



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 09:12 AM EDT

PDB ID : 4V6Z / pdb_00004v6z
EMDB ID : EMD-2472
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in classic pre-translocation state (pre1b)
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 : 12.00 Å (reported)
Based on initial models : 3I1O, 2K4C, 2HGP, 2WRI

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:

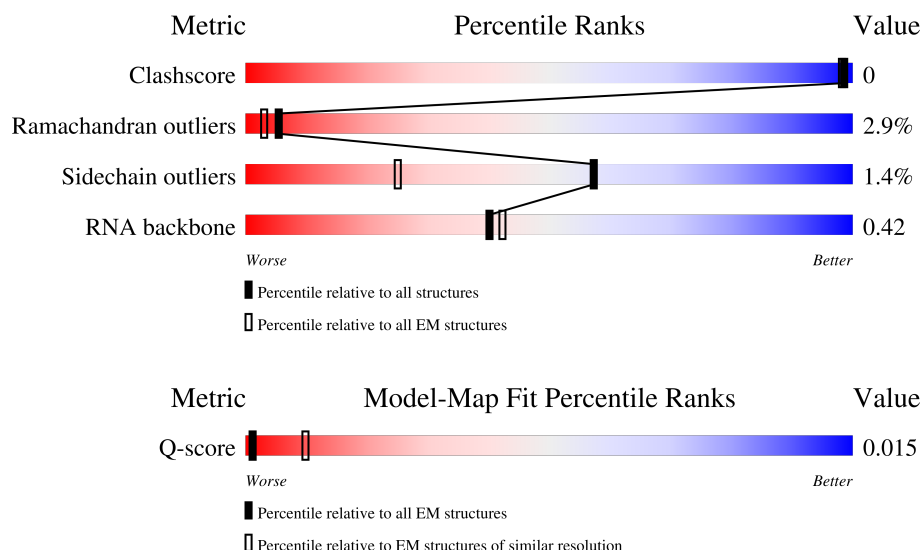
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 12.00 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	93 (11.50 - 12.50)

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	50% 95% 5%
2	AC	208	46% 96% .
3	AD	206	51% 95% 5%

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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	35% 60% 32% 7%
55	BB	118	23% 58% 38%
56	B5	234	60% 94% 5%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

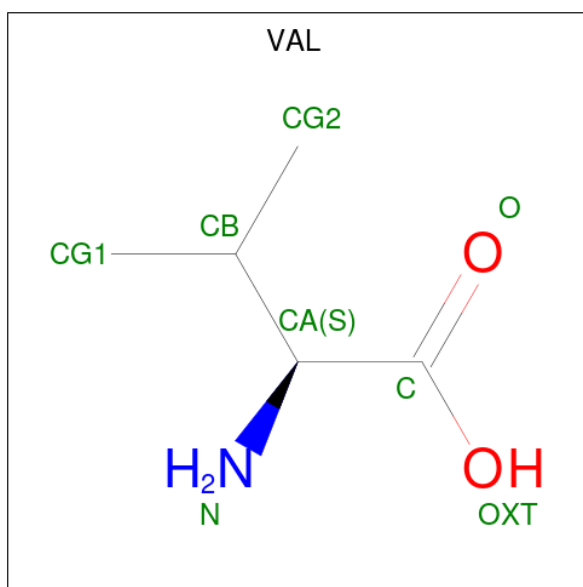
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

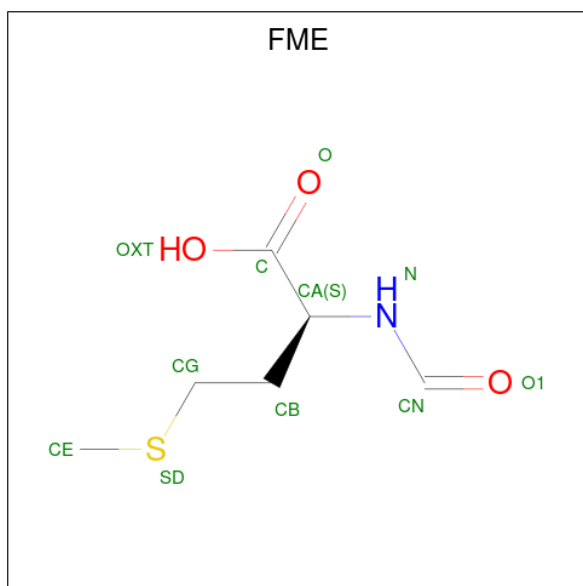
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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



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

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

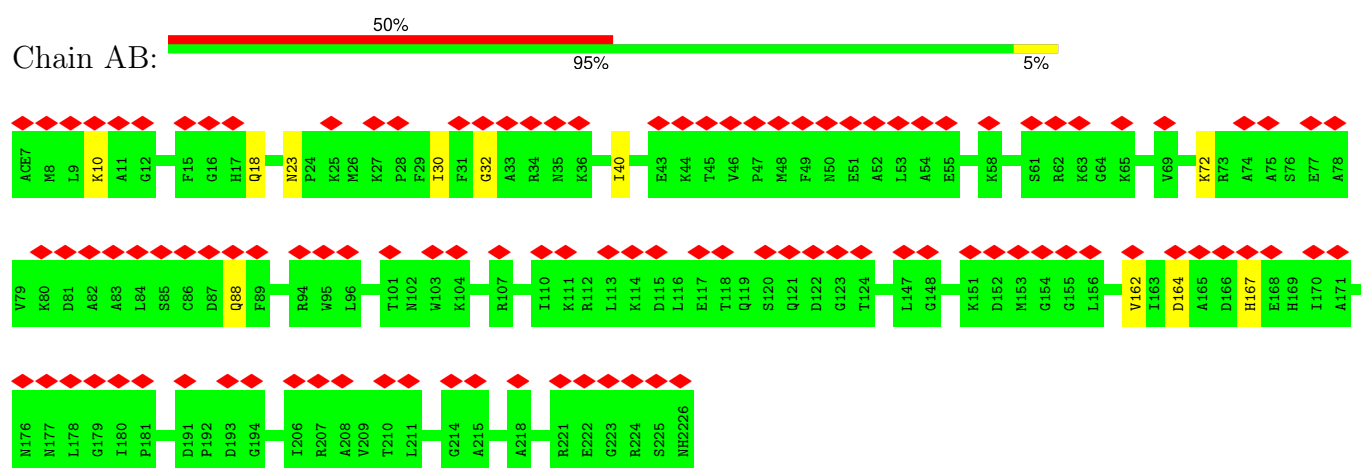


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

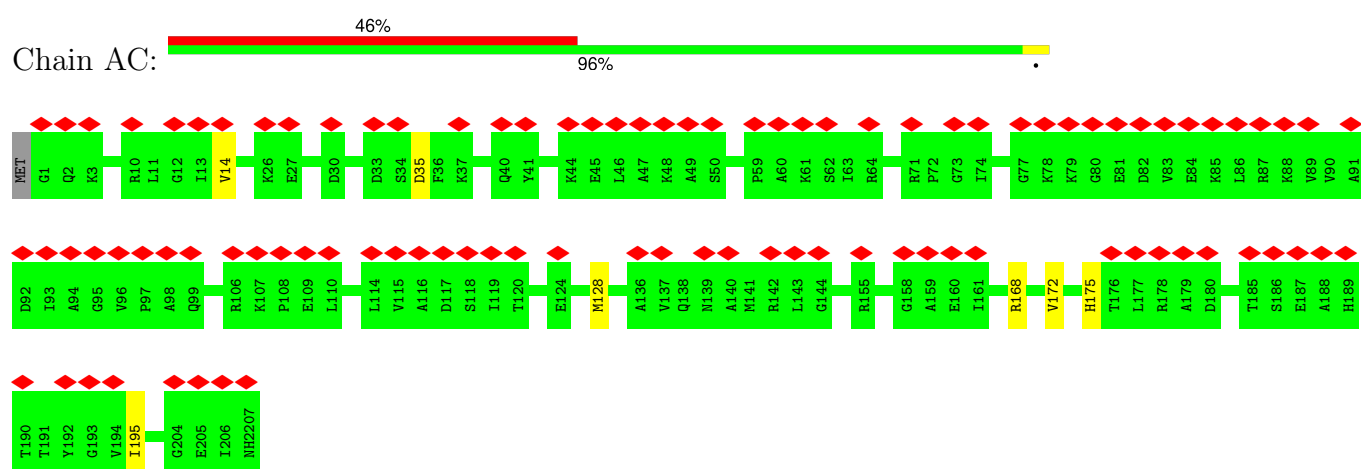
3 Residue-property plots

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

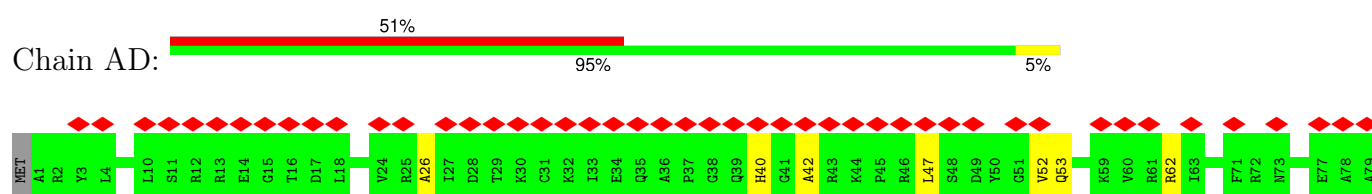
• Molecule 1: 30S ribosomal protein S2

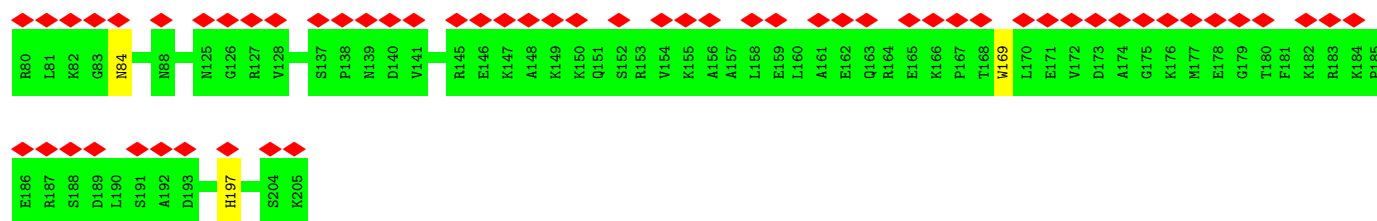


• Molecule 2: 30S ribosomal protein S3

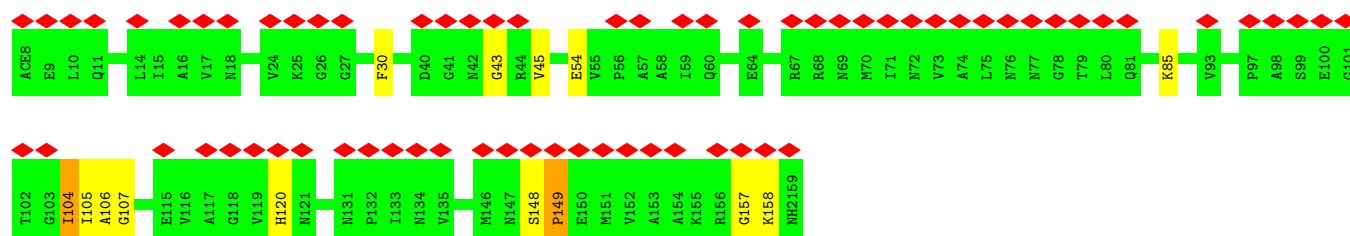


• Molecule 3: 30S ribosomal protein S4

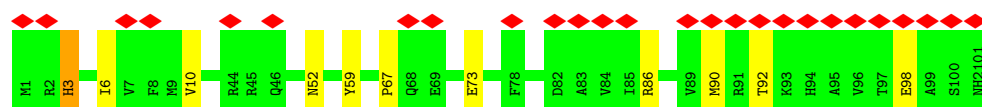
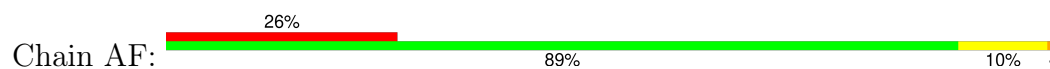




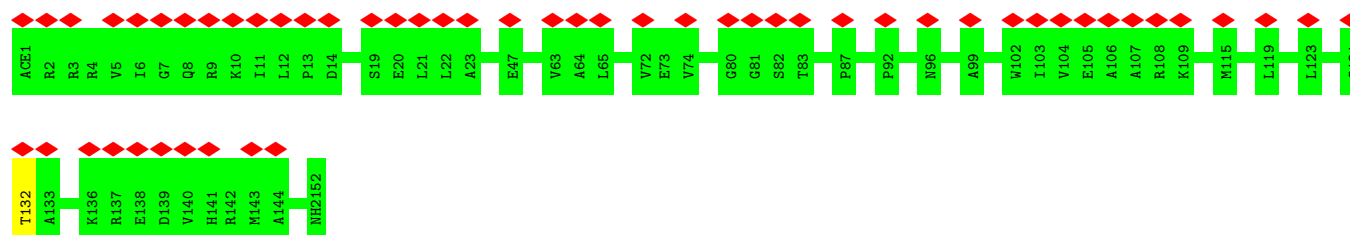
• Molecule 4: 30S ribosomal protein S5



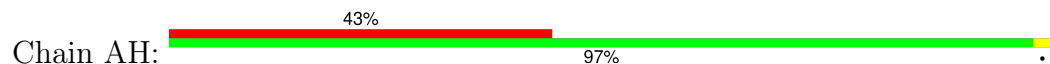
• Molecule 5: 30S ribosomal protein S6



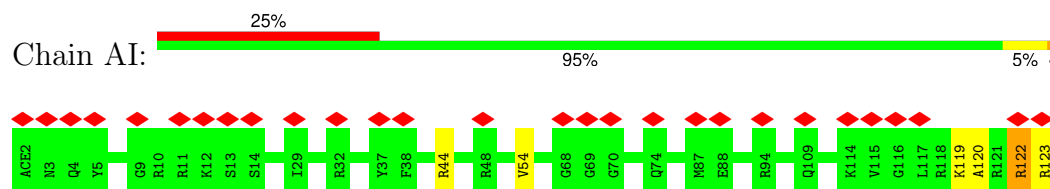
• Molecule 6: 30S ribosomal protein S7



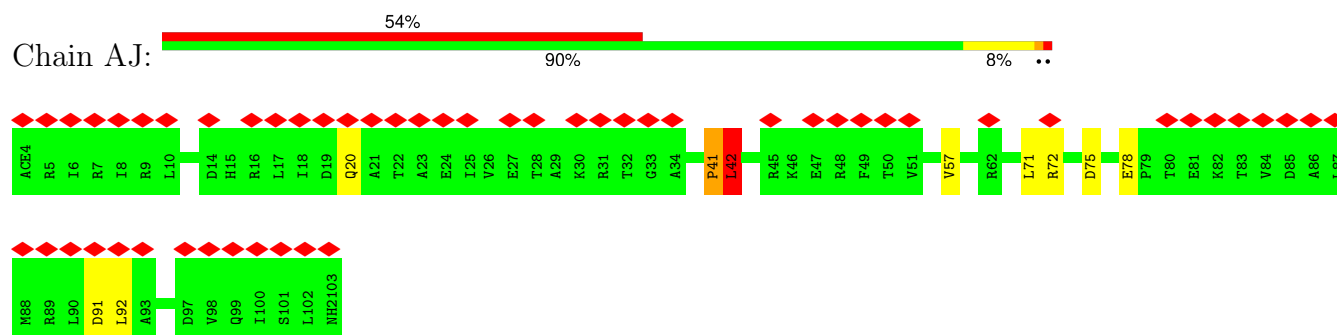
• Molecule 7: 30S ribosomal protein S8



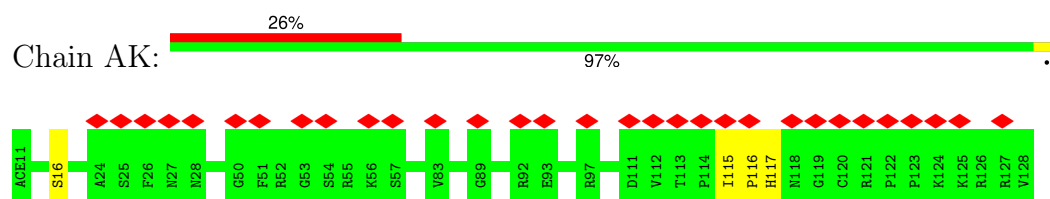
- Molecule 8: 30S ribosomal protein S9



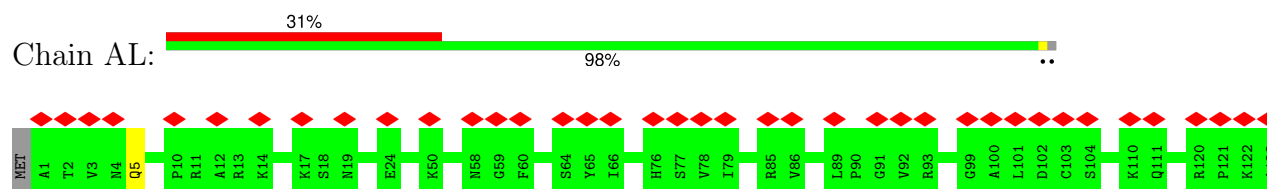
- Molecule 9: 30S ribosomal protein S10



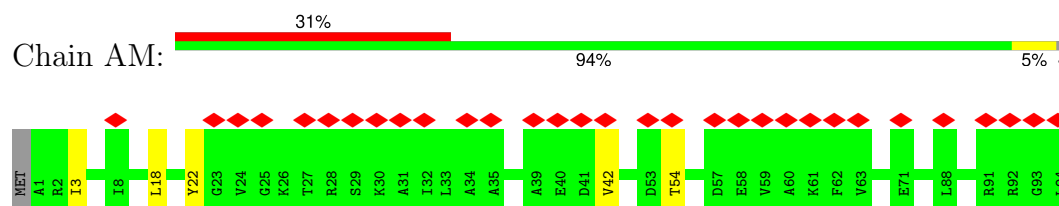
- Molecule 10: 30S ribosomal protein S11



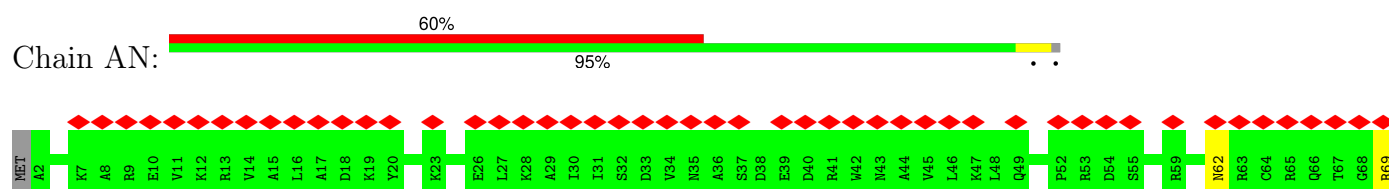
- Molecule 11: 30S ribosomal protein S12

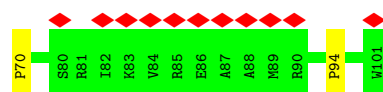


- Molecule 12: 30S ribosomal protein S13

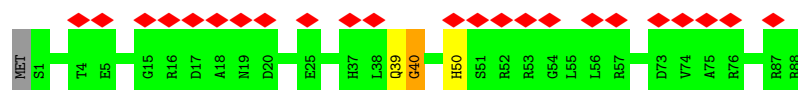


- Molecule 13: 30S ribosomal protein S14

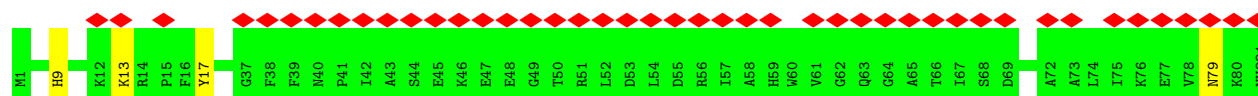




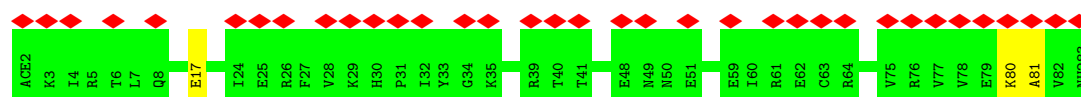
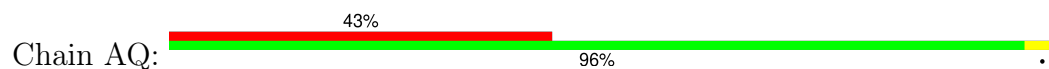
- Molecule 14: 30S ribosomal protein S15



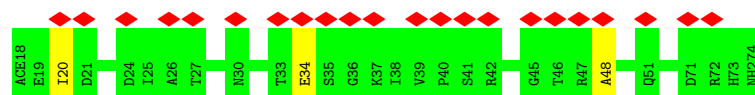
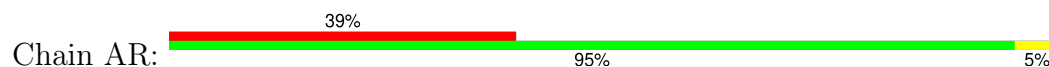
- Molecule 15: 30S ribosomal protein S16



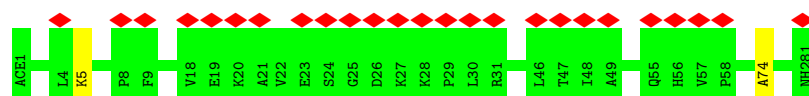
- Molecule 16: 30S ribosomal protein S17



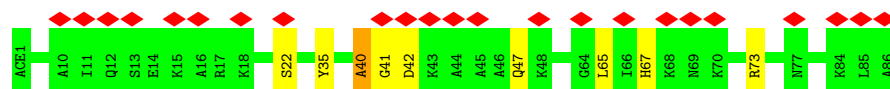
- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19

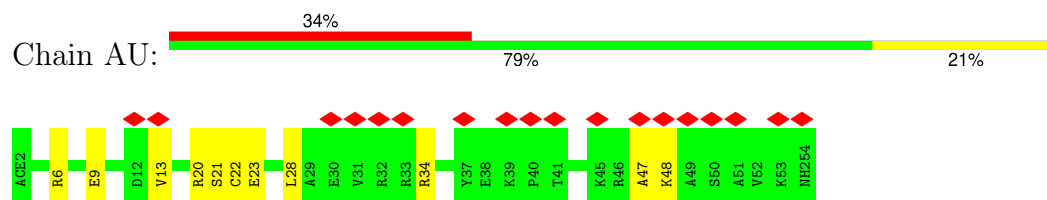


- Molecule 19: 30S ribosomal protein S20



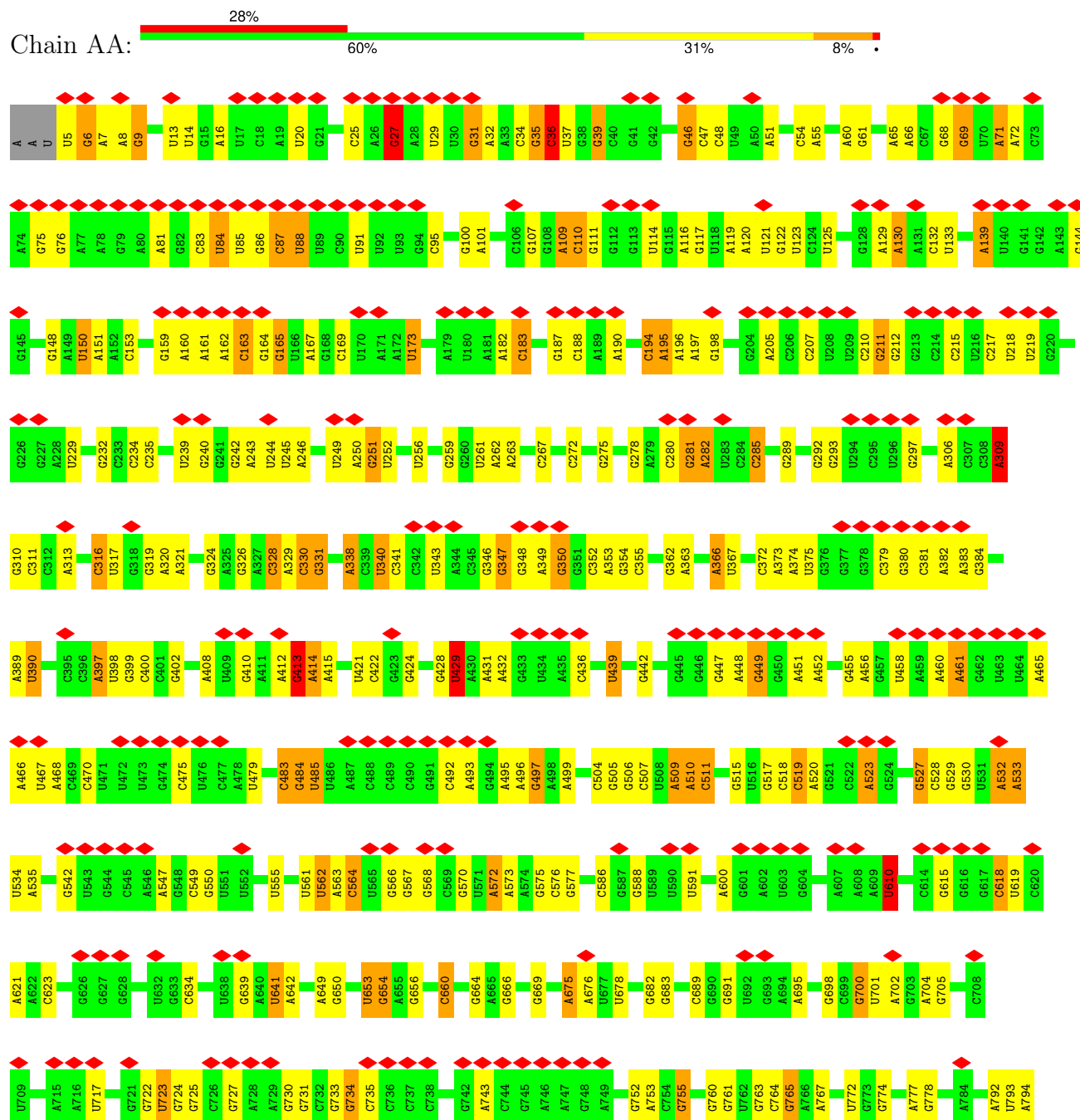
- Molecule 20: 30S ribosomal protein S21

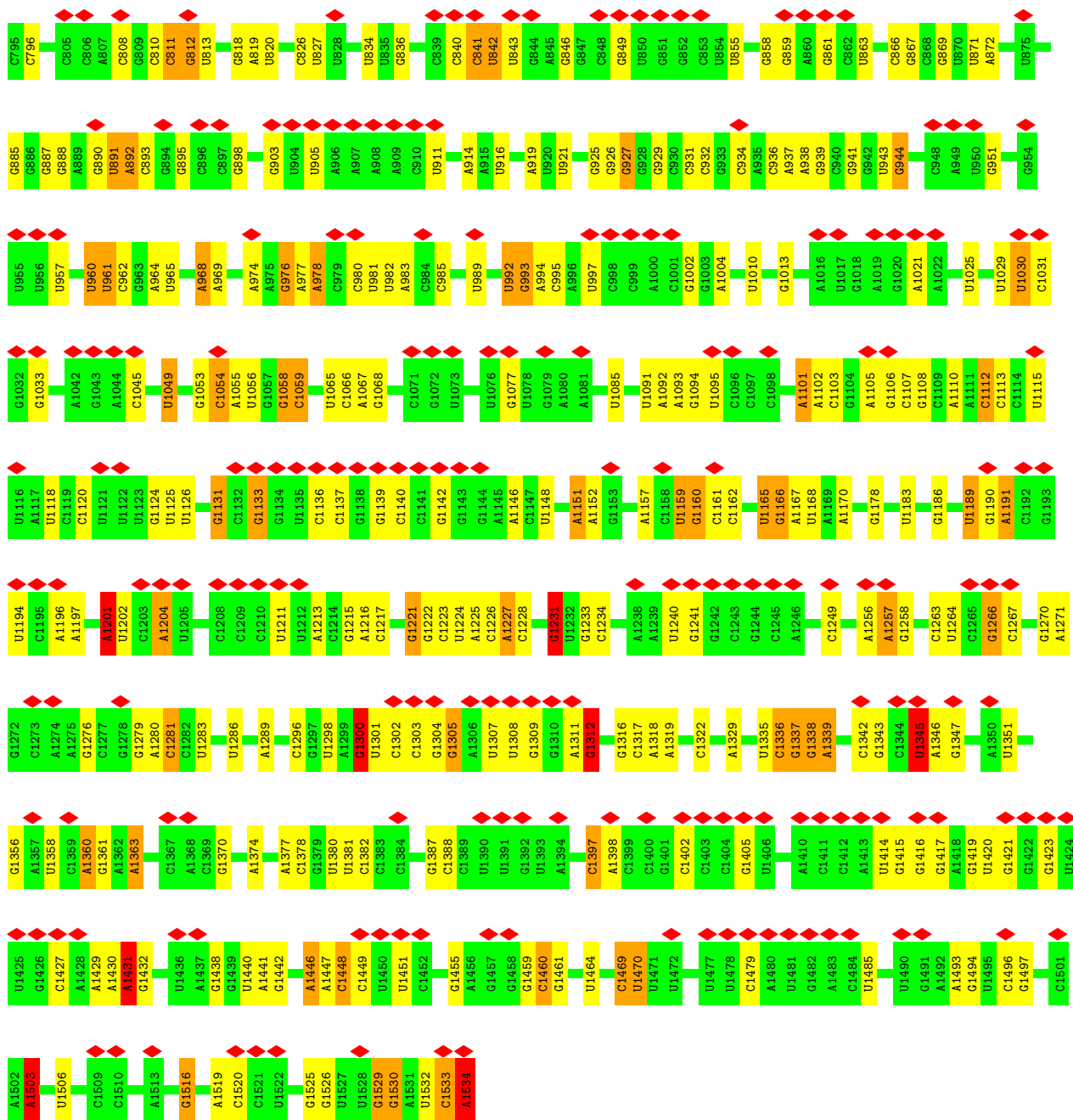
Chain AU:



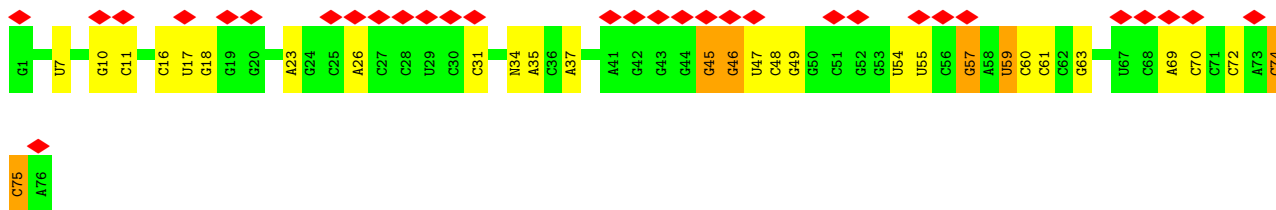
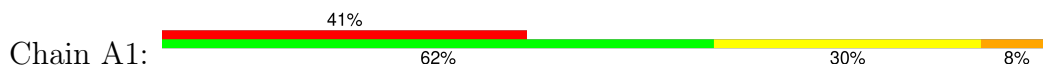
- Molecule 21: 16S ribosomal RNA

Chain AA:

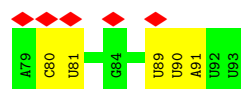




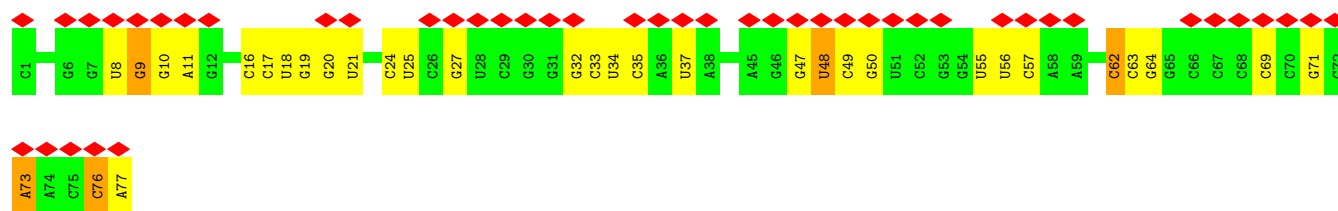
• Molecule 22: fMet-Val-tRNA-Val



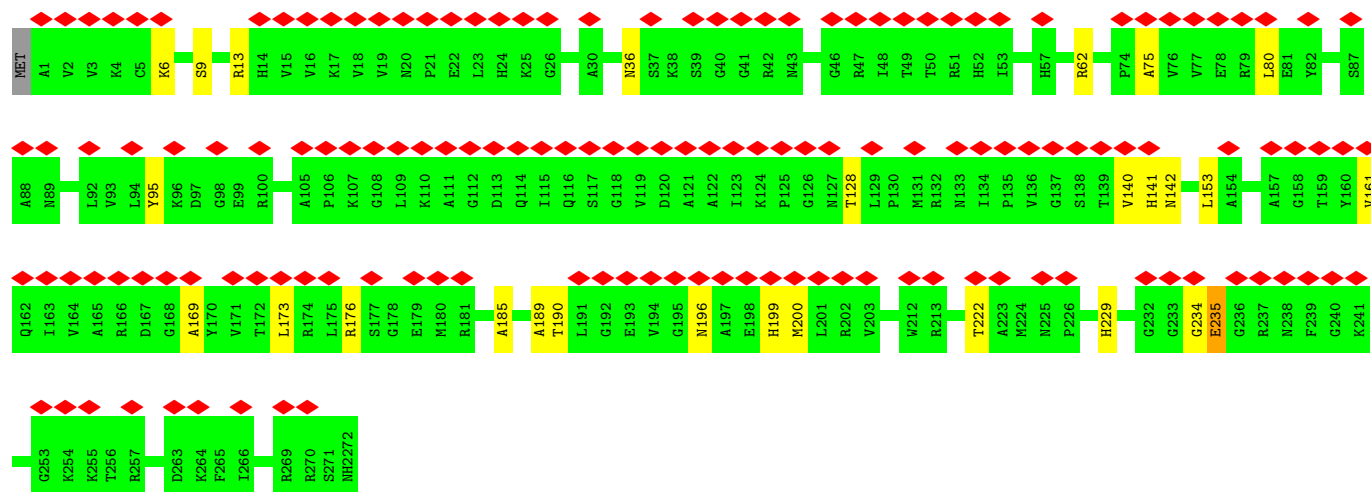
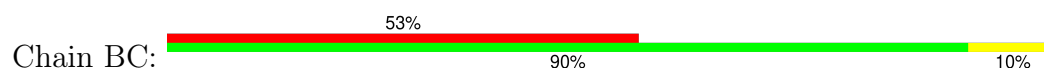
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'



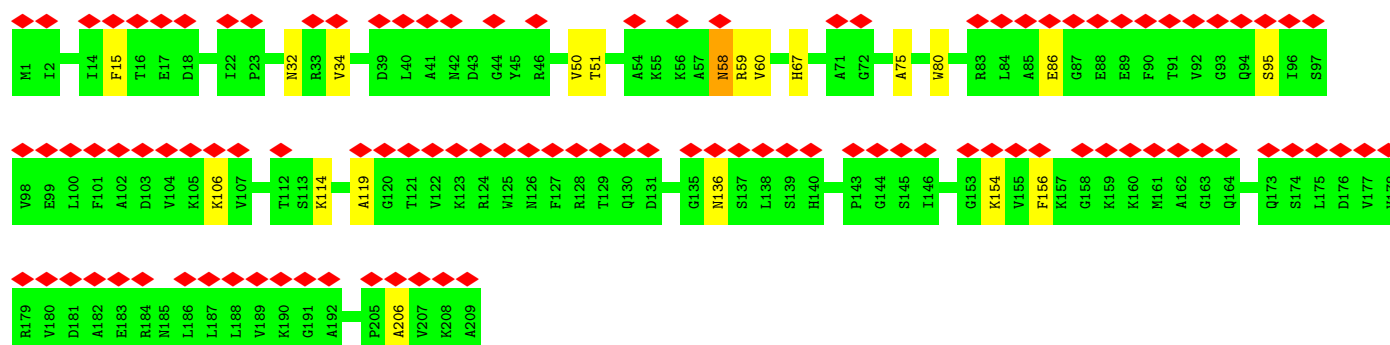
• Molecule 24: tRNA-fMet



• Molecule 25: 50S ribosomal protein L2

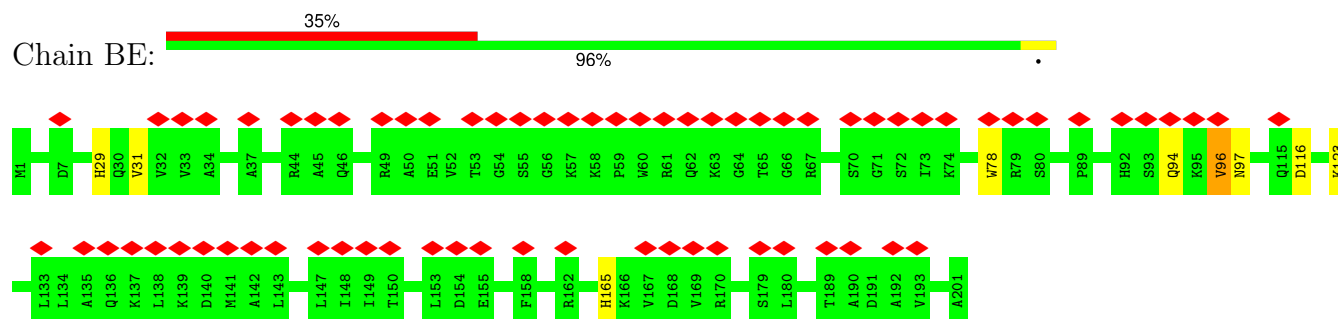


• Molecule 26: 50S ribosomal protein L3



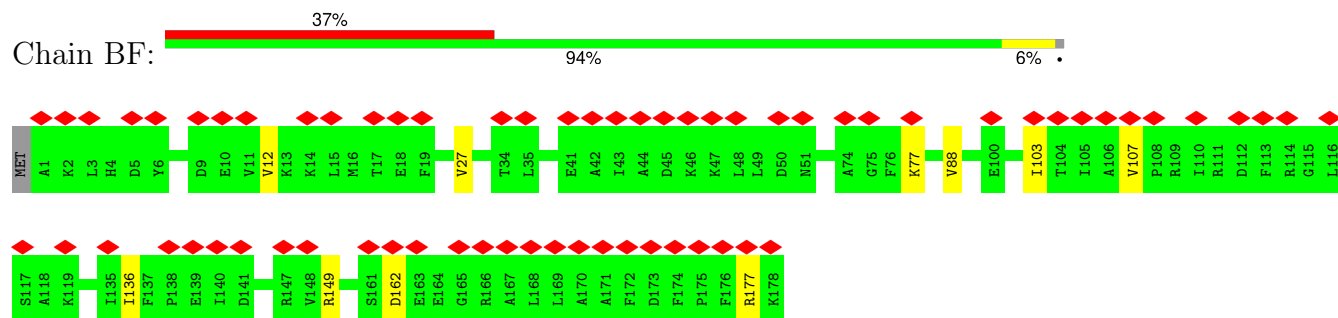
- Molecule 27: 50S ribosomal protein L4

Chain BE:



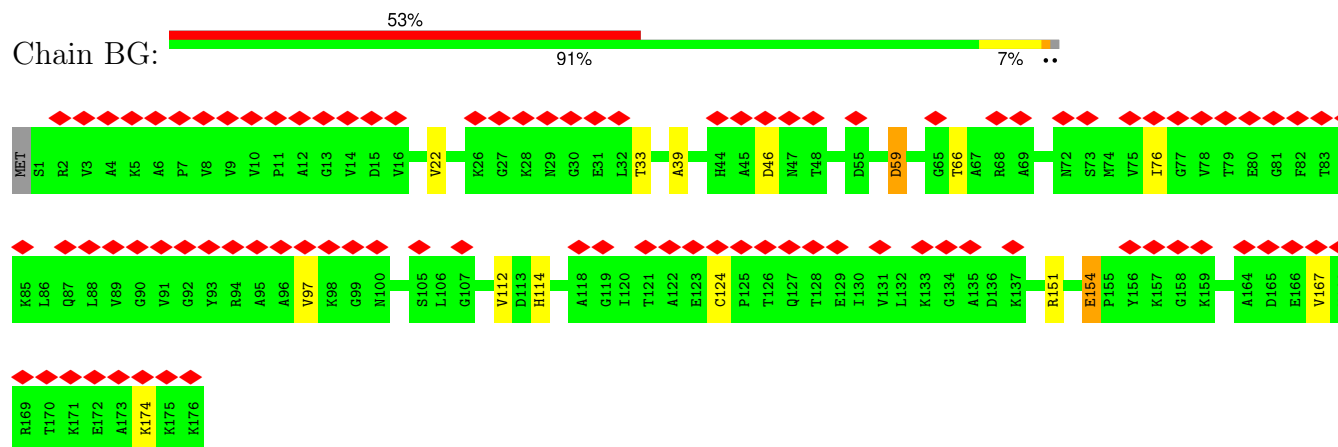
- Molecule 28: 50S ribosomal protein L5

Chain BF:



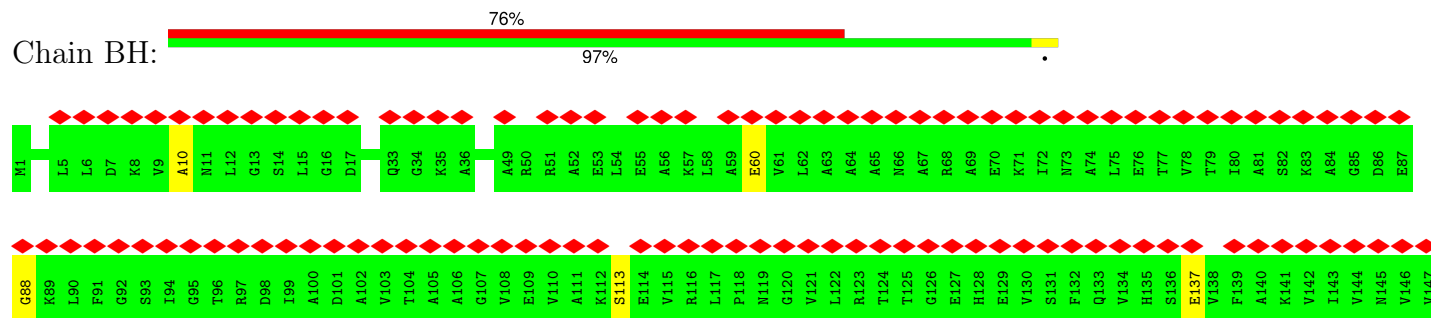
- Molecule 29: 50S ribosomal protein L6

Chain BG:



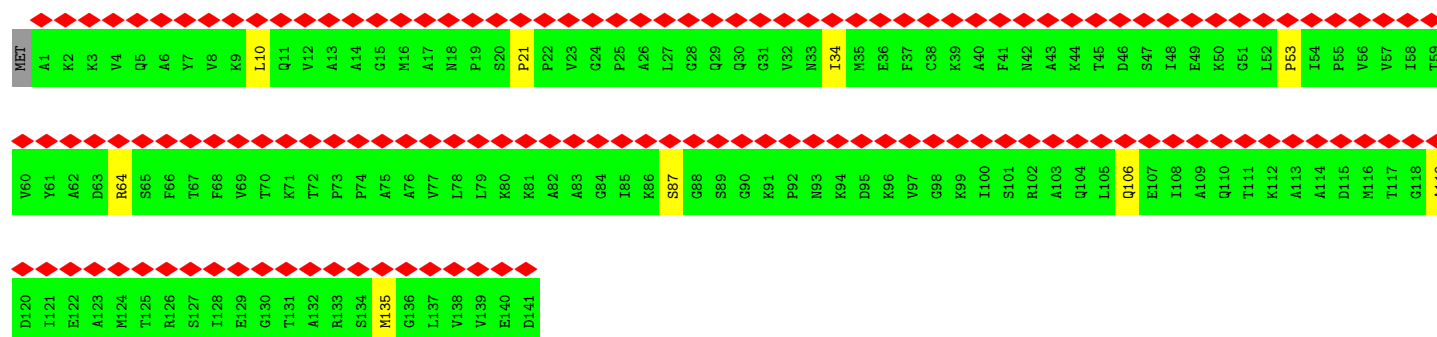
- Molecule 30: 50S ribosomal protein L9

Chain BH:

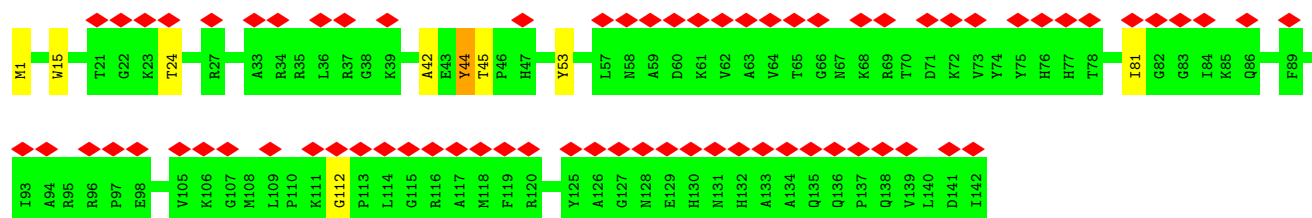




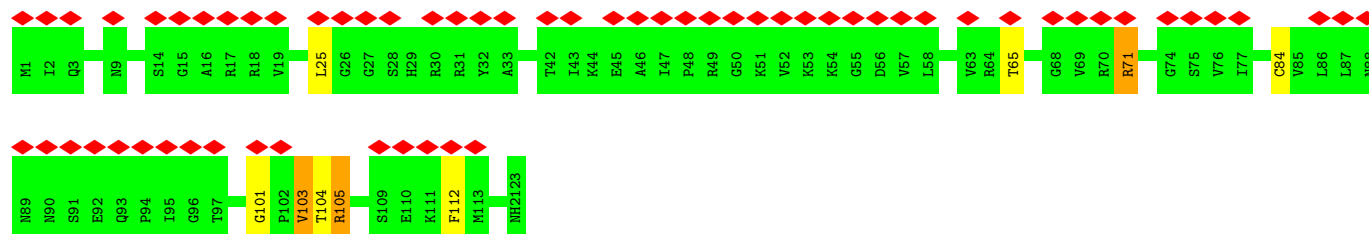
• Molecule 31: 50S ribosomal protein L11



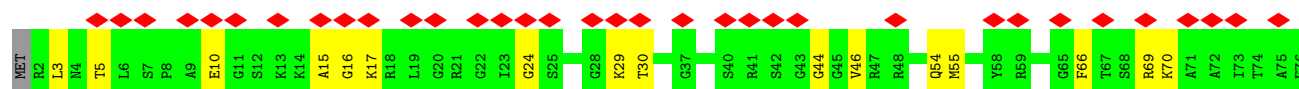
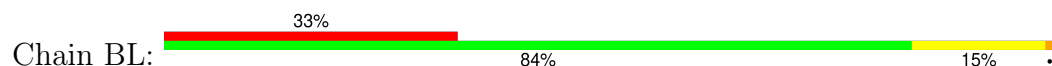
• Molecule 32: 50S ribosomal protein L13

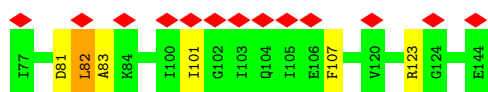


• Molecule 33: 50S ribosomal protein L14

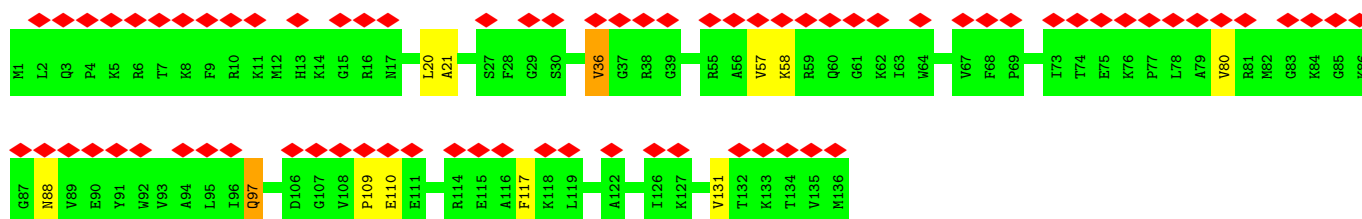


• Molecule 34: 50S ribosomal protein L15

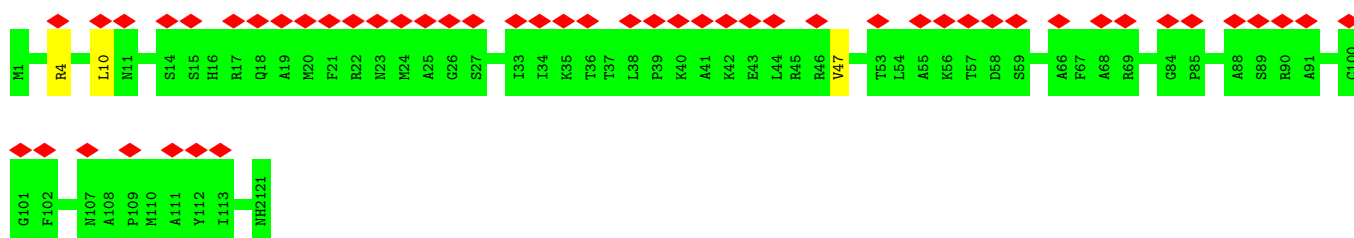
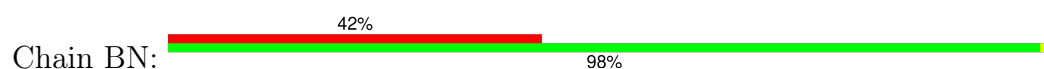




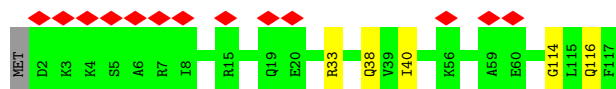
- Molecule 35: 50S ribosomal protein L16



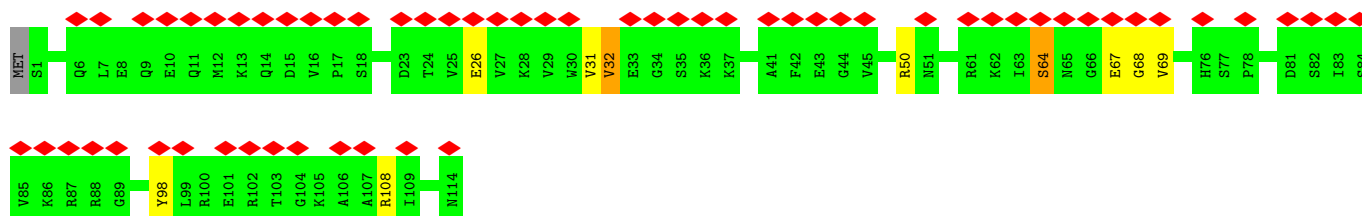
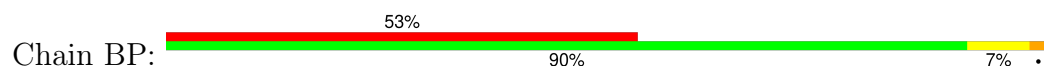
- Molecule 36: 50S ribosomal protein L17



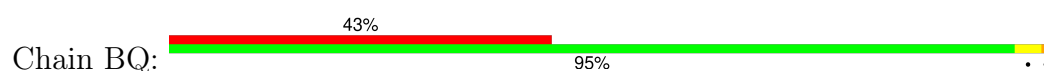
- Molecule 37: 50S ribosomal protein L18

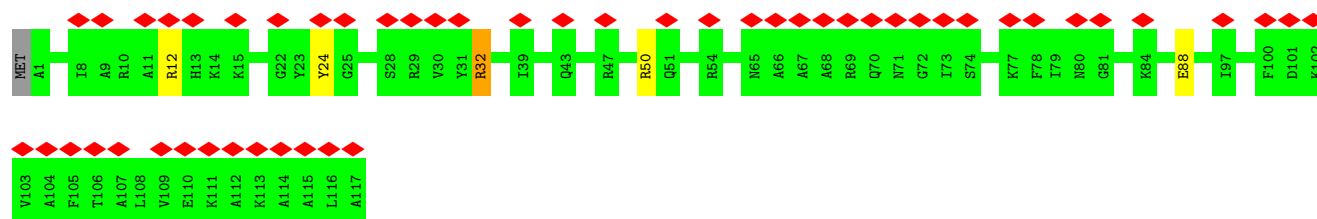


- Molecule 38: 50S ribosomal protein L19

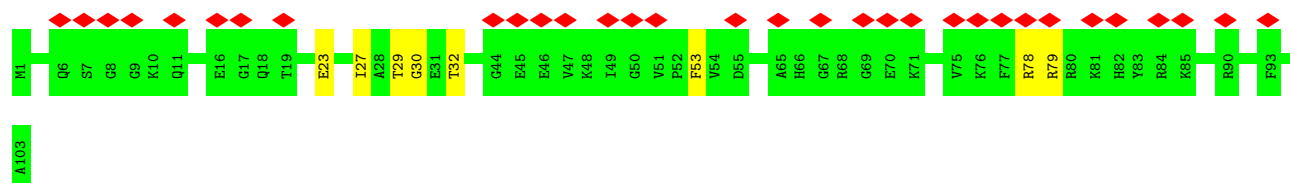


- Molecule 39: 50S ribosomal protein L20

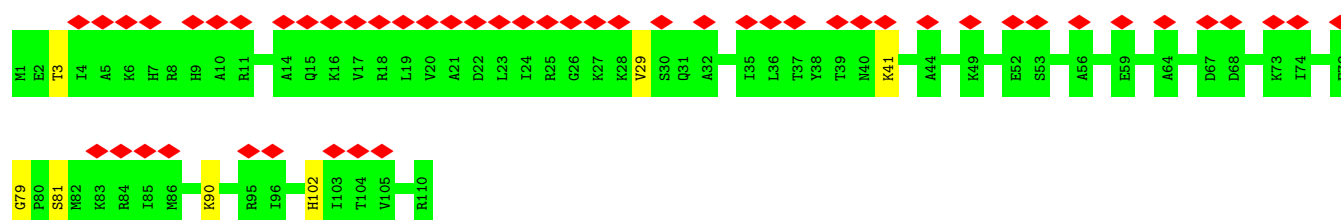




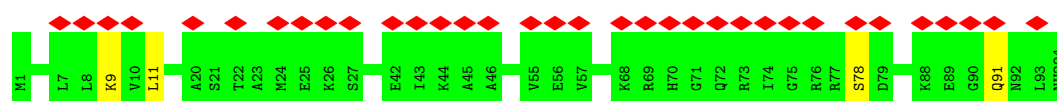
- Molecule 40: 50S ribosomal protein L21



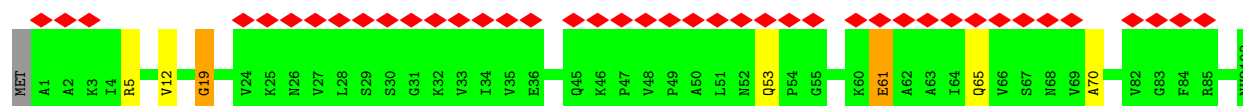
- Molecule 41: 50S ribosomal protein L22



- Molecule 42: 50S ribosomal protein L23

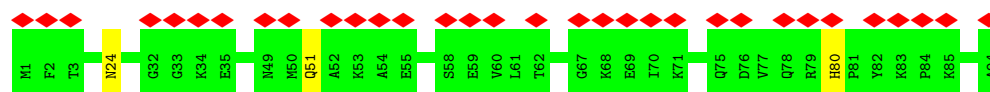


- Molecule 43: 50S ribosomal protein L24

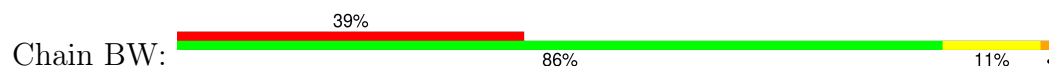


- Molecule 44: 50S ribosomal protein L25

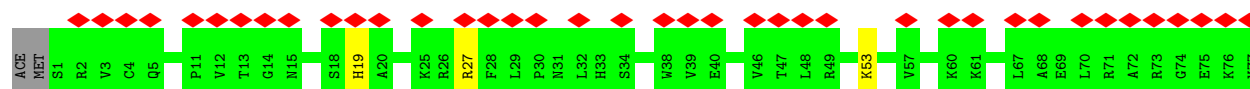




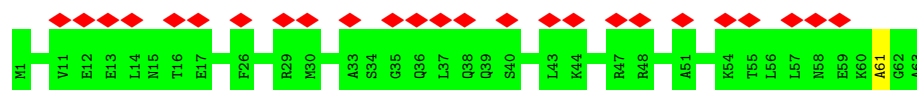
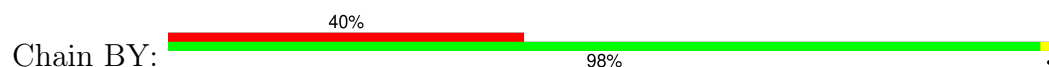
- Molecule 45: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L28



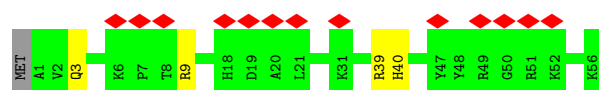
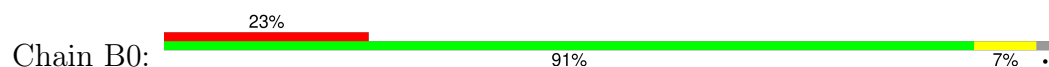
- Molecule 47: 50S ribosomal protein L29



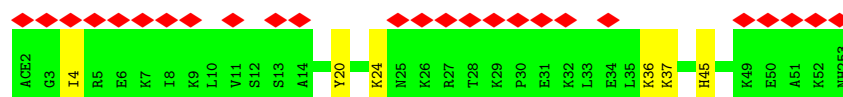
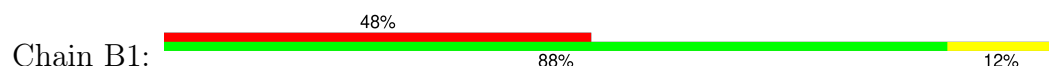
- Molecule 48: 50S ribosomal protein L30



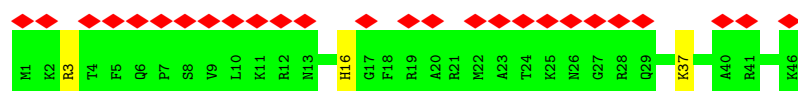
- Molecule 49: 50S ribosomal protein L32



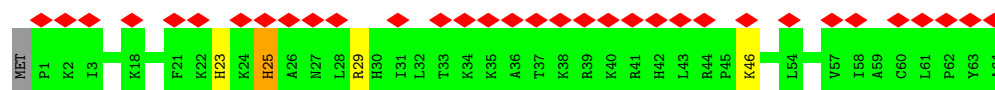
- Molecule 50: 50S ribosomal protein L33



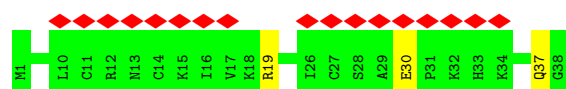
- Molecule 51: 50S ribosomal protein L34



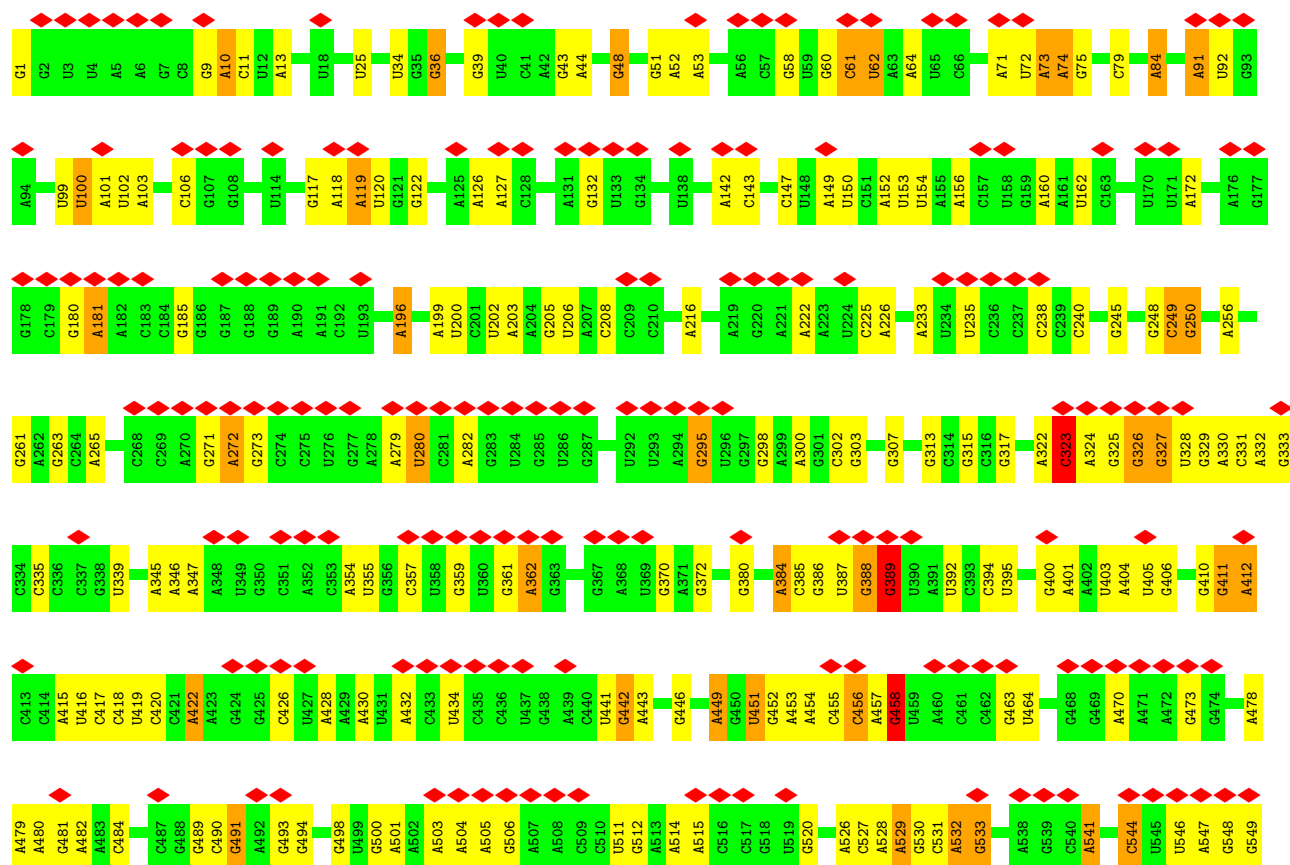
• Molecule 52: 50S ribosomal protein L35

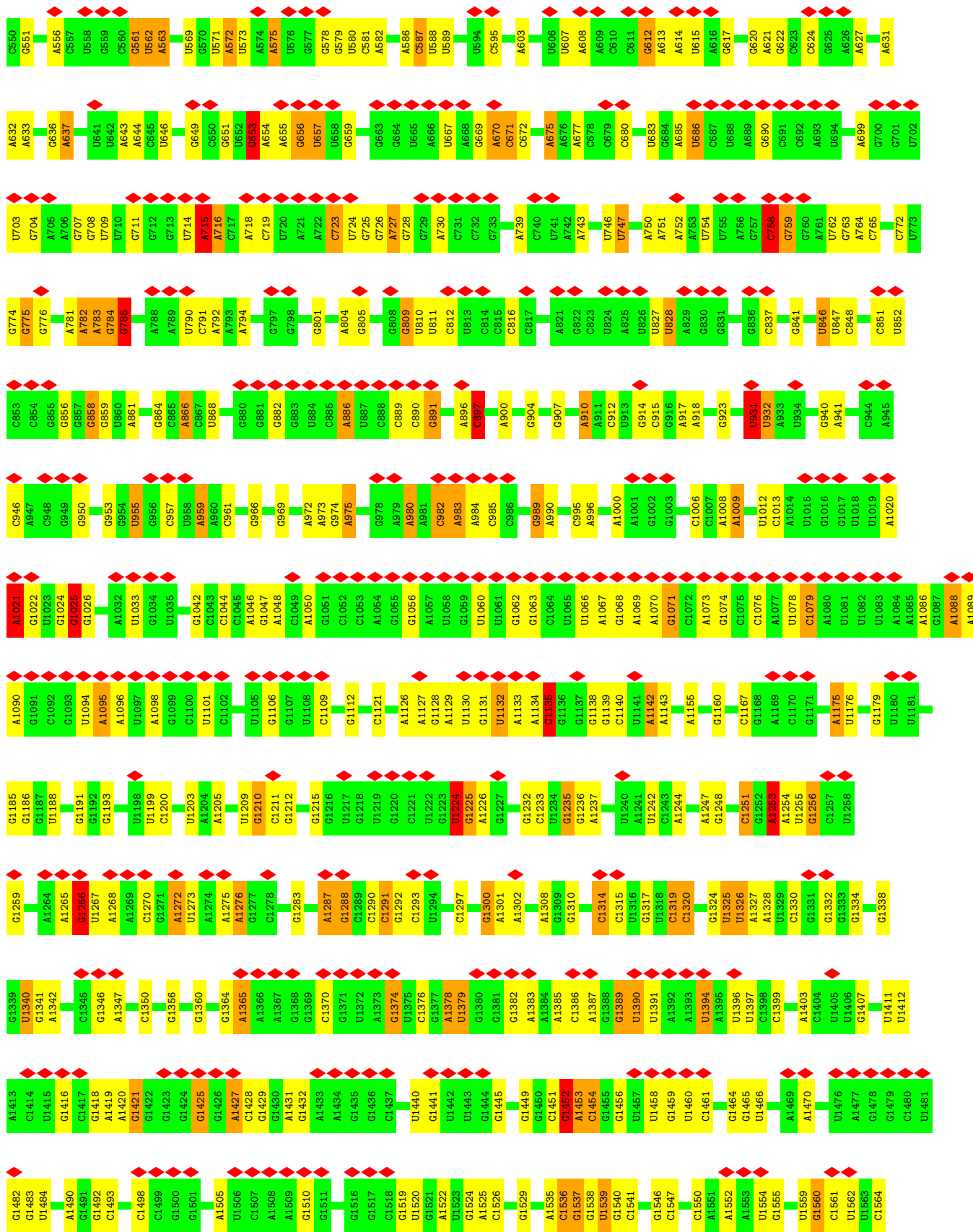


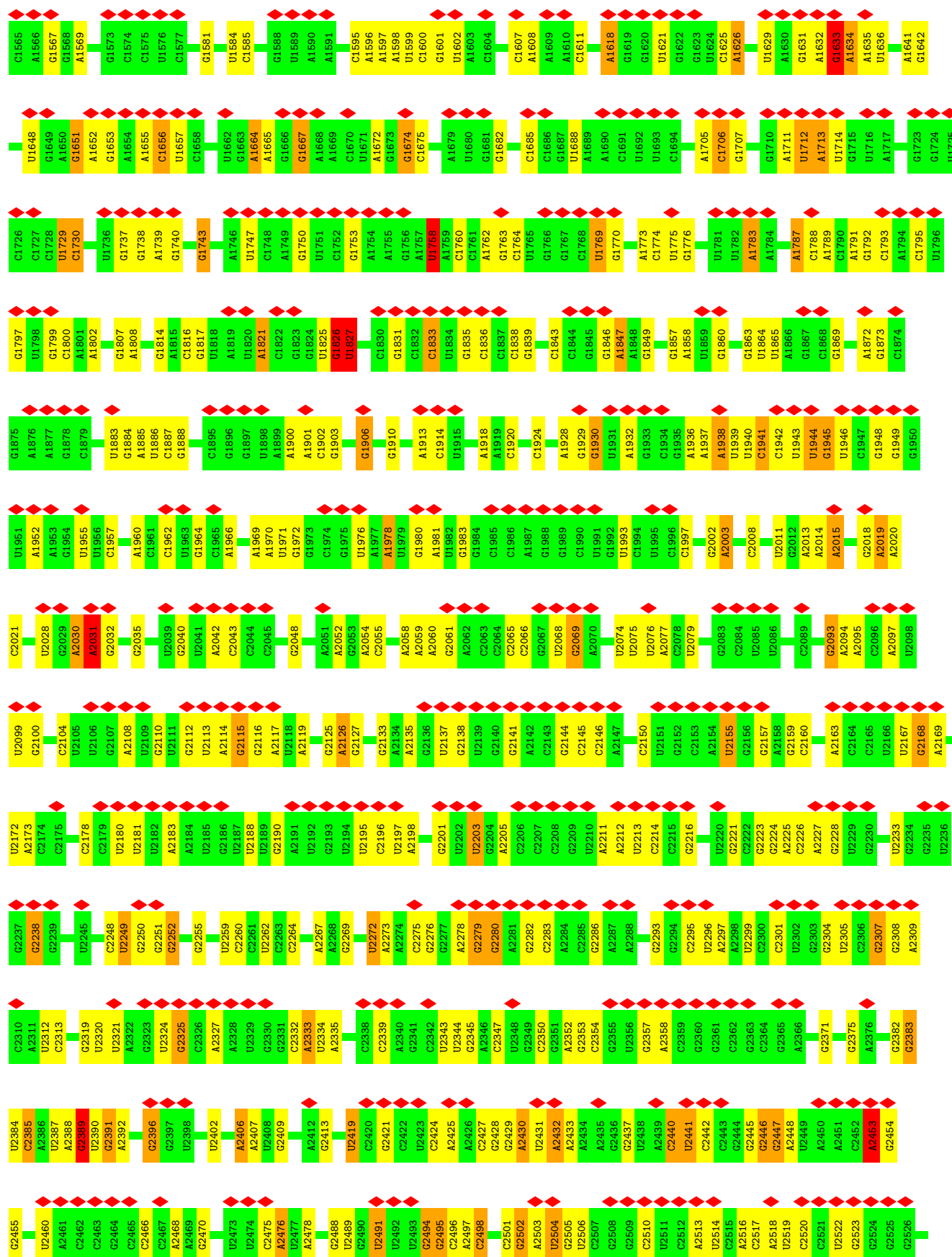
• Molecule 53: 50S ribosomal protein L36

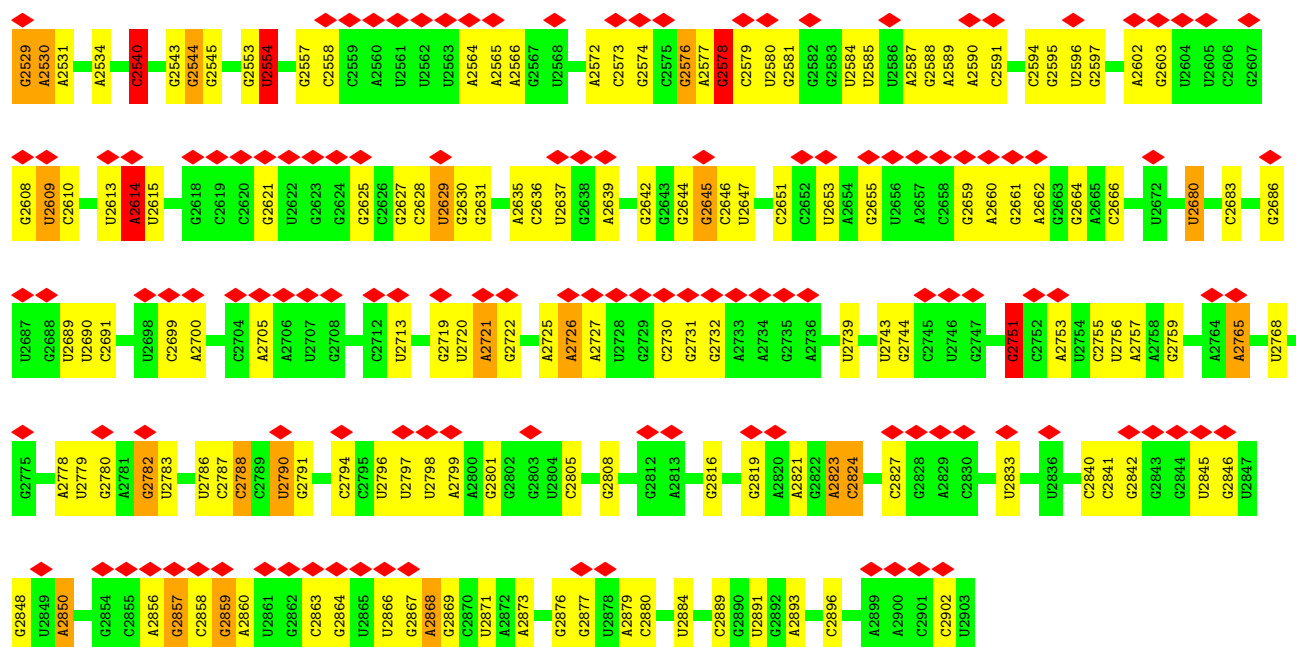


• Molecule 54: 23S ribosomal RNA

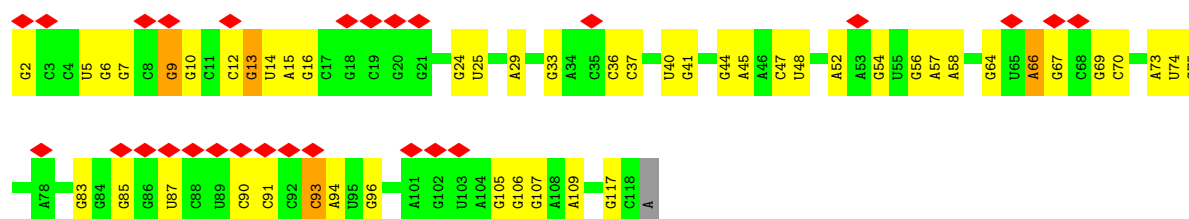




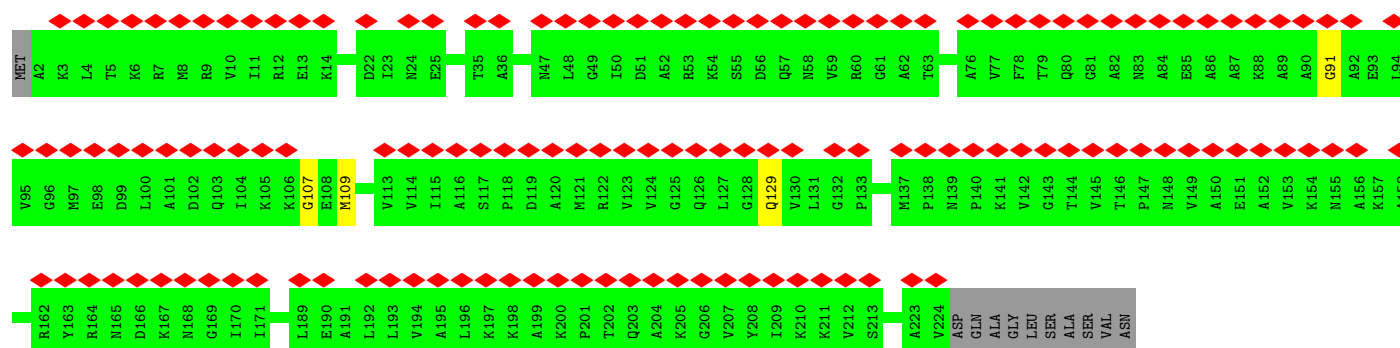




• Molecule 55: 5S ribosomal RNA



• Molecule 56: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13091	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	161000	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	191.487	Depositor
Minimum map value	-133.057	Depositor
Average map value	-0.914	Depositor
Map value standard deviation	20.362	Depositor
Recommended contour level	25	Depositor
Map size ($\text{\AA}$)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.8, 2.8, 2.8	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.98	0/1736	1.41	7/2340 (0.3%)
2	AC	1.04	0/1651	1.42	0/2225
3	AD	1.02	0/1665	1.50	12/2227 (0.5%)
4	AE	0.99	0/1119	1.48	18/1506 (1.2%)
5	AF	1.01	0/835	1.48	4/1128 (0.4%)
6	AG	1.01	0/1188	1.39	0/1593
7	AH	1.01	0/989	1.40	2/1326 (0.2%)
8	AI	1.06	0/1035	1.50	7/1377 (0.5%)
9	AJ	1.06	0/797	1.48	8/1079 (0.7%)
10	AK	1.09	0/894	1.44	3/1207 (0.2%)
11	AL	1.06	0/969	1.44	1/1300 (0.1%)
12	AM	1.09	0/884	1.51	2/1181 (0.2%)
13	AN	1.08	1/817 (0.1%)	1.46	3/1088 (0.3%)
14	AO	1.06	0/722	1.50	4/964 (0.4%)
15	AP	1.10	0/648	1.47	0/870
16	AQ	0.98	0/658	1.40	3/883 (0.3%)
17	AR	1.09	0/463	1.44	2/623 (0.3%)
18	AS	1.09	0/653	1.50	2/879 (0.2%)
19	AT	1.07	0/672	1.47	5/890 (0.6%)
20	AU	1.10	0/431	1.66	2/572 (0.3%)
21	AA	1.24	0/36759	1.20	107/57346 (0.2%)
22	A1	1.25	0/1668	1.22	8/2595 (0.3%)
23	A2	1.19	0/343	1.20	1/531 (0.2%)
24	A3	1.26	0/1722	1.20	6/2685 (0.2%)
25	BC	1.05	1/2121 (0.0%)	1.55	7/2852 (0.2%)
26	BD	0.98	0/1586	1.54	4/2134 (0.2%)
27	BE	0.95	0/1571	1.47	1/2113 (0.0%)
28	BF	0.99	0/1444	1.50	5/1937 (0.3%)
29	BG	0.96	0/1343	1.45	5/1816 (0.3%)
30	BH	0.92	0/1122	1.41	3/1515 (0.2%)
31	BI	0.95	1/1046 (0.1%)	1.48	2/1410 (0.1%)
32	BJ	1.00	0/1152	1.51	4/1551 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BK	1.01	0/947	1.50	5/1268 (0.4%)
34	BL	1.02	0/1054	1.61	11/1403 (0.8%)
35	BM	1.04	0/1093	1.54	9/1460 (0.6%)
36	BN	1.08	0/973	1.49	0/1301
37	BO	1.08	0/902	1.57	7/1209 (0.6%)
38	BP	1.04	0/929	1.57	3/1242 (0.2%)
39	BQ	1.03	0/960	1.48	6/1278 (0.5%)
40	BR	1.00	0/829	1.48	3/1107 (0.3%)
41	BS	0.99	0/864	1.53	6/1156 (0.5%)
42	BT	0.98	0/744	1.52	1/994 (0.1%)
43	BU	0.96	0/787	1.54	4/1051 (0.4%)
44	BV	0.97	0/766	1.48	1/1025 (0.1%)
45	BW	1.00	0/604	1.59	3/799 (0.4%)
46	BX	1.05	0/635	1.55	1/848 (0.1%)
47	BY	0.96	0/510	1.51	0/677
48	BZ	1.10	0/453	1.63	1/605 (0.2%)
49	B0	1.06	0/450	1.60	2/599 (0.3%)
50	B1	0.94	0/417	1.45	0/556
51	B2	1.14	0/380	1.61	2/498 (0.4%)
52	B3	0.99	0/513	1.56	3/676 (0.4%)
53	B4	1.04	0/303	1.51	3/397 (0.8%)
54	BA	1.13	0/69796	1.19	193/108888 (0.2%)
55	BB	1.13	0/2800	1.21	5/4367 (0.1%)
56	B5	0.95	0/1673	1.43	0/2255
All	All	1.13	3/160085 (0.0%)	1.28	507/239402 (0.2%)

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
2	AC	0	2
8	AI	0	1
10	AK	0	1
21	AA	0	365
22	A1	0	10
23	A2	0	1
24	A3	0	14
25	BC	0	2
33	BK	0	1
34	BL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	BA	0	666
55	BB	0	30
All	All	0	1094

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BI	53	PRO	CA-CB	-5.55	1.49	1.53
13	AN	69	ARG	CZ-NH2	-5.45	1.26	1.33
25	BC	176	ARG	CZ-NH2	-5.02	1.26	1.33

All (507) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AE	149	PRO	CA-N-CD	-8.80	99.68	112.00
26	BD	58	ASN	CA-C-N	8.62	137.21	121.70
26	BD	58	ASN	C-N-CA	8.62	137.21	121.70
25	BC	140	VAL	N-CA-C	8.45	118.29	111.62
54	BA	411	G	C2'-C3'-O3'	7.99	121.49	109.50
21	AA	1534	A	C1'-O4'-C4'	-7.68	102.02	109.70
31	BI	21	PRO	N-CA-C	7.58	119.95	110.70
20	AU	47	ALA	CA-C-N	7.41	135.04	121.70
20	AU	47	ALA	C-N-CA	7.41	135.04	121.70
54	BA	1769	U	C4'-C3'-C2'	-7.28	95.32	102.60
21	AA	1337	G	C1'-O4'-C4'	-7.20	102.70	109.90
21	AA	1231	G	C1'-O4'-C4'	-7.13	102.77	109.90
7	AH	53	ASP	CA-C-N	7.02	134.34	121.70
7	AH	53	ASP	C-N-CA	7.02	134.34	121.70
21	AA	36	C	C5'-C4'-C3'	-7.01	105.48	116.00
3	AD	52	VAL	CA-C-N	6.91	134.13	121.70
3	AD	52	VAL	C-N-CA	6.91	134.13	121.70
14	AO	40	GLY	CA-C-N	6.85	134.03	121.70
14	AO	40	GLY	C-N-CA	6.85	134.03	121.70
32	BJ	44	TYR	CA-C-N	6.80	133.94	121.70
32	BJ	44	TYR	C-N-CA	6.80	133.94	121.70
21	AA	413	G	C5'-C4'-C3'	-6.78	105.04	115.20
21	AA	331	G	O4'-C4'-C3'	6.73	110.73	104.00
28	BF	88	VAL	CA-C-N	6.66	130.29	120.90
28	BF	88	VAL	C-N-CA	6.66	130.29	120.90
3	AD	42	ALA	N-CA-C	6.53	118.48	111.36
54	BA	982	C	N1-C1'-C2'	6.45	121.67	112.00
3	AD	42	ALA	O-C-N	-6.40	114.86	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AI	122	ARG	NE-CZ-NH2	6.39	124.95	119.20
26	BD	50	VAL	N-CA-C	6.39	117.31	111.81
54	BA	984	A	O4'-C4'-C3'	6.38	110.38	104.00
54	BA	1942	C	O3'-P-O5'	6.33	113.50	104.00
21	AA	1516	G	O4'-C4'-C3'	6.33	110.33	104.00
4	AE	148	SER	CA-C-N	6.32	127.74	119.84
4	AE	148	SER	C-N-CA	6.32	127.74	119.84
54	BA	1674	G	C2'-C3'-O3'	-6.32	104.22	113.70
54	BA	932	U	O4'-C1'-N1	6.28	117.62	108.20
37	BO	33	ARG	NE-CZ-NH2	6.27	124.84	119.20
54	BA	323	C	O4'-C1'-N1	6.26	117.59	108.20
54	BA	931	U	O4'-C1'-N1	6.26	117.58	108.20
21	AA	755	G	O4'-C4'-C3'	6.24	110.24	104.00
4	AE	45	VAL	CA-C-N	6.20	126.46	122.18
4	AE	45	VAL	C-N-CA	6.20	126.46	122.18
3	AD	42	ALA	CA-C-N	6.20	132.86	121.70
3	AD	42	ALA	C-N-CA	6.20	132.86	121.70
21	AA	194	C	O4'-C4'-C3'	6.18	110.18	104.00
21	AA	1448	C	O4'-C4'-C3'	6.17	110.17	104.00
43	BU	53	GLN	OE1-CD-NE2	-6.16	116.44	122.60
54	BA	2280	G	C4'-C3'-C2'	-6.14	96.45	102.60
54	BA	1224	U	C4'-C3'-O3'	6.14	118.61	109.40
54	BA	2614	A	O3'-P-O5'	-6.14	94.78	104.00
21	AA	150	U	O4'-C4'-C3'	6.14	110.14	104.00
54	BA	677	A	O4'-C4'-C3'	6.14	110.14	104.00
21	AA	120	A	O4'-C4'-C3'	6.12	110.12	104.00
54	BA	2540	C	C1'-O4'-C4'	-6.11	103.79	109.90
54	BA	2755	C	O4'-C4'-C3'	6.11	110.11	104.00
54	BA	621	A	C5'-C4'-C3'	-6.10	106.85	116.00
54	BA	1378	A	C2'-C3'-O3'	6.09	118.63	109.50
54	BA	1826	G	C4'-C3'-C2'	-6.08	96.52	102.60
21	AA	1058	G	O4'-C4'-C3'	6.06	110.06	104.00
9	AJ	91	ASP	O-C-N	-6.04	115.26	123.24
34	BL	10	GLU	CA-C-N	6.03	132.56	121.70
34	BL	10	GLU	C-N-CA	6.03	132.56	121.70
54	BA	2371	G	C4'-C3'-C2'	-6.03	96.57	102.60
54	BA	1071	G	C5'-C4'-C3'	-6.02	106.97	116.00
22	A1	75	C	C1'-O4'-C4'	-6.01	103.89	109.90
54	BA	643	A	O4'-C1'-N9	6.01	117.52	108.50
21	AA	1112	C	O4'-C4'-C3'	6.01	110.01	104.00
54	BA	1776	G	C5'-C4'-C3'	-6.00	107.01	116.00
13	AN	69	ARG	NH1-CZ-NH2	-5.99	111.52	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AE	149	PRO	CA-C-N	5.98	132.47	121.70
4	AE	149	PRO	C-N-CA	5.98	132.47	121.70
54	BA	2823	A	O4'-C4'-C3'	5.97	109.97	104.00
54	BA	1787	A	O4'-C4'-C3'	5.95	109.95	104.00
21	AA	1166	G	O4'-C4'-C3'	5.94	109.94	104.00
21	AA	509	A	O4'-C4'-C3'	5.93	109.94	104.00
54	BA	1	G	C4'-C3'-C2'	-5.93	96.67	102.60
54	BA	126	A	C5'-C4'-C3'	-5.92	107.12	116.00
21	AA	964	A	O4'-C4'-C3'	5.91	109.91	104.00
16	AQ	81	ALA	O-C-N	-5.89	116.20	123.44
21	AA	932	C	C1'-O4'-C4'	-5.89	104.01	109.90
9	AJ	91	ASP	CA-C-N	5.88	132.28	121.70
9	AJ	91	ASP	C-N-CA	5.88	132.28	121.70
29	BG	114	HIS	CB-CG-CD2	-5.88	123.56	131.20
10	AK	117	HIS	CA-C-N	5.86	132.24	121.70
10	AK	117	HIS	C-N-CA	5.86	132.24	121.70
21	AA	1030	U	C1'-O4'-C4'	-5.84	103.86	109.70
55	BB	54	G	O3'-P-O5'	-5.84	95.25	104.00
19	AT	40	ALA	CA-C-N	5.83	132.20	121.70
19	AT	40	ALA	C-N-CA	5.83	132.20	121.70
24	A3	50	G	O4'-C4'-C3'	5.83	109.83	104.00
28	BF	177	ARG	NE-CZ-NH2	5.81	124.43	119.20
54	BA	1541	C	C4'-C3'-C2'	-5.81	96.79	102.60
54	BA	1109	C	C3'-C2'-C1'	5.81	107.11	101.30
54	BA	1762	A	O4'-C4'-C3'	5.81	109.81	104.00
21	AA	523	A	O4'-C4'-C3'	5.80	109.80	104.00
54	BA	2115	G	O4'-C4'-C3'	5.79	109.80	104.00
54	BA	2823	A	C3'-C2'-C1'	5.79	107.09	101.30
54	BA	1667	G	O4'-C4'-C3'	5.77	109.77	104.00
24	A3	69	C	C5'-C4'-C3'	-5.77	107.34	116.00
54	BA	752	A	O4'-C1'-N9	5.77	116.86	108.20
35	BM	88	ASN	OD1-CG-ND2	-5.76	116.84	122.60
54	BA	64	A	O4'-C4'-C3'	5.76	109.76	104.00
54	BA	750	A	O3'-P-O5'	5.76	112.64	104.00
54	BA	1095	A	O4'-C4'-C3'	5.75	109.75	104.00
21	AA	1186	G	O4'-C4'-C3'	5.74	109.74	104.00
24	A3	64	G	O4'-C4'-C3'	5.74	109.74	104.00
54	BA	1826	G	C2'-C3'-O3'	5.74	122.31	113.70
54	BA	1846	G	C2'-C3'-O3'	-5.74	105.08	113.70
54	BA	1634	A	C4'-C3'-O3'	5.74	118.01	109.40
54	BA	1597	A	C2'-C3'-O3'	-5.74	105.09	113.70
21	AA	455	G	O4'-C4'-C3'	5.74	109.74	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	B3	23	HIS	CA-C-N	5.73	129.77	120.60
52	B3	23	HIS	C-N-CA	5.73	129.77	120.60
54	BA	441	U	C4'-C3'-C2'	-5.73	96.87	102.60
3	AD	52	VAL	O-C-N	-5.73	115.41	122.57
21	AA	567	G	O4'-C4'-C3'	5.73	109.73	104.00
41	BS	102	HIS	CB-CG-CD2	-5.73	123.75	131.20
4	AE	85	LYS	CA-C-N	5.72	125.54	121.65
4	AE	85	LYS	C-N-CA	5.72	125.54	121.65
54	BA	886	A	C4'-C3'-C2'	-5.71	96.89	102.60
49	B0	9	ARG	NE-CZ-NH2	5.70	124.33	119.20
4	AE	104	ILE	O-C-N	-5.68	115.48	122.57
21	AA	139	A	O4'-C4'-C3'	5.67	109.67	104.00
21	AA	483	C	O4'-C4'-C3'	5.67	109.67	104.00
21	AA	1110	A	O4'-C4'-C3'	5.67	109.67	104.00
21	AA	1335	U	O4'-C4'-C3'	5.67	109.67	104.00
38	BP	108	ARG	NE-CZ-NH2	5.67	124.30	119.20
54	BA	2382	G	C2'-C3'-O3'	-5.66	105.20	113.70
37	BO	116	GLN	O-C-N	-5.66	115.93	122.95
54	BA	2504	U	O3'-P-O5'	5.66	112.48	104.00
54	BA	482	A	O4'-C4'-C3'	5.65	109.65	104.00
22	A1	69	A	O4'-C4'-C3'	5.65	109.65	104.00
54	BA	1429	G	O4'-C4'-C3'	5.65	109.65	104.00
21	AA	366	A	P-O3'-C3'	5.65	128.67	120.20
54	BA	1938	A	C1'-O4'-C4'	-5.65	104.05	109.70
54	BA	715	A	O4'-C4'-C3'	5.64	109.64	104.00
21	AA	414	A	O4'-C4'-C3'	5.64	109.64	104.00
54	BA	2095	A	C4'-C3'-C2'	-5.64	96.96	102.60
1	AB	167	HIS	CB-CG-CD2	-5.63	123.88	131.20
54	BA	670	A	C2'-C3'-O3'	5.63	117.95	109.50
54	BA	1338	G	O4'-C4'-C3'	5.63	109.63	104.00
54	BA	362	A	C5'-C4'-C3'	-5.63	107.55	116.00
21	AA	1092	A	O4'-C4'-C3'	5.63	109.63	104.00
54	BA	2751	G	O4'-C1'-N9	5.62	116.63	108.20
21	AA	492	C	O4'-C4'-C3'	5.62	109.62	104.00
16	AQ	81	ALA	CA-C-N	5.62	131.81	121.70
16	AQ	81	ALA	C-N-CA	5.62	131.81	121.70
54	BA	2052	A	O4'-C1'-C2'	-5.61	101.99	107.60
13	AN	94	PRO	CA-C-N	5.61	131.79	121.70
13	AN	94	PRO	C-N-CA	5.61	131.79	121.70
54	BA	1964	G	C3'-C2'-C1'	5.61	107.11	101.50
12	AM	111	PRO	CA-C-N	5.61	131.79	121.70
12	AM	111	PRO	C-N-CA	5.61	131.79	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1337	G	O3'-P-O5'	-5.60	95.60	104.00
54	BA	2554	U	C5'-C4'-C3'	-5.60	107.60	116.00
54	BA	897	C	O4'-C1'-C2'	-5.60	102.00	107.60
21	AA	483	C	C3'-C2'-C1'	5.58	106.89	101.30
4	AE	120	HIS	CB-CG-CD2	-5.58	123.95	131.20
21	AA	229	U	O4'-C4'-C3'	5.58	109.58	104.00
43	BU	19	GLY	CA-C-N	5.58	129.62	121.31
43	BU	19	GLY	C-N-CA	5.58	129.62	121.31
21	AA	495	A	C5'-C4'-C3'	-5.57	106.84	115.20
22	A1	45	G	O4'-C4'-C3'	5.57	109.57	104.00
54	BA	2275	C	C3'-C2'-C1'	5.57	106.87	101.30
54	BA	53	A	C4'-C3'-C2'	-5.56	97.04	102.60
21	AA	162	A	O4'-C4'-C3'	5.56	109.56	104.00
54	BA	91	A	O4'-C1'-N9	5.55	116.53	108.20
54	BA	2307	G	O4'-C1'-N9	5.55	116.53	108.20
21	AA	153	C	O4'-C4'-C3'	5.55	109.55	104.00
54	BA	2068	U	C1'-O4'-C4'	-5.54	104.36	109.90
3	AD	40	HIS	CB-CG-CD2	-5.54	123.99	131.20
54	BA	1706	C	C4'-C3'-O3'	5.54	117.72	109.40
24	A3	35	C	O4'-C4'-C3'	5.54	109.54	104.00
54	BA	380	G	C4'-C3'-C2'	-5.54	97.06	102.60
22	A1	18	G	O4'-C4'-C3'	5.54	109.53	104.00
21	AA	309	A	O4'-C4'-C3'	5.53	109.53	104.00
39	BQ	24	TYR	N-CA-C	5.53	118.83	111.75
54	BA	1872	A	O4'-C4'-C3'	5.53	109.53	104.00
11	AL	5	GLN	OE1-CD-NE2	-5.52	117.08	122.60
4	AE	149	PRO	O-C-N	-5.52	115.19	122.64
54	BA	2857	G	O4'-C4'-C3'	5.51	109.51	104.00
54	BA	723	C	C4'-C3'-C2'	-5.49	97.11	102.60
21	AA	129	A	O3'-P-O5'	-5.49	95.77	104.00
54	BA	1775	U	C4'-C3'-C2'	-5.49	97.11	102.60
54	BA	1253	A	C5'-C4'-C3'	-5.49	106.97	115.20
21	AA	532	A	C1'-O4'-C4'	-5.49	104.22	109.70
34	BL	54	GLN	OE1-CD-NE2	-5.48	117.12	122.60
37	BO	116	GLN	CA-C-N	5.48	131.57	121.70
37	BO	116	GLN	C-N-CA	5.48	131.57	121.70
54	BA	36	G	O4'-C4'-C3'	5.48	109.48	104.00
43	BU	65	GLN	OE1-CD-NE2	-5.48	117.12	122.60
5	AF	73	GLU	CA-C-N	5.48	128.38	120.38
5	AF	73	GLU	C-N-CA	5.48	128.38	120.38
54	BA	295	G	C5'-C4'-C3'	-5.48	107.78	116.00
21	AA	1338	G	C1'-O4'-C4'	-5.47	104.43	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	180	G	C2'-C3'-O3'	-5.47	105.49	113.70
21	AA	1339	A	O4'-C4'-C3'	5.46	109.46	104.00
54	BA	1021	A	O4'-C4'-C3'	5.46	109.45	104.00
54	BA	989	G	C4'-C3'-O3'	5.45	121.18	113.00
21	AA	460	A	O4'-C4'-C3'	5.45	109.45	104.00
21	AA	561	U	C3'-C2'-C1'	5.45	106.95	101.50
5	AF	67	PRO	N-CA-CB	5.44	108.40	103.34
54	BA	132	G	O4'-C4'-C3'	5.44	109.44	104.00
54	BA	2453	A	O4'-C4'-C3'	5.44	109.44	104.00
54	BA	2584	U	C4'-C3'-C2'	-5.44	97.16	102.60
54	BA	2902	C	C4'-C3'-C2'	-5.44	97.16	102.60
40	BR	78	ARG	NE-CZ-NH2	5.43	124.09	119.20
54	BA	2495	G	C5'-C4'-C3'	-5.43	107.85	116.00
54	BA	1325	U	O4'-C1'-C2'	-5.43	100.37	105.80
54	BA	2387	U	O4'-C4'-C3'	5.43	109.43	104.00
22	A1	16	C	O4'-C4'-C3'	5.43	109.43	104.00
54	BA	1611	C	O4'-C4'-C3'	5.43	109.43	104.00
28	BF	149	ARG	CA-C-N	5.42	126.18	120.43
28	BF	149	ARG	C-N-CA	5.42	126.18	120.43
54	BA	2860	A	O4'-C4'-C3'	5.42	109.42	104.00
4	AE	104	ILE	CA-C-N	5.42	131.45	121.70
4	AE	104	ILE	C-N-CA	5.42	131.45	121.70
21	AA	439	U	O4'-C4'-C3'	5.42	109.42	104.00
21	AA	374	A	O4'-C4'-C3'	5.41	109.41	104.00
21	AA	861	G	O4'-C4'-C3'	5.41	109.41	104.00
21	AA	1300	G	O4'-C4'-C3'	5.41	109.41	104.00
21	AA	282	A	C5'-C4'-C3'	-5.40	107.89	116.00
1	AB	10	LYS	CA-C-N	5.40	131.42	121.70
1	AB	10	LYS	C-N-CA	5.40	131.42	121.70
19	AT	47	GLN	CA-C-N	5.40	127.51	120.28
19	AT	47	GLN	C-N-CA	5.40	127.51	120.28
54	BA	44	A	O4'-C4'-C3'	5.39	109.39	104.00
54	BA	2031	A	C3'-C2'-C1'	5.39	106.69	101.30
21	AA	251	G	O4'-C1'-N9	5.39	116.28	108.20
54	BA	1425	G	O3'-P-O5'	5.39	112.08	104.00
14	AO	39	GLN	OE1-CD-NE2	-5.39	117.21	122.60
21	AA	449	G	O4'-C4'-C3'	5.39	109.39	104.00
21	AA	1105	A	O4'-C4'-C3'	5.39	109.39	104.00
54	BA	2272	U	O4'-C4'-C3'	5.38	109.38	104.00
10	AK	116	PRO	N-CA-CB	5.38	107.96	103.17
21	AA	1460	C	O4'-C4'-C3'	5.38	109.38	104.00
54	BA	1791	A	O4'-C4'-C3'	5.37	109.37	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	389	G	O4'-C4'-C3'	5.37	109.37	104.00
54	BA	1121	C	C4'-C3'-C2'	-5.37	97.23	102.60
21	AA	723	U	O3'-P-O5'	5.37	112.05	104.00
21	AA	993	G	C5'-C4'-C3'	-5.37	107.15	115.20
21	AA	1431	A	C3'-C2'-C1'	5.37	106.87	101.50
21	AA	519	C	C1'-O4'-C4'	-5.37	104.53	109.90
54	BA	1685	C	C4'-C3'-C2'	-5.36	97.24	102.60
54	BA	2031	A	O4'-C4'-C3'	5.36	109.36	104.00
54	BA	2114	A	O4'-C4'-C3'	5.36	109.36	104.00
21	AA	1133	G	O4'-C4'-C3'	5.36	109.36	104.00
41	BS	41	LYS	CA-C-N	5.36	127.72	120.38
41	BS	41	LYS	C-N-CA	5.36	127.72	120.38
55	BB	6	G	C4'-C3'-C2'	-5.36	97.24	102.60
8	AI	122	ARG	CA-C-N	5.35	127.83	120.39
8	AI	122	ARG	C-N-CA	5.35	127.83	120.39
54	BA	1235	G	O4'-C4'-C3'	5.35	109.35	104.00
54	BA	2059	A	O4'-C4'-C3'	5.35	109.35	104.00
54	BA	2319	G	O4'-C4'-C3'	5.35	109.35	104.00
54	BA	675	A	C4'-C3'-C2'	-5.35	97.25	102.60
54	BA	300	A	O4'-C4'-C3'	5.35	109.35	104.00
3	AD	197	HIS	CB-CG-CD2	-5.35	124.25	131.20
21	AA	1101	A	P-O3'-C3'	5.35	128.22	120.20
54	BA	2782	G	O4'-C4'-C3'	5.35	109.35	104.00
8	AI	54	VAL	CA-C-N	5.34	131.75	121.54
8	AI	54	VAL	C-N-CA	5.34	131.75	121.54
45	BW	39	GLN	OE1-CD-NE2	-5.34	117.26	122.60
54	BA	530	G	O4'-C4'-C3'	5.34	109.34	104.00
54	BA	1427	A	C2'-C3'-O3'	5.34	117.52	109.50
25	BC	229	HIS	CB-CG-CD2	-5.34	124.26	131.20
40	BR	79	ARG	CA-C-N	5.34	131.31	121.70
40	BR	79	ARG	C-N-CA	5.34	131.31	121.70
45	BW	38	ARG	CA-C-N	5.34	128.43	120.95
45	BW	38	ARG	C-N-CA	5.34	128.43	120.95
54	BA	422	A	O4'-C4'-C3'	5.34	109.34	104.00
21	AA	1148	U	O4'-C4'-C3'	5.34	109.34	104.00
52	B3	29	ARG	N-CA-C	5.34	119.94	113.38
33	BK	112	PHE	CA-C-N	5.33	127.42	120.28
33	BK	112	PHE	C-N-CA	5.33	127.42	120.28
42	BT	91	GLN	OE1-CD-NE2	-5.33	117.27	122.60
54	BA	1847	A	O4'-C1'-N9	5.33	116.50	108.50
54	BA	2680	U	C5'-C4'-C3'	-5.33	108.00	116.00
21	AA	442	G	O4'-C4'-C3'	5.33	109.33	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2279	G	C4'-C3'-C2'	-5.32	97.28	102.60
53	B4	30	GLU	CA-C-N	5.32	125.03	119.82
53	B4	30	GLU	C-N-CA	5.32	125.03	119.82
21	AA	379	C	O4'-C4'-C3'	5.32	109.32	104.00
54	BA	1758	U	O4'-C1'-N1	5.32	116.18	108.20
21	AA	1240	U	C5'-C4'-C3'	-5.32	108.03	116.00
54	BA	2755	C	C3'-C2'-C1'	5.31	106.61	101.30
54	BA	1795	C	C4'-C3'-C2'	-5.31	97.29	102.60
54	BA	1783	A	O4'-C4'-C3'	5.31	109.31	104.00
39	BQ	12	ARG	NE-CZ-NH2	5.30	123.97	119.20
54	BA	245	G	C5'-C4'-C3'	-5.30	108.05	116.00
54	BA	1634	A	C2'-C3'-O3'	5.30	117.45	109.50
54	BA	809	G	C4'-C3'-C2'	-5.30	97.30	102.60
54	BA	1564	C	O4'-C4'-C3'	5.29	109.29	104.00
54	BA	2167	U	O4'-C4'-C3'	5.29	109.29	104.00
54	BA	2788	C	C4'-C3'-C2'	-5.29	97.31	102.60
21	AA	1469	C	C3'-C2'-C1'	5.29	106.59	101.30
54	BA	1389	G	O4'-C4'-C3'	5.29	109.29	104.00
54	BA	1290	C	C4'-C3'-C2'	-5.28	97.32	102.60
21	AA	675	A	O4'-C4'-C3'	5.28	109.28	104.00
54	BA	2719	G	O4'-C4'-C3'	5.28	109.28	104.00
21	AA	311	C	C5'-C4'-C3'	-5.27	108.09	116.00
14	AO	50	HIS	CB-CG-CD2	-5.27	124.35	131.20
54	BA	2214	C	O4'-C4'-C3'	5.27	109.27	104.00
54	BA	2726	A	O4'-C1'-C2'	-5.27	100.53	105.80
3	AD	53	GLN	CA-C-N	5.27	127.65	120.54
3	AD	53	GLN	C-N-CA	5.27	127.65	120.54
21	AA	1216	A	C4'-C3'-C2'	-5.27	97.33	102.60
19	AT	73	ARG	NH1-CZ-NH2	-5.27	112.45	119.30
54	BA	653	U	O4'-C1'-N1	5.26	116.38	108.50
54	BA	1185	G	C2'-C3'-O3'	-5.26	105.81	113.70
24	A3	62	C	O4'-C4'-C3'	5.25	109.25	104.00
21	AA	610	U	C1'-O4'-C4'	-5.25	104.65	109.90
21	AA	1201	A	C5'-C4'-C3'	-5.25	107.32	115.20
5	AF	3	HIS	CB-CG-CD2	-5.25	124.38	131.20
21	AA	570	G	O4'-C4'-C3'	5.25	109.25	104.00
54	BA	1449	G	C4'-C3'-C2'	-5.25	97.35	102.60
39	BQ	50	ARG	NE-CZ-NH2	5.25	123.92	119.20
54	BA	575	A	C1'-O4'-C4'	-5.25	104.65	109.90
21	AA	207	C	O4'-C4'-C3'	5.25	109.25	104.00
35	BM	117	PHE	CA-C-N	5.25	127.56	120.38
35	BM	117	PHE	C-N-CA	5.25	127.56	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	BS	79	GLY	CA-C-N	5.24	125.41	119.90
41	BS	79	GLY	C-N-CA	5.24	125.41	119.90
49	B0	3	GLN	OE1-CD-NE2	-5.24	117.36	122.60
4	AE	157	GLY	CA-C-N	5.24	131.13	121.70
4	AE	157	GLY	C-N-CA	5.24	131.13	121.70
25	BC	199	HIS	CB-CG-CD2	-5.24	124.39	131.20
54	BA	1346	G	C4'-C3'-C2'	-5.24	97.36	102.60
21	AA	292	G	C5'-C4'-C3'	-5.24	108.14	116.00
1	AB	72	LYS	CA-C-N	5.24	127.55	120.38
1	AB	72	LYS	C-N-CA	5.24	127.55	120.38
54	BA	622	G	C5'-C4'-C3'	-5.24	108.14	116.00
9	AJ	20	GLN	OE1-CD-NE2	-5.24	117.36	122.60
54	BA	2529	G	O4'-C4'-C3'	5.24	109.24	104.00
54	BA	2666	C	O4'-C1'-N1	5.24	116.35	108.50
54	BA	2168	G	O4'-C4'-C3'	5.23	109.23	104.00
54	BA	1175	A	C5'-C4'-C3'	-5.23	108.16	116.00
51	B2	3	ARG	NE-CZ-NH2	5.23	123.91	119.20
44	BV	80	HIS	CB-CG-CD2	-5.22	124.41	131.20
54	BA	2642	G	C4'-C3'-C2'	-5.22	97.38	102.60
30	BH	60	GLU	CA-C-N	5.22	127.13	120.56
30	BH	60	GLU	C-N-CA	5.22	127.13	120.56
21	AA	944	G	O4'-C4'-C3'	5.21	109.22	104.00
54	BA	403	U	C2'-C3'-O3'	-5.21	105.88	113.70
54	BA	280	U	O4'-C1'-N1	5.21	116.31	108.50
54	BA	2333	A	O4'-C4'-C3'	5.21	109.21	104.00
23	A2	80	C	O4'-C4'-C3'	5.21	109.21	104.00
35	BM	97	GLN	CA-C-N	5.21	125.26	119.32
35	BM	97	GLN	C-N-CA	5.21	125.26	119.32
34	BL	16	GLY	CA-C-N	5.20	131.07	121.70
34	BL	16	GLY	C-N-CA	5.20	131.07	121.70
48	BZ	19	HIS	CB-CG-CD2	-5.20	124.44	131.20
21	AA	161	A	O4'-C4'-C3'	5.20	109.20	104.00
54	BA	1407	G	C4'-C3'-C2'	-5.20	97.41	102.60
30	BH	113	SER	N-CA-C	5.19	117.76	110.23
34	BL	24	GLY	CA-C-N	5.19	131.04	121.70
34	BL	24	GLY	C-N-CA	5.19	131.04	121.70
32	BJ	24	THR	CA-C-N	5.19	127.55	120.54
32	BJ	24	THR	C-N-CA	5.19	127.55	120.54
54	BA	1266	G	O3'-P-O5'	-5.19	96.22	104.00
54	BA	1930	G	C3'-C2'-C1'	-5.19	96.31	101.50
21	AA	447	G	O4'-C4'-C3'	5.18	109.19	104.00
9	AJ	41	PRO	CA-C-N	5.18	134.44	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AJ	41	PRO	C-N-CA	5.18	134.44	121.80
54	BA	1706	C	C2'-C3'-O3'	5.17	117.26	109.50
21	AA	641	U	C3'-C2'-C1'	5.17	106.67	101.50
37	BO	114	GLY	CA-C-N	5.17	128.19	120.90
37	BO	114	GLY	C-N-CA	5.17	128.19	120.90
21	AA	71	A	O4'-C4'-C3'	5.17	109.17	104.00
21	AA	338	A	O4'-C4'-C3'	5.16	109.16	104.00
21	AA	1402	C	O4'-C4'-C3'	5.16	109.16	104.00
22	A1	35	A	O4'-C4'-C3'	5.16	109.16	104.00
54	BA	1559	U	O4'-C1'-N1	5.16	115.94	108.20
21	AA	1066	C	O4'-C4'-C3'	5.16	109.16	104.00
25	BC	234	GLY	CA-C-N	5.16	130.99	121.70
25	BC	234	GLY	C-N-CA	5.16	130.99	121.70
54	BA	388	G	O4'-C4'-C3'	5.16	109.16	104.00
54	BA	2319	G	C5'-C4'-C3'	-5.16	108.26	116.00
31	BI	106	GLN	OE1-CD-NE2	-5.16	117.44	122.60
21	AA	190	A	O4'-C4'-C3'	5.16	109.16	104.00
54	BA	2110	G	C3'-C2'-C1'	-5.16	96.34	101.50
33	BK	71	ARG	CB-CA-C	5.16	120.33	110.17
54	BA	2019	A	O4'-C4'-C3'	5.16	109.16	104.00
55	BB	93	C	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	2578	G	C4'-C3'-C2'	-5.15	97.45	102.60
54	BA	2015	A	O4'-C4'-C3'	5.15	109.15	104.00
21	AA	1345	U	C1'-O4'-C4'	-5.15	104.55	109.70
54	BA	758	C	C4'-C3'-C2'	-5.15	97.45	102.60
1	AB	23	ASN	CA-C-N	5.15	124.81	119.56
1	AB	23	ASN	C-N-CA	5.15	124.81	119.56
35	BM	109	PRO	CA-C-N	5.15	131.37	121.54
35	BM	109	PRO	C-N-CA	5.15	131.37	121.54
3	AD	62	ARG	NH1-CZ-NH2	-5.14	112.61	119.30
54	BA	2293	G	O4'-C4'-C3'	5.14	109.14	104.00
17	AR	48	ALA	CA-C-N	5.14	127.42	120.38
17	AR	48	ALA	C-N-CA	5.14	127.42	120.38
21	AA	892	A	O4'-C4'-C3'	5.14	109.14	104.00
54	BA	394	C	C4'-C3'-C2'	-5.14	97.46	102.60
21	AA	1151	A	C5'-C4'-C3'	-5.14	108.30	116.00
54	BA	828	U	C5'-C4'-C3'	-5.13	108.30	116.00
54	BA	2389	G	O4'-C4'-C3'	5.13	109.14	104.00
4	AE	107	GLY	CA-C-N	5.13	125.78	120.03
4	AE	107	GLY	C-N-CA	5.13	125.78	120.03
21	AA	1503	A	C1'-O4'-C4'	-5.13	104.57	109.70
8	AI	123	ARG	CA-C-N	5.13	126.25	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AI	123	ARG	C-N-CA	5.13	126.25	119.84
54	BA	160	A	C4'-C3'-C2'	-5.13	97.47	102.60
54	BA	1978	A	O4'-C4'-C3'	5.13	109.13	104.00
34	BL	3	LEU	O-C-N	-5.13	117.00	122.85
54	BA	709	U	C4'-C3'-C2'	-5.13	97.47	102.60
54	BA	563	A	C5'-C4'-C3'	-5.13	108.31	116.00
54	BA	2578	G	C1'-O4'-C4'	-5.13	104.77	109.90
54	BA	1836	C	O4'-C4'-C3'	5.13	109.13	104.00
22	A1	63	G	O4'-C4'-C3'	5.12	109.12	104.00
54	BA	541	A	C4'-C3'-C2'	-5.12	97.48	102.60
41	BS	81	SER	N-CA-C	5.12	117.29	110.53
34	BL	81	ASP	CA-C-N	5.12	131.32	121.54
34	BL	81	ASP	C-N-CA	5.12	131.32	121.54
54	BA	2126	A	O4'-C1'-N9	5.11	115.87	108.20
54	BA	690	G	O4'-C4'-C3'	5.11	109.11	104.00
21	AA	39	G	C5'-C4'-C3'	-5.11	108.34	116.00
18	AS	74	ALA	CA-C-N	5.10	125.04	119.78
18	AS	74	ALA	C-N-CA	5.10	125.04	119.78
21	AA	1520	C	C5'-C4'-C3'	-5.10	108.34	116.00
54	BA	2496	C	C3'-C2'-C1'	5.10	106.40	101.30
21	AA	27	G	C5'-C4'-C3'	-5.10	108.35	116.00
54	BA	482	A	C3'-C2'-C1'	5.10	106.40	101.30
53	B4	37	GLN	OE1-CD-NE2	-5.10	117.50	122.60
54	BA	2732	G	O4'-C1'-C2'	-5.10	102.50	107.60
55	BB	5	U	C4'-C3'-C2'	-5.10	97.50	102.60
54	BA	2519	U	O3'-P-O5'	-5.09	96.36	104.00
25	BC	6	LYS	CA-C-N	5.09	126.21	119.84
25	BC	6	LYS	C-N-CA	5.09	126.21	119.84
26	BD	32	ASN	OD1-CG-ND2	-5.09	117.51	122.60
54	BA	2054	A	O4'-C4'-C3'	5.09	109.09	104.00
21	AA	320	A	O4'-C4'-C3'	5.09	109.09	104.00
54	BA	1596	A	C5'-C4'-C3'	-5.09	108.36	116.00
37	BO	38	GLN	OE1-CD-NE2	-5.09	117.51	122.60
24	A3	48	U	C5'-C4'-C3'	-5.09	107.57	115.20
54	BA	58	G	O4'-C4'-C3'	5.08	109.08	104.00
54	BA	1626	A	O4'-C4'-C3'	5.08	109.08	104.00
21	AA	390	U	C5'-C4'-C3'	-5.08	108.38	116.00
21	AA	1440	U	O4'-C4'-C3'	5.08	109.08	104.00
54	BA	747	U	O3'-P-O5'	-5.08	96.38	104.00
21	AA	46	G	O4'-C4'-C3'	5.08	109.08	104.00
39	BQ	32	ARG	NE-CZ-NH2	5.08	123.77	119.20
21	AA	167	A	C5'-C4'-C3'	-5.07	108.39	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BL	24	GLY	O-C-N	-5.07	118.09	122.91
54	BA	1664	A	O4'-C4'-C3'	5.07	109.07	104.00
54	BA	2768	U	C4'-C3'-C2'	-5.07	97.53	102.60
21	AA	510	A	O4'-C4'-C3'	5.07	109.07	104.00
21	AA	1374	A	C5'-C4'-C3'	-5.07	108.39	116.00
54	BA	1928	A	C2'-C3'-O3'	-5.07	106.09	113.70
33	BK	101	GLY	CA-C-N	5.07	124.68	119.56
33	BK	101	GLY	C-N-CA	5.07	124.68	119.56
54	BA	656	G	O4'-C4'-C3'	5.07	109.07	104.00
38	BP	68	GLY	CA-C-N	5.06	131.08	121.97
38	BP	68	GLY	C-N-CA	5.06	131.08	121.97
29	BG	124	CYS	CA-C-N	5.06	124.56	119.19
29	BG	124	CYS	C-N-CA	5.06	124.56	119.19
54	BA	2850	A	O4'-C1'-N9	5.06	116.09	108.50
21	AA	943	U	O4'-C4'-C3'	5.06	109.06	104.00
54	BA	2686	G	C4'-C3'-C2'	-5.06	97.54	102.60
29	BG	76	ILE	CA-C-N	5.05	125.59	119.98
29	BG	76	ILE	C-N-CA	5.05	125.59	119.98
54	BA	1456	G	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	2565	A	O4'-C4'-C3'	5.05	109.05	104.00
21	AA	572	A	C1'-O4'-C4'	-5.05	104.85	109.90
21	AA	1059	C	C5'-C4'-C3'	-5.05	108.43	116.00
54	BA	2195	U	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	2248	C	C4'-C3'-C2'	-5.05	97.55	102.60
21	AA	1165	U	O4'-C4'-C3'	5.05	109.05	104.00
54	BA	2419	U	O4'-C1'-N1	5.05	116.07	108.50
54	BA	846	U	O4'-C1'-N1	5.04	115.77	108.20
21	AA	1113	C	O4'-C4'-C3'	5.04	109.04	104.00
21	AA	1221	G	C5'-C4'-C3'	-5.04	108.44	116.00
54	BA	572	A	C4'-C3'-O3'	5.04	120.57	113.00
21	AA	373	A	C5'-C4'-C3'	-5.04	108.45	116.00
46	BX	19	HIS	CB-CG-CD2	-5.04	124.65	131.20
51	B2	16	HIS	CB-CG-CD2	-5.04	124.66	131.20
54	BA	1340	U	O4'-C1'-N1	5.04	115.75	108.20
54	BA	1365	A	O4'-C1'-C2'	-5.04	102.56	107.60
54	BA	1379	U	O4'-C4'-C3'	5.04	109.04	104.00
54	BA	715	A	C3'-C2'-C1'	5.03	106.33	101.30
55	BB	66	A	O4'-C4'-C3'	5.03	109.03	104.00
35	BM	20	LEU	CA-C-N	5.03	131.15	121.54
35	BM	20	LEU	C-N-CA	5.03	131.15	121.54
54	BA	1770	G	C4'-C3'-C2'	-5.03	97.57	102.60
54	BA	2476	A	C5'-C4'-C3'	-5.03	108.45	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AJ	78	GLU	CA-C-N	5.03	126.12	119.84
9	AJ	78	GLU	C-N-CA	5.03	126.12	119.84
27	BE	29	HIS	CB-CG-CD2	-5.03	124.67	131.20
39	BQ	88	GLU	CA-C-N	5.03	127.72	122.14
39	BQ	88	GLU	C-N-CA	5.03	127.72	122.14
54	BA	127	A	O4'-C4'-C3'	5.03	109.03	104.00
54	BA	866	A	O4'-C4'-C3'	5.03	109.03	104.00
54	BA	2522	U	O4'-C4'-C3'	5.02	109.02	104.00
21	AA	101	A	C5'-C4'-C3'	-5.02	108.47	116.00
54	BA	2787	C	C4'-C3'-C2'	-5.02	97.58	102.60
54	BA	1743	G	C4'-C3'-C2'	-5.02	97.58	102.60
21	AA	316	C	O4'-C4'-C3'	5.02	109.02	104.00
21	AA	793	U	C1'-O4'-C4'	-5.01	104.89	109.90
22	A1	69	A	C3'-C2'-C1'	5.01	106.31	101.30
21	AA	285	C	O4'-C4'-C3'	5.01	109.01	104.00
21	AA	1131	G	O4'-C4'-C3'	5.01	109.01	104.00
54	BA	2446	G	C4'-C3'-C2'	-5.01	97.59	102.60

There are no chirality outliers.

All (1094) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	23	A	Sidechain
22	A1	26	A	Sidechain
22	A1	31	C	Sidechain
22	A1	45	G	Sidechain
22	A1	49	G	Sidechain
22	A1	57	G	Sidechain
22	A1	59	U	Sidechain
22	A1	70	C	Sidechain
22	A1	72	C	Sidechain
22	A1	74	C	Sidechain
23	A2	81	U	Sidechain
24	A3	11	A	Sidechain
24	A3	24	C	Sidechain
24	A3	25	U	Sidechain
24	A3	27	G	Sidechain
24	A3	32	G	Sidechain
24	A3	34	U	Sidechain
24	A3	37	U	Sidechain
24	A3	47	G	Sidechain
24	A3	57	C	Sidechain

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Mol	Chain	Res	Type	Group
24	A3	71	G	Sidechain
24	A3	73	A	Sidechain
24	A3	76	C	Sidechain
24	A3	77	A	Sidechain
24	A3	9	G	Sidechain
21	AA	100	G	Sidechain
21	AA	1002	G	Sidechain
21	AA	1010	U	Sidechain
21	AA	1013	G	Sidechain
21	AA	1021	A	Sidechain
21	AA	1025	U	Sidechain
21	AA	1045	C	Sidechain
21	AA	1049	U	Sidechain
21	AA	1054	C	Sidechain
21	AA	1058	G	Sidechain
21	AA	1059	C	Sidechain
21	AA	1067	A	Sidechain
21	AA	107	G	Sidechain
21	AA	1077	G	Sidechain
21	AA	1085	U	Sidechain
21	AA	109	A	Sidechain
21	AA	1091	U	Sidechain
21	AA	1093	A	Sidechain
21	AA	110	C	Sidechain
21	AA	1103	C	Sidechain
21	AA	1106	G	Sidechain
21	AA	1107	C	Sidechain
21	AA	1108	G	Sidechain
21	AA	111	G	Sidechain
21	AA	1112	C	Sidechain
21	AA	1115	U	Sidechain
21	AA	1118	U	Sidechain
21	AA	1120	C	Sidechain
21	AA	1126	U	Sidechain
21	AA	1131	G	Sidechain
21	AA	1133	G	Sidechain
21	AA	1136	C	Sidechain
21	AA	114	U	Sidechain
21	AA	1142	G	Sidechain
21	AA	1146	A	Sidechain
21	AA	1159	U	Sidechain
21	AA	116	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1160	G	Sidechain
21	AA	1162	C	Sidechain
21	AA	1165	U	Sidechain
21	AA	1168	U	Sidechain
21	AA	117	G	Sidechain
21	AA	1170	A	Sidechain
21	AA	1178	G	Sidechain
21	AA	1189	U	Sidechain
21	AA	119	A	Sidechain
21	AA	1191	A	Sidechain
21	AA	1194	U	Sidechain
21	AA	1201	A	Sidechain
21	AA	1204	A	Sidechain
21	AA	1211	U	Sidechain
21	AA	1215	G	Sidechain
21	AA	122	G	Sidechain
21	AA	1221	G	Sidechain
21	AA	1223	C	Sidechain
21	AA	1224	U	Sidechain
21	AA	1227	A	Sidechain
21	AA	123	U	Sidechain
21	AA	1231	G	Sidechain
21	AA	1234	C	Sidechain
21	AA	1249	C	Sidechain
21	AA	125	U	Sidechain
21	AA	1257	A	Sidechain
21	AA	1263	C	Sidechain
21	AA	1264	U	Sidechain
21	AA	1266	G	Sidechain
21	AA	1267	C	Sidechain
21	AA	1270	G	Sidechain
21	AA	1271	A	Sidechain
21	AA	1276	G	Sidechain
21	AA	1279	G	Sidechain
21	AA	1281	C	Sidechain
21	AA	1283	U	Sidechain
21	AA	1289	A	Sidechain
21	AA	1296	C	Sidechain
21	AA	130	A	Sidechain
21	AA	1300	G	Sidechain
21	AA	1303	C	Sidechain
21	AA	1305	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1307	U	Sidechain
21	AA	1308	U	Sidechain
21	AA	1309	G	Sidechain
21	AA	1311	A	Sidechain
21	AA	1312	G	Sidechain
21	AA	1316	G	Sidechain
21	AA	1319	A	Sidechain
21	AA	1336	C	Sidechain
21	AA	1339	A	Sidechain
21	AA	1342	C	Sidechain
21	AA	1343	G	Sidechain
21	AA	1345	U	Sidechain
21	AA	1347	G	Sidechain
21	AA	1351	U	Sidechain
21	AA	1356	G	Sidechain
21	AA	1358	U	Sidechain
21	AA	1360	A	Sidechain
21	AA	1361	G	Sidechain
21	AA	1363	A	Sidechain
21	AA	1370	G	Sidechain
21	AA	1377	A	Sidechain
21	AA	1378	C	Sidechain
21	AA	1380	U	Sidechain
21	AA	1387	G	Sidechain
21	AA	1388	C	Sidechain
21	AA	139	A	Sidechain
21	AA	1397	C	Sidechain
21	AA	1405	G	Sidechain
21	AA	1414	U	Sidechain
21	AA	1415	G	Sidechain
21	AA	1416	G	Sidechain
21	AA	1417	G	Sidechain
21	AA	1420	U	Sidechain
21	AA	1421	G	Sidechain
21	AA	1423	G	Sidechain
21	AA	1427	C	Sidechain
21	AA	1430	A	Sidechain
21	AA	1431	A	Sidechain
21	AA	1438	G	Sidechain
21	AA	1441	A	Sidechain
21	AA	1442	G	Sidechain
21	AA	1446	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1449	C	Sidechain
21	AA	1451	U	Sidechain
21	AA	1455	G	Sidechain
21	AA	1459	G	Sidechain
21	AA	1460	C	Sidechain
21	AA	1461	G	Sidechain
21	AA	1464	U	Sidechain
21	AA	1470	U	Sidechain
21	AA	1479	C	Sidechain
21	AA	148	G	Sidechain
21	AA	1485	U	Sidechain
21	AA	1496	C	Sidechain
21	AA	150	U	Sidechain
21	AA	1503	A	Sidechain
21	AA	151	A	Sidechain
21	AA	1516	G	Sidechain
21	AA	1519	A	Sidechain
21	AA	1525	G	Sidechain
21	AA	1526	G	Sidechain
21	AA	1529	G	Sidechain
21	AA	1530	G	Sidechain
21	AA	1532	U	Sidechain
21	AA	1534	A	Sidechain
21	AA	163	C	Sidechain
21	AA	164	G	Sidechain
21	AA	165	G	Sidechain
21	AA	169	C	Sidechain
21	AA	173	U	Sidechain
21	AA	183	C	Sidechain
21	AA	187	G	Sidechain
21	AA	188	C	Sidechain
21	AA	195	A	Sidechain
21	AA	196	A	Sidechain
21	AA	20	U	Sidechain
21	AA	205	A	Sidechain
21	AA	210	C	Sidechain
21	AA	211	G	Sidechain
21	AA	215	C	Sidechain
21	AA	217	C	Sidechain
21	AA	218	U	Sidechain
21	AA	219	U	Sidechain
21	AA	232	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	234	C	Sidechain
21	AA	235	C	Sidechain
21	AA	242	G	Sidechain
21	AA	245	U	Sidechain
21	AA	25	C	Sidechain
21	AA	256	U	Sidechain
21	AA	259	G	Sidechain
21	AA	261	U	Sidechain
21	AA	262	A	Sidechain
21	AA	263	A	Sidechain
21	AA	267	C	Sidechain
21	AA	27	G	Sidechain
21	AA	278	G	Sidechain
21	AA	280	C	Sidechain
21	AA	281	G	Sidechain
21	AA	29	U	Sidechain
21	AA	297	G	Sidechain
21	AA	309	A	Sidechain
21	AA	31	G	Sidechain
21	AA	313	A	Sidechain
21	AA	319	G	Sidechain
21	AA	321	A	Sidechain
21	AA	324	G	Sidechain
21	AA	326	G	Sidechain
21	AA	328	C	Sidechain
21	AA	330	C	Sidechain
21	AA	331	G	Sidechain
21	AA	338	A	Sidechain
21	AA	340	U	Sidechain
21	AA	343	U	Sidechain
21	AA	346	G	Sidechain
21	AA	347	G	Sidechain
21	AA	349	A	Sidechain
21	AA	350	G	Sidechain
21	AA	353	A	Sidechain
21	AA	36	C	Sidechain
21	AA	362	G	Sidechain
21	AA	363	A	Sidechain
21	AA	37	U	Sidechain
21	AA	372	C	Sidechain
21	AA	375	U	Sidechain
21	AA	380	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	389	A	Sidechain
21	AA	390	U	Sidechain
21	AA	397	A	Sidechain
21	AA	399	G	Sidechain
21	AA	400	C	Sidechain
21	AA	402	G	Sidechain
21	AA	408	A	Sidechain
21	AA	413	G	Sidechain
21	AA	429	U	Sidechain
21	AA	431	A	Sidechain
21	AA	432	A	Sidechain
21	AA	436	C	Sidechain
21	AA	439	U	Sidechain
21	AA	448	A	Sidechain
21	AA	449	G	Sidechain
21	AA	458	U	Sidechain
21	AA	461	A	Sidechain
21	AA	465	A	Sidechain
21	AA	466	A	Sidechain
21	AA	475	C	Sidechain
21	AA	479	U	Sidechain
21	AA	483	C	Sidechain
21	AA	484	G	Sidechain
21	AA	485	U	Sidechain
21	AA	497	G	Sidechain
21	AA	499	A	Sidechain
21	AA	507	C	Sidechain
21	AA	511	C	Sidechain
21	AA	515	G	Sidechain
21	AA	517	G	Sidechain
21	AA	518	C	Sidechain
21	AA	519	C	Sidechain
21	AA	520	A	Sidechain
21	AA	527	G	Sidechain
21	AA	529	G	Sidechain
21	AA	530	G	Sidechain
21	AA	533	A	Sidechain
21	AA	54	C	Sidechain
21	AA	542	G	Sidechain
21	AA	549	C	Sidechain
21	AA	55	A	Sidechain
21	AA	555	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	562	U	Sidechain
21	AA	563	A	Sidechain
21	AA	564	C	Sidechain
21	AA	566	G	Sidechain
21	AA	568	G	Sidechain
21	AA	586	C	Sidechain
21	AA	588	G	Sidechain
21	AA	591	U	Sidechain
21	AA	6	G	Sidechain
21	AA	60	A	Sidechain
21	AA	600	A	Sidechain
21	AA	61	G	Sidechain
21	AA	610	U	Sidechain
21	AA	615	G	Sidechain
21	AA	618	C	Sidechain
21	AA	621	A	Sidechain
21	AA	623	C	Sidechain
21	AA	634	C	Sidechain
21	AA	639	G	Sidechain
21	AA	650	G	Sidechain
21	AA	653	U	Sidechain
21	AA	654	G	Sidechain
21	AA	656	G	Sidechain
21	AA	660	C	Sidechain
21	AA	664	G	Sidechain
21	AA	666	G	Sidechain
21	AA	669	G	Sidechain
21	AA	678	U	Sidechain
21	AA	68	G	Sidechain
21	AA	682	G	Sidechain
21	AA	683	G	Sidechain
21	AA	689	C	Sidechain
21	AA	69	G	Sidechain
21	AA	691	G	Sidechain
21	AA	695	A	Sidechain
21	AA	698	G	Sidechain
21	AA	700	G	Sidechain
21	AA	701	U	Sidechain
21	AA	702	A	Sidechain
21	AA	704	A	Sidechain
21	AA	705	G	Sidechain
21	AA	717	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	725	G	Sidechain
21	AA	727	G	Sidechain
21	AA	730	G	Sidechain
21	AA	734	G	Sidechain
21	AA	743	A	Sidechain
21	AA	75	G	Sidechain
21	AA	752	G	Sidechain
21	AA	753	A	Sidechain
21	AA	76	G	Sidechain
21	AA	760	G	Sidechain
21	AA	761	G	Sidechain
21	AA	763	G	Sidechain
21	AA	764	C	Sidechain
21	AA	765	G	Sidechain
21	AA	772	U	Sidechain
21	AA	774	G	Sidechain
21	AA	778	G	Sidechain
21	AA	796	C	Sidechain
21	AA	81	A	Sidechain
21	AA	810	C	Sidechain
21	AA	811	C	Sidechain
21	AA	812	G	Sidechain
21	AA	818	G	Sidechain
21	AA	820	U	Sidechain
21	AA	826	C	Sidechain
21	AA	827	U	Sidechain
21	AA	834	U	Sidechain
21	AA	836	G	Sidechain
21	AA	84	U	Sidechain
21	AA	841	C	Sidechain
21	AA	842	U	Sidechain
21	AA	849	G	Sidechain
21	AA	855	U	Sidechain
21	AA	858	G	Sidechain
21	AA	859	G	Sidechain
21	AA	863	U	Sidechain
21	AA	866	C	Sidechain
21	AA	869	G	Sidechain
21	AA	871	U	Sidechain
21	AA	88	U	Sidechain
21	AA	887	G	Sidechain
21	AA	888	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	890	G	Sidechain
21	AA	891	U	Sidechain
21	AA	895	G	Sidechain
21	AA	898	G	Sidechain
21	AA	9	G	Sidechain
21	AA	903	G	Sidechain
21	AA	905	U	Sidechain
21	AA	91	U	Sidechain
21	AA	911	U	Sidechain
21	AA	916	U	Sidechain
21	AA	919	A	Sidechain
21	AA	921	U	Sidechain
21	AA	927	G	Sidechain
21	AA	931	C	Sidechain
21	AA	936	C	Sidechain
21	AA	937	A	Sidechain
21	AA	938	A	Sidechain
21	AA	941	G	Sidechain
21	AA	944	G	Sidechain
21	AA	951	G	Sidechain
21	AA	957	U	Sidechain
21	AA	960	U	Sidechain
21	AA	961	U	Sidechain
21	AA	962	C	Sidechain
21	AA	968	A	Sidechain
21	AA	976	G	Sidechain
21	AA	977	A	Sidechain
21	AA	978	A	Sidechain
21	AA	982	U	Sidechain
21	AA	985	C	Sidechain
21	AA	989	U	Sidechain
21	AA	992	U	Sidechain
21	AA	995	C	Sidechain
21	AA	997	U	Sidechain
2	AC	168	ARG	Sidechain
2	AC	172	VAL	Peptide
8	AI	124	PRO	Peptide
10	AK	115	ILE	Peptide
54	BA	10	A	Sidechain
54	BA	100	U	Sidechain
54	BA	1000	A	Sidechain
54	BA	1006	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1009	A	Sidechain
54	BA	1020	A	Sidechain
54	BA	1025	G	Sidechain
54	BA	1026	G	Sidechain
54	BA	103	A	Sidechain
54	BA	1042	G	Sidechain
54	BA	1046	A	Sidechain
54	BA	1047	G	Sidechain
54	BA	1050	A	Sidechain
54	BA	1056	G	Sidechain
54	BA	106	C	Sidechain
54	BA	1066	U	Sidechain
54	BA	1069	A	Sidechain
54	BA	1074	G	Sidechain
54	BA	1079	C	Sidechain
54	BA	1086	A	Sidechain
54	BA	1088	A	Sidechain
54	BA	1095	A	Sidechain
54	BA	1098	A	Sidechain
54	BA	1101	U	Sidechain
54	BA	1106	G	Sidechain
54	BA	1127	A	Sidechain
54	BA	1130	U	Sidechain
54	BA	1131	G	Sidechain
54	BA	1132	U	Sidechain
54	BA	1133	A	Sidechain
54	BA	1135	C	Sidechain
54	BA	1138	G	Sidechain
54	BA	1139	G	Sidechain
54	BA	1140	C	Sidechain
54	BA	1160	G	Sidechain
54	BA	117	G	Sidechain
54	BA	1179	G	Sidechain
54	BA	1188	U	Sidechain
54	BA	119	A	Sidechain
54	BA	1191	G	Sidechain
54	BA	1193	G	Sidechain
54	BA	1199	U	Sidechain
54	BA	1200	C	Sidechain
54	BA	1203	U	Sidechain
54	BA	1209	U	Sidechain
54	BA	1210	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1212	G	Sidechain
54	BA	1215	G	Sidechain
54	BA	1224	U	Sidechain
54	BA	1225	G	Sidechain
54	BA	1226	A	Sidechain
54	BA	1232	G	Sidechain
54	BA	1233	C	Sidechain
54	BA	1235	G	Sidechain
54	BA	1236	G	Sidechain
54	BA	1237	A	Sidechain
54	BA	1244	A	Sidechain
54	BA	1248	G	Sidechain
54	BA	1251	C	Sidechain
54	BA	1253	A	Sidechain
54	BA	1256	G	Sidechain
54	BA	1259	G	Sidechain
54	BA	1266	G	Sidechain
54	BA	1268	A	Sidechain
54	BA	1270	C	Sidechain
54	BA	1272	A	Sidechain
54	BA	1276	A	Sidechain
54	BA	1283	G	Sidechain
54	BA	1287	A	Sidechain
54	BA	1288	G	Sidechain
54	BA	1291	C	Sidechain
54	BA	1292	G	Sidechain
54	BA	1293	C	Sidechain
54	BA	1297	C	Sidechain
54	BA	13	A	Sidechain
54	BA	1300	G	Sidechain
54	BA	1302	A	Sidechain
54	BA	1308	A	Sidechain
54	BA	1310	G	Sidechain
54	BA	1314	C	Sidechain
54	BA	1315	C	Sidechain
54	BA	1317	G	Sidechain
54	BA	1319	C	Sidechain
54	BA	1320	C	Sidechain
54	BA	1324	G	Sidechain
54	BA	1326	U	Sidechain
54	BA	1327	A	Sidechain
54	BA	1330	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1334	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1342	A	Sidechain
54	BA	1347	A	Sidechain
54	BA	1350	C	Sidechain
54	BA	1356	G	Sidechain
54	BA	1360	G	Sidechain
54	BA	1364	G	Sidechain
54	BA	1370	C	Sidechain
54	BA	1374	G	Sidechain
54	BA	1376	C	Sidechain
54	BA	1382	G	Sidechain
54	BA	1387	A	Sidechain
54	BA	1389	G	Sidechain
54	BA	1390	U	Sidechain
54	BA	1391	U	Sidechain
54	BA	1394	U	Sidechain
54	BA	1399	C	Sidechain
54	BA	1403	A	Sidechain
54	BA	1411	U	Sidechain
54	BA	1412	U	Sidechain
54	BA	1418	G	Sidechain
54	BA	1419	A	Sidechain
54	BA	1421	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1431	A	Sidechain
54	BA	1432	G	Sidechain
54	BA	1441	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1452	G	Sidechain
54	BA	1453	A	Sidechain
54	BA	1454	C	Sidechain
54	BA	1460	U	Sidechain
54	BA	1464	G	Sidechain
54	BA	147	C	Sidechain
54	BA	1470	A	Sidechain
54	BA	1483	G	Sidechain
54	BA	1484	U	Sidechain
54	BA	1492	G	Sidechain
54	BA	1498	C	Sidechain
54	BA	1505	A	Sidechain
54	BA	1510	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1519	G	Sidechain
54	BA	152	A	Sidechain
54	BA	1520	U	Sidechain
54	BA	1522	A	Sidechain
54	BA	1525	A	Sidechain
54	BA	1526	C	Sidechain
54	BA	1529	G	Sidechain
54	BA	153	U	Sidechain
54	BA	1536	C	Sidechain
54	BA	1537	G	Sidechain
54	BA	1539	U	Sidechain
54	BA	154	U	Sidechain
54	BA	1546	G	Sidechain
54	BA	1547	C	Sidechain
54	BA	1552	A	Sidechain
54	BA	1554	U	Sidechain
54	BA	1555	G	Sidechain
54	BA	156	A	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1562	U	Sidechain
54	BA	1567	G	Sidechain
54	BA	1581	G	Sidechain
54	BA	1585	C	Sidechain
54	BA	1595	C	Sidechain
54	BA	1600	C	Sidechain
54	BA	1601	G	Sidechain
54	BA	1602	U	Sidechain
54	BA	1618	A	Sidechain
54	BA	1621	U	Sidechain
54	BA	1632	A	Sidechain
54	BA	1633	G	Sidechain
54	BA	1636	U	Sidechain
54	BA	1641	A	Sidechain
54	BA	1642	G	Sidechain
54	BA	1651	G	Sidechain
54	BA	1653	G	Sidechain
54	BA	1655	A	Sidechain
54	BA	1656	C	Sidechain
54	BA	1657	U	Sidechain
54	BA	1664	A	Sidechain
54	BA	1665	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1667	G	Sidechain
54	BA	1672	A	Sidechain
54	BA	1682	G	Sidechain
54	BA	1688	U	Sidechain
54	BA	1705	A	Sidechain
54	BA	172	A	Sidechain
54	BA	1729	U	Sidechain
54	BA	1737	G	Sidechain
54	BA	1738	G	Sidechain
54	BA	1739	A	Sidechain
54	BA	1740	G	Sidechain
54	BA	1743	G	Sidechain
54	BA	1747	U	Sidechain
54	BA	1750	G	Sidechain
54	BA	1753	G	Sidechain
54	BA	1758	U	Sidechain
54	BA	1760	C	Sidechain
54	BA	1763	G	Sidechain
54	BA	1774	C	Sidechain
54	BA	1788	C	Sidechain
54	BA	1789	A	Sidechain
54	BA	1792	G	Sidechain
54	BA	1793	C	Sidechain
54	BA	1797	G	Sidechain
54	BA	1799	G	Sidechain
54	BA	1802	A	Sidechain
54	BA	1807	G	Sidechain
54	BA	181	A	Sidechain
54	BA	1814	G	Sidechain
54	BA	1817	G	Sidechain
54	BA	1821	A	Sidechain
54	BA	1825	U	Sidechain
54	BA	1827	U	Sidechain
54	BA	1831	G	Sidechain
54	BA	1833	C	Sidechain
54	BA	1835	G	Sidechain
54	BA	1838	C	Sidechain
54	BA	1839	G	Sidechain
54	BA	1843	C	Sidechain
54	BA	1849	G	Sidechain
54	BA	185	G	Sidechain
54	BA	1857	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1858	A	Sidechain
54	BA	1860	G	Sidechain
54	BA	1863	G	Sidechain
54	BA	1864	U	Sidechain
54	BA	1865	U	Sidechain
54	BA	1869	G	Sidechain
54	BA	1883	U	Sidechain
54	BA	1884	G	Sidechain
54	BA	1885	A	Sidechain
54	BA	1886	U	Sidechain
54	BA	1887	C	Sidechain
54	BA	1902	C	Sidechain
54	BA	1903	G	Sidechain
54	BA	1906	G	Sidechain
54	BA	1910	G	Sidechain
54	BA	1918	A	Sidechain
54	BA	1920	C	Sidechain
54	BA	1924	C	Sidechain
54	BA	1932	A	Sidechain
54	BA	1941	C	Sidechain
54	BA	1944	U	Sidechain
54	BA	1945	G	Sidechain
54	BA	1948	G	Sidechain
54	BA	1949	G	Sidechain
54	BA	1952	A	Sidechain
54	BA	1957	C	Sidechain
54	BA	196	A	Sidechain
54	BA	1960	A	Sidechain
54	BA	1962	C	Sidechain
54	BA	1966	A	Sidechain
54	BA	1969	A	Sidechain
54	BA	1976	U	Sidechain
54	BA	1978	A	Sidechain
54	BA	1983	G	Sidechain
54	BA	200	U	Sidechain
54	BA	2003	A	Sidechain
54	BA	2008	C	Sidechain
54	BA	2011	U	Sidechain
54	BA	2013	A	Sidechain
54	BA	2014	A	Sidechain
54	BA	2015	A	Sidechain
54	BA	2019	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	202	U	Sidechain
54	BA	2028	U	Sidechain
54	BA	203	A	Sidechain
54	BA	2030	A	Sidechain
54	BA	2031	A	Sidechain
54	BA	2035	G	Sidechain
54	BA	2040	G	Sidechain
54	BA	2042	A	Sidechain
54	BA	2048	G	Sidechain
54	BA	206	U	Sidechain
54	BA	2065	C	Sidechain
54	BA	2066	C	Sidechain
54	BA	2069	G	Sidechain
54	BA	2074	U	Sidechain
54	BA	2075	U	Sidechain
54	BA	2077	A	Sidechain
54	BA	2079	U	Sidechain
54	BA	208	C	Sidechain
54	BA	2093	G	Sidechain
54	BA	2094	A	Sidechain
54	BA	2097	A	Sidechain
54	BA	2099	U	Sidechain
54	BA	2100	G	Sidechain
54	BA	2104	C	Sidechain
54	BA	2108	A	Sidechain
54	BA	2116	G	Sidechain
54	BA	2125	G	Sidechain
54	BA	2141	G	Sidechain
54	BA	2145	C	Sidechain
54	BA	2155	U	Sidechain
54	BA	2163	A	Sidechain
54	BA	2168	G	Sidechain
54	BA	2178	C	Sidechain
54	BA	2180	U	Sidechain
54	BA	2183	A	Sidechain
54	BA	2188	U	Sidechain
54	BA	2190	G	Sidechain
54	BA	2196	C	Sidechain
54	BA	2201	G	Sidechain
54	BA	2203	U	Sidechain
54	BA	2205	A	Sidechain
54	BA	2221	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2223	G	Sidechain
54	BA	2224	G	Sidechain
54	BA	2227	A	Sidechain
54	BA	2228	G	Sidechain
54	BA	2233	U	Sidechain
54	BA	2238	G	Sidechain
54	BA	2249	U	Sidechain
54	BA	2252	G	Sidechain
54	BA	2255	G	Sidechain
54	BA	2259	U	Sidechain
54	BA	226	A	Sidechain
54	BA	2260	C	Sidechain
54	BA	2262	U	Sidechain
54	BA	2269	G	Sidechain
54	BA	2272	U	Sidechain
54	BA	2273	A	Sidechain
54	BA	2278	A	Sidechain
54	BA	2279	G	Sidechain
54	BA	2280	G	Sidechain
54	BA	2282	G	Sidechain
54	BA	2295	C	Sidechain
54	BA	2299	U	Sidechain
54	BA	2301	C	Sidechain
54	BA	2304	G	Sidechain
54	BA	2309	A	Sidechain
54	BA	2312	U	Sidechain
54	BA	2325	G	Sidechain
54	BA	2327	A	Sidechain
54	BA	2332	C	Sidechain
54	BA	2345	G	Sidechain
54	BA	235	U	Sidechain
54	BA	2354	C	Sidechain
54	BA	2357	G	Sidechain
54	BA	2358	A	Sidechain
54	BA	2375	G	Sidechain
54	BA	238	C	Sidechain
54	BA	2383	G	Sidechain
54	BA	2384	U	Sidechain
54	BA	2385	C	Sidechain
54	BA	2388	A	Sidechain
54	BA	2389	G	Sidechain
54	BA	2391	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2396	G	Sidechain
54	BA	240	C	Sidechain
54	BA	2406	A	Sidechain
54	BA	2413	G	Sidechain
54	BA	2421	G	Sidechain
54	BA	2424	C	Sidechain
54	BA	2427	C	Sidechain
54	BA	2428	G	Sidechain
54	BA	2430	A	Sidechain
54	BA	2432	A	Sidechain
54	BA	2437	G	Sidechain
54	BA	2440	C	Sidechain
54	BA	2442	C	Sidechain
54	BA	2445	G	Sidechain
54	BA	2446	G	Sidechain
54	BA	2447	G	Sidechain
54	BA	2453	A	Sidechain
54	BA	2455	G	Sidechain
54	BA	2460	U	Sidechain
54	BA	2466	C	Sidechain
54	BA	2468	A	Sidechain
54	BA	2470	G	Sidechain
54	BA	2475	C	Sidechain
54	BA	2478	A	Sidechain
54	BA	2488	G	Sidechain
54	BA	2489	U	Sidechain
54	BA	249	C	Sidechain
54	BA	2491	U	Sidechain
54	BA	2494	G	Sidechain
54	BA	2498	C	Sidechain
54	BA	25	U	Sidechain
54	BA	250	G	Sidechain
54	BA	2502	G	Sidechain
54	BA	2506	U	Sidechain
54	BA	2510	C	Sidechain
54	BA	2516	A	Sidechain
54	BA	2517	C	Sidechain
54	BA	2520	C	Sidechain
54	BA	2523	G	Sidechain
54	BA	2530	A	Sidechain
54	BA	2534	A	Sidechain
54	BA	2540	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2543	G	Sidechain
54	BA	2544	G	Sidechain
54	BA	2545	G	Sidechain
54	BA	2553	G	Sidechain
54	BA	2554	U	Sidechain
54	BA	256	A	Sidechain
54	BA	2564	A	Sidechain
54	BA	2574	G	Sidechain
54	BA	2576	G	Sidechain
54	BA	2577	A	Sidechain
54	BA	2578	G	Sidechain
54	BA	2579	C	Sidechain
54	BA	2580	U	Sidechain
54	BA	2585	U	Sidechain
54	BA	2587	A	Sidechain
54	BA	2588	G	Sidechain
54	BA	2589	A	Sidechain
54	BA	2590	A	Sidechain
54	BA	2591	C	Sidechain
54	BA	2594	C	Sidechain
54	BA	2595	G	Sidechain
54	BA	2596	U	Sidechain
54	BA	2597	G	Sidechain
54	BA	2602	A	Sidechain
54	BA	2603	G	Sidechain
54	BA	2608	G	Sidechain
54	BA	2609	U	Sidechain
54	BA	261	G	Sidechain
54	BA	2614	A	Sidechain
54	BA	2615	U	Sidechain
54	BA	2621	G	Sidechain
54	BA	2625	G	Sidechain
54	BA	2627	G	Sidechain
54	BA	2629	U	Sidechain
54	BA	2635	A	Sidechain
54	BA	2636	C	Sidechain
54	BA	2637	U	Sidechain
54	BA	2639	A	Sidechain
54	BA	2644	G	Sidechain
54	BA	2645	G	Sidechain
54	BA	265	A	Sidechain
54	BA	2651	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2653	U	Sidechain
54	BA	2659	G	Sidechain
54	BA	2661	G	Sidechain
54	BA	2662	A	Sidechain
54	BA	2664	G	Sidechain
54	BA	2680	U	Sidechain
54	BA	2699	C	Sidechain
54	BA	2700	A	Sidechain
54	BA	2705	A	Sidechain
54	BA	2713	U	Sidechain
54	BA	272	A	Sidechain
54	BA	2721	A	Sidechain
54	BA	2722	G	Sidechain
54	BA	2725	A	Sidechain
54	BA	2730	C	Sidechain
54	BA	2731	G	Sidechain
54	BA	2739	U	Sidechain
54	BA	2743	U	Sidechain
54	BA	2751	G	Sidechain
54	BA	2753	A	Sidechain
54	BA	2759	G	Sidechain
54	BA	2765	A	Sidechain
54	BA	2780	G	Sidechain
54	BA	2782	G	Sidechain
54	BA	2783	U	Sidechain
54	BA	2786	U	Sidechain
54	BA	2790	U	Sidechain
54	BA	2794	C	Sidechain
54	BA	2796	U	Sidechain
54	BA	2799	A	Sidechain
54	BA	2801	G	Sidechain
54	BA	2805	C	Sidechain
54	BA	2808	G	Sidechain
54	BA	2816	G	Sidechain
54	BA	2819	G	Sidechain
54	BA	282	A	Sidechain
54	BA	2824	C	Sidechain
54	BA	2827	C	Sidechain
54	BA	2840	C	Sidechain
54	BA	2841	C	Sidechain
54	BA	2842	G	Sidechain
54	BA	2845	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2848	G	Sidechain
54	BA	2850	A	Sidechain
54	BA	2856	A	Sidechain
54	BA	2857	G	Sidechain
54	BA	2859	G	Sidechain
54	BA	2863	C	Sidechain
54	BA	2864	G	Sidechain
54	BA	2866	U	Sidechain
54	BA	2868	A	Sidechain
54	BA	2869	G	Sidechain
54	BA	2871	U	Sidechain
54	BA	2873	A	Sidechain
54	BA	2876	G	Sidechain
54	BA	2877	G	Sidechain
54	BA	2879	A	Sidechain
54	BA	2889	C	Sidechain
54	BA	2891	U	Sidechain
54	BA	2893	A	Sidechain
54	BA	2896	C	Sidechain
54	BA	298	G	Sidechain
54	BA	302	C	Sidechain
54	BA	303	G	Sidechain
54	BA	307	G	Sidechain
54	BA	313	G	Sidechain
54	BA	315	G	Sidechain
54	BA	323	C	Sidechain
54	BA	325	G	Sidechain
54	BA	326	G	Sidechain
54	BA	327	G	Sidechain
54	BA	328	U	Sidechain
54	BA	333	G	Sidechain
54	BA	335	C	Sidechain
54	BA	339	U	Sidechain
54	BA	347	A	Sidechain
54	BA	354	A	Sidechain
54	BA	355	U	Sidechain
54	BA	357	C	Sidechain
54	BA	359	G	Sidechain
54	BA	361	G	Sidechain
54	BA	362	A	Sidechain
54	BA	384	A	Sidechain
54	BA	389	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	39	G	Sidechain
54	BA	392	U	Sidechain
54	BA	395	U	Sidechain
54	BA	400	G	Sidechain
54	BA	401	A	Sidechain
54	BA	410	G	Sidechain
54	BA	412	A	Sidechain
54	BA	415	A	Sidechain
54	BA	416	U	Sidechain
54	BA	417	C	Sidechain
54	BA	418	C	Sidechain
54	BA	419	U	Sidechain
54	BA	420	C	Sidechain
54	BA	422	A	Sidechain
54	BA	426	C	Sidechain
54	BA	43	G	Sidechain
54	BA	432	A	Sidechain
54	BA	434	U	Sidechain
54	BA	442	G	Sidechain
54	BA	446	G	Sidechain
54	BA	449	A	Sidechain
54	BA	456	C	Sidechain
54	BA	458	G	Sidechain
54	BA	463	G	Sidechain
54	BA	464	U	Sidechain
54	BA	470	A	Sidechain
54	BA	48	G	Sidechain
54	BA	489	G	Sidechain
54	BA	490	C	Sidechain
54	BA	491	G	Sidechain
54	BA	493	G	Sidechain
54	BA	494	G	Sidechain
54	BA	498	G	Sidechain
54	BA	500	G	Sidechain
54	BA	501	A	Sidechain
54	BA	503	A	Sidechain
54	BA	51	G	Sidechain
54	BA	511	U	Sidechain
54	BA	512	G	Sidechain
54	BA	514	A	Sidechain
54	BA	515	A	Sidechain
54	BA	528	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	529	A	Sidechain
54	BA	533	G	Sidechain
54	BA	541	A	Sidechain
54	BA	544	C	Sidechain
54	BA	551	G	Sidechain
54	BA	556	A	Sidechain
54	BA	561	G	Sidechain
54	BA	562	U	Sidechain
54	BA	563	A	Sidechain
54	BA	569	U	Sidechain
54	BA	571	U	Sidechain
54	BA	572	A	Sidechain
54	BA	578	G	Sidechain
54	BA	579	G	Sidechain
54	BA	580	U	Sidechain
54	BA	581	C	Sidechain
54	BA	582	A	Sidechain
54	BA	587	C	Sidechain
54	BA	588	U	Sidechain
54	BA	589	U	Sidechain
54	BA	595	C	Sidechain
54	BA	608	A	Sidechain
54	BA	612	G	Sidechain
54	BA	617	G	Sidechain
54	BA	624	C	Sidechain
54	BA	633	A	Sidechain
54	BA	636	G	Sidechain
54	BA	637	A	Sidechain
54	BA	644	A	Sidechain
54	BA	649	G	Sidechain
54	BA	653	U	Sidechain
54	BA	657	U	Sidechain
54	BA	659	G	Sidechain
54	BA	667	U	Sidechain
54	BA	669	G	Sidechain
54	BA	671	C	Sidechain
54	BA	680	C	Sidechain
54	BA	683	U	Sidechain
54	BA	686	U	Sidechain
54	BA	699	A	Sidechain
54	BA	703	U	Sidechain
54	BA	704	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	707	G	Sidechain
54	BA	708	G	Sidechain
54	BA	711	G	Sidechain
54	BA	714	U	Sidechain
54	BA	715	A	Sidechain
54	BA	716	A	Sidechain
54	BA	718	A	Sidechain
54	BA	723	C	Sidechain
54	BA	724	U	Sidechain
54	BA	725	G	Sidechain
54	BA	726	G	Sidechain
54	BA	727	A	Sidechain
54	BA	728	G	Sidechain
54	BA	73	A	Sidechain
54	BA	739	A	Sidechain
54	BA	74	A	Sidechain
54	BA	743	A	Sidechain
54	BA	746	U	Sidechain
54	BA	754	U	Sidechain
54	BA	758	C	Sidechain
54	BA	759	G	Sidechain
54	BA	772	C	Sidechain
54	BA	774	G	Sidechain
54	BA	775	G	Sidechain
54	BA	776	G	Sidechain
54	BA	782	A	Sidechain
54	BA	784	G	Sidechain
54	BA	785	G	Sidechain
54	BA	79	C	Sidechain
54	BA	801	G	Sidechain
54	BA	804	A	Sidechain
54	BA	810	U	Sidechain
54	BA	811	U	Sidechain
54	BA	816	C	Sidechain
54	BA	827	U	Sidechain
54	BA	828	U	Sidechain
54	BA	837	C	Sidechain
54	BA	84	A	Sidechain
54	BA	841	G	Sidechain
54	BA	851	C	Sidechain
54	BA	852	U	Sidechain
54	BA	856	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	858	G	Sidechain
54	BA	859	G	Sidechain
54	BA	861	A	Sidechain
54	BA	864	G	Sidechain
54	BA	868	U	Sidechain
54	BA	882	G	Sidechain
54	BA	886	A	Sidechain
54	BA	891	G	Sidechain
54	BA	897	C	Sidechain
54	BA	9	G	Sidechain
54	BA	900	A	Sidechain
54	BA	904	G	Sidechain
54	BA	91	A	Sidechain
54	BA	910	A	Sidechain
54	BA	912	C	Sidechain
54	BA	917	A	Sidechain
54	BA	918	A	Sidechain
54	BA	92	U	Sidechain
54	BA	923	G	Sidechain
54	BA	932	U	Sidechain
54	BA	940	G	Sidechain
54	BA	950	G	Sidechain
54	BA	953	G	Sidechain
54	BA	955	U	Sidechain
54	BA	957	C	Sidechain
54	BA	959	A	Sidechain
54	BA	966	G	Sidechain
54	BA	969	G	Sidechain
54	BA	975	A	Sidechain
54	BA	980	A	Sidechain
54	BA	983	A	Sidechain
54	BA	99	U	Sidechain
55	BB	10	G	Sidechain
55	BB	105	G	Sidechain
55	BB	106	G	Sidechain
55	BB	107	G	Sidechain
55	BB	117	G	Sidechain
55	BB	13	G	Sidechain
55	BB	14	U	Sidechain
55	BB	15	A	Sidechain
55	BB	2	G	Sidechain
55	BB	24	G	Sidechain

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Mol	Chain	Res	Type	Group
55	BB	25	U	Sidechain
55	BB	29	A	Sidechain
55	BB	33	G	Sidechain
55	BB	36	C	Sidechain
55	BB	40	U	Sidechain
55	BB	47	C	Sidechain
55	BB	48	U	Sidechain
55	BB	64	G	Sidechain
55	BB	66	A	Sidechain
55	BB	69	G	Sidechain
55	BB	7	G	Sidechain
55	BB	73	A	Sidechain
55	BB	75	G	Sidechain
55	BB	83	G	Sidechain
55	BB	85	G	Sidechain
55	BB	9	G	Sidechain
55	BB	91	C	Sidechain
55	BB	93	C	Sidechain
55	BB	94	A	Sidechain
55	BB	96	G	Sidechain
25	BC	142	ASN	Peptide
25	BC	62	ARG	Sidechain
33	BK	105	ARG	Sidechain
34	BL	123	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	1	0
19	AT	668	0	718	2	0
20	AU	429	0	453	0	0
21	AA	32828	0	15886	9	0
22	A1	1627	0	798	0	0
23	A2	309	0	156	0	0
24	A3	1642	0	801	1	0
25	BC	2083	0	2157	2	0
26	BD	1565	0	1616	3	0
27	BE	1552	0	1619	1	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	1	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	2	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	1	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	1	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	1	0
44	BV	753	0	780	0	0
45	BW	599	0	614	2	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	0
49	B0	444	0	461	0	0
50	B1	413	0	444	1	0
51	B2	377	0	418	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	30186	21	0
55	BB	2504	0	1181	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	97702	50	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 (50) 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)
19:AT:40:ALA:HB1	19:AT:41:GLY:HA2	1.81	0.62
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.76	0.51
26:BD:154:LYS:HE3	26:BD:156:PHE:CE1	2.46	0.51
54:BA:931:U:C5	54:BA:1167:C:H1'	2.46	0.50
21:AA:5:U:H4'	21:AA:6:G:C6	2.46	0.50
54:BA:1021:A:N6	54:BA:1142:A:H62	2.11	0.49
54:BA:1025:G:C4	54:BA:1135:C:H1'	2.48	0.48
26:BD:58:ASN:H	26:BD:59:ARG:HB2	1.79	0.46
54:BA:1451:C:H4'	54:BA:1452:G:C4	2.50	0.46
54:BA:36:G:H4'	54:BA:451:U:C4	2.50	0.46
54:BA:561:G:H2'	54:BA:562:U:H5''	1.98	0.45
45:BW:11:ASN:ND2	54:BA:2264:C:H41	2.14	0.45
21:AA:1533:C:H3'	21:AA:1534:A:H5''	1.98	0.44
24:A3:76:C:H1'	54:BA:2252:G:N2	2.33	0.44
21:AA:87:C:H2'	21:AA:88:U:C6	2.52	0.44
54:BA:2144:G:H2'	54:BA:2146:C:C5	2.52	0.44
33:BK:103:VAL:HG12	33:BK:104:THR:H	1.82	0.44
54:BA:2557:G:H2'	54:BA:2558:C:C6	2.53	0.44
40:BR:23:GLU:H	40:BR:23:GLU:CD	2.25	0.43
29:BG:154:GLU:H	29:BG:154:GLU:CD	2.26	0.43
33:BK:103:VAL:HG12	33:BK:104:THR:N	2.34	0.43
54:BA:783:A:C4	54:BA:785:G:H1'	2.54	0.43
27:BE:165:HIS:HA	54:BA:1205:A:C5	2.54	0.43
54:BA:1826:G:H2'	54:BA:1827:U:C6	2.54	0.43
19:AT:40:ALA:HB1	19:AT:41:GLY:CA	2.47	0.42
51:B2:37:LYS:HE3	54:BA:458:G:N7	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BA:532:A:C8	54:BA:2021:C:C4	3.07	0.42
50:B1:20:TYR:CE1	50:B1:37:LYS:HE3	2.55	0.42
1:AB:162:VAL:HG22	1:AB:164:ASP:H	1.85	0.42
21:AA:5:U:H4'	21:AA:6:G:C5	2.54	0.42
9:AJ:71:LEU:HD23	9:AJ:72:ARG:N	2.35	0.42
54:BA:2440:C:C5	54:BA:2441:U:H1'	2.55	0.41
9:AJ:42:LEU:HD22	9:AJ:42:LEU:C	2.46	0.41
25:BC:222:THR:HG22	54:BA:1826:G:H5''	2.03	0.41
54:BA:61:C:H3'	54:BA:62:U:H5''	2.03	0.41
26:BD:106:LYS:HE3	26:BD:206:ALA:O	2.20	0.41
54:BA:1729:U:C5	54:BA:1730:C:H1'	2.55	0.41
1:AB:30:ILE:HG22	1:AB:32:GLY:H	1.86	0.41
54:BA:1631:G:C2	54:BA:1633:G:H5''	2.56	0.41
18:AS:5:LYS:HE2	21:AA:1312:G:H5'	2.02	0.41
21:AA:6:G:H2'	21:AA:6:G:N3	2.36	0.41
21:AA:765:G:C8	21:AA:813:U:C4	3.08	0.41
43:BU:61:GLU:H	43:BU:61:GLU:CD	2.28	0.41
21:AA:35:G:H1'	21:AA:36:C:C6	2.56	0.41
37:BO:40:ILE:N	37:BO:40:ILE:HD12	2.36	0.41
21:AA:410:G:H2'	21:AA:429:U:C4	2.56	0.40
45:BW:10:ARG:C	45:BW:12:GLY:H	2.29	0.40
54:BA:1712:U:H3'	54:BA:1713:A:H3'	2.03	0.40
25:BC:75:ALA:HB2	25:BC:95:TYR:CD2	2.57	0.40
34:BL:70:LYS:HE2	34:BL:107:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AB	218/220 (99%)	195 (89%)	22 (10%)	1 (0%)	24 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	205/208 (99%)	191 (93%)	12 (6%)	2 (1%)	12	49
3	AD	203/206 (98%)	185 (91%)	15 (7%)	3 (2%)	8	40
4	AE	150/152 (99%)	134 (89%)	9 (6%)	7 (5%)	2	16
5	AF	99/101 (98%)	86 (87%)	6 (6%)	7 (7%)	1	11
6	AG	150/152 (99%)	143 (95%)	7 (5%)	0	100	100
7	AH	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
8	AI	126/128 (98%)	110 (87%)	12 (10%)	4 (3%)	3	21
9	AJ	98/100 (98%)	88 (90%)	5 (5%)	5 (5%)	1	15
10	AK	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	51
11	AL	121/124 (98%)	111 (92%)	10 (8%)	0	100	100
12	AM	112/115 (97%)	98 (88%)	12 (11%)	2 (2%)	6	34
13	AN	98/101 (97%)	90 (92%)	7 (7%)	1 (1%)	12	49
14	AO	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	10	44
15	AP	79/81 (98%)	68 (86%)	7 (9%)	4 (5%)	1	15
16	AQ	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	4	26
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	6	34
18	AS	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
19	AT	84/86 (98%)	74 (88%)	8 (10%)	2 (2%)	4	27
20	AU	51/53 (96%)	27 (53%)	14 (28%)	10 (20%)	0	2
25	BC	270/273 (99%)	238 (88%)	21 (8%)	11 (4%)	2	18
26	BD	207/209 (99%)	178 (86%)	18 (9%)	11 (5%)	1	15
27	BE	199/201 (99%)	177 (89%)	17 (8%)	5 (2%)	4	26
28	BF	176/179 (98%)	151 (86%)	21 (12%)	4 (2%)	5	28
29	BG	174/177 (98%)	152 (87%)	13 (8%)	9 (5%)	1	15
30	BH	147/149 (99%)	132 (90%)	13 (9%)	2 (1%)	9	40
31	BI	139/142 (98%)	125 (90%)	10 (7%)	4 (3%)	3	23
32	BJ	140/142 (99%)	125 (89%)	8 (6%)	7 (5%)	1	16
33	BK	121/123 (98%)	106 (88%)	12 (10%)	3 (2%)	4	26
34	BL	141/144 (98%)	117 (83%)	12 (8%)	12 (8%)	0	9
35	BM	134/136 (98%)	117 (87%)	12 (9%)	5 (4%)	2	20
36	BN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
38	BP	112/115 (97%)	91 (81%)	15 (13%)	6 (5%)	1	15
39	BQ	115/118 (98%)	100 (87%)	15 (13%)	0	100	100
40	BR	101/103 (98%)	94 (93%)	3 (3%)	4 (4%)	2	18
41	BS	108/110 (98%)	100 (93%)	6 (6%)	2 (2%)	6	32
42	BT	92/94 (98%)	78 (85%)	11 (12%)	3 (3%)	3	21
43	BU	101/104 (97%)	85 (84%)	12 (12%)	4 (4%)	2	18
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	65 (83%)	6 (8%)	7 (9%)	0	8
46	BX	75/79 (95%)	70 (93%)	3 (4%)	2 (3%)	4	25
47	BY	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	7	38
48	BZ	56/59 (95%)	50 (89%)	4 (7%)	2 (4%)	2	20
49	B0	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	6	32
50	B1	50/52 (96%)	43 (86%)	3 (6%)	4 (8%)	1	9
51	B2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
52	B3	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	3	21
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	210 (95%)	8 (4%)	3 (1%)	9	40
All	All	5876/6008 (98%)	5249 (89%)	458 (8%)	169 (3%)	5	23

All (169) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	149	PRO
8	AI	44	ARG
16	AQ	80	LYS
20	AU	6	ARG
20	AU	9	GLU
20	AU	13	VAL
25	BC	141	HIS
26	BD	80	TRP
27	BE	31	VAL
33	BK	71	ARG
33	BK	103	VAL
34	BL	55	MET
34	BL	66	PHE

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Mol	Chain	Res	Type
35	BM	21	ALA
35	BM	110	GLU
43	BU	70	ALA
49	B0	39	ARG
2	AC	195	ILE
3	AD	47	LEU
4	AE	54	GLU
4	AE	104	ILE
4	AE	105	ILE
5	AF	10	VAL
5	AF	59	TYR
8	AI	119	LYS
12	AM	22	TYR
12	AM	42	VAL
15	AP	17	TYR
19	AT	42	ASP
20	AU	22	CYS
20	AU	48	LYS
25	BC	161	VAL
25	BC	185	ALA
26	BD	51	THR
26	BD	60	VAL
26	BD	75	ALA
27	BE	96	VAL
28	BF	103	ILE
29	BG	46	ASP
29	BG	167	VAL
29	BG	174	LYS
31	BI	10	LEU
31	BI	119	ALA
32	BJ	15	TRP
33	BK	25	LEU
34	BL	82	LEU
34	BL	83	ALA
34	BL	101	ILE
36	BN	47	VAL
38	BP	69	VAL
40	BR	29	THR
40	BR	53	PHE
45	BW	10	ARG
45	BW	14	ASP
45	BW	23	LYS

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Mol	Chain	Res	Type
46	BX	27	ARG
50	B1	36	LYS
52	B3	46	LYS
4	AE	43	GLY
5	AF	6	ILE
5	AF	86	ARG
8	AI	120	ALA
9	AJ	41	PRO
9	AJ	57	VAL
9	AJ	75	ASP
10	AK	16	SER
20	AU	20	ARG
20	AU	34	ARG
25	BC	13	ARG
25	BC	36	ASN
26	BD	34	VAL
26	BD	86	GLU
26	BD	136	ASN
28	BF	77	LYS
29	BG	39	ALA
29	BG	59	ASP
30	BH	10	ALA
32	BJ	81	ILE
34	BL	15	ALA
34	BL	44	GLY
38	BP	26	GLU
38	BP	50	ARG
38	BP	64	SER
40	BR	30	GLY
42	BT	11	LEU
43	BU	5	ARG
45	BW	41	GLY
45	BW	74	LYS
50	B1	45	HIS
56	B5	109	MET
1	AB	18	GLN
5	AF	90	MET
8	AI	122	ARG
15	AP	9	HIS
15	AP	79	ASN
16	AQ	17	GLU
19	AT	65	LEU

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Mol	Chain	Res	Type
20	AU	21	SER
25	BC	189	ALA
25	BC	196	ASN
26	BD	95	SER
26	BD	114	LYS
27	BE	94	GLN
27	BE	97	ASN
27	BE	123	LYS
28	BF	136	ILE
29	BG	22	VAL
29	BG	151	ARG
30	BH	88	GLY
31	BI	135	MET
32	BJ	44	TYR
32	BJ	45	THR
34	BL	5	THR
34	BL	29	LYS
34	BL	30	THR
35	BM	36	VAL
35	BM	58	LYS
38	BP	32	VAL
42	BT	78	SER
45	BW	11	ASN
47	BY	61	ALA
48	BZ	3	THR
50	B1	24	LYS
52	B3	25	HIS
3	AD	26	ALA
3	AD	84	ASN
4	AE	106	ALA
5	AF	92	THR
5	AF	98	GLU
9	AJ	42	LEU
9	AJ	92	LEU
15	AP	13	LYS
20	AU	28	LEU
25	BC	153	LEU
26	BD	15	PHE
28	BF	107	VAL
31	BI	64	ARG
32	BJ	53	TYR
34	BL	17	LYS

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Mol	Chain	Res	Type
34	BL	69	ARG
36	BN	10	LEU
41	BS	90	LYS
43	BU	12	VAL
45	BW	44	PHE
46	BX	53	LYS
4	AE	158	LYS
13	AN	70	PRO
20	AU	23	GLU
25	BC	169	ALA
25	BC	235	GLU
26	BD	119	ALA
32	BJ	42	ALA
35	BM	80	VAL
42	BT	9	LYS
50	B1	4	ILE
32	BJ	112	GLY
56	B5	91	GLY
56	B5	107	GLY
38	BP	31	VAL
2	AC	14	VAL
25	BC	9	SER
29	BG	112	VAL
48	BZ	31	ILE
14	AO	40	GLY
17	AR	20	ILE
40	BR	27	ILE
41	BS	29	VAL
43	BU	19	GLY
29	BG	97	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%)	178 (99%)	2 (1%)	65 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/171 (99%)	167 (98%)	3 (2%)	51	68
3	AD	172/173 (99%)	171 (99%)	1 (1%)	78	83
4	AE	113/113 (100%)	112 (99%)	1 (1%)	70	79
5	AF	87/87 (100%)	85 (98%)	2 (2%)	44	64
6	AG	123/123 (100%)	122 (99%)	1 (1%)	73	80
7	AH	104/105 (99%)	102 (98%)	2 (2%)	50	67
8	AI	105/105 (100%)	105 (100%)	0	100	100
9	AJ	86/86 (100%)	85 (99%)	1 (1%)	63	75
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	88 (97%)	3 (3%)	33	55
13	AN	83/84 (99%)	82 (99%)	1 (1%)	63	75
14	AO	76/77 (99%)	76 (100%)	0	100	100
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	47 (98%)	1 (2%)	47	65
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	62 (95%)	3 (5%)	24	45
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	210 (97%)	6 (3%)	38	60
26	BD	164/164 (100%)	163 (99%)	1 (1%)	78	83
27	BE	165/165 (100%)	162 (98%)	3 (2%)	51	68
28	BF	149/150 (99%)	146 (98%)	3 (2%)	48	66
29	BG	137/138 (99%)	133 (97%)	4 (3%)	37	58
30	BH	114/114 (100%)	113 (99%)	1 (1%)	70	79
31	BI	109/110 (99%)	107 (98%)	2 (2%)	51	68
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%)	100 (98%)	2 (2%)	48	66
35	BM	109/109 (100%)	105 (96%)	4 (4%)	30	51
36	BN	100/100 (100%)	99 (99%)	1 (1%)	68	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BO	86/87 (99%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	95 (96%)	4 (4%)	28	49
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	65	76
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
43	BU	83/84 (99%)	82 (99%)	1 (1%)	63	75
44	BV	78/78 (100%)	76 (97%)	2 (3%)	40	62
45	BW	59/59 (100%)	58 (98%)	1 (2%)	53	69
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	47	65
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	50 (98%)	1 (2%)	48	66
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%)	4775 (99%)	67 (1%)	57	72

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	40	ILE
1	AB	88	GLN
2	AC	35	ASP
2	AC	128	MET
2	AC	175	HIS
3	AD	169	TRP
4	AE	30	PHE
5	AF	3	HIS
5	AF	52	ASN
6	AG	132	THR
7	AH	76	ARG
7	AH	104	SER
9	AJ	42	LEU

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Mol	Chain	Res	Type
12	AM	3	ILE
12	AM	18	LEU
12	AM	54	THR
13	AN	62	ASN
17	AR	34	GLU
19	AT	22	SER
19	AT	35	TYR
19	AT	67	HIS
25	BC	80	LEU
25	BC	128	THR
25	BC	173	LEU
25	BC	190	THR
25	BC	200	MET
25	BC	235	GLU
26	BD	67	HIS
27	BE	78	TRP
27	BE	96	VAL
27	BE	116	ASP
28	BF	12	VAL
28	BF	27	VAL
28	BF	162	ASP
29	BG	33	THR
29	BG	59	ASP
29	BG	66	THR
29	BG	154	GLU
30	BH	137	GLU
31	BI	34	ILE
31	BI	87	SER
32	BJ	1	MET
33	BK	65	THR
33	BK	84	CYS
33	BK	105	ARG
34	BL	46	VAL
34	BL	82	LEU
35	BM	36	VAL
35	BM	57	VAL
35	BM	97	GLN
35	BM	131	VAL
36	BN	4	ARG
38	BP	32	VAL
38	BP	64	SER
38	BP	67	GLU

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Mol	Chain	Res	Type
38	BP	98	TYR
39	BQ	32	ARG
40	BR	32	THR
41	BS	3	THR
43	BU	61	GLU
44	BV	24	ASN
44	BV	51	GLN
45	BW	31	LEU
49	B0	40	HIS
52	B3	25	HIS
53	B4	19	ARG
56	B5	129	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	18	GLN
1	AB	38	HIS
1	AB	145	ASN
1	AB	177	ASN
2	AC	40	GLN
3	AD	163	GLN
5	AF	63	ASN
6	AG	67	ASN
6	AG	85	GLN
6	AG	129	ASN
6	AG	147	ASN
8	AI	4	GLN
8	AI	74	GLN
8	AI	125	GLN
10	AK	23	HIS
10	AK	37	GLN
11	AL	19	ASN
13	AN	66	GLN
14	AO	37	HIS
14	AO	79	GLN
15	AP	18	GLN
17	AR	53	GLN
18	AS	51	HIS
18	AS	56	HIS
19	AT	74	HIS
25	BC	250	GLN

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Mol	Chain	Res	Type
26	BD	36	GLN
27	BE	29	HIS
27	BE	62	GLN
28	BF	26	GLN
29	BG	21	GLN
29	BG	37	ASN
29	BG	63	GLN
30	BH	2	GLN
30	BH	11	ASN
30	BH	28	ASN
31	BI	5	GLN
31	BI	29	GLN
32	BJ	76	HIS
32	BJ	77	HIS
37	BO	104	GLN
39	BQ	71	ASN
40	BR	87	GLN
40	BR	89	HIS
41	BS	7	HIS
41	BS	15	GLN
41	BS	57	ASN
44	BV	51	GLN
44	BV	80	HIS
45	BW	11	ASN
46	BX	15	ASN
52	B3	23	HIS
56	B5	155	ASN
56	B5	160	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	270 (17%)	72 (4%)
22	A1	75/76 (98%)	10 (13%)	6 (8%)
23	A2	14/15 (93%)	3 (21%)	1 (7%)
24	A3	76/77 (98%)	12 (15%)	6 (7%)
54	BA	2902/2903 (99%)	493 (16%)	132 (4%)
55	BB	116/118 (98%)	18 (15%)	3 (2%)
All	All	4712/4722 (99%)	806 (17%)	220 (4%)

All (806) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	16	A
21	AA	27	G
21	AA	31	G
21	AA	32	A
21	AA	34	C
21	AA	35	G
21	AA	39	G
21	AA	46	G
21	AA	47	C
21	AA	48	C
21	AA	51	A
21	AA	65	A
21	AA	66	A
21	AA	69	G
21	AA	71	A
21	AA	72	A
21	AA	83	C
21	AA	84	U
21	AA	85	U
21	AA	86	G
21	AA	87	C
21	AA	95	C
21	AA	109	A
21	AA	110	C
21	AA	121	U
21	AA	130	A
21	AA	132	C
21	AA	133	U
21	AA	144	G
21	AA	159	G
21	AA	160	A
21	AA	163	C
21	AA	165	G
21	AA	182	A
21	AA	183	C
21	AA	194	C
21	AA	195	A
21	AA	197	A

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Mol	Chain	Res	Type
21	AA	198	G
21	AA	211	G
21	AA	212	G
21	AA	239	U
21	AA	240	G
21	AA	243	A
21	AA	244	U
21	AA	246	A
21	AA	249	U
21	AA	250	A
21	AA	251	G
21	AA	252	U
21	AA	272	C
21	AA	275	G
21	AA	282	A
21	AA	285	C
21	AA	289	G
21	AA	293	G
21	AA	306	A
21	AA	309	A
21	AA	310	G
21	AA	316	C
21	AA	317	U
21	AA	328	C
21	AA	329	A
21	AA	330	C
21	AA	340	U
21	AA	341	C
21	AA	347	G
21	AA	348	G
21	AA	352	C
21	AA	354	G
21	AA	355	C
21	AA	367	U
21	AA	381	C
21	AA	382	A
21	AA	383	A
21	AA	384	G
21	AA	397	A
21	AA	398	U
21	AA	412	A
21	AA	413	G

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Mol	Chain	Res	Type
21	AA	414	A
21	AA	415	A
21	AA	421	U
21	AA	422	C
21	AA	424	G
21	AA	428	G
21	AA	429	U
21	AA	452	A
21	AA	456	A
21	AA	461	A
21	AA	467	U
21	AA	468	A
21	AA	470	C
21	AA	484	G
21	AA	485	U
21	AA	493	A
21	AA	496	A
21	AA	497	G
21	AA	504	C
21	AA	505	G
21	AA	506	G
21	AA	509	A
21	AA	510	A
21	AA	511	C
21	AA	523	A
21	AA	527	G
21	AA	528	C
21	AA	532	A
21	AA	533	A
21	AA	534	U
21	AA	547	A
21	AA	550	G
21	AA	562	U
21	AA	564	C
21	AA	572	A
21	AA	573	A
21	AA	575	G
21	AA	576	C
21	AA	577	G
21	AA	610	U
21	AA	618	C
21	AA	619	U

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Mol	Chain	Res	Type
21	AA	641	U
21	AA	642	A
21	AA	649	A
21	AA	653	U
21	AA	654	G
21	AA	660	C
21	AA	675	A
21	AA	676	A
21	AA	700	G
21	AA	722	G
21	AA	723	U
21	AA	724	G
21	AA	731	G
21	AA	733	G
21	AA	734	G
21	AA	735	C
21	AA	755	G
21	AA	767	A
21	AA	777	A
21	AA	794	A
21	AA	808	C
21	AA	811	C
21	AA	812	G
21	AA	819	A
21	AA	840	C
21	AA	841	C
21	AA	842	U
21	AA	843	U
21	AA	846	G
21	AA	867	G
21	AA	872	A
21	AA	885	G
21	AA	891	U
21	AA	892	A
21	AA	893	C
21	AA	914	A
21	AA	925	G
21	AA	926	G
21	AA	927	G
21	AA	929	G
21	AA	934	C
21	AA	939	G

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Mol	Chain	Res	Type
21	AA	960	U
21	AA	961	U
21	AA	968	A
21	AA	969	A
21	AA	974	A
21	AA	976	G
21	AA	978	A
21	AA	980	C
21	AA	981	U
21	AA	983	A
21	AA	992	U
21	AA	993	G
21	AA	994	A
21	AA	1004	A
21	AA	1030	U
21	AA	1031	C
21	AA	1033	G
21	AA	1053	G
21	AA	1054	C
21	AA	1055	A
21	AA	1056	U
21	AA	1065	U
21	AA	1068	G
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1124	G
21	AA	1125	U
21	AA	1137	C
21	AA	1139	G
21	AA	1140	C
21	AA	1152	A
21	AA	1157	A
21	AA	1159	U
21	AA	1160	G
21	AA	1161	C
21	AA	1166	G
21	AA	1167	A
21	AA	1183	U
21	AA	1189	U
21	AA	1190	G

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Mol	Chain	Res	Type
21	AA	1191	A
21	AA	1196	A
21	AA	1197	A
21	AA	1201	A
21	AA	1202	U
21	AA	1204	A
21	AA	1213	A
21	AA	1217	C
21	AA	1222	G
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1228	C
21	AA	1241	G
21	AA	1256	A
21	AA	1257	A
21	AA	1258	G
21	AA	1266	G
21	AA	1280	A
21	AA	1281	C
21	AA	1286	U
21	AA	1300	G
21	AA	1301	U
21	AA	1302	C
21	AA	1304	G
21	AA	1305	G
21	AA	1312	G
21	AA	1317	C
21	AA	1318	A
21	AA	1322	C
21	AA	1329	A
21	AA	1336	C
21	AA	1337	G
21	AA	1338	G
21	AA	1345	U
21	AA	1346	A
21	AA	1360	A
21	AA	1363	A
21	AA	1381	U
21	AA	1382	C
21	AA	1397	C
21	AA	1398	A

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Mol	Chain	Res	Type
21	AA	1419	G
21	AA	1431	A
21	AA	1432	G
21	AA	1446	A
21	AA	1447	A
21	AA	1448	C
21	AA	1469	C
21	AA	1470	U
21	AA	1493	A
21	AA	1494	G
21	AA	1497	G
21	AA	1503	A
21	AA	1506	U
21	AA	1529	G
21	AA	1530	G
21	AA	1533	C
21	AA	1534	A
22	A1	10	G
22	A1	11	C
22	A1	17	U
22	A1	47	U
22	A1	48	C
22	A1	57	G
22	A1	60	C
22	A1	61	C
22	A1	74	C
22	A1	75	C
23	A2	89	U
23	A2	90	U
23	A2	91	A
24	A3	9	G
24	A3	10	G
24	A3	16	C
24	A3	17	C
24	A3	18	U
24	A3	19	G
24	A3	20	G
24	A3	48	U
24	A3	49	C
24	A3	62	C
24	A3	63	C
24	A3	73	A

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Mol	Chain	Res	Type
54	BA	10	A
54	BA	11	C
54	BA	34	U
54	BA	48	G
54	BA	52	A
54	BA	61	C
54	BA	62	U
54	BA	71	A
54	BA	72	U
54	BA	73	A
54	BA	75	G
54	BA	84	A
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	122	G
54	BA	142	A
54	BA	143	C
54	BA	149	A
54	BA	150	U
54	BA	162	U
54	BA	181	A
54	BA	196	A
54	BA	199	A
54	BA	205	G
54	BA	216	A
54	BA	222	A
54	BA	225	C
54	BA	233	A
54	BA	248	G
54	BA	249	C
54	BA	250	G
54	BA	263	G
54	BA	271	G
54	BA	272	A
54	BA	273	G
54	BA	279	A
54	BA	280	U
54	BA	295	G

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Mol	Chain	Res	Type
54	BA	317	G
54	BA	323	C
54	BA	324	A
54	BA	326	G
54	BA	327	G
54	BA	329	G
54	BA	330	A
54	BA	331	C
54	BA	332	A
54	BA	345	A
54	BA	346	A
54	BA	370	G
54	BA	372	G
54	BA	384	A
54	BA	385	C
54	BA	386	G
54	BA	388	G
54	BA	389	G
54	BA	404	A
54	BA	405	U
54	BA	406	G
54	BA	412	A
54	BA	428	A
54	BA	430	A
54	BA	443	A
54	BA	449	A
54	BA	451	U
54	BA	452	G
54	BA	453	A
54	BA	454	A
54	BA	455	C
54	BA	456	C
54	BA	457	A
54	BA	458	G
54	BA	473	G
54	BA	478	A
54	BA	479	A
54	BA	480	A
54	BA	481	G
54	BA	484	C
54	BA	491	G
54	BA	504	A

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Mol	Chain	Res	Type
54	BA	505	A
54	BA	520	G
54	BA	526	A
54	BA	527	C
54	BA	529	A
54	BA	531	C
54	BA	532	A
54	BA	533	G
54	BA	544	C
54	BA	546	U
54	BA	547	A
54	BA	548	G
54	BA	549	G
54	BA	573	U
54	BA	575	A
54	BA	586	A
54	BA	587	C
54	BA	603	A
54	BA	607	U
54	BA	612	G
54	BA	613	A
54	BA	614	A
54	BA	615	U
54	BA	620	G
54	BA	627	A
54	BA	631	A
54	BA	632	A
54	BA	637	A
54	BA	646	U
54	BA	653	U
54	BA	654	A
54	BA	655	A
54	BA	656	G
54	BA	657	U
54	BA	671	C
54	BA	672	C
54	BA	685	A
54	BA	686	U
54	BA	715	A
54	BA	716	A
54	BA	719	C
54	BA	727	A

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Mol	Chain	Res	Type
54	BA	730	A
54	BA	747	U
54	BA	751	A
54	BA	758	C
54	BA	759	G
54	BA	763	G
54	BA	764	A
54	BA	765	C
54	BA	775	G
54	BA	781	A
54	BA	782	A
54	BA	783	A
54	BA	784	G
54	BA	785	G
54	BA	790	U
54	BA	791	C
54	BA	792	A
54	BA	794	A
54	BA	805	G
54	BA	809	G
54	BA	812	C
54	BA	847	U
54	BA	848	C
54	BA	858	G
54	BA	866	A
54	BA	889	C
54	BA	890	C
54	BA	891	G
54	BA	896	A
54	BA	897	C
54	BA	907	G
54	BA	910	A
54	BA	914	G
54	BA	915	C
54	BA	931	U
54	BA	941	A
54	BA	946	C
54	BA	955	U
54	BA	959	A
54	BA	961	C
54	BA	972	A
54	BA	974	G

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Mol	Chain	Res	Type
54	BA	975	A
54	BA	980	A
54	BA	982	C
54	BA	983	A
54	BA	985	C
54	BA	990	A
54	BA	995	C
54	BA	996	A
54	BA	1008	A
54	BA	1009	A
54	BA	1012	U
54	BA	1013	C
54	BA	1021	A
54	BA	1022	G
54	BA	1024	G
54	BA	1025	G
54	BA	1033	U
54	BA	1044	C
54	BA	1048	A
54	BA	1060	U
54	BA	1062	G
54	BA	1063	G
54	BA	1067	A
54	BA	1068	G
54	BA	1070	A
54	BA	1071	G
54	BA	1073	A
54	BA	1076	C
54	BA	1078	U
54	BA	1079	C
54	BA	1088	A
54	BA	1089	A
54	BA	1090	A
54	BA	1094	U
54	BA	1096	A
54	BA	1112	G
54	BA	1126	A
54	BA	1128	G
54	BA	1129	A
54	BA	1132	U
54	BA	1134	A
54	BA	1135	C

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Mol	Chain	Res	Type
54	BA	1142	A
54	BA	1143	A
54	BA	1155	A
54	BA	1175	A
54	BA	1176	U
54	BA	1186	G
54	BA	1210	G
54	BA	1211	C
54	BA	1225	G
54	BA	1242	U
54	BA	1247	A
54	BA	1251	C
54	BA	1253	A
54	BA	1254	A
54	BA	1255	U
54	BA	1256	G
54	BA	1265	A
54	BA	1266	G
54	BA	1267	U
54	BA	1272	A
54	BA	1273	U
54	BA	1275	A
54	BA	1276	A
54	BA	1287	A
54	BA	1291	C
54	BA	1300	G
54	BA	1301	A
54	BA	1314	C
54	BA	1319	C
54	BA	1320	C
54	BA	1325	U
54	BA	1326	U
54	BA	1328	A
54	BA	1332	G
54	BA	1341	G
54	BA	1365	A
54	BA	1374	G
54	BA	1379	U
54	BA	1383	A
54	BA	1385	A
54	BA	1386	C
54	BA	1390	U

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Mol	Chain	Res	Type
54	BA	1394	U
54	BA	1396	U
54	BA	1397	U
54	BA	1416	G
54	BA	1420	A
54	BA	1421	G
54	BA	1427	A
54	BA	1428	C
54	BA	1440	U
54	BA	1452	G
54	BA	1453	A
54	BA	1454	C
54	BA	1458	U
54	BA	1459	G
54	BA	1461	C
54	BA	1466	U
54	BA	1482	G
54	BA	1490	A
54	BA	1493	C
54	BA	1524	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	1550	C
54	BA	1560	G
54	BA	1569	A
54	BA	1584	U
54	BA	1598	A
54	BA	1599	U
54	BA	1607	C
54	BA	1608	A
54	BA	1618	A
54	BA	1625	C
54	BA	1626	A
54	BA	1629	U
54	BA	1633	G
54	BA	1634	A
54	BA	1635	A
54	BA	1648	U

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Mol	Chain	Res	Type
54	BA	1651	G
54	BA	1652	A
54	BA	1656	C
54	BA	1674	G
54	BA	1675	C
54	BA	1707	G
54	BA	1712	U
54	BA	1714	U
54	BA	1730	C
54	BA	1758	U
54	BA	1764	C
54	BA	1773	A
54	BA	1800	C
54	BA	1808	A
54	BA	1816	C
54	BA	1821	A
54	BA	1827	U
54	BA	1833	C
54	BA	1847	A
54	BA	1873	G
54	BA	1888	G
54	BA	1900	A
54	BA	1901	A
54	BA	1906	G
54	BA	1913	A
54	BA	1914	C
54	BA	1929	G
54	BA	1930	G
54	BA	1937	A
54	BA	1938	A
54	BA	1939	U
54	BA	1940	U
54	BA	1941	C
54	BA	1943	U
54	BA	1944	U
54	BA	1945	G
54	BA	1946	U
54	BA	1955	U
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1981	A

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Mol	Chain	Res	Type
54	BA	1993	U
54	BA	1997	C
54	BA	2002	G
54	BA	2003	A
54	BA	2018	G
54	BA	2020	A
54	BA	2030	A
54	BA	2031	A
54	BA	2032	G
54	BA	2043	C
54	BA	2055	C
54	BA	2058	A
54	BA	2060	A
54	BA	2061	G
54	BA	2069	G
54	BA	2076	U
54	BA	2093	G
54	BA	2112	G
54	BA	2113	U
54	BA	2115	G
54	BA	2117	A
54	BA	2119	A
54	BA	2126	A
54	BA	2127	G
54	BA	2133	G
54	BA	2135	A
54	BA	2137	U
54	BA	2138	G
54	BA	2155	U
54	BA	2157	G
54	BA	2159	G
54	BA	2160	C
54	BA	2169	A
54	BA	2172	U
54	BA	2173	A
54	BA	2181	U
54	BA	2198	A
54	BA	2203	U
54	BA	2211	A
54	BA	2212	A
54	BA	2213	U
54	BA	2216	G

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Mol	Chain	Res	Type
54	BA	2225	A
54	BA	2226	C
54	BA	2238	G
54	BA	2250	G
54	BA	2251	G
54	BA	2267	A
54	BA	2276	G
54	BA	2283	C
54	BA	2296	U
54	BA	2297	A
54	BA	2305	U
54	BA	2307	G
54	BA	2308	G
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2324	U
54	BA	2325	G
54	BA	2333	A
54	BA	2334	U
54	BA	2335	A
54	BA	2339	C
54	BA	2343	U
54	BA	2344	U
54	BA	2347	C
54	BA	2350	C
54	BA	2352	A
54	BA	2353	G
54	BA	2383	G
54	BA	2385	C
54	BA	2389	G
54	BA	2390	U
54	BA	2391	G
54	BA	2392	A
54	BA	2396	G
54	BA	2402	U
54	BA	2406	A
54	BA	2407	A
54	BA	2409	G
54	BA	2419	U
54	BA	2425	A
54	BA	2429	G

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Mol	Chain	Res	Type
54	BA	2430	A
54	BA	2431	U
54	BA	2432	A
54	BA	2433	A
54	BA	2441	U
54	BA	2447	G
54	BA	2448	A
54	BA	2453	A
54	BA	2454	G
54	BA	2476	A
54	BA	2491	U
54	BA	2494	G
54	BA	2495	G
54	BA	2498	C
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2504	U
54	BA	2505	G
54	BA	2513	A
54	BA	2514	U
54	BA	2518	A
54	BA	2529	G
54	BA	2530	A
54	BA	2531	A
54	BA	2540	C
54	BA	2544	G
54	BA	2554	U
54	BA	2566	A
54	BA	2573	C
54	BA	2576	G
54	BA	2578	G
54	BA	2581	G
54	BA	2609	U
54	BA	2610	C
54	BA	2613	U
54	BA	2614	A
54	BA	2628	C
54	BA	2629	U
54	BA	2630	G
54	BA	2631	G
54	BA	2645	G

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Mol	Chain	Res	Type
54	BA	2646	C
54	BA	2647	U
54	BA	2655	G
54	BA	2660	A
54	BA	2683	C
54	BA	2689	U
54	BA	2690	U
54	BA	2691	C
54	BA	2721	A
54	BA	2726	A
54	BA	2727	A
54	BA	2744	G
54	BA	2751	G
54	BA	2757	A
54	BA	2765	A
54	BA	2778	A
54	BA	2779	U
54	BA	2791	G
54	BA	2797	U
54	BA	2798	U
54	BA	2821	A
54	BA	2823	A
54	BA	2824	C
54	BA	2833	U
54	BA	2846	G
54	BA	2858	C
54	BA	2859	G
54	BA	2867	G
54	BA	2868	A
54	BA	2880	C
54	BA	2884	U
55	BB	9	G
55	BB	12	C
55	BB	13	G
55	BB	16	G
55	BB	37	C
55	BB	41	G
55	BB	44	G
55	BB	45	A
55	BB	52	A
55	BB	56	G
55	BB	57	A

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Mol	Chain	Res	Type
55	BB	58	A
55	BB	67	G
55	BB	70	C
55	BB	74	U
55	BB	87	U
55	BB	90	C
55	BB	109	A

All (220) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	13	U
21	AA	34	C
21	AA	46	G
21	AA	65	A
21	AA	85	U
21	AA	109	A
21	AA	132	C
21	AA	173	U
21	AA	194	C
21	AA	211	G
21	AA	243	A
21	AA	251	G
21	AA	281	G
21	AA	309	A
21	AA	316	C
21	AA	328	C
21	AA	340	U
21	AA	350	G
21	AA	354	G
21	AA	366	A
21	AA	382	A
21	AA	383	A
21	AA	414	A
21	AA	451	A
21	AA	496	A
21	AA	504	C
21	AA	509	A
21	AA	527	G
21	AA	532	A
21	AA	535	A
21	AA	575	G

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Mol	Chain	Res	Type
21	AA	641	U
21	AA	653	U
21	AA	675	A
21	AA	733	G
21	AA	734	G
21	AA	792	A
21	AA	811	C
21	AA	840	C
21	AA	891	U
21	AA	892	A
21	AA	925	G
21	AA	965	U
21	AA	983	A
21	AA	1029	U
21	AA	1030	U
21	AA	1049	U
21	AA	1101	A
21	AA	1124	G
21	AA	1139	G
21	AA	1151	A
21	AA	1166	G
21	AA	1190	G
21	AA	1196	A
21	AA	1201	A
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1231	G
21	AA	1233	G
21	AA	1257	A
21	AA	1298	U
21	AA	1300	G
21	AA	1304	G
21	AA	1305	G
21	AA	1336	C
21	AA	1345	U
21	AA	1381	U
21	AA	1429	A
21	AA	1431	A
21	AA	1447	A
21	AA	1469	C
22	A1	10	G

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Mol	Chain	Res	Type
22	A1	46	7MG
22	A1	47	U
22	A1	59	U
22	A1	60	C
22	A1	74	C
23	A2	90	U
24	A3	9	G
24	A3	16	C
24	A3	17	C
24	A3	19	G
24	A3	48	U
24	A3	62	C
54	BA	10	A
54	BA	60	G
54	BA	71	A
54	BA	72	U
54	BA	74	A
54	BA	101	A
54	BA	149	A
54	BA	196	A
54	BA	249	C
54	BA	279	A
54	BA	322	A
54	BA	323	C
54	BA	329	G
54	BA	345	A
54	BA	384	A
54	BA	387	U
54	BA	388	G
54	BA	405	U
54	BA	411	G
54	BA	428	A
54	BA	442	G
54	BA	455	C
54	BA	456	C
54	BA	457	A
54	BA	506	G
54	BA	547	A
54	BA	548	G
54	BA	613	A
54	BA	627	A
54	BA	631	A

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Mol	Chain	Res	Type
54	BA	651	G
54	BA	654	A
54	BA	656	G
54	BA	670	A
54	BA	675	A
54	BA	685	A
54	BA	715	A
54	BA	762	U
54	BA	764	A
54	BA	782	A
54	BA	790	U
54	BA	846	U
54	BA	847	U
54	BA	866	A
54	BA	931	U
54	BA	973	A
54	BA	989	G
54	BA	1008	A
54	BA	1021	A
54	BA	1089	A
54	BA	1128	G
54	BA	1132	U
54	BA	1134	A
54	BA	1142	A
54	BA	1224	U
54	BA	1254	A
54	BA	1266	G
54	BA	1288	G
54	BA	1300	G
54	BA	1320	C
54	BA	1325	U
54	BA	1332	G
54	BA	1378	A
54	BA	1385	A
54	BA	1396	U
54	BA	1397	U
54	BA	1420	A
54	BA	1427	A
54	BA	1453	A
54	BA	1465	G
54	BA	1490	A
54	BA	1535	A

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Mol	Chain	Res	Type
54	BA	1539	U
54	BA	1607	C
54	BA	1625	C
54	BA	1634	A
54	BA	1651	G
54	BA	1674	G
54	BA	1706	C
54	BA	1711	A
54	BA	1713	A
54	BA	1769	U
54	BA	1783	A
54	BA	1787	A
54	BA	1826	G
54	BA	1913	A
54	BA	1936	A
54	BA	1938	A
54	BA	1940	U
54	BA	1943	U
54	BA	1945	G
54	BA	1955	U
54	BA	1971	U
54	BA	1980	G
54	BA	2002	G
54	BA	2030	A
54	BA	2031	A
54	BA	2060	A
54	BA	2126	A
54	BA	2150	C
54	BA	2172	U
54	BA	2197	U
54	BA	2212	A
54	BA	2225	A
54	BA	2249	U
54	BA	2286	G
54	BA	2296	U
54	BA	2324	U
54	BA	2343	U
54	BA	2389	G
54	BA	2391	G
54	BA	2429	G
54	BA	2447	G
54	BA	2453	A

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Mol	Chain	Res	Type
54	BA	2494	G
54	BA	2497	A
54	BA	2503	A
54	BA	2513	A
54	BA	2529	G
54	BA	2572	A
54	BA	2576	G
54	BA	2609	U
54	BA	2628	C
54	BA	2630	G
54	BA	2720	U
54	BA	2721	A
54	BA	2726	A
54	BA	2751	G
54	BA	2756	U
54	BA	2788	C
54	BA	2790	U
54	BA	2823	A
55	BB	12	C
55	BB	56	G
55	BB	57	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	4SU	A1	7	22	18,21,22	1.58	2 (11%)	25,30,33	1.13	2 (8%)
24	OMC	A3	33	24	19,22,23	0.95	0	25,31,34	1.18	2 (8%)
22	7MG	A1	46	22	23,26,27	4.17	2 (8%)	27,39,42	1.59	3 (11%)
22	5MU	A1	54	22	19,22,23	0.80	0	27,32,35	1.62	6 (22%)
24	5MU	A3	55	24	19,22,23	0.91	0	27,32,35	1.55	4 (14%)
24	4SU	A3	8	24	18,21,22	1.70	3 (16%)	25,30,33	0.84	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PSU	A3	56	24	18,21,22	1.05	1 (5%)	21,30,33	1.67	4 (19%)
22	CM0	A1	34	23,22	21,26,27	1.49	2 (9%)	26,37,40	1.36	3 (11%)
22	PSU	A1	55	22	18,21,22	1.01	1 (5%)	21,30,33	1.39	2 (9%)
24	H2U	A3	21	24	18,21,22	1.40	2 (11%)	19,30,33	1.14	3 (15%)
22	6MZ	A1	37	22	22,25,26	0.69	0	29,36,39	1.25	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/7/25/26	0/2/2/2
24	PSU	A3	56	24	-	2/7/25/26	0/2/2/2
22	CM0	A1	34	23,22	-	2/12/30/31	0/2/2/2
22	PSU	A1	55	22	-	0/7/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
22	6MZ	A1	37	22	-	0/9/27/28	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-19.48	1.33	1.45
24	A3	8	4SU	C5-C4	-5.69	1.35	1.42
22	A1	34	CM0	O5-C5	-5.14	1.24	1.36
22	A1	7	4SU	C5-C4	-5.08	1.36	1.42
24	A3	21	H2U	C2-N3	-3.66	1.31	1.38
24	A3	21	H2U	C4-N3	-3.14	1.32	1.37
22	A1	7	4SU	C4-S4	-2.75	1.63	1.68
22	A1	55	PSU	O4'-C1'	-2.70	1.40	1.43
24	A3	8	4SU	C4-S4	-2.69	1.64	1.68
22	A1	46	7MG	C8-N7	-2.48	1.30	1.42
24	A3	56	PSU	C4-N3	-2.38	1.34	1.38
24	A3	8	4SU	O4'-C4'	-2.36	1.39	1.45
22	A1	34	CM0	O8-C8	-2.33	1.23	1.30

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	6.40	112.43	103.37
22	A1	37	6MZ	C9-N6-C6	5.01	127.49	122.85
22	A1	55	PSU	C6-C5-C4	4.17	120.99	118.17
22	A1	34	CM0	C7-O5-C5	4.14	122.76	117.48
22	A1	54	5MU	C5M-C5-C6	-4.12	117.27	122.85
24	A3	55	5MU	C5M-C5-C6	-4.07	117.34	122.85
24	A3	56	PSU	C6-C5-C4	3.95	120.84	118.17
22	A1	54	5MU	C6-C5-C4	3.62	121.00	118.02
24	A3	55	5MU	C5M-C5-C4	3.29	122.29	118.78
24	A3	33	OMC	O2-C2-N3	-3.20	117.29	122.33
22	A1	7	4SU	C6-C5-C4	2.99	122.54	119.95
22	A1	54	5MU	C5-C6-N1	-2.95	120.11	123.31
24	A3	21	H2U	N3-C2-N1	2.89	119.55	116.65
24	A3	55	5MU	C6-C5-C4	2.84	120.36	118.02
24	A3	56	PSU	N1-C2-N3	2.83	118.15	115.17
24	A3	56	PSU	O4'-C1'-C2'	2.76	108.97	105.15
22	A1	54	5MU	C5M-C5-C4	2.75	121.72	118.78
24	A3	33	OMC	C2'-C1'-N1	-2.52	109.45	114.24
22	A1	7	4SU	O4'-C1'-N1	2.46	113.93	108.36
24	A3	55	5MU	C5-C6-N1	-2.36	120.75	123.31
24	A3	21	H2U	C5-C4-N3	2.33	119.17	116.69
22	A1	54	5MU	C4-N3-C2	-2.30	124.32	127.34
22	A1	55	PSU	O4'-C1'-C2'	2.29	108.32	105.15
24	A3	21	H2U	O2-C2-N3	-2.21	117.42	121.49
22	A1	54	5MU	N3-C2-N1	2.18	117.73	114.89
24	A3	56	PSU	O4-C4-N3	-2.09	116.19	120.11
22	A1	46	7MG	C4-C5-N7	2.05	107.80	105.38
22	A1	34	CM0	O2-C2-N1	2.04	125.46	122.80
22	A1	46	7MG	O4'-C4'-C3'	2.03	109.18	105.15
22	A1	34	CM0	O2-C2-N3	-2.02	117.75	121.49
24	A3	8	4SU	C6-C5-C4	2.01	121.69	119.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A3	56	PSU	O4'-C1'-C5-C4
24	A3	56	PSU	O4'-C1'-C5-C6
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9
22	A1	46	7MG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	FME	BA	3001	57	8,9,10	0.74	0	8,9,11	1.05	0
57	VAL	A1	101	58,22	4,6,7	0.80	0	6,7,9	1.10	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	FME	BA	3001	57	-	1/7/9/11	-
57	VAL	A1	101	58,22	-	0/5/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-2.67	117.91	124.77

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.

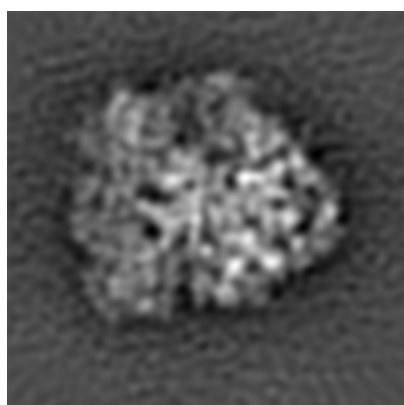
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2472. These allow visual inspection of the internal detail of the map and identification of artifacts.

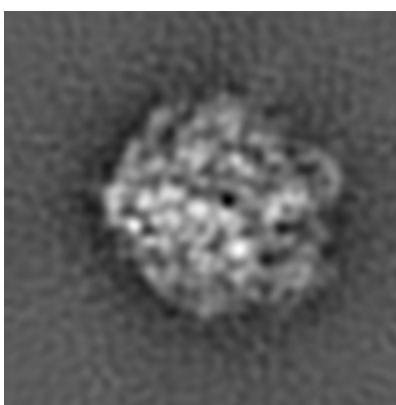
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

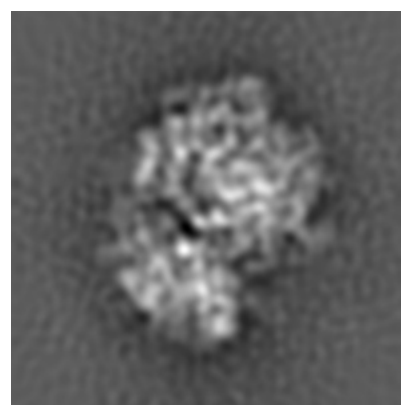
6.1.1 Primary map



X



Y

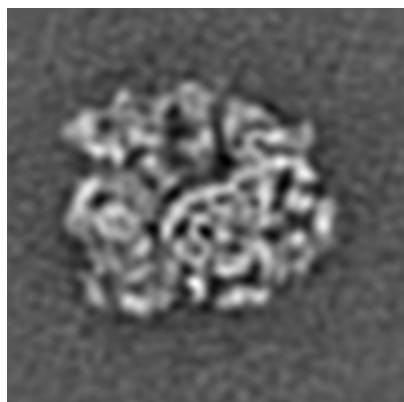


Z

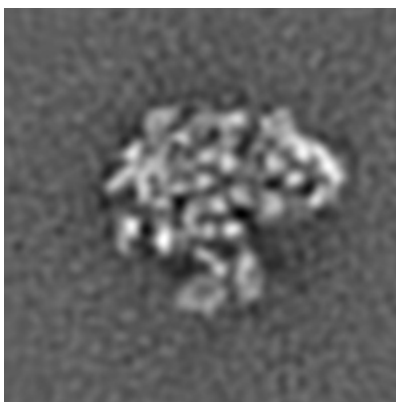
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

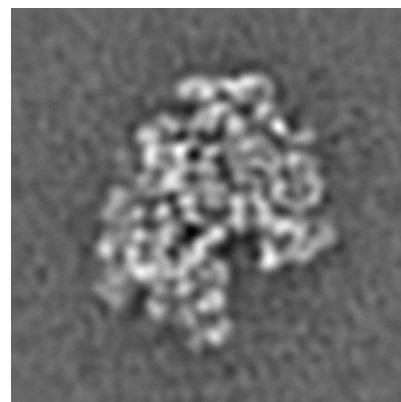
6.2.1 Primary map



X Index: 64



Y Index: 64

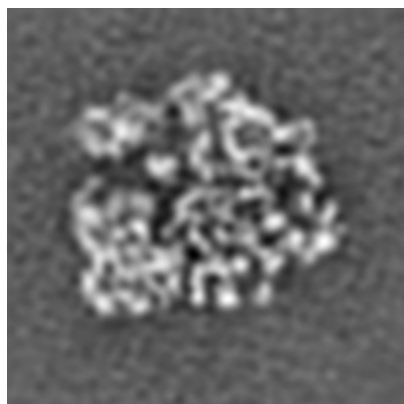


Z Index: 64

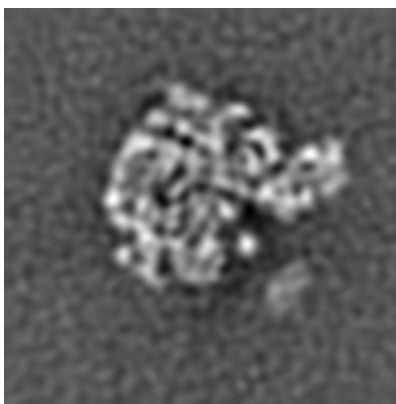
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

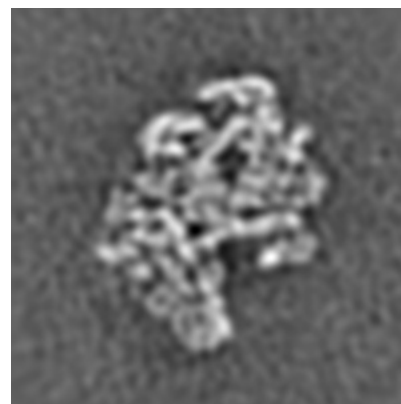
6.3.1 Primary map



X Index: 67



Y Index: 71

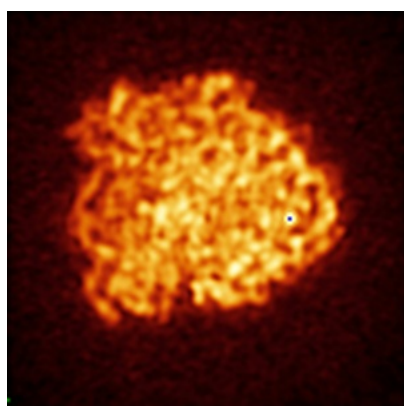


Z Index: 61

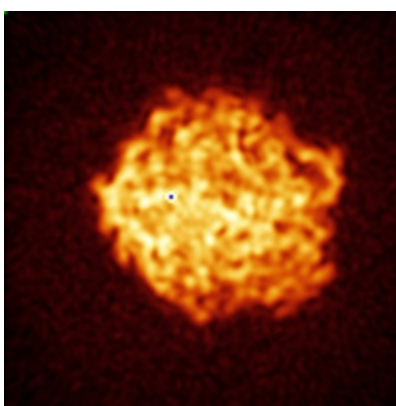
The images above show the largest variance slices of the map in three orthogonal directions.

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

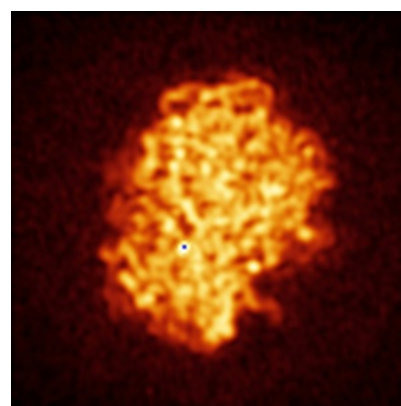
6.4.1 Primary map



X



Y

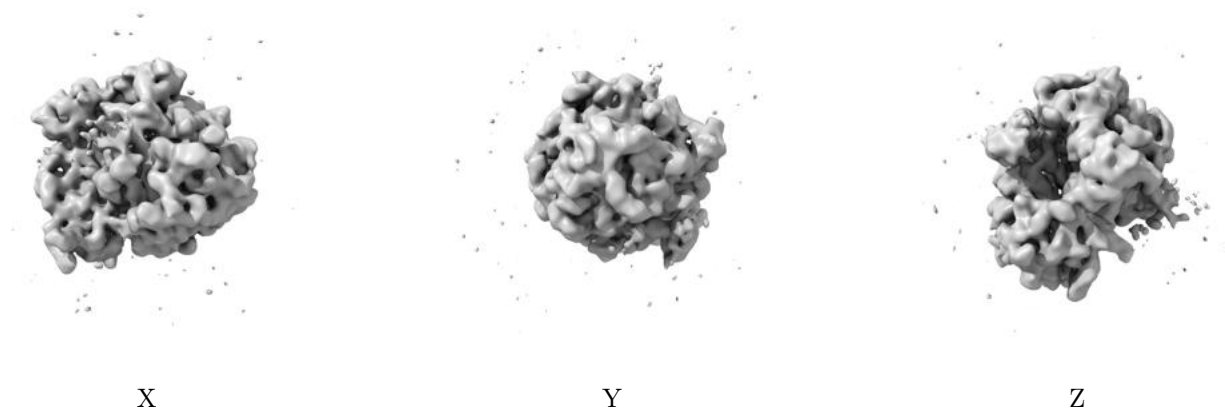


Z

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

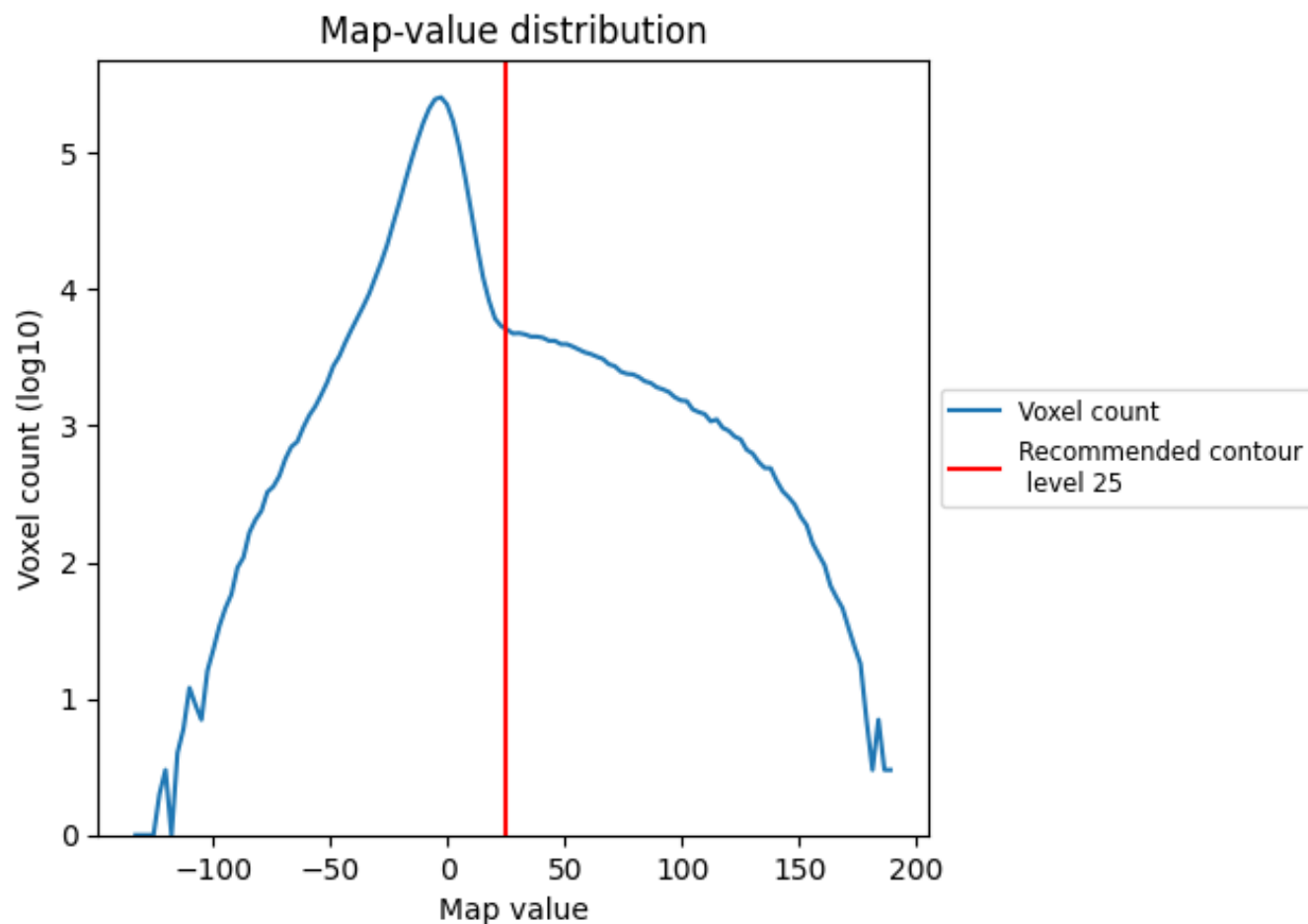
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

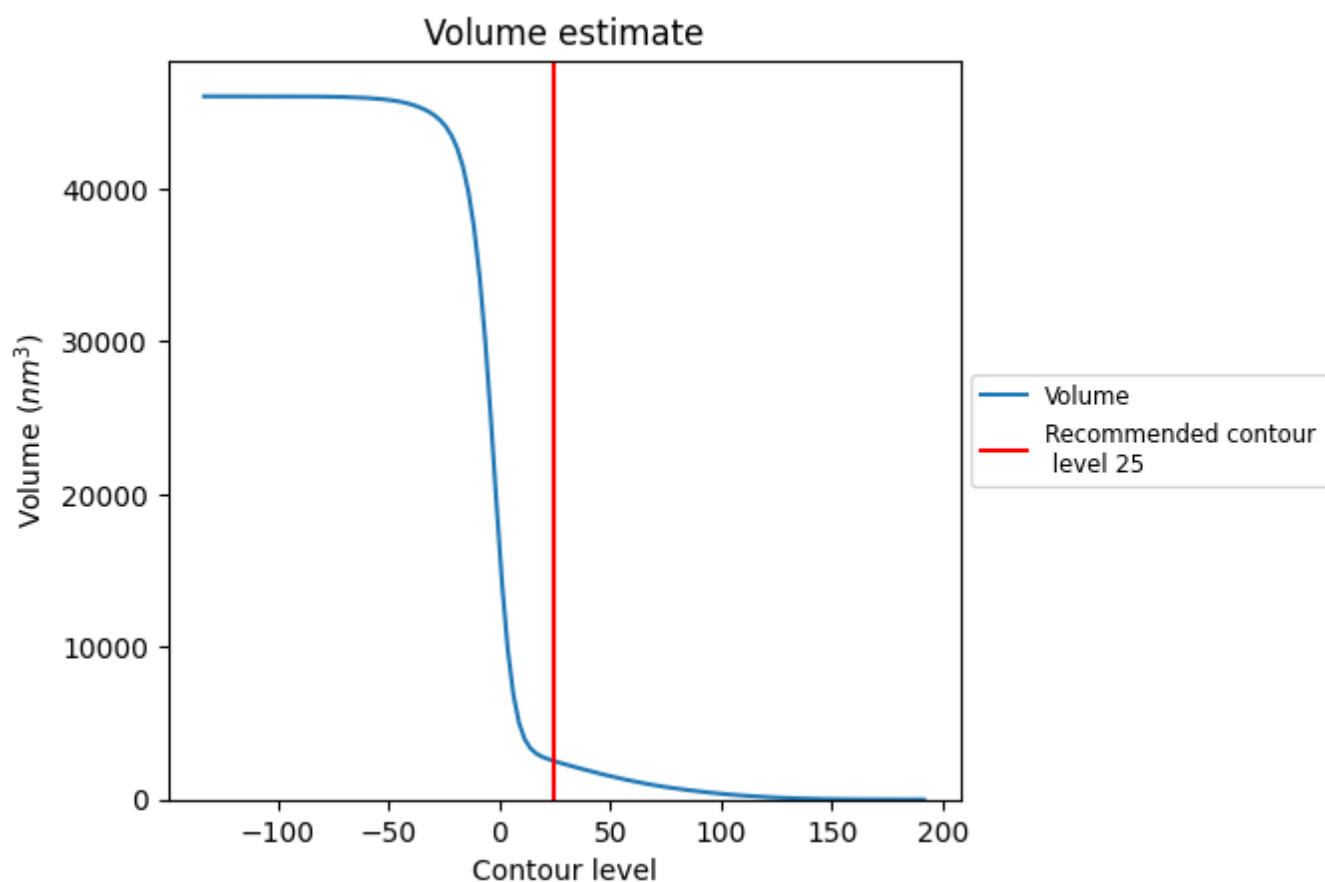
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

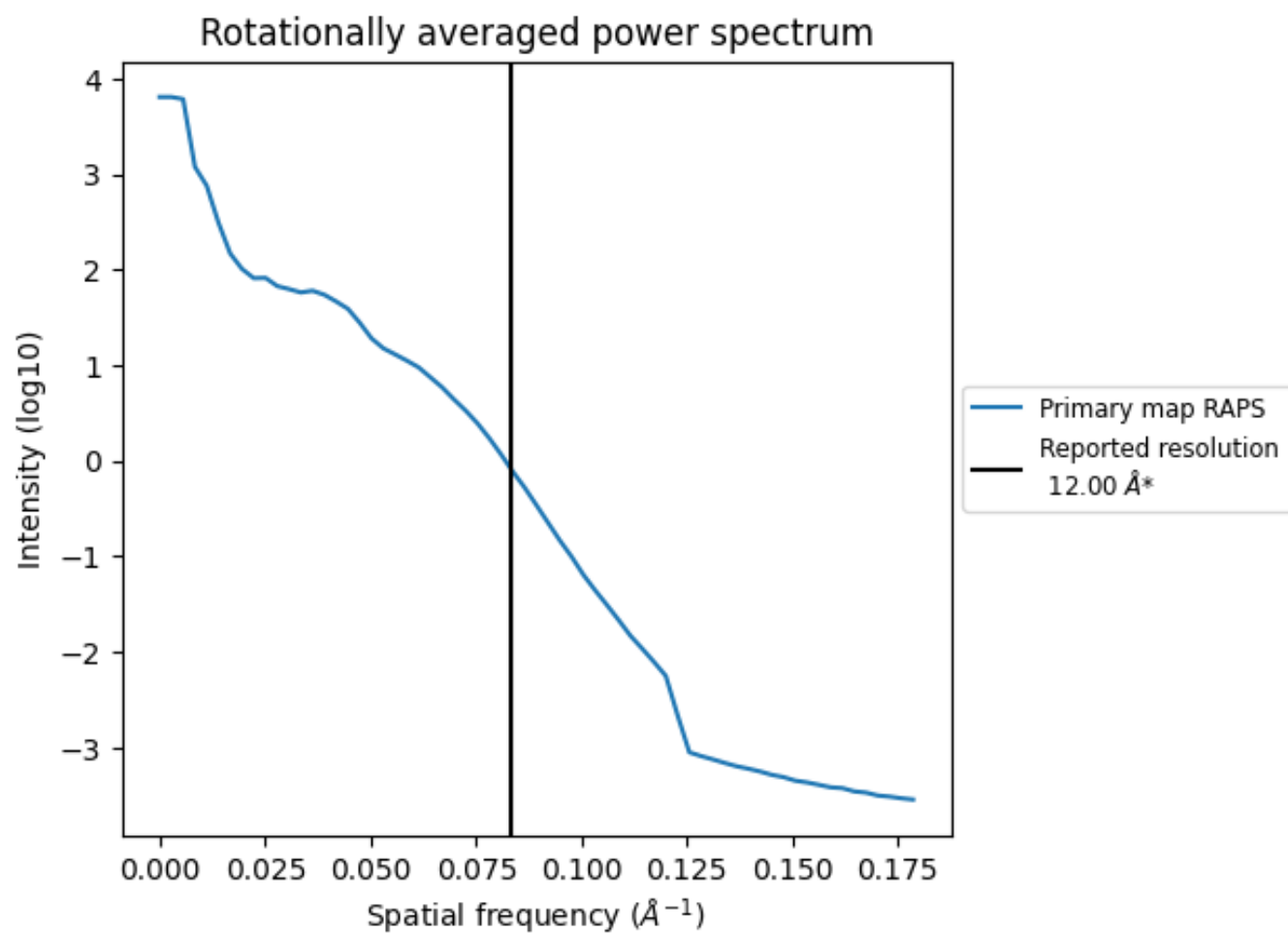
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2507 nm³; this corresponds to an approximate mass of 2264 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 0.083 Å⁻¹

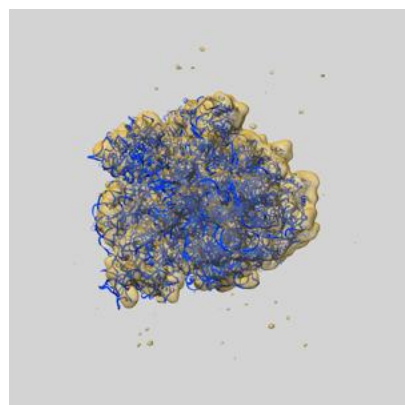
8 Fourier-Shell correlation

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

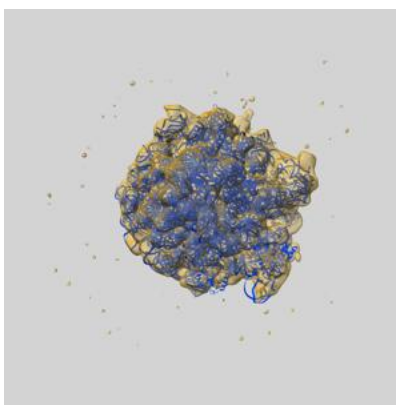
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2472 and PDB model 4V6Z. Per-residue inclusion information can be found in section [3](#) on page [18](#).

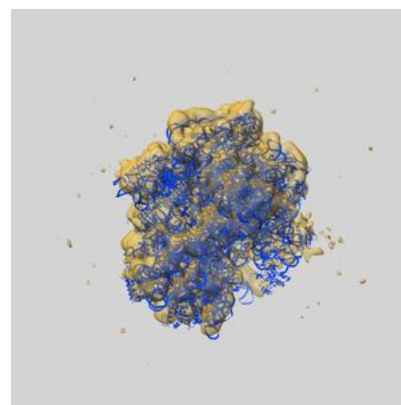
9.1 Map-model overlay [i](#)



X



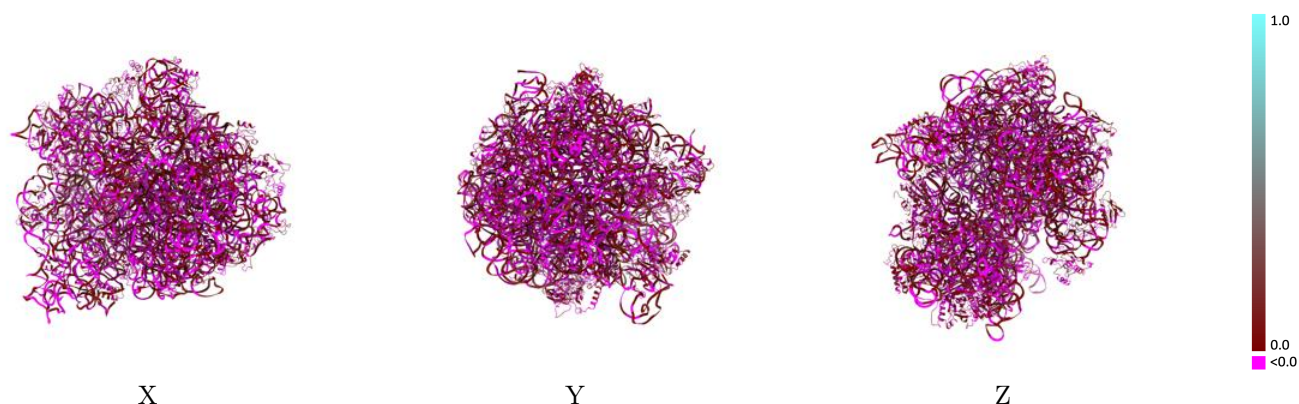
Y



Z

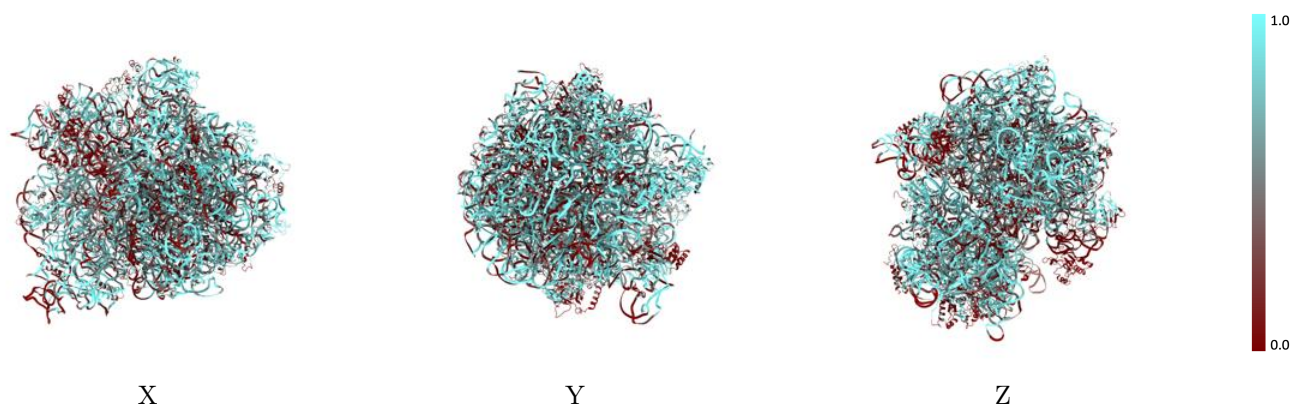
The images above show the 3D surface view of the map at the recommended contour level 25.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



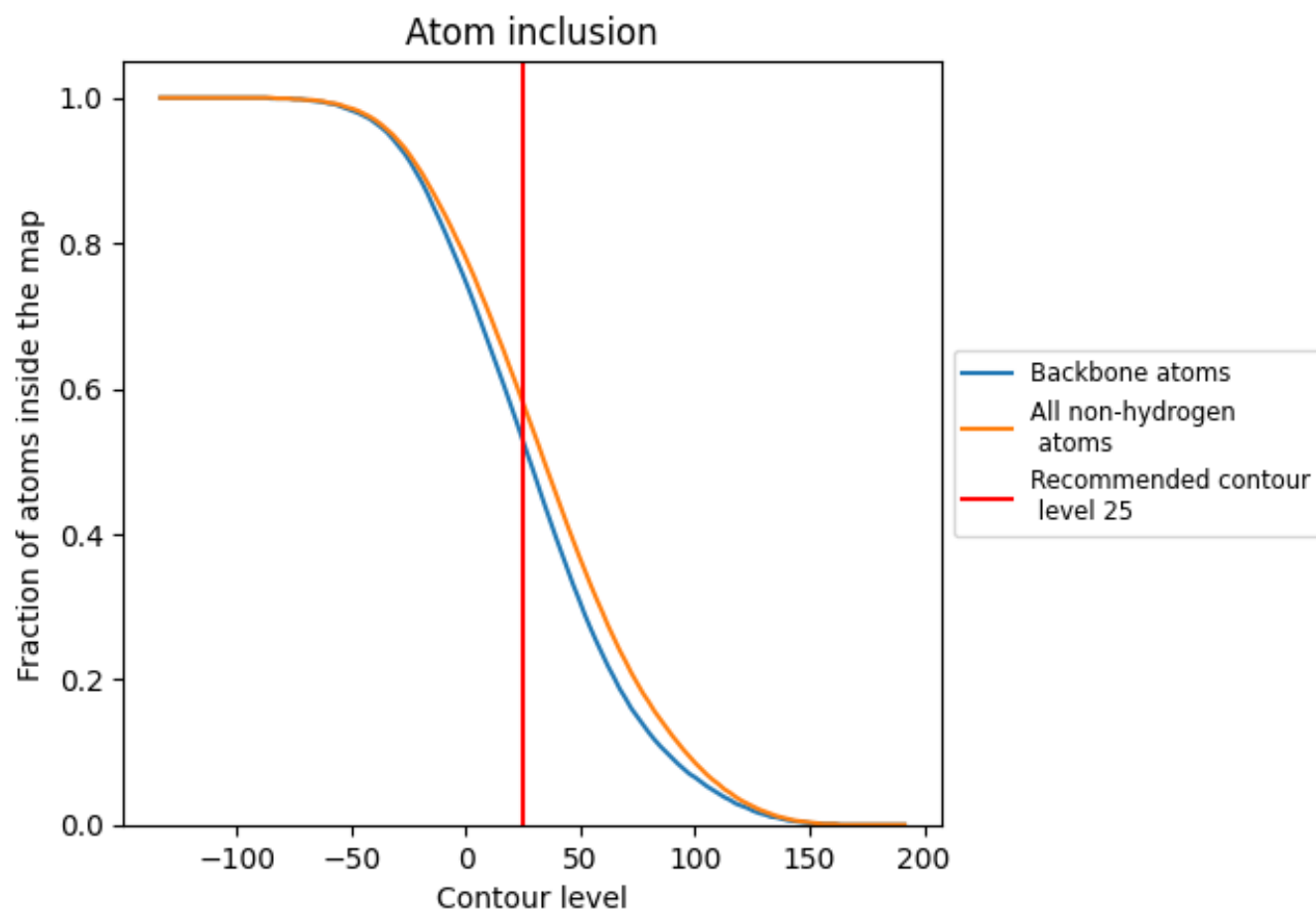
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5810	 0.0150
A1	 0.5160	 0.0210
A2	 0.4760	 -0.0030
A3	 0.3830	 -0.0050
AA	 0.6610	 0.0230
AB	 0.4760	 0.0520
AC	 0.5210	 0.0080
AD	 0.4340	 0.0110
AE	 0.5200	 0.0300
AF	 0.7140	 0.0380
AG	 0.5950	 0.0120
AH	 0.5110	 0.0070
AI	 0.7070	 0.0030
AJ	 0.4240	 0.0020
AK	 0.6720	 0.0330
AL	 0.6300	 0.0140
AM	 0.6530	 0.0320
AN	 0.3420	 -0.0380
AO	 0.7130	 0.0190
AP	 0.4340	 0.0050
AQ	 0.5450	 0.0230
AR	 0.5810	 0.0020
AS	 0.6650	 0.0190
AT	 0.7030	 0.0010
AU	 0.5820	 0.0460
B0	 0.7100	 0.0380
B1	 0.5120	 0.0350
B2	 0.4170	 -0.0450
B3	 0.4130	 -0.0030
B4	 0.5100	 -0.0030
B5	 0.3460	 -0.0020
BA	 0.5880	 0.0150
BB	 0.7180	 0.0320
BC	 0.4310	 -0.0150
BD	 0.4710	 0.0100



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Chain	Atom inclusion	Q-score
BE	 0.5910	 -0.0060
BF	 0.5840	 0.0210
BG	 0.4590	 0.0220
BH	 0.2250	 0.0250
BI	 0.0000	 -0.0030
BJ	 0.4790	 -0.0040
BK	 0.4540	 0.0030
BL	 0.6080	 -0.0140
BM	 0.4260	 0.0170
BN	 0.5740	 -0.0180
BO	 0.8410	 0.0280
BP	 0.4290	 -0.0060
BQ	 0.5300	 -0.0060
BR	 0.6140	 -0.0070
BS	 0.4800	 0.0010
BT	 0.6280	 -0.0100
BU	 0.5690	 0.0050
BV	 0.6310	 0.0560
BW	 0.6220	 0.0220
BX	 0.4460	 -0.0480
BY	 0.5490	 0.0070
BZ	 0.4460	 0.0020