



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 12:25 AM EDT

PDB ID : 4V76 / pdb_00004v76
EMDB ID : EMD-1722
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post2a)
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 : 17.00 Å(reported)
Based on initial models : 2WRI, 3I1O, 2K4C, 2HGP

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:

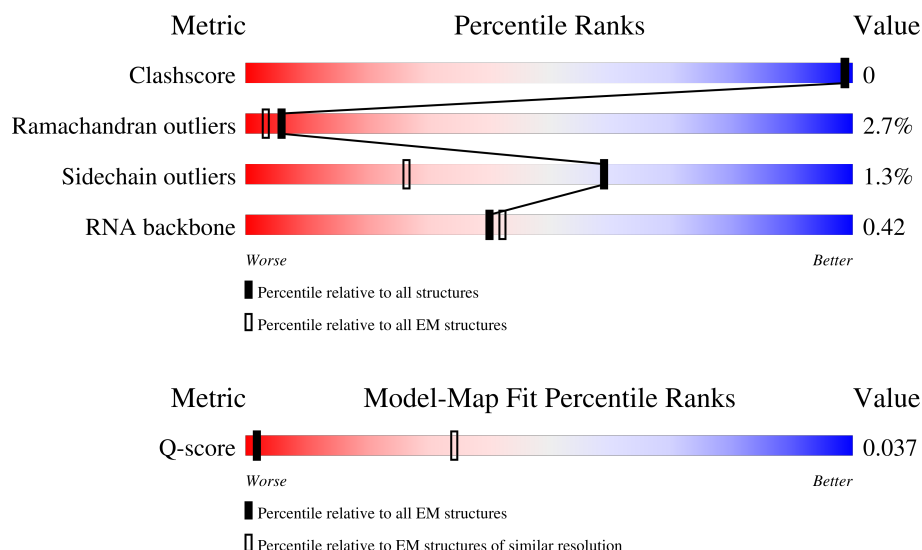
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 17.00 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	38 (16.50 - 17.50)

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	54% 97% .
2	AC	208	50% 96% .
3	AD	206	52% 95% ..

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Mol	Chain	Length	Quality of chain
4	AE	152	
5	AF	101	
6	AG	152	
7	AH	130	
8	AI	128	
9	AJ	100	
10	AK	118	
11	AL	124	
12	AM	115	
13	AN	101	
14	AO	89	
15	AP	81	
16	AQ	82	
17	AR	57	
18	AS	81	
19	AT	86	
20	AU	53	
21	AA	1533	
22	A1	76	
23	A2	15	
24	A3	77	
25	BC	273	
26	BD	209	
27	BE	201	
28	BF	179	

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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	20% 62% 31% 7%
55	BB	118	13% 69% 28%
56	B5	234	57% 92% 5%

2 Entry composition [i](#)

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		

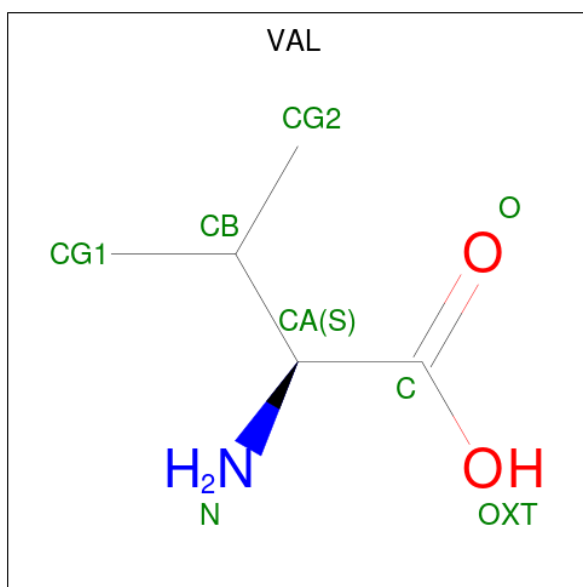
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

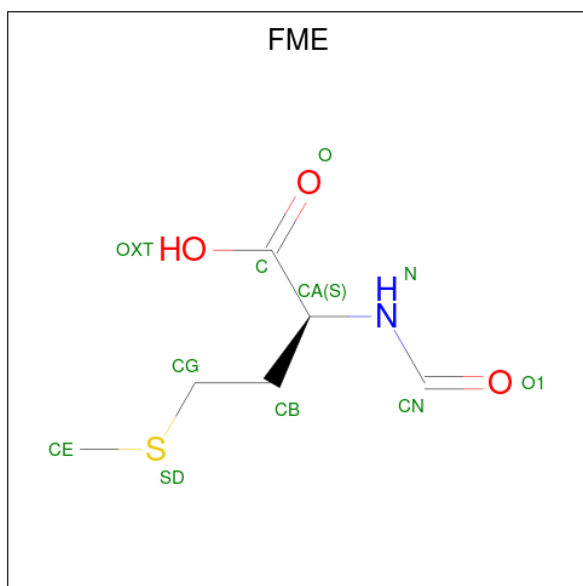
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- 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).

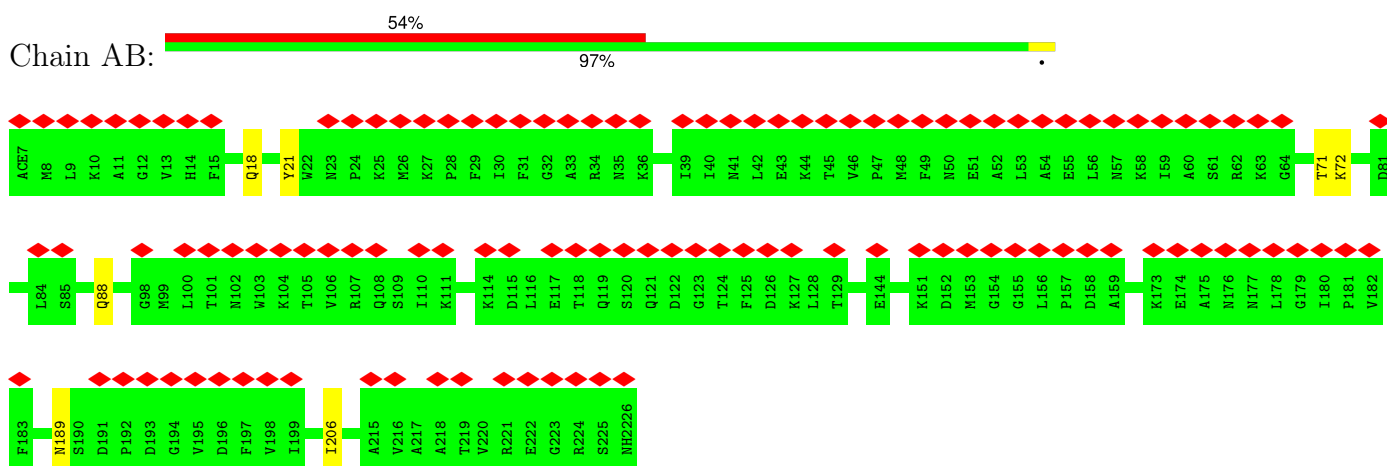


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

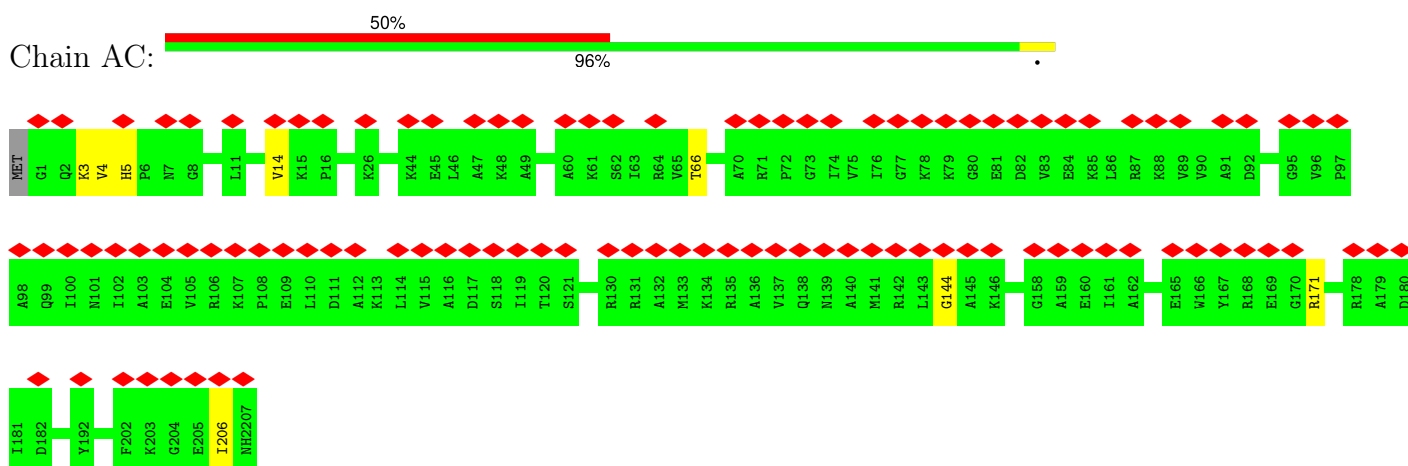
3 Residue-property plots

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.

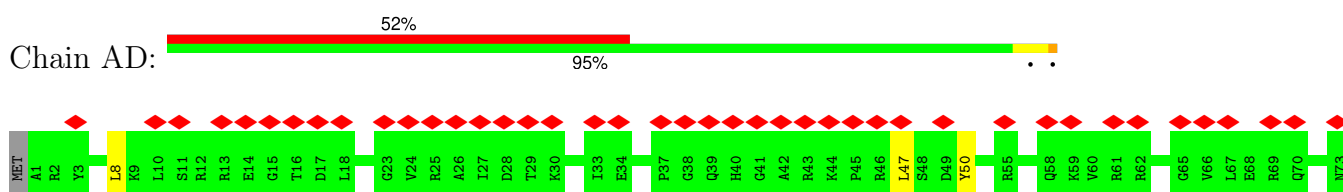
• Molecule 1: 30S ribosomal protein S2

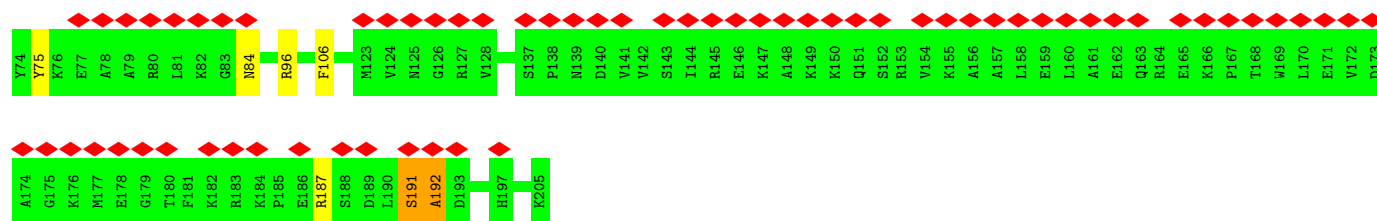


• Molecule 2: 30S ribosomal protein S3

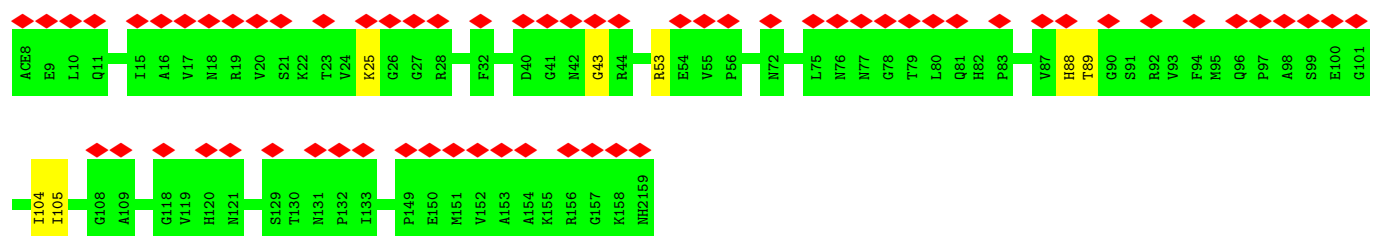
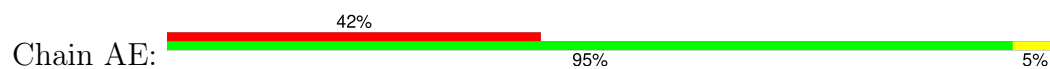


• Molecule 3: 30S ribosomal protein S4

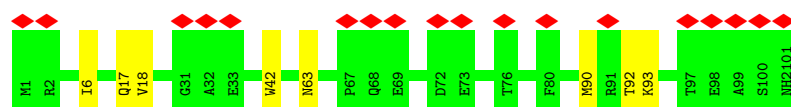




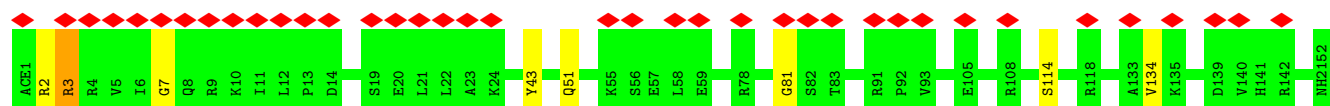
• Molecule 4: 30S ribosomal protein S5



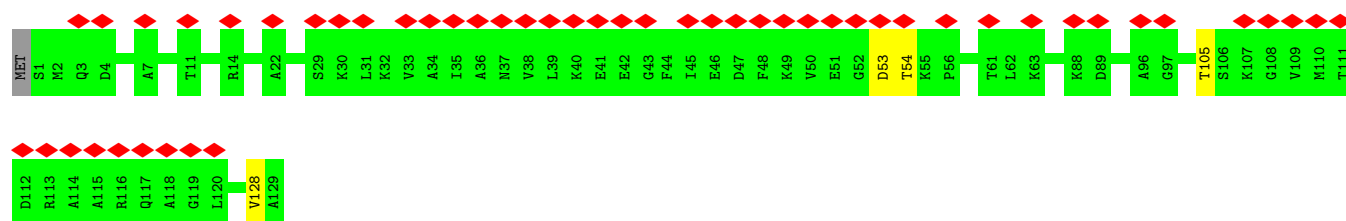
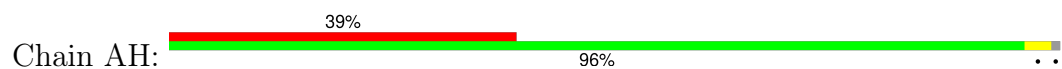
• Molecule 5: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S7

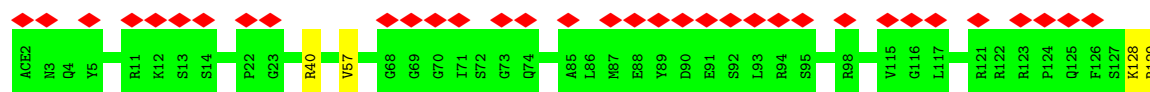


• Molecule 7: 30S ribosomal protein S8

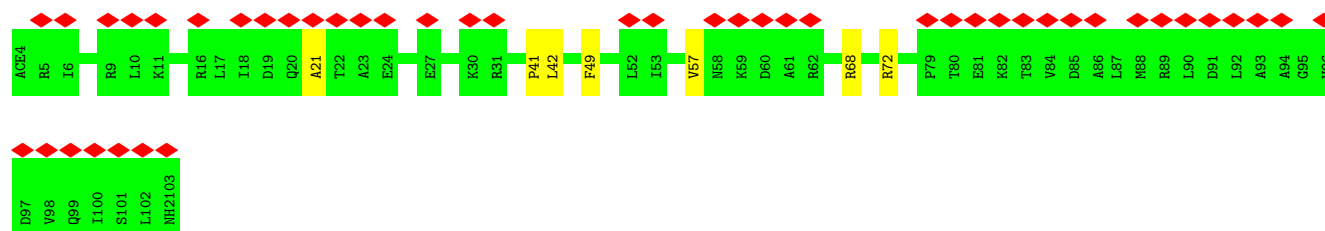


• Molecule 8: 30S ribosomal protein S9

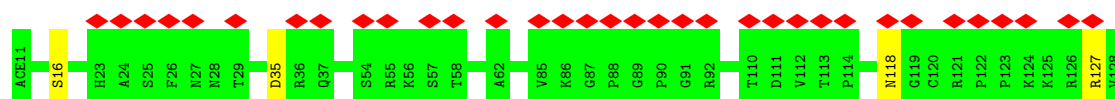




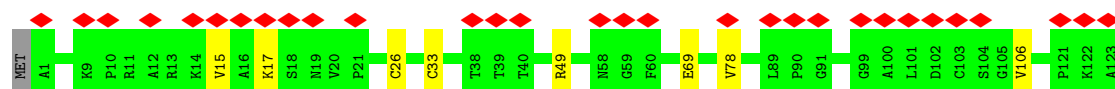
- Molecule 9: 30S ribosomal protein S10



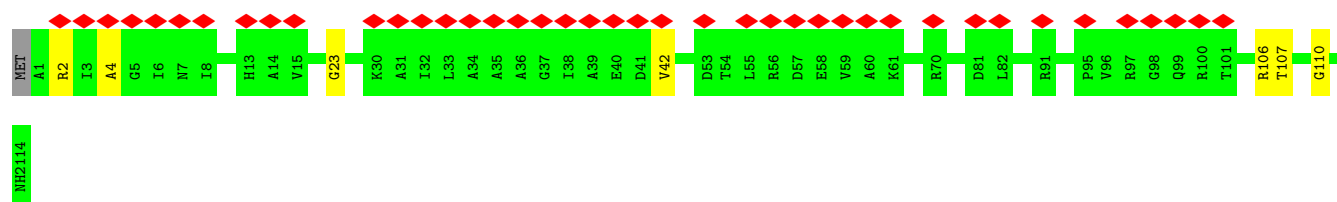
- Molecule 10: 30S ribosomal protein S11



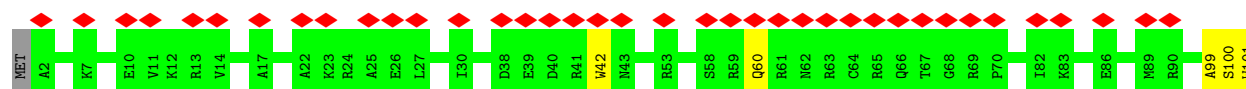
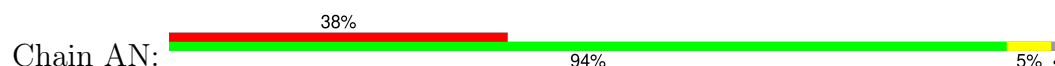
- Molecule 11: 30S ribosomal protein S12



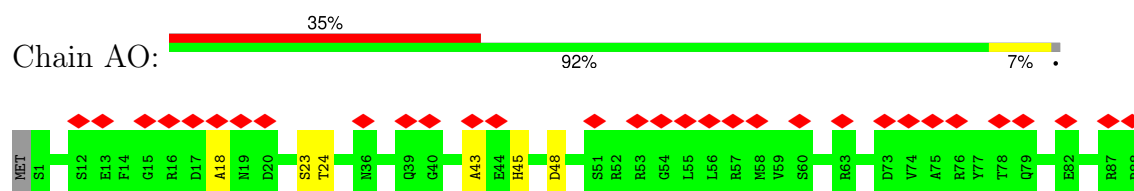
- Molecule 12: 30S ribosomal protein S13



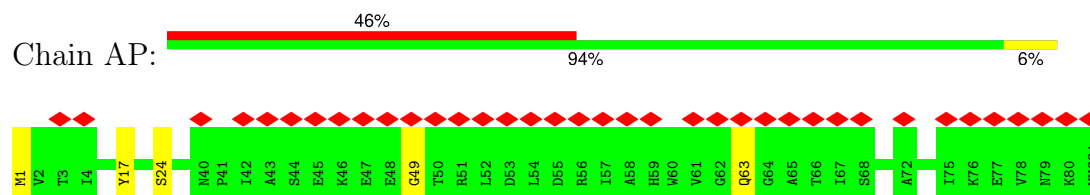
- Molecule 13: 30S ribosomal protein S14



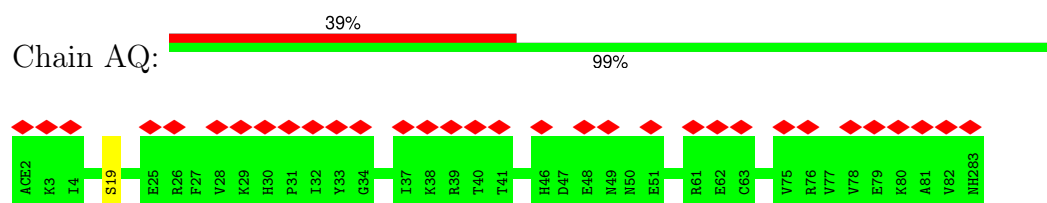
- Molecule 14: 30S ribosomal protein S15



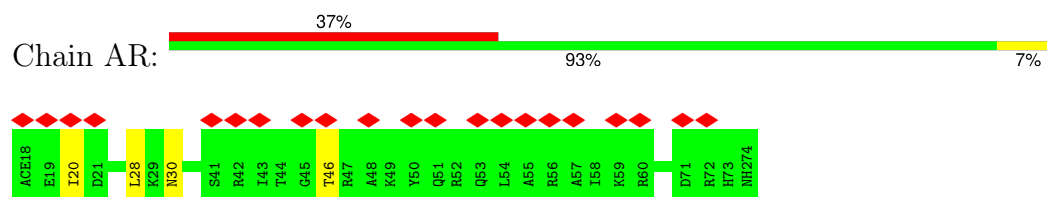
- Molecule 15: 30S ribosomal protein S16



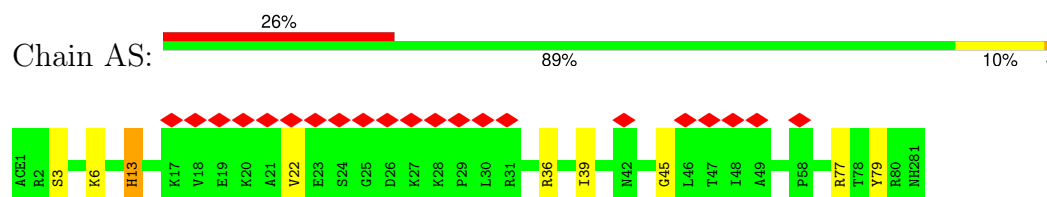
- Molecule 16: 30S ribosomal protein S17



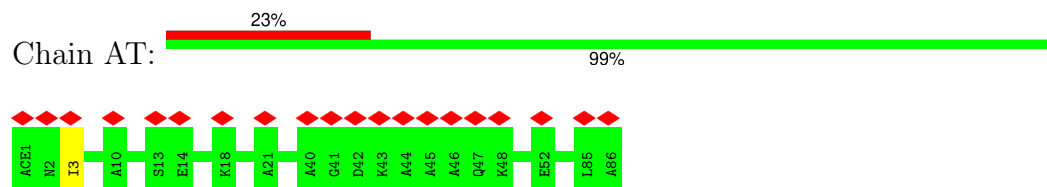
- Molecule 17: 30S ribosomal protein S18



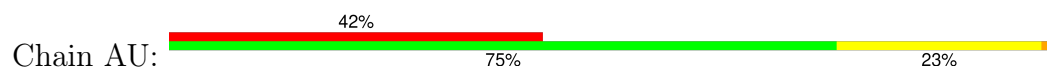
- Molecule 18: 30S ribosomal protein S19

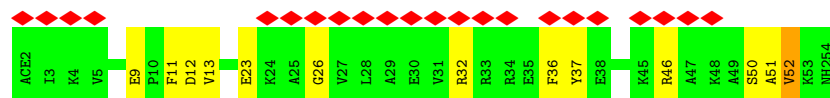


- Molecule 19: 30S ribosomal protein S20

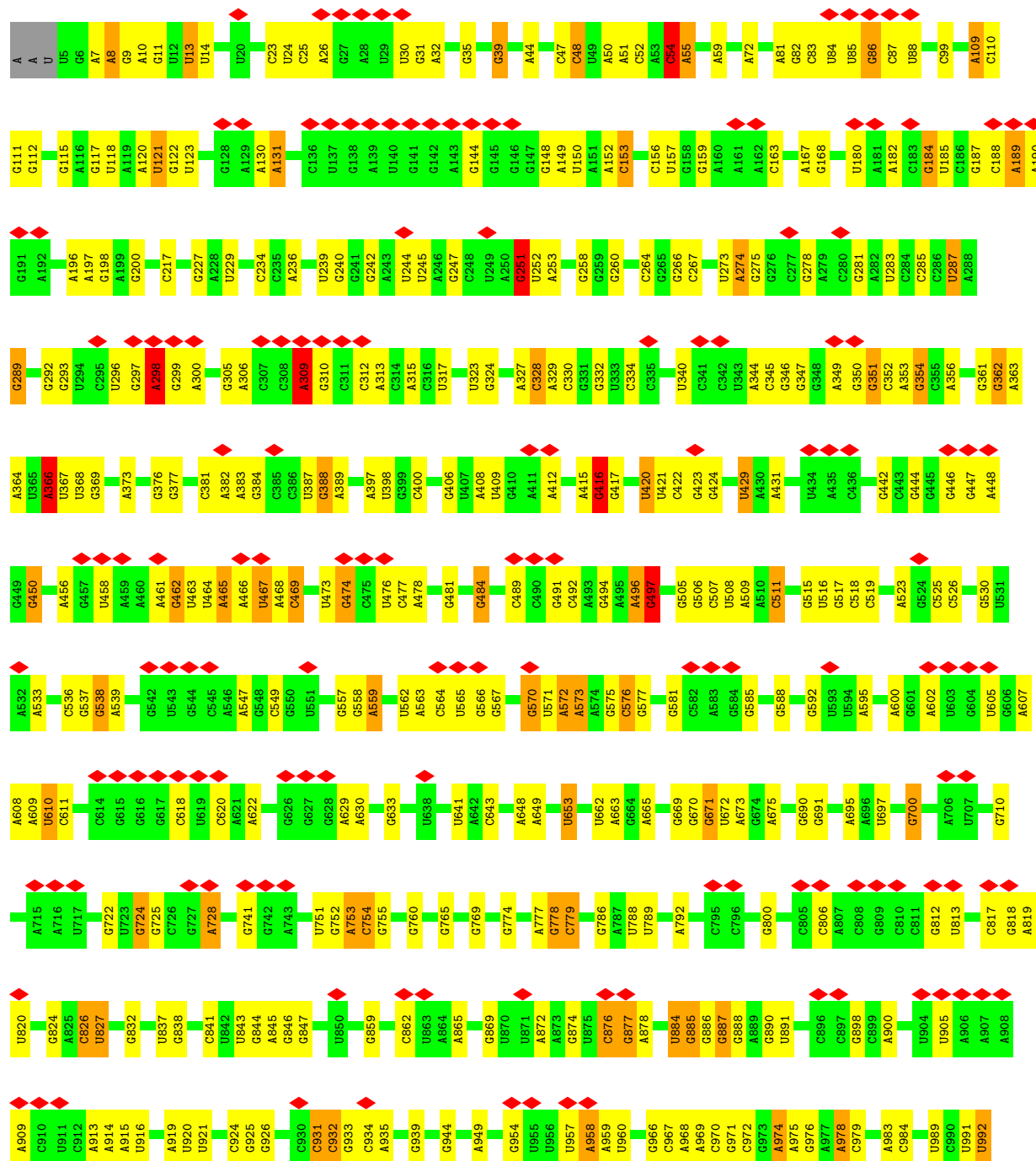


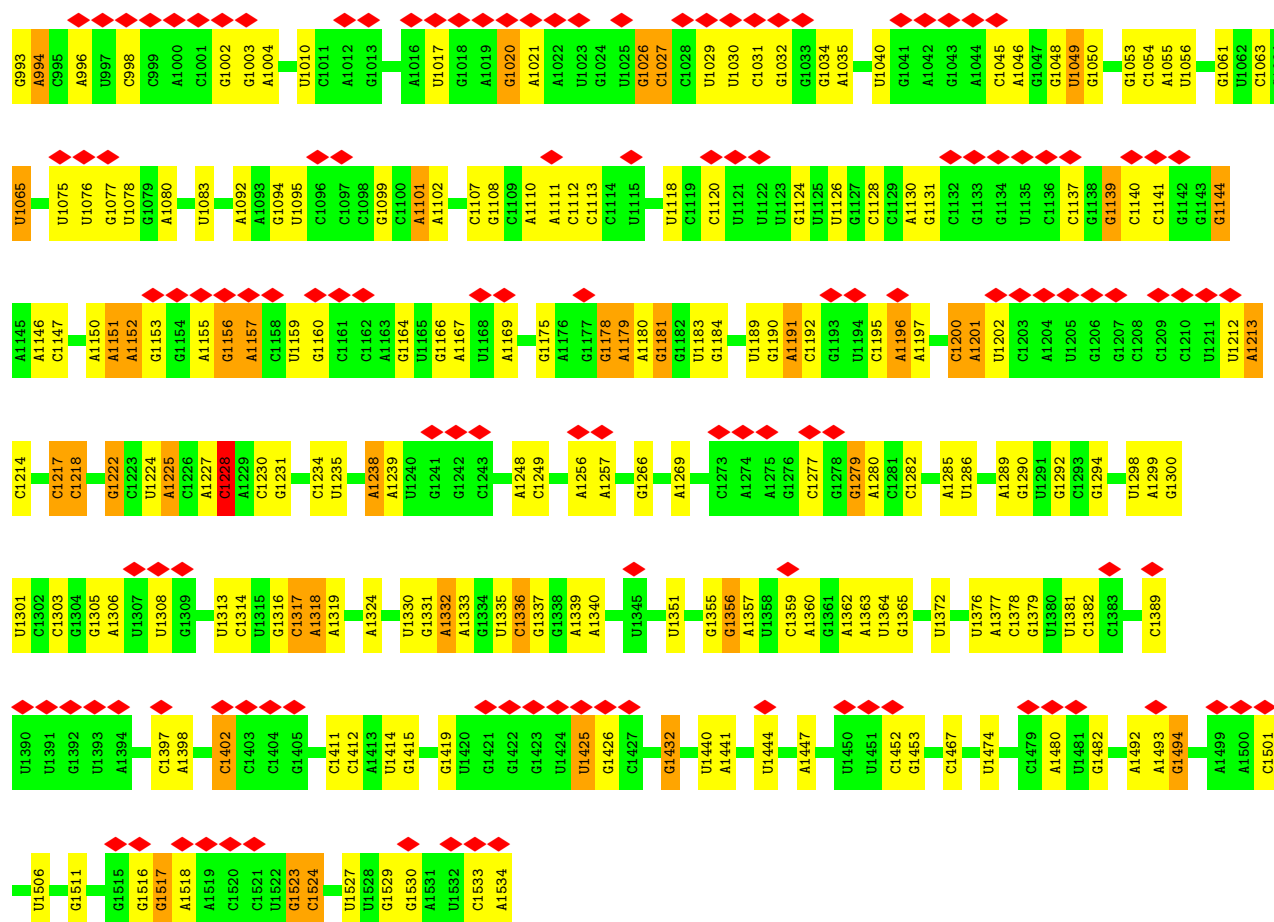
- Molecule 20: 30S ribosomal protein S21



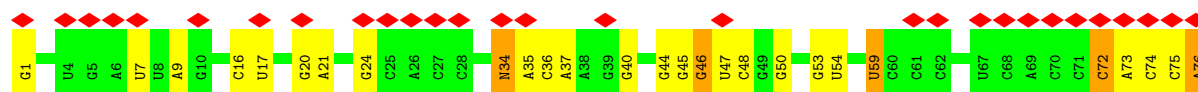
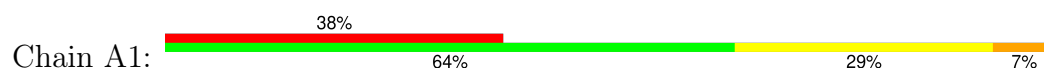


• Molecule 21: 16S ribosomal RNA

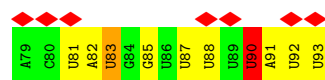




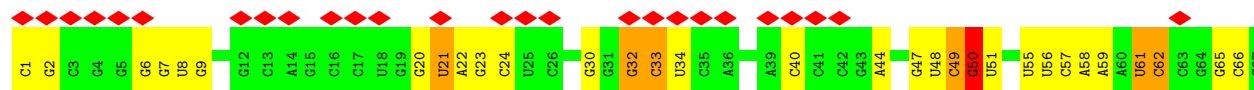
• Molecule 22: fMet-Val-tRNA-Val

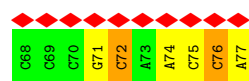


• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

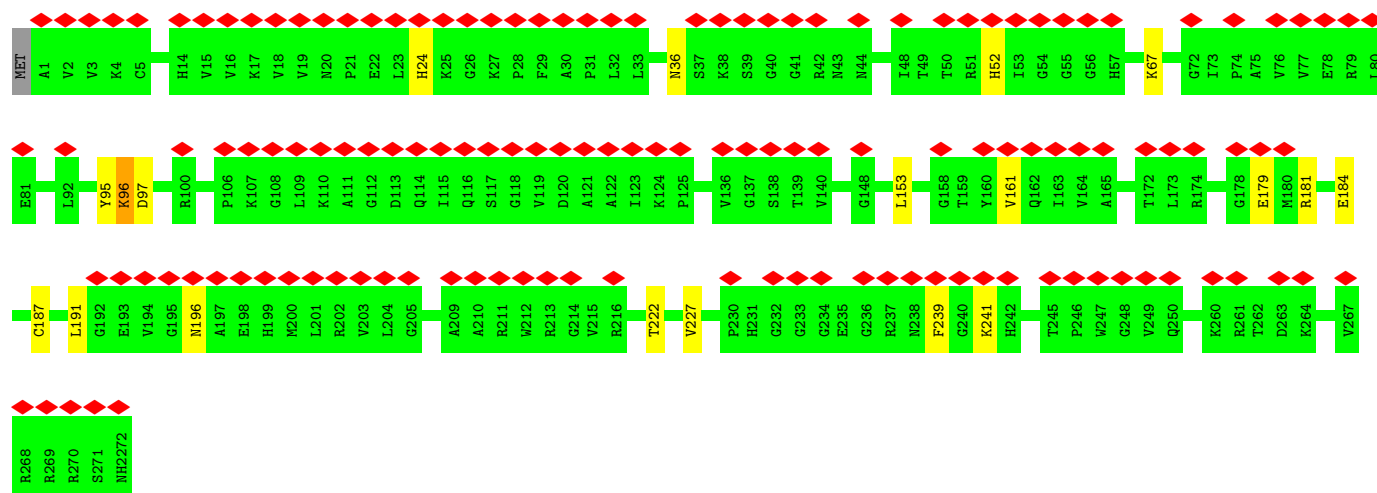


• Molecule 24: tRNA-fMet

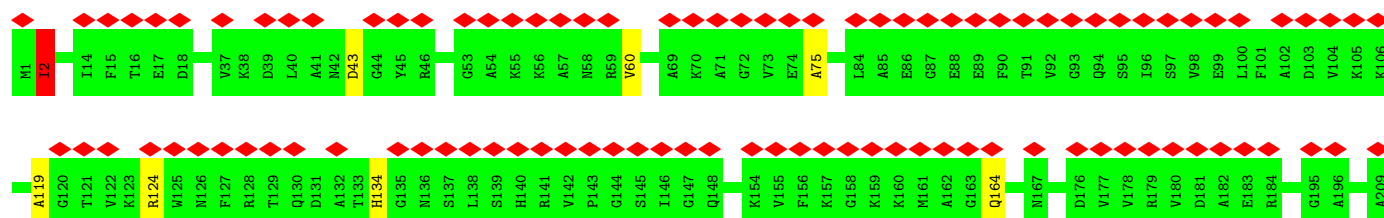




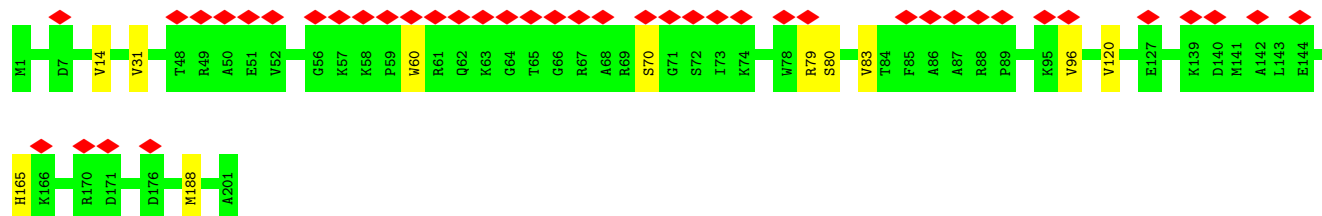
• Molecule 25: 50S ribosomal protein L2



• Molecule 26: 50S ribosomal protein L3

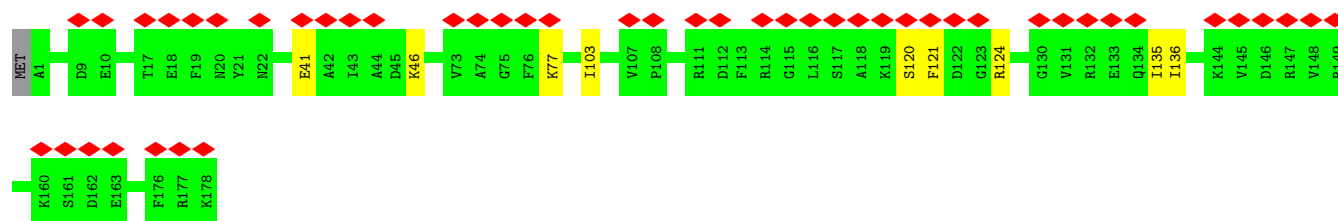


• Molecule 27: 50S ribosomal protein L4



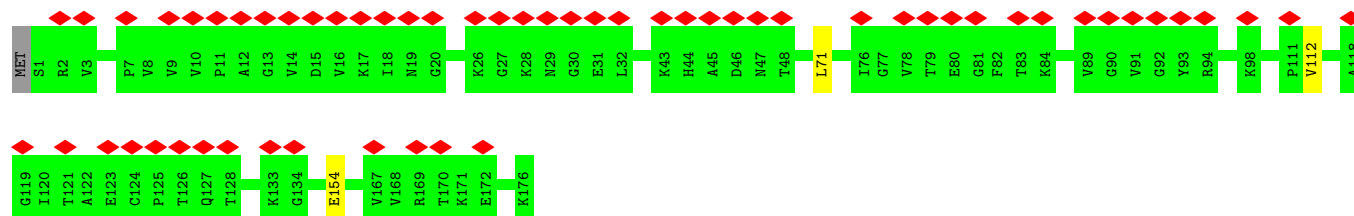
• Molecule 28: 50S ribosomal protein L5





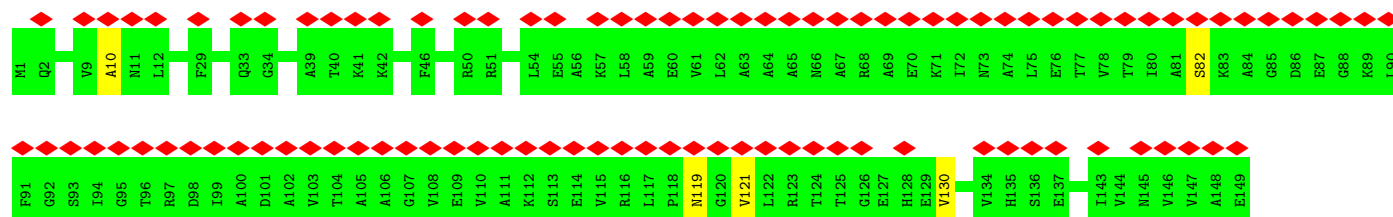
- Molecule 29: 50S ribosomal protein L6

Chain BG: 33% 98%



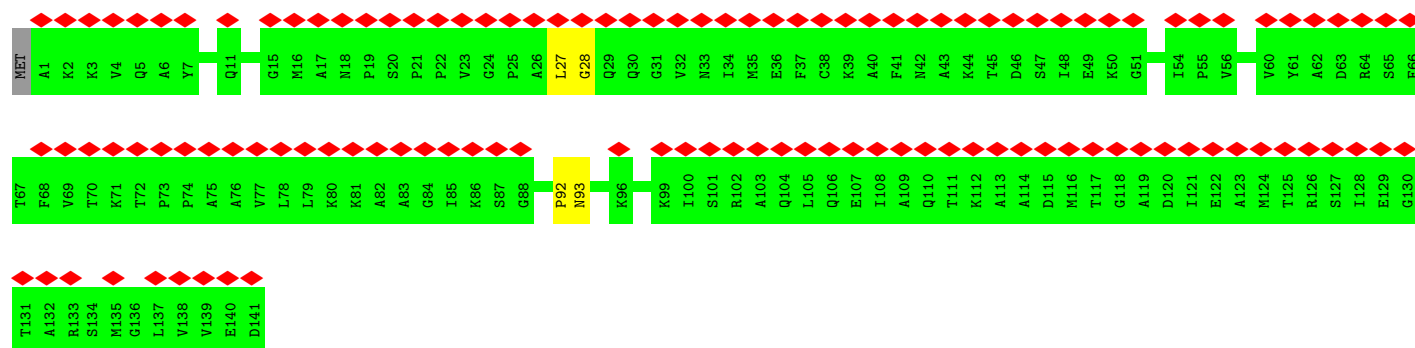
- Molecule 30: 50S ribosomal protein L9

Chain BH: 66% 97%



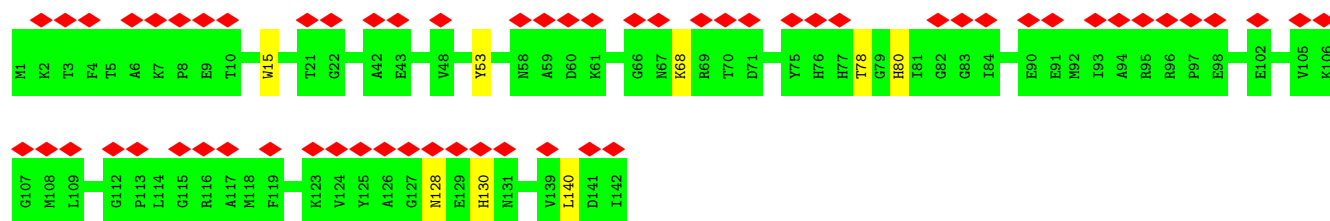
- Molecule 31: 50S ribosomal protein L11

Chain BI: 83% 96%



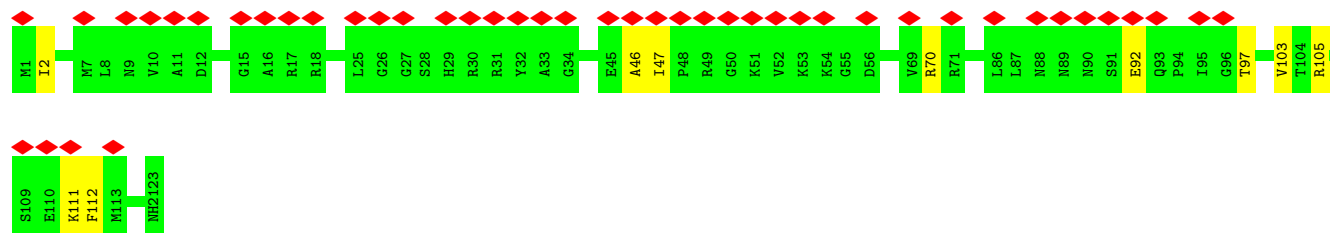
- Molecule 32: 50S ribosomal protein L13

Chain BJ: 42% 94% 6%



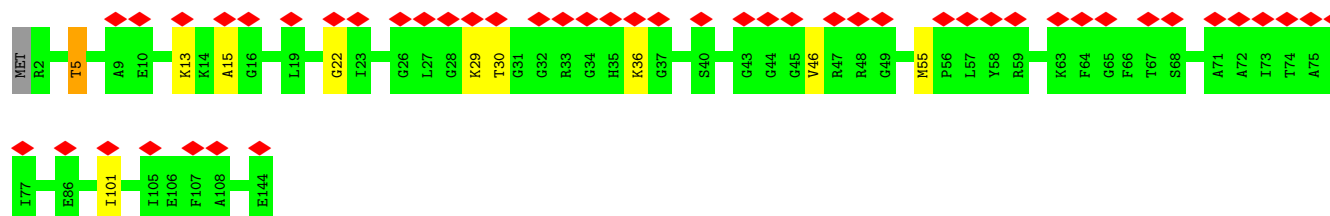
- Molecule 33: 50S ribosomal protein L14

Chain BK: 37% 92% 8%



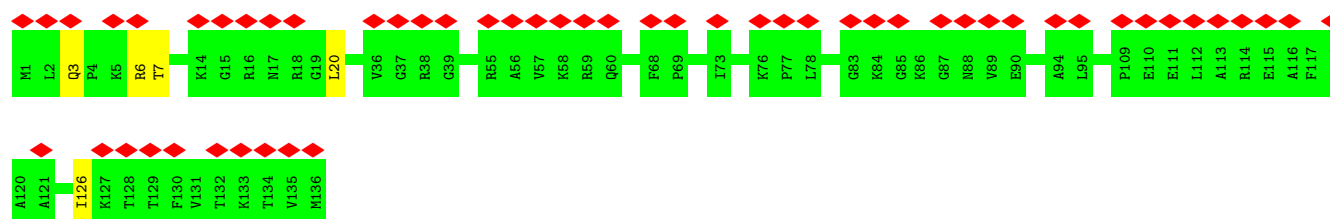
- Molecule 34: 50S ribosomal protein L15

Chain BL: 33% 92% 6% ..



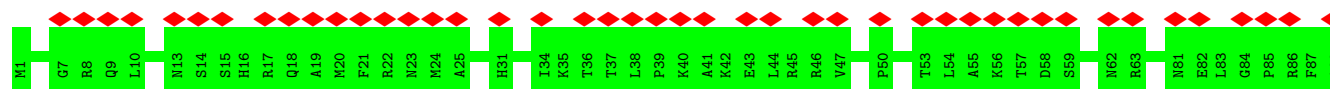
- Molecule 35: 50S ribosomal protein L16

Chain BM: 40% 96% .



- Molecule 36: 50S ribosomal protein L17

Chain BN: 46% 98% .

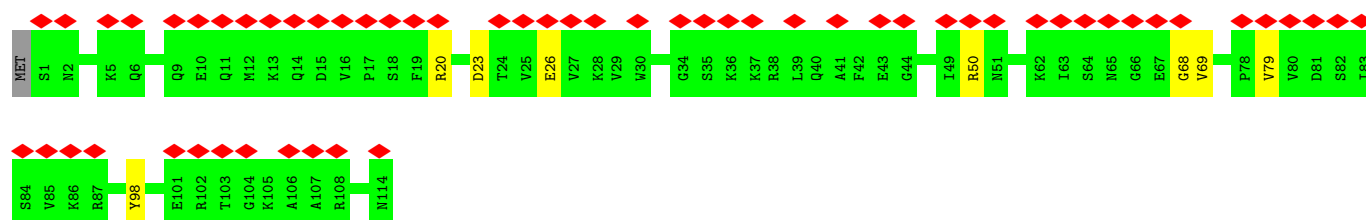




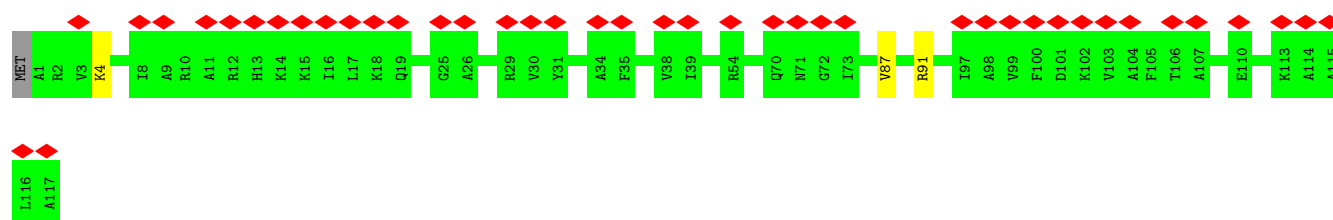
- Molecule 37: 50S ribosomal protein L18



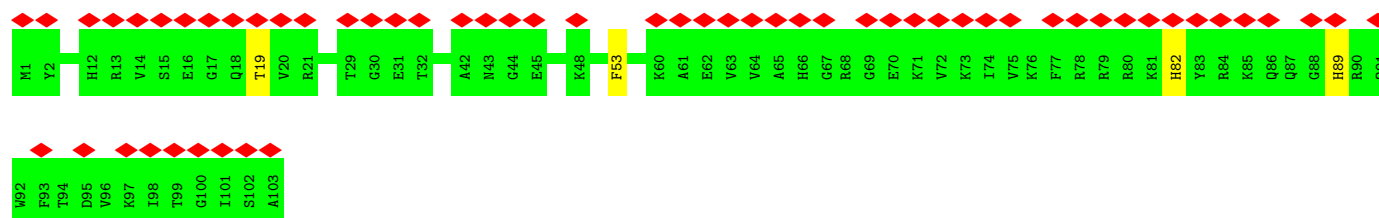
- Molecule 38: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L20

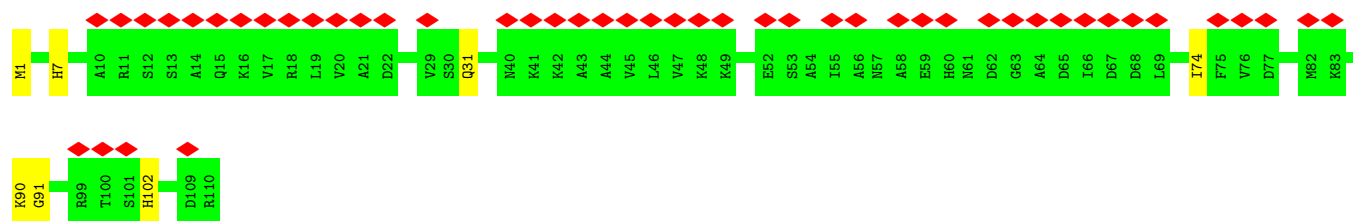


- Molecule 40: 50S ribosomal protein L21



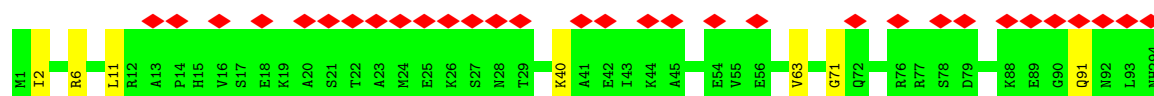
- Molecule 41: 50S ribosomal protein L22





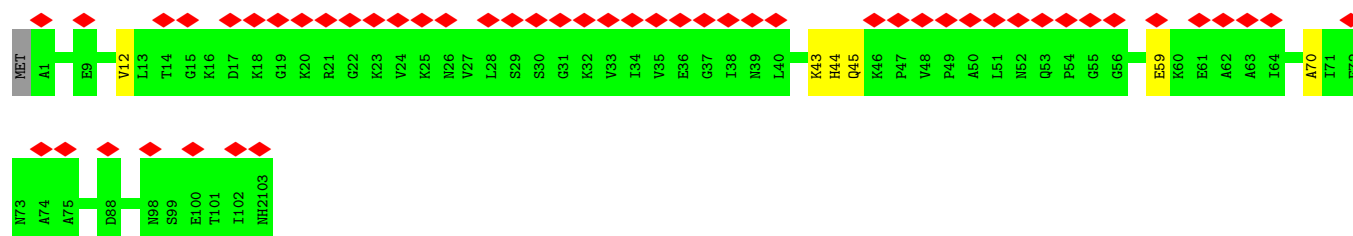
- Molecule 42: 50S ribosomal protein L23

Chain BT:



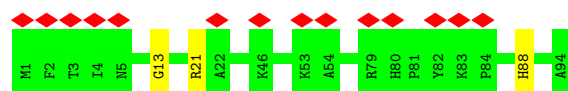
- Molecule 43: 50S ribosomal protein L24

Chain BU:



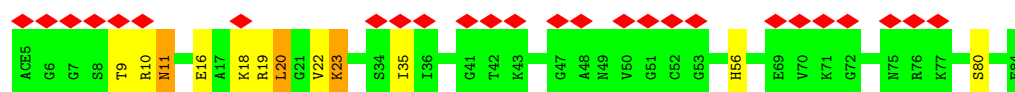
- Molecule 44: 50S ribosomal protein L25

Chain BV:



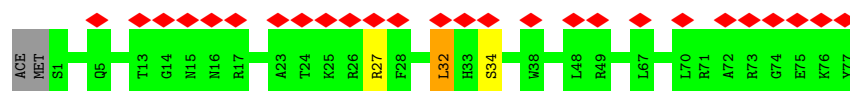
- Molecule 45: 50S ribosomal protein L27

Chain BW:

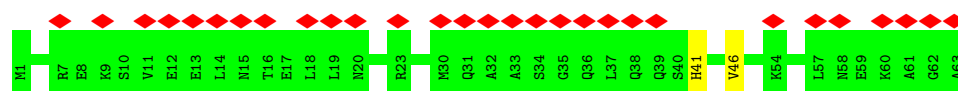


- Molecule 46: 50S ribosomal protein L28

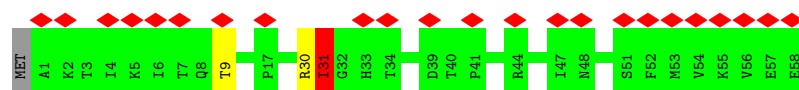
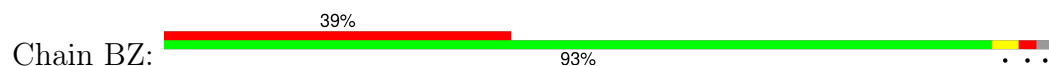
Chain BX:



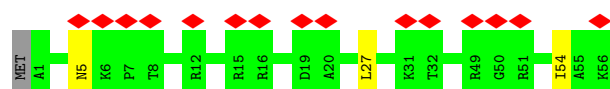
- Molecule 47: 50S ribosomal protein L29



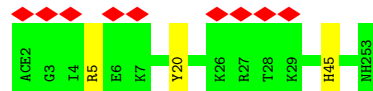
- Molecule 48: 50S ribosomal protein L30



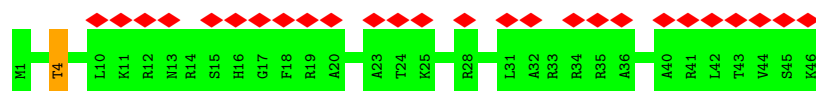
- Molecule 49: 50S ribosomal protein L32



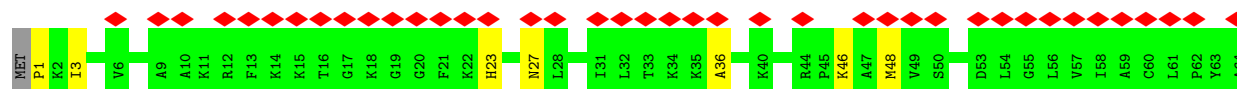
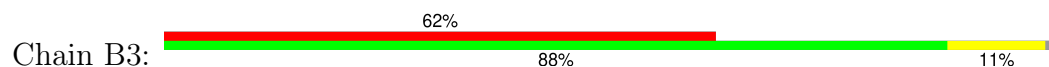
- Molecule 50: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L34

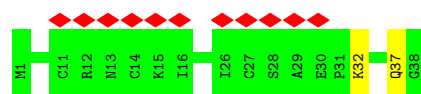


- Molecule 52: 50S ribosomal protein L35

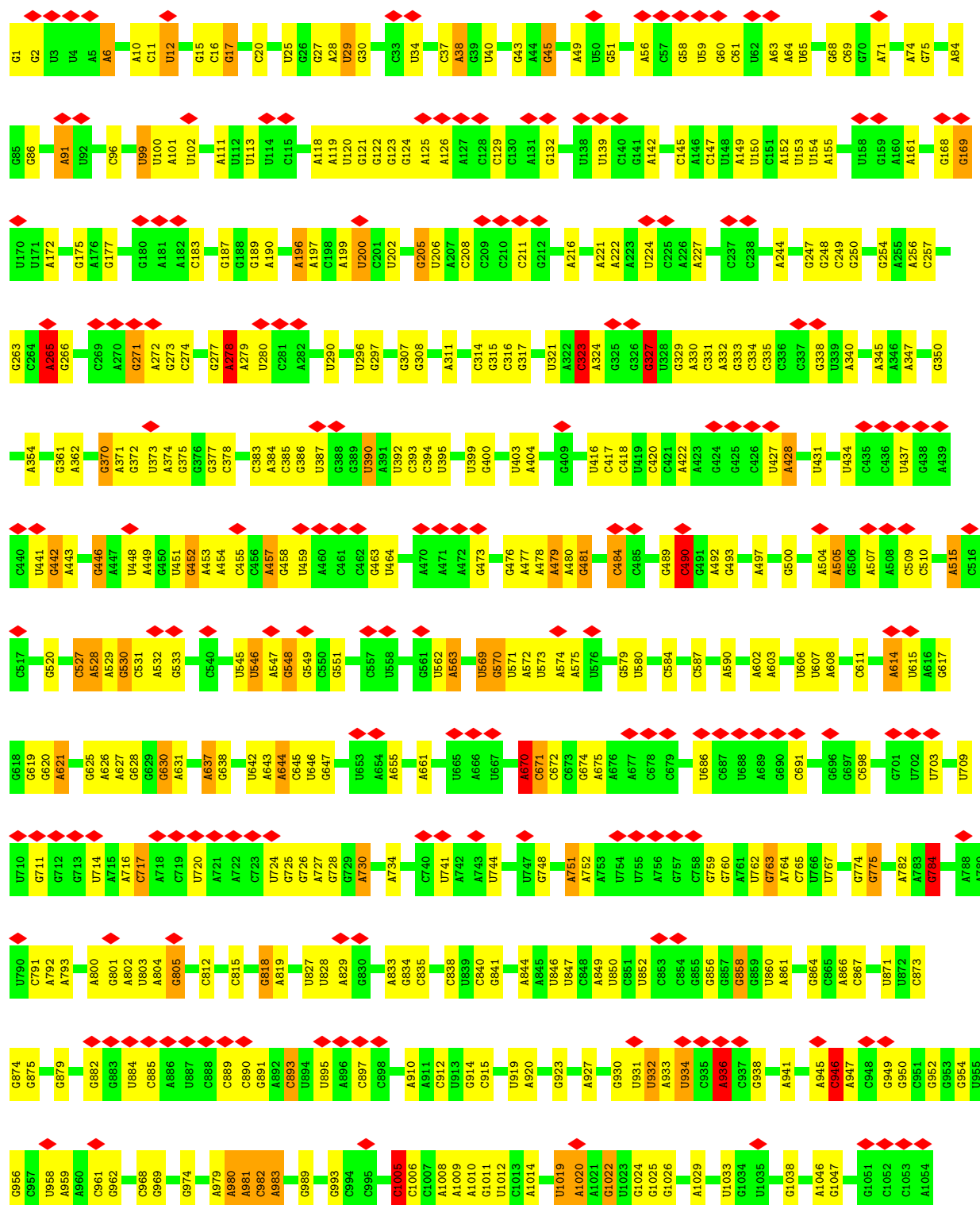


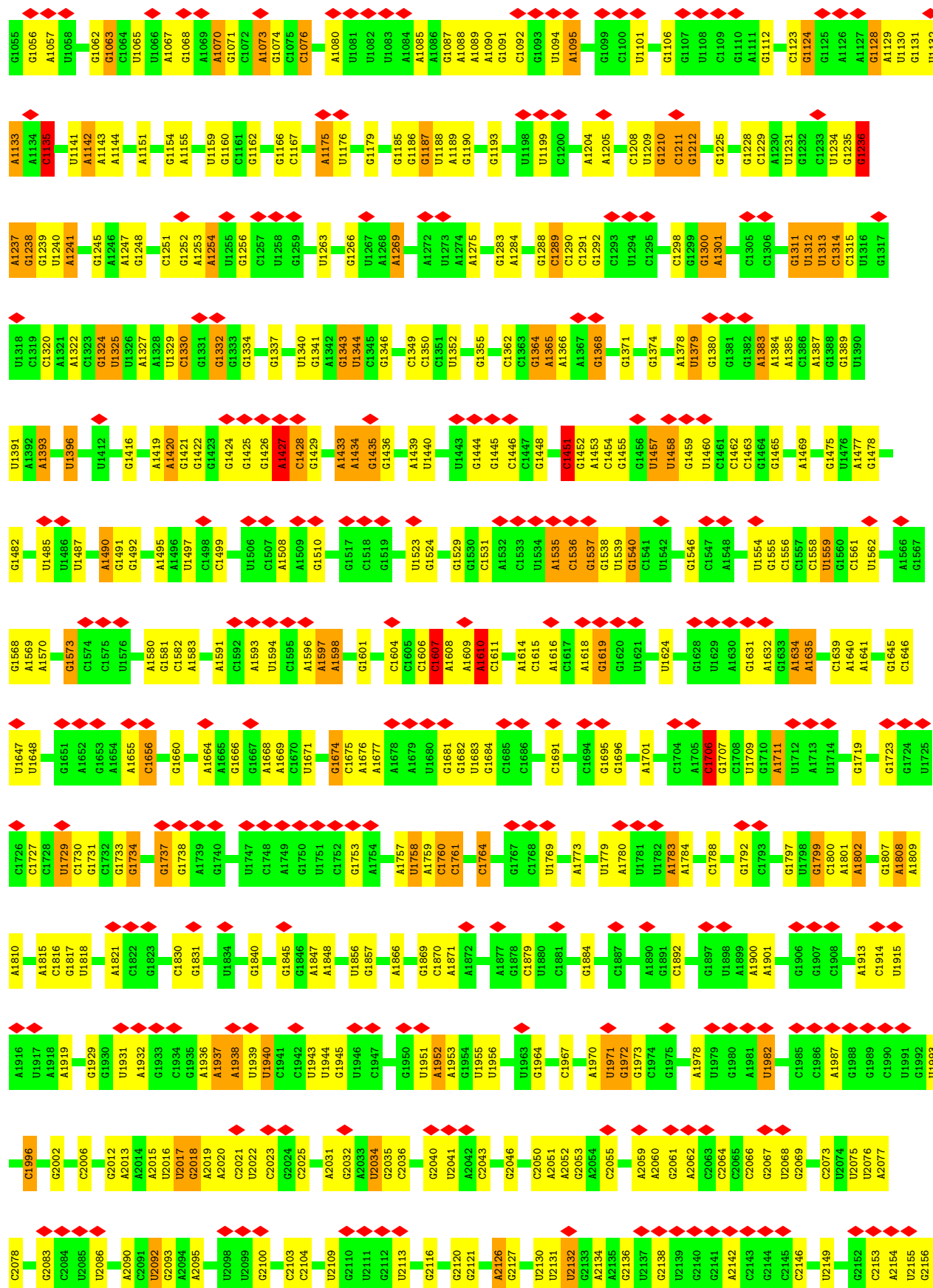
- Molecule 53: 50S ribosomal protein L36

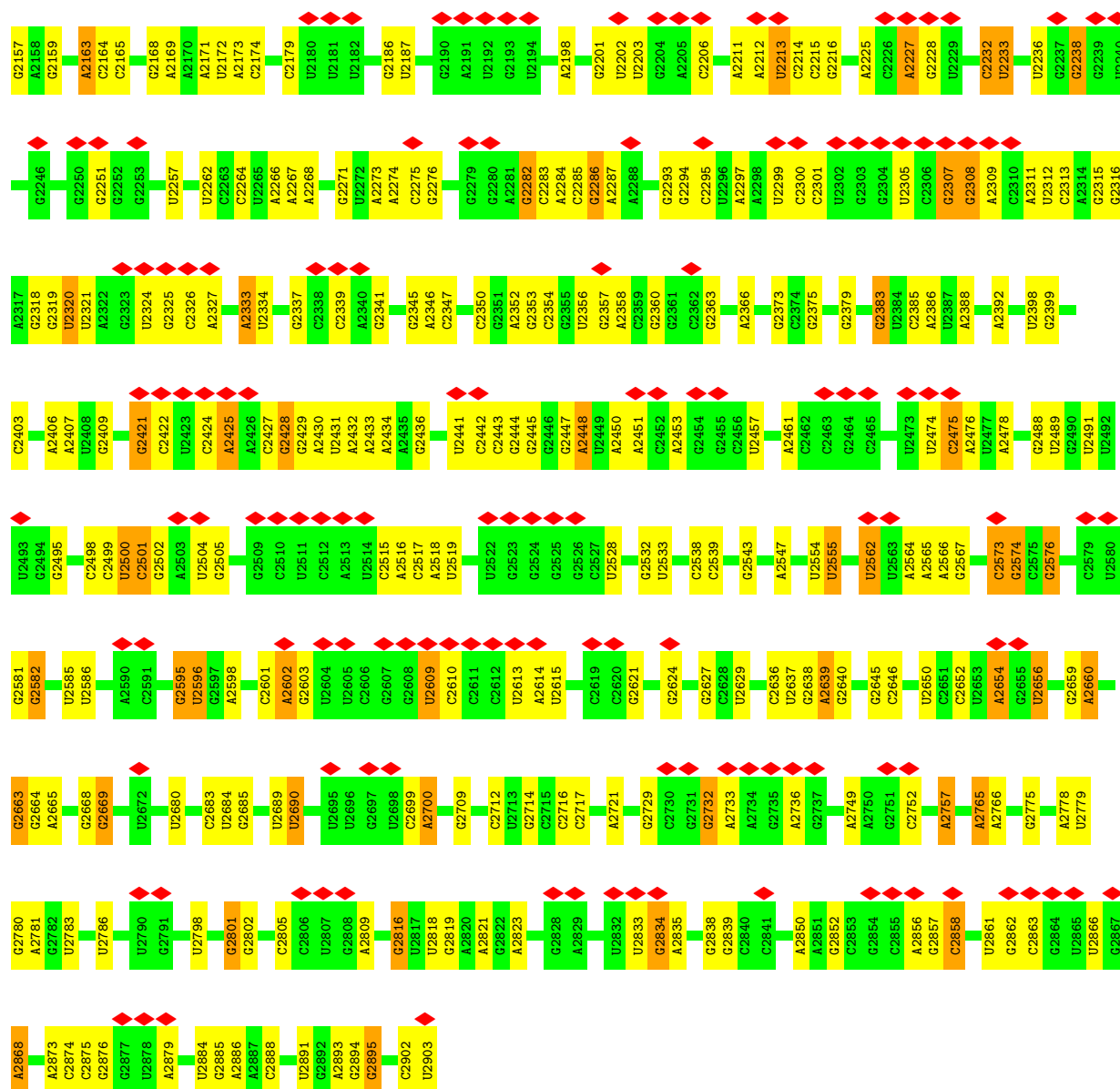


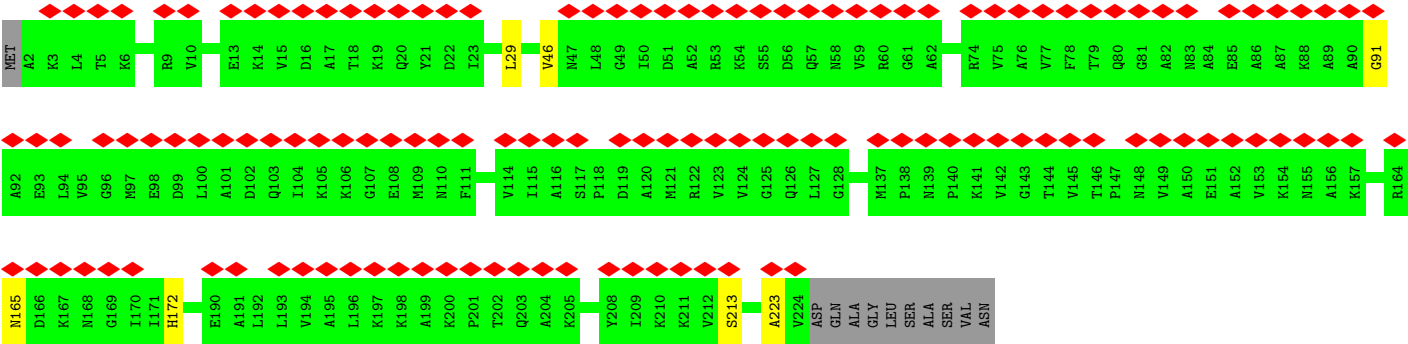


• Molecule 54: 23S ribosomal RNA









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5656	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	local	Depositor
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	162740	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	172.869	Depositor
Minimum map value	-108.132	Depositor
Average map value	-1.067	Depositor
Map value standard deviation	18.681	Depositor
Recommended contour level	22	Depositor
Map size ($\text{\AA}$)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90, 90, 90	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: 6MZ, ACE, NH2, H2U, 5MU, FME, 7MG, CM0, PSU, 4SU, OMC

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	0.91	0/1736	1.35	4/2340 (0.2%)
2	AC	0.91	0/1651	1.35	1/2225 (0.0%)
3	AD	0.93	0/1665	1.45	8/2227 (0.4%)
4	AE	0.89	0/1119	1.39	3/1506 (0.2%)
5	AF	0.93	0/835	1.43	1/1128 (0.1%)
6	AG	0.94	0/1188	1.37	1/1593 (0.1%)
7	AH	0.90	0/989	1.39	3/1326 (0.2%)
8	AI	0.93	0/1035	1.38	2/1377 (0.1%)
9	AJ	0.96	0/797	1.38	2/1079 (0.2%)
10	AK	0.96	0/894	1.38	0/1207
11	AL	0.95	0/969	1.41	0/1300
12	AM	0.98	0/884	1.51	8/1181 (0.7%)
13	AN	0.96	0/817	1.45	4/1088 (0.4%)
14	AO	0.91	0/722	1.45	0/964
15	AP	0.98	0/648	1.39	0/870
16	AQ	0.91	0/658	1.31	0/883
17	AR	0.96	0/463	1.36	2/623 (0.3%)
18	AS	0.95	0/653	1.55	7/879 (0.8%)
19	AT	0.89	0/672	1.38	0/890
20	AU	0.96	0/431	1.78	15/572 (2.6%)
21	AA	1.01	0/36759	1.15	68/57346 (0.1%)
22	A1	1.01	0/1668	1.16	0/2595
23	A2	1.05	0/343	1.36	2/531 (0.4%)
24	A3	1.01	0/1722	1.18	4/2685 (0.1%)
25	BC	0.92	0/2121	1.49	6/2852 (0.2%)
26	BD	0.86	0/1586	1.49	2/2134 (0.1%)
27	BE	0.84	0/1571	1.45	3/2113 (0.1%)
28	BF	0.86	0/1444	1.42	4/1937 (0.2%)
29	BG	0.86	0/1343	1.47	0/1816
30	BH	0.83	0/1122	1.46	2/1515 (0.1%)
31	BI	0.85	0/1046	1.46	2/1410 (0.1%)
32	BJ	0.89	0/1152	1.49	6/1551 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BK	0.90	0/947	1.46	0/1268
34	BL	0.93	0/1054	1.56	4/1403 (0.3%)
35	BM	0.91	0/1093	1.48	1/1460 (0.1%)
36	BN	0.92	0/973	1.50	0/1301
37	BO	0.87	0/902	1.42	1/1209 (0.1%)
38	BP	0.89	0/929	1.44	2/1242 (0.2%)
39	BQ	0.89	0/960	1.45	0/1278
40	BR	0.85	0/829	1.46	1/1107 (0.1%)
41	BS	0.86	0/864	1.53	5/1156 (0.4%)
42	BT	0.83	0/744	1.47	4/994 (0.4%)
43	BU	0.85	0/787	1.45	0/1051
44	BV	0.85	0/766	1.43	4/1025 (0.4%)
45	BW	0.90	0/604	1.59	5/799 (0.6%)
46	BX	0.91	0/635	1.49	0/848
47	BY	0.85	0/510	1.43	0/677
48	BZ	0.90	0/453	1.51	1/605 (0.2%)
49	B0	0.96	0/450	1.56	0/599
50	B1	0.84	0/417	1.34	0/556
51	B2	0.95	0/380	1.46	0/498
52	B3	0.94	0/513	1.53	3/676 (0.4%)
53	B4	0.85	0/303	1.44	0/397
54	BA	0.85	0/69796	1.15	148/108888 (0.1%)
55	BB	0.86	0/2800	1.14	1/4367 (0.0%)
56	B5	0.83	0/1673	1.39	1/2255 (0.0%)
All	All	0.91	0/160085	1.24	341/239402 (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
3	AD	0	2
4	AE	0	1
8	AI	0	1
9	AJ	0	1
11	AL	0	1
18	AS	0	1
21	AA	0	346
22	A1	0	12
23	A2	0	4
24	A3	0	13

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	BP	0	1
50	B1	0	1
54	BA	0	647
55	BB	0	19
56	B5	0	1
All	All	0	1051

There are no bond length outliers.

All (341) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	872	A	C1'-O4'-C4'	-8.94	100.96	109.90
12	AM	106	ARG	CA-C-N	8.67	137.30	121.70
12	AM	106	ARG	C-N-CA	8.67	137.30	121.70
54	BA	1451	C	C2'-C3'-O3'	8.27	121.91	109.50
7	AH	53	ASP	CA-C-N	7.78	135.71	121.70
7	AH	53	ASP	C-N-CA	7.78	135.71	121.70
54	BA	614	A	O4'-C1'-N9	7.78	120.17	108.50
54	BA	818	G	C4'-C3'-O3'	7.76	124.64	113.00
8	AI	128	LYS	CA-C-N	7.59	135.35	121.70
8	AI	128	LYS	C-N-CA	7.59	135.35	121.70
12	AM	106	ARG	CD-NE-CZ	7.28	134.59	124.40
20	AU	51	ALA	CA-C-N	7.21	134.67	121.70
20	AU	51	ALA	C-N-CA	7.21	134.67	121.70
1	AB	206	ILE	CA-C-N	7.07	134.42	121.70
1	AB	206	ILE	C-N-CA	7.07	134.42	121.70
54	BA	1809	A	O3'-P-O5'	-7.05	93.43	104.00
54	BA	548	G	O4'-C1'-N9	6.90	118.55	108.20
21	AA	465	A	C1'-O4'-C4'	-6.83	102.87	109.70
54	BA	1428	C	C4'-C3'-O3'	6.83	119.65	109.40
18	AS	3	SER	CA-C-N	6.82	133.98	121.70
18	AS	3	SER	C-N-CA	6.82	133.98	121.70
3	AD	191	SER	CA-C-N	6.81	133.95	121.70
3	AD	191	SER	C-N-CA	6.81	133.95	121.70
54	BA	1312	U	C2'-C3'-O3'	6.78	119.67	109.50
4	AE	104	ILE	CA-C-N	6.77	133.89	121.70
4	AE	104	ILE	C-N-CA	6.77	133.89	121.70
54	BA	1645	G	C2'-C3'-O3'	-6.74	103.59	113.70
24	A3	76	C	C1'-O4'-C4'	-6.71	103.19	109.90
54	BA	315	G	C2'-C3'-O3'	-6.58	103.83	113.70
18	AS	22	VAL	CA-C-N	6.56	133.52	121.70
18	AS	22	VAL	C-N-CA	6.56	133.52	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AS	77	ARG	NE-CZ-NH2	6.38	124.94	119.20
21	AA	476	U	P-O3'-C3'	6.33	129.69	120.20
44	BV	21	ARG	NE-CZ-NH2	6.32	124.88	119.20
54	BA	2257	U	C4'-C3'-O3'	-6.28	103.58	113.00
24	A3	61	U	O4'-C4'-C3'	6.21	110.21	104.00
21	AA	168	G	C5'-C4'-C3'	-6.20	106.69	116.00
54	BA	1792	G	C5'-C4'-C3'	-6.19	106.72	116.00
21	AA	1049	U	P-O3'-C3'	6.13	129.39	120.20
54	BA	1458	U	C1'-O4'-C4'	-6.10	103.80	109.90
54	BA	1300	G	C4'-C3'-O3'	6.07	118.51	109.40
21	AA	1501	C	O4'-C4'-C3'	6.07	110.07	104.00
34	BL	22	GLY	CA-C-N	6.04	132.56	121.70
34	BL	22	GLY	C-N-CA	6.04	132.56	121.70
54	BA	196	A	O4'-C1'-N9	6.03	117.25	108.20
21	AA	305	G	C5'-C4'-C3'	-6.03	106.16	115.20
54	BA	2624	G	C5'-C4'-C3'	-6.03	106.96	116.00
3	AD	106	PHE	CA-C-N	6.02	125.75	121.65
3	AD	106	PHE	C-N-CA	6.02	125.75	121.65
54	BA	481	G	O4'-C1'-N9	6.02	117.23	108.20
26	BD	124	ARG	CD-NE-CZ	6.01	132.82	124.40
54	BA	1799	G	C2'-C3'-O3'	6.01	118.51	109.50
21	AA	351	G	O4'-C4'-C3'	6.01	110.01	104.00
54	BA	280	U	O4'-C1'-N1	5.97	117.45	108.50
3	AD	50	TYR	CA-C-N	5.96	126.72	119.99
3	AD	50	TYR	C-N-CA	5.96	126.72	119.99
54	BA	1071	G	O4'-C4'-C3'	5.95	109.95	104.00
21	AA	416	G	C5'-C4'-C3'	-5.93	107.10	116.00
54	BA	1393	A	C4'-C3'-C2'	-5.93	96.67	102.60
18	AS	13	HIS	CB-CG-CD2	-5.93	123.49	131.20
54	BA	1189	A	C4'-C3'-C2'	-5.93	96.67	102.60
54	BA	490	C	O4'-C1'-N1	5.91	117.37	108.50
44	BV	13	GLY	CA-C-N	5.89	128.98	120.79
44	BV	13	GLY	C-N-CA	5.89	128.98	120.79
25	BC	67	LYS	CA-C-N	5.89	129.12	120.82
25	BC	67	LYS	C-N-CA	5.89	129.12	120.82
55	BB	24	G	O4'-C4'-C3'	5.88	109.88	104.00
54	BA	2320	U	O4'-C1'-N1	5.86	117.29	108.50
21	AA	958	A	O4'-C4'-C3'	5.85	109.85	104.00
52	B3	1	PRO	CA-N-CD	-5.83	103.84	112.00
28	BF	121	PHE	CA-C-N	5.82	132.18	121.70
28	BF	121	PHE	C-N-CA	5.82	132.18	121.70
54	BA	1490	A	O4'-C1'-N9	5.82	116.93	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	BS	7	HIS	CB-CG-CD2	-5.82	123.64	131.20
21	AA	388	G	O4'-C4'-C3'	5.82	109.82	104.00
32	BJ	140	LEU	CA-C-N	5.81	132.15	121.70
32	BJ	140	LEU	C-N-CA	5.81	132.15	121.70
54	BA	443	A	O4'-C4'-C3'	5.81	109.81	104.00
54	BA	570	G	O4'-C4'-C3'	5.80	109.81	104.00
54	BA	1427	A	P-O3'-C3'	5.79	128.88	120.20
54	BA	2171	A	C2'-C3'-O3'	5.79	118.18	109.50
54	BA	1938	A	C1'-O4'-C4'	-5.78	103.92	109.70
54	BA	834	G	O3'-P-O5'	5.78	112.67	104.00
24	A3	50	G	O4'-C4'-C3'	5.77	109.77	104.00
21	AA	1356	G	O4'-C4'-C3'	5.76	109.76	104.00
54	BA	2136	G	O4'-C4'-C3'	5.76	109.76	104.00
54	BA	1314	C	N1-C1'-C2'	5.74	120.60	112.00
41	BS	91	GLY	CA-C-N	5.72	132.01	121.70
41	BS	91	GLY	C-N-CA	5.72	132.01	121.70
54	BA	1236	G	O4'-C4'-C3'	5.72	109.72	104.00
54	BA	621	A	C5'-C4'-C3'	-5.72	107.42	116.00
54	BA	1691	C	C4'-C3'-C2'	-5.71	96.89	102.60
26	BD	2	ILE	CA-CB-CG1	5.70	120.09	110.40
54	BA	1154	G	C2'-C3'-O3'	-5.70	105.15	113.70
54	BA	478	A	O4'-C4'-C3'	5.70	109.70	104.00
54	BA	2264	C	C4'-C3'-C2'	-5.70	96.90	102.60
21	AA	724	G	C5'-C4'-C3'	-5.69	107.47	116.00
54	BA	323	C	O4'-C1'-N1	5.68	116.72	108.20
25	BC	96	LYS	CA-C-N	5.67	130.83	121.99
25	BC	96	LYS	C-N-CA	5.67	130.83	121.99
54	BA	850	U	O4'-C4'-C3'	5.66	109.66	104.00
21	AA	1101	A	P-O3'-C3'	5.66	128.69	120.20
54	BA	1427	A	C2'-C3'-O3'	5.65	117.98	109.50
54	BA	670	A	C2'-C3'-O3'	5.64	117.96	109.50
54	BA	1128	G	C1'-O4'-C4'	-5.62	104.08	109.70
3	AD	84	ASN	CA-C-N	5.62	128.08	120.38
3	AD	84	ASN	C-N-CA	5.62	128.08	120.38
54	BA	278	A	N9-C1'-C2'	5.61	120.41	112.00
54	BA	1313	U	O4'-C4'-C3'	5.60	109.60	104.00
54	BA	1076	C	C1'-O4'-C4'	-5.59	104.31	109.90
54	BA	1210	G	C2'-C3'-O3'	5.58	117.87	109.50
54	BA	2130	U	O4'-C4'-C3'	5.58	109.58	104.00
54	BA	1607	C	O4'-C1'-N1	5.58	116.57	108.20
54	BA	1610	A	C1'-O4'-C4'	-5.58	104.32	109.90
21	AA	1144	G	O4'-C4'-C3'	5.58	109.58	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	364	A	O4'-C4'-C3'	5.58	109.58	104.00
54	BA	759	G	C4'-C3'-C2'	-5.57	97.03	102.60
13	AN	42	TRP	CA-C-N	5.57	131.72	121.70
13	AN	42	TRP	C-N-CA	5.57	131.72	121.70
54	BA	2757	A	C5'-C4'-C3'	-5.55	107.67	116.00
54	BA	614	A	C1'-O4'-C4'	-5.54	104.36	109.90
54	BA	265	A	O4'-C1'-N9	5.54	116.51	108.20
54	BA	2489	U	O4'-C4'-C3'	5.53	109.53	104.00
54	BA	1352	U	C4'-C3'-C2'	-5.53	97.07	102.60
21	AA	476	U	C5'-C4'-C3'	-5.53	107.71	116.00
31	BI	92	PRO	CA-C-N	5.52	132.09	121.54
31	BI	92	PRO	C-N-CA	5.52	132.09	121.54
54	BA	2652	C	O4'-C4'-C3'	5.52	109.52	104.00
21	AA	382	A	O4'-C4'-C3'	5.51	109.51	104.00
37	BO	38	GLN	OE1-CD-NE2	-5.51	117.09	122.60
54	BA	1915	U	O4'-C4'-C3'	5.50	109.50	104.00
54	BA	2874	C	O4'-C4'-C3'	5.50	109.50	104.00
21	AA	189	A	O4'-C4'-C3'	5.50	109.50	104.00
54	BA	2562	U	C5'-C4'-C3'	-5.48	107.78	116.00
54	BA	2227	A	C4'-C3'-C2'	-5.48	97.12	102.60
54	BA	884	U	C2'-C3'-O3'	-5.47	105.49	113.70
54	BA	2669	G	C4'-C3'-C2'	-5.47	97.13	102.60
32	BJ	78	THR	CA-C-N	5.46	131.53	121.70
32	BJ	78	THR	C-N-CA	5.46	131.53	121.70
54	BA	2169	A	O4'-C1'-N9	5.46	116.69	108.50
54	BA	2595	G	C4'-C3'-C2'	-5.46	97.14	102.60
12	AM	106	ARG	O-C-N	-5.45	115.85	122.22
20	AU	50	SER	CA-C-N	5.44	131.50	121.70
20	AU	50	SER	C-N-CA	5.44	131.50	121.70
34	BL	5	THR	CA-C-N	5.44	131.50	121.70
34	BL	5	THR	C-N-CA	5.44	131.50	121.70
54	BA	515	A	O4'-C4'-C3'	5.43	109.43	104.00
48	BZ	31	ILE	CA-CB-CG1	5.43	119.62	110.40
54	BA	2213	U	O4'-C1'-N1	5.43	116.34	108.20
54	BA	1073	A	O4'-C1'-N9	5.42	116.34	108.20
54	BA	2120	G	O4'-C4'-C3'	5.42	109.42	104.00
21	AA	695	A	O4'-C4'-C3'	5.42	109.42	104.00
54	BA	2126	A	O4'-C1'-N9	5.42	116.33	108.20
54	BA	1210	G	C4'-C3'-O3'	5.42	117.53	109.40
12	AM	106	ARG	N-CA-C	5.41	117.94	111.71
21	AA	728	A	O4'-C4'-C3'	5.41	109.41	104.00
54	BA	2092	U	O4'-C1'-N1	5.41	116.31	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AM	110	GLY	CA-C-N	5.40	125.41	119.90
12	AM	110	GLY	C-N-CA	5.40	125.41	119.90
21	AA	366	A	O4'-C4'-C3'	5.40	109.40	104.00
21	AA	54	C	C1'-O4'-C4'	-5.40	104.30	109.70
21	AA	1197	A	O4'-C4'-C3'	5.40	109.40	104.00
23	A2	90	U	O4'-C4'-C3'	-5.40	98.60	104.00
54	BA	1451	C	C4'-C3'-O3'	5.40	117.50	109.40
54	BA	1706	C	C4'-C3'-O3'	5.40	117.50	109.40
25	BC	52	HIS	CB-CG-CD2	-5.39	124.19	131.20
54	BA	893	C	C4'-C3'-C2'	-5.39	97.21	102.60
21	AA	1228	C	C1'-O4'-C4'	-5.38	104.31	109.70
21	AA	196	A	O4'-C4'-C3'	5.38	109.38	104.00
54	BA	2282	G	C4'-C3'-O3'	5.37	121.06	113.00
21	AA	1201	A	P-O3'-C3'	5.37	128.25	120.20
21	AA	1518	A	O4'-C4'-C3'	5.37	109.36	104.00
54	BA	1761	C	O4'-C4'-C3'	5.36	109.36	104.00
42	BT	71	GLY	CA-C-N	5.36	131.34	121.70
42	BT	71	GLY	C-N-CA	5.36	131.34	121.70
54	BA	828	U	C5'-C4'-C3'	-5.35	107.97	116.00
21	AA	497	G	O4'-C4'-C3'	5.33	109.33	104.00
54	BA	1135	C	O4'-C4'-C3'	5.33	109.33	104.00
54	BA	2202	U	C4'-C3'-C2'	-5.33	97.27	102.60
54	BA	936	A	C1'-O4'-C4'	-5.33	104.57	109.90
54	BA	1389	G	O4'-C4'-C3'	5.33	109.33	104.00
21	AA	298	A	C5'-C4'-C3'	-5.32	108.02	116.00
21	AA	1178	G	O4'-C4'-C3'	5.32	109.32	104.00
45	BW	22	VAL	CA-C-N	5.32	131.71	121.54
45	BW	22	VAL	C-N-CA	5.32	131.71	121.54
4	AE	104	ILE	O-C-N	-5.32	115.92	122.57
21	AA	1318	A	O4'-C4'-C3'	5.32	109.32	104.00
9	AJ	21	ALA	CA-C-N	5.32	127.67	120.38
9	AJ	21	ALA	C-N-CA	5.32	127.67	120.38
27	BE	60	TRP	CA-C-N	5.32	131.28	121.70
27	BE	60	TRP	C-N-CA	5.32	131.28	121.70
54	BA	29	U	O4'-C1'-C2'	-5.32	102.28	107.60
54	BA	2700	A	O4'-C4'-C3'	5.32	109.32	104.00
54	BA	2660	A	O4'-C4'-C3'	5.31	109.31	104.00
32	BJ	68	LYS	N-CA-CB	-5.31	103.39	111.15
56	B5	172	HIS	CB-CG-CD2	-5.31	124.29	131.20
54	BA	1314	C	O4'-C1'-C2'	-5.31	102.29	107.60
54	BA	527	C	C2'-C3'-O3'	5.31	117.46	109.50
54	BA	1737	G	O4'-C4'-C3'	5.31	109.31	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AF	17	GLN	OE1-CD-NE2	-5.31	117.29	122.60
54	BA	572	A	O4'-C4'-C3'	5.31	109.31	104.00
21	AA	1357	A	O4'-C4'-C3'	5.30	109.30	104.00
54	BA	2432	A	C1'-O4'-C4'	-5.30	104.60	109.90
21	AA	13	U	C1'-O4'-C4'	-5.30	104.40	109.70
25	BC	24	HIS	CB-CG-CD2	-5.30	124.32	131.20
23	A2	93	U	C1'-O4'-C4'	-5.29	104.41	109.70
45	BW	23	LYS	N-CA-C	5.29	122.07	110.80
54	BA	1313	U	N1-C1'-C2'	5.29	119.93	112.00
21	AA	630	A	O4'-C4'-C3'	5.29	109.29	104.00
21	AA	570	G	O4'-C4'-C3'	5.28	109.28	104.00
44	BV	88	HIS	CB-CG-CD2	-5.27	124.35	131.20
21	AA	292	G	O4'-C4'-C3'	5.27	109.27	104.00
2	AC	5	HIS	CB-CG-CD2	-5.26	124.36	131.20
7	AH	53	ASP	O-C-N	-5.26	115.70	121.76
21	AA	1425	U	P-O3'-C3'	5.26	128.09	120.20
54	BA	1063	G	C1'-O4'-C4'	-5.26	104.64	109.90
54	BA	1235	G	O4'-C4'-C3'	5.25	109.25	104.00
54	BA	638	G	C5'-C4'-C3'	-5.25	108.12	116.00
54	BA	1193	G	C4'-C3'-C2'	-5.25	97.35	102.60
21	AA	1467	C	O4'-C4'-C3'	5.25	109.25	104.00
21	AA	383	A	O4'-C4'-C3'	5.25	109.25	104.00
54	BA	2783	U	O4'-C4'-C3'	5.25	109.25	104.00
54	BA	1598	A	O4'-C4'-C3'	5.24	109.23	104.00
21	AA	1280	A	C1'-O4'-C4'	-5.22	104.47	109.70
20	AU	46	ARG	CA-C-N	5.22	131.10	121.70
20	AU	46	ARG	C-N-CA	5.22	131.10	121.70
54	BA	1634	A	C5'-C4'-C3'	-5.22	108.17	116.00
42	BT	6	ARG	NE-CZ-NH2	5.21	123.89	119.20
20	AU	11	PHE	CA-C-N	5.21	131.07	121.70
20	AU	11	PHE	C-N-CA	5.21	131.07	121.70
21	AA	1156	G	O4'-C4'-C3'	5.20	109.20	104.00
17	AR	28	LEU	CA-C-N	5.19	127.49	120.38
17	AR	28	LEU	C-N-CA	5.19	127.49	120.38
21	AA	229	U	O4'-C4'-C3'	5.19	109.19	104.00
13	AN	100	SER	CA-C-N	5.19	131.04	121.70
13	AN	100	SER	C-N-CA	5.19	131.04	121.70
54	BA	549	G	O4'-C4'-C3'	5.19	109.19	104.00
21	AA	239	U	C5'-C4'-C3'	-5.18	107.43	115.20
20	AU	36	PHE	CA-C-N	5.18	131.44	121.54
20	AU	36	PHE	C-N-CA	5.18	131.44	121.54
21	AA	1523	G	O4'-C4'-C3'	5.18	109.18	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1426	G	C2'-C3'-O3'	-5.17	105.94	113.70
54	BA	1731	G	O4'-C1'-N9	5.17	115.96	108.20
21	AA	900	A	O4'-C4'-C3'	5.17	109.17	104.00
54	BA	2574	G	O4'-C4'-C3'	5.17	109.17	104.00
41	BS	102	HIS	CB-CG-CD2	-5.17	124.48	131.20
54	BA	37	C	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	802	A	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	1596	A	C4'-C3'-C2'	-5.17	97.43	102.60
21	AA	826	C	O4'-C4'-C3'	5.16	109.16	104.00
27	BE	14	VAL	N-CA-C	5.16	115.68	110.05
54	BA	1764	C	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	211	C	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	1606	C	O4'-C1'-N1	5.16	116.24	108.50
21	AA	1511	G	O4'-C4'-C3'	5.16	109.16	104.00
54	BA	784	G	O4'-C1'-N9	5.15	116.23	108.50
21	AA	876	C	P-O3'-C3'	5.15	127.93	120.20
54	BA	751	A	O4'-C4'-C3'	5.15	109.15	104.00
18	AS	36	ARG	NE-CZ-NH2	5.15	123.83	119.20
54	BA	2858	C	O4'-C1'-N1	5.15	115.93	108.20
12	AM	2	ARG	NE-CZ-NH2	5.15	123.83	119.20
54	BA	6	A	C5'-C4'-C3'	-5.15	108.28	116.00
21	AA	251	G	P-O3'-C3'	5.14	127.91	120.20
54	BA	45	G	O4'-C4'-C3'	5.14	109.14	104.00
54	BA	1225	G	O4'-C4'-C3'	5.14	109.14	104.00
54	BA	1573	G	O4'-C4'-C3'	5.14	109.14	104.00
21	AA	283	U	O4'-C4'-C3'	5.13	109.13	104.00
54	BA	254	G	C4'-C3'-C2'	-5.13	97.47	102.60
21	AA	1534	A	C1'-O4'-C4'	-5.13	104.57	109.70
54	BA	1301	A	O4'-C1'-C2'	-5.12	100.68	105.80
54	BA	1769	U	C4'-C3'-C2'	-5.12	97.48	102.60
6	AG	51	GLN	OE1-CD-NE2	-5.12	117.48	122.60
54	BA	1619	G	O4'-C4'-C3'	5.12	109.12	104.00
54	BA	2685	G	C4'-C3'-C2'	-5.11	97.49	102.60
54	BA	327	G	C5'-C4'-C3'	-5.11	108.34	116.00
21	AA	876	C	C5'-C4'-C3'	-5.11	108.34	116.00
54	BA	2656	U	C4'-C3'-C2'	-5.11	97.49	102.60
28	BF	135	ILE	CA-C-N	5.11	131.16	121.97
28	BF	135	ILE	C-N-CA	5.11	131.16	121.97
21	AA	1402	C	O4'-C4'-C3'	5.10	109.10	104.00
54	BA	1289	C	C3'-C2'-C1'	5.10	106.40	101.30
54	BA	2861	U	C4'-C3'-C2'	-5.10	97.50	102.60
1	AB	72	LYS	CA-C-N	5.09	128.46	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AB	72	LYS	C-N-CA	5.09	128.46	120.82
21	AA	1078	U	O4'-C4'-C3'	5.09	109.09	104.00
45	BW	20	LEU	CA-C-N	5.09	125.51	120.31
45	BW	20	LEU	C-N-CA	5.09	125.51	120.31
32	BJ	78	THR	N-CA-C	5.09	118.65	112.23
54	BA	2576	G	O4'-C4'-C3'	5.09	109.09	104.00
21	AA	1040	U	C5'-C4'-C3'	-5.09	108.37	116.00
54	BA	2308	G	O4'-C1'-N9	5.08	115.83	108.20
54	BA	1952	A	O4'-C1'-C2'	-5.08	100.72	105.80
54	BA	1384	A	O4'-C4'-C3'	5.08	109.08	104.00
35	BM	3	GLN	N-CA-C	5.08	112.79	108.22
54	BA	1010	A	O4'-C4'-C3'	5.08	109.08	104.00
21	AA	227	G	C5'-C4'-C3'	-5.07	108.39	116.00
21	AA	600	A	C5'-C4'-C3'	-5.07	108.40	116.00
54	BA	1005	C	C3'-C2'-C1'	5.06	106.56	101.50
54	BA	1760	C	O4'-C4'-C3'	5.06	109.06	104.00
20	AU	23	GLU	CA-C-N	5.06	131.20	121.54
20	AU	23	GLU	C-N-CA	5.06	131.20	121.54
54	BA	856	G	O4'-C4'-C3'	5.06	109.06	104.00
54	BA	1379	U	O4'-C4'-C3'	5.06	109.06	104.00
54	BA	2421	G	C2'-C3'-O3'	5.06	117.08	109.50
21	AA	600	A	O3'-P-O5'	-5.06	96.42	104.00
54	BA	946	C	C5'-C4'-C3'	-5.05	108.42	116.00
54	BA	394	C	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	644	A	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	113	U	O4'-C4'-C3'	5.05	109.05	104.00
21	AA	450	G	O4'-C4'-C3'	5.05	109.05	104.00
54	BA	169	G	O4'-C4'-C3'	5.05	109.05	104.00
41	BS	31	GLN	OE1-CD-NE2	-5.05	117.55	122.60
42	BT	40	LYS	N-CA-C	5.04	118.20	111.75
54	BA	1870	C	O4'-C4'-C3'	5.04	109.04	104.00
21	AA	1269	A	O4'-C4'-C3'	5.04	109.04	104.00
54	BA	1597	A	C3'-C2'-C1'	5.04	106.34	101.30
21	AA	309	A	O4'-C4'-C3'	5.04	109.04	104.00
54	BA	1523	U	O4'-C1'-N1	5.04	115.76	108.20
20	AU	32	ARG	CA-C-N	5.04	130.76	121.70
20	AU	32	ARG	C-N-CA	5.04	130.76	121.70
21	AA	1179	A	C3'-C2'-C1'	5.04	106.53	101.50
21	AA	328	C	C2'-C3'-O3'	5.03	117.05	109.50
54	BA	1783	A	C2'-C3'-O3'	-5.03	106.15	113.70
54	BA	2311	A	O4'-C4'-C3'	5.03	109.03	104.00
20	AU	26	GLY	O-C-N	-5.03	117.96	124.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	958	A	C3'-C2'-C1'	5.03	106.33	101.30
24	A3	66	C	O4'-C4'-C3'	5.03	109.03	104.00
40	BR	89	HIS	CB-CG-CD2	-5.03	124.66	131.20
54	BA	1971	U	N1-C1'-C2'	5.02	119.53	112.00
38	BP	68	GLY	CA-C-N	5.02	131.00	121.97
38	BP	68	GLY	C-N-CA	5.02	131.00	121.97
54	BA	91	A	O4'-C1'-N9	5.02	115.73	108.20
21	AA	1111	A	O4'-C4'-C3'	5.01	109.02	104.00
52	B3	36	ALA	CA-C-N	5.01	127.25	120.38
52	B3	36	ALA	C-N-CA	5.01	127.25	120.38
54	BA	2017	U	O4'-C4'-C3'	5.01	109.01	104.00
21	AA	753	A	P-O3'-C3'	5.00	127.71	120.20
30	BH	119	ASN	CA-C-N	5.00	125.41	120.31
30	BH	119	ASN	C-N-CA	5.00	125.41	120.31
21	AA	932	C	O4'-C4'-C3'	5.00	109.00	104.00
54	BA	1677	A	C4'-C3'-C2'	-5.00	97.60	102.60

There are no chirality outliers.

All (1051) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	1	G	Sidechain
22	A1	24	G	Sidechain
22	A1	36	C	Sidechain
22	A1	40	G	Sidechain
22	A1	44	G	Sidechain
22	A1	45	G	Sidechain
22	A1	47	U	Sidechain
22	A1	50	G	Sidechain
22	A1	53	G	Sidechain
22	A1	59	U	Sidechain
22	A1	72	C	Sidechain
22	A1	76	A	Sidechain
23	A2	81	U	Sidechain
23	A2	83	U	Sidechain
23	A2	85	G	Sidechain
23	A2	90	U	Sidechain
24	A3	24	C	Sidechain
24	A3	32	G	Sidechain
24	A3	34	U	Sidechain
24	A3	44	A	Sidechain
24	A3	49	C	Sidechain

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Mol	Chain	Res	Type	Group
24	A3	50	G	Sidechain
24	A3	57	C	Sidechain
24	A3	6	G	Sidechain
24	A3	62	C	Sidechain
24	A3	65	G	Sidechain
24	A3	7	G	Sidechain
24	A3	72	C	Sidechain
24	A3	75	C	Sidechain
21	AA	1002	G	Sidechain
21	AA	1003	G	Sidechain
21	AA	1010	U	Sidechain
21	AA	1020	G	Sidechain
21	AA	1021	A	Sidechain
21	AA	1026	G	Sidechain
21	AA	1027	C	Sidechain
21	AA	1029	U	Sidechain
21	AA	1034	G	Sidechain
21	AA	1046	A	Sidechain
21	AA	1048	G	Sidechain
21	AA	1054	C	Sidechain
21	AA	1055	A	Sidechain
21	AA	1061	G	Sidechain
21	AA	1063	C	Sidechain
21	AA	1065	U	Sidechain
21	AA	1075	U	Sidechain
21	AA	1076	U	Sidechain
21	AA	1077	G	Sidechain
21	AA	1080	A	Sidechain
21	AA	1083	U	Sidechain
21	AA	109	A	Sidechain
21	AA	1092	A	Sidechain
21	AA	1099	G	Sidechain
21	AA	11	G	Sidechain
21	AA	110	C	Sidechain
21	AA	1107	C	Sidechain
21	AA	1108	G	Sidechain
21	AA	111	G	Sidechain
21	AA	1110	A	Sidechain
21	AA	1112	C	Sidechain
21	AA	1113	C	Sidechain
21	AA	1118	U	Sidechain
21	AA	112	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1120	C	Sidechain
21	AA	1128	C	Sidechain
21	AA	1131	G	Sidechain
21	AA	1139	G	Sidechain
21	AA	1141	C	Sidechain
21	AA	1144	G	Sidechain
21	AA	115	G	Sidechain
21	AA	1150	A	Sidechain
21	AA	1151	A	Sidechain
21	AA	1152	A	Sidechain
21	AA	1153	G	Sidechain
21	AA	1155	A	Sidechain
21	AA	1157	A	Sidechain
21	AA	1164	G	Sidechain
21	AA	1166	G	Sidechain
21	AA	117	G	Sidechain
21	AA	1175	G	Sidechain
21	AA	118	U	Sidechain
21	AA	1180	A	Sidechain
21	AA	1181	G	Sidechain
21	AA	1192	C	Sidechain
21	AA	1195	C	Sidechain
21	AA	1196	A	Sidechain
21	AA	1200	C	Sidechain
21	AA	121	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1217	C	Sidechain
21	AA	1218	C	Sidechain
21	AA	1222	G	Sidechain
21	AA	1225	A	Sidechain
21	AA	1228	C	Sidechain
21	AA	123	U	Sidechain
21	AA	1230	C	Sidechain
21	AA	1234	C	Sidechain
21	AA	1235	U	Sidechain
21	AA	1238	A	Sidechain
21	AA	1239	A	Sidechain
21	AA	1248	A	Sidechain
21	AA	1249	C	Sidechain
21	AA	1266	G	Sidechain
21	AA	1277	C	Sidechain
21	AA	1279	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1282	C	Sidechain
21	AA	1289	A	Sidechain
21	AA	1290	G	Sidechain
21	AA	1292	G	Sidechain
21	AA	1294	G	Sidechain
21	AA	130	A	Sidechain
21	AA	1306	A	Sidechain
21	AA	1308	U	Sidechain
21	AA	131	A	Sidechain
21	AA	1313	U	Sidechain
21	AA	1314	C	Sidechain
21	AA	1316	G	Sidechain
21	AA	1317	C	Sidechain
21	AA	1324	A	Sidechain
21	AA	1330	U	Sidechain
21	AA	1331	G	Sidechain
21	AA	1332	A	Sidechain
21	AA	1333	A	Sidechain
21	AA	1336	C	Sidechain
21	AA	1339	A	Sidechain
21	AA	1351	U	Sidechain
21	AA	1355	G	Sidechain
21	AA	1356	G	Sidechain
21	AA	1359	C	Sidechain
21	AA	1360	A	Sidechain
21	AA	1362	A	Sidechain
21	AA	1372	U	Sidechain
21	AA	1376	U	Sidechain
21	AA	1377	A	Sidechain
21	AA	1378	C	Sidechain
21	AA	1389	C	Sidechain
21	AA	1397	C	Sidechain
21	AA	1402	C	Sidechain
21	AA	1412	C	Sidechain
21	AA	1414	U	Sidechain
21	AA	1415	G	Sidechain
21	AA	1432	G	Sidechain
21	AA	1444	U	Sidechain
21	AA	1474	U	Sidechain
21	AA	148	G	Sidechain
21	AA	1480	A	Sidechain
21	AA	1482	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1494	G	Sidechain
21	AA	150	U	Sidechain
21	AA	1516	G	Sidechain
21	AA	1517	G	Sidechain
21	AA	152	A	Sidechain
21	AA	1524	C	Sidechain
21	AA	1527	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1533	C	Sidechain
21	AA	156	C	Sidechain
21	AA	157	U	Sidechain
21	AA	159	G	Sidechain
21	AA	163	C	Sidechain
21	AA	167	A	Sidechain
21	AA	180	U	Sidechain
21	AA	182	A	Sidechain
21	AA	184	G	Sidechain
21	AA	187	G	Sidechain
21	AA	197	A	Sidechain
21	AA	200	G	Sidechain
21	AA	217	C	Sidechain
21	AA	23	C	Sidechain
21	AA	234	C	Sidechain
21	AA	236	A	Sidechain
21	AA	24	U	Sidechain
21	AA	242	G	Sidechain
21	AA	251	G	Sidechain
21	AA	258	G	Sidechain
21	AA	26	A	Sidechain
21	AA	260	G	Sidechain
21	AA	264	C	Sidechain
21	AA	267	C	Sidechain
21	AA	273	U	Sidechain
21	AA	274	A	Sidechain
21	AA	278	G	Sidechain
21	AA	285	C	Sidechain
21	AA	287	U	Sidechain
21	AA	289	G	Sidechain
21	AA	296	U	Sidechain
21	AA	297	G	Sidechain
21	AA	298	A	Sidechain
21	AA	30	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	300	A	Sidechain
21	AA	306	A	Sidechain
21	AA	309	A	Sidechain
21	AA	312	C	Sidechain
21	AA	313	A	Sidechain
21	AA	315	A	Sidechain
21	AA	323	U	Sidechain
21	AA	324	G	Sidechain
21	AA	330	C	Sidechain
21	AA	334	C	Sidechain
21	AA	340	U	Sidechain
21	AA	345	C	Sidechain
21	AA	349	A	Sidechain
21	AA	35	G	Sidechain
21	AA	353	A	Sidechain
21	AA	354	G	Sidechain
21	AA	356	A	Sidechain
21	AA	361	G	Sidechain
21	AA	362	G	Sidechain
21	AA	366	A	Sidechain
21	AA	376	G	Sidechain
21	AA	377	G	Sidechain
21	AA	387	U	Sidechain
21	AA	388	G	Sidechain
21	AA	39	G	Sidechain
21	AA	400	C	Sidechain
21	AA	415	A	Sidechain
21	AA	416	G	Sidechain
21	AA	417	G	Sidechain
21	AA	420	U	Sidechain
21	AA	423	G	Sidechain
21	AA	429	U	Sidechain
21	AA	431	A	Sidechain
21	AA	44	A	Sidechain
21	AA	442	G	Sidechain
21	AA	444	G	Sidechain
21	AA	446	G	Sidechain
21	AA	447	G	Sidechain
21	AA	448	A	Sidechain
21	AA	450	G	Sidechain
21	AA	456	A	Sidechain
21	AA	458	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	462	G	Sidechain
21	AA	467	U	Sidechain
21	AA	469	C	Sidechain
21	AA	473	U	Sidechain
21	AA	474	G	Sidechain
21	AA	478	A	Sidechain
21	AA	48	C	Sidechain
21	AA	481	G	Sidechain
21	AA	484	G	Sidechain
21	AA	489	C	Sidechain
21	AA	491	G	Sidechain
21	AA	492	C	Sidechain
21	AA	494	G	Sidechain
21	AA	496	A	Sidechain
21	AA	497	G	Sidechain
21	AA	50	A	Sidechain
21	AA	505	G	Sidechain
21	AA	506	G	Sidechain
21	AA	507	C	Sidechain
21	AA	508	U	Sidechain
21	AA	511	C	Sidechain
21	AA	515	G	Sidechain
21	AA	516	U	Sidechain
21	AA	517	G	Sidechain
21	AA	518	C	Sidechain
21	AA	519	C	Sidechain
21	AA	526	C	Sidechain
21	AA	530	G	Sidechain
21	AA	533	A	Sidechain
21	AA	536	C	Sidechain
21	AA	537	G	Sidechain
21	AA	538	G	Sidechain
21	AA	54	C	Sidechain
21	AA	549	C	Sidechain
21	AA	55	A	Sidechain
21	AA	557	G	Sidechain
21	AA	558	G	Sidechain
21	AA	559	A	Sidechain
21	AA	570	G	Sidechain
21	AA	571	U	Sidechain
21	AA	572	A	Sidechain
21	AA	573	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	576	C	Sidechain
21	AA	581	G	Sidechain
21	AA	585	G	Sidechain
21	AA	588	G	Sidechain
21	AA	59	A	Sidechain
21	AA	592	G	Sidechain
21	AA	595	A	Sidechain
21	AA	602	A	Sidechain
21	AA	605	U	Sidechain
21	AA	610	U	Sidechain
21	AA	611	C	Sidechain
21	AA	618	C	Sidechain
21	AA	622	A	Sidechain
21	AA	629	A	Sidechain
21	AA	633	G	Sidechain
21	AA	641	U	Sidechain
21	AA	643	C	Sidechain
21	AA	653	U	Sidechain
21	AA	662	U	Sidechain
21	AA	663	A	Sidechain
21	AA	669	G	Sidechain
21	AA	670	G	Sidechain
21	AA	671	G	Sidechain
21	AA	673	A	Sidechain
21	AA	675	A	Sidechain
21	AA	690	G	Sidechain
21	AA	691	G	Sidechain
21	AA	697	U	Sidechain
21	AA	700	G	Sidechain
21	AA	710	G	Sidechain
21	AA	72	A	Sidechain
21	AA	722	G	Sidechain
21	AA	725	G	Sidechain
21	AA	728	A	Sidechain
21	AA	741	G	Sidechain
21	AA	751	U	Sidechain
21	AA	752	G	Sidechain
21	AA	754	C	Sidechain
21	AA	760	G	Sidechain
21	AA	765	G	Sidechain
21	AA	769	G	Sidechain
21	AA	774	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	778	G	Sidechain
21	AA	779	C	Sidechain
21	AA	786	G	Sidechain
21	AA	788	U	Sidechain
21	AA	789	U	Sidechain
21	AA	792	A	Sidechain
21	AA	8	A	Sidechain
21	AA	800	G	Sidechain
21	AA	806	C	Sidechain
21	AA	81	A	Sidechain
21	AA	813	U	Sidechain
21	AA	818	G	Sidechain
21	AA	82	G	Sidechain
21	AA	820	U	Sidechain
21	AA	824	G	Sidechain
21	AA	827	U	Sidechain
21	AA	83	C	Sidechain
21	AA	832	G	Sidechain
21	AA	837	U	Sidechain
21	AA	838	G	Sidechain
21	AA	859	G	Sidechain
21	AA	86	G	Sidechain
21	AA	862	C	Sidechain
21	AA	865	A	Sidechain
21	AA	869	G	Sidechain
21	AA	874	G	Sidechain
21	AA	877	G	Sidechain
21	AA	878	A	Sidechain
21	AA	88	U	Sidechain
21	AA	884	U	Sidechain
21	AA	885	G	Sidechain
21	AA	886	G	Sidechain
21	AA	887	G	Sidechain
21	AA	888	G	Sidechain
21	AA	898	G	Sidechain
21	AA	905	U	Sidechain
21	AA	909	A	Sidechain
21	AA	915	A	Sidechain
21	AA	916	U	Sidechain
21	AA	919	A	Sidechain
21	AA	921	U	Sidechain
21	AA	924	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	925	G	Sidechain
21	AA	926	G	Sidechain
21	AA	931	C	Sidechain
21	AA	932	C	Sidechain
21	AA	933	G	Sidechain
21	AA	944	G	Sidechain
21	AA	949	A	Sidechain
21	AA	954	G	Sidechain
21	AA	957	U	Sidechain
21	AA	974	A	Sidechain
21	AA	978	A	Sidechain
21	AA	989	U	Sidechain
21	AA	99	C	Sidechain
21	AA	991	U	Sidechain
21	AA	992	U	Sidechain
21	AA	994	A	Sidechain
21	AA	996	A	Sidechain
21	AA	998	C	Sidechain
3	AD	75	TYR	Sidechain
3	AD	96	ARG	Sidechain
4	AE	53	ARG	Sidechain
8	AI	129	ARG	Sidechain
9	AJ	72	ARG	Sidechain
11	AL	26	CYS	Peptide
18	AS	79	TYR	Sidechain
50	B1	5	ARG	Sidechain
56	B5	223	ALA	Mainchain
54	BA	1	G	Sidechain
54	BA	10	A	Sidechain
54	BA	1005	C	Sidechain
54	BA	1014	A	Sidechain
54	BA	1019	U	Sidechain
54	BA	1020	A	Sidechain
54	BA	1022	G	Sidechain
54	BA	1029	A	Sidechain
54	BA	1038	G	Sidechain
54	BA	1056	G	Sidechain
54	BA	1057	A	Sidechain
54	BA	1062	G	Sidechain
54	BA	1065	U	Sidechain
54	BA	1070	A	Sidechain
54	BA	1074	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1080	A	Sidechain
54	BA	1085	A	Sidechain
54	BA	1090	A	Sidechain
54	BA	1091	G	Sidechain
54	BA	1095	A	Sidechain
54	BA	11	C	Sidechain
54	BA	1101	U	Sidechain
54	BA	1106	G	Sidechain
54	BA	111	A	Sidechain
54	BA	1124	G	Sidechain
54	BA	1133	A	Sidechain
54	BA	1135	C	Sidechain
54	BA	1142	A	Sidechain
54	BA	1143	A	Sidechain
54	BA	1151	A	Sidechain
54	BA	1159	U	Sidechain
54	BA	1160	G	Sidechain
54	BA	1162	G	Sidechain
54	BA	1166	G	Sidechain
54	BA	1167	C	Sidechain
54	BA	1175	A	Sidechain
54	BA	1179	G	Sidechain
54	BA	1185	G	Sidechain
54	BA	1186	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	1190	G	Sidechain
54	BA	1199	U	Sidechain
54	BA	12	U	Sidechain
54	BA	1208	C	Sidechain
54	BA	1209	U	Sidechain
54	BA	1211	C	Sidechain
54	BA	1212	G	Sidechain
54	BA	123	G	Sidechain
54	BA	1231	U	Sidechain
54	BA	1234	U	Sidechain
54	BA	1236	G	Sidechain
54	BA	1237	A	Sidechain
54	BA	1238	G	Sidechain
54	BA	1239	G	Sidechain
54	BA	124	G	Sidechain
54	BA	1241	A	Sidechain
54	BA	1245	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1248	G	Sidechain
54	BA	1251	C	Sidechain
54	BA	1254	A	Sidechain
54	BA	1256	G	Sidechain
54	BA	1263	U	Sidechain
54	BA	1269	A	Sidechain
54	BA	1275	A	Sidechain
54	BA	1283	G	Sidechain
54	BA	1284	A	Sidechain
54	BA	129	C	Sidechain
54	BA	1291	C	Sidechain
54	BA	1292	G	Sidechain
54	BA	1298	C	Sidechain
54	BA	1311	G	Sidechain
54	BA	1315	C	Sidechain
54	BA	132	G	Sidechain
54	BA	1320	C	Sidechain
54	BA	1322	A	Sidechain
54	BA	1324	G	Sidechain
54	BA	1327	A	Sidechain
54	BA	1330	C	Sidechain
54	BA	1332	G	Sidechain
54	BA	1334	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1343	G	Sidechain
54	BA	1344	U	Sidechain
54	BA	1346	G	Sidechain
54	BA	1350	C	Sidechain
54	BA	1355	G	Sidechain
54	BA	1362	C	Sidechain
54	BA	1364	G	Sidechain
54	BA	1366	A	Sidechain
54	BA	1368	G	Sidechain
54	BA	1371	G	Sidechain
54	BA	1387	A	Sidechain
54	BA	1396	U	Sidechain
54	BA	142	A	Sidechain
54	BA	1420	A	Sidechain
54	BA	1424	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1427	A	Sidechain
54	BA	1433	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1434	A	Sidechain
54	BA	1435	G	Sidechain
54	BA	1436	G	Sidechain
54	BA	1439	A	Sidechain
54	BA	1444	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1446	C	Sidechain
54	BA	1448	G	Sidechain
54	BA	1451	C	Sidechain
54	BA	1457	U	Sidechain
54	BA	1460	U	Sidechain
54	BA	1462	C	Sidechain
54	BA	1463	C	Sidechain
54	BA	1465	G	Sidechain
54	BA	1469	A	Sidechain
54	BA	1475	G	Sidechain
54	BA	1477	A	Sidechain
54	BA	1478	G	Sidechain
54	BA	1485	U	Sidechain
54	BA	1487	U	Sidechain
54	BA	1492	G	Sidechain
54	BA	1497	U	Sidechain
54	BA	1499	C	Sidechain
54	BA	15	G	Sidechain
54	BA	152	A	Sidechain
54	BA	1524	G	Sidechain
54	BA	1529	G	Sidechain
54	BA	153	U	Sidechain
54	BA	1531	C	Sidechain
54	BA	1535	A	Sidechain
54	BA	1536	C	Sidechain
54	BA	1537	G	Sidechain
54	BA	154	U	Sidechain
54	BA	1540	G	Sidechain
54	BA	1546	G	Sidechain
54	BA	1554	U	Sidechain
54	BA	1555	G	Sidechain
54	BA	1556	C	Sidechain
54	BA	1559	U	Sidechain
54	BA	1561	C	Sidechain
54	BA	1562	U	Sidechain
54	BA	1570	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1573	G	Sidechain
54	BA	1580	A	Sidechain
54	BA	1581	G	Sidechain
54	BA	1582	C	Sidechain
54	BA	1583	A	Sidechain
54	BA	1591	A	Sidechain
54	BA	1593	A	Sidechain
54	BA	1594	U	Sidechain
54	BA	1601	G	Sidechain
54	BA	1604	C	Sidechain
54	BA	1607	C	Sidechain
54	BA	1609	A	Sidechain
54	BA	161	A	Sidechain
54	BA	1610	A	Sidechain
54	BA	1614	A	Sidechain
54	BA	1619	G	Sidechain
54	BA	1624	U	Sidechain
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1635	A	Sidechain
54	BA	1640	A	Sidechain
54	BA	1641	A	Sidechain
54	BA	1646	C	Sidechain
54	BA	1656	C	Sidechain
54	BA	1660	G	Sidechain
54	BA	1666	G	Sidechain
54	BA	1671	U	Sidechain
54	BA	1674	G	Sidechain
54	BA	1676	A	Sidechain
54	BA	168	G	Sidechain
54	BA	1681	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1683	U	Sidechain
54	BA	1684	G	Sidechain
54	BA	169	G	Sidechain
54	BA	1695	G	Sidechain
54	BA	1696	G	Sidechain
54	BA	17	G	Sidechain
54	BA	1706	C	Sidechain
54	BA	1709	U	Sidechain
54	BA	1711	A	Sidechain
54	BA	1719	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1723	G	Sidechain
54	BA	1727	C	Sidechain
54	BA	1729	U	Sidechain
54	BA	1734	G	Sidechain
54	BA	1737	G	Sidechain
54	BA	1738	G	Sidechain
54	BA	175	G	Sidechain
54	BA	1753	G	Sidechain
54	BA	1758	U	Sidechain
54	BA	1759	A	Sidechain
54	BA	177	G	Sidechain
54	BA	1779	U	Sidechain
54	BA	1788	C	Sidechain
54	BA	1797	G	Sidechain
54	BA	1801	A	Sidechain
54	BA	1802	A	Sidechain
54	BA	1807	G	Sidechain
54	BA	1808	A	Sidechain
54	BA	1817	G	Sidechain
54	BA	1818	U	Sidechain
54	BA	1821	A	Sidechain
54	BA	183	C	Sidechain
54	BA	1830	C	Sidechain
54	BA	1831	G	Sidechain
54	BA	1840	G	Sidechain
54	BA	1845	G	Sidechain
54	BA	1856	U	Sidechain
54	BA	1857	G	Sidechain
54	BA	1866	A	Sidechain
54	BA	1869	G	Sidechain
54	BA	187	G	Sidechain
54	BA	1871	A	Sidechain
54	BA	1879	C	Sidechain
54	BA	1884	G	Sidechain
54	BA	189	G	Sidechain
54	BA	1892	C	Sidechain
54	BA	190	A	Sidechain
54	BA	1929	G	Sidechain
54	BA	1931	U	Sidechain
54	BA	1932	A	Sidechain
54	BA	1937	A	Sidechain
54	BA	1940	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1951	U	Sidechain
54	BA	1953	A	Sidechain
54	BA	197	A	Sidechain
54	BA	1972	G	Sidechain
54	BA	1973	G	Sidechain
54	BA	1978	A	Sidechain
54	BA	1982	U	Sidechain
54	BA	1987	A	Sidechain
54	BA	1996	C	Sidechain
54	BA	2	G	Sidechain
54	BA	200	U	Sidechain
54	BA	2012	G	Sidechain
54	BA	2013	A	Sidechain
54	BA	2015	A	Sidechain
54	BA	2016	U	Sidechain
54	BA	2018	G	Sidechain
54	BA	2019	A	Sidechain
54	BA	202	U	Sidechain
54	BA	2020	A	Sidechain
54	BA	2021	C	Sidechain
54	BA	2022	U	Sidechain
54	BA	2025	C	Sidechain
54	BA	2034	U	Sidechain
54	BA	2036	C	Sidechain
54	BA	2040	G	Sidechain
54	BA	2041	U	Sidechain
54	BA	2046	G	Sidechain
54	BA	205	G	Sidechain
54	BA	2050	C	Sidechain
54	BA	2052	A	Sidechain
54	BA	2053	G	Sidechain
54	BA	2059	A	Sidechain
54	BA	206	U	Sidechain
54	BA	2064	C	Sidechain
54	BA	2066	C	Sidechain
54	BA	2067	G	Sidechain
54	BA	2073	C	Sidechain
54	BA	2075	U	Sidechain
54	BA	2076	U	Sidechain
54	BA	2077	A	Sidechain
54	BA	2078	C	Sidechain
54	BA	208	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2083	G	Sidechain
54	BA	2086	U	Sidechain
54	BA	2090	A	Sidechain
54	BA	2095	A	Sidechain
54	BA	2100	G	Sidechain
54	BA	2103	C	Sidechain
54	BA	2104	C	Sidechain
54	BA	2109	U	Sidechain
54	BA	2116	G	Sidechain
54	BA	2121	G	Sidechain
54	BA	2132	U	Sidechain
54	BA	2134	A	Sidechain
54	BA	2142	A	Sidechain
54	BA	2146	C	Sidechain
54	BA	2149	U	Sidechain
54	BA	2153	C	Sidechain
54	BA	2154	A	Sidechain
54	BA	2156	G	Sidechain
54	BA	2157	G	Sidechain
54	BA	2163	A	Sidechain
54	BA	2165	C	Sidechain
54	BA	2168	G	Sidechain
54	BA	2179	C	Sidechain
54	BA	2186	G	Sidechain
54	BA	2187	U	Sidechain
54	BA	2201	G	Sidechain
54	BA	2206	C	Sidechain
54	BA	2215	C	Sidechain
54	BA	2225	A	Sidechain
54	BA	2228	G	Sidechain
54	BA	2232	C	Sidechain
54	BA	2233	U	Sidechain
54	BA	2236	U	Sidechain
54	BA	2238	G	Sidechain
54	BA	227	A	Sidechain
54	BA	2271	G	Sidechain
54	BA	2273	A	Sidechain
54	BA	2274	A	Sidechain
54	BA	2284	A	Sidechain
54	BA	2285	C	Sidechain
54	BA	2286	G	Sidechain
54	BA	2287	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2293	G	Sidechain
54	BA	2294	G	Sidechain
54	BA	2295	C	Sidechain
54	BA	2297	A	Sidechain
54	BA	2299	U	Sidechain
54	BA	2300	C	Sidechain
54	BA	2301	C	Sidechain
54	BA	2305	U	Sidechain
54	BA	2307	G	Sidechain
54	BA	2315	G	Sidechain
54	BA	2316	G	Sidechain
54	BA	2318	G	Sidechain
54	BA	2319	G	Sidechain
54	BA	2324	U	Sidechain
54	BA	2327	A	Sidechain
54	BA	2333	A	Sidechain
54	BA	2337	G	Sidechain
54	BA	2341	G	Sidechain
54	BA	2345	G	Sidechain
54	BA	2354	C	Sidechain
54	BA	2356	U	Sidechain
54	BA	2357	G	Sidechain
54	BA	2358	A	Sidechain
54	BA	2360	G	Sidechain
54	BA	2363	G	Sidechain
54	BA	2366	A	Sidechain
54	BA	2375	G	Sidechain
54	BA	2383	G	Sidechain
54	BA	2386	A	Sidechain
54	BA	2392	A	Sidechain
54	BA	2398	U	Sidechain
54	BA	2399	G	Sidechain
54	BA	2421	G	Sidechain
54	BA	2425	A	Sidechain
54	BA	2427	C	Sidechain
54	BA	2428	G	Sidechain
54	BA	2429	G	Sidechain
54	BA	2433	A	Sidechain
54	BA	2434	A	Sidechain
54	BA	2436	G	Sidechain
54	BA	244	A	Sidechain
54	BA	2442	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2443	C	Sidechain
54	BA	2444	G	Sidechain
54	BA	2445	G	Sidechain
54	BA	2448	A	Sidechain
54	BA	2453	A	Sidechain
54	BA	2457	U	Sidechain
54	BA	2461	A	Sidechain
54	BA	247	G	Sidechain
54	BA	2475	C	Sidechain
54	BA	2478	A	Sidechain
54	BA	2488	G	Sidechain
54	BA	2495	G	Sidechain
54	BA	25	U	Sidechain
54	BA	250	G	Sidechain
54	BA	2500	U	Sidechain
54	BA	2501	C	Sidechain
54	BA	2515	C	Sidechain
54	BA	2516	A	Sidechain
54	BA	2517	C	Sidechain
54	BA	2538	C	Sidechain
54	BA	2543	G	Sidechain
54	BA	2555	U	Sidechain
54	BA	256	A	Sidechain
54	BA	2562	U	Sidechain
54	BA	257	C	Sidechain
54	BA	2573	C	Sidechain
54	BA	2574	G	Sidechain
54	BA	2582	G	Sidechain
54	BA	2595	G	Sidechain
54	BA	2596	U	Sidechain
54	BA	2598	A	Sidechain
54	BA	2601	C	Sidechain
54	BA	2602	A	Sidechain
54	BA	2609	U	Sidechain
54	BA	2615	U	Sidechain
54	BA	2621	G	Sidechain
54	BA	2627	G	Sidechain
54	BA	263	G	Sidechain
54	BA	2636	C	Sidechain
54	BA	2637	U	Sidechain
54	BA	2638	G	Sidechain
54	BA	2639	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2645	G	Sidechain
54	BA	265	A	Sidechain
54	BA	2650	U	Sidechain
54	BA	2654	A	Sidechain
54	BA	2659	G	Sidechain
54	BA	2660	A	Sidechain
54	BA	2663	G	Sidechain
54	BA	2664	G	Sidechain
54	BA	2668	G	Sidechain
54	BA	2680	U	Sidechain
54	BA	2690	U	Sidechain
54	BA	2699	C	Sidechain
54	BA	27	G	Sidechain
54	BA	2700	A	Sidechain
54	BA	2709	G	Sidechain
54	BA	271	G	Sidechain
54	BA	2712	C	Sidechain
54	BA	2716	C	Sidechain
54	BA	2721	A	Sidechain
54	BA	2729	G	Sidechain
54	BA	273	G	Sidechain
54	BA	2732	G	Sidechain
54	BA	2736	A	Sidechain
54	BA	274	C	Sidechain
54	BA	2749	A	Sidechain
54	BA	2752	C	Sidechain
54	BA	2757	A	Sidechain
54	BA	2765	A	Sidechain
54	BA	2775	G	Sidechain
54	BA	2779	U	Sidechain
54	BA	278	A	Sidechain
54	BA	2781	A	Sidechain
54	BA	2786	U	Sidechain
54	BA	28	A	Sidechain
54	BA	2801	G	Sidechain
54	BA	2802	G	Sidechain
54	BA	2805	C	Sidechain
54	BA	2809	A	Sidechain
54	BA	2816	G	Sidechain
54	BA	2818	U	Sidechain
54	BA	2819	G	Sidechain
54	BA	2834	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2838	G	Sidechain
54	BA	2839	G	Sidechain
54	BA	2852	G	Sidechain
54	BA	2856	A	Sidechain
54	BA	2857	G	Sidechain
54	BA	2862	G	Sidechain
54	BA	2863	C	Sidechain
54	BA	2866	U	Sidechain
54	BA	2868	A	Sidechain
54	BA	2873	A	Sidechain
54	BA	2875	C	Sidechain
54	BA	2885	G	Sidechain
54	BA	2888	C	Sidechain
54	BA	2891	U	Sidechain
54	BA	2893	A	Sidechain
54	BA	2894	G	Sidechain
54	BA	2895	G	Sidechain
54	BA	290	U	Sidechain
54	BA	2902	C	Sidechain
54	BA	2903	U	Sidechain
54	BA	296	U	Sidechain
54	BA	307	G	Sidechain
54	BA	308	G	Sidechain
54	BA	311	A	Sidechain
54	BA	314	C	Sidechain
54	BA	317	G	Sidechain
54	BA	321	U	Sidechain
54	BA	323	C	Sidechain
54	BA	327	G	Sidechain
54	BA	329	G	Sidechain
54	BA	333	G	Sidechain
54	BA	334	C	Sidechain
54	BA	340	A	Sidechain
54	BA	345	A	Sidechain
54	BA	347	A	Sidechain
54	BA	350	G	Sidechain
54	BA	354	A	Sidechain
54	BA	361	G	Sidechain
54	BA	362	A	Sidechain
54	BA	370	G	Sidechain
54	BA	371	A	Sidechain
54	BA	375	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	38	A	Sidechain
54	BA	383	C	Sidechain
54	BA	384	A	Sidechain
54	BA	385	C	Sidechain
54	BA	390	U	Sidechain
54	BA	392	U	Sidechain
54	BA	393	C	Sidechain
54	BA	395	U	Sidechain
54	BA	399	U	Sidechain
54	BA	40	U	Sidechain
54	BA	400	G	Sidechain
54	BA	403	U	Sidechain
54	BA	416	U	Sidechain
54	BA	417	C	Sidechain
54	BA	418	C	Sidechain
54	BA	420	C	Sidechain
54	BA	422	A	Sidechain
54	BA	427	U	Sidechain
54	BA	428	A	Sidechain
54	BA	43	G	Sidechain
54	BA	431	U	Sidechain
54	BA	434	U	Sidechain
54	BA	437	U	Sidechain
54	BA	442	G	Sidechain
54	BA	446	G	Sidechain
54	BA	448	U	Sidechain
54	BA	449	A	Sidechain
54	BA	45	G	Sidechain
54	BA	452	G	Sidechain
54	BA	453	A	Sidechain
54	BA	457	A	Sidechain
54	BA	463	G	Sidechain
54	BA	464	U	Sidechain
54	BA	476	G	Sidechain
54	BA	477	A	Sidechain
54	BA	479	A	Sidechain
54	BA	480	A	Sidechain
54	BA	484	C	Sidechain
54	BA	489	G	Sidechain
54	BA	49	A	Sidechain
54	BA	490	C	Sidechain
54	BA	492	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	493	G	Sidechain
54	BA	497	A	Sidechain
54	BA	500	G	Sidechain
54	BA	505	A	Sidechain
54	BA	507	A	Sidechain
54	BA	51	G	Sidechain
54	BA	515	A	Sidechain
54	BA	520	G	Sidechain
54	BA	528	A	Sidechain
54	BA	530	G	Sidechain
54	BA	531	C	Sidechain
54	BA	545	U	Sidechain
54	BA	546	U	Sidechain
54	BA	551	G	Sidechain
54	BA	56	A	Sidechain
54	BA	562	U	Sidechain
54	BA	563	A	Sidechain
54	BA	569	U	Sidechain
54	BA	571	U	Sidechain
54	BA	579	G	Sidechain
54	BA	58	G	Sidechain
54	BA	580	U	Sidechain
54	BA	584	C	Sidechain
54	BA	59	U	Sidechain
54	BA	602	A	Sidechain
54	BA	606	U	Sidechain
54	BA	607	U	Sidechain
54	BA	608	A	Sidechain
54	BA	611	C	Sidechain
54	BA	619	G	Sidechain
54	BA	621	A	Sidechain
54	BA	626	A	Sidechain
54	BA	628	G	Sidechain
54	BA	63	A	Sidechain
54	BA	630	G	Sidechain
54	BA	631	A	Sidechain
54	BA	637	A	Sidechain
54	BA	642	U	Sidechain
54	BA	644	A	Sidechain
54	BA	646	U	Sidechain
54	BA	647	G	Sidechain
54	BA	65	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	670	A	Sidechain
54	BA	671	C	Sidechain
54	BA	674	G	Sidechain
54	BA	675	A	Sidechain
54	BA	68	G	Sidechain
54	BA	69	C	Sidechain
54	BA	691	C	Sidechain
54	BA	698	C	Sidechain
54	BA	703	U	Sidechain
54	BA	709	U	Sidechain
54	BA	711	G	Sidechain
54	BA	714	U	Sidechain
54	BA	717	C	Sidechain
54	BA	720	U	Sidechain
54	BA	725	G	Sidechain
54	BA	726	G	Sidechain
54	BA	727	A	Sidechain
54	BA	728	G	Sidechain
54	BA	730	A	Sidechain
54	BA	734	A	Sidechain
54	BA	741	U	Sidechain
54	BA	744	U	Sidechain
54	BA	760	G	Sidechain
54	BA	763	G	Sidechain
54	BA	767	U	Sidechain
54	BA	774	G	Sidechain
54	BA	775	G	Sidechain
54	BA	784	G	Sidechain
54	BA	793	A	Sidechain
54	BA	800	A	Sidechain
54	BA	801	G	Sidechain
54	BA	803	U	Sidechain
54	BA	804	A	Sidechain
54	BA	805	G	Sidechain
54	BA	829	A	Sidechain
54	BA	833	A	Sidechain
54	BA	835	C	Sidechain
54	BA	838	C	Sidechain
54	BA	84	A	Sidechain
54	BA	840	C	Sidechain
54	BA	841	G	Sidechain
54	BA	844	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	849	A	Sidechain
54	BA	852	U	Sidechain
54	BA	858	G	Sidechain
54	BA	86	G	Sidechain
54	BA	861	A	Sidechain
54	BA	864	G	Sidechain
54	BA	873	C	Sidechain
54	BA	874	G	Sidechain
54	BA	875	G	Sidechain
54	BA	879	G	Sidechain
54	BA	882	G	Sidechain
54	BA	891	G	Sidechain
54	BA	893	C	Sidechain
54	BA	895	U	Sidechain
54	BA	897	C	Sidechain
54	BA	912	C	Sidechain
54	BA	914	G	Sidechain
54	BA	919	U	Sidechain
54	BA	920	A	Sidechain
54	BA	923	G	Sidechain
54	BA	927	A	Sidechain
54	BA	930	G	Sidechain
54	BA	932	U	Sidechain
54	BA	933	A	Sidechain
54	BA	934	U	Sidechain
54	BA	936	A	Sidechain
54	BA	941	A	Sidechain
54	BA	946	C	Sidechain
54	BA	947	A	Sidechain
54	BA	949	G	Sidechain
54	BA	950	G	Sidechain
54	BA	952	G	Sidechain
54	BA	954	G	Sidechain
54	BA	956	G	Sidechain
54	BA	968	C	Sidechain
54	BA	969	G	Sidechain
54	BA	979	A	Sidechain
54	BA	980	A	Sidechain
54	BA	981	A	Sidechain
54	BA	982	C	Sidechain
54	BA	983	A	Sidechain
54	BA	989	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	99	U	Sidechain
54	BA	993	G	Sidechain
55	BB	105	G	Sidechain
55	BB	106	G	Sidechain
55	BB	107	G	Sidechain
55	BB	112	G	Sidechain
55	BB	13	G	Sidechain
55	BB	26	C	Sidechain
55	BB	32	U	Sidechain
55	BB	38	C	Sidechain
55	BB	41	G	Sidechain
55	BB	47	C	Sidechain
55	BB	48	U	Sidechain
55	BB	54	G	Sidechain
55	BB	57	A	Sidechain
55	BB	61	G	Sidechain
55	BB	62	C	Sidechain
55	BB	64	G	Sidechain
55	BB	75	G	Sidechain
55	BB	83	G	Sidechain
55	BB	96	G	Sidechain
38	BP	98	TYR	Sidechain

5.2 Too-close contacts

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	16520	3	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	841	0	0
25	BC	2083	0	2157	2	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	0	0
31	BI	1032	0	1088	1	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	1	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	0	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	1	0
48	BZ	449	0	491	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	BA	62317	0	31298	6	0
55	BB	2504	0	1269	0	0
56	B5	1658	0	1751	1	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99612	18	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 (18) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AL:69:GLU:H	11:AL:106:VAL:HG13	1.75	0.52
54:BA:1349:C:N4	54:BA:1383:A:H61	2.11	0.49
54:BA:1324:G:H3'	54:BA:1325:U:H5''	1.97	0.46
4:AE:88:HIS:CG	4:AE:89:THR:H	2.32	0.45
33:BK:111:LYS:HE3	33:BK:112:PHE:CZ	2.52	0.45
47:BY:41:HIS:CG	54:BA:96:C:H4'	2.51	0.45
21:AA:1191:A:C8	21:AA:1191:A:C5'	3.01	0.44
54:BA:441:U:H2'	54:BA:442:G:C8	2.52	0.44
56:B5:29:LEU:C	56:B5:29:LEU:HD13	2.43	0.44
25:BC:95:TYR:C	25:BC:97:ASP:H	2.26	0.43
11:AL:15:VAL:HG21	11:AL:17:LYS:HE3	2.01	0.43
11:AL:49:ARG:CZ	21:AA:523:A:H61	2.31	0.43
3:AD:191:SER:HA	3:AD:192:ALA:HB3	2.02	0.41
31:BI:27:LEU:HD12	31:BI:28:GLY:N	2.36	0.41
34:BL:13:LYS:HE3	54:BA:661:A:H4'	2.03	0.41
54:BA:1364:G:H2'	54:BA:1365:A:H5'	2.03	0.41
21:AA:1191:A:C8	21:AA:1191:A:H5'	2.57	0.40
25:BC:239:PHE:CE2	25:BC:241:LYS:HE3	2.56	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%)	201 (92%)	15 (7%)	2 (1%)	14	51
2	AC	205/208 (99%)	190 (93%)	9 (4%)	6 (3%)	3	23
3	AD	203/206 (98%)	191 (94%)	9 (4%)	3 (2%)	8	40
4	AE	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	6	31
5	AF	99/101 (98%)	87 (88%)	7 (7%)	5 (5%)	1	15
6	AG	150/152 (99%)	136 (91%)	8 (5%)	6 (4%)	2	18
7	AH	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	16	54
8	AI	126/128 (98%)	110 (87%)	15 (12%)	1 (1%)	16	54
9	AJ	98/100 (98%)	86 (88%)	8 (8%)	4 (4%)	2	18
10	AK	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	14	51
11	AL	121/124 (98%)	110 (91%)	9 (7%)	2 (2%)	7	36
12	AM	112/115 (97%)	92 (82%)	16 (14%)	4 (4%)	2	20
13	AN	98/101 (97%)	92 (94%)	4 (4%)	2 (2%)	6	31
14	AO	86/89 (97%)	76 (88%)	5 (6%)	5 (6%)	1	14
15	AP	79/81 (98%)	69 (87%)	6 (8%)	4 (5%)	1	15
16	AQ	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	6	34
18	AS	79/81 (98%)	69 (87%)	7 (9%)	3 (4%)	2	19
19	AT	84/86 (98%)	80 (95%)	3 (4%)	1 (1%)	10	44
20	AU	51/53 (96%)	38 (74%)	9 (18%)	4 (8%)	1	10
25	BC	270/273 (99%)	235 (87%)	27 (10%)	8 (3%)	3	23
26	BD	207/209 (99%)	185 (89%)	16 (8%)	6 (3%)	3	23
27	BE	199/201 (99%)	180 (90%)	11 (6%)	8 (4%)	2	18
28	BF	176/179 (98%)	157 (89%)	13 (7%)	6 (3%)	3	21
29	BG	174/177 (98%)	155 (89%)	18 (10%)	1 (1%)	21	59
30	BH	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	6	31
31	BI	139/142 (98%)	129 (93%)	9 (6%)	1 (1%)	18	56
32	BJ	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	3	23
33	BK	121/123 (98%)	103 (85%)	13 (11%)	5 (4%)	2	18
34	BL	141/144 (98%)	109 (77%)	24 (17%)	8 (6%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BM	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	8	40
36	BN	119/121 (98%)	105 (88%)	13 (11%)	1 (1%)	16	54
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	14	51
38	BP	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	2	20
39	BQ	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	4	25
40	BR	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	6	31
41	BS	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	6	32
42	BT	92/94 (98%)	79 (86%)	9 (10%)	4 (4%)	2	17
43	BU	101/104 (97%)	87 (86%)	9 (9%)	5 (5%)	1	16
44	BV	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
45	BW	78/80 (98%)	54 (69%)	15 (19%)	9 (12%)	0	5
46	BX	75/79 (95%)	64 (85%)	8 (11%)	3 (4%)	2	18
47	BY	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	7	38
48	BZ	56/59 (95%)	52 (93%)	1 (2%)	3 (5%)	1	15
49	B0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	1	14
50	B1	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
51	B2	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5	28
52	B3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	3	21
53	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	24
56	B5	221/234 (94%)	210 (95%)	8 (4%)	3 (1%)	9	40
All	All	5876/6008 (98%)	5259 (90%)	459 (8%)	158 (3%)	6	25

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AM	107	THR
14	AO	45	HIS
20	AU	9	GLU
20	AU	37	TYR
25	BC	181	ARG
25	BC	191	LEU
26	BD	2	ILE
27	BE	70	SER
28	BF	136	ILE
29	BG	112	VAL

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Mol	Chain	Res	Type
34	BL	101	ILE
43	BU	70	ALA
45	BW	18	LYS
45	BW	23	LYS
48	BZ	30	ARG
49	B0	5	ASN
49	B0	54	ILE
2	AC	14	VAL
4	AE	105	ILE
5	AF	6	ILE
5	AF	63	ASN
6	AG	3	ARG
9	AJ	57	VAL
13	AN	99	ALA
14	AO	48	ASP
15	AP	17	TYR
25	BC	36	ASN
25	BC	187	CYS
26	BD	60	VAL
27	BE	188	MET
30	BH	10	ALA
31	BI	93	ASN
33	BK	92	GLU
33	BK	103	VAL
34	BL	29	LYS
34	BL	46	VAL
36	BN	102	PHE
41	BS	74	ILE
41	BS	90	LYS
42	BT	63	VAL
42	BT	91	GLN
43	BU	43	LYS
51	B2	4	THR
52	B3	3	ILE
56	B5	46	VAL
56	B5	213	SER
1	AB	18	GLN
1	AB	21	TYR
2	AC	171	ARG
3	AD	47	LEU
4	AE	25	LYS
5	AF	90	MET

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Mol	Chain	Res	Type
5	AF	93	LYS
6	AG	114	SER
18	AS	6	LYS
19	AT	3	ILE
26	BD	43	ASP
27	BE	80	SER
27	BE	120	VAL
28	BF	77	LYS
30	BH	121	VAL
32	BJ	15	TRP
32	BJ	80	HIS
32	BJ	128	ASN
33	BK	46	ALA
34	BL	36	LYS
39	BQ	4	LYS
39	BQ	91	ARG
40	BR	82	HIS
42	BT	2	ILE
42	BT	11	LEU
45	BW	10	ARG
45	BW	19	ARG
45	BW	20	LEU
45	BW	56	HIS
46	BX	27	ARG
46	BX	32	LEU
48	BZ	9	THR
52	B3	46	LYS
3	AD	187	ARG
4	AE	43	GLY
6	AG	43	TYR
6	AG	134	VAL
7	AH	105	THR
9	AJ	42	LEU
10	AK	16	SER
12	AM	4	ALA
12	AM	42	VAL
13	AN	60	GLN
14	AO	18	ALA
14	AO	43	ALA
15	AP	24	SER
15	AP	49	GLY
15	AP	63	GLN

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Mol	Chain	Res	Type
18	AS	45	GLY
20	AU	12	ASP
20	AU	52	VAL
25	BC	96	LYS
25	BC	161	VAL
25	BC	196	ASN
26	BD	119	ALA
27	BE	96	VAL
28	BF	46	LYS
32	BJ	53	TYR
34	BL	15	ALA
40	BR	53	PHE
43	BU	45	GLN
43	BU	59	GLU
45	BW	11	ASN
45	BW	16	GLU
49	B0	27	LEU
56	B5	91	GLY
2	AC	3	LYS
3	AD	192	ALA
5	AF	92	THR
6	AG	7	GLY
9	AJ	68	ARG
11	AL	78	VAL
14	AO	23	SER
25	BC	153	LEU
26	BD	75	ALA
27	BE	165	HIS
28	BF	120	SER
33	BK	2	ILE
34	BL	30	THR
35	BM	6	ARG
35	BM	20	LEU
38	BP	26	GLU
38	BP	69	VAL
38	BP	79	VAL
39	BQ	87	VAL
45	BW	35	ILE
47	BY	46	VAL
11	AL	33	CYS
26	BD	134	HIS
28	BF	41	GLU

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Mol	Chain	Res	Type
34	BL	5	THR
34	BL	55	MET
37	BO	23	ALA
46	BX	34	SER
48	BZ	31	ILE
53	B4	37	GLN
2	AC	4	VAL
6	AG	81	GLY
12	AM	23	GLY
17	AR	20	ILE
18	AS	39	ILE
30	BH	130	VAL
38	BP	20	ARG
2	AC	144	GLY
28	BF	103	ILE
9	AJ	41	PRO
43	BU	12	VAL
2	AC	206	ILE
8	AI	57	VAL
27	BE	83	VAL
33	BK	47	ILE
27	BE	31	VAL

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%)	177 (98%)	3 (2%)	53	69
2	AC	170/171 (99%)	169 (99%)	1 (1%)	78	83
3	AD	172/173 (99%)	171 (99%)	1 (1%)	78	83
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	85 (98%)	2 (2%)	44	64
6	AG	123/123 (100%)	121 (98%)	2 (2%)	55	70
7	AH	104/105 (99%)	102 (98%)	2 (2%)	50	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AI	105/105 (100%)	104 (99%)	1 (1%)	68	78
9	AJ	86/86 (100%)	85 (99%)	1 (1%)	63	75
10	AK	90/90 (100%)	87 (97%)	3 (3%)	33	55
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	82 (99%)	1 (1%)	63	75
14	AO	76/77 (99%)	75 (99%)	1 (1%)	61	74
15	AP	65/65 (100%)	64 (98%)	1 (2%)	57	72
16	AQ	74/74 (100%)	73 (99%)	1 (1%)	59	72
17	AR	48/48 (100%)	46 (96%)	2 (4%)	26	48
18	AS	70/70 (100%)	69 (99%)	1 (1%)	59	72
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%)	212 (98%)	4 (2%)	50	67
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%)	115 (99%)	1 (1%)	70	79
33	BK	103/103 (100%)	100 (97%)	3 (3%)	37	58
34	BL	102/103 (99%)	102 (100%)	0	100	100
35	BM	109/109 (100%)	107 (98%)	2 (2%)	51	68
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%)	97 (98%)	2 (2%)	48	66
39	BQ	89/90 (99%)	89 (100%)	0	100	100
40	BR	84/84 (100%)	83 (99%)	1 (1%)	63	75
41	BS	93/93 (100%)	92 (99%)	1 (1%)	65	76
42	BT	80/80 (100%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BU	83/84 (99%)	82 (99%)	1 (1%)	63	75
44	BV	78/78 (100%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	56 (95%)	3 (5%)	21	42
46	BX	67/68 (98%)	66 (98%)	1 (2%)	57	72
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	47 (98%)	1 (2%)	47	65
49	B0	47/48 (98%)	47 (100%)	0	100	100
50	B1	45/45 (100%)	43 (96%)	2 (4%)	25	47
51	B2	38/38 (100%)	37 (97%)	1 (3%)	40	62
52	B3	51/52 (98%)	48 (94%)	3 (6%)	18	39
53	B4	34/34 (100%)	33 (97%)	1 (3%)	37	58
56	B5	173/181 (96%)	172 (99%)	1 (1%)	78	83
All	All	4842/4870 (99%)	4780 (99%)	62 (1%)	59	74

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	71	THR
1	AB	88	GLN
1	AB	189	ASN
2	AC	66	THR
3	AD	8	LEU
5	AF	18	VAL
5	AF	42	TRP
6	AG	2	ARG
6	AG	3	ARG
7	AH	54	THR
7	AH	128	VAL
8	AI	40	ARG
9	AJ	49	PHE
10	AK	35	ASP
10	AK	118	ASN
10	AK	127	ARG
13	AN	101	TRP
14	AO	24	THR
15	AP	1	MET
16	AQ	19	SER
17	AR	30	ASN

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Mol	Chain	Res	Type
17	AR	46	THR
18	AS	13	HIS
20	AU	13	VAL
20	AU	52	VAL
25	BC	179	GLU
25	BC	184	GLU
25	BC	222	THR
25	BC	227	VAL
26	BD	2	ILE
26	BD	164	GLN
27	BE	79	ARG
28	BF	124	ARG
29	BG	71	LEU
29	BG	154	GLU
30	BH	82	SER
32	BJ	130	HIS
33	BK	70	ARG
33	BK	97	THR
33	BK	105	ARG
35	BM	7	THR
35	BM	126	ILE
36	BN	98	LEU
37	BO	31	THR
38	BP	23	ASP
38	BP	50	ARG
40	BR	19	THR
41	BS	1	MET
43	BU	44	HIS
45	BW	9	THR
45	BW	11	ASN
45	BW	80	SER
46	BX	32	LEU
48	BZ	31	ILE
50	B1	20	TYR
50	B1	45	HIS
51	B2	4	THR
52	B3	23	HIS
52	B3	27	ASN
52	B3	48	MET
53	B4	32	LYS
56	B5	165	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61)

such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	57	ASN
1	AB	108	GLN
1	AB	189	ASN
2	AC	31	ASN
2	AC	40	GLN
2	AC	68	HIS
2	AC	189	HIS
3	AD	35	GLN
3	AD	197	HIS
4	AE	60	GLN
4	AE	81	GLN
4	AE	121	ASN
5	AF	63	ASN
6	AG	129	ASN
8	AI	4	GLN
8	AI	74	GLN
9	AJ	70	HIS
12	AM	51	GLN
12	AM	90	HIS
18	AS	13	HIS
18	AS	55	GLN
19	AT	60	GLN
25	BC	14	HIS
25	BC	89	ASN
26	BD	148	GLN
27	BE	163	ASN
27	BE	165	HIS
27	BE	195	GLN
29	BG	44	HIS
30	BH	145	ASN
31	BI	11	GLN
31	BI	30	GLN
32	BJ	76	HIS
32	BJ	77	HIS
33	BK	5	GLN
33	BK	88	ASN
34	BL	38	GLN
34	BL	93	ASN
37	BO	100	HIS
37	BO	104	GLN
38	BP	6	GLN
38	BP	11	GLN

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Mol	Chain	Res	Type
39	BQ	58	GLN
39	BQ	65	ASN
43	BU	45	GLN
43	BU	98	ASN
44	BV	87	GLN
45	BW	39	GLN
45	BW	56	HIS
46	BX	5	GLN
46	BX	16	ASN
46	BX	31	ASN
46	BX	35	HIS
47	BY	39	GLN
48	BZ	8	GLN
49	B0	3	GLN
50	B1	18	HIS
51	B2	13	ASN
52	B3	42	HIS
56	B5	83	ASN
56	B5	168	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	273 (17%)	92 (6%)
22	A1	75/76 (98%)	15 (20%)	2 (2%)
23	A2	14/15 (93%)	7 (50%)	3 (21%)
24	A3	77/77 (100%)	22 (28%)	8 (10%)
54	BA	2902/2903 (99%)	498 (17%)	130 (4%)
55	BB	116/118 (98%)	17 (14%)	3 (2%)
All	All	4713/4722 (99%)	832 (17%)	238 (5%)

All (832) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	10	A
21	AA	13	U
21	AA	14	U
21	AA	25	C

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Mol	Chain	Res	Type
21	AA	31	G
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	51	A
21	AA	52	C
21	AA	54	C
21	AA	55	A
21	AA	84	U
21	AA	85	U
21	AA	86	G
21	AA	87	C
21	AA	109	A
21	AA	120	A
21	AA	121	U
21	AA	122	G
21	AA	131	A
21	AA	144	G
21	AA	149	A
21	AA	153	C
21	AA	184	G
21	AA	185	U
21	AA	188	C
21	AA	189	A
21	AA	190	A
21	AA	198	G
21	AA	240	G
21	AA	244	U
21	AA	245	U
21	AA	247	G
21	AA	251	G
21	AA	252	U
21	AA	253	A
21	AA	266	G
21	AA	274	A
21	AA	275	G
21	AA	281	G
21	AA	287	U
21	AA	289	G
21	AA	293	G
21	AA	298	A

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Mol	Chain	Res	Type
21	AA	299	G
21	AA	309	A
21	AA	310	G
21	AA	317	U
21	AA	328	C
21	AA	329	A
21	AA	332	G
21	AA	344	A
21	AA	346	G
21	AA	347	G
21	AA	350	G
21	AA	351	G
21	AA	352	C
21	AA	354	G
21	AA	362	G
21	AA	363	A
21	AA	367	U
21	AA	368	U
21	AA	369	G
21	AA	373	A
21	AA	381	C
21	AA	384	G
21	AA	389	A
21	AA	397	A
21	AA	398	U
21	AA	406	G
21	AA	408	A
21	AA	409	U
21	AA	412	A
21	AA	416	G
21	AA	420	U
21	AA	421	U
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	461	A
21	AA	462	G
21	AA	463	U
21	AA	464	U
21	AA	466	A
21	AA	467	U
21	AA	468	A

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Mol	Chain	Res	Type
21	AA	469	C
21	AA	474	G
21	AA	477	C
21	AA	484	G
21	AA	496	A
21	AA	497	G
21	AA	509	A
21	AA	511	C
21	AA	525	C
21	AA	538	G
21	AA	539	A
21	AA	547	A
21	AA	559	A
21	AA	562	U
21	AA	563	A
21	AA	564	C
21	AA	565	U
21	AA	566	G
21	AA	567	G
21	AA	572	A
21	AA	573	A
21	AA	575	G
21	AA	576	C
21	AA	577	G
21	AA	607	A
21	AA	608	A
21	AA	609	A
21	AA	610	U
21	AA	620	C
21	AA	648	A
21	AA	649	A
21	AA	653	U
21	AA	665	A
21	AA	671	G
21	AA	672	U
21	AA	700	G
21	AA	724	G
21	AA	754	C
21	AA	755	G
21	AA	777	A
21	AA	778	G
21	AA	779	C

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Mol	Chain	Res	Type
21	AA	812	G
21	AA	817	C
21	AA	819	A
21	AA	826	C
21	AA	827	U
21	AA	841	C
21	AA	843	U
21	AA	844	G
21	AA	845	A
21	AA	846	G
21	AA	847	G
21	AA	877	G
21	AA	884	U
21	AA	885	G
21	AA	887	G
21	AA	890	G
21	AA	891	U
21	AA	914	A
21	AA	920	U
21	AA	931	C
21	AA	934	C
21	AA	935	A
21	AA	939	G
21	AA	958	A
21	AA	959	A
21	AA	960	U
21	AA	966	G
21	AA	967	C
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	972	C
21	AA	974	A
21	AA	975	A
21	AA	976	G
21	AA	978	A
21	AA	979	C
21	AA	983	A
21	AA	984	C
21	AA	992	U
21	AA	993	G
21	AA	994	A

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Mol	Chain	Res	Type
21	AA	1004	A
21	AA	1017	U
21	AA	1020	G
21	AA	1026	G
21	AA	1027	C
21	AA	1030	U
21	AA	1031	C
21	AA	1032	G
21	AA	1035	A
21	AA	1045	C
21	AA	1049	U
21	AA	1050	G
21	AA	1056	U
21	AA	1065	U
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1126	U
21	AA	1130	A
21	AA	1137	C
21	AA	1139	G
21	AA	1140	C
21	AA	1146	A
21	AA	1147	C
21	AA	1151	A
21	AA	1152	A
21	AA	1156	G
21	AA	1157	A
21	AA	1159	U
21	AA	1160	G
21	AA	1167	A
21	AA	1169	A
21	AA	1178	G
21	AA	1179	A
21	AA	1181	G
21	AA	1183	U
21	AA	1184	G
21	AA	1189	U
21	AA	1190	G
21	AA	1191	A
21	AA	1196	A

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Mol	Chain	Res	Type
21	AA	1201	A
21	AA	1202	U
21	AA	1212	U
21	AA	1213	A
21	AA	1218	C
21	AA	1222	G
21	AA	1224	U
21	AA	1225	A
21	AA	1227	A
21	AA	1228	C
21	AA	1231	G
21	AA	1238	A
21	AA	1256	A
21	AA	1257	A
21	AA	1279	G
21	AA	1285	A
21	AA	1286	U
21	AA	1298	U
21	AA	1299	A
21	AA	1300	G
21	AA	1301	U
21	AA	1303	C
21	AA	1305	G
21	AA	1317	C
21	AA	1318	A
21	AA	1319	A
21	AA	1332	A
21	AA	1335	U
21	AA	1336	C
21	AA	1337	G
21	AA	1340	A
21	AA	1363	A
21	AA	1364	U
21	AA	1365	G
21	AA	1379	G
21	AA	1381	U
21	AA	1382	C
21	AA	1398	A
21	AA	1411	C
21	AA	1419	G
21	AA	1426	G
21	AA	1432	G

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Mol	Chain	Res	Type
21	AA	1440	U
21	AA	1441	A
21	AA	1447	A
21	AA	1452	C
21	AA	1453	G
21	AA	1492	A
21	AA	1493	A
21	AA	1494	G
21	AA	1506	U
21	AA	1517	G
21	AA	1523	G
21	AA	1524	C
21	AA	1529	G
21	AA	1530	G
22	A1	9	A
22	A1	16	C
22	A1	17	U
22	A1	20	G
22	A1	21	A
22	A1	34	CM0
22	A1	35	A
22	A1	46	7MG
22	A1	48	C
22	A1	59	U
22	A1	72	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	87	U
23	A2	88	U
23	A2	90	U
23	A2	91	A
23	A2	92	U
24	A3	2	G
24	A3	9	G
24	A3	20	G
24	A3	21	H2U
24	A3	22	A
24	A3	23	G

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Mol	Chain	Res	Type
24	A3	30	G
24	A3	32	G
24	A3	33	OMC
24	A3	40	C
24	A3	48	U
24	A3	49	C
24	A3	50	G
24	A3	51	U
24	A3	58	A
24	A3	59	A
24	A3	61	U
24	A3	62	C
24	A3	71	G
24	A3	72	C
24	A3	76	C
24	A3	77	A
54	BA	6	A
54	BA	12	U
54	BA	17	G
54	BA	20	C
54	BA	29	U
54	BA	30	G
54	BA	34	U
54	BA	38	A
54	BA	60	G
54	BA	61	C
54	BA	64	A
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	99	U
54	BA	100	U
54	BA	101	A
54	BA	102	U
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	125	A
54	BA	126	A
54	BA	139	U

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Mol	Chain	Res	Type
54	BA	145	C
54	BA	147	C
54	BA	149	A
54	BA	150	U
54	BA	155	A
54	BA	172	A
54	BA	196	A
54	BA	199	A
54	BA	200	U
54	BA	205	G
54	BA	216	A
54	BA	222	A
54	BA	224	U
54	BA	248	G
54	BA	249	C
54	BA	265	A
54	BA	266	G
54	BA	271	G
54	BA	272	A
54	BA	277	G
54	BA	278	A
54	BA	279	A
54	BA	297	G
54	BA	316	C
54	BA	323	C
54	BA	324	A
54	BA	327	G
54	BA	330	A
54	BA	331	C
54	BA	332	A
54	BA	335	C
54	BA	338	G
54	BA	370	G
54	BA	372	G
54	BA	373	U
54	BA	374	A
54	BA	377	G
54	BA	378	C
54	BA	386	G
54	BA	387	U
54	BA	390	U
54	BA	404	A

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Mol	Chain	Res	Type
54	BA	428	A
54	BA	451	U
54	BA	452	G
54	BA	454	A
54	BA	455	C
54	BA	457	A
54	BA	458	G
54	BA	459	U
54	BA	473	G
54	BA	481	G
54	BA	484	C
54	BA	490	C
54	BA	504	A
54	BA	505	A
54	BA	509	C
54	BA	510	C
54	BA	528	A
54	BA	529	A
54	BA	530	G
54	BA	532	A
54	BA	533	G
54	BA	546	U
54	BA	547	A
54	BA	548	G
54	BA	563	A
54	BA	569	U
54	BA	570	G
54	BA	573	U
54	BA	574	A
54	BA	575	A
54	BA	587	C
54	BA	590	A
54	BA	603	A
54	BA	614	A
54	BA	615	U
54	BA	617	G
54	BA	620	G
54	BA	627	A
54	BA	630	G
54	BA	637	A
54	BA	643	A
54	BA	645	C

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Mol	Chain	Res	Type
54	BA	655	A
54	BA	671	C
54	BA	672	C
54	BA	686	U
54	BA	716	A
54	BA	717	C
54	BA	724	U
54	BA	730	A
54	BA	748	G
54	BA	751	A
54	BA	752	A
54	BA	763	G
54	BA	764	A
54	BA	765	C
54	BA	775	G
54	BA	782	A
54	BA	784	G
54	BA	791	C
54	BA	792	A
54	BA	805	G
54	BA	812	C
54	BA	815	C
54	BA	819	A
54	BA	827	U
54	BA	846	U
54	BA	847	U
54	BA	858	G
54	BA	860	U
54	BA	866	A
54	BA	867	C
54	BA	871	U
54	BA	885	C
54	BA	889	C
54	BA	890	C
54	BA	910	A
54	BA	915	C
54	BA	931	U
54	BA	932	U
54	BA	934	U
54	BA	936	A
54	BA	938	G
54	BA	945	A

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Mol	Chain	Res	Type
54	BA	946	C
54	BA	958	U
54	BA	959	A
54	BA	961	C
54	BA	974	G
54	BA	980	A
54	BA	981	A
54	BA	982	C
54	BA	983	A
54	BA	1005	C
54	BA	1006	C
54	BA	1008	A
54	BA	1009	A
54	BA	1011	G
54	BA	1012	U
54	BA	1019	U
54	BA	1020	A
54	BA	1022	G
54	BA	1024	G
54	BA	1025	G
54	BA	1026	G
54	BA	1033	U
54	BA	1046	A
54	BA	1047	G
54	BA	1063	G
54	BA	1067	A
54	BA	1068	G
54	BA	1070	A
54	BA	1073	A
54	BA	1076	C
54	BA	1087	G
54	BA	1088	A
54	BA	1092	C
54	BA	1094	U
54	BA	1095	A
54	BA	1112	G
54	BA	1123	C
54	BA	1124	G
54	BA	1129	A
54	BA	1131	G
54	BA	1132	U
54	BA	1133	A

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Mol	Chain	Res	Type
54	BA	1135	C
54	BA	1141	U
54	BA	1142	A
54	BA	1144	A
54	BA	1155	A
54	BA	1175	A
54	BA	1176	U
54	BA	1187	G
54	BA	1188	U
54	BA	1204	A
54	BA	1205	A
54	BA	1211	C
54	BA	1212	G
54	BA	1229	C
54	BA	1236	G
54	BA	1237	A
54	BA	1238	G
54	BA	1240	U
54	BA	1241	A
54	BA	1247	A
54	BA	1252	G
54	BA	1253	A
54	BA	1254	A
54	BA	1266	G
54	BA	1269	A
54	BA	1288	G
54	BA	1289	C
54	BA	1290	C
54	BA	1300	G
54	BA	1301	A
54	BA	1311	G
54	BA	1312	U
54	BA	1313	U
54	BA	1314	C
54	BA	1325	U
54	BA	1329	U
54	BA	1330	C
54	BA	1332	G
54	BA	1337	G
54	BA	1341	G
54	BA	1343	G
54	BA	1344	U

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Mol	Chain	Res	Type
54	BA	1365	A
54	BA	1368	G
54	BA	1374	G
54	BA	1378	A
54	BA	1379	U
54	BA	1380	G
54	BA	1383	A
54	BA	1385	A
54	BA	1391	U
54	BA	1393	A
54	BA	1396	U
54	BA	1416	G
54	BA	1419	A
54	BA	1420	A
54	BA	1421	G
54	BA	1422	G
54	BA	1427	A
54	BA	1428	C
54	BA	1429	G
54	BA	1434	A
54	BA	1435	G
54	BA	1440	U
54	BA	1452	G
54	BA	1453	A
54	BA	1454	C
54	BA	1455	G
54	BA	1457	U
54	BA	1458	U
54	BA	1459	G
54	BA	1482	G
54	BA	1490	A
54	BA	1491	G
54	BA	1495	A
54	BA	1510	G
54	BA	1535	A
54	BA	1536	C
54	BA	1537	G
54	BA	1538	G
54	BA	1539	U
54	BA	1540	G
54	BA	1558	C
54	BA	1559	U

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Mol	Chain	Res	Type
54	BA	1568	G
54	BA	1569	A
54	BA	1597	A
54	BA	1598	A
54	BA	1607	C
54	BA	1608	A
54	BA	1610	A
54	BA	1611	C
54	BA	1618	A
54	BA	1634	A
54	BA	1635	A
54	BA	1639	C
54	BA	1647	U
54	BA	1648	U
54	BA	1656	C
54	BA	1664	A
54	BA	1668	A
54	BA	1669	A
54	BA	1674	G
54	BA	1675	C
54	BA	1701	A
54	BA	1707	G
54	BA	1711	A
54	BA	1729	U
54	BA	1730	C
54	BA	1733	G
54	BA	1734	G
54	BA	1757	A
54	BA	1758	U
54	BA	1760	C
54	BA	1761	C
54	BA	1764	C
54	BA	1773	A
54	BA	1780	A
54	BA	1784	A
54	BA	1799	G
54	BA	1800	C
54	BA	1802	A
54	BA	1808	A
54	BA	1810	A
54	BA	1815	A
54	BA	1816	C

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Mol	Chain	Res	Type
54	BA	1847	A
54	BA	1848	A
54	BA	1900	A
54	BA	1901	A
54	BA	1913	A
54	BA	1914	C
54	BA	1919	A
54	BA	1937	A
54	BA	1938	A
54	BA	1939	U
54	BA	1940	U
54	BA	1943	U
54	BA	1944	U
54	BA	1945	G
54	BA	1952	A
54	BA	1955	U
54	BA	1956	U
54	BA	1964	G
54	BA	1967	C
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1982	U
54	BA	1993	U
54	BA	1996	C
54	BA	2002	G
54	BA	2006	C
54	BA	2017	U
54	BA	2018	G
54	BA	2023	C
54	BA	2031	A
54	BA	2032	G
54	BA	2034	U
54	BA	2043	C
54	BA	2051	A
54	BA	2055	C
54	BA	2060	A
54	BA	2061	G
54	BA	2062	A
54	BA	2068	U
54	BA	2069	G
54	BA	2092	U

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Mol	Chain	Res	Type
54	BA	2093	G
54	BA	2113	U
54	BA	2126	A
54	BA	2127	G
54	BA	2131	U
54	BA	2132	U
54	BA	2138	G
54	BA	2155	U
54	BA	2159	G
54	BA	2163	A
54	BA	2164	C
54	BA	2172	U
54	BA	2173	A
54	BA	2174	C
54	BA	2198	A
54	BA	2203	U
54	BA	2211	A
54	BA	2212	A
54	BA	2213	U
54	BA	2214	C
54	BA	2216	G
54	BA	2227	A
54	BA	2232	C
54	BA	2238	G
54	BA	2251	G
54	BA	2262	U
54	BA	2266	A
54	BA	2267	A
54	BA	2268	A
54	BA	2275	C
54	BA	2276	G
54	BA	2283	C
54	BA	2307	G
54	BA	2308	G
54	BA	2309	A
54	BA	2312	U
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2326	C
54	BA	2333	A

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Mol	Chain	Res	Type
54	BA	2334	U
54	BA	2339	C
54	BA	2346	A
54	BA	2347	C
54	BA	2350	C
54	BA	2353	G
54	BA	2379	G
54	BA	2383	G
54	BA	2385	C
54	BA	2388	A
54	BA	2403	C
54	BA	2406	A
54	BA	2407	A
54	BA	2409	G
54	BA	2422	C
54	BA	2424	C
54	BA	2425	A
54	BA	2428	G
54	BA	2431	U
54	BA	2441	U
54	BA	2447	G
54	BA	2448	A
54	BA	2450	A
54	BA	2451	A
54	BA	2474	U
54	BA	2475	C
54	BA	2476	A
54	BA	2491	U
54	BA	2498	C
54	BA	2499	C
54	BA	2500	U
54	BA	2501	C
54	BA	2502	G
54	BA	2504	U
54	BA	2505	G
54	BA	2518	A
54	BA	2519	U
54	BA	2533	U
54	BA	2539	C
54	BA	2547	A
54	BA	2554	U
54	BA	2555	U

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Mol	Chain	Res	Type
54	BA	2564	A
54	BA	2565	A
54	BA	2566	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	2586	U
54	BA	2596	U
54	BA	2602	A
54	BA	2603	G
54	BA	2609	U
54	BA	2610	C
54	BA	2613	U
54	BA	2614	A
54	BA	2629	U
54	BA	2639	A
54	BA	2640	G
54	BA	2646	C
54	BA	2654	A
54	BA	2656	U
54	BA	2663	G
54	BA	2665	A
54	BA	2669	G
54	BA	2683	C
54	BA	2684	U
54	BA	2689	U
54	BA	2690	U
54	BA	2714	G
54	BA	2717	C
54	BA	2732	G
54	BA	2733	A
54	BA	2765	A
54	BA	2766	A
54	BA	2778	A
54	BA	2798	U
54	BA	2801	G
54	BA	2816	G
54	BA	2821	A
54	BA	2823	A

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Mol	Chain	Res	Type
54	BA	2833	U
54	BA	2834	G
54	BA	2835	A
54	BA	2850	A
54	BA	2868	A
54	BA	2876	G
54	BA	2879	A
54	BA	2884	U
54	BA	2886	A
54	BA	2895	G
55	BB	13	G
55	BB	14	U
55	BB	15	A
55	BB	16	G
55	BB	25	U
55	BB	31	C
55	BB	36	C
55	BB	37	C
55	BB	41	G
55	BB	42	C
55	BB	44	G
55	BB	45	A
55	BB	61	G
55	BB	84	G
55	BB	87	U
55	BB	90	C
55	BB	109	A

All (238) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	13	U
21	AA	51	A
21	AA	54	C
21	AA	85	U
21	AA	120	A
21	AA	184	G
21	AA	189	A
21	AA	251	G
21	AA	274	A
21	AA	281	G

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Mol	Chain	Res	Type
21	AA	298	A
21	AA	309	A
21	AA	327	A
21	AA	328	C
21	AA	346	G
21	AA	351	G
21	AA	362	G
21	AA	366	A
21	AA	368	U
21	AA	408	A
21	AA	420	U
21	AA	461	A
21	AA	462	G
21	AA	463	U
21	AA	465	A
21	AA	496	A
21	AA	538	G
21	AA	563	A
21	AA	567	G
21	AA	572	A
21	AA	575	G
21	AA	576	C
21	AA	607	A
21	AA	609	A
21	AA	648	A
21	AA	671	G
21	AA	753	A
21	AA	777	A
21	AA	778	G
21	AA	826	C
21	AA	843	U
21	AA	845	A
21	AA	876	C
21	AA	884	U
21	AA	890	G
21	AA	913	A
21	AA	958	A
21	AA	960	U
21	AA	970	C
21	AA	971	G
21	AA	978	A
21	AA	983	A

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Mol	Chain	Res	Type
21	AA	992	U
21	AA	1026	G
21	AA	1030	U
21	AA	1049	U
21	AA	1053	G
21	AA	1101	A
21	AA	1124	G
21	AA	1139	G
21	AA	1146	A
21	AA	1151	A
21	AA	1156	G
21	AA	1159	U
21	AA	1178	G
21	AA	1179	A
21	AA	1183	U
21	AA	1190	G
21	AA	1191	A
21	AA	1196	A
21	AA	1200	C
21	AA	1201	A
21	AA	1212	U
21	AA	1214	C
21	AA	1217	C
21	AA	1222	G
21	AA	1225	A
21	AA	1227	A
21	AA	1298	U
21	AA	1318	A
21	AA	1335	U
21	AA	1337	G
21	AA	1363	A
21	AA	1364	U
21	AA	1381	U
21	AA	1425	U
21	AA	1440	U
21	AA	1452	C
21	AA	1492	A
21	AA	1523	G
21	AA	1529	G
22	A1	72	C
22	A1	75	C
23	A2	82	A

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Mol	Chain	Res	Type
23	A2	87	U
23	A2	90	U
24	A3	1	C
24	A3	22	A
24	A3	47	G
24	A3	50	G
24	A3	58	A
24	A3	61	U
24	A3	71	G
24	A3	74	A
54	BA	16	C
54	BA	29	U
54	BA	60	G
54	BA	91	A
54	BA	99	U
54	BA	101	A
54	BA	149	A
54	BA	199	A
54	BA	221	A
54	BA	265	A
54	BA	271	G
54	BA	277	G
54	BA	278	A
54	BA	330	A
54	BA	372	G
54	BA	374	A
54	BA	377	G
54	BA	446	G
54	BA	451	U
54	BA	458	G
54	BA	479	A
54	BA	481	G
54	BA	510	C
54	BA	527	C
54	BA	530	G
54	BA	569	U
54	BA	587	C
54	BA	614	A
54	BA	625	G
54	BA	670	A
54	BA	751	A
54	BA	762	U

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Mol	Chain	Res	Type
54	BA	764	A
54	BA	818	G
54	BA	931	U
54	BA	958	U
54	BA	962	G
54	BA	974	G
54	BA	980	A
54	BA	981	A
54	BA	982	C
54	BA	983	A
54	BA	1019	U
54	BA	1073	A
54	BA	1089	A
54	BA	1123	C
54	BA	1128	G
54	BA	1130	U
54	BA	1133	A
54	BA	1141	U
54	BA	1142	A
54	BA	1187	G
54	BA	1210	G
54	BA	1228	G
54	BA	1236	G
54	BA	1238	G
54	BA	1240	U
54	BA	1252	G
54	BA	1253	A
54	BA	1289	C
54	BA	1300	G
54	BA	1312	U
54	BA	1313	U
54	BA	1329	U
54	BA	1343	G
54	BA	1379	U
54	BA	1419	A
54	BA	1420	A
54	BA	1421	G
54	BA	1427	A
54	BA	1428	C
54	BA	1433	A
54	BA	1434	A
54	BA	1451	C

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Mol	Chain	Res	Type
54	BA	1453	A
54	BA	1454	C
54	BA	1457	U
54	BA	1508	A
54	BA	1539	U
54	BA	1568	G
54	BA	1597	A
54	BA	1615	C
54	BA	1616	A
54	BA	1634	A
54	BA	1655	A
54	BA	1668	A
54	BA	1706	C
54	BA	1733	G
54	BA	1757	A
54	BA	1760	C
54	BA	1783	A
54	BA	1799	G
54	BA	1847	A
54	BA	1900	A
54	BA	1913	A
54	BA	1914	C
54	BA	1936	A
54	BA	1938	A
54	BA	1943	U
54	BA	1955	U
54	BA	1970	A
54	BA	2017	U
54	BA	2035	G
54	BA	2131	U
54	BA	2163	A
54	BA	2172	U
54	BA	2213	U
54	BA	2233	U
54	BA	2267	A
54	BA	2275	C
54	BA	2282	G
54	BA	2286	G
54	BA	2312	U
54	BA	2352	A
54	BA	2373	G
54	BA	2430	A

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Mol	Chain	Res	Type
54	BA	2450	A
54	BA	2499	C
54	BA	2500	U
54	BA	2528	U
54	BA	2532	G
54	BA	2566	A
54	BA	2581	G
54	BA	2585	U
54	BA	2669	G
54	BA	2689	U
54	BA	2780	G
54	BA	2833	U
54	BA	2858	C
54	BA	2879	A
55	BB	12	C
55	BB	15	A
55	BB	56	G

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	$\# Z > 2$
24	OMC	A3	33	24	19,22,23	0.74	0	25,31,34	0.98	1 (4%)
24	PSU	A3	56	24	18,21,22	0.95	0	21,30,33	1.27	2 (9%)
22	4SU	A1	7	22	18,21,22	1.42	2 (11%)	25,30,33	1.00	2 (8%)
22	7MG	A1	46	22	23,26,27	4.01	2 (8%)	27,39,42	1.48	1 (3%)
22	PSU	A1	55	22	18,21,22	0.79	0	21,30,33	1.06	0
24	4SU	A3	8	24	18,21,22	1.44	2 (11%)	25,30,33	0.87	1 (4%)
22	6MZ	A1	37	22	22,25,26	0.68	0	29,36,39	1.08	2 (6%)
24	H2U	A3	21	24	18,21,22	1.35	2 (11%)	19,30,33	1.23	3 (15%)
24	5MU	A3	55	24	19,22,23	0.68	0	27,32,35	1.34	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	5MU	A1	54	22	19,22,23	0.72	0	27,32,35	1.39	3 (11%)
22	CM0	A1	34	23,22	21,26,27	1.35	2 (9%)	26,37,40	1.57	3 (11%)

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
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2
24	PSU	A3	56	24	-	0/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3
22	PSU	A1	55	22	-	1/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/7/25/26	0/2/2/2
22	6MZ	A1	37	22	-	2/9/27/28	0/3/3/3
24	H2U	A3	21	24	-	0/7/38/39	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	CM0	A1	34	23,22	-	3/12/30/31	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	-18.86	1.33	1.45
24	A3	8	4SU	C5-C4	-5.18	1.36	1.42
22	A1	7	4SU	C5-C4	-5.05	1.36	1.42
22	A1	34	CM0	O5-C5	-4.87	1.25	1.36
24	A3	21	H2U	C4-N3	-3.27	1.32	1.37
24	A3	21	H2U	C2-N3	-3.21	1.32	1.38
22	A1	46	7MG	C8-N7	-2.41	1.30	1.42
22	A1	7	4SU	C4-S4	-2.25	1.64	1.68
24	A3	8	4SU	C4-S4	-2.11	1.65	1.68
22	A1	34	CM0	O8-C8	-2.08	1.23	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	5.74	111.49	103.37
22	A1	34	CM0	C7-O5-C5	5.63	124.65	117.48
22	A1	37	6MZ	C9-N6-C6	3.87	126.44	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5M-C5-C6	-3.73	117.80	122.85
24	A3	55	5MU	C5M-C5-C6	-3.63	117.94	122.85
22	A1	54	5MU	C6-C5-C4	3.10	120.58	118.02
24	A3	21	H2U	N3-C2-N1	2.96	119.62	116.65
24	A3	56	PSU	C6-C5-C4	2.96	120.17	118.17
24	A3	33	OMC	O2-C2-N3	-2.91	117.75	122.33
24	A3	55	5MU	C6-C5-C4	2.87	120.38	118.02
24	A3	56	PSU	O4'-C1'-C2'	2.75	108.95	105.15
24	A3	55	5MU	C5M-C5-C4	2.71	121.67	118.78
22	A1	54	5MU	C5M-C5-C4	2.66	121.63	118.78
22	A1	7	4SU	C6-C5-C4	2.48	122.10	119.95
22	A1	7	4SU	O4'-C4'-C3'	2.27	109.67	105.15
24	A3	21	H2U	C5-C4-N3	2.26	119.09	116.69
22	A1	34	CM0	O4'-C4'-C3'	2.21	109.53	105.15
22	A1	37	6MZ	C4-C5-C6	-2.18	114.97	116.78
24	A3	8	4SU	C6-C5-C4	2.09	121.76	119.95
24	A3	21	H2U	O2-C2-N3	-2.09	117.64	121.49
22	A1	34	CM0	C3'-C2'-C1'	2.08	105.39	101.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	37	6MZ	C5-C6-N6-C9
22	A1	37	6MZ	N1-C6-N6-C9
22	A1	46	7MG	C4'-C5'-O5'-P
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9
22	A1	55	PSU	O4'-C1'-C5-C4
22	A1	34	CM0	C6-C5-O5-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
57	VAL	A1	101	58,22	4,6,7	0.65	0	6,7,9	0.91	0
58	FME	BA	3001	57	8,9,10	0.73	0	8,9,11	1.77	2 (25%)

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
57	VAL	A1	101	58,22	-	0/5/6/8	-
58	FME	BA	3001	57	-	1/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	FME	CA-N-CN	3.33	127.95	122.82
58	BA	3001	FME	C-CA-N	2.64	114.59	109.50

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	FME	O1-CN-N-CA

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.

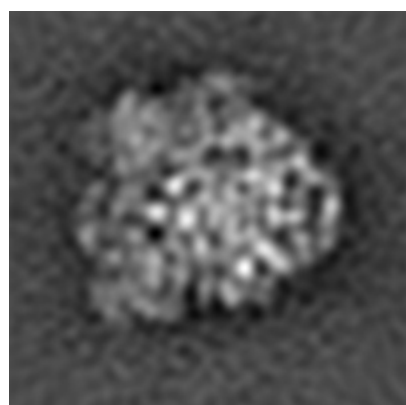
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1722. These allow visual inspection of the internal detail of the map and identification of artifacts.

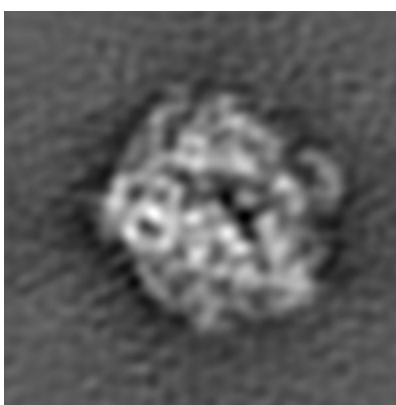
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

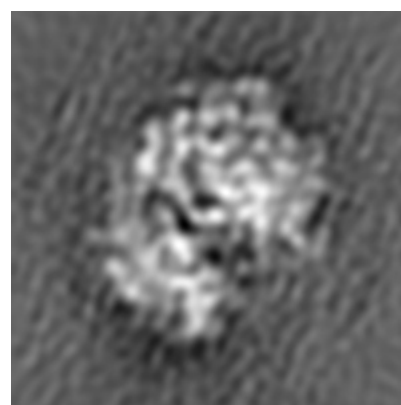
6.1.1 Primary map



X



Y

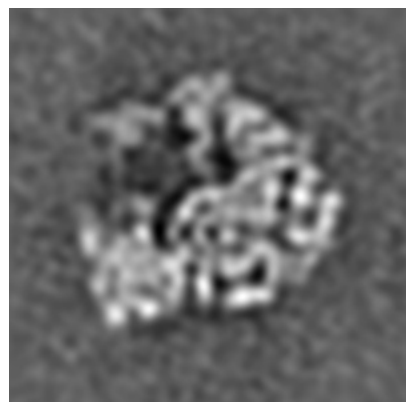


Z

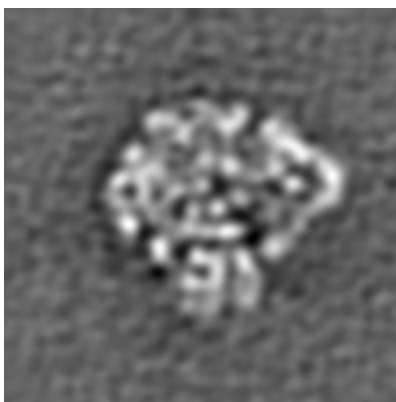
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

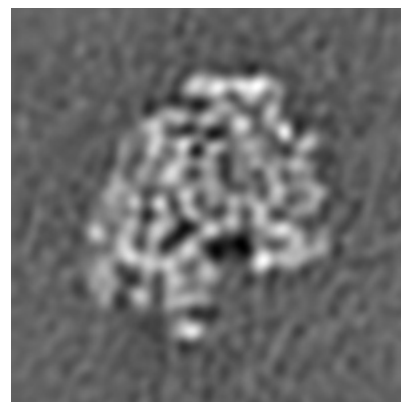
6.2.1 Primary map



X Index: 64



Y Index: 64



Z Index: 64

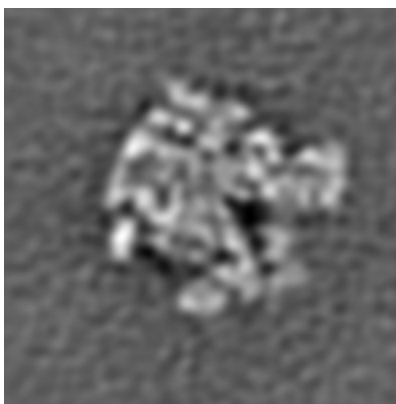
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

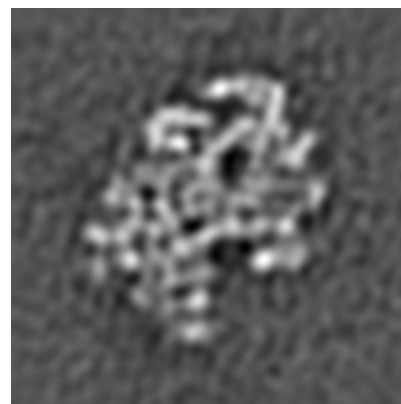
6.3.1 Primary map



X Index: 62



Y Index: 69

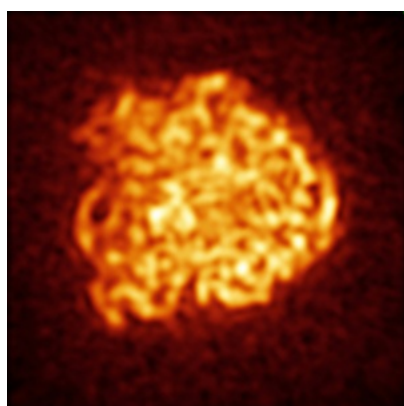


Z Index: 61

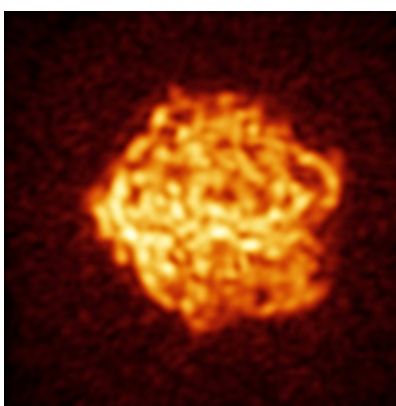
The images above show the largest variance slices of the map in three orthogonal directions.

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

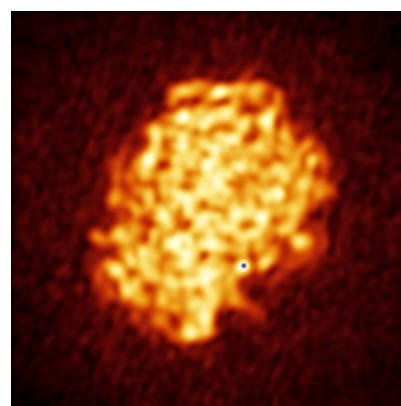
6.4.1 Primary map



X



Y

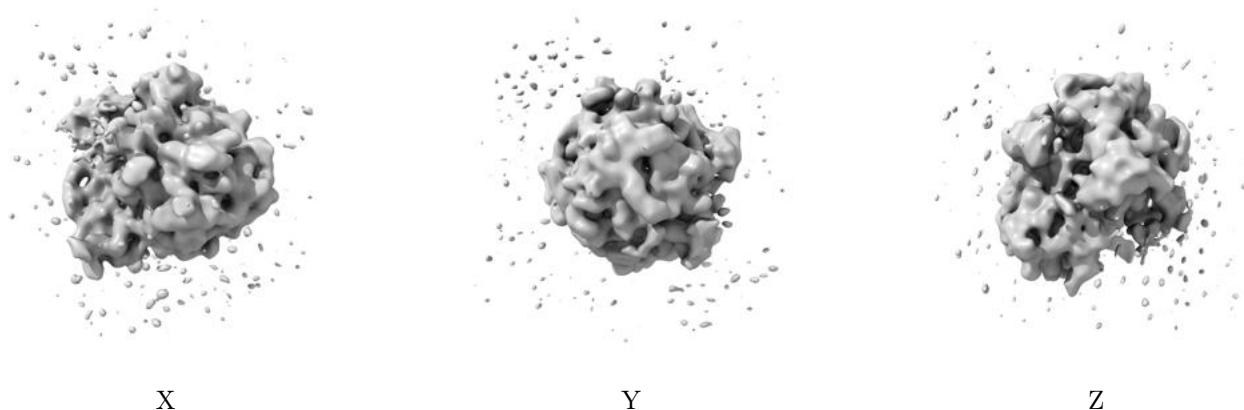


Z

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 22.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

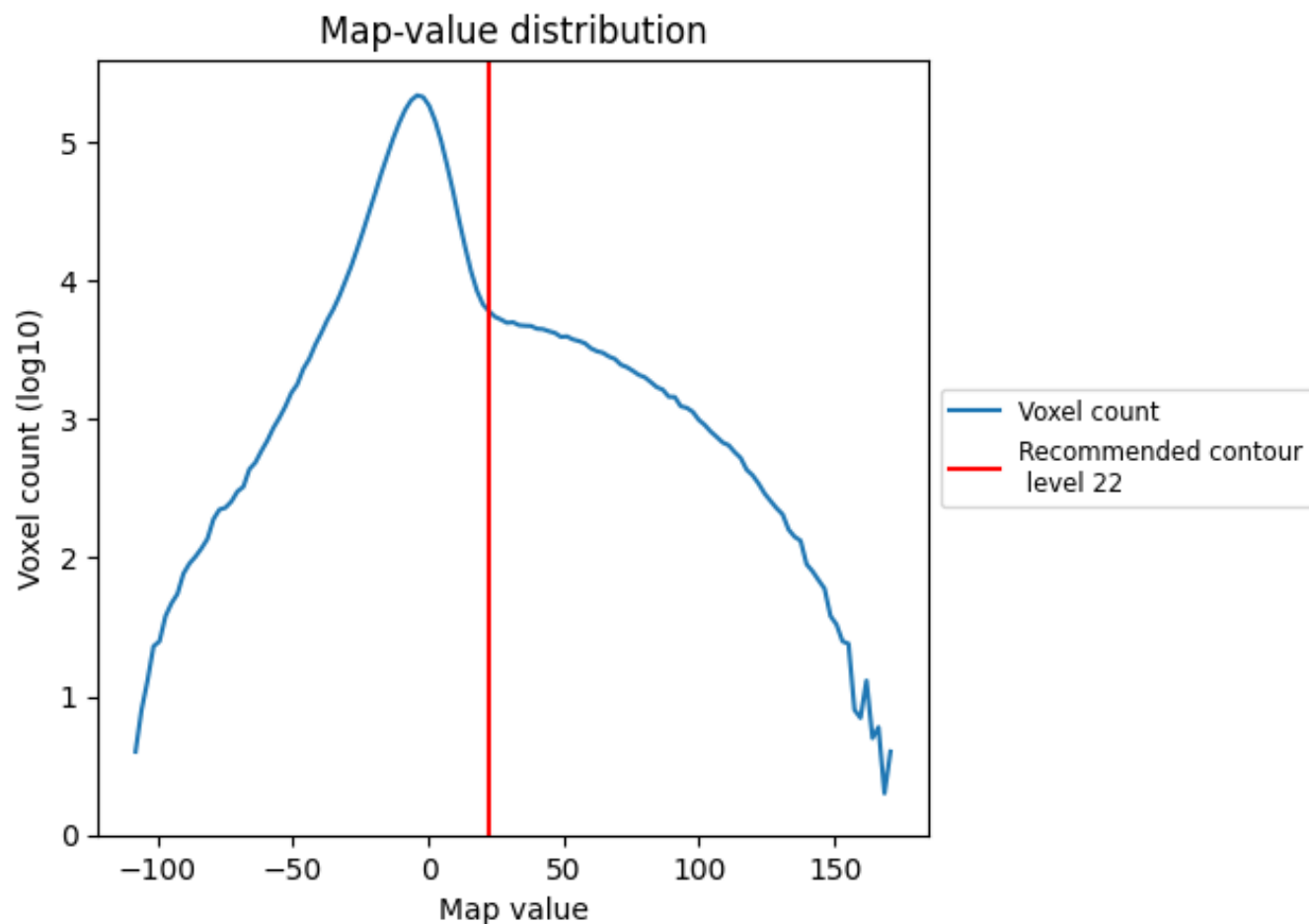
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

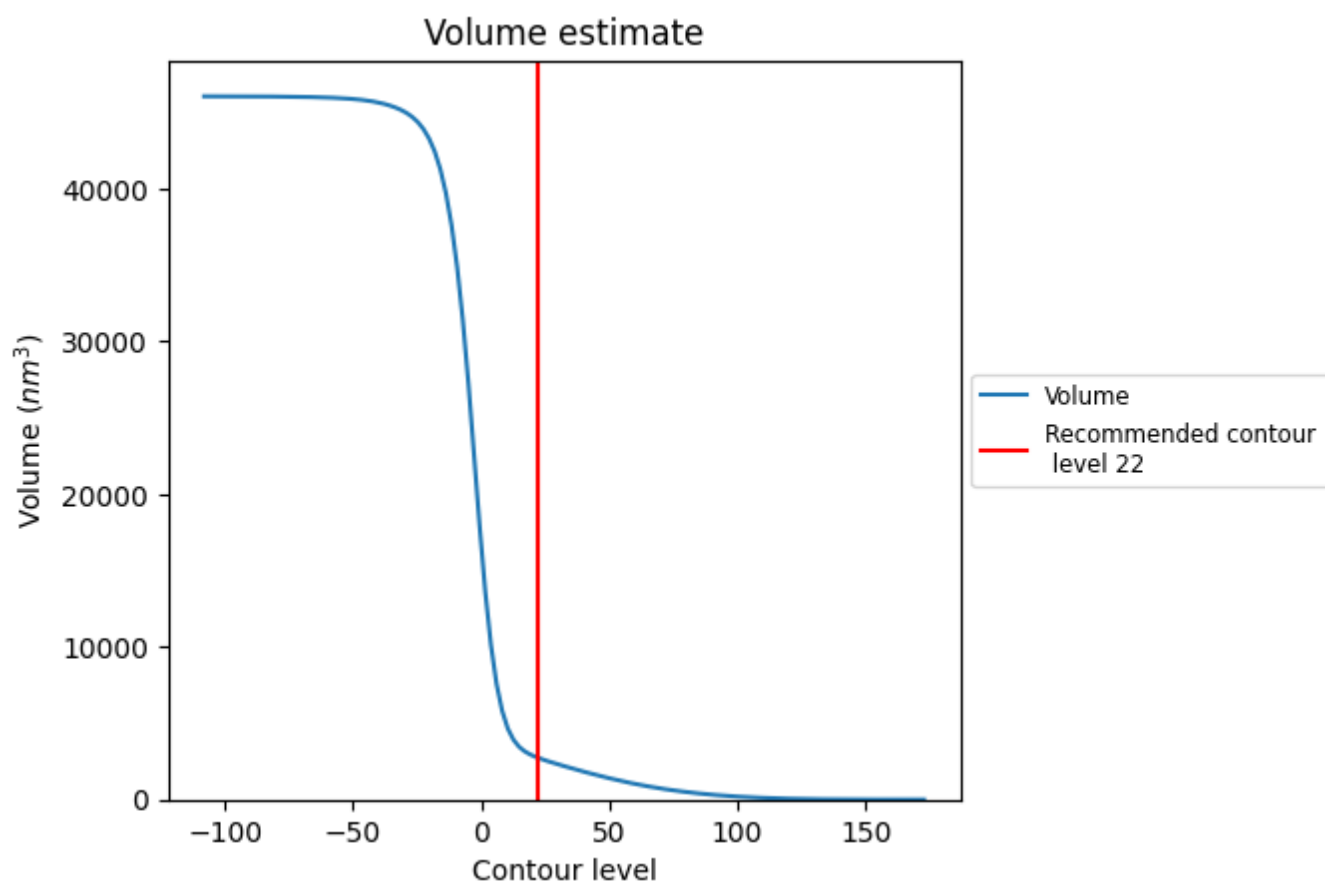
This section contains the results of statistical analysis of the map.

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.

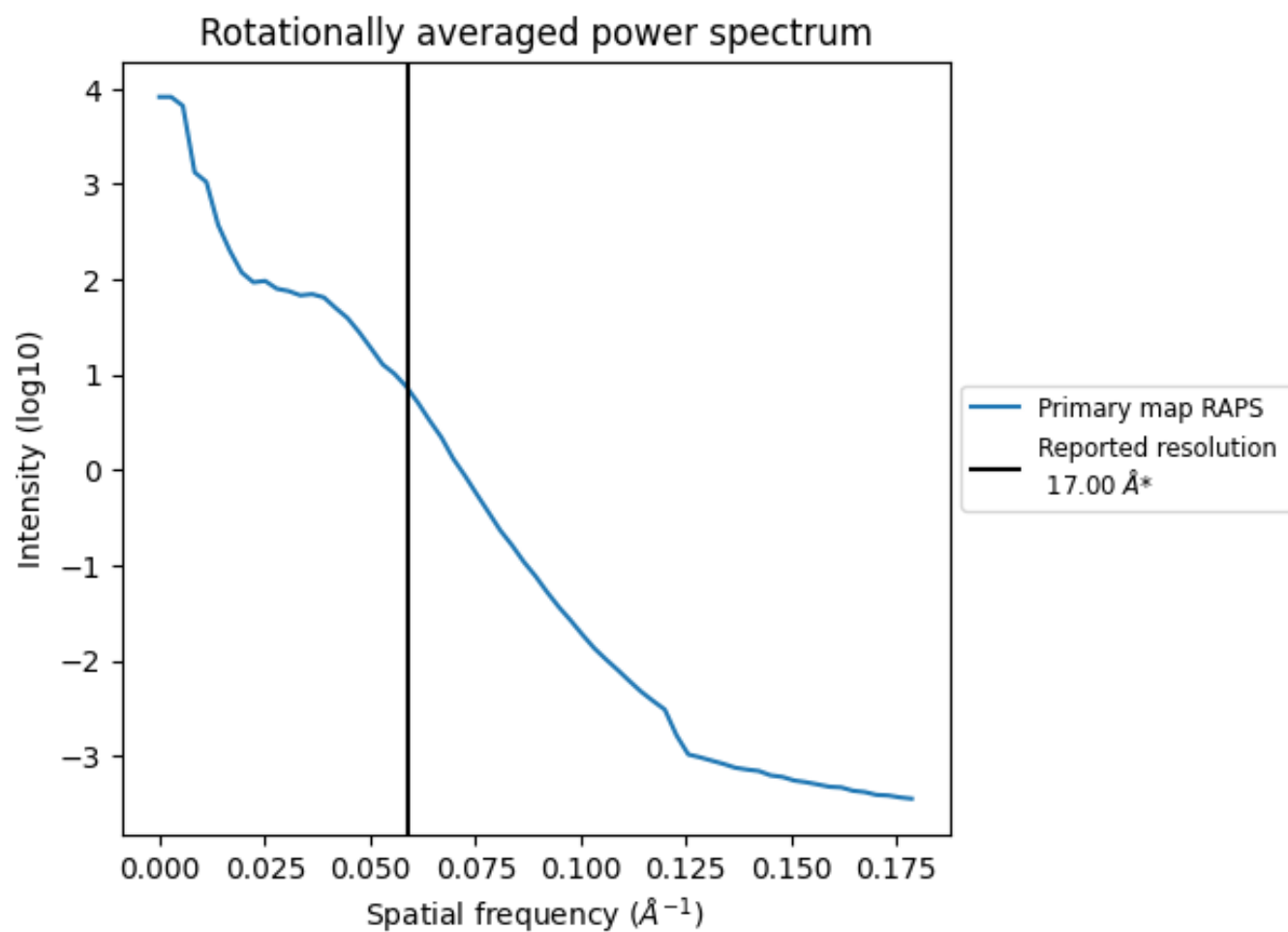
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2749 nm³; this corresponds to an approximate mass of 2483 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 0.059 Å⁻¹

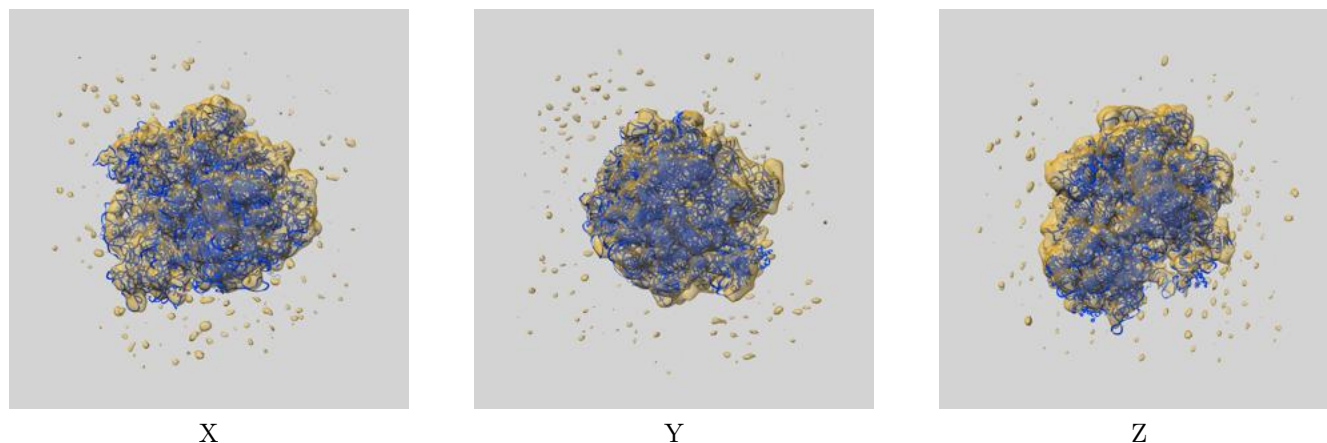
8 Fourier-Shell correlation

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-1722 and PDB model 4V76. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



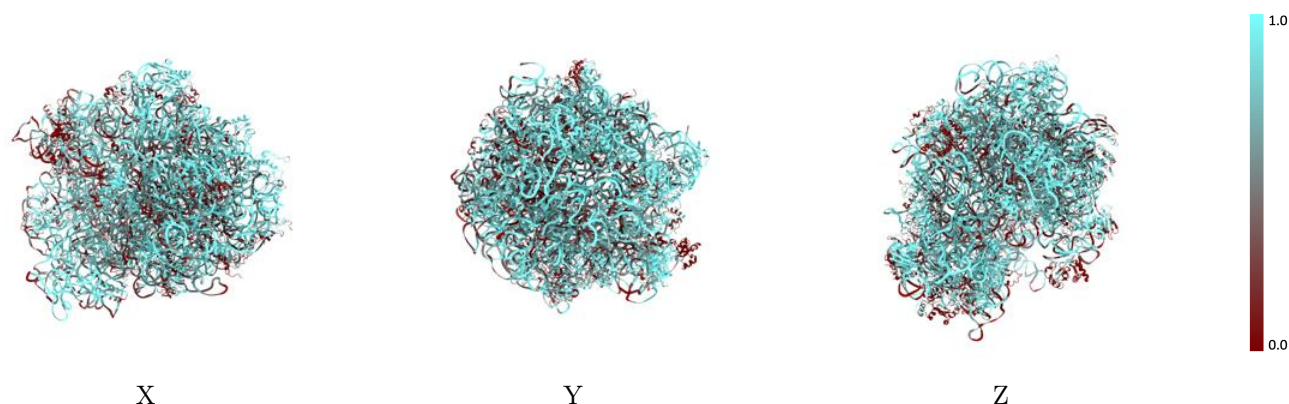
The images above show the 3D surface view of the map at the recommended contour level 22.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



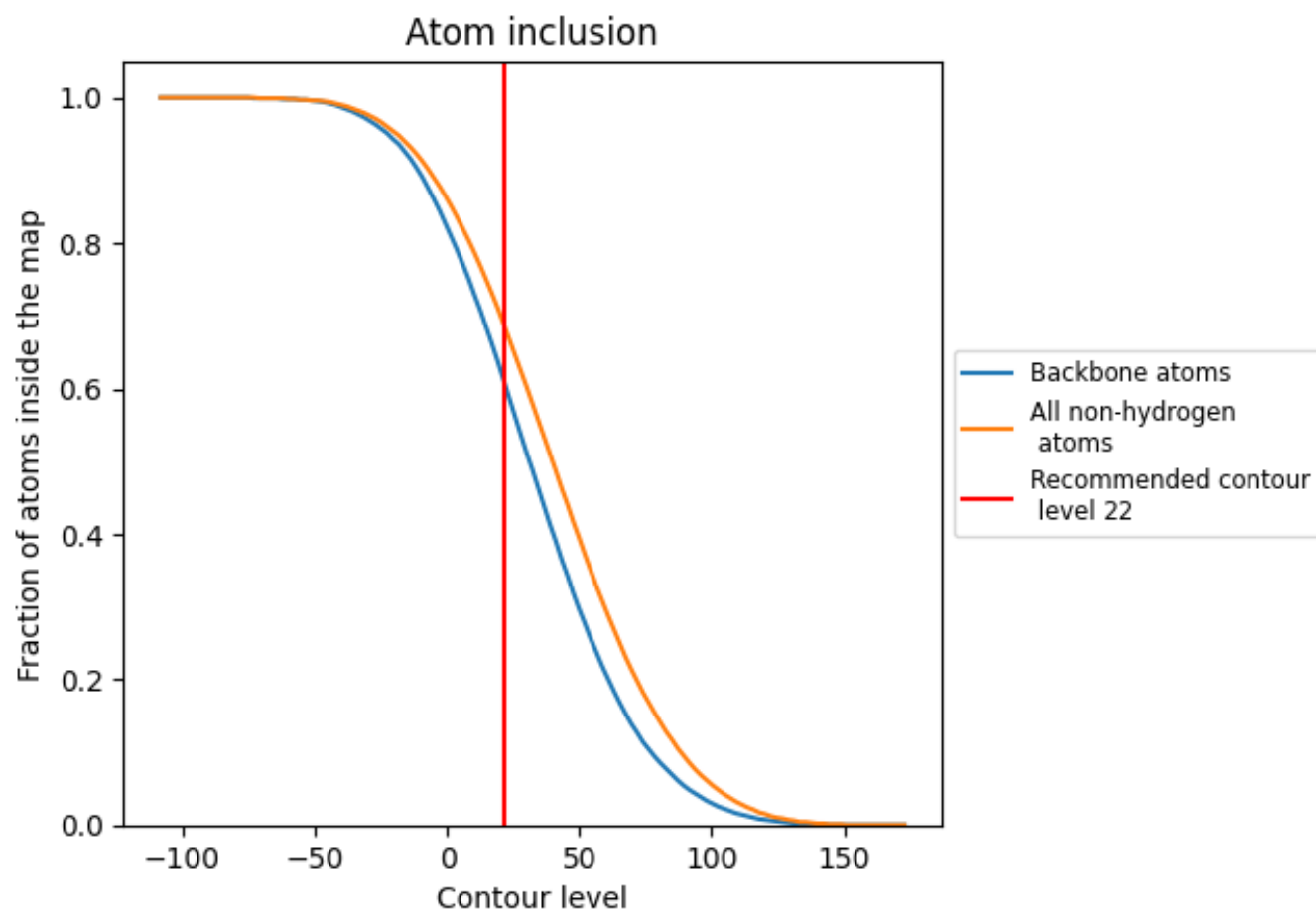
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6840	 0.0370
A1	 0.5760	 0.0450
A2	 0.4820	 -0.0220
A3	 0.5150	 0.0290
AA	 0.7520	 0.0460
AB	 0.4450	 0.0190
AC	 0.4720	 0.0350
AD	 0.4490	 0.0100
AE	 0.5510	 0.0400
AF	 0.8170	 0.0540
AG	 0.7100	 0.0210
AH	 0.5710	 0.0210
AI	 0.7320	 0.0200
AJ	 0.5130	 0.0170
AK	 0.6700	 0.0270
AL	 0.7000	 0.0340
AM	 0.6070	 0.0290
AN	 0.5880	 0.0120
AO	 0.6320	 0.0260
AP	 0.5300	 0.0040
AQ	 0.5400	 0.0080
AR	 0.6060	 -0.0260
AS	 0.7400	 0.0290
AT	 0.7300	 -0.0140
AU	 0.5670	 -0.0090
B0	 0.7010	 0.0580
B1	 0.7720	 0.0440
B2	 0.3780	 -0.0020
B3	 0.3770	 -0.0360
B4	 0.6780	 0.0220
B5	 0.3780	 0.0000
BA	 0.7390	 0.0460
BB	 0.7890	 0.0500
BC	 0.4730	 0.0120
BD	 0.5070	 0.0100



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Chain	Atom inclusion	Q-score
BE	 0.7430	 0.0260
BF	 0.6980	 0.0560
BG	 0.6350	 0.0470
BH	 0.3300	 0.0120
BI	 0.1420	 0.0320
BJ	 0.5140	 0.0170
BK	 0.5770	 0.0300
BL	 0.6140	 -0.0030
BM	 0.5580	 0.0190
BN	 0.5220	 -0.0100
BO	 0.8640	 0.0310
BP	 0.4820	 0.0120
BQ	 0.6350	 0.0180
BR	 0.4180	 -0.0060
BS	 0.5270	 -0.0100
BT	 0.6200	 0.0130
BU	 0.5060	 0.0190
BV	 0.7520	 0.0480
BW	 0.6600	 0.0160
BX	 0.5940	 0.0040
BY	 0.5410	 0.0370
BZ	 0.5400	 0.0060