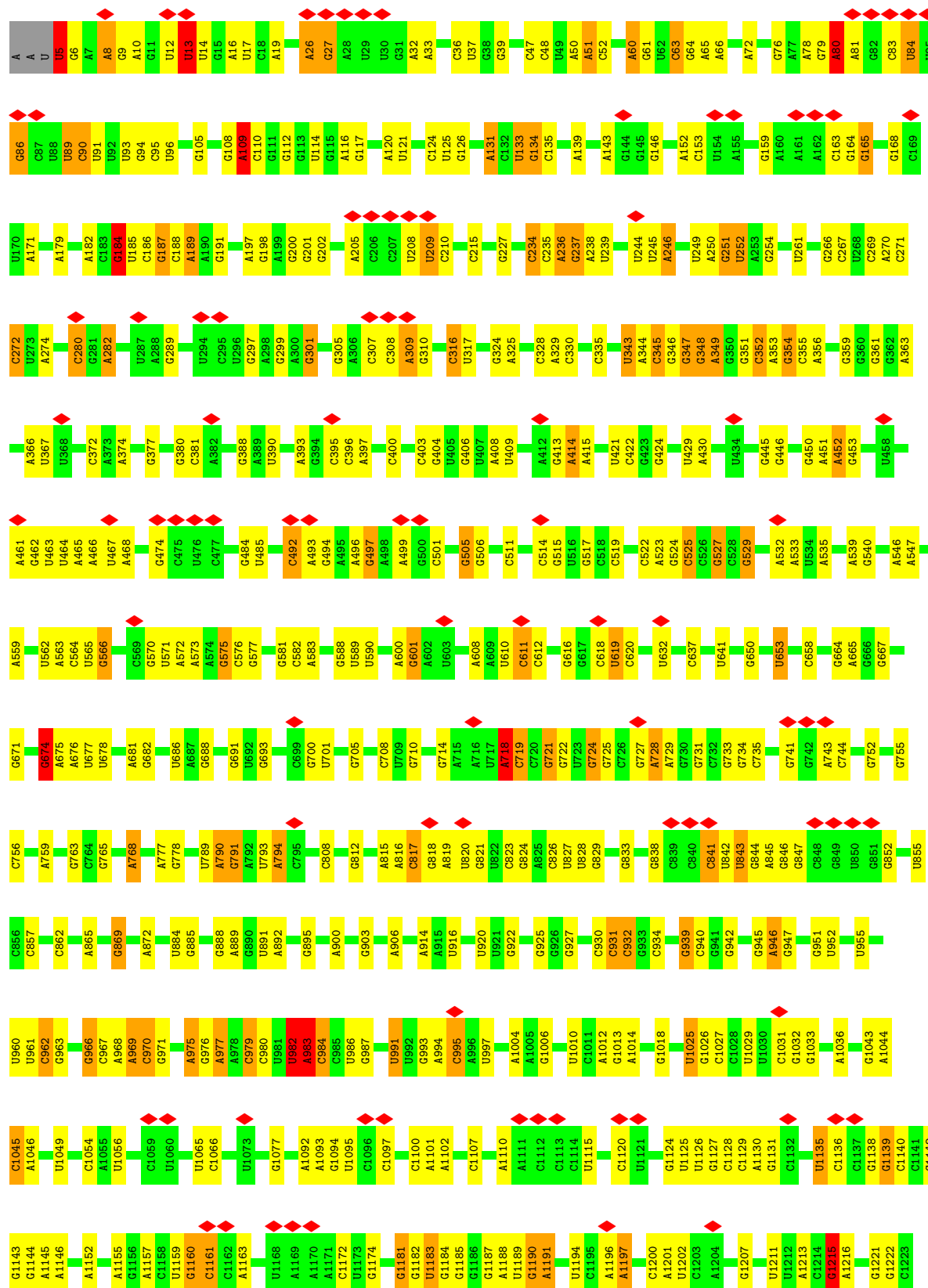


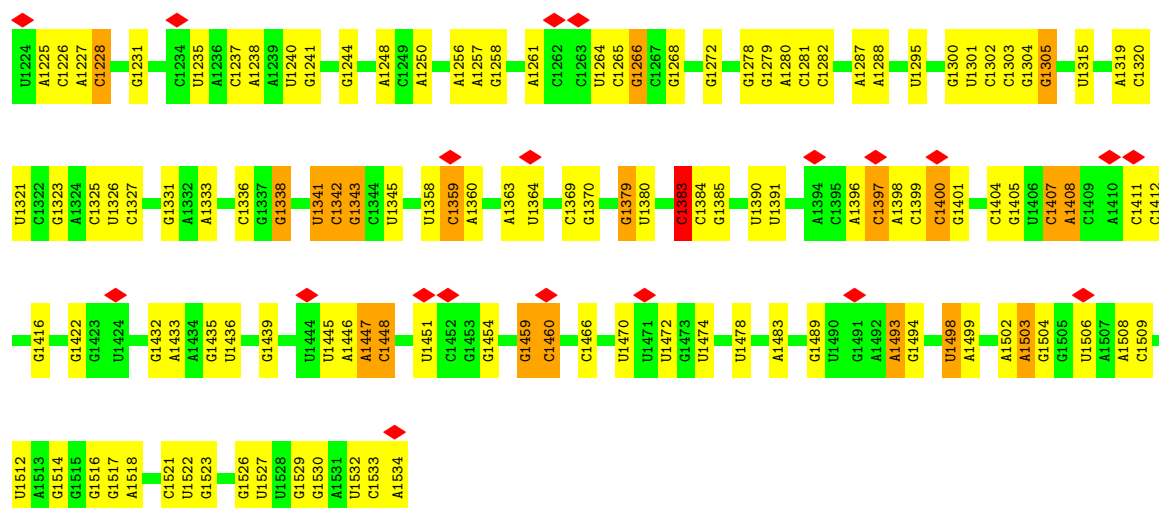
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA



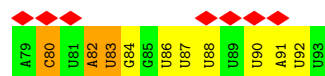




• Molecule 22: fMet-Val-tRNA-Val



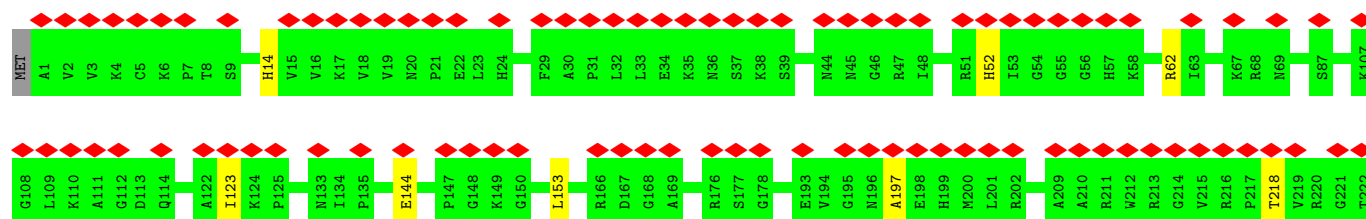
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

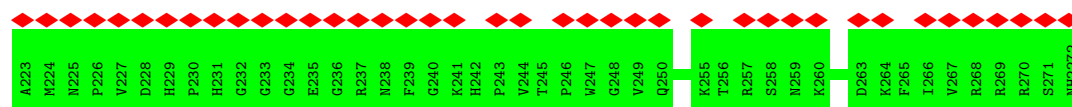


• Molecule 24: tRNA-fMet

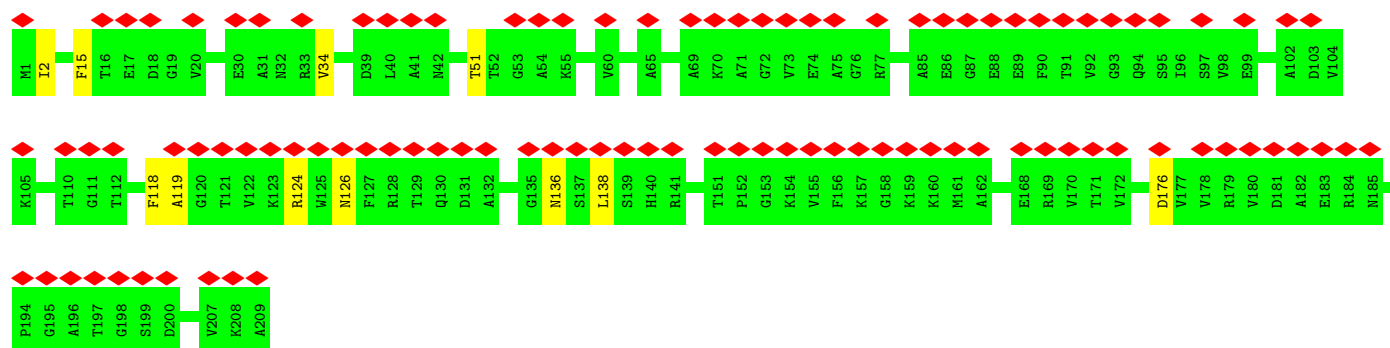


• Molecule 25: 50S ribosomal protein L2

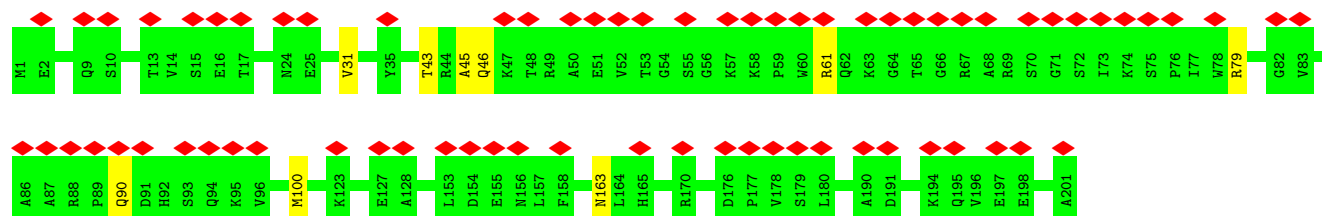




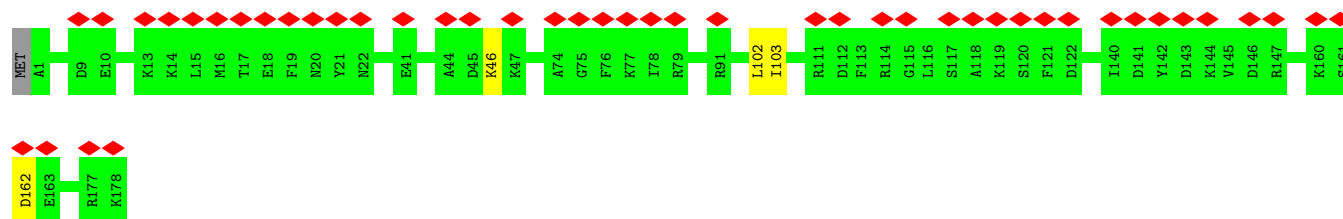
• Molecule 26: 50S ribosomal protein L3



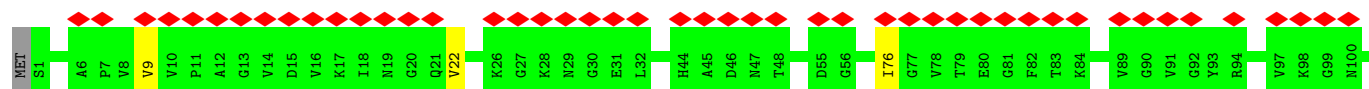
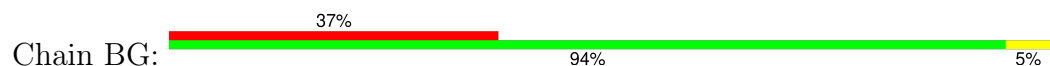
• Molecule 27: 50S ribosomal protein L4



• Molecule 28: 50S ribosomal protein L5



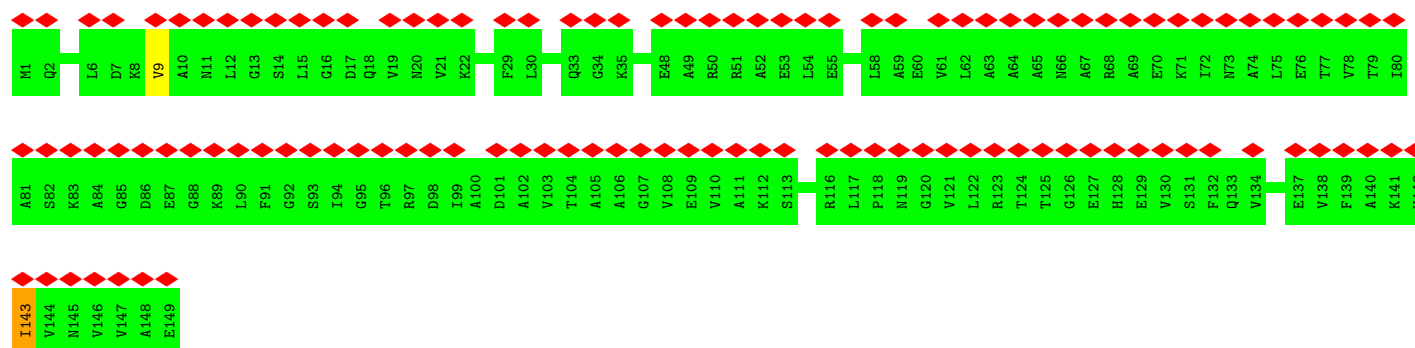
• Molecule 29: 50S ribosomal protein L6





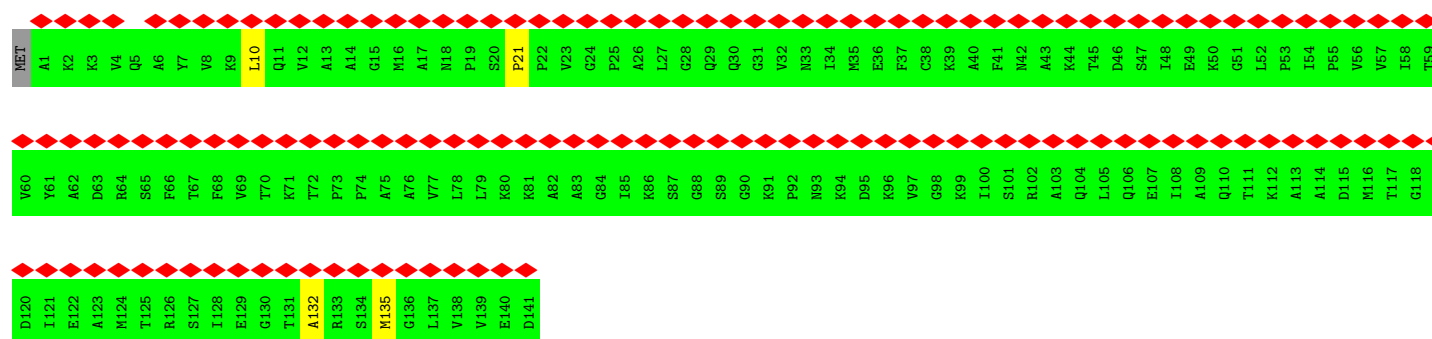
- Molecule 30: 50S ribosomal protein L9

Chain BH: 77% 99%



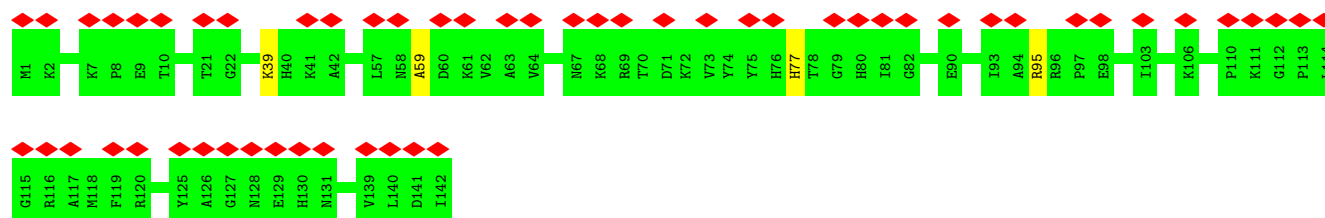
- Molecule 31: 50S ribosomal protein L11

Chain BI: 99% 96%



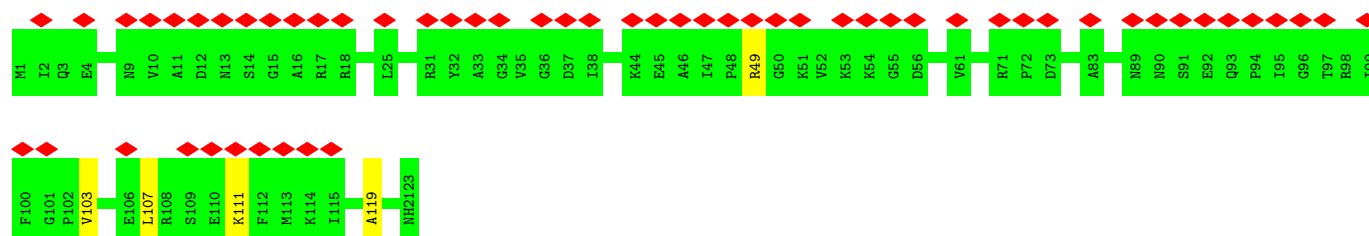
- Molecule 32: 50S ribosomal protein L13

Chain BJ: 39% 97%

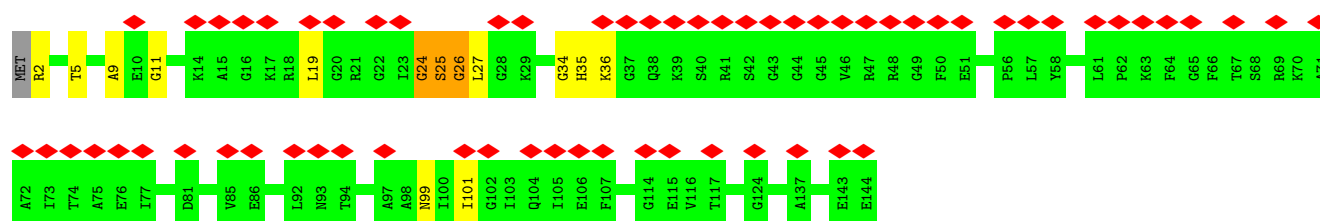
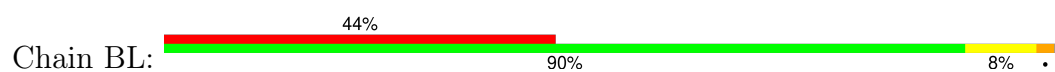


- Molecule 33: 50S ribosomal protein L14

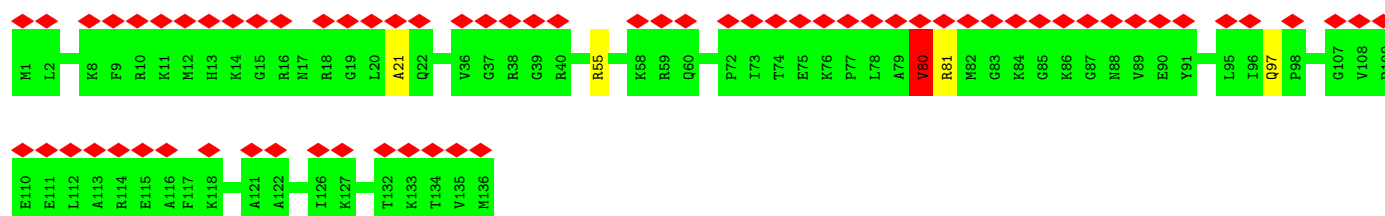
Chain BK: 46% 96%



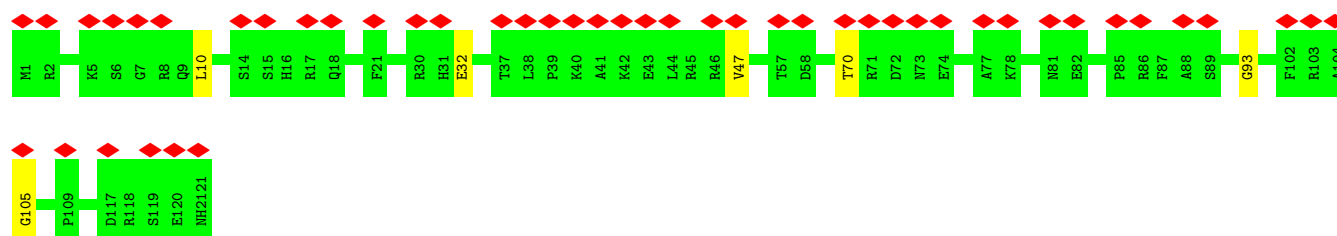
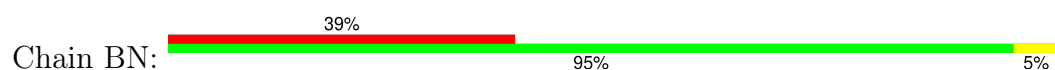
• Molecule 34: 50S ribosomal protein L15



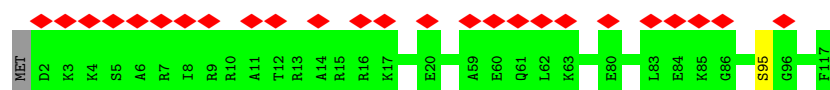
• Molecule 35: 50S ribosomal protein L16



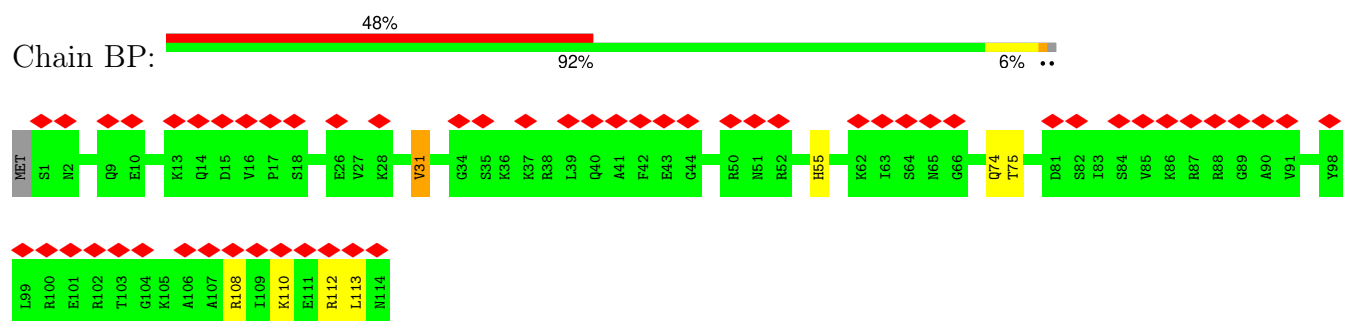
• Molecule 36: 50S ribosomal protein L17



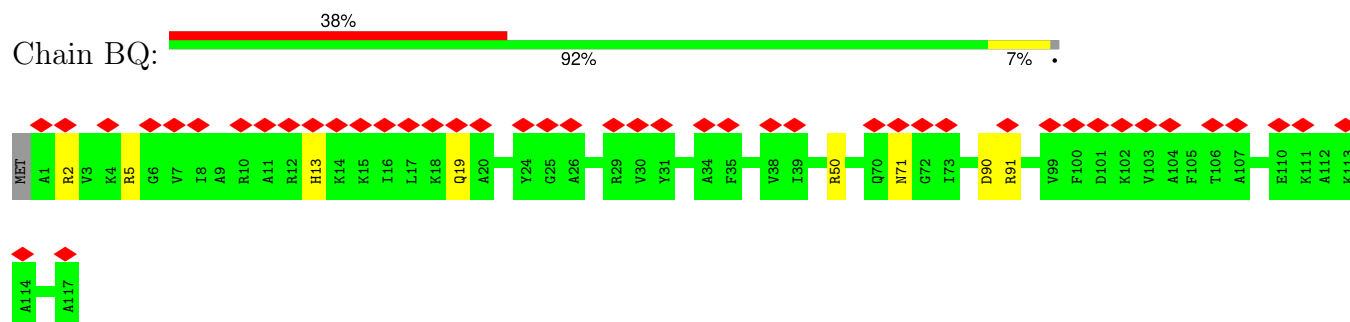
• Molecule 37: 50S ribosomal protein L18



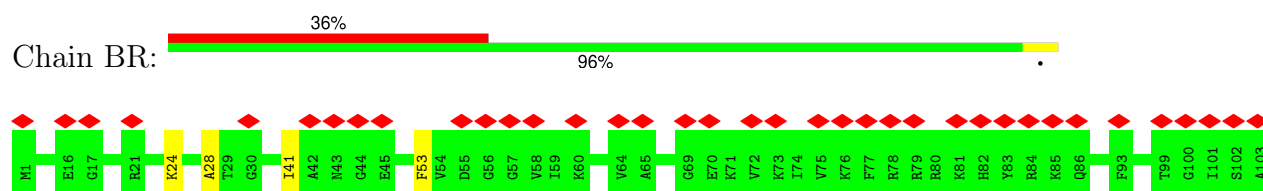
• Molecule 38: 50S ribosomal protein L19



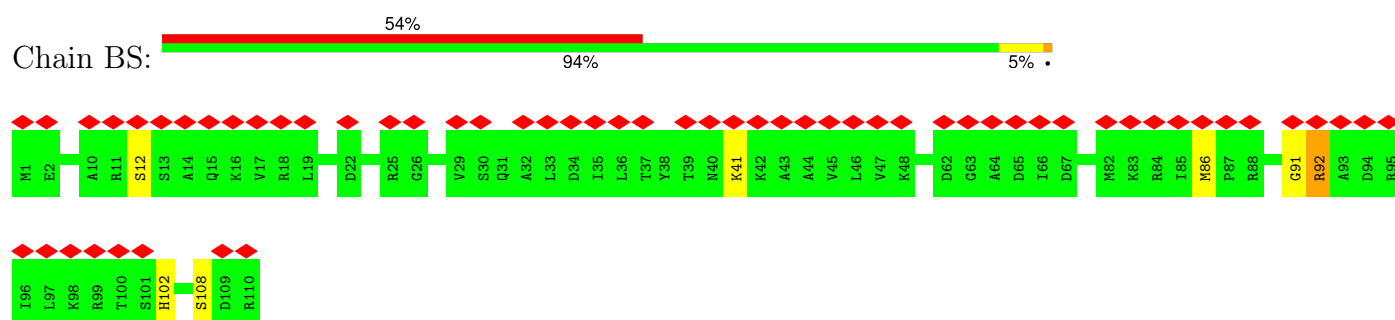
- Molecule 39: 50S ribosomal protein L20



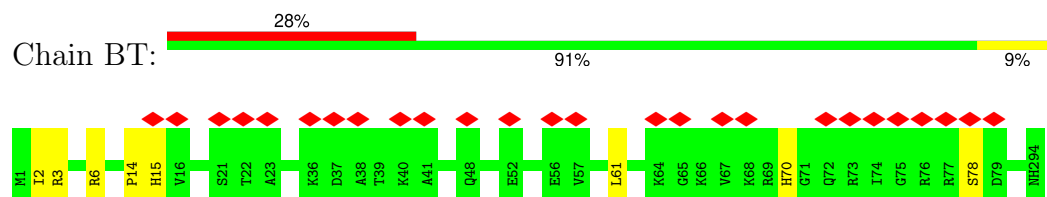
- Molecule 40: 50S ribosomal protein L21



- Molecule 41: 50S ribosomal protein L22

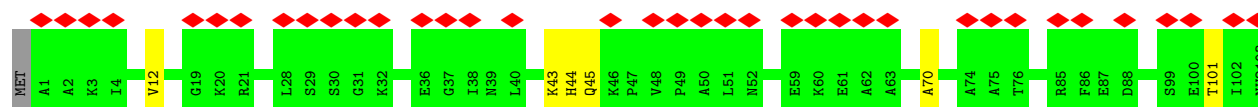


- Molecule 42: 50S ribosomal protein L23

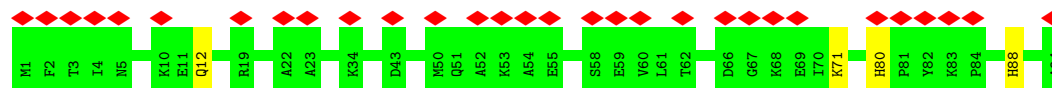


- Molecule 43: 50S ribosomal protein L24

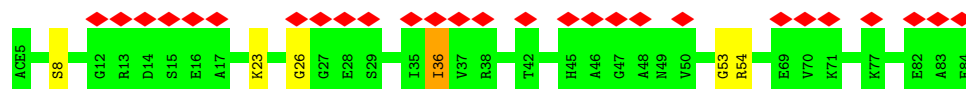




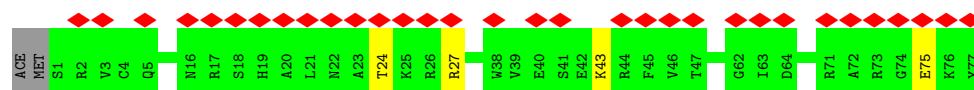
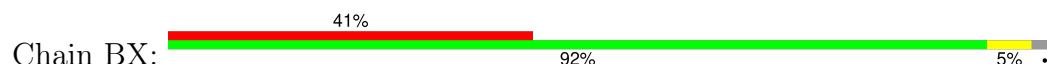
- Molecule 44: 50S ribosomal protein L25



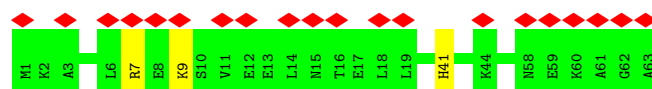
- Molecule 45: 50S ribosomal protein L27



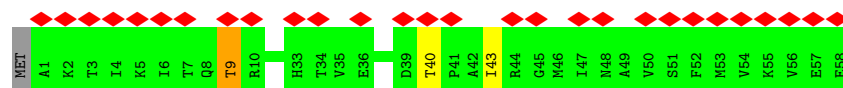
- Molecule 46: 50S ribosomal protein L28



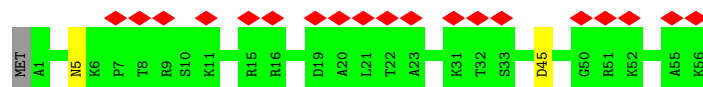
- Molecule 47: 50S ribosomal protein L29



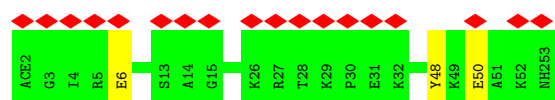
- Molecule 48: 50S ribosomal protein L30



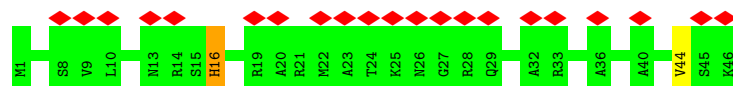
- Molecule 49: 50S ribosomal protein L32



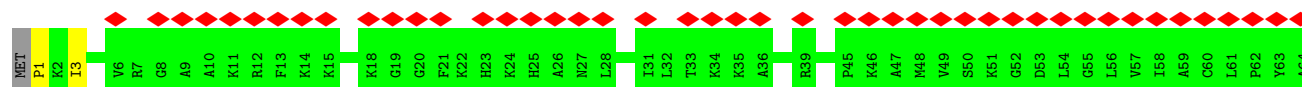
- Molecule 50: 50S ribosomal protein L33



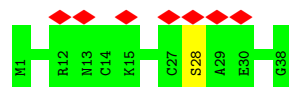
- Molecule 51: 50S ribosomal protein L34



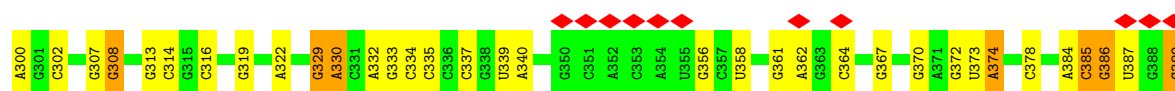
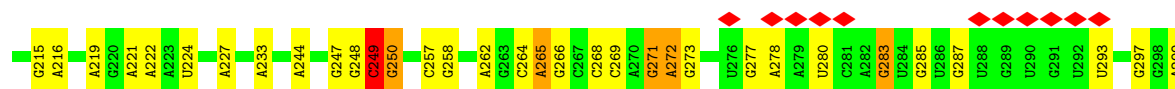
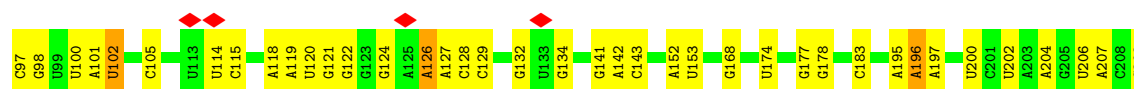
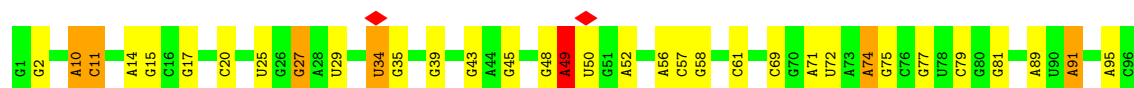
- Molecule 52: 50S ribosomal protein L35

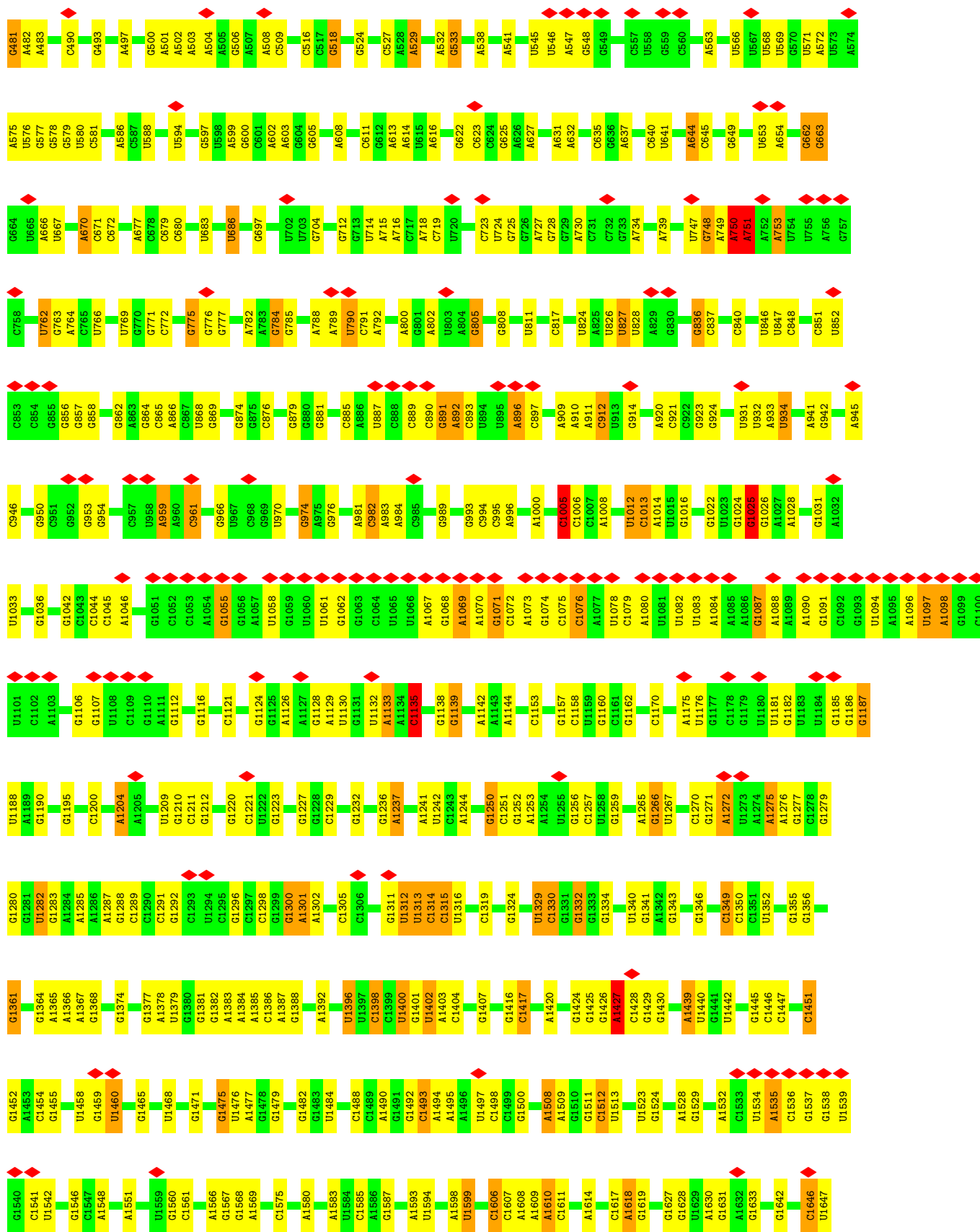


- Molecule 53: 50S ribosomal protein L36

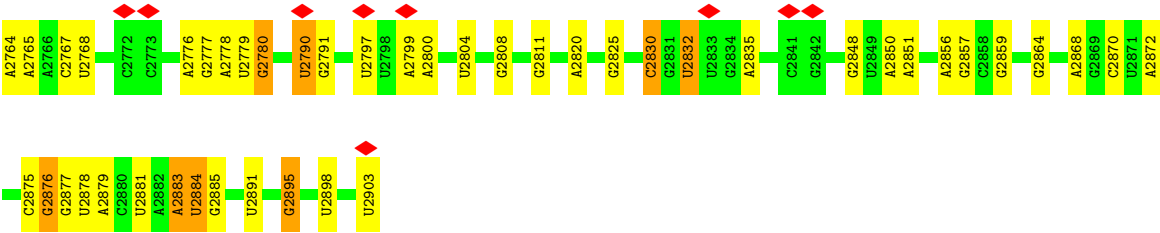


- Molecule 54: 23S ribosomal RNA

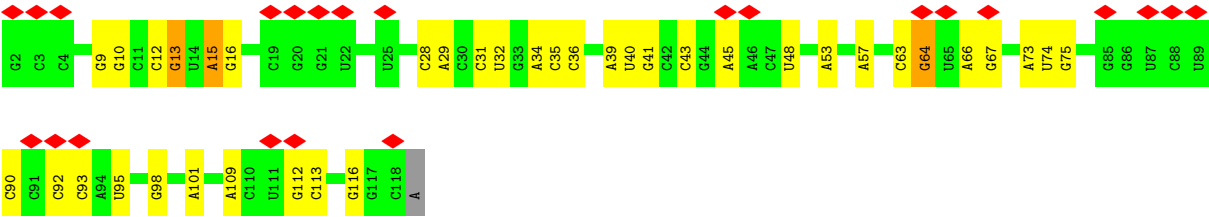




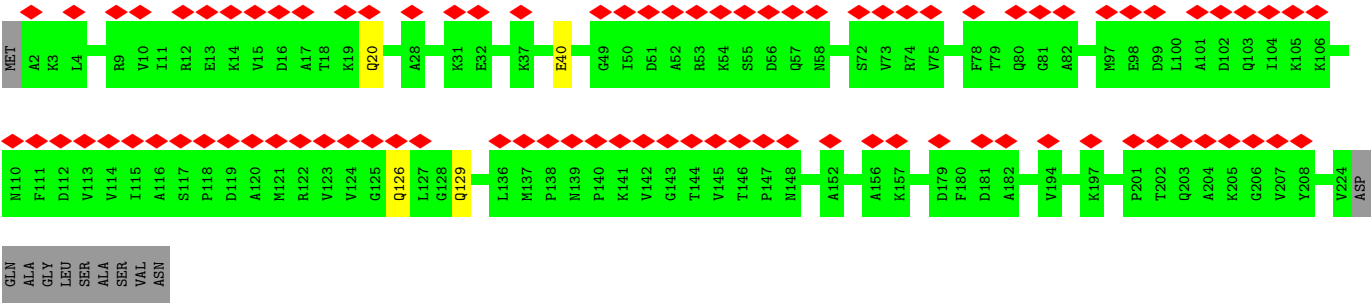
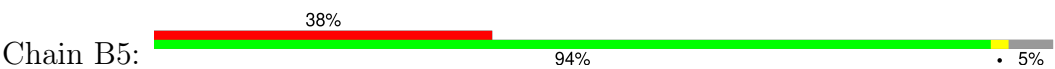
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A2701	U2535	C2291	C2291	C2291	U2203	A2058	G1974	U1716		
A2702	C2536	C2292	C2292	C2292	U2206	G2059	A1978	A1717		
A2703	U2537	C2293	C2293	C2293	C2206	A2060	U1979	G1723		
A2704	C2538	C2294	C2294	C2294	A2211	G2061	G1980	G1724		
A2705	U2539	C2295	C2295	C2295	A2212	A2062	U1981	C1727		
A2706	C2540	C2296	C2296	C2296	A2213	C2063	G1982	G1728		
A2707	U2541	C2297	C2297	C2297	A2214	C2064	U1983	U1729		
A2708	C2542	C2298	C2298	C2298	A2215	C2065	U1984	G1814		
A2709	U2543	C2299	C2299	C2299	A2216	C2066	G1985	G1815		
A2710	C2544	C2300	C2300	C2300	A2217	G2067	C1986	G1816		
A2711	U2545	C2301	C2301	C2301	U2220	U2068	C1987	G1817		
A2712	C2546	C2302	C2302	C2302	G2223			C1731		
A2713	U2547	C2303	C2303	C2303				G1732		
A2714	C2548	C2304	C2304	C2304				U1818		
A2715	U2549	C2305	C2305	C2305				A1819		
A2716	C2550	C2306	C2306	C2306						
A2717	U2551	C2307	C2307	C2307						
A2718	C2552	C2308	C2308	C2308						
A2719	U2553	C2309	C2309	C2309						
A2720	C2554	C2310	C2310	C2310						
A2721	U2555	C2311	C2311	C2311						
A2722	C2556	C2312	C2312	C2312						
A2723	U2557	C2313	C2313	C2313						
A2724	C2558	C2314	C2314	C2314						
A2725	U2559	C2315	C2315	C2315						
A2726	C2560	C2316	C2316	C2316						
A2727	U2561	C2317	C2317	C2317						
A2728	C2562	C2318	C2318	C2318						
A2729	U2563	C2319	C2319	C2319						
A2730	C2564	C2320	C2320	C2320						
A2731	U2565	C2321	C2321	C2321						
A2732	C2566	C2322	C2322	C2322						
A2733	U2567	C2323	C2323	C2323						
A2734	C2568	C2324	C2324	C2324						
A2735	U2569	C2325	C2325	C2325						
A2736	C2570	C2326	C2326	C2326						
A2737	U2571	C2327	C2327	C2327						
A2738	C2572	C2328	C2328	C2328						
A2739	U2573	C2329	C2329	C2329						
A2740	C2574	C2330	C2330	C2330						
A2741	U2575	C2331	C2331	C2331						
A2742	C2576	C2332	C2332	C2332						
A2743	U2577	C2333	C2333	C2333						
A2744	C2578	C2334	C2334	C2334						
A2745	U2579	C2335	C2335	C2335						
A2746	C2580	C2336	C2336	C2336						
A2747	U2581	C2337	C2337	C2337						
A2748	C2582	C2338	C2338	C2338						
A2749	U2583	C2339	C2339	C2339						
A2750	C2584	C2340	C2340	C2340						
A2751	U2585	C2341	C2341	C2341						
A2752	C2586	C2342	C2342	C2342						
A2753	U2587	C2343	C2343	C2343						
A2754	C2588	C2344	C2344	C2344						
A2755	U2589	C2345	C2345	C2345						
A2756	C2590	C2346	C2346	C2346						
A2757	U2591	C2347	C2347	C2347						
A2758	C2592	C2348	C2348	C2348						
A2759	U2593	C2349	C2349	C2349						
A2760	C2594	C2350	C2350	C2350						
A2761	U2595	C2351	C2351	C2351						
A2762	C2596	C2352	C2352	C2352						
A2763	U2597	C2353	C2353	C2353						
A2764	C2598	C2354	C2354	C2354						
A2765	U2599	C2355	C2355	C2355						
A2766	C2600	C2356	C2356	C2356						
A2767	U2601	C2357	C2357	C2357						
A2768	C2602	C2358	C2358	C2358						
A2769	U2603	C2359	C2359	C2359						
A2770	C2604	C2360	C2360	C2360						
A2771	U2605	C2361	C2361	C2361						
A2772	C2606	C2362	C2362	C2362						
A2773	U2607	C2363	C2363	C2363						
A2774	C2608	C2364	C2364	C2364						
A2775	U2609	C2365	C2365	C2365						
A2776	C2610	C2366	C2366	C2366						
A2777	U2611	C2367	C2367	C2367						
A2778	C2612	C2368	C2368	C2368						
A2779	U2613	C2369	C2369	C2369						
A2780	C2614	C2370	C2370	C2370						
A2781	U2615	C2371	C2371	C2371						
A2782	C2616	C2372	C2372	C2372						
A2783	U2617	C2373	C2373	C2373						
A2784	C2618	C2374	C2374	C2374						
A2785	U2619	C2375	C2375	C2375						
A2786	C2620	C2376	C2376	C2376						
A2787	U2621	C2377	C2377	C2377						
A2788	C2622	C2378	C2378	C2378						
A2789	U2623	C2379	C2379	C2379						
A2790	C2624	C2380	C2380	C2380						
A2791	U2625	C2381	C2381	C2381						
A2792	C2626	C2382	C2382	C2382						
A2793	U2627	C2383	C2383	C2383						
A2794	C2628	C2384	C2384	C2384						
A2795	U2629	C2385	C2385	C2385						
A2796	C2630	C2386	C2386	C2386						
A2797	U2631	C2387	C2387	C2387						
A2798	C2632	C2388	C2388	C2388						
A2799	U2633	C2389	C2389	C2389						
A2800	C2634	C2390	C2390	C2390						
A2801	U2635	C2391	C2391	C2391						
A2802	C2636	C2392	C2392	C2392						
A2803	U2637	C2393	C2393	C2393						
A2804	C2638	C2394	C2394	C2394						
A2805	U2639	C2395	C2395	C2395						
A2806	C2640	C2396	C2396	C2396						
A2807	U2641	C2397	C2397	C2397						



● Molecule 55: 5S ribosomal RNA



● Molecule 56: 50S ribosomal protein L1



GLN
ALA
GLY
LEU
SER
SER
VAL
ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4705	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	161000	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	176.039	Depositor
Minimum map value	-108.322	Depositor
Average map value	-0.887	Depositor
Map value standard deviation	18.782	Depositor
Recommended contour level	25	Depositor
Map size ($\text{\AA}$)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.8, 2.8, 2.8	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU, NH2, 7MG, CM0, H2U, OMC, 4SU, ACE, FME, 6MZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AB	0.95	0/1736	1.34	6/2340 (0.3%)
2	AC	0.95	0/1651	1.32	0/2225
3	AD	0.98	0/1665	1.40	6/2227 (0.3%)
4	AE	0.96	0/1119	1.44	8/1506 (0.5%)
5	AF	0.97	0/835	1.39	1/1128 (0.1%)
6	AG	0.98	0/1188	1.41	3/1593 (0.2%)
7	AH	0.95	0/989	1.33	2/1326 (0.2%)
8	AI	1.00	0/1035	1.47	4/1377 (0.3%)
9	AJ	0.99	0/797	1.34	0/1079
10	AK	1.01	0/894	1.44	3/1207 (0.2%)
11	AL	1.01	0/969	1.48	6/1300 (0.5%)
12	AM	1.01	0/884	1.57	5/1181 (0.4%)
13	AN	0.98	0/817	1.39	3/1088 (0.3%)
14	AO	0.97	0/722	1.36	0/964
15	AP	1.01	0/648	1.40	0/870
16	AQ	0.93	0/658	1.31	2/883 (0.2%)
17	AR	1.00	0/463	1.39	3/623 (0.5%)
18	AS	1.01	0/653	1.49	2/879 (0.2%)
19	AT	0.92	0/672	1.33	0/890
20	AU	1.03	0/431	1.66	3/572 (0.5%)
21	AA	0.98	0/36759	1.16	78/57346 (0.1%)
22	A1	1.01	0/1668	1.20	6/2595 (0.2%)
23	A2	1.00	0/343	1.36	4/531 (0.8%)
24	A3	1.00	0/1722	1.15	4/2685 (0.1%)
25	BC	0.96	0/2121	1.50	1/2852 (0.0%)
26	BD	0.88	0/1586	1.43	0/2134
27	BE	0.88	0/1571	1.46	5/2113 (0.2%)
28	BF	0.89	0/1444	1.40	0/1937
29	BG	0.89	0/1343	1.46	5/1816 (0.3%)
30	BH	0.87	0/1122	1.42	0/1515
31	BI	0.89	0/1046	1.45	1/1410 (0.1%)
32	BJ	0.94	0/1152	1.42	5/1551 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BK	0.95	0/947	1.47	2/1268 (0.2%)
34	BL	0.94	0/1054	1.64	13/1403 (0.9%)
35	BM	0.93	0/1093	1.55	3/1460 (0.2%)
36	BN	0.96	0/973	1.53	0/1301
37	BO	0.92	0/902	1.44	0/1209
38	BP	0.95	0/929	1.52	3/1242 (0.2%)
39	BQ	0.93	0/960	1.46	2/1278 (0.2%)
40	BR	0.90	0/829	1.40	0/1107
41	BS	0.88	0/864	1.41	4/1156 (0.3%)
42	BT	0.88	0/744	1.42	1/994 (0.1%)
43	BU	0.91	0/787	1.44	1/1051 (0.1%)
44	BV	0.94	0/766	1.43	2/1025 (0.2%)
45	BW	0.95	0/604	1.54	4/799 (0.5%)
46	BX	0.97	0/635	1.42	0/848
47	BY	0.87	0/510	1.42	1/677 (0.1%)
48	BZ	0.93	0/453	1.44	1/605 (0.2%)
49	B0	1.01	0/450	1.55	0/599
50	B1	0.93	0/417	1.47	0/556
51	B2	0.99	0/380	1.51	1/498 (0.2%)
52	B3	1.02	0/513	1.53	1/676 (0.1%)
53	B4	0.96	0/303	1.49	1/397 (0.3%)
54	BA	0.83	0/69796	1.14	116/108888 (0.1%)
55	BB	0.83	0/2800	1.15	3/4367 (0.1%)
56	B5	0.88	0/1673	1.41	2/2255 (0.1%)
All	All	0.91	0/160085	1.23	327/239402 (0.1%)

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
10	AK	0	1
21	AA	0	358
22	A1	0	15
23	A2	0	5
24	A3	0	9
26	BD	0	1
41	BS	0	1
50	B1	0	1
54	BA	0	709
55	BB	0	21
All	All	0	1121

There are no bond length outliers.

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AM	106	ARG	CA-C-N	11.09	141.67	121.70
12	AM	106	ARG	C-N-CA	11.09	141.67	121.70
21	AA	1391	U	C1'-O4'-C4'	-9.18	100.72	109.90
18	AS	3	SER	CA-C-N	8.89	137.70	121.70
18	AS	3	SER	C-N-CA	8.89	137.70	121.70
8	AI	124	PRO	CA-N-CD	-8.30	100.38	112.00
54	BA	1714	U	O4'-C1'-N1	7.64	119.66	108.20
45	BW	53	GLY	CA-C-N	7.64	135.45	121.70
45	BW	53	GLY	C-N-CA	7.64	135.45	121.70
13	AN	100	SER	CA-C-N	7.51	135.22	121.70
13	AN	100	SER	C-N-CA	7.51	135.22	121.70
21	AA	872	A	C1'-O4'-C4'	-7.45	102.45	109.90
32	BJ	95	ARG	NE-CZ-NH2	7.37	125.83	119.20
3	AD	48	SER	CA-C-N	7.32	134.87	121.70
3	AD	48	SER	C-N-CA	7.32	134.87	121.70
12	AM	111	PRO	CA-C-N	7.13	134.54	121.70
12	AM	111	PRO	C-N-CA	7.13	134.54	121.70
54	BA	546	U	O4'-C1'-N1	7.13	119.20	108.50
42	BT	6	ARG	NE-CZ-NH2	6.96	125.46	119.20
22	A1	73	A	P-O3'-C3'	6.95	130.63	120.20
35	BM	80	VAL	CA-C-N	6.92	134.15	121.70
35	BM	80	VAL	C-N-CA	6.92	134.15	121.70
8	AI	113	LYS	CA-C-N	6.88	134.09	121.70
8	AI	113	LYS	C-N-CA	6.88	134.09	121.70
39	BQ	50	ARG	NE-CZ-NH2	6.85	125.36	119.20
54	BA	1314	C	O4'-C1'-C2'	-6.72	100.88	107.60
4	AE	45	VAL	CA-C-N	6.72	128.27	121.35
4	AE	45	VAL	C-N-CA	6.72	128.27	121.35
54	BA	271	G	C4'-C3'-O3'	6.61	119.32	109.40
54	BA	1314	C	N1-C1'-C2'	6.59	121.88	112.00
17	AR	70	THR	CA-C-N	6.49	133.39	121.70
17	AR	70	THR	C-N-CA	6.49	133.39	121.70
41	BS	92	ARG	NE-CZ-NH2	6.41	124.97	119.20
54	BA	49	A	C4'-C3'-O3'	6.40	118.99	109.40
1	AB	10	LYS	CA-C-N	6.36	133.15	121.70
1	AB	10	LYS	C-N-CA	6.36	133.15	121.70
54	BA	2600	A	C5'-C4'-C3'	6.36	125.54	116.00
54	BA	330	A	O4'-C1'-N9	6.28	117.61	108.20
54	BA	1936	A	C2'-C3'-O3'	6.21	118.81	109.50
4	AE	104	ILE	CA-C-N	6.13	132.74	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AE	104	ILE	C-N-CA	6.13	132.74	121.70
34	BL	5	THR	CA-C-N	6.13	132.74	121.70
34	BL	5	THR	C-N-CA	6.13	132.74	121.70
38	BP	108	ARG	NE-CZ-NH2	6.13	124.72	119.20
54	BA	2644	G	O4'-C4'-C3'	6.12	110.12	104.00
21	AA	13	U	O4'-C4'-C3'	6.11	110.11	104.00
21	AA	1341	U	O4'-C4'-C3'	6.10	110.10	104.00
21	AA	1342	C	C5'-C4'-C3'	-6.09	106.87	116.00
41	BS	102	HIS	CB-CG-CD2	-6.08	123.29	131.20
54	BA	2473	U	O4'-C1'-N1	6.08	117.32	108.20
22	A1	47	U	C1'-O4'-C4'	-6.08	103.62	109.70
54	BA	670	A	C2'-C3'-O3'	6.07	118.60	109.50
54	BA	2600	A	C4'-C3'-O3'	6.01	122.02	113.00
54	BA	625	G	C4'-C3'-C2'	-6.00	96.60	102.60
4	AE	107	GLY	CA-C-N	5.98	126.73	120.03
4	AE	107	GLY	C-N-CA	5.98	126.73	120.03
11	AL	17	LYS	CA-C-N	5.98	132.46	121.70
11	AL	17	LYS	C-N-CA	5.98	132.46	121.70
54	BA	1069	A	O4'-C1'-N9	5.97	117.16	108.20
54	BA	308	G	O4'-C4'-C3'	5.96	109.96	104.00
21	AA	414	A	O4'-C4'-C3'	5.95	109.95	104.00
20	AU	47	ALA	CA-C-N	5.94	132.38	121.70
20	AU	47	ALA	C-N-CA	5.94	132.38	121.70
54	BA	2667	C	O4'-C4'-C3'	5.94	109.94	104.00
21	AA	234	C	C4'-C3'-C2'	-5.93	96.67	102.60
21	AA	335	C	C5'-C4'-C3'	-5.93	107.11	116.00
11	AL	120	ARG	NE-CZ-NH2	5.92	124.53	119.20
21	AA	492	C	O4'-C4'-C3'	5.91	109.91	104.00
34	BL	25	SER	CA-C-N	5.88	132.28	121.70
34	BL	25	SER	C-N-CA	5.88	132.28	121.70
21	AA	674	G	O4'-C4'-C3'	5.88	109.88	104.00
54	BA	2489	U	O4'-C4'-C3'	5.86	109.86	104.00
32	BJ	39	LYS	CA-C-N	5.86	131.12	121.99
32	BJ	39	LYS	C-N-CA	5.86	131.12	121.99
21	AA	1338	G	C1'-O4'-C4'	-5.85	104.05	109.90
54	BA	1005	C	O4'-C4'-C3'	5.85	109.85	104.00
54	BA	480	A	C5'-C4'-C3'	-5.84	107.25	116.00
54	BA	1880	U	O4'-C4'-C3'	5.84	109.84	104.00
29	BG	76	ILE	CA-C-N	5.82	126.55	120.03
29	BG	76	ILE	C-N-CA	5.82	126.55	120.03
54	BA	2503	A	C2'-C3'-O3'	5.82	118.23	109.50
39	BQ	13	HIS	CB-CG-CD2	-5.81	123.65	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	249	C	C2'-C3'-O3'	5.80	118.20	109.50
44	BV	80	HIS	CB-CG-CD2	-5.80	123.67	131.20
21	AA	343	U	O4'-C4'-C3'	5.79	109.80	104.00
54	BA	2283	C	C4'-C3'-C2'	-5.77	96.83	102.60
12	AM	106	ARG	O-C-N	-5.76	114.93	122.59
54	BA	1312	U	C2'-C3'-O3'	5.76	118.14	109.50
21	AA	345	C	C1'-O4'-C4'	-5.75	103.94	109.70
34	BL	2	ARG	CA-C-N	5.74	132.04	121.70
34	BL	2	ARG	C-N-CA	5.74	132.04	121.70
44	BV	88	HIS	CB-CG-CD2	-5.72	123.77	131.20
10	AK	91	GLY	CA-C-N	5.72	129.84	120.63
10	AK	91	GLY	C-N-CA	5.72	129.84	120.63
21	AA	852	G	O4'-C4'-C3'	5.71	109.71	104.00
54	BA	1758	U	O4'-C1'-N1	5.71	116.76	108.20
21	AA	1383	C	O4'-C4'-C3'	5.70	109.70	104.00
54	BA	1609	A	C1'-O4'-C4'	-5.70	104.20	109.90
54	BA	2277	G	C5'-C4'-C3'	-5.70	107.45	116.00
17	AR	70	THR	O-C-N	-5.70	116.98	123.48
3	AD	106	PHE	CA-C-N	5.70	127.22	121.35
3	AD	106	PHE	C-N-CA	5.70	127.22	121.35
54	BA	1759	A	O4'-C4'-C3'	5.69	109.69	104.00
54	BA	49	A	C2'-C3'-O3'	5.68	118.02	109.50
21	AA	653	U	O4'-C1'-N1	5.68	116.72	108.20
21	AA	250	A	O4'-C4'-C3'	5.67	109.67	104.00
54	BA	2881	U	O4'-C4'-C3'	5.67	109.67	104.00
21	AA	208	U	O4'-C4'-C3'	5.67	109.67	104.00
21	AA	189	A	O4'-C4'-C3'	5.67	109.67	104.00
45	BW	36	ILE	CA-CB-CG1	5.66	120.02	110.40
54	BA	2549	G	C5'-C4'-C3'	-5.63	107.55	116.00
33	BK	49	ARG	CA-C-N	5.63	125.69	120.34
33	BK	49	ARG	C-N-CA	5.63	125.69	120.34
21	AA	5	U	C1'-O4'-C4'	-5.62	104.28	109.90
21	AA	869	G	O4'-C4'-C3'	5.62	109.62	104.00
21	AA	187	G	C1'-O4'-C4'	-5.62	104.28	109.90
54	BA	751	A	C1'-O4'-C4'	-5.62	104.28	109.90
21	AA	982	U	P-O3'-C3'	5.62	128.62	120.20
22	A1	3	G	C5'-C4'-O4'	5.61	118.22	109.80
34	BL	26	GLY	CA-C-N	5.61	131.79	121.70
34	BL	26	GLY	C-N-CA	5.61	131.79	121.70
54	BA	2132	U	O4'-C1'-N1	5.61	116.61	108.20
21	AA	109	A	C1'-O4'-C4'	-5.61	104.09	109.70
21	AA	1197	A	O4'-C4'-C3'	5.60	109.60	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	750	A	N9-C1'-C2'	5.59	120.39	112.00
31	BI	21	PRO	N-CA-C	5.59	117.52	110.70
21	AA	793	U	C1'-O4'-C4'	-5.59	104.31	109.90
41	BS	91	GLY	CA-C-N	5.58	131.75	121.70
41	BS	91	GLY	C-N-CA	5.58	131.75	121.70
29	BG	174	LYS	CA-C-N	5.58	131.74	121.70
29	BG	174	LYS	C-N-CA	5.58	131.74	121.70
21	AA	316	C	O4'-C4'-C3'	5.58	109.58	104.00
21	AA	1190	G	O4'-C4'-C3'	5.58	109.58	104.00
54	BA	409	G	O4'-C4'-C3'	5.58	109.58	104.00
54	BA	1313	U	O4'-C4'-C3'	5.58	109.58	104.00
21	AA	63	C	O4'-C4'-C3'	5.57	109.57	104.00
21	AA	89	U	O4'-C4'-C3'	5.57	109.57	104.00
54	BA	1427	A	C2'-C3'-O3'	5.54	117.80	109.50
54	BA	762	U	C2'-C3'-O3'	5.52	117.78	109.50
54	BA	2586	U	C2'-C3'-O3'	5.51	121.97	113.70
21	AA	5	U	O4'-C1'-N1	5.51	116.76	108.50
21	AA	1304	G	O4'-C4'-C3'	5.51	109.51	104.00
54	BA	1195	G	C4'-C3'-C2'	-5.50	97.09	102.60
54	BA	1204	A	O4'-C1'-N9	5.49	116.44	108.20
54	BA	649	G	O4'-C4'-C3'	5.49	109.49	104.00
21	AA	682	G	C5'-C4'-C3'	-5.48	107.78	116.00
21	AA	1261	A	O4'-C4'-C3'	5.48	109.48	104.00
54	BA	1084	A	O4'-C1'-N9	5.47	116.71	108.50
54	BA	2058	A	O4'-C4'-C3'	5.47	109.47	104.00
21	AA	497	G	O4'-C4'-C3'	5.47	109.47	104.00
54	BA	126	A	O4'-C4'-C3'	5.46	109.46	104.00
35	BM	55	ARG	NE-CZ-NH2	5.45	124.11	119.20
54	BA	1682	G	O4'-C4'-C3'	5.45	109.44	104.00
55	BB	13	G	O4'-C1'-N9	5.44	116.36	108.20
54	BA	2017	U	O4'-C4'-C3'	5.44	109.44	104.00
22	A1	56	C	O4'-C4'-C3'	5.43	109.43	104.00
54	BA	424	G	C4'-C3'-C2'	-5.43	97.17	102.60
54	BA	1475	G	C2'-C3'-O3'	5.43	117.64	109.50
21	AA	575	G	P-O3'-C3'	5.43	128.34	120.20
54	BA	1352	U	O4'-C1'-N1	5.42	116.63	108.50
3	AD	186	GLU	CA-C-N	5.42	131.89	121.54
3	AD	186	GLU	C-N-CA	5.42	131.89	121.54
24	A3	75	C	C5'-C4'-C3'	-5.41	107.88	116.00
54	BA	1401	G	C2'-C3'-O3'	-5.40	105.61	113.70
21	AA	363	A	O4'-C4'-C3'	5.39	109.39	104.00
21	AA	1191	A	O4'-C4'-C3'	5.38	109.38	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1268	G	O4'-C4'-C3'	5.38	109.38	104.00
21	AA	970	C	O4'-C4'-C3'	5.38	109.38	104.00
5	AF	66	ALA	N-CA-C	5.37	112.85	108.07
21	AA	445	G	O4'-C4'-C3'	5.36	109.36	104.00
23	A2	82	A	C5'-C4'-C3'	-5.35	107.97	116.00
54	BA	2212	A	O4'-C1'-N9	5.35	116.53	108.50
23	A2	80	C	C5'-C4'-C3'	-5.34	107.98	116.00
54	BA	196	A	O4'-C1'-N9	5.34	116.52	108.50
54	BA	1157	G	O4'-C4'-C3'	5.34	109.34	104.00
21	AA	975	A	C2'-C3'-O3'	5.34	117.51	109.50
16	AQ	46	HIS	CB-CG-CD2	-5.34	124.26	131.20
21	AA	120	A	O4'-C4'-C3'	5.34	109.34	104.00
21	AA	817	C	C1'-O4'-C4'	-5.33	104.37	109.70
34	BL	9	ALA	O-C-N	-5.33	116.54	122.09
6	AG	74	VAL	O-C-N	-5.33	117.73	122.69
21	AA	718	A	O4'-C4'-C3'	5.33	109.33	104.00
11	AL	16	ALA	CA-C-N	5.32	131.71	121.54
11	AL	16	ALA	C-N-CA	5.32	131.71	121.54
25	BC	52	HIS	CB-CG-CD2	-5.32	124.28	131.20
21	AA	790	A	O4'-C4'-C3'	5.32	109.32	104.00
54	BA	102	U	O4'-C1'-N1	5.32	116.18	108.20
22	A1	61	C	O4'-C4'-C3'	5.31	109.31	104.00
54	BA	2430	A	O4'-C4'-C3'	5.31	109.31	104.00
54	BA	2463	C	C4'-C3'-C2'	-5.31	97.29	102.60
21	AA	967	C	O4'-C4'-C3'	5.31	109.31	104.00
55	BB	66	A	O4'-C4'-C3'	5.31	109.31	104.00
54	BA	1899	A	O4'-C4'-C3'	5.30	109.30	104.00
54	BA	2586	U	C4'-C3'-C2'	-5.30	97.30	102.60
34	BL	24	GLY	CA-C-N	5.29	131.23	121.70
34	BL	24	GLY	C-N-CA	5.29	131.23	121.70
7	AH	117	GLN	OE1-CD-NE2	-5.29	117.31	122.60
21	AA	80	A	O4'-C4'-C3'	5.29	109.29	104.00
54	BA	1349	C	O4'-C4'-C3'	5.29	109.29	104.00
21	AA	1407	C	O4'-C4'-C3'	5.29	109.29	104.00
43	BU	44	HIS	CB-CG-CD2	-5.29	124.33	131.20
54	BA	2212	A	C1'-O4'-C4'	-5.29	104.61	109.90
27	BE	46	GLN	OE1-CD-NE2	-5.28	117.32	122.60
54	BA	1282	U	O4'-C4'-C3'	5.28	109.28	104.00
21	AA	983	A	O4'-C4'-C3'	5.28	109.28	104.00
21	AA	570	G	O4'-C4'-C3'	5.28	109.28	104.00
21	AA	184	G	C5'-C4'-C3'	-5.27	108.09	116.00
21	AA	931	C	O4'-C4'-C3'	5.27	109.27	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1377	G	O3'-P-O5'	-5.26	96.11	104.00
38	BP	55	HIS	CB-CG-CD2	-5.26	124.36	131.20
20	AU	8	ASN	CA-CB-CG	5.26	117.86	112.60
21	AA	719	C	O4'-C4'-C3'	5.25	109.25	104.00
21	AA	343	U	O3'-P-O5'	-5.25	96.13	104.00
34	BL	35	HIS	CB-CG-CD2	-5.25	124.38	131.20
54	BA	2644	G	C3'-C2'-C1'	5.25	106.55	101.30
21	AA	388	G	O4'-C4'-C3'	5.25	109.25	104.00
54	BA	2898	U	C4'-C3'-C2'	-5.24	97.36	102.60
21	AA	13	U	C4'-C3'-O3'	-5.24	105.14	113.00
54	BA	1429	G	O4'-C4'-C3'	5.23	109.23	104.00
21	AA	17	U	C5'-C4'-C3'	-5.23	108.16	116.00
34	BL	2	ARG	NE-CZ-NH2	5.23	123.90	119.20
21	AA	374	A	O4'-C4'-C3'	5.22	109.22	104.00
54	BA	2438	U	O4'-C4'-C3'	5.22	109.22	104.00
21	AA	611	C	O4'-C4'-C3'	5.22	109.22	104.00
54	BA	2602	A	O4'-C1'-C2'	-5.21	102.39	107.60
54	BA	2197	U	O3'-P-O5'	-5.21	96.18	104.00
7	AH	87	ARG	NE-CZ-NH2	5.21	123.89	119.20
54	BA	572	A	O4'-C4'-C3'	5.21	109.21	104.00
21	AA	841	C	O4'-C4'-C3'	5.21	109.21	104.00
54	BA	280	U	O4'-C1'-N1	5.20	116.30	108.50
23	A2	87	U	O4'-C4'-C3'	5.20	109.20	104.00
54	BA	57	C	C4'-C3'-C2'	-5.20	97.41	102.60
13	AN	100	SER	O-C-N	-5.19	115.69	122.59
21	AA	37	U	C5'-C4'-C3'	-5.19	108.22	116.00
54	BA	91	A	O4'-C1'-N9	5.19	115.98	108.20
21	AA	546	A	O4'-C4'-C3'	5.18	109.18	104.00
21	AA	1215	G	O4'-C4'-C3'	5.18	109.19	104.00
32	BJ	59	ALA	N-CA-C	5.18	119.09	112.87
21	AA	1445	U	O4'-C4'-C3'	5.17	109.17	104.00
54	BA	2129	C	O4'-C1'-N1	5.17	116.26	108.50
54	BA	2830	C	C3'-C2'-O2'	5.17	118.46	110.70
21	AA	505	G	O4'-C4'-C3'	5.17	109.17	104.00
21	AA	1006	G	C5'-C4'-C3'	-5.17	108.25	116.00
56	B5	20	GLN	OE1-CD-NE2	-5.17	117.43	122.60
54	BA	2076	U	O4'-C1'-N1	5.17	115.95	108.20
23	A2	83	U	O3'-P-O5'	-5.16	96.26	104.00
54	BA	1633	G	O4'-C4'-C3'	5.16	109.16	104.00
54	BA	2382	G	O3'-P-O5'	-5.15	96.28	104.00
54	BA	837	C	O4'-C4'-C3'	5.14	109.14	104.00
54	BA	1790	C	O4'-C4'-C3'	5.14	109.14	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	750	A	O4'-C1'-C2'	-5.14	102.46	107.60
53	B4	28	SER	N-CA-C	5.14	117.62	111.71
54	BA	2680	U	C5'-C4'-C3'	-5.13	108.30	116.00
54	BA	2661	G	O4'-C4'-C3'	5.13	109.13	104.00
1	AB	23	ASN	CA-C-N	5.13	124.79	119.56
1	AB	23	ASN	C-N-CA	5.13	124.79	119.56
10	AK	23	HIS	CB-CG-CD2	-5.12	124.54	131.20
45	BW	54	ARG	NE-CZ-NH2	5.12	123.81	119.20
55	BB	95	U	C5'-C4'-C3'	-5.12	108.32	116.00
21	AA	1152	A	O4'-C4'-C3'	5.12	109.12	104.00
54	BA	1497	U	O4'-C1'-C2'	-5.11	100.69	105.80
54	BA	2279	G	C4'-C3'-C2'	-5.11	97.49	102.60
21	AA	209	U	O4'-C4'-C3'	5.11	109.11	104.00
54	BA	1270	C	O4'-C4'-C3'	5.11	109.11	104.00
54	BA	1301	A	O4'-C1'-C2'	-5.11	100.69	105.80
38	BP	31	VAL	N-CA-C	5.11	119.96	109.34
54	BA	1447	C	C4'-C3'-C2'	-5.11	97.49	102.60
11	AL	95	HIS	CB-CG-CD2	-5.10	124.57	131.20
29	BG	114	HIS	CB-CG-CD2	-5.10	124.57	131.20
24	A3	34	U	O4'-C4'-C3'	5.09	109.09	104.00
54	BA	1451	C	O4'-C1'-N1	5.09	115.84	108.20
6	AG	48	THR	CA-C-N	5.09	127.06	120.44
6	AG	48	THR	C-N-CA	5.09	127.06	120.44
48	BZ	43	ILE	CA-CB-CG1	5.09	119.05	110.40
54	BA	1097	U	O4'-C1'-C2'	-5.09	100.71	105.80
54	BA	196	A	C1'-O4'-C4'	-5.08	104.82	109.90
21	AA	1237	C	O4'-C4'-C3'	5.08	109.08	104.00
54	BA	293	U	O3'-P-O5'	5.08	111.62	104.00
54	BA	2116	G	O4'-C4'-C3'	5.08	109.08	104.00
54	BA	2439	A	O4'-C1'-N9	5.07	115.81	108.20
21	AA	112	G	C5'-C4'-C3'	-5.07	108.40	116.00
54	BA	1936	A	C4'-C3'-O3'	5.07	117.00	109.40
16	AQ	62	GLU	OE1-CD-OE2	-5.06	110.75	122.90
54	BA	2029	G	O4'-C4'-C3'	5.06	109.06	104.00
54	BA	2223	G	C5'-C4'-C3'	-5.06	108.41	116.00
54	BA	576	U	O4'-C4'-C3'	5.06	109.06	104.00
4	AE	106	ALA	CA-C-N	5.05	125.95	120.44
4	AE	106	ALA	C-N-CA	5.05	125.95	120.44
8	AI	109	GLN	OE1-CD-NE2	-5.05	117.55	122.60
21	AA	1369	C	O4'-C4'-C3'	5.05	109.06	104.00
54	BA	748	G	O4'-C4'-C3'	5.05	109.06	104.00
21	AA	1359	C	O4'-C4'-C3'	5.05	109.05	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BJ	77	HIS	CB-CG-CD2	-5.05	124.63	131.20
54	BA	1937	A	O4'-C1'-N9	5.05	115.77	108.20
22	A1	70	C	P-O3'-C3'	5.05	127.77	120.20
54	BA	1298	C	O4'-C4'-C3'	5.04	109.05	104.00
21	AA	601	G	O4'-C4'-C3'	5.04	109.04	104.00
54	BA	827	U	C2'-C3'-O3'	-5.04	106.14	113.70
27	BE	45	ALA	CA-C-N	5.04	127.92	120.82
27	BE	45	ALA	C-N-CA	5.04	127.92	120.82
54	BA	1583	A	O4'-C4'-C3'	5.04	109.04	104.00
54	BA	1606	C	O4'-C1'-N1	5.04	116.06	108.50
54	BA	777	G	C5'-C4'-C3'	-5.04	108.44	116.00
54	BA	1475	G	P-O3'-C3'	5.04	127.76	120.20
54	BA	300	A	O4'-C4'-C3'	5.04	109.03	104.00
54	BA	1812	U	C4'-C3'-C2'	-5.03	97.57	102.60
54	BA	1679	A	C4'-C3'-C2'	-5.03	97.57	102.60
24	A3	50	G	O4'-C4'-C3'	5.03	109.03	104.00
21	AA	768	A	O3'-P-O5'	5.02	111.53	104.00
24	A3	10	G	C5'-C4'-C3'	-5.02	108.47	116.00
54	BA	715	A	C2'-C3'-O3'	-5.02	106.17	113.70
54	BA	1923	U	C4'-C3'-C2'	-5.02	97.58	102.60
1	AB	223	GLY	CA-C-N	5.01	130.73	121.70
1	AB	223	GLY	C-N-CA	5.01	130.73	121.70
21	AA	451	A	O3'-P-O5'	5.01	111.52	104.00
52	B3	1	PRO	CA-N-CD	-5.01	104.98	112.00
21	AA	78	A	O4'-C4'-C3'	5.01	109.01	104.00
47	BY	41	HIS	CB-CG-CD2	-5.01	124.68	131.20
21	AA	355	C	O4'-C4'-C3'	5.01	109.01	104.00
51	B2	16	HIS	CB-CG-CD2	-5.01	124.69	131.20
56	B5	126	GLN	OE1-CD-NE2	-5.01	117.59	122.60
27	BE	100	MET	CA-C-N	5.01	126.95	120.44
27	BE	100	MET	C-N-CA	5.01	126.95	120.44
54	BA	1398	C	O4'-C4'-C3'	5.01	109.01	104.00
54	BA	2895	G	O4'-C4'-C3'	5.01	109.01	104.00
54	BA	2342	C	C4'-C3'-C2'	-5.01	97.59	102.60
54	BA	1535	A	O4'-C4'-C3'	5.00	109.00	104.00

There are no chirality outliers.

All (1121) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	10	G	Sidechain
22	A1	16	C	Sidechain

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Mol	Chain	Res	Type	Group
22	A1	18	G	Sidechain
22	A1	2	G	Sidechain
22	A1	21	A	Sidechain
22	A1	24	G	Sidechain
22	A1	27	C	Sidechain
22	A1	45	G	Sidechain
22	A1	52	G	Sidechain
22	A1	61	C	Sidechain
22	A1	64	U	Sidechain
22	A1	67	U	Sidechain
22	A1	72	C	Sidechain
22	A1	76	A	Sidechain
22	A1	9	A	Sidechain
23	A2	80	C	Sidechain
23	A2	86	U	Sidechain
23	A2	88	U	Sidechain
23	A2	90	U	Sidechain
23	A2	91	A	Sidechain
24	A3	1	C	Sidechain
24	A3	2	G	Sidechain
24	A3	34	U	Sidechain
24	A3	44	A	Sidechain
24	A3	58	A	Sidechain
24	A3	60	A	Sidechain
24	A3	69	C	Sidechain
24	A3	72	C	Sidechain
24	A3	73	A	Sidechain
21	AA	10	A	Sidechain
21	AA	1010	U	Sidechain
21	AA	1012	A	Sidechain
21	AA	1013	G	Sidechain
21	AA	1014	A	Sidechain
21	AA	1018	G	Sidechain
21	AA	1025	U	Sidechain
21	AA	1027	C	Sidechain
21	AA	1029	U	Sidechain
21	AA	1033	G	Sidechain
21	AA	1036	A	Sidechain
21	AA	1043	G	Sidechain
21	AA	1045	C	Sidechain
21	AA	1046	A	Sidechain
21	AA	105	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1066	C	Sidechain
21	AA	1077	G	Sidechain
21	AA	108	G	Sidechain
21	AA	109	A	Sidechain
21	AA	1092	A	Sidechain
21	AA	1093	A	Sidechain
21	AA	1095	U	Sidechain
21	AA	1097	C	Sidechain
21	AA	1100	C	Sidechain
21	AA	1107	C	Sidechain
21	AA	1110	A	Sidechain
21	AA	1115	U	Sidechain
21	AA	1120	C	Sidechain
21	AA	1124	G	Sidechain
21	AA	1125	U	Sidechain
21	AA	1128	C	Sidechain
21	AA	1131	G	Sidechain
21	AA	1135	U	Sidechain
21	AA	1139	G	Sidechain
21	AA	114	U	Sidechain
21	AA	1142	G	Sidechain
21	AA	1144	G	Sidechain
21	AA	1145	A	Sidechain
21	AA	1155	A	Sidechain
21	AA	1157	A	Sidechain
21	AA	116	A	Sidechain
21	AA	1160	G	Sidechain
21	AA	1161	C	Sidechain
21	AA	1163	A	Sidechain
21	AA	117	G	Sidechain
21	AA	1172	C	Sidechain
21	AA	1174	G	Sidechain
21	AA	1181	G	Sidechain
21	AA	1183	U	Sidechain
21	AA	1185	G	Sidechain
21	AA	1187	G	Sidechain
21	AA	1194	U	Sidechain
21	AA	12	U	Sidechain
21	AA	1200	C	Sidechain
21	AA	1207	G	Sidechain
21	AA	1211	U	Sidechain
21	AA	1213	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1215	G	Sidechain
21	AA	1216	A	Sidechain
21	AA	1221	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1228	C	Sidechain
21	AA	1235	U	Sidechain
21	AA	124	C	Sidechain
21	AA	1244	G	Sidechain
21	AA	1248	A	Sidechain
21	AA	1250	A	Sidechain
21	AA	1258	G	Sidechain
21	AA	126	G	Sidechain
21	AA	1264	U	Sidechain
21	AA	1265	C	Sidechain
21	AA	1266	G	Sidechain
21	AA	1272	G	Sidechain
21	AA	1278	G	Sidechain
21	AA	1288	A	Sidechain
21	AA	1295	U	Sidechain
21	AA	13	U	Sidechain
21	AA	1301	U	Sidechain
21	AA	1305	G	Sidechain
21	AA	131	A	Sidechain
21	AA	1315	U	Sidechain
21	AA	1325	C	Sidechain
21	AA	1326	U	Sidechain
21	AA	1327	C	Sidechain
21	AA	133	U	Sidechain
21	AA	1331	G	Sidechain
21	AA	1333	A	Sidechain
21	AA	1336	C	Sidechain
21	AA	1338	G	Sidechain
21	AA	134	G	Sidechain
21	AA	1343	G	Sidechain
21	AA	1345	U	Sidechain
21	AA	135	C	Sidechain
21	AA	1358	U	Sidechain
21	AA	1359	C	Sidechain
21	AA	1364	U	Sidechain
21	AA	1370	G	Sidechain
21	AA	1379	G	Sidechain
21	AA	1383	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1385	G	Sidechain
21	AA	139	A	Sidechain
21	AA	1396	A	Sidechain
21	AA	1397	C	Sidechain
21	AA	1400	C	Sidechain
21	AA	1404	C	Sidechain
21	AA	1405	G	Sidechain
21	AA	1408	A	Sidechain
21	AA	1411	C	Sidechain
21	AA	1412	C	Sidechain
21	AA	1416	G	Sidechain
21	AA	1422	G	Sidechain
21	AA	143	A	Sidechain
21	AA	1435	G	Sidechain
21	AA	1436	U	Sidechain
21	AA	1439	G	Sidechain
21	AA	1447	A	Sidechain
21	AA	1448	C	Sidechain
21	AA	1451	U	Sidechain
21	AA	1459	G	Sidechain
21	AA	146	G	Sidechain
21	AA	1460	C	Sidechain
21	AA	1466	C	Sidechain
21	AA	1470	U	Sidechain
21	AA	1472	U	Sidechain
21	AA	1474	U	Sidechain
21	AA	1478	U	Sidechain
21	AA	1483	A	Sidechain
21	AA	1489	G	Sidechain
21	AA	1493	A	Sidechain
21	AA	1498	U	Sidechain
21	AA	1502	A	Sidechain
21	AA	1503	A	Sidechain
21	AA	1508	A	Sidechain
21	AA	1509	C	Sidechain
21	AA	1512	U	Sidechain
21	AA	1514	G	Sidechain
21	AA	1516	G	Sidechain
21	AA	1517	G	Sidechain
21	AA	1518	A	Sidechain
21	AA	152	A	Sidechain
21	AA	1521	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1522	U	Sidechain
21	AA	1526	G	Sidechain
21	AA	1527	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1532	U	Sidechain
21	AA	1533	C	Sidechain
21	AA	1534	A	Sidechain
21	AA	159	G	Sidechain
21	AA	164	G	Sidechain
21	AA	165	G	Sidechain
21	AA	168	G	Sidechain
21	AA	171	A	Sidechain
21	AA	179	A	Sidechain
21	AA	184	G	Sidechain
21	AA	186	C	Sidechain
21	AA	189	A	Sidechain
21	AA	19	A	Sidechain
21	AA	197	A	Sidechain
21	AA	200	G	Sidechain
21	AA	202	G	Sidechain
21	AA	215	C	Sidechain
21	AA	227	G	Sidechain
21	AA	234	C	Sidechain
21	AA	236	A	Sidechain
21	AA	237	G	Sidechain
21	AA	246	A	Sidechain
21	AA	249	U	Sidechain
21	AA	251	G	Sidechain
21	AA	252	U	Sidechain
21	AA	254	G	Sidechain
21	AA	26	A	Sidechain
21	AA	261	U	Sidechain
21	AA	267	C	Sidechain
21	AA	269	C	Sidechain
21	AA	27	G	Sidechain
21	AA	270	A	Sidechain
21	AA	271	C	Sidechain
21	AA	272	C	Sidechain
21	AA	274	A	Sidechain
21	AA	280	C	Sidechain
21	AA	282	A	Sidechain
21	AA	297	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	299	G	Sidechain
21	AA	301	G	Sidechain
21	AA	305	G	Sidechain
21	AA	309	A	Sidechain
21	AA	324	G	Sidechain
21	AA	325	A	Sidechain
21	AA	346	G	Sidechain
21	AA	347	G	Sidechain
21	AA	348	G	Sidechain
21	AA	349	A	Sidechain
21	AA	352	C	Sidechain
21	AA	353	A	Sidechain
21	AA	354	G	Sidechain
21	AA	359	G	Sidechain
21	AA	372	C	Sidechain
21	AA	377	G	Sidechain
21	AA	380	G	Sidechain
21	AA	390	U	Sidechain
21	AA	393	A	Sidechain
21	AA	395	C	Sidechain
21	AA	396	C	Sidechain
21	AA	400	C	Sidechain
21	AA	403	C	Sidechain
21	AA	404	G	Sidechain
21	AA	408	A	Sidechain
21	AA	409	U	Sidechain
21	AA	430	A	Sidechain
21	AA	446	G	Sidechain
21	AA	450	G	Sidechain
21	AA	452	A	Sidechain
21	AA	464	U	Sidechain
21	AA	474	G	Sidechain
21	AA	485	U	Sidechain
21	AA	494	G	Sidechain
21	AA	496	A	Sidechain
21	AA	497	G	Sidechain
21	AA	499	A	Sidechain
21	AA	5	U	Sidechain
21	AA	501	C	Sidechain
21	AA	505	G	Sidechain
21	AA	506	G	Sidechain
21	AA	51	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	514	C	Sidechain
21	AA	515	G	Sidechain
21	AA	517	G	Sidechain
21	AA	519	C	Sidechain
21	AA	522	C	Sidechain
21	AA	523	A	Sidechain
21	AA	525	C	Sidechain
21	AA	527	G	Sidechain
21	AA	529	G	Sidechain
21	AA	533	A	Sidechain
21	AA	535	A	Sidechain
21	AA	539	A	Sidechain
21	AA	540	G	Sidechain
21	AA	562	U	Sidechain
21	AA	565	U	Sidechain
21	AA	566	G	Sidechain
21	AA	571	U	Sidechain
21	AA	581	G	Sidechain
21	AA	582	C	Sidechain
21	AA	583	A	Sidechain
21	AA	589	U	Sidechain
21	AA	590	U	Sidechain
21	AA	6	G	Sidechain
21	AA	60	A	Sidechain
21	AA	600	A	Sidechain
21	AA	601	G	Sidechain
21	AA	608	A	Sidechain
21	AA	610	U	Sidechain
21	AA	616	G	Sidechain
21	AA	618	C	Sidechain
21	AA	619	U	Sidechain
21	AA	63	C	Sidechain
21	AA	632	U	Sidechain
21	AA	637	C	Sidechain
21	AA	641	U	Sidechain
21	AA	650	G	Sidechain
21	AA	658	C	Sidechain
21	AA	66	A	Sidechain
21	AA	664	G	Sidechain
21	AA	667	G	Sidechain
21	AA	671	G	Sidechain
21	AA	676	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	677	U	Sidechain
21	AA	678	U	Sidechain
21	AA	681	A	Sidechain
21	AA	686	U	Sidechain
21	AA	688	G	Sidechain
21	AA	691	G	Sidechain
21	AA	693	G	Sidechain
21	AA	701	U	Sidechain
21	AA	705	G	Sidechain
21	AA	708	C	Sidechain
21	AA	710	G	Sidechain
21	AA	714	G	Sidechain
21	AA	718	A	Sidechain
21	AA	721	G	Sidechain
21	AA	722	G	Sidechain
21	AA	724	G	Sidechain
21	AA	725	G	Sidechain
21	AA	727	G	Sidechain
21	AA	728	A	Sidechain
21	AA	741	G	Sidechain
21	AA	743	A	Sidechain
21	AA	744	C	Sidechain
21	AA	752	G	Sidechain
21	AA	759	A	Sidechain
21	AA	76	G	Sidechain
21	AA	763	G	Sidechain
21	AA	768	A	Sidechain
21	AA	778	G	Sidechain
21	AA	789	U	Sidechain
21	AA	79	G	Sidechain
21	AA	791	G	Sidechain
21	AA	794	A	Sidechain
21	AA	8	A	Sidechain
21	AA	80	A	Sidechain
21	AA	808	C	Sidechain
21	AA	815	A	Sidechain
21	AA	816	A	Sidechain
21	AA	820	U	Sidechain
21	AA	823	C	Sidechain
21	AA	824	G	Sidechain
21	AA	826	C	Sidechain
21	AA	83	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	833	G	Sidechain
21	AA	838	G	Sidechain
21	AA	84	U	Sidechain
21	AA	843	U	Sidechain
21	AA	847	G	Sidechain
21	AA	855	U	Sidechain
21	AA	857	C	Sidechain
21	AA	86	G	Sidechain
21	AA	862	C	Sidechain
21	AA	865	A	Sidechain
21	AA	869	G	Sidechain
21	AA	888	G	Sidechain
21	AA	889	A	Sidechain
21	AA	891	U	Sidechain
21	AA	892	A	Sidechain
21	AA	895	G	Sidechain
21	AA	90	C	Sidechain
21	AA	900	A	Sidechain
21	AA	903	G	Sidechain
21	AA	906	A	Sidechain
21	AA	91	U	Sidechain
21	AA	916	U	Sidechain
21	AA	920	U	Sidechain
21	AA	922	G	Sidechain
21	AA	925	G	Sidechain
21	AA	93	U	Sidechain
21	AA	931	C	Sidechain
21	AA	932	C	Sidechain
21	AA	939	G	Sidechain
21	AA	946	A	Sidechain
21	AA	947	G	Sidechain
21	AA	951	G	Sidechain
21	AA	952	U	Sidechain
21	AA	955	U	Sidechain
21	AA	961	U	Sidechain
21	AA	962	C	Sidechain
21	AA	963	G	Sidechain
21	AA	966	G	Sidechain
21	AA	969	A	Sidechain
21	AA	977	A	Sidechain
21	AA	979	C	Sidechain
21	AA	982	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	983	A	Sidechain
21	AA	984	C	Sidechain
21	AA	986	U	Sidechain
21	AA	987	G	Sidechain
21	AA	991	U	Sidechain
21	AA	995	C	Sidechain
21	AA	997	U	Sidechain
10	AK	115	ILE	Peptide
50	B1	48	TYR	Sidechain
54	BA	10	A	Sidechain
54	BA	1000	A	Sidechain
54	BA	1005	C	Sidechain
54	BA	1012	U	Sidechain
54	BA	1013	C	Sidechain
54	BA	1014	A	Sidechain
54	BA	1016	G	Sidechain
54	BA	102	U	Sidechain
54	BA	1025	G	Sidechain
54	BA	1031	G	Sidechain
54	BA	1036	G	Sidechain
54	BA	1042	G	Sidechain
54	BA	105	C	Sidechain
54	BA	1055	G	Sidechain
54	BA	1061	U	Sidechain
54	BA	1062	G	Sidechain
54	BA	1071	G	Sidechain
54	BA	1074	G	Sidechain
54	BA	1075	C	Sidechain
54	BA	1076	C	Sidechain
54	BA	1078	U	Sidechain
54	BA	1079	C	Sidechain
54	BA	1080	A	Sidechain
54	BA	1082	U	Sidechain
54	BA	1083	U	Sidechain
54	BA	1087	G	Sidechain
54	BA	1091	G	Sidechain
54	BA	1094	U	Sidechain
54	BA	1096	A	Sidechain
54	BA	1098	A	Sidechain
54	BA	11	C	Sidechain
54	BA	1106	G	Sidechain
54	BA	1107	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1116	G	Sidechain
54	BA	1121	C	Sidechain
54	BA	1133	A	Sidechain
54	BA	1135	C	Sidechain
54	BA	1138	G	Sidechain
54	BA	1139	G	Sidechain
54	BA	114	U	Sidechain
54	BA	1142	A	Sidechain
54	BA	115	C	Sidechain
54	BA	1153	C	Sidechain
54	BA	1158	C	Sidechain
54	BA	1160	G	Sidechain
54	BA	1162	G	Sidechain
54	BA	1170	C	Sidechain
54	BA	1181	U	Sidechain
54	BA	1182	G	Sidechain
54	BA	1186	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	1200	C	Sidechain
54	BA	1209	U	Sidechain
54	BA	1212	G	Sidechain
54	BA	1220	G	Sidechain
54	BA	1221	C	Sidechain
54	BA	1223	G	Sidechain
54	BA	1229	C	Sidechain
54	BA	1236	G	Sidechain
54	BA	1237	A	Sidechain
54	BA	124	G	Sidechain
54	BA	1241	A	Sidechain
54	BA	1244	A	Sidechain
54	BA	1250	G	Sidechain
54	BA	1257	C	Sidechain
54	BA	1259	G	Sidechain
54	BA	1265	A	Sidechain
54	BA	1266	G	Sidechain
54	BA	1267	U	Sidechain
54	BA	1271	G	Sidechain
54	BA	1272	A	Sidechain
54	BA	1275	A	Sidechain
54	BA	1277	G	Sidechain
54	BA	1279	G	Sidechain
54	BA	1280	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1285	A	Sidechain
54	BA	129	C	Sidechain
54	BA	1296	G	Sidechain
54	BA	1300	G	Sidechain
54	BA	1305	C	Sidechain
54	BA	1311	G	Sidechain
54	BA	1315	C	Sidechain
54	BA	1316	U	Sidechain
54	BA	1319	C	Sidechain
54	BA	132	G	Sidechain
54	BA	1324	G	Sidechain
54	BA	1329	U	Sidechain
54	BA	1330	C	Sidechain
54	BA	1332	G	Sidechain
54	BA	1334	G	Sidechain
54	BA	134	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1343	G	Sidechain
54	BA	1346	G	Sidechain
54	BA	1355	G	Sidechain
54	BA	1356	G	Sidechain
54	BA	1361	G	Sidechain
54	BA	1364	G	Sidechain
54	BA	1367	A	Sidechain
54	BA	1374	G	Sidechain
54	BA	1381	G	Sidechain
54	BA	1387	A	Sidechain
54	BA	1396	U	Sidechain
54	BA	1398	C	Sidechain
54	BA	14	A	Sidechain
54	BA	1400	U	Sidechain
54	BA	1402	U	Sidechain
54	BA	1403	A	Sidechain
54	BA	1404	C	Sidechain
54	BA	1407	G	Sidechain
54	BA	141	G	Sidechain
54	BA	1417	C	Sidechain
54	BA	1424	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1426	G	Sidechain
54	BA	1427	A	Sidechain
54	BA	143	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1430	G	Sidechain
54	BA	1439	A	Sidechain
54	BA	1442	U	Sidechain
54	BA	1445	G	Sidechain
54	BA	1446	C	Sidechain
54	BA	1460	U	Sidechain
54	BA	1465	G	Sidechain
54	BA	1468	U	Sidechain
54	BA	1471	G	Sidechain
54	BA	1477	A	Sidechain
54	BA	1479	G	Sidechain
54	BA	1484	U	Sidechain
54	BA	1488	C	Sidechain
54	BA	1492	G	Sidechain
54	BA	1493	C	Sidechain
54	BA	1494	A	Sidechain
54	BA	1495	A	Sidechain
54	BA	1498	C	Sidechain
54	BA	1500	G	Sidechain
54	BA	1508	A	Sidechain
54	BA	1512	C	Sidechain
54	BA	1513	U	Sidechain
54	BA	152	A	Sidechain
54	BA	1524	G	Sidechain
54	BA	1529	G	Sidechain
54	BA	153	U	Sidechain
54	BA	1542	U	Sidechain
54	BA	1546	G	Sidechain
54	BA	1548	A	Sidechain
54	BA	1551	A	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1567	G	Sidechain
54	BA	1575	C	Sidechain
54	BA	1580	A	Sidechain
54	BA	1585	C	Sidechain
54	BA	1587	G	Sidechain
54	BA	1593	A	Sidechain
54	BA	1594	U	Sidechain
54	BA	1599	U	Sidechain
54	BA	1606	C	Sidechain
54	BA	1607	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1610	A	Sidechain
54	BA	1618	A	Sidechain
54	BA	1628	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1642	G	Sidechain
54	BA	1646	C	Sidechain
54	BA	1657	U	Sidechain
54	BA	1659	G	Sidechain
54	BA	1669	A	Sidechain
54	BA	1671	U	Sidechain
54	BA	1672	A	Sidechain
54	BA	1678	A	Sidechain
54	BA	168	G	Sidechain
54	BA	1681	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1687	G	Sidechain
54	BA	1692	U	Sidechain
54	BA	1695	G	Sidechain
54	BA	1698	A	Sidechain
54	BA	17	G	Sidechain
54	BA	1705	A	Sidechain
54	BA	1706	C	Sidechain
54	BA	1707	G	Sidechain
54	BA	1708	C	Sidechain
54	BA	1709	U	Sidechain
54	BA	1717	A	Sidechain
54	BA	1723	G	Sidechain
54	BA	1724	G	Sidechain
54	BA	1727	C	Sidechain
54	BA	1729	U	Sidechain
54	BA	1731	G	Sidechain
54	BA	1732	C	Sidechain
54	BA	1736	U	Sidechain
54	BA	1738	G	Sidechain
54	BA	174	U	Sidechain
54	BA	1748	C	Sidechain
54	BA	1749	A	Sidechain
54	BA	1752	C	Sidechain
54	BA	1753	G	Sidechain
54	BA	1757	A	Sidechain
54	BA	1760	C	Sidechain
54	BA	1765	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	177	G	Sidechain
54	BA	1772	A	Sidechain
54	BA	1774	C	Sidechain
54	BA	1779	U	Sidechain
54	BA	178	G	Sidechain
54	BA	1781	U	Sidechain
54	BA	1784	A	Sidechain
54	BA	1788	C	Sidechain
54	BA	1790	C	Sidechain
54	BA	1802	A	Sidechain
54	BA	1805	A	Sidechain
54	BA	1808	A	Sidechain
54	BA	1811	G	Sidechain
54	BA	1812	U	Sidechain
54	BA	1817	G	Sidechain
54	BA	1818	U	Sidechain
54	BA	1820	U	Sidechain
54	BA	1824	G	Sidechain
54	BA	1828	G	Sidechain
54	BA	183	C	Sidechain
54	BA	1830	C	Sidechain
54	BA	1831	G	Sidechain
54	BA	1833	C	Sidechain
54	BA	1834	U	Sidechain
54	BA	1842	G	Sidechain
54	BA	1845	G	Sidechain
54	BA	1849	G	Sidechain
54	BA	1860	G	Sidechain
54	BA	1865	U	Sidechain
54	BA	1869	G	Sidechain
54	BA	1870	C	Sidechain
54	BA	1878	G	Sidechain
54	BA	1882	U	Sidechain
54	BA	1885	A	Sidechain
54	BA	1893	C	Sidechain
54	BA	1903	G	Sidechain
54	BA	1904	G	Sidechain
54	BA	1906	G	Sidechain
54	BA	1908	C	Sidechain
54	BA	1909	C	Sidechain
54	BA	1910	G	Sidechain
54	BA	1912	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1916	A	Sidechain
54	BA	1918	A	Sidechain
54	BA	1925	C	Sidechain
54	BA	1927	A	Sidechain
54	BA	1928	A	Sidechain
54	BA	1931	U	Sidechain
54	BA	1933	G	Sidechain
54	BA	1937	A	Sidechain
54	BA	1938	A	Sidechain
54	BA	1941	C	Sidechain
54	BA	1943	U	Sidechain
54	BA	1945	G	Sidechain
54	BA	1946	U	Sidechain
54	BA	195	A	Sidechain
54	BA	1950	G	Sidechain
54	BA	1956	U	Sidechain
54	BA	1957	C	Sidechain
54	BA	1958	C	Sidechain
54	BA	1959	G	Sidechain
54	BA	1962	C	Sidechain
54	BA	1964	G	Sidechain
54	BA	1969	A	Sidechain
54	BA	1973	G	Sidechain
54	BA	1974	C	Sidechain
54	BA	1978	A	Sidechain
54	BA	1983	G	Sidechain
54	BA	1984	G	Sidechain
54	BA	1989	G	Sidechain
54	BA	1996	C	Sidechain
54	BA	2	G	Sidechain
54	BA	2001	C	Sidechain
54	BA	2003	A	Sidechain
54	BA	2007	U	Sidechain
54	BA	2009	A	Sidechain
54	BA	2013	A	Sidechain
54	BA	202	U	Sidechain
54	BA	2020	A	Sidechain
54	BA	2022	U	Sidechain
54	BA	2025	C	Sidechain
54	BA	2027	G	Sidechain
54	BA	2029	G	Sidechain
54	BA	2031	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2034	U	Sidechain
54	BA	2037	A	Sidechain
54	BA	2040	G	Sidechain
54	BA	2041	U	Sidechain
54	BA	2043	C	Sidechain
54	BA	2044	C	Sidechain
54	BA	2046	G	Sidechain
54	BA	2057	G	Sidechain
54	BA	2059	A	Sidechain
54	BA	206	U	Sidechain
54	BA	2061	G	Sidechain
54	BA	2064	C	Sidechain
54	BA	2065	C	Sidechain
54	BA	2066	C	Sidechain
54	BA	207	A	Sidechain
54	BA	2080	A	Sidechain
54	BA	2083	G	Sidechain
54	BA	209	C	Sidechain
54	BA	2093	G	Sidechain
54	BA	2103	C	Sidechain
54	BA	2108	A	Sidechain
54	BA	2111	U	Sidechain
54	BA	2115	G	Sidechain
54	BA	2117	A	Sidechain
54	BA	2118	U	Sidechain
54	BA	2132	U	Sidechain
54	BA	2136	G	Sidechain
54	BA	2147	A	Sidechain
54	BA	215	G	Sidechain
54	BA	2155	U	Sidechain
54	BA	2163	A	Sidechain
54	BA	2165	C	Sidechain
54	BA	2168	G	Sidechain
54	BA	2170	A	Sidechain
54	BA	2172	U	Sidechain
54	BA	2178	C	Sidechain
54	BA	219	A	Sidechain
54	BA	2197	U	Sidechain
54	BA	2199	A	Sidechain
54	BA	2202	U	Sidechain
54	BA	221	A	Sidechain
54	BA	2211	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2212	A	Sidechain
54	BA	2213	U	Sidechain
54	BA	2215	C	Sidechain
54	BA	2217	G	Sidechain
54	BA	2238	G	Sidechain
54	BA	2240	U	Sidechain
54	BA	2242	G	Sidechain
54	BA	2243	U	Sidechain
54	BA	2257	U	Sidechain
54	BA	2259	U	Sidechain
54	BA	2266	A	Sidechain
54	BA	2267	A	Sidechain
54	BA	227	A	Sidechain
54	BA	2271	G	Sidechain
54	BA	2276	G	Sidechain
54	BA	2277	G	Sidechain
54	BA	2278	A	Sidechain
54	BA	2286	G	Sidechain
54	BA	2287	A	Sidechain
54	BA	2293	G	Sidechain
54	BA	2294	G	Sidechain
54	BA	2295	C	Sidechain
54	BA	2297	A	Sidechain
54	BA	2300	C	Sidechain
54	BA	2301	C	Sidechain
54	BA	2304	G	Sidechain
54	BA	2311	A	Sidechain
54	BA	2313	C	Sidechain
54	BA	2315	G	Sidechain
54	BA	2320	U	Sidechain
54	BA	2324	U	Sidechain
54	BA	233	A	Sidechain
54	BA	2336	A	Sidechain
54	BA	2338	C	Sidechain
54	BA	2339	C	Sidechain
54	BA	2348	U	Sidechain
54	BA	2349	G	Sidechain
54	BA	2357	G	Sidechain
54	BA	2362	C	Sidechain
54	BA	2375	G	Sidechain
54	BA	2389	G	Sidechain
54	BA	2391	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2393	U	Sidechain
54	BA	2411	A	Sidechain
54	BA	2413	G	Sidechain
54	BA	2415	G	Sidechain
54	BA	2416	C	Sidechain
54	BA	2418	A	Sidechain
54	BA	2422	C	Sidechain
54	BA	2424	C	Sidechain
54	BA	2431	U	Sidechain
54	BA	2434	A	Sidechain
54	BA	244	A	Sidechain
54	BA	2442	C	Sidechain
54	BA	2443	C	Sidechain
54	BA	2444	G	Sidechain
54	BA	2447	G	Sidechain
54	BA	2450	A	Sidechain
54	BA	2452	C	Sidechain
54	BA	2453	A	Sidechain
54	BA	2454	G	Sidechain
54	BA	2461	A	Sidechain
54	BA	2464	G	Sidechain
54	BA	2465	C	Sidechain
54	BA	2466	C	Sidechain
54	BA	2468	A	Sidechain
54	BA	2469	A	Sidechain
54	BA	247	G	Sidechain
54	BA	2476	A	Sidechain
54	BA	2477	U	Sidechain
54	BA	2478	A	Sidechain
54	BA	2479	U	Sidechain
54	BA	2487	G	Sidechain
54	BA	2488	G	Sidechain
54	BA	249	C	Sidechain
54	BA	2490	G	Sidechain
54	BA	2491	U	Sidechain
54	BA	2492	U	Sidechain
54	BA	2496	C	Sidechain
54	BA	2498	C	Sidechain
54	BA	25	U	Sidechain
54	BA	250	G	Sidechain
54	BA	2501	C	Sidechain
54	BA	2510	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2514	U	Sidechain
54	BA	2517	C	Sidechain
54	BA	2521	C	Sidechain
54	BA	2530	A	Sidechain
54	BA	2535	G	Sidechain
54	BA	2539	C	Sidechain
54	BA	2548	U	Sidechain
54	BA	2549	G	Sidechain
54	BA	2550	G	Sidechain
54	BA	2552	U	Sidechain
54	BA	2555	U	Sidechain
54	BA	2561	U	Sidechain
54	BA	2564	A	Sidechain
54	BA	2566	A	Sidechain
54	BA	257	C	Sidechain
54	BA	2571	U	Sidechain
54	BA	2575	C	Sidechain
54	BA	2579	C	Sidechain
54	BA	258	G	Sidechain
54	BA	2581	G	Sidechain
54	BA	2588	G	Sidechain
54	BA	2595	G	Sidechain
54	BA	2608	G	Sidechain
54	BA	2613	U	Sidechain
54	BA	2615	U	Sidechain
54	BA	2617	U	Sidechain
54	BA	262	A	Sidechain
54	BA	2622	U	Sidechain
54	BA	2623	G	Sidechain
54	BA	2624	G	Sidechain
54	BA	2627	G	Sidechain
54	BA	2628	C	Sidechain
54	BA	2637	U	Sidechain
54	BA	264	C	Sidechain
54	BA	2640	G	Sidechain
54	BA	2646	C	Sidechain
54	BA	2647	U	Sidechain
54	BA	265	A	Sidechain
54	BA	2656	U	Sidechain
54	BA	2657	A	Sidechain
54	BA	2661	G	Sidechain
54	BA	2666	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2668	G	Sidechain
54	BA	2669	G	Sidechain
54	BA	2673	G	Sidechain
54	BA	268	C	Sidechain
54	BA	2680	U	Sidechain
54	BA	2682	A	Sidechain
54	BA	2684	U	Sidechain
54	BA	2688	G	Sidechain
54	BA	2689	U	Sidechain
54	BA	269	C	Sidechain
54	BA	2692	G	Sidechain
54	BA	2693	G	Sidechain
54	BA	27	G	Sidechain
54	BA	2703	C	Sidechain
54	BA	2715	C	Sidechain
54	BA	2716	C	Sidechain
54	BA	2717	C	Sidechain
54	BA	2718	G	Sidechain
54	BA	272	A	Sidechain
54	BA	2722	G	Sidechain
54	BA	2723	C	Sidechain
54	BA	2727	A	Sidechain
54	BA	2728	U	Sidechain
54	BA	2729	G	Sidechain
54	BA	2731	G	Sidechain
54	BA	2739	U	Sidechain
54	BA	2747	G	Sidechain
54	BA	2751	G	Sidechain
54	BA	2755	C	Sidechain
54	BA	2764	A	Sidechain
54	BA	2765	A	Sidechain
54	BA	2767	C	Sidechain
54	BA	2768	U	Sidechain
54	BA	277	G	Sidechain
54	BA	2779	U	Sidechain
54	BA	2780	G	Sidechain
54	BA	2790	U	Sidechain
54	BA	2797	U	Sidechain
54	BA	2804	U	Sidechain
54	BA	2808	G	Sidechain
54	BA	2811	G	Sidechain
54	BA	2825	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	283	G	Sidechain
54	BA	2830	C	Sidechain
54	BA	2832	U	Sidechain
54	BA	2835	A	Sidechain
54	BA	2848	G	Sidechain
54	BA	285	G	Sidechain
54	BA	2851	A	Sidechain
54	BA	2856	A	Sidechain
54	BA	2857	G	Sidechain
54	BA	2859	G	Sidechain
54	BA	2864	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	287	G	Sidechain
54	BA	2870	C	Sidechain
54	BA	2876	G	Sidechain
54	BA	2877	G	Sidechain
54	BA	2878	U	Sidechain
54	BA	2879	A	Sidechain
54	BA	2883	A	Sidechain
54	BA	2884	U	Sidechain
54	BA	2885	G	Sidechain
54	BA	2891	U	Sidechain
54	BA	29	U	Sidechain
54	BA	2903	U	Sidechain
54	BA	297	G	Sidechain
54	BA	307	G	Sidechain
54	BA	313	G	Sidechain
54	BA	314	C	Sidechain
54	BA	319	G	Sidechain
54	BA	322	A	Sidechain
54	BA	329	G	Sidechain
54	BA	333	G	Sidechain
54	BA	334	C	Sidechain
54	BA	337	C	Sidechain
54	BA	339	U	Sidechain
54	BA	34	U	Sidechain
54	BA	340	A	Sidechain
54	BA	356	G	Sidechain
54	BA	358	U	Sidechain
54	BA	361	G	Sidechain
54	BA	362	A	Sidechain
54	BA	364	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	367	G	Sidechain
54	BA	374	A	Sidechain
54	BA	378	C	Sidechain
54	BA	385	C	Sidechain
54	BA	386	G	Sidechain
54	BA	389	G	Sidechain
54	BA	39	G	Sidechain
54	BA	391	A	Sidechain
54	BA	392	U	Sidechain
54	BA	393	C	Sidechain
54	BA	394	C	Sidechain
54	BA	395	U	Sidechain
54	BA	401	A	Sidechain
54	BA	403	U	Sidechain
54	BA	405	U	Sidechain
54	BA	417	C	Sidechain
54	BA	418	C	Sidechain
54	BA	419	U	Sidechain
54	BA	423	A	Sidechain
54	BA	425	G	Sidechain
54	BA	426	C	Sidechain
54	BA	43	G	Sidechain
54	BA	430	A	Sidechain
54	BA	437	U	Sidechain
54	BA	443	A	Sidechain
54	BA	446	G	Sidechain
54	BA	448	U	Sidechain
54	BA	453	A	Sidechain
54	BA	455	C	Sidechain
54	BA	457	A	Sidechain
54	BA	458	G	Sidechain
54	BA	460	A	Sidechain
54	BA	461	C	Sidechain
54	BA	463	G	Sidechain
54	BA	464	U	Sidechain
54	BA	477	A	Sidechain
54	BA	48	G	Sidechain
54	BA	480	A	Sidechain
54	BA	481	G	Sidechain
54	BA	49	A	Sidechain
54	BA	493	G	Sidechain
54	BA	497	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	500	G	Sidechain
54	BA	501	A	Sidechain
54	BA	502	A	Sidechain
54	BA	516	C	Sidechain
54	BA	518	G	Sidechain
54	BA	52	A	Sidechain
54	BA	524	G	Sidechain
54	BA	529	A	Sidechain
54	BA	533	G	Sidechain
54	BA	538	A	Sidechain
54	BA	541	A	Sidechain
54	BA	545	U	Sidechain
54	BA	547	A	Sidechain
54	BA	56	A	Sidechain
54	BA	568	U	Sidechain
54	BA	569	U	Sidechain
54	BA	577	G	Sidechain
54	BA	578	G	Sidechain
54	BA	579	G	Sidechain
54	BA	58	G	Sidechain
54	BA	580	U	Sidechain
54	BA	581	C	Sidechain
54	BA	594	U	Sidechain
54	BA	597	G	Sidechain
54	BA	599	A	Sidechain
54	BA	600	G	Sidechain
54	BA	602	A	Sidechain
54	BA	605	G	Sidechain
54	BA	608	A	Sidechain
54	BA	61	C	Sidechain
54	BA	611	C	Sidechain
54	BA	613	A	Sidechain
54	BA	616	A	Sidechain
54	BA	622	G	Sidechain
54	BA	623	C	Sidechain
54	BA	631	A	Sidechain
54	BA	632	A	Sidechain
54	BA	635	C	Sidechain
54	BA	640	C	Sidechain
54	BA	641	U	Sidechain
54	BA	644	A	Sidechain
54	BA	654	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	662	G	Sidechain
54	BA	663	G	Sidechain
54	BA	666	A	Sidechain
54	BA	667	U	Sidechain
54	BA	672	C	Sidechain
54	BA	677	A	Sidechain
54	BA	679	C	Sidechain
54	BA	680	C	Sidechain
54	BA	683	U	Sidechain
54	BA	686	U	Sidechain
54	BA	69	C	Sidechain
54	BA	697	G	Sidechain
54	BA	704	G	Sidechain
54	BA	712	G	Sidechain
54	BA	714	U	Sidechain
54	BA	718	A	Sidechain
54	BA	72	U	Sidechain
54	BA	723	C	Sidechain
54	BA	724	U	Sidechain
54	BA	725	G	Sidechain
54	BA	734	A	Sidechain
54	BA	739	A	Sidechain
54	BA	74	A	Sidechain
54	BA	748	G	Sidechain
54	BA	750	A	Sidechain
54	BA	751	A	Sidechain
54	BA	753	A	Sidechain
54	BA	766	U	Sidechain
54	BA	769	U	Sidechain
54	BA	77	G	Sidechain
54	BA	771	G	Sidechain
54	BA	772	C	Sidechain
54	BA	775	G	Sidechain
54	BA	784	G	Sidechain
54	BA	788	A	Sidechain
54	BA	79	C	Sidechain
54	BA	790	U	Sidechain
54	BA	800	A	Sidechain
54	BA	802	A	Sidechain
54	BA	805	G	Sidechain
54	BA	808	G	Sidechain
54	BA	81	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	817	C	Sidechain
54	BA	826	U	Sidechain
54	BA	836	G	Sidechain
54	BA	840	C	Sidechain
54	BA	851	C	Sidechain
54	BA	852	U	Sidechain
54	BA	857	G	Sidechain
54	BA	862	G	Sidechain
54	BA	864	G	Sidechain
54	BA	865	C	Sidechain
54	BA	868	U	Sidechain
54	BA	869	G	Sidechain
54	BA	874	G	Sidechain
54	BA	876	C	Sidechain
54	BA	879	G	Sidechain
54	BA	881	G	Sidechain
54	BA	885	C	Sidechain
54	BA	887	U	Sidechain
54	BA	89	A	Sidechain
54	BA	891	G	Sidechain
54	BA	892	A	Sidechain
54	BA	893	C	Sidechain
54	BA	896	A	Sidechain
54	BA	912	C	Sidechain
54	BA	920	A	Sidechain
54	BA	921	C	Sidechain
54	BA	923	G	Sidechain
54	BA	924	G	Sidechain
54	BA	934	U	Sidechain
54	BA	942	G	Sidechain
54	BA	945	A	Sidechain
54	BA	95	A	Sidechain
54	BA	950	G	Sidechain
54	BA	953	G	Sidechain
54	BA	954	G	Sidechain
54	BA	959	A	Sidechain
54	BA	961	C	Sidechain
54	BA	966	G	Sidechain
54	BA	97	C	Sidechain
54	BA	970	U	Sidechain
54	BA	974	G	Sidechain
54	BA	976	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	982	C	Sidechain
54	BA	984	A	Sidechain
54	BA	989	G	Sidechain
54	BA	993	G	Sidechain
55	BB	10	G	Sidechain
55	BB	101	A	Sidechain
55	BB	112	G	Sidechain
55	BB	113	C	Sidechain
55	BB	116	G	Sidechain
55	BB	15	A	Sidechain
55	BB	28	C	Sidechain
55	BB	29	A	Sidechain
55	BB	31	C	Sidechain
55	BB	32	U	Sidechain
55	BB	39	A	Sidechain
55	BB	40	U	Sidechain
55	BB	41	G	Sidechain
55	BB	43	C	Sidechain
55	BB	48	U	Sidechain
55	BB	57	A	Sidechain
55	BB	64	G	Sidechain
55	BB	75	G	Sidechain
55	BB	92	C	Sidechain
55	BB	93	C	Sidechain
55	BB	98	G	Sidechain
26	BD	124	ARG	Sidechain
41	BS	86	MET	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	3	0
6	AG	1178	0	1234	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	1	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16522	2	0
22	A1	1627	0	832	1	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	1	0
25	BC	2083	0	2157	1	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	1	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	2	0
35	BM	1074	0	1157	1	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31345	6	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99665	16	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 0.

All (16) 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)
30:BH:143:ILE:H	30:BH:143:ILE:HD13	1.72	0.54
24:A3:72:C:C5	24:A3:73:A:C8	2.98	0.51
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.33	0.47
35:BM:80:VAL:H	35:BM:81:ARG:HA	1.81	0.46
22:A1:76:A:H62	54:BA:2600:A:H3'	1.82	0.44
54:BA:308:G:H21	54:BA:329:G:N2	2.15	0.43
54:BA:2306:C:H3'	54:BA:2307:G:H5''	2.01	0.43
21:AA:979:C:N4	21:AA:1360:A:H62	2.16	0.42
54:BA:1771:C:H2'	54:BA:1772:A:C8	2.53	0.42
54:BA:1025:G:C5	54:BA:1135:C:H1'	2.55	0.41
5:AF:94:HIS:CG	5:AF:95:ALA:N	2.89	0.41
11:AL:115:LYS:HE3	11:AL:116:TYR:CE2	2.55	0.41
5:AF:49:TYR:CE1	21:AA:674:G:H5''	2.55	0.41
25:BC:14:HIS:CE1	54:BA:1830:C:H5'	2.56	0.40
34:BL:25:SER:CB	34:BL:26:GLY:CA	2.99	0.40
34:BL:24:GLY:HA2	34:BL:25:SER:C	2.46	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	AB	218/220 (99%)	202 (93%)	13 (6%)	3 (1%)	9	40
2	AC	205/208 (99%)	189 (92%)	13 (6%)	3 (2%)	8	40
3	AD	203/206 (98%)	192 (95%)	6 (3%)	5 (2%)	4	26
4	AE	150/152 (99%)	136 (91%)	10 (7%)	4 (3%)	4	25
5	AF	99/101 (98%)	85 (86%)	8 (8%)	6 (6%)	1	13
6	AG	150/152 (99%)	139 (93%)	9 (6%)	2 (1%)	9	42
7	AH	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
8	AI	126/128 (98%)	112 (89%)	10 (8%)	4 (3%)	3	21
9	AJ	98/100 (98%)	90 (92%)	4 (4%)	4 (4%)	2	18
10	AK	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
11	AL	121/124 (98%)	109 (90%)	7 (6%)	5 (4%)	2	18
12	AM	112/115 (97%)	93 (83%)	17 (15%)	2 (2%)	6	34
13	AN	98/101 (97%)	85 (87%)	9 (9%)	4 (4%)	2	18
14	AO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	28
15	AP	79/81 (98%)	67 (85%)	10 (13%)	2 (2%)	4	26
16	AQ	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	9	42
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	6	34
18	AS	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	9	42
19	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	AU	51/53 (96%)	34 (67%)	9 (18%)	8 (16%)	0	3
25	BC	270/273 (99%)	245 (91%)	21 (8%)	4 (2%)	8	40
26	BD	207/209 (99%)	182 (88%)	17 (8%)	8 (4%)	2	19
27	BE	199/201 (99%)	183 (92%)	11 (6%)	5 (2%)	4	26
28	BF	176/179 (98%)	156 (89%)	17 (10%)	3 (2%)	7	36
29	BG	174/177 (98%)	156 (90%)	14 (8%)	4 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BH	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	18	56
31	BI	139/142 (98%)	125 (90%)	11 (8%)	3 (2%)	5	29
32	BJ	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
33	BK	121/123 (98%)	109 (90%)	9 (7%)	3 (2%)	4	26
34	BL	141/144 (98%)	124 (88%)	10 (7%)	7 (5%)	1	16
35	BM	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	8	40
36	BN	119/121 (98%)	101 (85%)	13 (11%)	5 (4%)	2	17
37	BO	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
38	BP	112/115 (97%)	98 (88%)	9 (8%)	5 (4%)	2	17
39	BQ	115/118 (98%)	103 (90%)	8 (7%)	4 (4%)	3	20
40	BR	101/103 (98%)	95 (94%)	3 (3%)	3 (3%)	3	23
41	BS	108/110 (98%)	95 (88%)	11 (10%)	2 (2%)	6	32
42	BT	92/94 (98%)	73 (79%)	12 (13%)	7 (8%)	1	10
43	BU	101/104 (97%)	85 (84%)	11 (11%)	5 (5%)	1	16
44	BV	92/94 (98%)	89 (97%)	2 (2%)	1 (1%)	11	46
45	BW	78/80 (98%)	58 (74%)	17 (22%)	3 (4%)	2	19
46	BX	75/79 (95%)	60 (80%)	11 (15%)	4 (5%)	1	15
47	BY	61/63 (97%)	57 (93%)	2 (3%)	2 (3%)	3	21
48	BZ	56/59 (95%)	49 (88%)	6 (11%)	1 (2%)	6	34
49	B0	54/57 (95%)	50 (93%)	3 (6%)	1 (2%)	6	32
50	B1	50/52 (96%)	43 (86%)	5 (10%)	2 (4%)	2	18
51	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	28
52	B3	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	7	38
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	210 (95%)	11 (5%)	0	100	100
All	All	5876/6008 (98%)	5290 (90%)	442 (8%)	144 (2%)	6	26

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AF	86	ARG
8	AI	124	PRO
12	AM	42	VAL

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Mol	Chain	Res	Type
13	AN	56	SER
17	AR	20	ILE
20	AU	17	ARG
20	AU	24	LYS
26	BD	2	ILE
26	BD	51	THR
26	BD	119	ALA
27	BE	61	ARG
30	BH	9	VAL
33	BK	103	VAL
36	BN	47	VAL
38	BP	31	VAL
43	BU	70	ALA
52	B3	3	ILE
5	AF	63	ASN
9	AJ	75	ASP
11	AL	17	LYS
11	AL	78	VAL
13	AN	99	ALA
15	AP	17	TYR
16	AQ	35	LYS
20	AU	22	CYS
20	AU	30	GLU
25	BC	153	LEU
25	BC	197	ALA
26	BD	118	PHE
27	BE	43	THR
27	BE	90	GLN
28	BF	103	ILE
31	BI	10	LEU
34	BL	27	LEU
34	BL	34	GLY
36	BN	10	LEU
38	BP	110	LYS
40	BR	24	LYS
40	BR	53	PHE
42	BT	2	ILE
42	BT	3	ARG
42	BT	70	HIS
43	BU	43	LYS
43	BU	45	GLN
44	BV	71	LYS

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Mol	Chain	Res	Type
46	BX	24	THR
47	BY	7	ARG
48	BZ	9	THR
49	B0	5	ASN
50	B1	6	GLU
51	B2	44	VAL
1	AB	10	LYS
3	AD	4	LEU
3	AD	47	LEU
3	AD	187	ARG
4	AE	43	GLY
4	AE	54	GLU
4	AE	105	ILE
5	AF	52	ASN
5	AF	82	ASP
6	AG	147	ASN
8	AI	55	ASP
9	AJ	41	PRO
9	AJ	57	VAL
9	AJ	58	ASN
11	AL	33	CYS
11	AL	112	ALA
13	AN	100	SER
15	AP	79	ASN
20	AU	15	LEU
26	BD	15	PHE
26	BD	136	ASN
26	BD	138	LEU
33	BK	111	LYS
34	BL	99	ASN
36	BN	32	GLU
39	BQ	91	ARG
41	BS	41	LYS
41	BS	92	ARG
42	BT	61	LEU
45	BW	23	LYS
46	BX	27	ARG
46	BX	75	GLU
1	AB	18	GLN
3	AD	84	ASN
5	AF	6	ILE
5	AF	94	HIS

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Mol	Chain	Res	Type
6	AG	43	TYR
8	AI	41	GLU
8	AI	114	LYS
14	AO	43	ALA
20	AU	25	ALA
25	BC	144	GLU
28	BF	46	LYS
29	BG	9	VAL
31	BI	132	ALA
31	BI	135	MET
33	BK	119	ALA
35	BM	21	ALA
36	BN	93	GLY
38	BP	74	GLN
38	BP	113	LEU
39	BQ	90	ASP
40	BR	28	ALA
42	BT	14	PRO
42	BT	15	HIS
42	BT	78	SER
43	BU	12	VAL
45	BW	8	SER
45	BW	26	GLY
46	BX	43	LYS
47	BY	9	LYS
50	B1	50	GLU
1	AB	11	ALA
3	AD	29	THR
4	AE	24	VAL
11	AL	11	ARG
13	AN	58	SER
26	BD	34	VAL
27	BE	79	ARG
29	BG	22	VAL
29	BG	164	ALA
34	BL	19	LEU
34	BL	36	LYS
38	BP	112	ARG
2	AC	144	GLY
14	AO	74	VAL
18	AS	39	ILE
20	AU	27	VAL

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Mol	Chain	Res	Type
20	AU	48	LYS
28	BF	102	LEU
29	BG	112	VAL
36	BN	105	GLY
39	BQ	2	ARG
39	BQ	5	ARG
43	BU	101	THR
34	BL	11	GLY
2	AC	195	ILE
25	BC	123	ILE
27	BE	31	VAL
34	BL	101	ILE
35	BM	80	VAL
2	AC	206	ILE
12	AM	8	ILE

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	AB	180/180 (100%)	178 (99%)	2 (1%)	65	76
2	AC	170/171 (99%)	168 (99%)	2 (1%)	63	75
3	AD	172/173 (99%)	171 (99%)	1 (1%)	78	83
4	AE	113/113 (100%)	112 (99%)	1 (1%)	70	79
5	AF	87/87 (100%)	87 (100%)	0	100	100
6	AG	123/123 (100%)	122 (99%)	1 (1%)	73	80
7	AH	104/105 (99%)	101 (97%)	3 (3%)	37	58
8	AI	105/105 (100%)	104 (99%)	1 (1%)	68	78
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	44	64
10	AK	90/90 (100%)	89 (99%)	1 (1%)	65	76
11	AL	103/104 (99%)	101 (98%)	2 (2%)	50	67
12	AM	91/92 (99%)	89 (98%)	2 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AN	83/84 (99%)	82 (99%)	1 (1%)	63	75
14	AO	76/77 (99%)	74 (97%)	2 (3%)	40	62
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	39	61
17	AR	48/48 (100%)	47 (98%)	1 (2%)	47	65
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	42 (96%)	2 (4%)	24	46
25	BC	216/217 (100%)	214 (99%)	2 (1%)	70	79
26	BD	164/164 (100%)	162 (99%)	2 (1%)	63	75
27	BE	165/165 (100%)	164 (99%)	1 (1%)	78	83
28	BF	149/150 (99%)	148 (99%)	1 (1%)	76	81
29	BG	137/138 (99%)	135 (98%)	2 (2%)	57	72
30	BH	114/114 (100%)	113 (99%)	1 (1%)	70	79
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	116 (100%)	0	100	100
33	BK	103/103 (100%)	102 (99%)	1 (1%)	68	78
34	BL	102/103 (99%)	102 (100%)	0	100	100
35	BM	109/109 (100%)	108 (99%)	1 (1%)	70	79
36	BN	100/100 (100%)	99 (99%)	1 (1%)	68	78
37	BO	86/87 (99%)	85 (99%)	1 (1%)	63	75
38	BP	99/100 (99%)	98 (99%)	1 (1%)	68	78
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	45	64
40	BR	84/84 (100%)	83 (99%)	1 (1%)	63	75
41	BS	93/93 (100%)	91 (98%)	2 (2%)	45	64
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	83 (100%)	0	100	100
44	BV	78/78 (100%)	77 (99%)	1 (1%)	61	74
45	BW	59/59 (100%)	58 (98%)	1 (2%)	53	69
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BZ	48/49 (98%)	46 (96%)	2 (4%)	26	48
49	B0	47/48 (98%)	46 (98%)	1 (2%)	47	65
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	37 (97%)	1 (3%)	40	62
52	B3	51/52 (98%)	51 (100%)	0	100	100
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	171 (99%)	2 (1%)	63	75
All	All	4842/4870 (99%)	4789 (99%)	53 (1%)	63	76

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

Mol	Chain	Res	Type
1	AB	57	ASN
1	AB	88	GLN
2	AC	2	GLN
2	AC	175	HIS
3	AD	14	GLU
4	AE	99	SER
6	AG	3	ARG
7	AH	20	ASN
7	AH	77	VAL
7	AH	100	ILE
8	AI	129	ARG
9	AJ	44	THR
9	AJ	87	LEU
10	AK	60	PHE
11	AL	28	GLN
11	AL	71	HIS
12	AM	90	HIS
12	AM	106	ARG
13	AN	100	SER
14	AO	45	HIS
14	AO	73	ASP
16	AQ	62	GLU
16	AQ	64	ARG
17	AR	71	ASP
20	AU	8	ASN
20	AU	17	ARG
25	BC	62	ARG
25	BC	218	THR

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Mol	Chain	Res	Type
26	BD	126	ASN
26	BD	176	ASP
27	BE	163	ASN
28	BF	162	ASP
29	BG	105	SER
29	BG	115	GLN
30	BH	143	ILE
33	BK	107	LEU
35	BM	97	GLN
36	BN	70	THR
37	BO	95	SER
38	BP	75	THR
39	BQ	19	GLN
39	BQ	71	ASN
40	BR	41	ILE
41	BS	12	SER
41	BS	108	SER
44	BV	12	GLN
45	BW	36	ILE
48	BZ	9	THR
48	BZ	40	THR
49	B0	45	ASP
51	B2	16	HIS
56	B5	40	GLU
56	B5	129	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	35	ASN
1	AB	145	ASN
1	AB	177	ASN
2	AC	24	ASN
2	AC	68	HIS
2	AC	99	GLN
3	AD	40	HIS
4	AE	147	ASN
5	AF	58	HIS
5	AF	81	ASN
8	AI	3	ASN
8	AI	24	ASN
8	AI	74	GLN

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Mol	Chain	Res	Type
9	AJ	15	HIS
9	AJ	64	GLN
9	AJ	99	GLN
10	AK	37	GLN
11	AL	19	ASN
14	AO	19	ASN
19	AT	81	GLN
25	BC	24	HIS
25	BC	36	ASN
25	BC	85	ASN
25	BC	199	HIS
25	BC	250	GLN
26	BD	49	GLN
27	BE	156	ASN
28	BF	22	ASN
28	BF	62	GLN
29	BG	110	HIS
29	BG	115	GLN
30	BH	119	ASN
33	BK	90	ASN
34	BL	35	HIS
35	BM	60	GLN
36	BN	31	HIS
36	BN	73	ASN
37	BO	29	HIS
37	BO	38	GLN
38	BP	2	ASN
38	BP	114	ASN
39	BQ	19	GLN
39	BQ	71	ASN
40	BR	6	GLN
40	BR	11	GLN
40	BR	66	HIS
43	BU	53	GLN
44	BV	87	GLN
51	B2	13	ASN
56	B5	57	GLN
56	B5	172	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	279 (18%)	88 (5%)
22	A1	75/76 (98%)	14 (18%)	7 (9%)
23	A2	14/15 (93%)	4 (28%)	1 (7%)
24	A3	76/77 (98%)	14 (18%)	4 (5%)
54	BA	2902/2903 (99%)	517 (17%)	125 (4%)
55	BB	116/118 (98%)	15 (12%)	5 (4%)
All	All	4713/4722 (99%)	843 (17%)	230 (4%)

All (843) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	16	A
21	AA	26	A
21	AA	27	G
21	AA	32	A
21	AA	33	A
21	AA	36	C
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	50	A
21	AA	51	A
21	AA	52	C
21	AA	61	G
21	AA	64	G
21	AA	65	A
21	AA	72	A
21	AA	80	A
21	AA	81	A
21	AA	84	U
21	AA	86	G
21	AA	89	U
21	AA	90	C
21	AA	94	G
21	AA	95	C
21	AA	96	U
21	AA	109	A
21	AA	110	C
21	AA	121	U

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Mol	Chain	Res	Type
21	AA	125	U
21	AA	131	A
21	AA	134	G
21	AA	163	C
21	AA	165	G
21	AA	182	A
21	AA	184	G
21	AA	185	U
21	AA	187	G
21	AA	188	C
21	AA	191	G
21	AA	198	G
21	AA	201	G
21	AA	209	U
21	AA	210	C
21	AA	235	C
21	AA	236	A
21	AA	237	G
21	AA	238	A
21	AA	239	U
21	AA	244	U
21	AA	245	U
21	AA	251	G
21	AA	252	U
21	AA	266	G
21	AA	272	C
21	AA	280	C
21	AA	282	A
21	AA	289	G
21	AA	301	G
21	AA	307	C
21	AA	308	C
21	AA	309	A
21	AA	310	G
21	AA	317	U
21	AA	328	C
21	AA	329	A
21	AA	330	C
21	AA	343	U
21	AA	344	A
21	AA	347	G
21	AA	348	G

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Mol	Chain	Res	Type
21	AA	349	A
21	AA	351	G
21	AA	352	C
21	AA	354	G
21	AA	356	A
21	AA	361	G
21	AA	366	A
21	AA	367	U
21	AA	381	C
21	AA	397	A
21	AA	406	G
21	AA	413	G
21	AA	414	A
21	AA	415	A
21	AA	421	U
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	452	A
21	AA	453	G
21	AA	461	A
21	AA	462	G
21	AA	463	U
21	AA	465	A
21	AA	466	A
21	AA	467	U
21	AA	468	A
21	AA	484	G
21	AA	492	C
21	AA	493	A
21	AA	511	C
21	AA	524	G
21	AA	525	C
21	AA	527	G
21	AA	529	G
21	AA	532	A
21	AA	547	A
21	AA	559	A
21	AA	564	C
21	AA	566	G
21	AA	572	A
21	AA	573	A

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Mol	Chain	Res	Type
21	AA	575	G
21	AA	576	C
21	AA	577	G
21	AA	588	G
21	AA	611	C
21	AA	612	C
21	AA	619	U
21	AA	620	C
21	AA	653	U
21	AA	665	A
21	AA	674	G
21	AA	675	A
21	AA	700	G
21	AA	718	A
21	AA	719	C
21	AA	721	G
21	AA	724	G
21	AA	728	A
21	AA	729	A
21	AA	731	G
21	AA	733	G
21	AA	734	G
21	AA	735	C
21	AA	755	G
21	AA	756	C
21	AA	765	G
21	AA	777	A
21	AA	790	A
21	AA	791	G
21	AA	794	A
21	AA	812	G
21	AA	817	C
21	AA	818	G
21	AA	819	A
21	AA	821	G
21	AA	827	U
21	AA	828	U
21	AA	829	G
21	AA	841	C
21	AA	842	U
21	AA	843	U
21	AA	844	G

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Mol	Chain	Res	Type
21	AA	845	A
21	AA	846	G
21	AA	884	U
21	AA	885	G
21	AA	914	A
21	AA	927	G
21	AA	930	C
21	AA	932	C
21	AA	934	C
21	AA	939	G
21	AA	940	C
21	AA	942	G
21	AA	945	G
21	AA	946	A
21	AA	960	U
21	AA	962	C
21	AA	966	G
21	AA	968	A
21	AA	969	A
21	AA	970	C
21	AA	971	G
21	AA	976	G
21	AA	977	A
21	AA	980	C
21	AA	983	A
21	AA	984	C
21	AA	993	G
21	AA	994	A
21	AA	995	C
21	AA	1004	A
21	AA	1025	U
21	AA	1026	G
21	AA	1031	C
21	AA	1032	G
21	AA	1045	C
21	AA	1054	C
21	AA	1056	U
21	AA	1065	U
21	AA	1094	G
21	AA	1101	A
21	AA	1102	A
21	AA	1126	U

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Mol	Chain	Res	Type
21	AA	1127	G
21	AA	1129	C
21	AA	1130	A
21	AA	1135	U
21	AA	1136	C
21	AA	1138	G
21	AA	1139	G
21	AA	1140	C
21	AA	1143	G
21	AA	1146	A
21	AA	1159	U
21	AA	1160	G
21	AA	1161	C
21	AA	1181	G
21	AA	1182	G
21	AA	1183	U
21	AA	1184	G
21	AA	1188	A
21	AA	1189	U
21	AA	1190	G
21	AA	1191	A
21	AA	1196	A
21	AA	1197	A
21	AA	1201	A
21	AA	1202	U
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1228	C
21	AA	1238	A
21	AA	1240	U
21	AA	1241	G
21	AA	1256	A
21	AA	1257	A
21	AA	1266	G
21	AA	1279	G
21	AA	1280	A
21	AA	1281	C
21	AA	1282	C
21	AA	1287	A
21	AA	1300	G
21	AA	1302	C

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Mol	Chain	Res	Type
21	AA	1303	C
21	AA	1305	G
21	AA	1320	C
21	AA	1321	U
21	AA	1323	G
21	AA	1341	U
21	AA	1343	G
21	AA	1363	A
21	AA	1379	G
21	AA	1380	U
21	AA	1383	C
21	AA	1384	C
21	AA	1390	U
21	AA	1397	C
21	AA	1398	A
21	AA	1399	C
21	AA	1400	C
21	AA	1401	G
21	AA	1407	C
21	AA	1408	A
21	AA	1432	G
21	AA	1433	A
21	AA	1446	A
21	AA	1447	A
21	AA	1448	C
21	AA	1454	G
21	AA	1459	G
21	AA	1460	C
21	AA	1493	A
21	AA	1494	G
21	AA	1499	A
21	AA	1503	A
21	AA	1504	G
21	AA	1506	U
21	AA	1523	G
21	AA	1529	G
21	AA	1530	G
22	A1	3	G
22	A1	4	U
22	A1	17	U
22	A1	18	G
22	A1	43	G

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Mol	Chain	Res	Type
22	A1	44	G
22	A1	46	7MG
22	A1	48	C
22	A1	60	C
22	A1	71	C
22	A1	73	A
22	A1	74	C
22	A1	75	C
22	A1	76	A
23	A2	82	A
23	A2	83	U
23	A2	84	G
23	A2	92	U
24	A3	2	G
24	A3	9	G
24	A3	10	G
24	A3	11	A
24	A3	16	C
24	A3	17	C
24	A3	18	U
24	A3	22	A
24	A3	36	A
24	A3	48	U
24	A3	49	C
24	A3	60	A
24	A3	72	C
24	A3	73	A
54	BA	10	A
54	BA	11	C
54	BA	15	G
54	BA	20	C
54	BA	27	G
54	BA	34	U
54	BA	35	G
54	BA	45	G
54	BA	50	U
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	91	A
54	BA	98	G
54	BA	100	U

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Mol	Chain	Res	Type
54	BA	101	A
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	126	A
54	BA	127	A
54	BA	128	C
54	BA	142	A
54	BA	196	A
54	BA	197	A
54	BA	200	U
54	BA	204	A
54	BA	216	A
54	BA	222	A
54	BA	224	U
54	BA	248	G
54	BA	250	G
54	BA	265	A
54	BA	266	G
54	BA	271	G
54	BA	272	A
54	BA	273	G
54	BA	278	A
54	BA	283	G
54	BA	299	A
54	BA	302	C
54	BA	316	C
54	BA	330	A
54	BA	332	A
54	BA	335	C
54	BA	370	G
54	BA	372	G
54	BA	373	U
54	BA	374	A
54	BA	385	C
54	BA	386	G
54	BA	387	U
54	BA	389	G
54	BA	392	U
54	BA	396	G

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Mol	Chain	Res	Type
54	BA	404	A
54	BA	411	G
54	BA	428	A
54	BA	429	A
54	BA	430	A
54	BA	436	C
54	BA	446	G
54	BA	447	A
54	BA	448	U
54	BA	451	U
54	BA	453	A
54	BA	454	A
54	BA	457	A
54	BA	458	G
54	BA	473	G
54	BA	481	G
54	BA	482	A
54	BA	483	A
54	BA	490	C
54	BA	503	A
54	BA	504	A
54	BA	506	G
54	BA	508	A
54	BA	518	G
54	BA	527	C
54	BA	529	A
54	BA	532	A
54	BA	533	G
54	BA	548	G
54	BA	563	A
54	BA	566	U
54	BA	571	U
54	BA	575	A
54	BA	586	A
54	BA	588	U
54	BA	614	A
54	BA	627	A
54	BA	637	A
54	BA	644	A
54	BA	645	C
54	BA	653	U
54	BA	662	G

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Mol	Chain	Res	Type
54	BA	663	G
54	BA	670	A
54	BA	671	C
54	BA	686	U
54	BA	716	A
54	BA	719	C
54	BA	727	A
54	BA	728	G
54	BA	730	A
54	BA	747	U
54	BA	750	A
54	BA	751	A
54	BA	753	A
54	BA	762	U
54	BA	763	G
54	BA	764	A
54	BA	775	G
54	BA	776	G
54	BA	782	A
54	BA	784	G
54	BA	785	G
54	BA	789	A
54	BA	790	U
54	BA	791	C
54	BA	792	A
54	BA	805	G
54	BA	811	U
54	BA	824	U
54	BA	827	U
54	BA	828	U
54	BA	836	G
54	BA	846	U
54	BA	847	U
54	BA	848	C
54	BA	856	G
54	BA	858	G
54	BA	866	A
54	BA	889	C
54	BA	890	C
54	BA	891	G
54	BA	892	A
54	BA	896	A

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Mol	Chain	Res	Type
54	BA	897	C
54	BA	910	A
54	BA	911	A
54	BA	912	C
54	BA	914	G
54	BA	931	U
54	BA	932	U
54	BA	934	U
54	BA	941	A
54	BA	946	C
54	BA	959	A
54	BA	961	C
54	BA	974	G
54	BA	981	A
54	BA	982	C
54	BA	983	A
54	BA	994	C
54	BA	995	C
54	BA	996	A
54	BA	1005	C
54	BA	1006	C
54	BA	1008	A
54	BA	1012	U
54	BA	1013	C
54	BA	1022	G
54	BA	1024	G
54	BA	1025	G
54	BA	1026	G
54	BA	1028	A
54	BA	1033	U
54	BA	1044	C
54	BA	1045	C
54	BA	1046	A
54	BA	1055	G
54	BA	1058	U
54	BA	1067	A
54	BA	1068	G
54	BA	1069	A
54	BA	1070	A
54	BA	1071	G
54	BA	1072	C
54	BA	1073	A

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Mol	Chain	Res	Type
54	BA	1076	C
54	BA	1087	G
54	BA	1088	A
54	BA	1090	A
54	BA	1097	U
54	BA	1098	A
54	BA	1112	G
54	BA	1124	G
54	BA	1126	A
54	BA	1128	G
54	BA	1129	A
54	BA	1130	U
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1139	G
54	BA	1144	A
54	BA	1175	A
54	BA	1176	U
54	BA	1185	G
54	BA	1187	G
54	BA	1188	U
54	BA	1190	G
54	BA	1204	A
54	BA	1210	G
54	BA	1211	C
54	BA	1227	G
54	BA	1237	A
54	BA	1242	U
54	BA	1250	G
54	BA	1251	C
54	BA	1252	G
54	BA	1253	A
54	BA	1256	G
54	BA	1266	G
54	BA	1272	A
54	BA	1275	A
54	BA	1276	A
54	BA	1282	U
54	BA	1283	G
54	BA	1287	A
54	BA	1288	G

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Mol	Chain	Res	Type
54	BA	1289	C
54	BA	1291	C
54	BA	1292	G
54	BA	1300	G
54	BA	1301	A
54	BA	1302	A
54	BA	1313	U
54	BA	1314	C
54	BA	1315	C
54	BA	1329	U
54	BA	1330	C
54	BA	1332	G
54	BA	1341	G
54	BA	1349	C
54	BA	1350	C
54	BA	1361	G
54	BA	1365	A
54	BA	1366	A
54	BA	1368	G
54	BA	1378	A
54	BA	1379	U
54	BA	1382	G
54	BA	1383	A
54	BA	1384	A
54	BA	1385	A
54	BA	1386	C
54	BA	1388	G
54	BA	1392	A
54	BA	1400	U
54	BA	1402	U
54	BA	1416	G
54	BA	1417	C
54	BA	1420	A
54	BA	1427	A
54	BA	1428	C
54	BA	1439	A
54	BA	1440	U
54	BA	1451	C
54	BA	1452	G
54	BA	1454	C
54	BA	1455	G
54	BA	1458	U

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Mol	Chain	Res	Type
54	BA	1459	G
54	BA	1460	U
54	BA	1476	U
54	BA	1482	G
54	BA	1490	A
54	BA	1493	C
54	BA	1508	A
54	BA	1509	A
54	BA	1512	C
54	BA	1523	U
54	BA	1528	A
54	BA	1532	A
54	BA	1534	U
54	BA	1535	A
54	BA	1536	C
54	BA	1537	G
54	BA	1538	G
54	BA	1539	U
54	BA	1541	C
54	BA	1566	A
54	BA	1568	G
54	BA	1569	A
54	BA	1598	A
54	BA	1599	U
54	BA	1608	A
54	BA	1610	A
54	BA	1611	C
54	BA	1614	A
54	BA	1617	C
54	BA	1618	A
54	BA	1619	G
54	BA	1627	G
54	BA	1630	A
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1651	G
54	BA	1654	A
54	BA	1656	C
54	BA	1668	A
54	BA	1669	A
54	BA	1670	C

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Mol	Chain	Res	Type
54	BA	1674	G
54	BA	1675	C
54	BA	1696	G
54	BA	1699	G
54	BA	1700	A
54	BA	1712	U
54	BA	1714	U
54	BA	1715	G
54	BA	1730	C
54	BA	1758	U
54	BA	1760	C
54	BA	1761	C
54	BA	1763	G
54	BA	1764	C
54	BA	1773	A
54	BA	1780	A
54	BA	1782	U
54	BA	1789	A
54	BA	1800	C
54	BA	1807	G
54	BA	1808	A
54	BA	1809	A
54	BA	1813	G
54	BA	1814	G
54	BA	1815	A
54	BA	1816	C
54	BA	1820	U
54	BA	1821	A
54	BA	1829	A
54	BA	1830	C
54	BA	1877	A
54	BA	1884	G
54	BA	1900	A
54	BA	1912	A
54	BA	1913	A
54	BA	1914	C
54	BA	1926	U
54	BA	1937	A
54	BA	1940	U
54	BA	1945	G
54	BA	1946	U
54	BA	1952	A

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Mol	Chain	Res	Type
54	BA	1955	U
54	BA	1963	U
54	BA	1967	C
54	BA	1971	U
54	BA	1972	G
54	BA	1982	U
54	BA	1983	G
54	BA	1993	U
54	BA	1997	C
54	BA	2021	C
54	BA	2022	U
54	BA	2023	C
54	BA	2026	U
54	BA	2030	A
54	BA	2031	A
54	BA	2032	G
54	BA	2034	U
54	BA	2043	C
54	BA	2055	C
54	BA	2059	A
54	BA	2061	G
54	BA	2062	A
54	BA	2063	C
54	BA	2093	G
54	BA	2094	A
54	BA	2112	G
54	BA	2113	U
54	BA	2114	A
54	BA	2116	G
54	BA	2117	A
54	BA	2118	U
54	BA	2119	A
54	BA	2126	A
54	BA	2127	G
54	BA	2129	C
54	BA	2131	U
54	BA	2132	U
54	BA	2137	U
54	BA	2138	G
54	BA	2157	G
54	BA	2159	G
54	BA	2165	C

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Mol	Chain	Res	Type
54	BA	2172	U
54	BA	2173	A
54	BA	2174	C
54	BA	2181	U
54	BA	2194	U
54	BA	2203	U
54	BA	2211	A
54	BA	2212	A
54	BA	2216	G
54	BA	2225	A
54	BA	2238	G
54	BA	2239	G
54	BA	2261	C
54	BA	2269	G
54	BA	2275	C
54	BA	2277	G
54	BA	2283	C
54	BA	2288	A
54	BA	2289	G
54	BA	2297	A
54	BA	2305	U
54	BA	2307	G
54	BA	2309	A
54	BA	2311	A
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2333	A
54	BA	2334	U
54	BA	2335	A
54	BA	2347	C
54	BA	2353	G
54	BA	2367	G
54	BA	2383	G
54	BA	2385	C
54	BA	2386	A
54	BA	2402	U
54	BA	2406	A
54	BA	2423	U
54	BA	2425	A
54	BA	2429	G

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Mol	Chain	Res	Type
54	BA	2430	A
54	BA	2431	U
54	BA	2432	A
54	BA	2441	U
54	BA	2448	A
54	BA	2449	U
54	BA	2473	U
54	BA	2474	U
54	BA	2476	A
54	BA	2478	A
54	BA	2480	C
54	BA	2488	G
54	BA	2489	U
54	BA	2490	G
54	BA	2491	U
54	BA	2492	U
54	BA	2498	C
54	BA	2499	C
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2504	U
54	BA	2505	G
54	BA	2513	A
54	BA	2518	A
54	BA	2519	U
54	BA	2529	G
54	BA	2531	A
54	BA	2540	C
54	BA	2542	A
54	BA	2543	G
54	BA	2547	A
54	BA	2567	G
54	BA	2573	C
54	BA	2576	G
54	BA	2581	G
54	BA	2582	G
54	BA	2585	U
54	BA	2587	A
54	BA	2588	G
54	BA	2603	G
54	BA	2609	U

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Mol	Chain	Res	Type
54	BA	2610	C
54	BA	2611	C
54	BA	2628	C
54	BA	2629	U
54	BA	2644	G
54	BA	2645	G
54	BA	2660	A
54	BA	2661	G
54	BA	2663	G
54	BA	2668	G
54	BA	2681	C
54	BA	2683	C
54	BA	2689	U
54	BA	2690	U
54	BA	2714	G
54	BA	2718	G
54	BA	2726	A
54	BA	2729	G
54	BA	2732	G
54	BA	2733	A
54	BA	2750	A
54	BA	2751	G
54	BA	2756	U
54	BA	2776	A
54	BA	2777	G
54	BA	2778	A
54	BA	2780	G
54	BA	2790	U
54	BA	2791	G
54	BA	2799	A
54	BA	2800	A
54	BA	2820	A
54	BA	2832	U
54	BA	2850	A
54	BA	2872	A
54	BA	2875	C
54	BA	2876	G
54	BA	2883	A
54	BA	2884	U
54	BA	2895	G
55	BB	9	G
55	BB	12	C

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Mol	Chain	Res	Type
55	BB	13	G
55	BB	15	A
55	BB	16	G
55	BB	35	C
55	BB	36	C
55	BB	45	A
55	BB	53	A
55	BB	64	G
55	BB	67	G
55	BB	73	A
55	BB	74	U
55	BB	90	C
55	BB	109	A

All (230) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	26	A
21	AA	32	A
21	AA	51	A
21	AA	60	A
21	AA	64	G
21	AA	80	A
21	AA	89	U
21	AA	94	G
21	AA	95	C
21	AA	109	A
21	AA	133	U
21	AA	184	G
21	AA	205	A
21	AA	209	U
21	AA	236	A
21	AA	238	A
21	AA	244	U
21	AA	246	A
21	AA	251	G
21	AA	307	C
21	AA	309	A
21	AA	316	C
21	AA	329	A
21	AA	343	U

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Mol	Chain	Res	Type
21	AA	344	A
21	AA	345	C
21	AA	347	G
21	AA	366	A
21	AA	452	A
21	AA	465	A
21	AA	492	C
21	AA	524	G
21	AA	563	A
21	AA	575	G
21	AA	611	C
21	AA	619	U
21	AA	674	G
21	AA	718	A
21	AA	728	A
21	AA	733	G
21	AA	734	G
21	AA	755	G
21	AA	790	A
21	AA	817	C
21	AA	818	G
21	AA	827	U
21	AA	841	C
21	AA	843	U
21	AA	844	G
21	AA	845	A
21	AA	884	U
21	AA	945	G
21	AA	970	C
21	AA	975	A
21	AA	982	U
21	AA	983	A
21	AA	991	U
21	AA	994	A
21	AA	1025	U
21	AA	1044	A
21	AA	1049	U
21	AA	1101	A
21	AA	1126	U
21	AA	1129	C
21	AA	1159	U
21	AA	1181	G

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Mol	Chain	Res	Type
21	AA	1188	A
21	AA	1190	G
21	AA	1196	A
21	AA	1201	A
21	AA	1215	G
21	AA	1227	A
21	AA	1231	G
21	AA	1238	A
21	AA	1280	A
21	AA	1300	G
21	AA	1319	A
21	AA	1342	C
21	AA	1379	G
21	AA	1383	C
21	AA	1399	C
21	AA	1407	C
21	AA	1446	A
21	AA	1447	A
21	AA	1459	G
21	AA	1493	A
21	AA	1498	U
22	A1	3	G
22	A1	17	U
22	A1	43	G
22	A1	47	U
22	A1	60	C
22	A1	70	C
22	A1	73	A
23	A2	83	U
24	A3	10	G
24	A3	16	C
24	A3	48	U
24	A3	61	U
54	BA	49	A
54	BA	118	A
54	BA	121	G
54	BA	126	A
54	BA	249	C
54	BA	271	G
54	BA	272	A
54	BA	278	A
54	BA	384	A

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Mol	Chain	Res	Type
54	BA	428	A
54	BA	446	G
54	BA	448	U
54	BA	453	A
54	BA	481	G
54	BA	482	A
54	BA	503	A
54	BA	506	G
54	BA	509	C
54	BA	532	A
54	BA	603	A
54	BA	670	A
54	BA	749	A
54	BA	750	A
54	BA	762	U
54	BA	784	G
54	BA	789	A
54	BA	791	C
54	BA	827	U
54	BA	847	U
54	BA	890	C
54	BA	896	A
54	BA	909	A
54	BA	911	A
54	BA	931	U
54	BA	933	A
54	BA	981	A
54	BA	994	C
54	BA	1005	C
54	BA	1033	U
54	BA	1068	G
54	BA	1070	A
54	BA	1072	C
54	BA	1097	U
54	BA	1128	G
54	BA	1129	A
54	BA	1132	U
54	BA	1187	G
54	BA	1232	G
54	BA	1282	U
54	BA	1287	A
54	BA	1288	G

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Mol	Chain	Res	Type
54	BA	1300	G
54	BA	1301	A
54	BA	1312	U
54	BA	1313	U
54	BA	1314	C
54	BA	1329	U
54	BA	1349	C
54	BA	1385	A
54	BA	1396	U
54	BA	1427	A
54	BA	1428	C
54	BA	1451	C
54	BA	1460	U
54	BA	1475	G
54	BA	1508	A
54	BA	1511	G
54	BA	1534	U
54	BA	1536	C
54	BA	1598	A
54	BA	1610	A
54	BA	1617	C
54	BA	1618	A
54	BA	1655	A
54	BA	1668	A
54	BA	1674	G
54	BA	1699	G
54	BA	1713	A
54	BA	1760	C
54	BA	1808	A
54	BA	1813	G
54	BA	1820	U
54	BA	1912	A
54	BA	1913	A
54	BA	1936	A
54	BA	1945	G
54	BA	1951	U
54	BA	1952	A
54	BA	1963	U
54	BA	2021	C
54	BA	2030	A
54	BA	2062	A
54	BA	2092	U

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Mol	Chain	Res	Type
54	BA	2113	U
54	BA	2117	A
54	BA	2126	A
54	BA	2211	A
54	BA	2282	G
54	BA	2286	G
54	BA	2288	A
54	BA	2321	U
54	BA	2346	A
54	BA	2391	G
54	BA	2429	G
54	BA	2430	A
54	BA	2439	A
54	BA	2473	U
54	BA	2489	U
54	BA	2497	A
54	BA	2501	C
54	BA	2503	A
54	BA	2504	U
54	BA	2518	A
54	BA	2542	A
54	BA	2569	G
54	BA	2581	G
54	BA	2586	U
54	BA	2609	U
54	BA	2644	G
54	BA	2680	U
54	BA	2689	U
54	BA	2732	G
54	BA	2776	A
54	BA	2790	U
54	BA	2875	C
55	BB	15	A
55	BB	34	A
55	BB	35	C
55	BB	63	C
55	BB	73	A

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	6MZ	A1	37	22	22,25,26	0.64	0	29,36,39	1.22	2 (6%)
22	CM0	A1	34	22	21,26,27	1.24	2 (9%)	26,37,40	1.44	1 (3%)
24	5MU	A3	55	24	19,22,23	0.72	0	27,32,35	1.33	4 (14%)
22	5MU	A1	54	22	19,22,23	0.73	0	27,32,35	1.33	3 (11%)
22	7MG	A1	46	22	23,26,27	4.01	2 (8%)	27,39,42	1.40	2 (7%)
24	PSU	A3	56	24	18,21,22	0.82	0	21,30,33	1.39	2 (9%)
22	4SU	A1	7	22	18,21,22	1.41	2 (11%)	25,30,33	0.97	2 (8%)
22	PSU	A1	55	22	18,21,22	0.84	0	21,30,33	1.41	3 (14%)
24	4SU	A3	8	24	18,21,22	1.53	2 (11%)	25,30,33	0.83	1 (4%)
24	H2U	A3	21	24	18,21,22	1.40	2 (11%)	19,30,33	1.37	3 (15%)
24	OMC	A3	33	24	19,22,23	0.73	0	25,31,34	1.01	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	6MZ	A1	37	22	-	0/9/27/28	0/3/3/3
22	CM0	A1	34	22	-	2/12/30/31	0/2/2/2
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3
24	PSU	A3	56	24	-	2/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2
22	PSU	A1	55	22	-	3/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/7/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-18.78	1.33	1.45
24	A3	8	4SU	C5-C4	-5.32	1.36	1.42
22	A1	7	4SU	C5-C4	-5.02	1.36	1.42
22	A1	34	CM0	O5-C5	-4.45	1.26	1.36
24	A3	21	H2U	C2-N3	-3.57	1.31	1.38
24	A3	21	H2U	C4-N3	-3.53	1.31	1.37
22	A1	46	7MG	C8-N7	-2.37	1.30	1.42
24	A3	8	4SU	C4-S4	-2.18	1.64	1.68
22	A1	7	4SU	C4-S4	-2.13	1.65	1.68
22	A1	34	CM0	O8-C8	-2.06	1.24	1.30

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	5.72	111.47	103.37
22	A1	34	CM0	C7-O5-C5	5.51	124.50	117.48
22	A1	55	PSU	C6-C5-C4	4.11	120.95	118.17
22	A1	37	6MZ	C9-N6-C6	4.10	126.65	122.85
24	A3	21	H2U	N3-C2-N1	3.61	120.27	116.65
24	A3	55	5MU	C5M-C5-C6	-3.45	118.18	122.85
24	A3	56	PSU	C6-C5-C4	3.45	120.50	118.17
22	A1	54	5MU	C5M-C5-C6	-3.43	118.20	122.85
22	A1	54	5MU	C6-C5-C4	3.00	120.49	118.02
24	A3	33	OMC	O2-C2-N3	-2.97	117.65	122.33
24	A3	55	5MU	C6-C5-C4	2.95	120.45	118.02
24	A3	56	PSU	O4'-C1'-C2'	2.86	109.11	105.15
24	A3	21	H2U	C5-C4-N3	2.66	119.51	116.69
22	A1	55	PSU	O4'-C1'-C2'	2.60	108.75	105.15
22	A1	37	6MZ	C4-C5-C6	-2.53	114.68	116.78
24	A3	21	H2U	O2-C2-N3	-2.52	116.84	121.49
24	A3	55	5MU	C5M-C5-C4	2.41	121.36	118.78
22	A1	54	5MU	C5M-C5-C4	2.36	121.30	118.78
22	A1	55	PSU	N1-C2-N3	2.29	117.58	115.17
22	A1	7	4SU	C6-C5-C4	2.20	121.86	119.95
22	A1	7	4SU	O4'-C4'-C3'	2.18	109.48	105.15
24	A3	55	5MU	C5-C6-N1	-2.17	120.96	123.31
24	A3	8	4SU	C6-C5-C4	2.11	121.78	119.95
22	A1	46	7MG	C4-C5-N7	2.05	107.79	105.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	46	7MG	C4'-C5'-O5'-P
22	A1	55	PSU	C2'-C1'-C5-C4
24	A3	56	PSU	O4'-C1'-C5-C4
24	A3	56	PSU	O4'-C1'-C5-C6
22	A1	34	CM0	O5-C7-C8-O9
22	A1	34	CM0	O5-C7-C8-O8
22	A1	55	PSU	O4'-C1'-C5-C4
22	A1	55	PSU	O4'-C1'-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
58	FME	BA	3001	57	8,9,10	0.77	0	8,9,11	2.22	3 (37%)
57	VAL	A1	101	58,22	4,6,7	0.87	0	6,7,9	0.98	1 (16%)

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
58	FME	BA	3001	57	-	0/7/9/11	-
57	VAL	A1	101	58,22	-	3/5/6/8	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
58	BA	3001	FME	C-CA-N	4.00	117.22	109.50
58	BA	3001	FME	CA-N-CN	3.74	128.57	122.82
57	A1	101	VAL	O-C-CA	-2.37	118.68	124.77
58	BA	3001	FME	O-C-CA	-2.33	118.78	124.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A1	101	VAL	O-C-CA-CB
57	A1	101	VAL	C-CA-CB-CG1
57	A1	101	VAL	C-CA-CB-CG2

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.

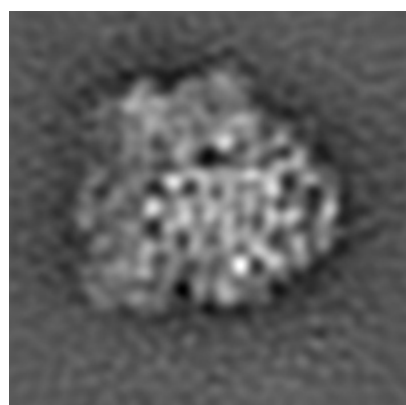
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2473. These allow visual inspection of the internal detail of the map and identification of artifacts.

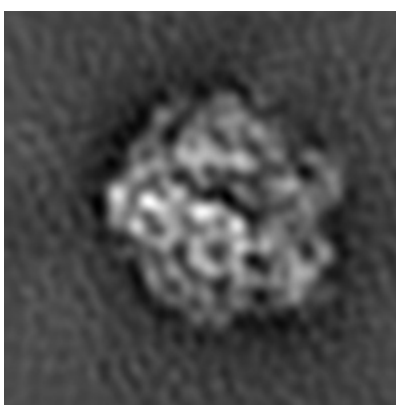
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

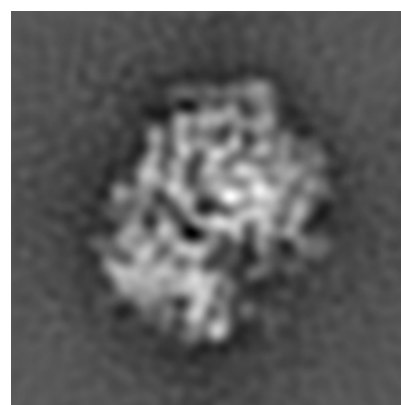
6.1.1 Primary map



X



Y

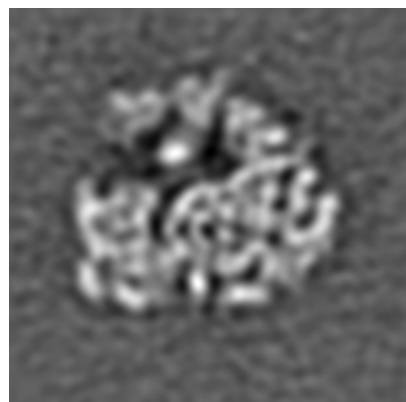


Z

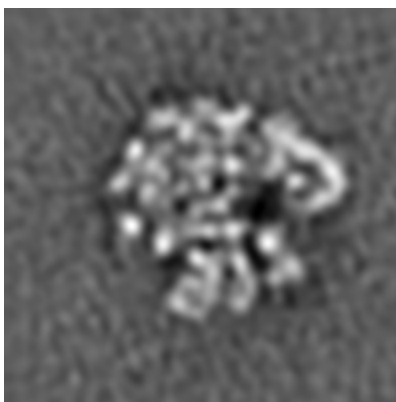
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

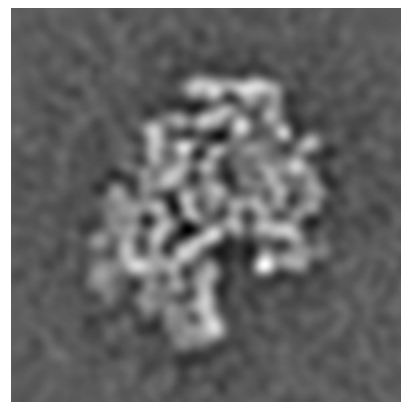
6.2.1 Primary map



X Index: 64



Y Index: 64

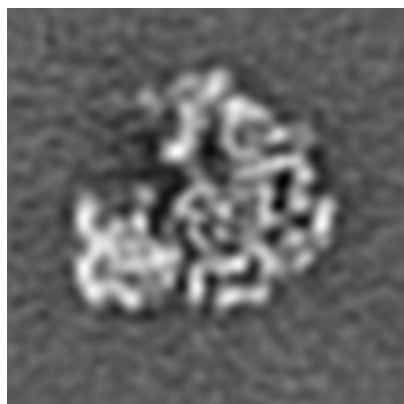


Z Index: 64

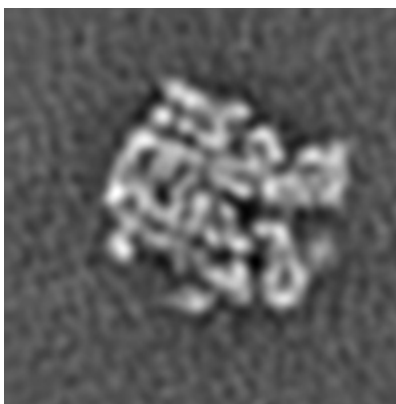
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 66



Y Index: 69

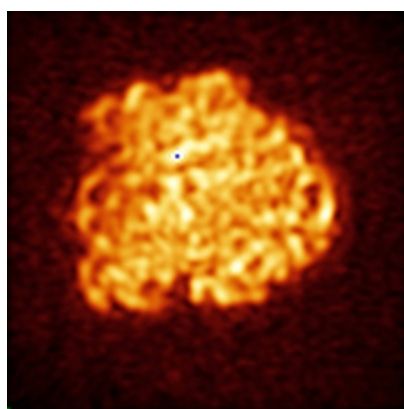


Z Index: 62

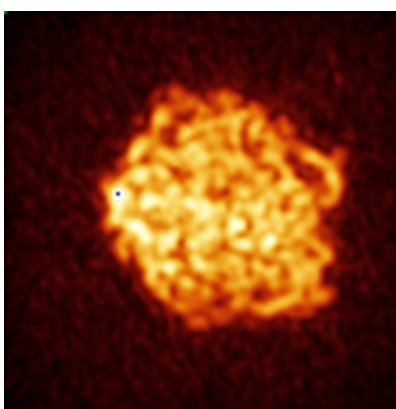
The images above show the largest variance slices of the map in three orthogonal directions.

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

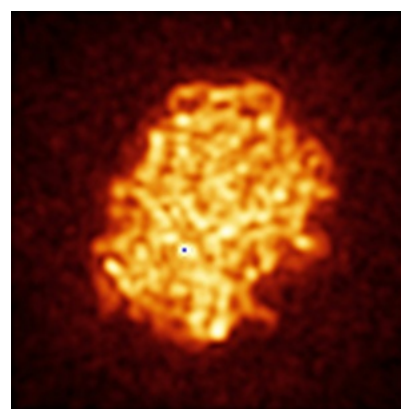
6.4.1 Primary map



X



Y

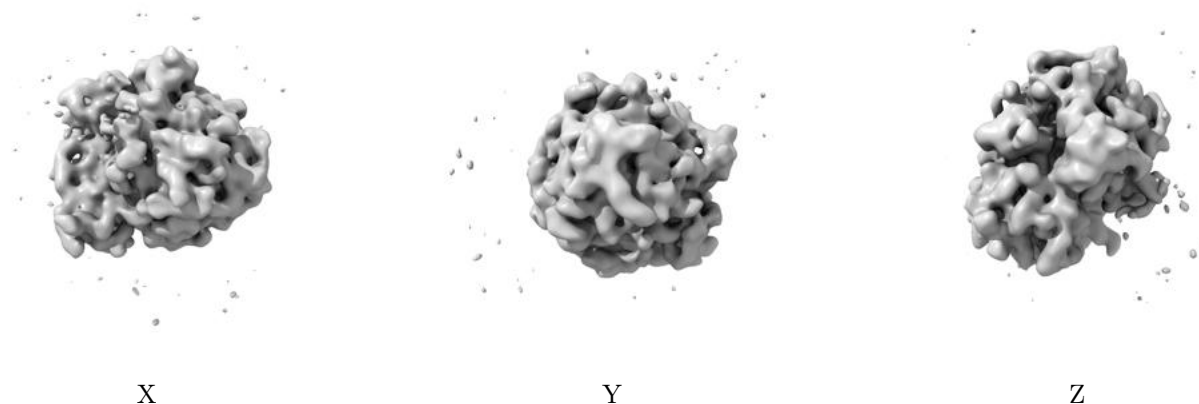


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 25.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

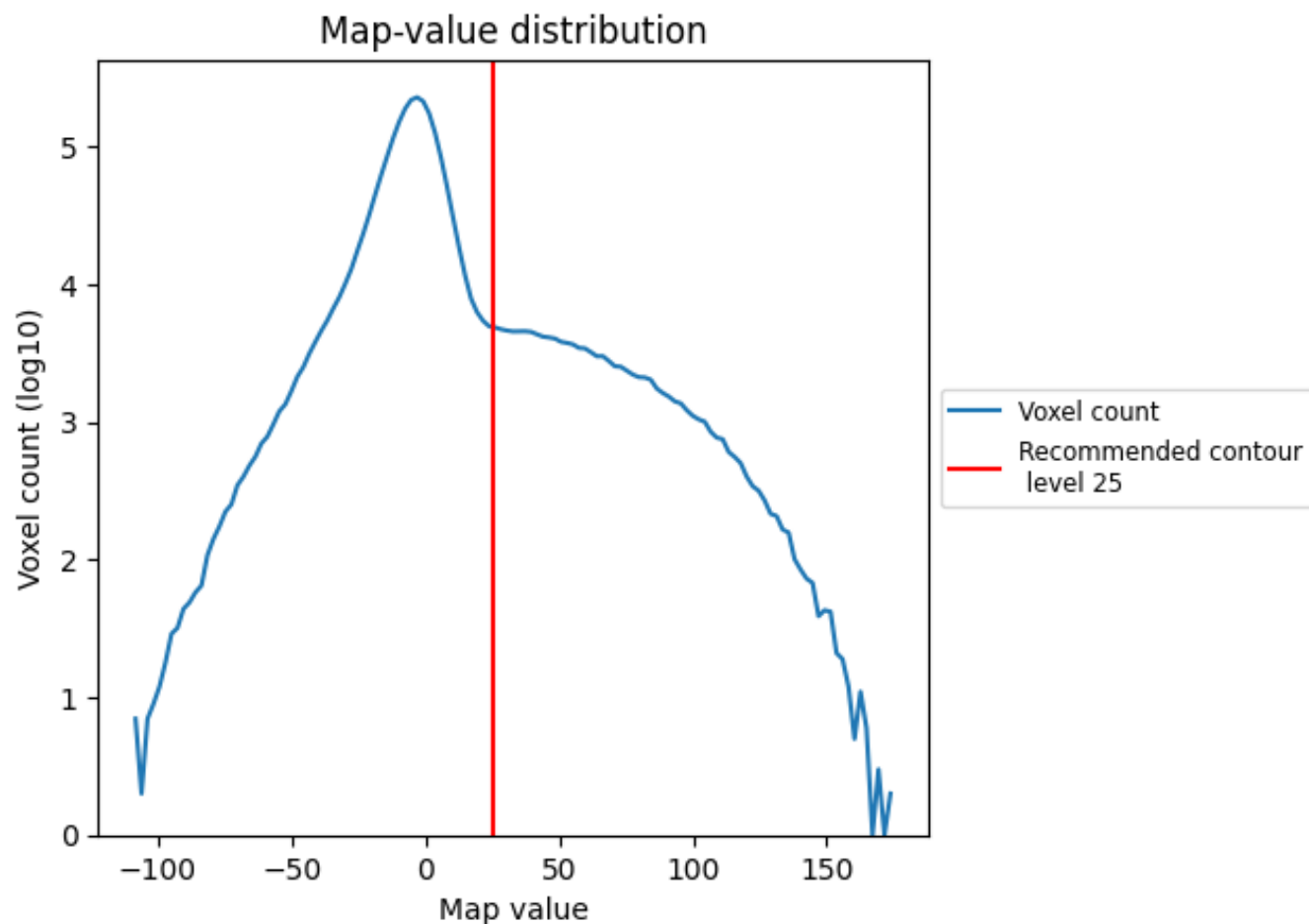
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

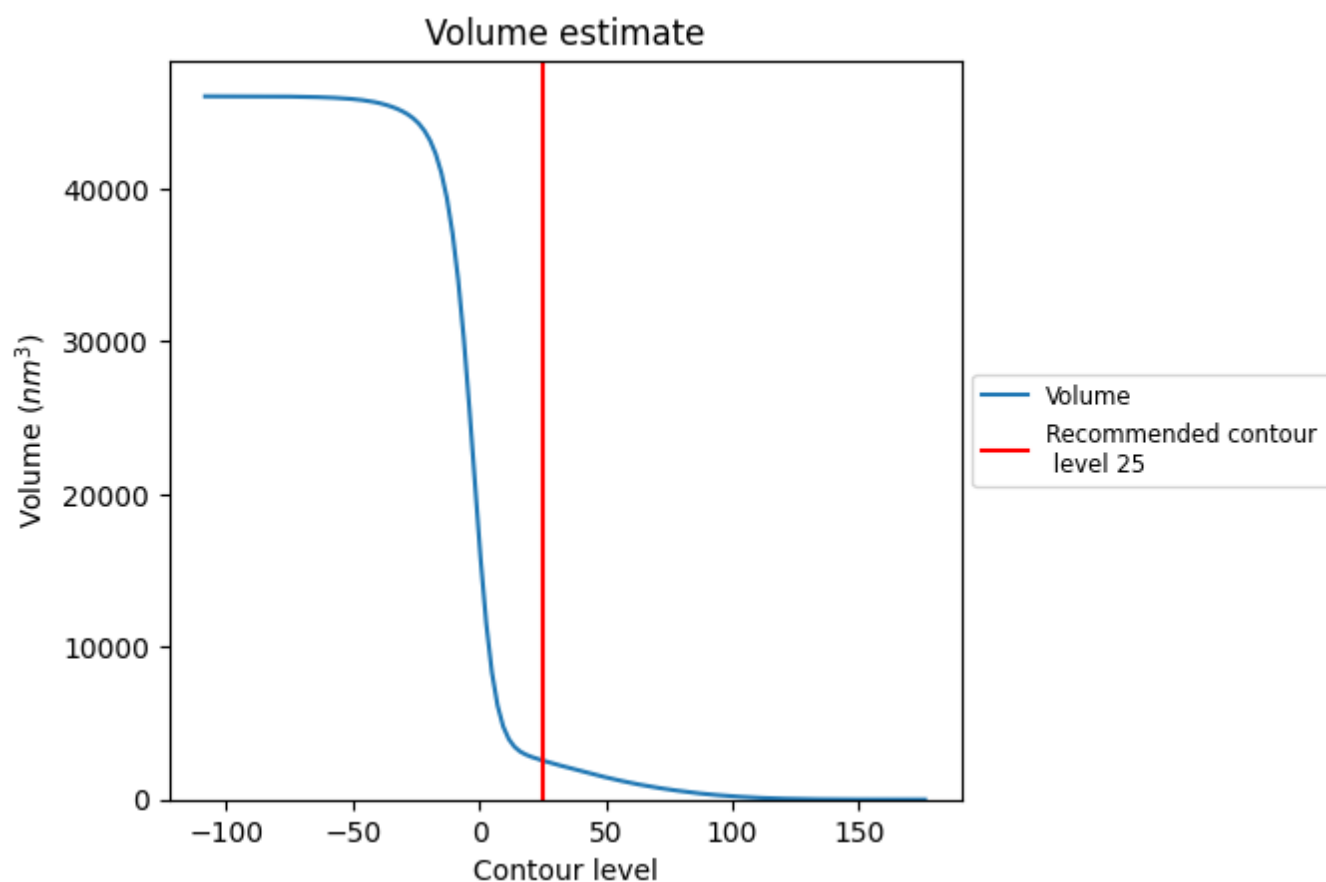
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

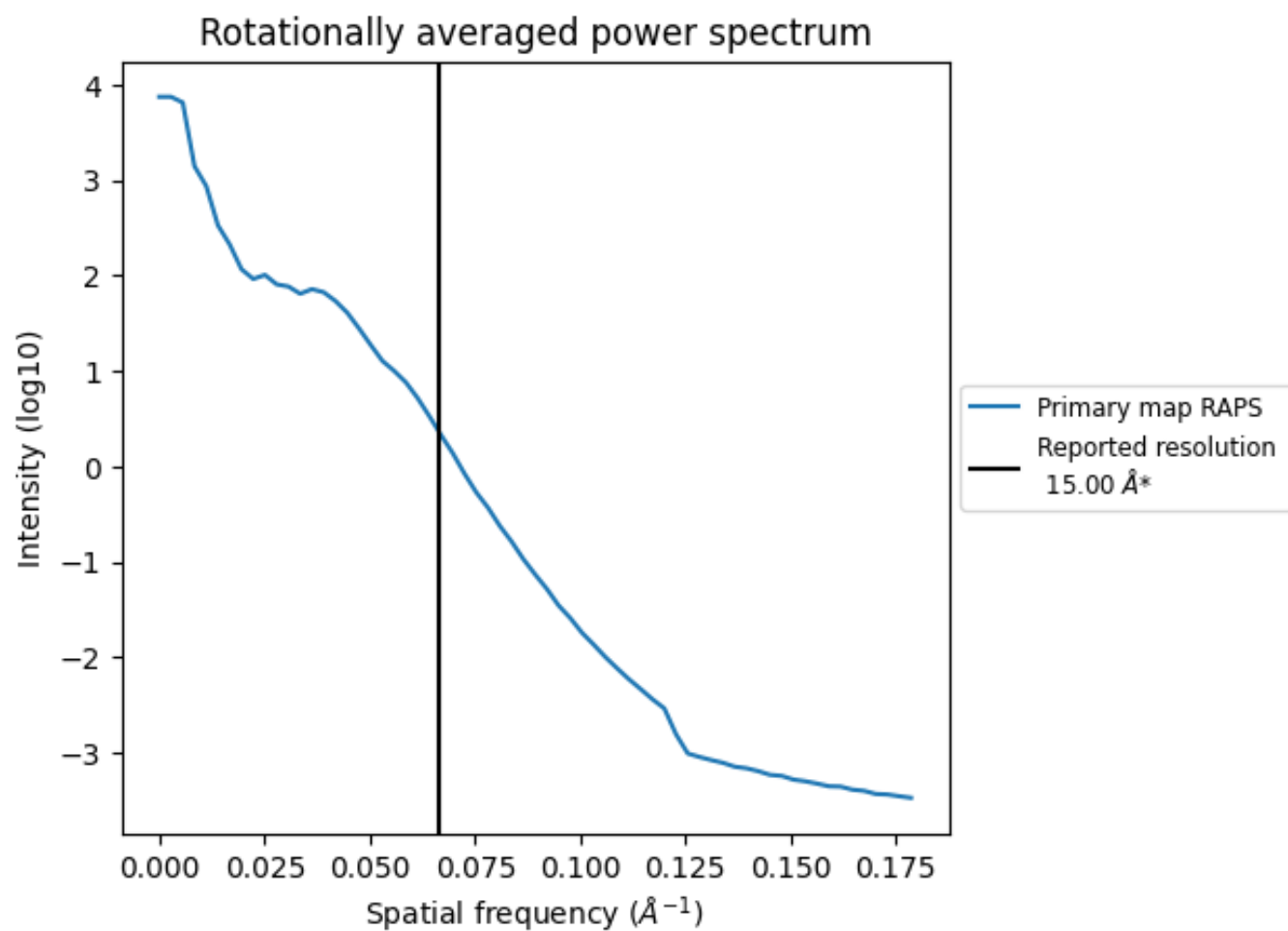
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2557 nm³; this corresponds to an approximate mass of 2310 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 0.067 $\text{\AA}^{-1}$

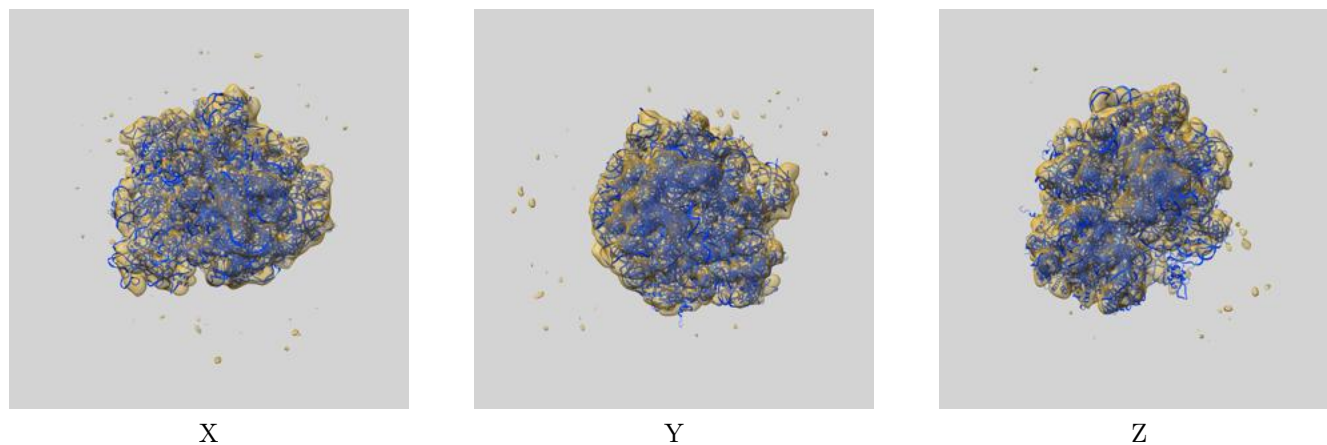
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

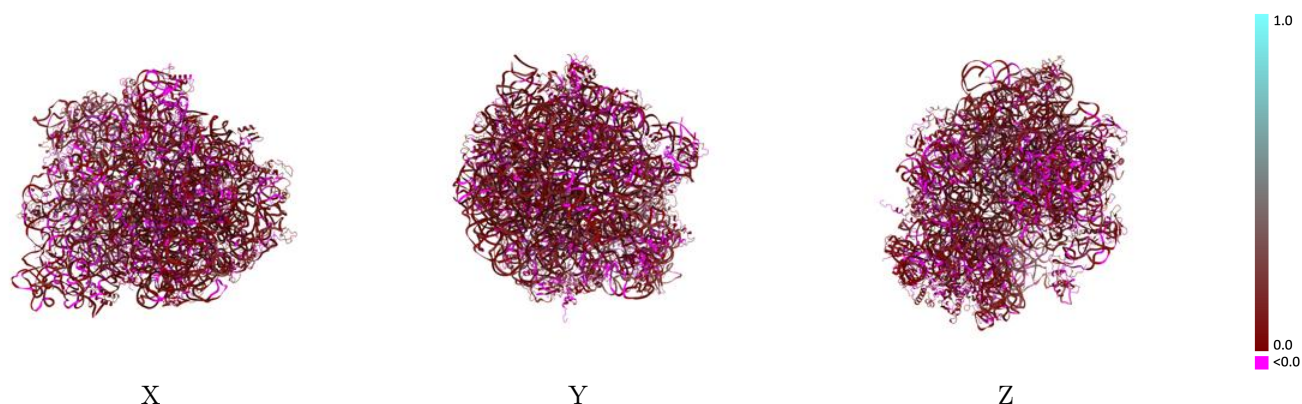
This section contains information regarding the fit between EMDB map EMD-2473 and PDB model 4V73. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



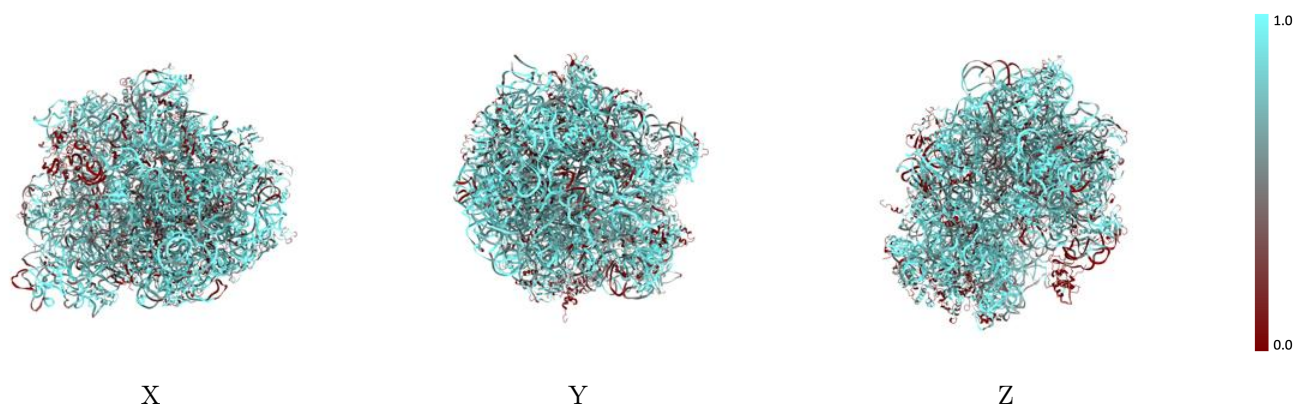
The images above show the 3D surface view of the map at the recommended contour level 25.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



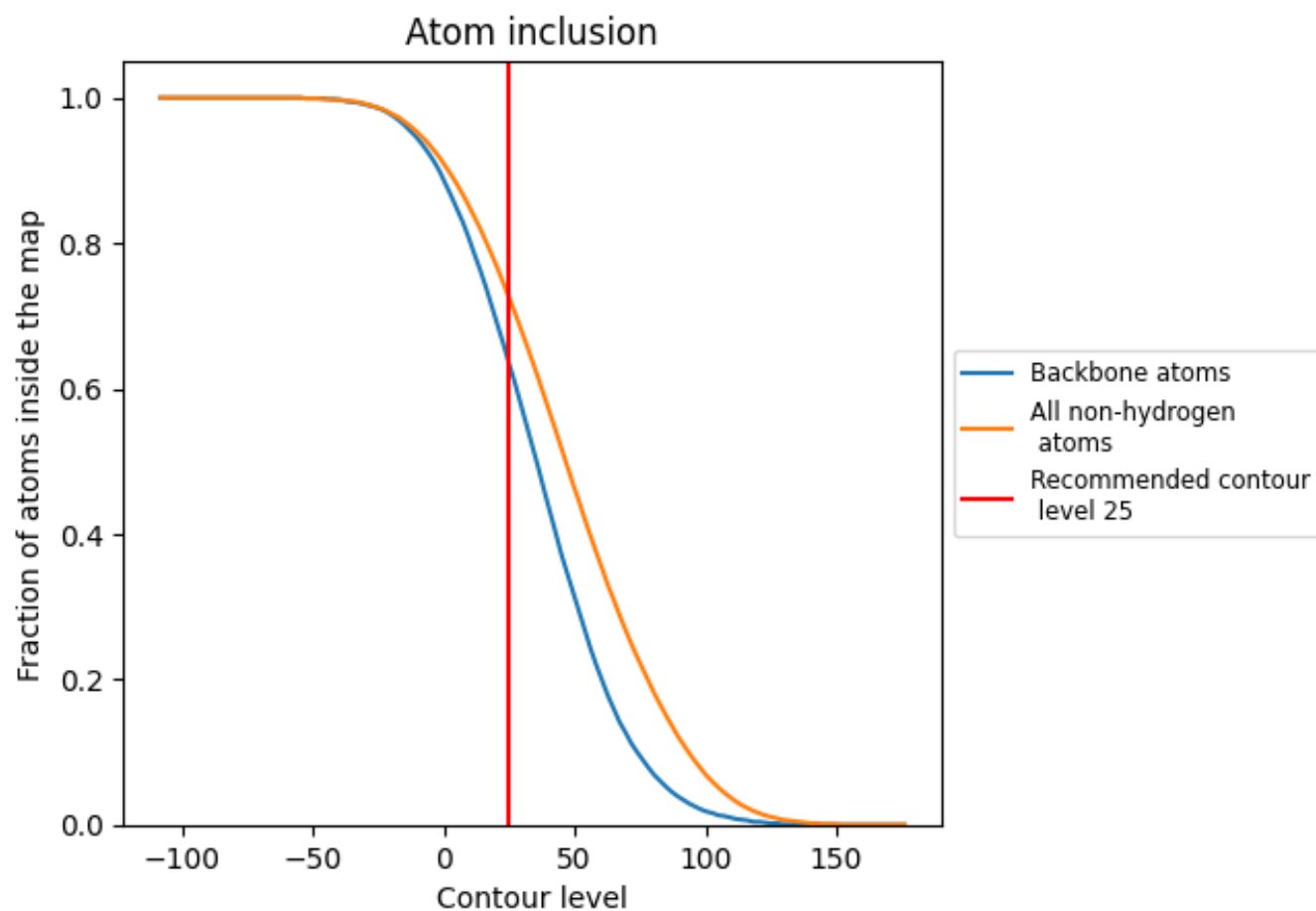
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 72% 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 (25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7240	 0.0610
A1	 0.7610	 0.0870
A2	 0.5110	 0.0570
A3	 0.7080	 0.0630
AA	 0.8180	 0.0730
AB	 0.5310	 0.0480
AC	 0.5630	 0.0370
AD	 0.5450	 0.0320
AE	 0.6820	 0.0660
AF	 0.6600	 0.0440
AG	 0.6550	 0.0420
AH	 0.5820	 0.0360
AI	 0.7220	 0.0440
AJ	 0.6620	 0.0350
AK	 0.5630	 0.0450
AL	 0.5780	 0.0480
AM	 0.6530	 0.0560
AN	 0.6300	 0.0480
AO	 0.6220	 0.0160
AP	 0.5610	 -0.0080
AQ	 0.5700	 0.0270
AR	 0.6220	 0.0070
AS	 0.8540	 0.0480
AT	 0.7550	 0.0110
AU	 0.4570	 -0.0040
B0	 0.6260	 0.0390
B1	 0.6630	 0.0590
B2	 0.4960	 0.0090
B3	 0.2870	 -0.0110
B4	 0.7570	 0.0450
B5	 0.5740	 0.0150
BA	 0.7880	 0.0770
BB	 0.7360	 0.0390
BC	 0.4830	 0.0130
BD	 0.5040	 0.0230



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Chain	Atom inclusion	Q-score
BE	 0.6320	 0.0390
BF	 0.6980	 0.0490
BG	 0.6020	 0.0550
BH	 0.2370	 0.0420
BI	 0.0070	 0.0200
BJ	 0.5770	 0.0280
BK	 0.4750	 0.0430
BL	 0.5160	 0.0010
BM	 0.4840	 0.0400
BN	 0.6080	 0.0190
BO	 0.7660	 0.0120
BP	 0.4850	 0.0390
BQ	 0.6050	 0.0190
BR	 0.6160	 0.0240
BS	 0.4440	 0.0110
BT	 0.6720	 0.0310
BU	 0.6170	 0.0390
BV	 0.6400	 0.0330
BW	 0.5670	 0.0130
BX	 0.5390	 0.0090
BY	 0.6780	 0.0540
BZ	 0.4620	 0.0210