



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 09:44 AM EDT

PDB ID : 4V79 / pdb_00004v79
EMDB ID : EMD-1723
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post3b)
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on : 2013-10-14
Resolution : 15.00 Å(reported)
Based on initial models : 2HGP, 2WRI, 2K4C, 3I1O

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

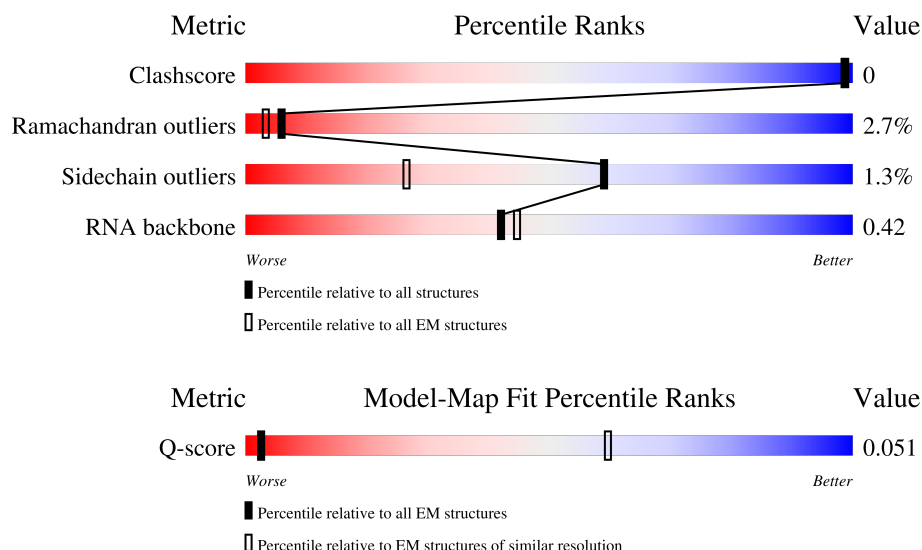
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 15.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	37 (14.50 - 15.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AB	220	42% 95% .
2	AC	208	54% 96% .
3	AD	206	48% 96% ..

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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	21% 61% 32% 6%
55	BB	118	7% 65% 25% 8%
56	B5	234	54% 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		

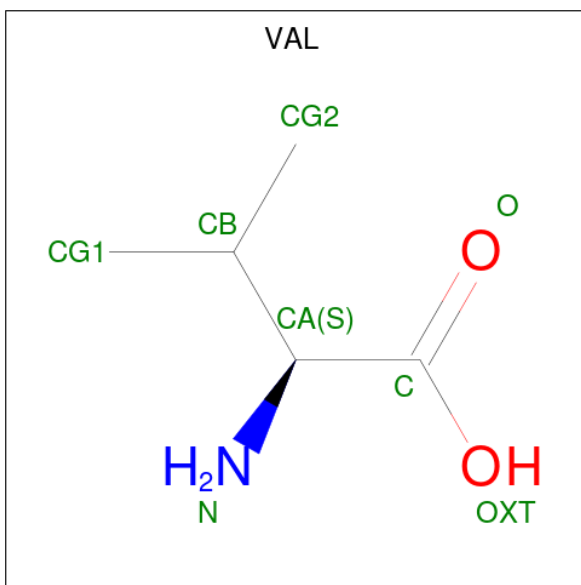
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

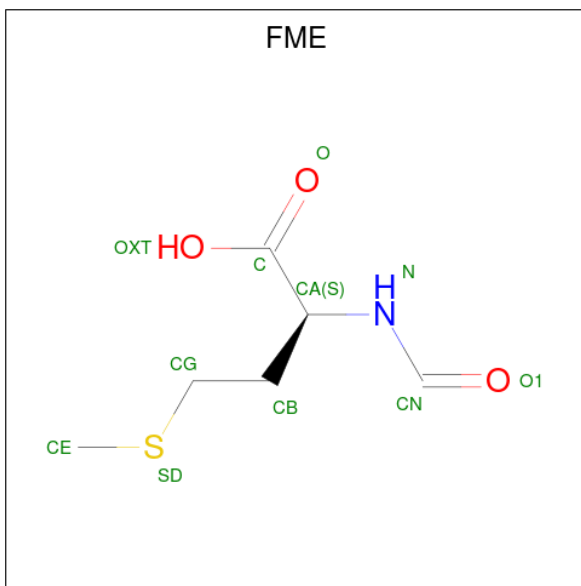
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- 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).

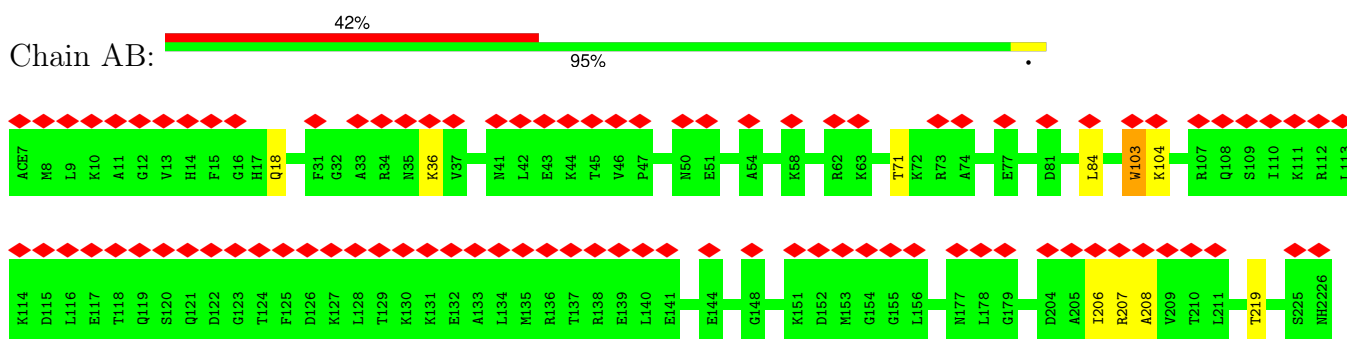


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

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.

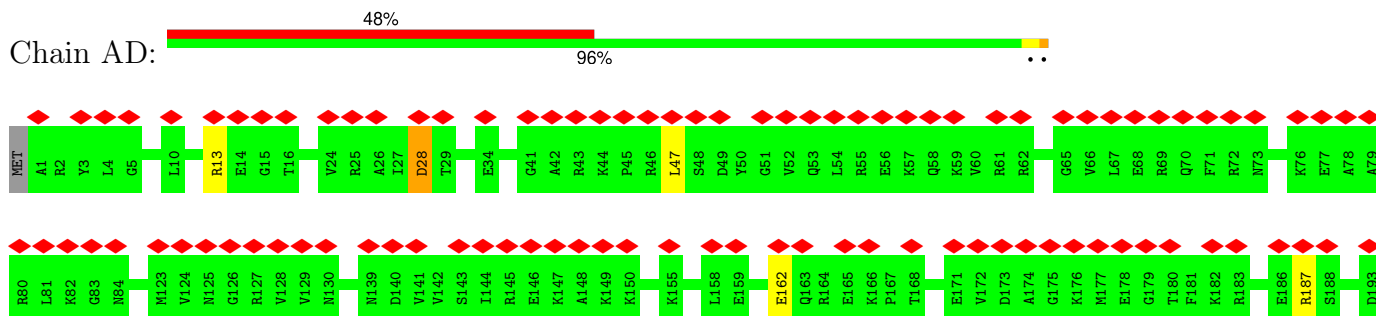
• Molecule 1: 30S ribosomal protein S2

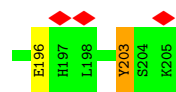


• Molecule 2: 30S ribosomal protein S3



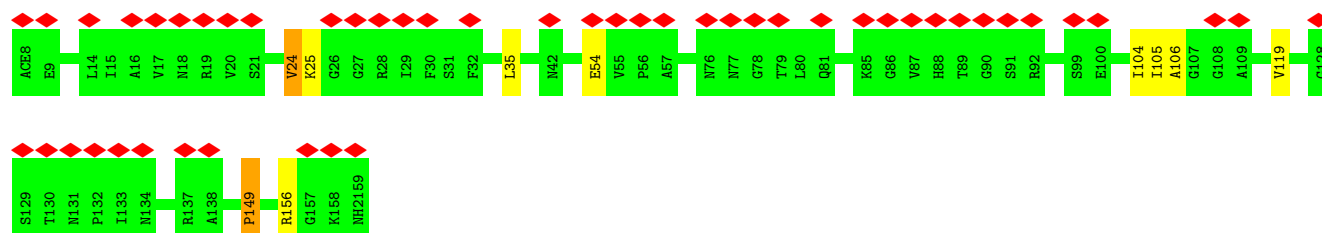
• Molecule 3: 30S ribosomal protein S4





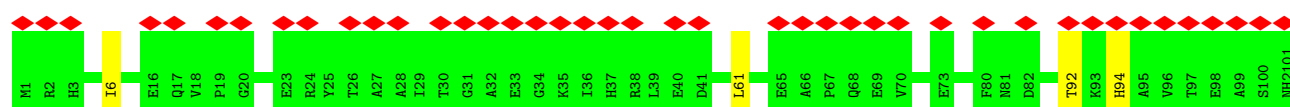
• Molecule 4: 30S ribosomal protein S5

Chain AE: 32% 93% 5% •



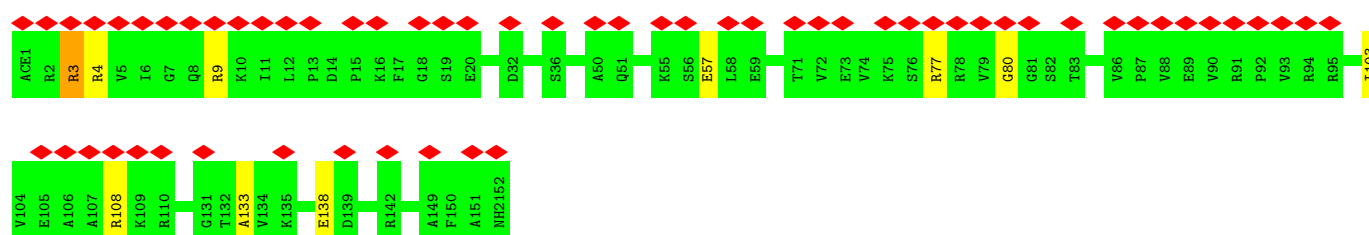
• Molecule 5: 30S ribosomal protein S6

Chain AF: 42% 96% •



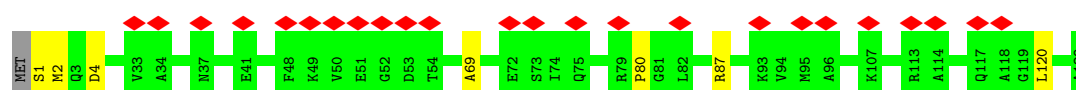
• Molecule 6: 30S ribosomal protein S7

Chain AG: 39% 93% 6% •



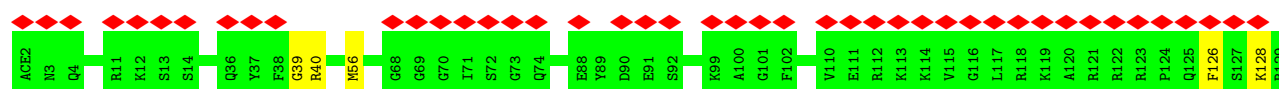
• Molecule 7: 30S ribosomal protein S8

Chain AH: 18% 94% 5% •

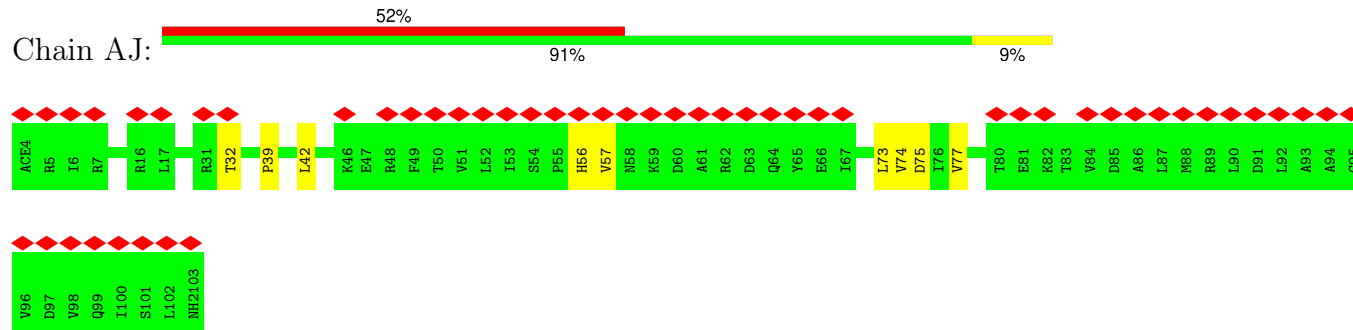


• Molecule 8: 30S ribosomal protein S9

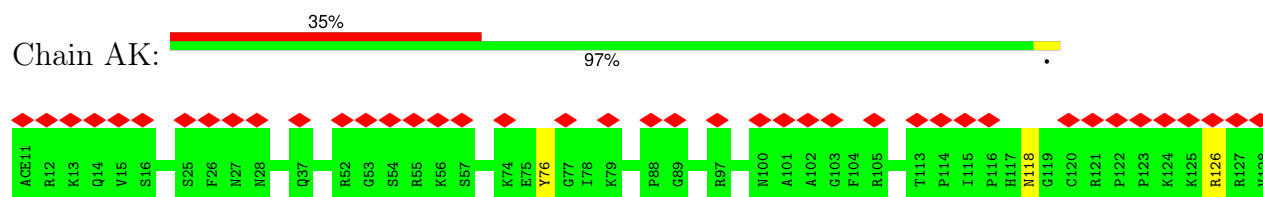
Chain AI: 34% 96% •



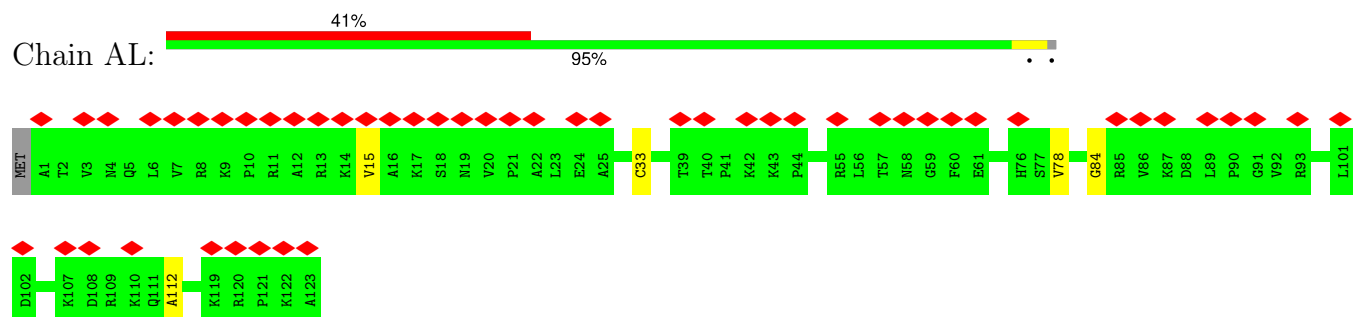
- Molecule 9: 30S ribosomal protein S10



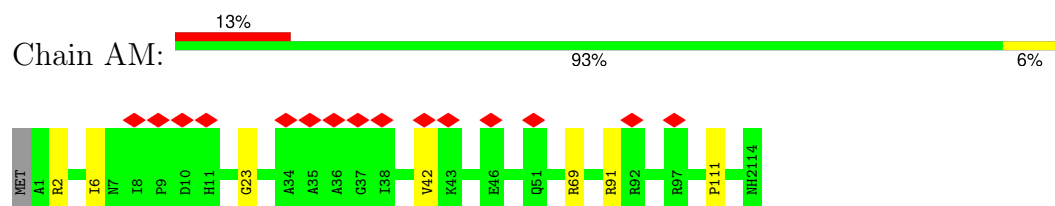
- Molecule 10: 30S ribosomal protein S11



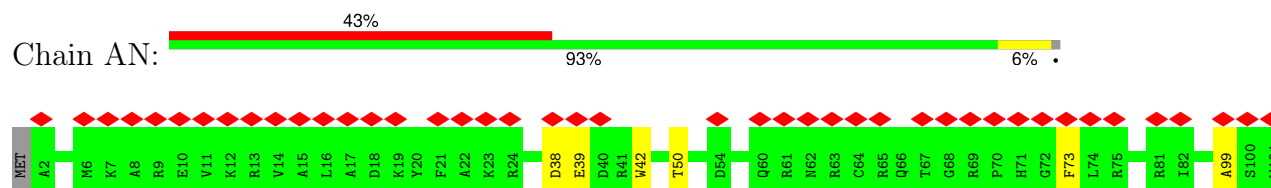
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13

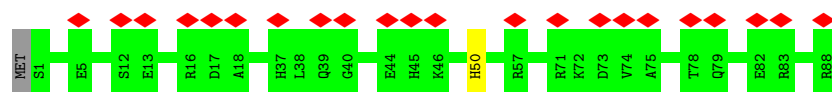


- Molecule 13: 30S ribosomal protein S14

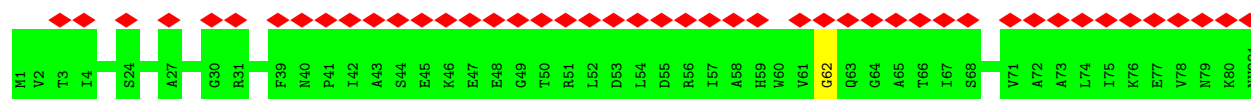


- Molecule 14: 30S ribosomal protein S15

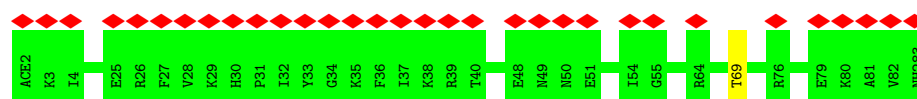




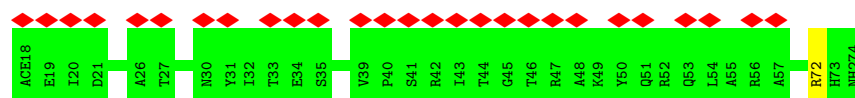
- Molecule 15: 30S ribosomal protein S16



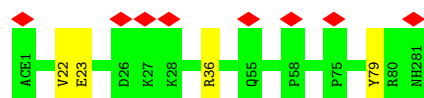
- Molecule 16: 30S ribosomal protein S17



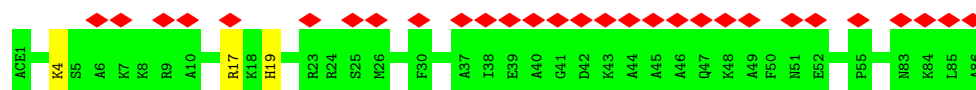
- Molecule 17: 30S ribosomal protein S18



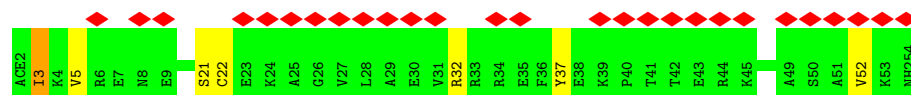
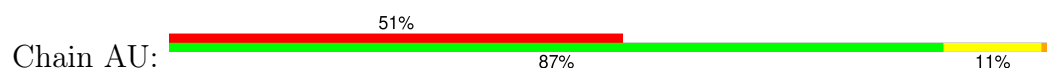
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20

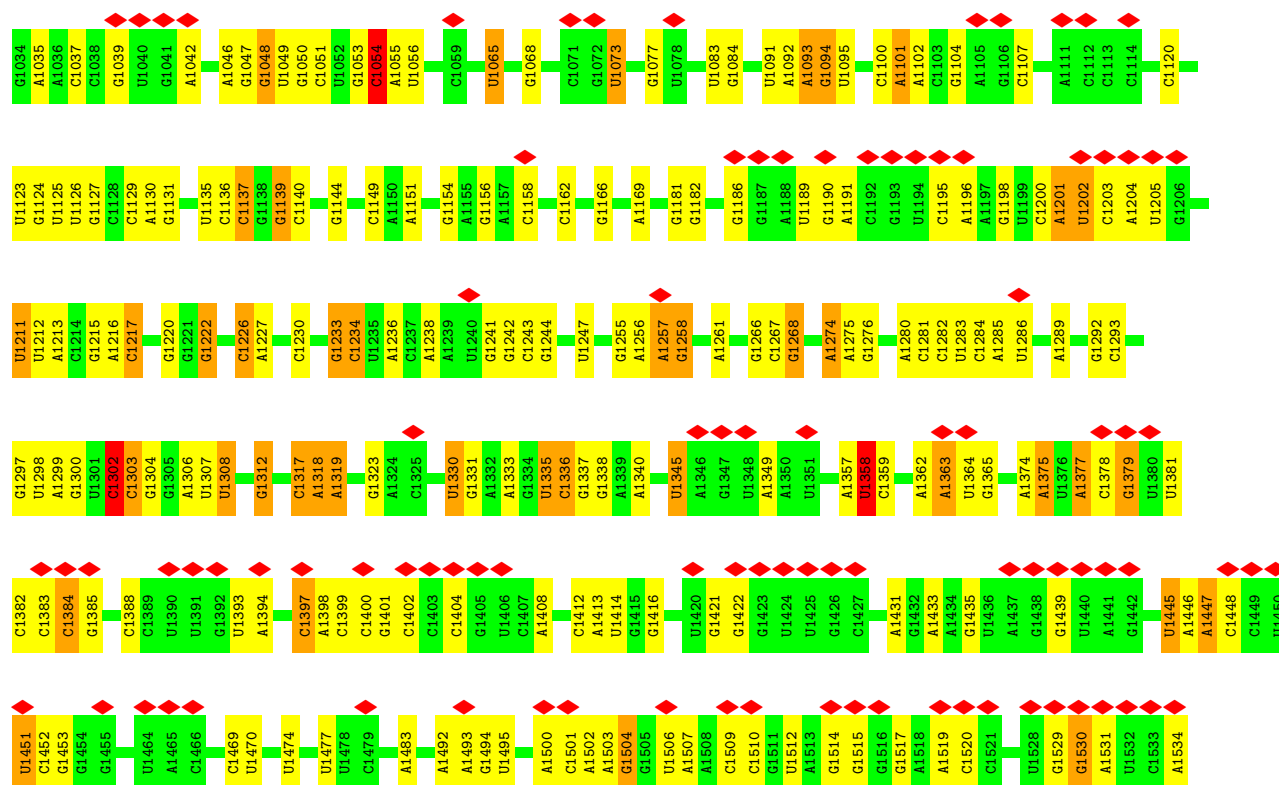


- Molecule 20: 30S ribosomal protein S21

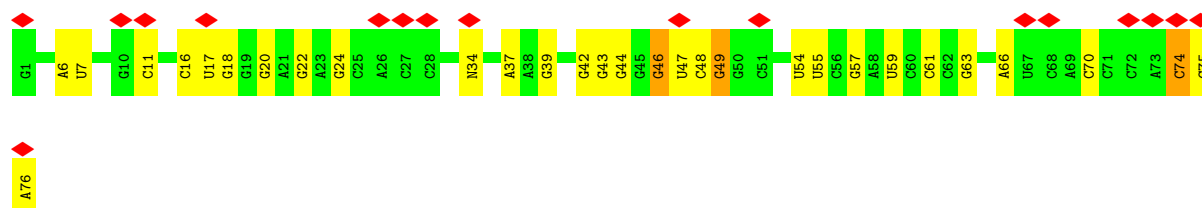


Chain AA:





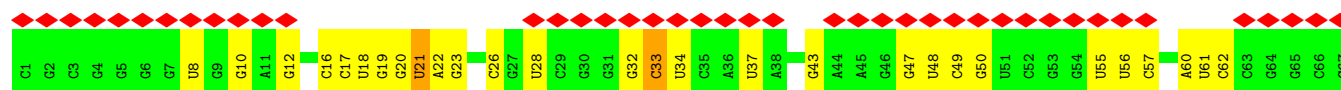
• Molecule 22: fMet-Val-tRNA-Val

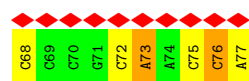


• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

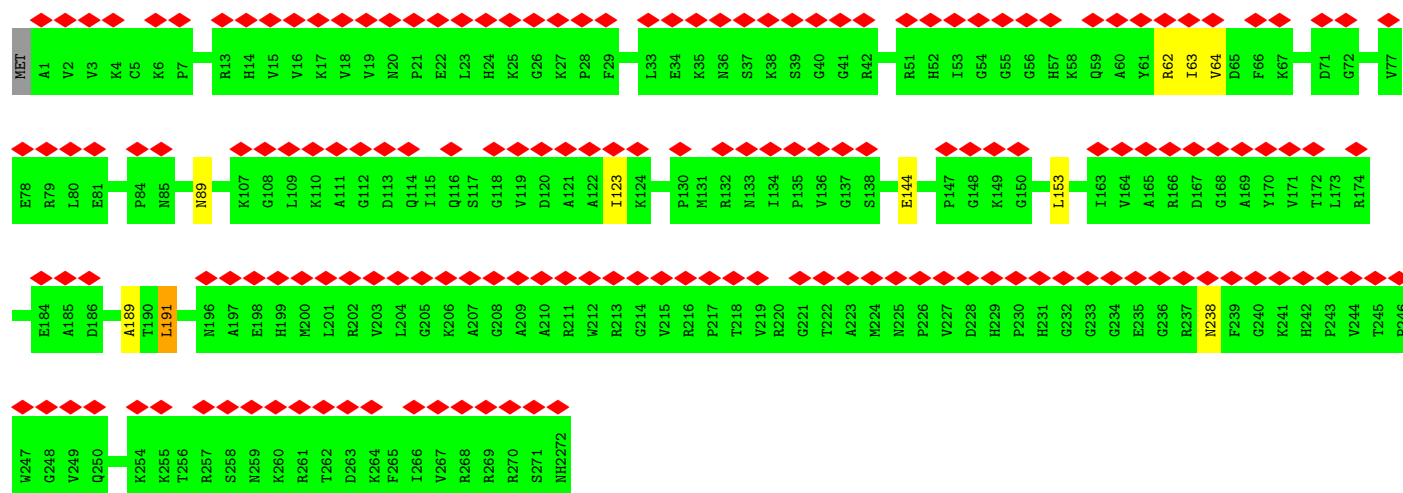


• Molecule 24: tRNA-fMet

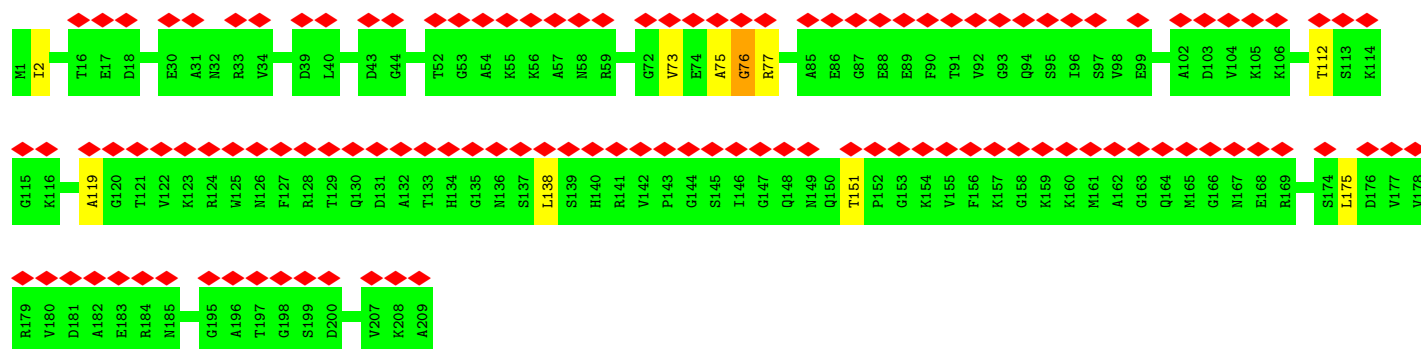




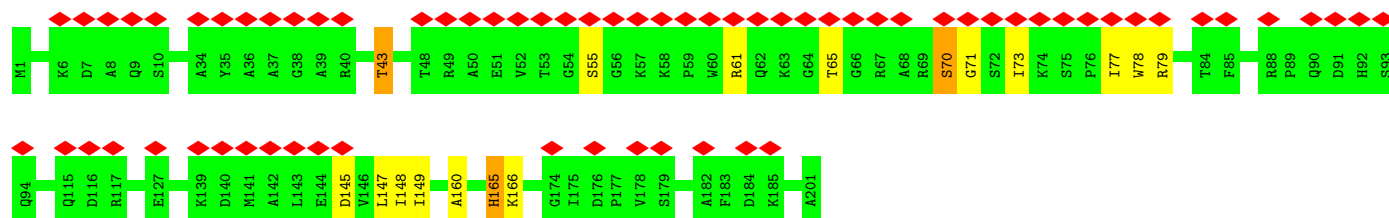
• Molecule 25: 50S ribosomal protein L2



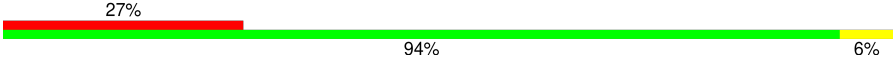
• Molecule 26: 50S ribosomal protein L3

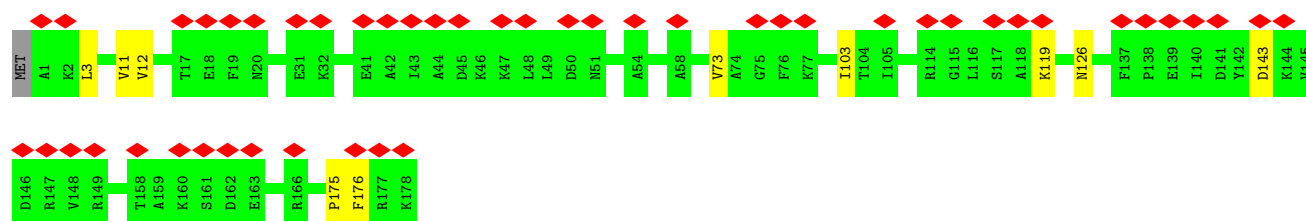


• Molecule 27: 50S ribosomal protein L4

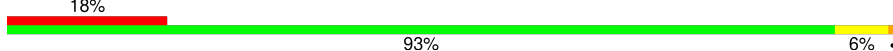


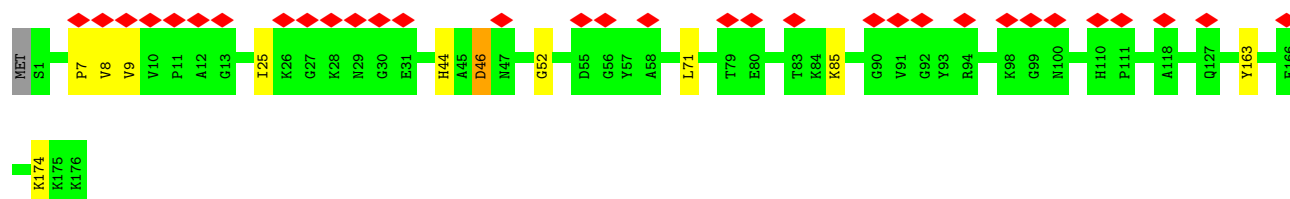
• Molecule 28: 50S ribosomal protein L5

Chain BF: 

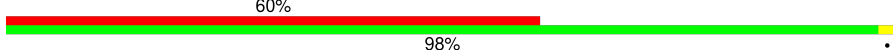


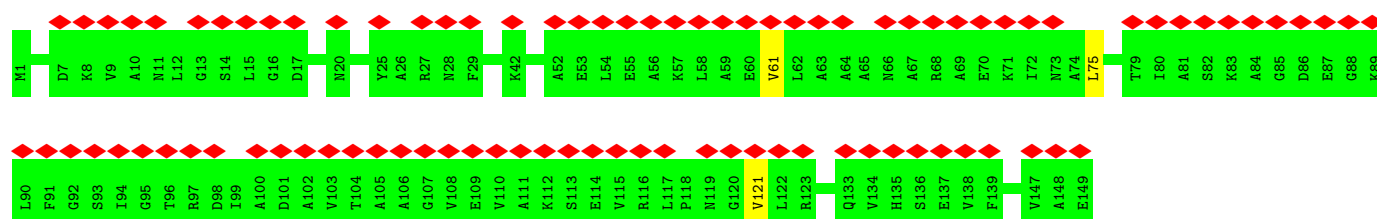
- Molecule 29: 50S ribosomal protein L6

Chain BG: 



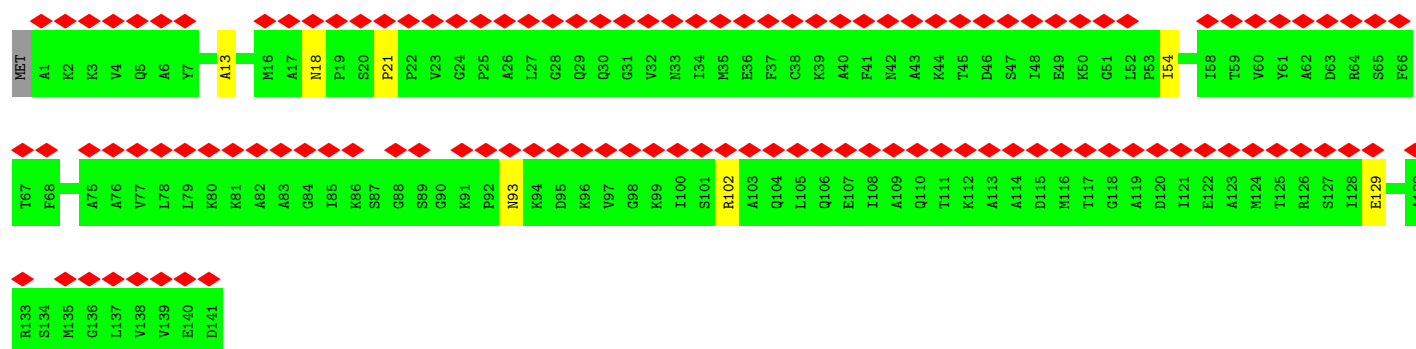
- Molecule 30: 50S ribosomal protein L9

Chain BH: 

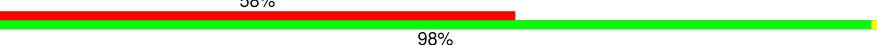


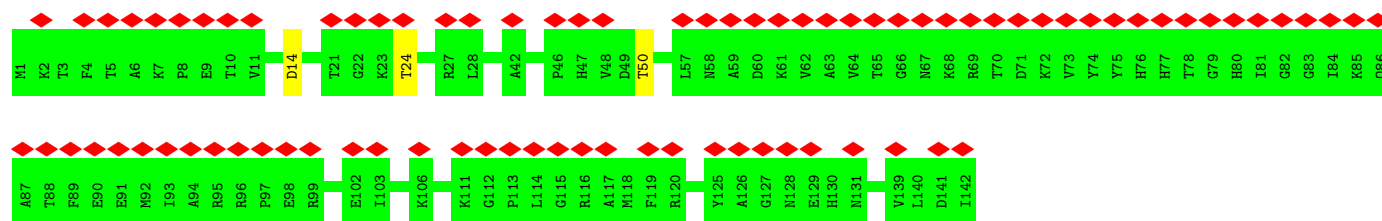
- Molecule 31: 50S ribosomal protein L11

Chain BI: 

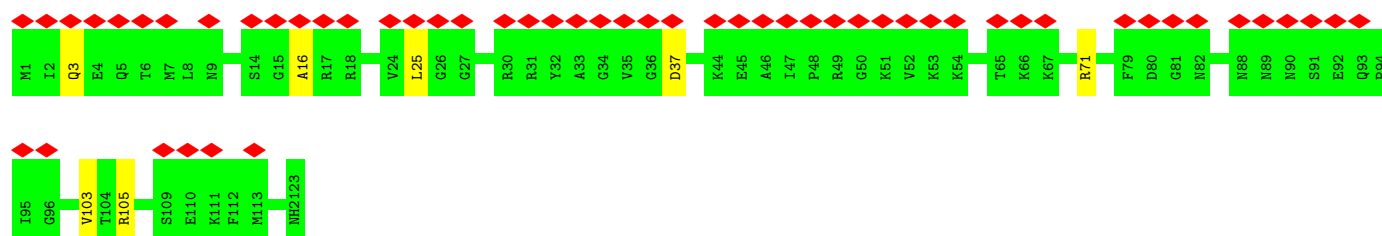


- Molecule 32: 50S ribosomal protein L13

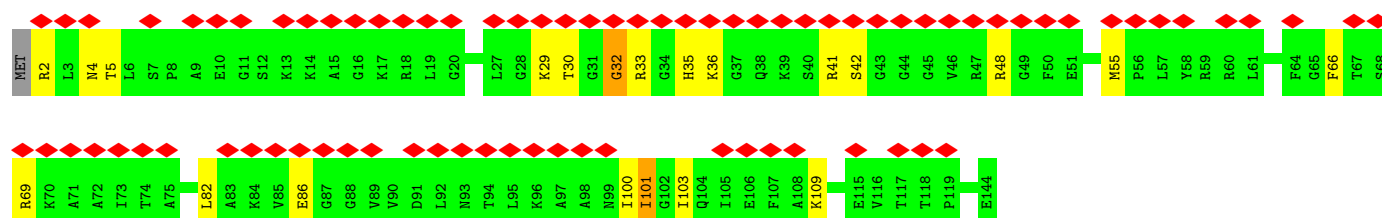
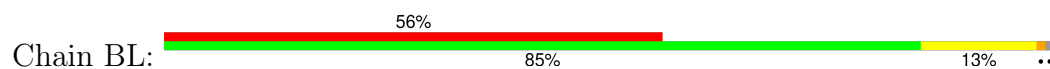
Chain BJ: 



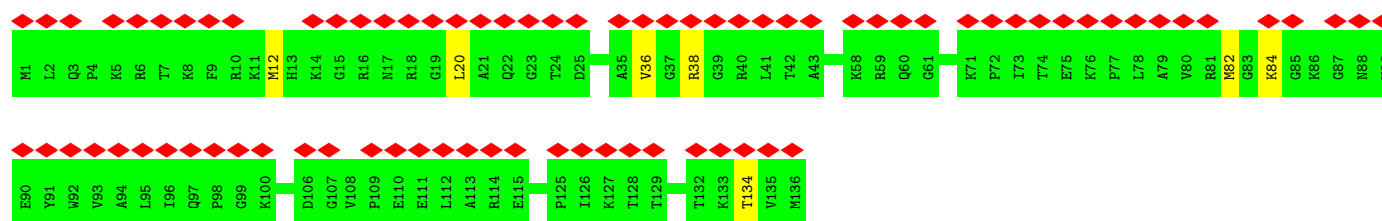
• Molecule 33: 50S ribosomal protein L14



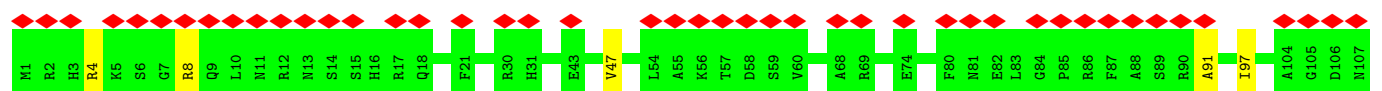
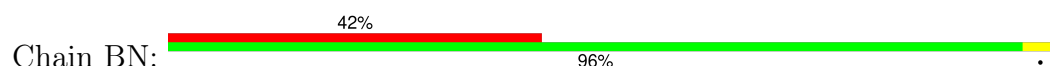
• Molecule 34: 50S ribosomal protein L15

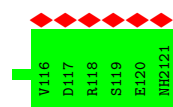


• Molecule 35: 50S ribosomal protein L16

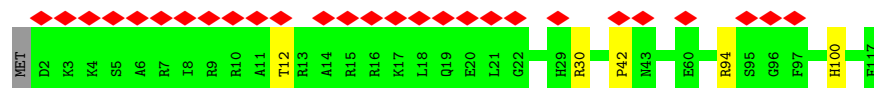


• Molecule 36: 50S ribosomal protein L17

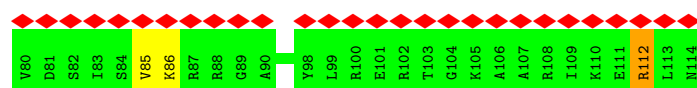




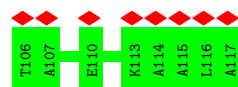
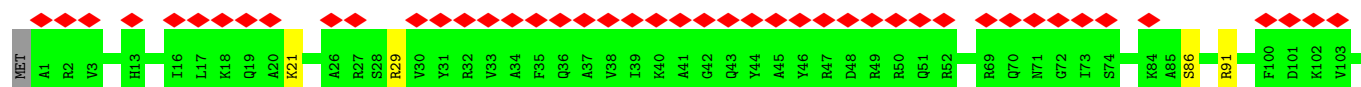
- Molecule 37: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L19



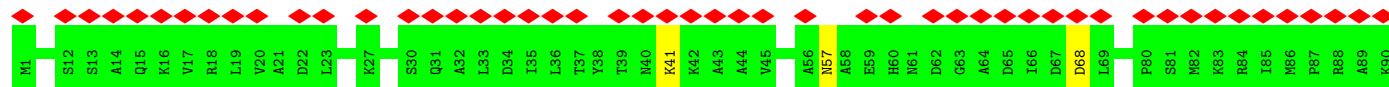
- Molecule 39: 50S ribosomal protein L20

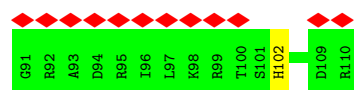


- Molecule 40: 50S ribosomal protein L21

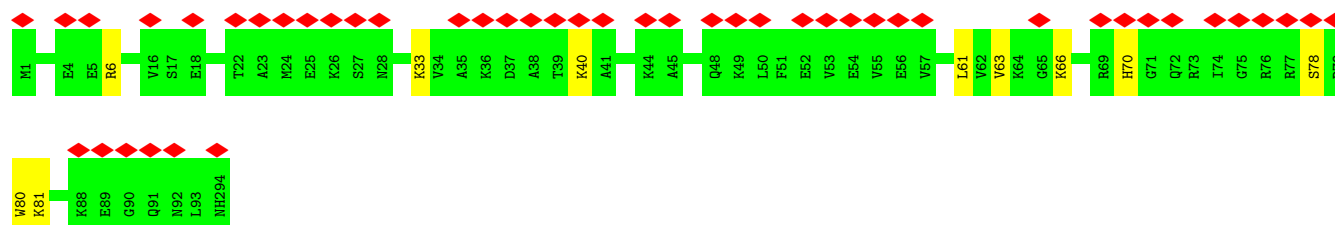
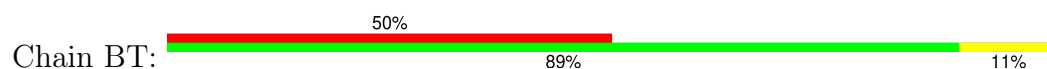


- Molecule 41: 50S ribosomal protein L22

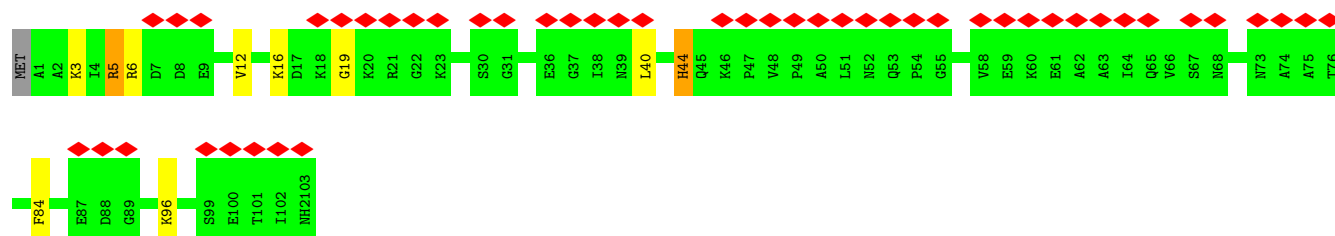
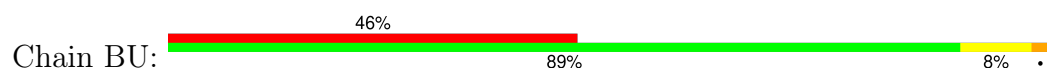




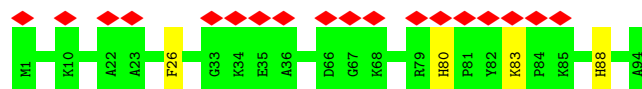
- Molecule 42: 50S ribosomal protein L23



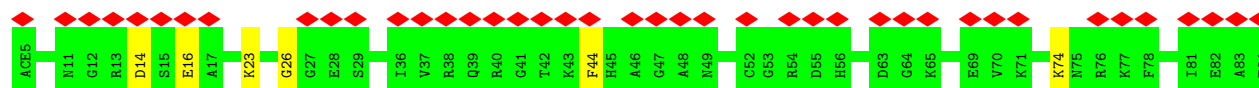
- Molecule 43: 50S ribosomal protein L24



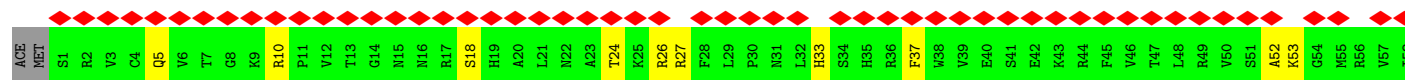
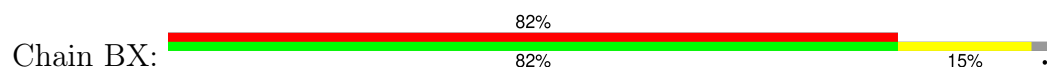
- Molecule 44: 50S ribosomal protein L25

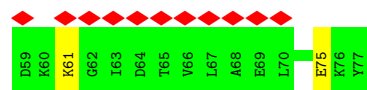


- Molecule 45: 50S ribosomal protein L27

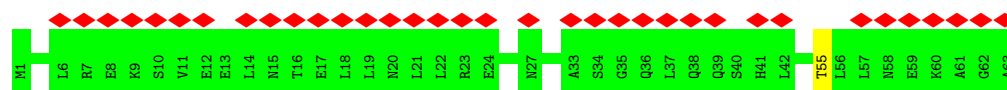


- Molecule 46: 50S ribosomal protein L28

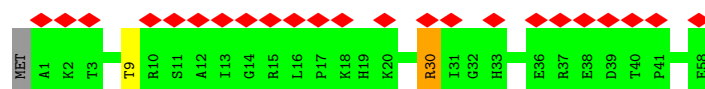




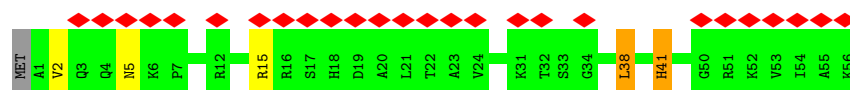
- Molecule 47: 50S ribosomal protein L29



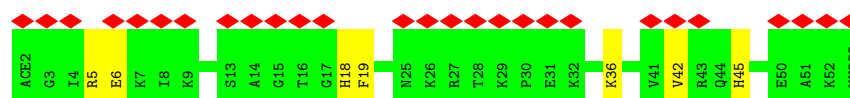
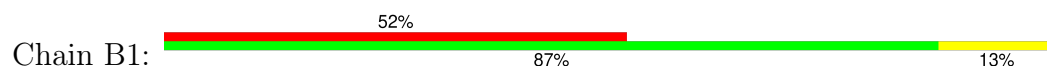
- Molecule 48: 50S ribosomal protein L30



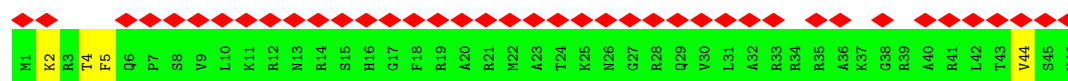
- Molecule 49: 50S ribosomal protein L32



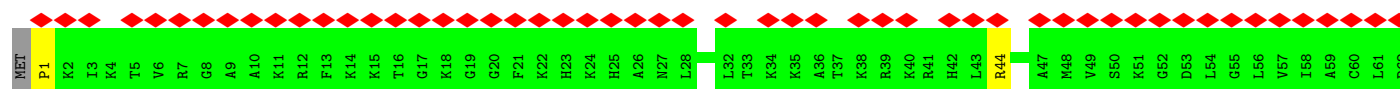
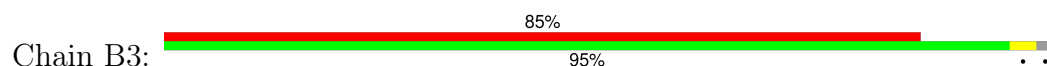
- Molecule 50: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L34

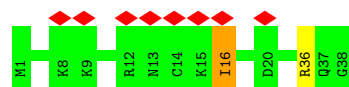


- Molecule 52: 50S ribosomal protein L35

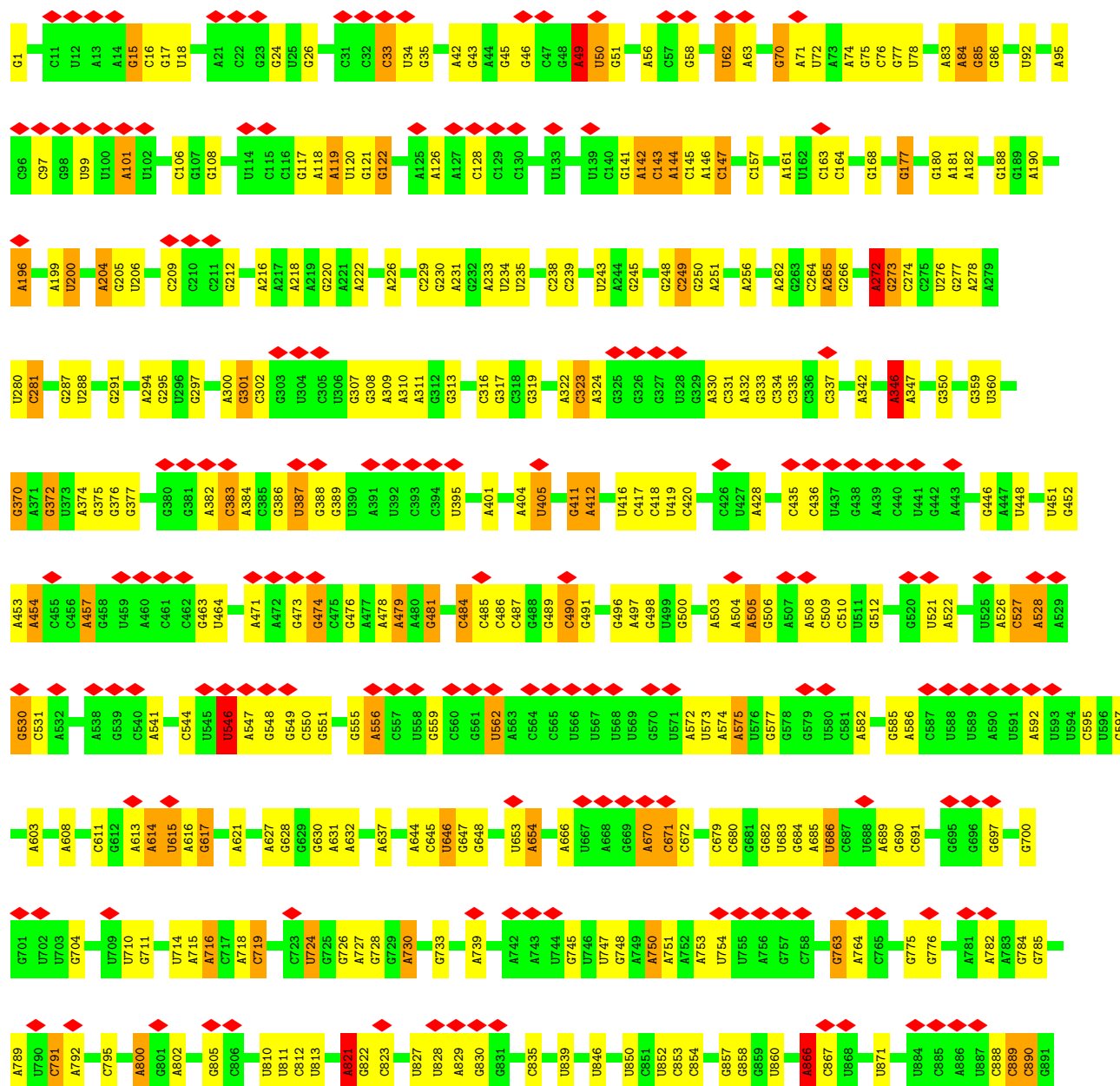


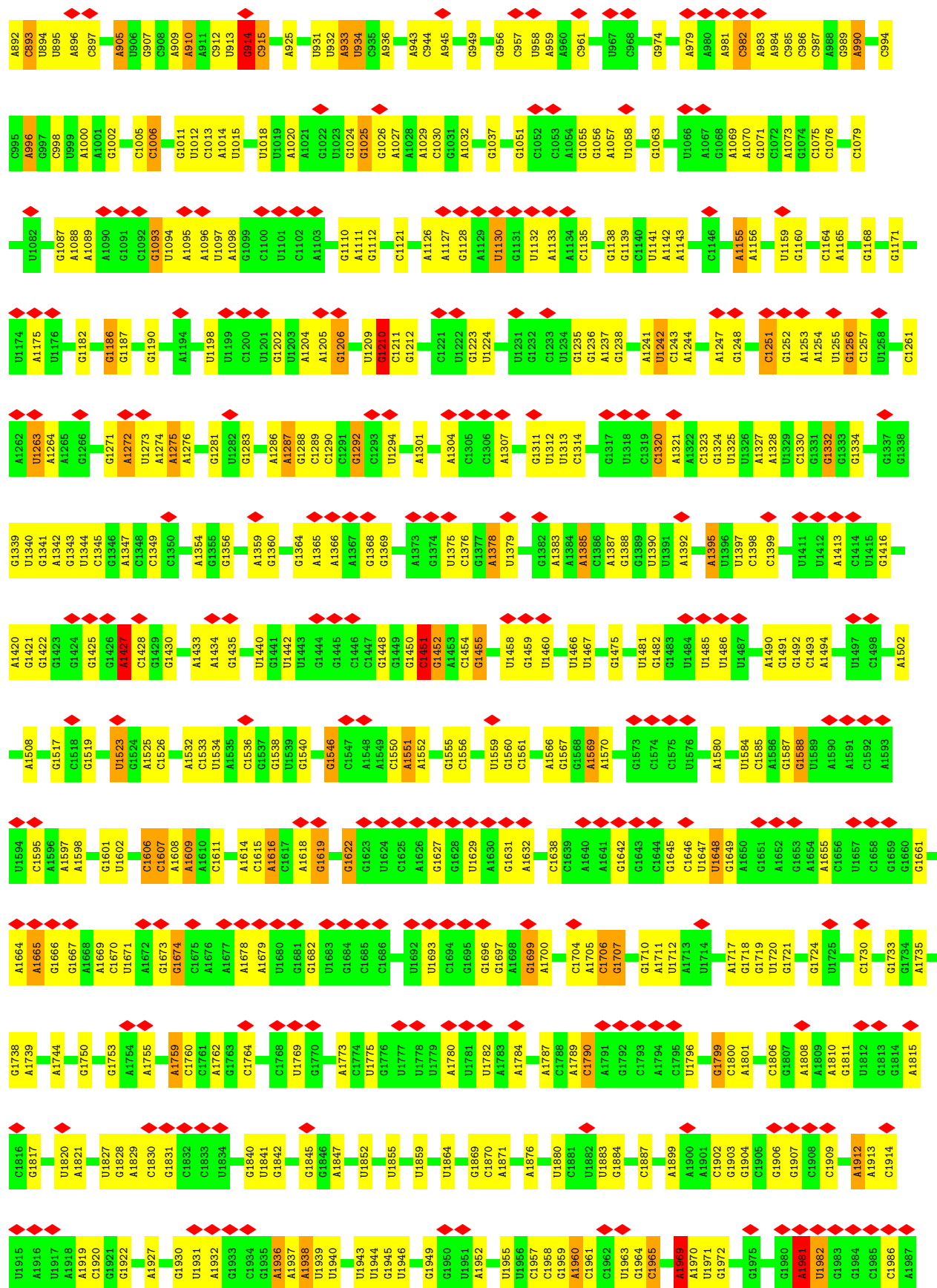


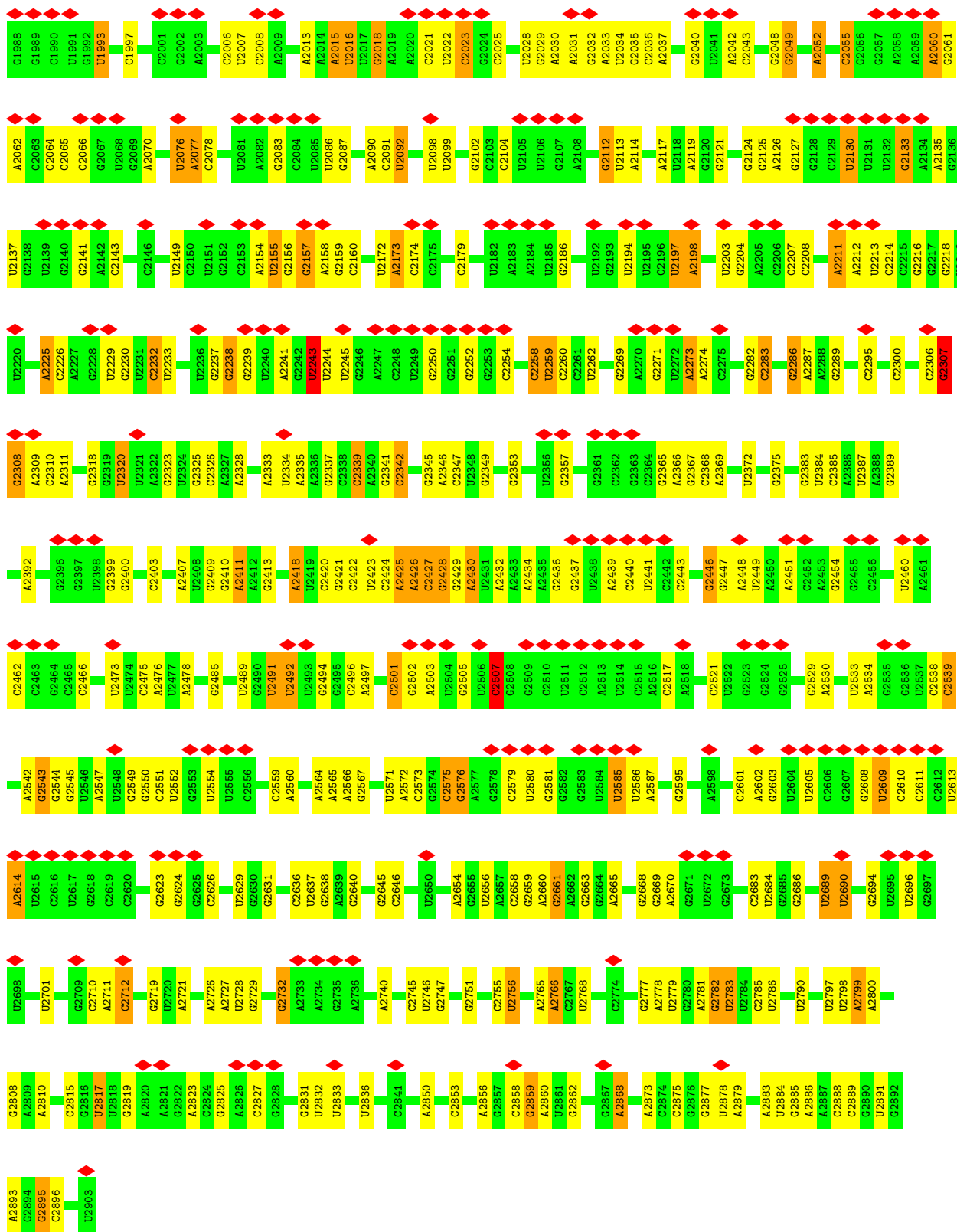
- Molecule 53: 50S ribosomal protein L36



- Molecule 54: 23S ribosomal RNA

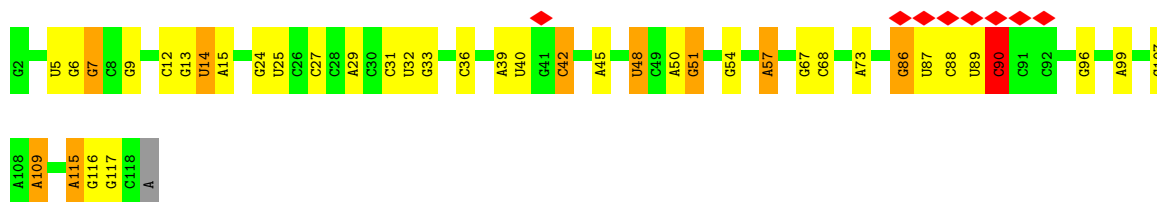






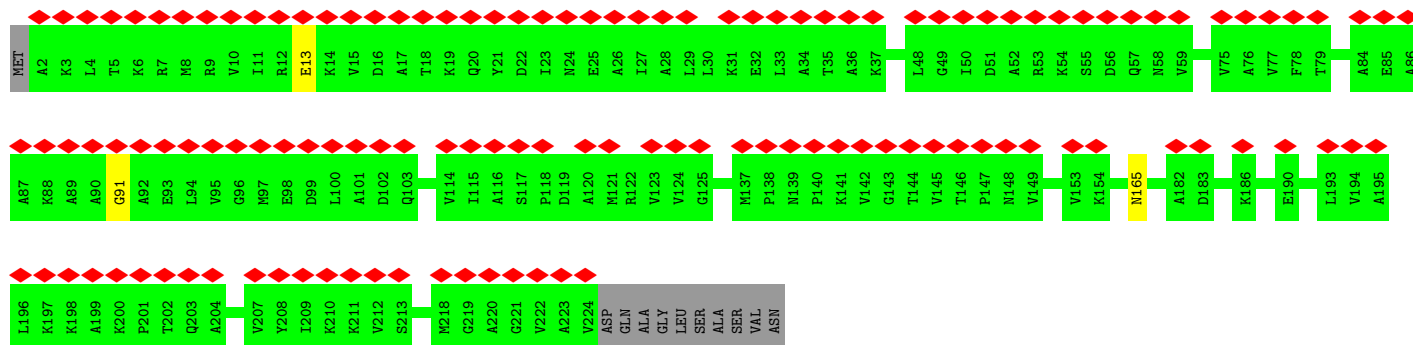
• Molecule 55: 5S ribosomal RNA





- Molecule 56: 50S ribosomal protein L1

Chain B5: 54% 94% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5083	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	162740	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	300.566	Depositor
Minimum map value	-221.637	Depositor
Average map value	-0.135	Depositor
Map value standard deviation	28.849	Depositor
Recommended contour level	30	Depositor
Map size ($\text{\AA}$)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	2.8, 2.8, 2.8	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AB	0.91	0/1736	1.37	5/2340 (0.2%)
2	AC	0.91	0/1651	1.37	0/2225
3	AD	0.92	0/1665	1.43	4/2227 (0.2%)
4	AE	0.90	0/1119	1.51	15/1506 (1.0%)
5	AF	0.92	0/835	1.40	1/1128 (0.1%)
6	AG	0.94	0/1188	1.47	7/1593 (0.4%)
7	AH	0.87	0/989	1.40	9/1326 (0.7%)
8	AI	0.94	0/1035	1.38	2/1377 (0.1%)
9	AJ	0.95	0/797	1.41	5/1079 (0.5%)
10	AK	0.95	0/894	1.41	2/1207 (0.2%)
11	AL	0.95	0/969	1.48	0/1300
12	AM	0.98	0/884	1.53	8/1181 (0.7%)
13	AN	0.95	0/817	1.42	4/1088 (0.4%)
14	AO	0.92	0/722	1.43	1/964 (0.1%)
15	AP	0.96	0/648	1.45	2/870 (0.2%)
16	AQ	0.86	0/658	1.32	0/883
17	AR	1.00	0/463	1.44	2/623 (0.3%)
18	AS	0.93	0/653	1.43	4/879 (0.5%)
19	AT	0.91	0/672	1.41	1/890 (0.1%)
20	AU	0.97	0/431	1.67	8/572 (1.4%)
21	AA	1.00	0/36759	1.15	72/57346 (0.1%)
22	A1	1.01	0/1668	1.14	2/2595 (0.1%)
23	A2	0.97	0/343	1.20	0/531
24	A3	0.99	0/1722	1.19	6/2685 (0.2%)
25	BC	0.95	0/2121	1.50	0/2852
26	BD	0.86	0/1586	1.46	2/2134 (0.1%)
27	BE	0.84	0/1571	1.47	4/2113 (0.2%)
28	BF	0.87	0/1444	1.41	2/1937 (0.1%)
29	BG	0.87	0/1343	1.45	4/1816 (0.2%)
30	BH	0.83	0/1122	1.42	0/1515
31	BI	0.86	0/1046	1.46	1/1410 (0.1%)
32	BJ	0.90	0/1152	1.48	3/1551 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BK	0.94	0/947	1.52	1/1268 (0.1%)
34	BL	0.93	0/1054	1.74	18/1403 (1.3%)
35	BM	0.88	0/1093	1.44	0/1460
36	BN	0.92	0/973	1.49	4/1301 (0.3%)
37	BO	0.90	0/902	1.42	0/1209
38	BP	0.89	0/929	1.51	4/1242 (0.3%)
39	BQ	0.88	0/960	1.46	1/1278 (0.1%)
40	BR	0.90	0/829	1.49	1/1107 (0.1%)
41	BS	0.86	0/864	1.48	3/1156 (0.3%)
42	BT	0.83	0/744	1.47	1/994 (0.1%)
43	BU	0.89	0/787	1.58	2/1051 (0.2%)
44	BV	0.84	0/766	1.39	1/1025 (0.1%)
45	BW	0.92	0/604	1.49	0/799
46	BX	0.92	0/635	1.60	4/848 (0.5%)
47	BY	0.85	0/510	1.39	0/677
48	BZ	0.89	0/453	1.49	1/605 (0.2%)
49	B0	0.94	0/450	1.56	3/599 (0.5%)
50	B1	0.82	0/417	1.46	1/556 (0.2%)
51	B2	0.96	0/380	1.57	3/498 (0.6%)
52	B3	0.92	0/513	1.44	0/676
53	B4	0.94	0/303	1.55	0/397
54	BA	0.85	0/69796	1.14	114/108888 (0.1%)
55	BB	0.87	0/2800	1.12	2/4367 (0.0%)
56	B5	0.84	0/1673	1.43	0/2255
All	All	0.90	0/160085	1.24	340/239402 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AD	0	1
21	AA	0	359
22	A1	0	16
23	A2	0	5
24	A3	0	8
36	BN	0	1
37	BO	0	1
38	BP	0	2
46	BX	0	1
54	BA	0	692

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	29
All	All	0	1115

There are no bond length outliers.

All (340) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AB	206	ILE	CA-C-N	10.32	140.28	121.70
1	AB	206	ILE	C-N-CA	10.32	140.28	121.70
34	BL	4	ASN	CA-C-N	9.34	138.51	121.70
34	BL	4	ASN	C-N-CA	9.34	138.51	121.70
18	AS	22	VAL	CA-C-N	9.03	137.96	121.70
18	AS	22	VAL	C-N-CA	9.03	137.96	121.70
15	AP	62	GLY	CA-C-N	8.40	136.82	121.70
15	AP	62	GLY	C-N-CA	8.40	136.82	121.70
20	AU	3	ILE	CA-C-N	8.19	136.44	121.70
20	AU	3	ILE	C-N-CA	8.19	136.44	121.70
10	AK	126	ARG	CA-C-N	8.16	136.39	121.70
10	AK	126	ARG	C-N-CA	8.16	136.39	121.70
4	AE	104	ILE	O-C-N	-8.03	115.74	122.97
34	BL	48	ARG	N-CA-C	8.00	121.00	111.33
4	AE	24	VAL	CA-C-N	7.99	136.07	121.70
4	AE	24	VAL	C-N-CA	7.99	136.07	121.70
12	AM	91	ARG	CA-C-N	7.91	135.95	121.70
12	AM	91	ARG	C-N-CA	7.91	135.95	121.70
17	AR	72	ARG	CA-C-N	7.80	135.74	121.70
17	AR	72	ARG	C-N-CA	7.80	135.74	121.70
20	AU	21	SER	CA-C-N	7.76	135.68	121.70
20	AU	21	SER	C-N-CA	7.76	135.68	121.70
24	A3	76	C	O3'-P-O5'	-7.63	92.56	104.00
7	AH	80	PRO	CA-C-N	7.61	135.39	121.70
7	AH	80	PRO	C-N-CA	7.61	135.39	121.70
31	BI	21	PRO	N-CA-C	7.55	119.91	110.70
54	BA	527	C	C2'-C3'-O3'	7.53	120.79	109.50
54	BA	1981	A	O4'-C1'-N9	7.45	119.37	108.20
4	AE	104	ILE	CA-C-N	7.41	135.03	121.70
4	AE	104	ILE	C-N-CA	7.41	135.03	121.70
6	AG	108	ARG	CA-C-N	7.30	134.84	121.70
6	AG	108	ARG	C-N-CA	7.30	134.84	121.70
21	AA	130	A	C1'-O4'-C4'	-7.11	102.59	109.70
34	BL	32	GLY	CA-C-N	7.01	134.32	121.70
34	BL	32	GLY	C-N-CA	7.01	134.32	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	872	A	C1'-O4'-C4'	-6.95	102.75	109.70
54	BA	323	C	O4'-C1'-N1	6.80	118.40	108.20
54	BA	2258	C	C2'-C3'-O3'	6.79	119.69	109.50
32	BJ	24	THR	CA-C-N	6.76	133.87	121.70
32	BJ	24	THR	C-N-CA	6.76	133.87	121.70
4	AE	149	PRO	CA-C-N	6.69	133.74	121.70
4	AE	149	PRO	C-N-CA	6.69	133.74	121.70
54	BA	2543	G	C5'-C4'-C3'	-6.67	106.00	116.00
1	AB	206	ILE	O-C-N	-6.66	115.70	122.23
4	AE	106	ALA	CA-C-N	6.57	126.22	119.92
4	AE	106	ALA	C-N-CA	6.57	126.22	119.92
21	AA	1054	C	C1'-O4'-C4'	-6.47	103.23	109.70
54	BA	2018	G	O4'-C4'-C3'	6.45	110.45	104.00
54	BA	265	A	O4'-C1'-N9	6.45	117.87	108.20
21	AA	884	U	C1'-O4'-C4'	-6.39	103.31	109.70
6	AG	9	ARG	CA-C-N	6.38	133.19	121.70
6	AG	9	ARG	C-N-CA	6.38	133.19	121.70
21	AA	262	A	C1'-O4'-C4'	-6.36	103.54	109.90
54	BA	2076	U	O4'-C1'-N1	6.30	117.65	108.20
21	AA	792	A	C1'-O4'-C4'	-6.28	103.42	109.70
34	BL	2	ARG	CA-C-N	6.28	133.00	121.70
34	BL	2	ARG	C-N-CA	6.28	133.00	121.70
7	AH	120	LEU	CA-C-N	6.26	127.08	121.82
7	AH	120	LEU	C-N-CA	6.26	127.08	121.82
46	BX	26	ARG	NE-CZ-NH2	6.25	124.82	119.20
21	AA	575	G	C1'-O4'-C4'	-6.23	103.47	109.70
54	BA	99	U	O4'-C1'-N1	6.21	117.52	108.20
54	BA	889	C	C2'-C3'-O3'	6.17	118.75	109.50
22	A1	59	U	C1'-O4'-C4'	-6.13	103.77	109.90
54	BA	2307	G	O4'-C1'-N9	6.13	117.40	108.20
54	BA	1912	A	O4'-C4'-C3'	6.05	110.06	104.00
24	A3	47	G	C1'-O4'-C4'	-6.04	103.86	109.90
38	BP	25	VAL	N-CA-C	6.02	116.99	111.81
54	BA	1943	U	O4'-C1'-N1	6.00	117.20	108.20
21	AA	54	C	P-O3'-C3'	5.99	129.18	120.20
21	AA	771	G	C1'-O4'-C4'	-5.98	103.92	109.90
39	BQ	29	ARG	NE-CZ-NH2	5.98	124.58	119.20
12	AM	2	ARG	NE-CZ-NH2	5.97	124.58	119.20
54	BA	346	A	O4'-C1'-C2'	-5.96	101.64	107.60
32	BJ	24	THR	O-C-N	-5.95	115.39	122.65
12	AM	111	PRO	CA-C-N	5.93	132.38	121.70
12	AM	111	PRO	C-N-CA	5.93	132.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AE	149	PRO	CA-N-CD	-5.92	103.71	112.00
20	AU	52	VAL	CA-C-N	5.92	132.35	121.70
20	AU	52	VAL	C-N-CA	5.92	132.35	121.70
54	BA	684	G	C5'-C4'-C3'	-5.92	107.13	116.00
54	BA	1210	G	C2'-C3'-O3'	5.91	118.37	109.50
54	BA	412	A	O4'-C4'-C3'	5.91	109.91	104.00
21	AA	339	C	C5'-C4'-C3'	-5.90	107.15	116.00
19	AT	17	ARG	NE-CZ-NH2	5.89	124.50	119.20
54	BA	614	A	O4'-C1'-N9	5.88	117.02	108.20
54	BA	1609	A	C1'-O4'-C4'	-5.87	103.83	109.70
54	BA	2711	A	C4'-C3'-C2'	-5.83	96.77	102.60
48	BZ	30	ARG	NE-CZ-NH2	5.83	124.45	119.20
21	AA	315	A	O4'-C4'-C3'	5.82	109.82	104.00
54	BA	1093	G	O4'-C4'-C3'	5.82	109.82	104.00
54	BA	272	A	C1'-O4'-C4'	-5.80	103.90	109.70
21	AA	255	G	C5'-C4'-C3'	-5.77	107.34	116.00
41	BS	41	LYS	CA-C-N	5.76	128.27	120.38
41	BS	41	LYS	C-N-CA	5.76	128.27	120.38
21	AA	6	G	C1'-O4'-C4'	-5.74	104.16	109.90
21	AA	795	C	O4'-C4'-C3'	5.74	109.73	104.00
54	BA	143	C	C1'-O4'-C4'	-5.74	103.97	109.70
21	AA	1384	C	P-O3'-C3'	5.73	128.80	120.20
6	AG	3	ARG	CA-C-N	5.73	132.48	121.54
6	AG	3	ARG	C-N-CA	5.73	132.48	121.54
21	AA	1303	C	C5'-C4'-C3'	-5.72	107.42	116.00
21	AA	1181	G	C5'-C4'-C3'	-5.71	106.63	115.20
54	BA	1606	C	C1'-O4'-C4'	-5.71	104.00	109.70
54	BA	243	U	O4'-C4'-C3'	5.70	109.70	104.00
4	AE	24	VAL	O-C-N	-5.70	115.45	122.57
13	AN	42	TRP	CA-C-N	5.66	131.88	121.70
13	AN	42	TRP	C-N-CA	5.66	131.88	121.70
18	AS	22	VAL	O-C-N	-5.65	115.51	122.57
44	BV	88	HIS	CB-CG-CD2	-5.65	123.85	131.20
54	BA	233	A	O4'-C4'-C3'	5.64	109.64	104.00
54	BA	1927	A	O4'-C4'-C3'	5.63	109.64	104.00
13	AN	50	THR	CA-C-N	5.63	127.13	120.09
13	AN	50	THR	C-N-CA	5.63	127.13	120.09
54	BA	1427	A	C2'-C3'-O3'	5.63	117.95	109.50
54	BA	147	C	C1'-O4'-C4'	-5.62	104.28	109.90
22	A1	59	U	O4'-C1'-N1	5.62	116.92	108.50
28	BF	11	VAL	CA-C-N	5.61	132.06	121.97
28	BF	11	VAL	C-N-CA	5.61	132.06	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2016	U	O4'-C4'-C3'	5.61	109.61	104.00
21	AA	58	C	C5'-C4'-C3'	-5.60	106.79	115.20
54	BA	2507	C	O4'-C1'-C2'	-5.60	102.00	107.60
54	BA	2768	U	C4'-C3'-C2'	-5.60	97.00	102.60
55	BB	24	G	O4'-C4'-C3'	5.60	109.60	104.00
21	AA	250	A	P-O3'-C3'	5.59	128.58	120.20
21	AA	1375	A	O4'-C4'-C3'	5.58	109.58	104.00
54	BA	2719	G	O4'-C4'-C3'	5.58	109.58	104.00
54	BA	2273	A	C5'-C4'-C3'	-5.57	107.64	116.00
21	AA	6	G	O4'-C1'-N9	5.56	116.84	108.50
40	BR	84	ARG	NE-CZ-NH2	5.55	124.20	119.20
21	AA	1258	G	C1'-O4'-C4'	-5.55	104.35	109.90
54	BA	2766	A	O4'-C4'-C3'	5.55	109.55	104.00
54	BA	2384	U	C2'-C3'-O3'	5.55	117.82	109.50
54	BA	1597	A	C2'-C3'-O3'	-5.55	105.38	113.70
9	AJ	56	HIS	CA-C-N	5.54	131.94	121.97
9	AJ	56	HIS	C-N-CA	5.54	131.94	121.97
21	AA	1268	G	O4'-C4'-C3'	5.54	109.54	104.00
21	AA	182	A	C5'-C4'-C3'	-5.53	107.70	116.00
54	BA	1452	G	O4'-C4'-C3'	5.52	109.52	104.00
21	AA	1005	A	O4'-C4'-C3'	5.52	109.52	104.00
34	BL	48	ARG	CA-C-N	5.51	131.62	121.70
34	BL	48	ARG	C-N-CA	5.51	131.62	121.70
7	AH	1	SER	CA-C-N	5.51	131.62	121.70
7	AH	1	SER	C-N-CA	5.51	131.62	121.70
49	B0	38	LEU	CA-C-N	5.50	128.42	120.38
49	B0	38	LEU	C-N-CA	5.50	128.42	120.38
21	AA	1377	A	O4'-C4'-C3'	5.49	109.49	104.00
54	BA	1332	G	C5'-C4'-C3'	-5.49	106.97	115.20
54	BA	1427	A	P-O3'-C3'	5.49	128.43	120.20
24	A3	10	G	O4'-C4'-C3'	5.47	109.47	104.00
34	BL	41	ARG	CA-C-N	5.47	131.54	121.70
34	BL	41	ARG	C-N-CA	5.47	131.54	121.70
6	AG	77	ARG	NE-CZ-NH2	5.47	124.12	119.20
54	BA	2158	A	O3'-P-O5'	-5.46	95.81	104.00
54	BA	1523	U	O4'-C1'-N1	5.46	116.69	108.50
54	BA	546	U	O4'-C1'-N1	5.46	116.69	108.50
54	BA	1210	G	C4'-C3'-O3'	5.46	117.59	109.40
54	BA	1810	A	O4'-C4'-C3'	5.45	109.45	104.00
42	BT	6	ARG	NE-CZ-NH2	5.45	124.10	119.20
33	BK	3	GLN	OE1-CD-NE2	-5.45	117.15	122.60
54	BA	1648	U	C5'-C4'-C3'	-5.44	107.85	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	845	A	C1'-O4'-C4'	-5.42	104.48	109.90
41	BS	102	HIS	CB-CG-CD2	-5.42	124.16	131.20
54	BA	1328	A	O4'-C4'-C3'	5.42	109.42	104.00
54	BA	280	U	O4'-C1'-N1	5.41	116.32	108.20
34	BL	35	HIS	CA-C-N	5.41	131.87	121.54
34	BL	35	HIS	C-N-CA	5.41	131.87	121.54
51	B2	5	PHE	CA-C-N	5.41	131.44	121.70
51	B2	5	PHE	C-N-CA	5.41	131.44	121.70
34	BL	101	ILE	N-CA-C	5.40	120.57	109.34
21	AA	1530	G	C1'-O4'-C4'	-5.40	104.50	109.90
51	B2	4	THR	N-CA-C	5.40	117.92	111.71
4	AE	156	ARG	NE-CZ-NH2	5.40	124.06	119.20
54	BA	1799	G	C2'-C3'-O3'	5.40	117.60	109.50
21	AA	839	C	O4'-C4'-C3'	5.39	109.39	104.00
7	AH	87	ARG	NE-CZ-NH2	5.39	124.05	119.20
54	BA	1699	G	O4'-C1'-N9	5.39	116.28	108.20
4	AE	54	GLU	CA-C-N	5.38	124.63	120.33
4	AE	54	GLU	C-N-CA	5.38	124.63	120.33
54	BA	1332	G	O4'-C1'-N9	5.38	116.27	108.20
21	AA	81	A	C5'-C4'-C3'	-5.37	107.94	116.00
54	BA	646	U	C4'-C3'-C2'	-5.37	97.23	102.60
7	AH	4	ASP	CA-C-N	5.37	125.03	119.56
7	AH	4	ASP	C-N-CA	5.37	125.03	119.56
54	BA	1141	U	C3'-C2'-C1'	5.37	106.67	101.30
54	BA	2547	A	C1'-O4'-C4'	-5.36	104.55	109.90
21	AA	701	U	C4'-C3'-O3'	5.35	117.42	109.40
24	A3	73	A	O4'-C4'-C3'	5.35	109.35	104.00
21	AA	6	G	P-O3'-C3'	5.34	128.22	120.20
21	AA	1093	A	O4'-C4'-C3'	5.34	109.34	104.00
27	BE	165	HIS	CA-C-N	5.34	131.74	121.54
27	BE	165	HIS	C-N-CA	5.34	131.74	121.54
54	BA	1546	G	C4'-C3'-O3'	5.34	121.01	113.00
54	BA	387	U	C1'-O4'-C4'	-5.34	104.36	109.70
54	BA	1606	C	O4'-C1'-N1	5.34	116.20	108.20
21	AA	1445	U	O4'-C4'-C3'	5.33	109.33	104.00
54	BA	2243	U	C4'-C3'-C2'	-5.33	97.27	102.60
3	AD	28	ASP	CA-C-N	5.33	131.72	121.54
3	AD	28	ASP	C-N-CA	5.33	131.72	121.54
21	AA	948	C	O3'-P-O5'	5.33	111.99	104.00
54	BA	1551	A	O4'-C4'-C3'	5.33	109.33	104.00
12	AM	69	ARG	CA-C-N	5.32	128.15	120.38
12	AM	69	ARG	C-N-CA	5.32	128.15	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	526	A	O4'-C4'-C3'	5.32	109.32	104.00
54	BA	1395	A	O4'-C4'-C3'	5.32	109.32	104.00
29	BG	52	GLY	CA-C-N	5.31	125.21	119.85
29	BG	52	GLY	C-N-CA	5.31	125.21	119.85
8	AI	40	ARG	CA-C-N	5.31	128.41	120.87
8	AI	40	ARG	C-N-CA	5.31	128.41	120.87
54	BA	49	A	C4'-C3'-O3'	5.30	117.36	109.40
54	BA	1969	A	O4'-C4'-C3'	5.30	109.30	104.00
54	BA	2154	A	C2'-C3'-O3'	-5.30	105.75	113.70
21	AA	577	G	O4'-C4'-C3'	5.30	109.30	104.00
24	A3	50	G	O4'-C4'-C3'	5.30	109.30	104.00
29	BG	7	PRO	CA-C-N	5.30	131.50	121.97
29	BG	7	PRO	C-N-CA	5.30	131.50	121.97
54	BA	1138	G	C2'-C3'-O3'	-5.30	105.75	113.70
21	AA	1302	C	O4'-C4'-C3'	5.29	109.29	104.00
54	BA	2389	G	O4'-C4'-C3'	5.29	109.29	104.00
54	BA	931	U	O4'-C1'-N1	5.29	116.43	108.50
21	AA	382	A	O4'-C4'-C3'	5.28	109.28	104.00
54	BA	2875	C	O4'-C4'-C3'	5.28	109.28	104.00
54	BA	309	A	O4'-C4'-C3'	5.28	109.28	104.00
54	BA	763	G	C5'-C4'-C3'	-5.27	108.09	116.00
54	BA	1141	U	O4'-C4'-C3'	5.27	109.27	104.00
54	BA	1706	C	C4'-C3'-O3'	5.27	117.30	109.40
21	AA	718	A	O4'-C4'-C3'	5.26	109.27	104.00
21	AA	1127	G	O4'-C4'-C3'	5.26	109.26	104.00
54	BA	16	C	O4'-C4'-C3'	5.26	109.26	104.00
54	BA	142	A	C2'-C3'-O3'	5.26	117.38	109.50
21	AA	1201	A	P-O3'-C3'	5.25	128.08	120.20
21	AA	587	G	O4'-C4'-C3'	5.25	109.25	104.00
54	BA	2501	C	O4'-C1'-C2'	-5.25	100.55	105.80
21	AA	1379	G	O4'-C4'-C3'	5.24	109.24	104.00
54	BA	2782	G	O4'-C4'-C3'	5.24	109.24	104.00
3	AD	203	TYR	CA-C-N	5.24	131.13	121.70
3	AD	203	TYR	C-N-CA	5.24	131.13	121.70
21	AA	320	A	C5'-C4'-C3'	-5.24	108.14	116.00
54	BA	2810	A	C4'-C3'-C2'	-5.24	97.36	102.60
26	BD	76	GLY	CA-C-N	5.24	131.54	121.54
26	BD	76	GLY	C-N-CA	5.24	131.54	121.54
54	BA	2624	G	C4'-C3'-C2'	-5.24	97.36	102.60
21	AA	1048	G	O4'-C4'-C3'	5.23	109.23	104.00
54	BA	220	G	O4'-C4'-C3'	5.23	109.23	104.00
54	BA	933	A	O4'-C1'-N9	5.23	116.04	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	485	U	O4'-C4'-C3'	5.22	109.22	104.00
21	AA	14	U	O4'-C4'-C3'	5.21	109.21	104.00
34	BL	42	SER	CA-C-N	5.21	131.07	121.70
34	BL	42	SER	C-N-CA	5.21	131.07	121.70
50	B1	5	ARG	NE-CZ-NH2	5.21	123.89	119.20
4	AE	149	PRO	O-C-N	-5.20	115.62	122.64
54	BA	2342	C	C4'-C3'-C2'	-5.20	97.40	102.60
54	BA	1160	G	O4'-C4'-C3'	5.20	109.20	104.00
36	BN	91	ALA	CA-C-N	5.20	127.79	120.57
36	BN	91	ALA	C-N-CA	5.20	127.79	120.57
54	BA	2339	C	O4'-C1'-N1	5.20	116.29	108.50
54	BA	985	C	O4'-C4'-C3'	5.19	109.19	104.00
38	BP	85	VAL	CA-C-N	5.19	127.19	120.44
38	BP	85	VAL	C-N-CA	5.19	127.19	120.44
54	BA	1378	A	O3'-P-O5'	-5.19	96.21	104.00
21	AA	120	A	O4'-C4'-C3'	5.19	109.19	104.00
54	BA	2451	A	O4'-C4'-C3'	5.18	109.18	104.00
54	BA	821	A	O4'-C4'-C3'	5.18	109.18	104.00
43	BU	44	HIS	CB-CG-CD2	-5.17	124.47	131.20
54	BA	49	A	C2'-C3'-O3'	5.17	117.26	109.50
54	BA	670	A	C2'-C3'-O3'	5.17	117.26	109.50
21	AA	397	A	C5'-C4'-C3'	-5.17	108.25	116.00
21	AA	725	G	C5'-C4'-C3'	-5.17	108.25	116.00
38	BP	86	LYS	N-CA-C	5.16	116.59	111.07
54	BA	2287	A	O3'-P-O5'	5.16	111.74	104.00
21	AA	1345	U	C1'-O4'-C4'	-5.16	104.74	109.90
49	B0	15	ARG	NE-CZ-NH2	5.16	123.84	119.20
54	BA	1588	G	C4'-C3'-C2'	-5.16	97.44	102.60
21	AA	1026	G	O4'-C4'-C3'	5.15	109.15	104.00
21	AA	647	C	O4'-C4'-C3'	5.15	109.15	104.00
54	BA	2790	U	O4'-C1'-C2'	-5.15	100.65	105.80
46	BX	53	LYS	CA-C-N	5.14	125.69	119.98
46	BX	53	LYS	C-N-CA	5.14	125.69	119.98
54	BA	1155	A	O4'-C4'-C3'	5.14	109.14	104.00
21	AA	1236	A	O4'-C4'-C3'	5.14	109.14	104.00
54	BA	1025	G	O3'-P-O5'	5.14	111.72	104.00
21	AA	492	C	O4'-C4'-C3'	5.14	109.14	104.00
21	AA	1101	A	C2'-C3'-O3'	5.14	117.21	109.50
14	AO	50	HIS	CB-CG-CD2	-5.13	124.53	131.20
54	BA	2143	C	C4'-C3'-C2'	-5.13	97.47	102.60
12	AM	91	ARG	N-CA-C	5.13	116.73	111.03
9	AJ	73	LEU	CA-C-N	5.13	131.20	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AJ	73	LEU	C-N-CA	5.13	131.20	121.97
36	BN	8	ARG	CA-C-N	5.12	127.46	120.54
36	BN	8	ARG	C-N-CA	5.12	127.46	120.54
20	AU	22	CYS	CA-C-N	5.12	131.33	121.54
20	AU	22	CYS	C-N-CA	5.12	131.33	121.54
1	AB	207	ARG	CA-C-N	5.12	131.32	121.54
1	AB	207	ARG	C-N-CA	5.12	131.32	121.54
54	BA	474	G	O4'-C1'-N9	5.12	115.88	108.20
34	BL	100	ILE	CA-C-N	5.12	131.18	121.97
34	BL	100	ILE	C-N-CA	5.12	131.18	121.97
54	BA	750	A	C5'-C4'-C3'	-5.12	108.33	116.00
54	BA	2547	A	O4'-C1'-N9	5.11	116.17	108.50
21	AA	483	C	O4'-C4'-C3'	5.11	109.11	104.00
18	AS	36	ARG	NE-CZ-NH2	5.11	123.80	119.20
21	AA	1501	C	O4'-C4'-C3'	5.10	109.10	104.00
21	AA	1255	G	O4'-C4'-C3'	5.10	109.10	104.00
43	BU	6	ARG	NE-CZ-NH2	5.10	123.79	119.20
21	AA	722	G	C5'-C4'-C3'	-5.10	108.36	116.00
21	AA	945	G	O4'-C4'-C3'	5.09	109.09	104.00
54	BA	2130	U	O4'-C4'-C3'	5.09	109.09	104.00
21	AA	110	C	O4'-C4'-C3'	5.09	109.09	104.00
21	AA	6	G	C4'-C3'-O3'	5.08	120.61	113.00
21	AA	343	U	O4'-C4'-C3'	5.07	109.07	104.00
21	AA	938	A	C5'-C4'-C3'	-5.06	108.41	116.00
21	AA	485	U	C3'-C2'-C1'	5.06	106.36	101.30
54	BA	337	C	C4'-C3'-C2'	-5.06	97.54	102.60
24	A3	43	G	C5'-C4'-C3'	-5.05	108.42	116.00
54	BA	527	C	O3'-P-O5'	5.05	111.58	104.00
54	BA	2411	A	O4'-C4'-C3'	5.05	109.05	104.00
54	BA	530	G	O3'-P-O5'	-5.04	96.43	104.00
54	BA	86	G	C5'-C4'-C3'	-5.04	108.44	116.00
54	BA	141	G	C4'-C3'-C2'	-5.04	97.56	102.60
5	AF	94	HIS	CB-CG-CD2	-5.04	124.65	131.20
54	BA	2229	U	C4'-C3'-C2'	-5.03	97.57	102.60
21	AA	397	A	O3'-P-O5'	-5.03	96.45	104.00
9	AJ	39	PRO	N-CA-CB	5.03	107.65	103.17
21	AA	758	C	O4'-C4'-C3'	5.03	109.03	104.00
21	AA	1470	U	C5'-C4'-C3'	-5.03	108.46	116.00
21	AA	723	U	O4'-C4'-C3'	5.02	109.02	104.00
27	BE	65	THR	CA-C-N	5.02	126.42	120.14
27	BE	65	THR	C-N-CA	5.02	126.42	120.14
54	BA	823	C	O4'-C4'-C3'	5.02	109.02	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BX	10	ARG	N-CA-C	5.02	114.07	108.25
54	BA	2289	G	O4'-C4'-C3'	5.01	109.02	104.00
54	BA	1759	A	O4'-C4'-C3'	5.01	109.01	104.00
21	AA	764	C	O4'-C4'-C3'	5.01	109.01	104.00
55	BB	99	A	C5'-C4'-C3'	-5.01	108.48	116.00
54	BA	1451	C	O4'-C1'-N1	5.01	115.71	108.20
21	AA	1358	U	O4'-C4'-C3'	5.01	109.01	104.00
54	BA	2732	G	C5'-C4'-C3'	-5.00	108.49	116.00
54	BA	1555	G	O4'-C4'-C3'	5.00	109.00	104.00
54	BA	1986	C	C4'-C3'-C2'	-5.00	97.60	102.60
54	BA	2425	A	C4'-C3'-O3'	5.00	116.90	109.40

There are no chirality outliers.

All (1115) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	11	C	Sidechain
22	A1	17	U	Sidechain
22	A1	22	G	Sidechain
22	A1	24	G	Sidechain
22	A1	39	G	Sidechain
22	A1	42	G	Sidechain
22	A1	43	G	Sidechain
22	A1	44	G	Sidechain
22	A1	49	G	Sidechain
22	A1	57	G	Sidechain
22	A1	6	A	Sidechain
22	A1	61	C	Sidechain
22	A1	63	G	Sidechain
22	A1	66	A	Sidechain
22	A1	70	C	Sidechain
22	A1	74	C	Sidechain
23	A2	83	U	Sidechain
23	A2	85	G	Sidechain
23	A2	86	U	Sidechain
23	A2	92	U	Sidechain
23	A2	93	U	Sidechain
24	A3	12	G	Sidechain
24	A3	23	G	Sidechain
24	A3	28	U	Sidechain
24	A3	34	U	Sidechain
24	A3	37	U	Sidechain

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Mol	Chain	Res	Type	Group
24	A3	57	C	Sidechain
24	A3	60	A	Sidechain
24	A3	68	C	Sidechain
21	AA	100	G	Sidechain
21	AA	1000	A	Sidechain
21	AA	1001	C	Sidechain
21	AA	1002	G	Sidechain
21	AA	1007	U	Sidechain
21	AA	1008	U	Sidechain
21	AA	1010	U	Sidechain
21	AA	1013	G	Sidechain
21	AA	1017	U	Sidechain
21	AA	103	U	Sidechain
21	AA	1031	C	Sidechain
21	AA	1033	G	Sidechain
21	AA	1035	A	Sidechain
21	AA	1039	G	Sidechain
21	AA	1042	A	Sidechain
21	AA	1046	A	Sidechain
21	AA	1047	G	Sidechain
21	AA	1048	G	Sidechain
21	AA	1049	U	Sidechain
21	AA	105	G	Sidechain
21	AA	1053	G	Sidechain
21	AA	1054	C	Sidechain
21	AA	1065	U	Sidechain
21	AA	1068	G	Sidechain
21	AA	1073	U	Sidechain
21	AA	1077	G	Sidechain
21	AA	108	G	Sidechain
21	AA	1083	U	Sidechain
21	AA	1084	G	Sidechain
21	AA	1091	U	Sidechain
21	AA	1092	A	Sidechain
21	AA	1093	A	Sidechain
21	AA	1094	G	Sidechain
21	AA	1095	U	Sidechain
21	AA	1100	C	Sidechain
21	AA	1104	G	Sidechain
21	AA	1107	C	Sidechain
21	AA	111	G	Sidechain
21	AA	112	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1120	C	Sidechain
21	AA	1131	G	Sidechain
21	AA	1135	U	Sidechain
21	AA	1137	C	Sidechain
21	AA	1139	G	Sidechain
21	AA	1144	G	Sidechain
21	AA	1149	C	Sidechain
21	AA	115	G	Sidechain
21	AA	1151	A	Sidechain
21	AA	1154	G	Sidechain
21	AA	1156	G	Sidechain
21	AA	1158	C	Sidechain
21	AA	1162	C	Sidechain
21	AA	1166	G	Sidechain
21	AA	1169	A	Sidechain
21	AA	117	G	Sidechain
21	AA	1186	G	Sidechain
21	AA	1198	G	Sidechain
21	AA	1200	C	Sidechain
21	AA	1202	U	Sidechain
21	AA	1205	U	Sidechain
21	AA	1211	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1215	G	Sidechain
21	AA	1216	A	Sidechain
21	AA	1217	C	Sidechain
21	AA	1220	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1226	C	Sidechain
21	AA	1230	C	Sidechain
21	AA	1233	G	Sidechain
21	AA	1234	C	Sidechain
21	AA	124	C	Sidechain
21	AA	1241	G	Sidechain
21	AA	1242	G	Sidechain
21	AA	1243	C	Sidechain
21	AA	1244	G	Sidechain
21	AA	1247	U	Sidechain
21	AA	1257	A	Sidechain
21	AA	1261	A	Sidechain
21	AA	1266	G	Sidechain
21	AA	1267	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	127	G	Sidechain
21	AA	1274	A	Sidechain
21	AA	1275	A	Sidechain
21	AA	1276	G	Sidechain
21	AA	1282	C	Sidechain
21	AA	1283	U	Sidechain
21	AA	1284	C	Sidechain
21	AA	1289	A	Sidechain
21	AA	1292	G	Sidechain
21	AA	1293	C	Sidechain
21	AA	1297	G	Sidechain
21	AA	1302	C	Sidechain
21	AA	1304	G	Sidechain
21	AA	1306	A	Sidechain
21	AA	1307	U	Sidechain
21	AA	1308	U	Sidechain
21	AA	1312	G	Sidechain
21	AA	1317	C	Sidechain
21	AA	1318	A	Sidechain
21	AA	1319	A	Sidechain
21	AA	1323	G	Sidechain
21	AA	1330	U	Sidechain
21	AA	1333	A	Sidechain
21	AA	1335	U	Sidechain
21	AA	1336	C	Sidechain
21	AA	1337	G	Sidechain
21	AA	1349	A	Sidechain
21	AA	1357	A	Sidechain
21	AA	1358	U	Sidechain
21	AA	1362	A	Sidechain
21	AA	1363	A	Sidechain
21	AA	1379	G	Sidechain
21	AA	138	G	Sidechain
21	AA	1381	U	Sidechain
21	AA	1383	C	Sidechain
21	AA	1388	C	Sidechain
21	AA	1393	U	Sidechain
21	AA	1397	C	Sidechain
21	AA	14	U	Sidechain
21	AA	1402	C	Sidechain
21	AA	1404	C	Sidechain
21	AA	1408	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1412	C	Sidechain
21	AA	1413	A	Sidechain
21	AA	1416	G	Sidechain
21	AA	1421	G	Sidechain
21	AA	1422	G	Sidechain
21	AA	1431	A	Sidechain
21	AA	1433	A	Sidechain
21	AA	1435	G	Sidechain
21	AA	1439	G	Sidechain
21	AA	1451	U	Sidechain
21	AA	1474	U	Sidechain
21	AA	1477	U	Sidechain
21	AA	1483	A	Sidechain
21	AA	149	A	Sidechain
21	AA	1495	U	Sidechain
21	AA	150	U	Sidechain
21	AA	1500	A	Sidechain
21	AA	1504	G	Sidechain
21	AA	1509	C	Sidechain
21	AA	1510	C	Sidechain
21	AA	1512	U	Sidechain
21	AA	1514	G	Sidechain
21	AA	1515	G	Sidechain
21	AA	1517	G	Sidechain
21	AA	1519	A	Sidechain
21	AA	153	C	Sidechain
21	AA	1531	A	Sidechain
21	AA	156	C	Sidechain
21	AA	157	U	Sidechain
21	AA	159	G	Sidechain
21	AA	165	G	Sidechain
21	AA	166	U	Sidechain
21	AA	181	A	Sidechain
21	AA	185	U	Sidechain
21	AA	186	C	Sidechain
21	AA	187	G	Sidechain
21	AA	188	C	Sidechain
21	AA	190	A	Sidechain
21	AA	191	G	Sidechain
21	AA	193	C	Sidechain
21	AA	194	C	Sidechain
21	AA	195	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	196	A	Sidechain
21	AA	197	A	Sidechain
21	AA	204	G	Sidechain
21	AA	205	A	Sidechain
21	AA	207	C	Sidechain
21	AA	212	G	Sidechain
21	AA	213	G	Sidechain
21	AA	222	C	Sidechain
21	AA	229	U	Sidechain
21	AA	236	A	Sidechain
21	AA	253	A	Sidechain
21	AA	255	G	Sidechain
21	AA	273	U	Sidechain
21	AA	277	C	Sidechain
21	AA	278	G	Sidechain
21	AA	286	C	Sidechain
21	AA	287	U	Sidechain
21	AA	288	A	Sidechain
21	AA	295	C	Sidechain
21	AA	297	G	Sidechain
21	AA	309	A	Sidechain
21	AA	310	G	Sidechain
21	AA	312	C	Sidechain
21	AA	324	G	Sidechain
21	AA	325	A	Sidechain
21	AA	328	C	Sidechain
21	AA	330	C	Sidechain
21	AA	331	G	Sidechain
21	AA	339	C	Sidechain
21	AA	340	U	Sidechain
21	AA	362	G	Sidechain
21	AA	364	A	Sidechain
21	AA	366	A	Sidechain
21	AA	37	U	Sidechain
21	AA	373	A	Sidechain
21	AA	375	U	Sidechain
21	AA	39	G	Sidechain
21	AA	391	G	Sidechain
21	AA	395	C	Sidechain
21	AA	399	G	Sidechain
21	AA	401	C	Sidechain
21	AA	409	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	416	G	Sidechain
21	AA	425	G	Sidechain
21	AA	426	U	Sidechain
21	AA	430	A	Sidechain
21	AA	431	A	Sidechain
21	AA	432	A	Sidechain
21	AA	433	G	Sidechain
21	AA	435	A	Sidechain
21	AA	438	U	Sidechain
21	AA	442	G	Sidechain
21	AA	453	G	Sidechain
21	AA	454	G	Sidechain
21	AA	464	U	Sidechain
21	AA	466	A	Sidechain
21	AA	467	U	Sidechain
21	AA	468	A	Sidechain
21	AA	479	U	Sidechain
21	AA	48	C	Sidechain
21	AA	482	A	Sidechain
21	AA	487	A	Sidechain
21	AA	491	G	Sidechain
21	AA	492	C	Sidechain
21	AA	496	A	Sidechain
21	AA	503	C	Sidechain
21	AA	512	U	Sidechain
21	AA	517	G	Sidechain
21	AA	523	A	Sidechain
21	AA	524	G	Sidechain
21	AA	527	G	Sidechain
21	AA	529	G	Sidechain
21	AA	532	A	Sidechain
21	AA	534	U	Sidechain
21	AA	536	C	Sidechain
21	AA	537	G	Sidechain
21	AA	539	A	Sidechain
21	AA	547	A	Sidechain
21	AA	552	U	Sidechain
21	AA	560	A	Sidechain
21	AA	561	U	Sidechain
21	AA	564	C	Sidechain
21	AA	569	C	Sidechain
21	AA	573	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	575	G	Sidechain
21	AA	576	C	Sidechain
21	AA	58	C	Sidechain
21	AA	580	C	Sidechain
21	AA	583	A	Sidechain
21	AA	588	G	Sidechain
21	AA	589	U	Sidechain
21	AA	59	A	Sidechain
21	AA	592	G	Sidechain
21	AA	596	A	Sidechain
21	AA	598	U	Sidechain
21	AA	6	G	Sidechain
21	AA	600	A	Sidechain
21	AA	606	G	Sidechain
21	AA	607	A	Sidechain
21	AA	609	A	Sidechain
21	AA	610	U	Sidechain
21	AA	614	C	Sidechain
21	AA	618	C	Sidechain
21	AA	65	A	Sidechain
21	AA	652	U	Sidechain
21	AA	656	G	Sidechain
21	AA	66	A	Sidechain
21	AA	666	G	Sidechain
21	AA	67	C	Sidechain
21	AA	673	A	Sidechain
21	AA	674	G	Sidechain
21	AA	677	U	Sidechain
21	AA	68	G	Sidechain
21	AA	682	G	Sidechain
21	AA	683	G	Sidechain
21	AA	687	A	Sidechain
21	AA	690	G	Sidechain
21	AA	697	U	Sidechain
21	AA	698	G	Sidechain
21	AA	699	C	Sidechain
21	AA	704	A	Sidechain
21	AA	712	A	Sidechain
21	AA	718	A	Sidechain
21	AA	722	G	Sidechain
21	AA	73	C	Sidechain
21	AA	749	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	751	U	Sidechain
21	AA	752	G	Sidechain
21	AA	754	C	Sidechain
21	AA	759	A	Sidechain
21	AA	765	G	Sidechain
21	AA	77	A	Sidechain
21	AA	775	G	Sidechain
21	AA	778	G	Sidechain
21	AA	780	A	Sidechain
21	AA	789	U	Sidechain
21	AA	790	A	Sidechain
21	AA	792	A	Sidechain
21	AA	802	A	Sidechain
21	AA	812	G	Sidechain
21	AA	816	A	Sidechain
21	AA	819	A	Sidechain
21	AA	821	G	Sidechain
21	AA	822	U	Sidechain
21	AA	826	C	Sidechain
21	AA	827	U	Sidechain
21	AA	828	U	Sidechain
21	AA	83	C	Sidechain
21	AA	836	G	Sidechain
21	AA	838	G	Sidechain
21	AA	842	U	Sidechain
21	AA	844	G	Sidechain
21	AA	845	A	Sidechain
21	AA	850	U	Sidechain
21	AA	855	U	Sidechain
21	AA	856	C	Sidechain
21	AA	858	G	Sidechain
21	AA	869	G	Sidechain
21	AA	870	U	Sidechain
21	AA	871	U	Sidechain
21	AA	873	A	Sidechain
21	AA	874	G	Sidechain
21	AA	877	G	Sidechain
21	AA	88	U	Sidechain
21	AA	881	G	Sidechain
21	AA	892	A	Sidechain
21	AA	898	G	Sidechain
21	AA	90	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	91	U	Sidechain
21	AA	914	A	Sidechain
21	AA	918	A	Sidechain
21	AA	919	A	Sidechain
21	AA	922	G	Sidechain
21	AA	924	C	Sidechain
21	AA	928	G	Sidechain
21	AA	937	A	Sidechain
21	AA	94	G	Sidechain
21	AA	940	C	Sidechain
21	AA	946	A	Sidechain
21	AA	948	C	Sidechain
21	AA	949	A	Sidechain
21	AA	951	G	Sidechain
21	AA	956	U	Sidechain
21	AA	958	A	Sidechain
21	AA	961	U	Sidechain
21	AA	962	C	Sidechain
21	AA	965	U	Sidechain
21	AA	970	C	Sidechain
21	AA	974	A	Sidechain
21	AA	975	A	Sidechain
21	AA	988	G	Sidechain
21	AA	99	C	Sidechain
21	AA	991	U	Sidechain
21	AA	998	C	Sidechain
3	AD	13	ARG	Sidechain
54	BA	1	G	Sidechain
54	BA	1000	A	Sidechain
54	BA	1002	G	Sidechain
54	BA	1006	C	Sidechain
54	BA	101	A	Sidechain
54	BA	1014	A	Sidechain
54	BA	1015	U	Sidechain
54	BA	1018	U	Sidechain
54	BA	1020	A	Sidechain
54	BA	1027	A	Sidechain
54	BA	1029	A	Sidechain
54	BA	1030	C	Sidechain
54	BA	1032	A	Sidechain
54	BA	1037	G	Sidechain
54	BA	1051	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1055	G	Sidechain
54	BA	1056	G	Sidechain
54	BA	106	C	Sidechain
54	BA	1063	G	Sidechain
54	BA	1069	A	Sidechain
54	BA	1075	C	Sidechain
54	BA	108	G	Sidechain
54	BA	1087	G	Sidechain
54	BA	1098	A	Sidechain
54	BA	1110	G	Sidechain
54	BA	1111	A	Sidechain
54	BA	1121	C	Sidechain
54	BA	1130	U	Sidechain
54	BA	1143	A	Sidechain
54	BA	1159	U	Sidechain
54	BA	1164	C	Sidechain
54	BA	1165	A	Sidechain
54	BA	1168	G	Sidechain
54	BA	117	G	Sidechain
54	BA	1171	G	Sidechain
54	BA	1175	A	Sidechain
54	BA	1182	G	Sidechain
54	BA	1186	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	119	A	Sidechain
54	BA	1190	G	Sidechain
54	BA	1198	U	Sidechain
54	BA	1202	G	Sidechain
54	BA	1206	G	Sidechain
54	BA	1210	G	Sidechain
54	BA	1212	G	Sidechain
54	BA	122	G	Sidechain
54	BA	1223	G	Sidechain
54	BA	1224	U	Sidechain
54	BA	1235	G	Sidechain
54	BA	1236	G	Sidechain
54	BA	1244	A	Sidechain
54	BA	1247	A	Sidechain
54	BA	1248	G	Sidechain
54	BA	1251	C	Sidechain
54	BA	1254	A	Sidechain
54	BA	1256	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1257	C	Sidechain
54	BA	1261	C	Sidechain
54	BA	1263	U	Sidechain
54	BA	1264	A	Sidechain
54	BA	1272	A	Sidechain
54	BA	1275	A	Sidechain
54	BA	1281	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	1287	A	Sidechain
54	BA	1292	G	Sidechain
54	BA	1294	U	Sidechain
54	BA	1307	A	Sidechain
54	BA	1320	C	Sidechain
54	BA	1323	C	Sidechain
54	BA	1327	A	Sidechain
54	BA	1330	C	Sidechain
54	BA	1339	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1342	A	Sidechain
54	BA	1343	G	Sidechain
54	BA	1344	U	Sidechain
54	BA	1345	C	Sidechain
54	BA	1347	A	Sidechain
54	BA	1349	C	Sidechain
54	BA	1354	A	Sidechain
54	BA	1356	G	Sidechain
54	BA	1359	A	Sidechain
54	BA	1364	G	Sidechain
54	BA	1366	A	Sidechain
54	BA	1369	G	Sidechain
54	BA	1375	U	Sidechain
54	BA	1376	C	Sidechain
54	BA	1385	A	Sidechain
54	BA	1387	A	Sidechain
54	BA	1390	U	Sidechain
54	BA	1392	A	Sidechain
54	BA	1395	A	Sidechain
54	BA	1399	C	Sidechain
54	BA	1413	A	Sidechain
54	BA	1421	G	Sidechain
54	BA	1422	G	Sidechain
54	BA	1425	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1427	A	Sidechain
54	BA	1430	G	Sidechain
54	BA	1433	A	Sidechain
54	BA	1434	A	Sidechain
54	BA	144	A	Sidechain
54	BA	1442	U	Sidechain
54	BA	1448	G	Sidechain
54	BA	1450	G	Sidechain
54	BA	1451	C	Sidechain
54	BA	1455	G	Sidechain
54	BA	1459	G	Sidechain
54	BA	1466	U	Sidechain
54	BA	1467	U	Sidechain
54	BA	1481	U	Sidechain
54	BA	1490	A	Sidechain
54	BA	1491	G	Sidechain
54	BA	1492	G	Sidechain
54	BA	1494	A	Sidechain
54	BA	15	G	Sidechain
54	BA	1502	A	Sidechain
54	BA	1517	G	Sidechain
54	BA	1519	G	Sidechain
54	BA	1525	A	Sidechain
54	BA	1526	C	Sidechain
54	BA	1532	A	Sidechain
54	BA	1533	C	Sidechain
54	BA	1534	U	Sidechain
54	BA	1540	G	Sidechain
54	BA	1546	G	Sidechain
54	BA	1550	C	Sidechain
54	BA	1551	A	Sidechain
54	BA	1552	A	Sidechain
54	BA	1556	C	Sidechain
54	BA	1561	C	Sidechain
54	BA	1569	A	Sidechain
54	BA	157	C	Sidechain
54	BA	1570	A	Sidechain
54	BA	1580	A	Sidechain
54	BA	1584	U	Sidechain
54	BA	1587	G	Sidechain
54	BA	1588	G	Sidechain
54	BA	1595	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1601	G	Sidechain
54	BA	1602	U	Sidechain
54	BA	1607	C	Sidechain
54	BA	1611	C	Sidechain
54	BA	1615	C	Sidechain
54	BA	1616	A	Sidechain
54	BA	1619	G	Sidechain
54	BA	1622	G	Sidechain
54	BA	1627	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1638	C	Sidechain
54	BA	1642	G	Sidechain
54	BA	1645	G	Sidechain
54	BA	1649	G	Sidechain
54	BA	1655	A	Sidechain
54	BA	1661	G	Sidechain
54	BA	1665	A	Sidechain
54	BA	1666	G	Sidechain
54	BA	1667	G	Sidechain
54	BA	1669	A	Sidechain
54	BA	1671	U	Sidechain
54	BA	1673	G	Sidechain
54	BA	1674	G	Sidechain
54	BA	1678	A	Sidechain
54	BA	1679	A	Sidechain
54	BA	168	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1693	U	Sidechain
54	BA	1697	G	Sidechain
54	BA	17	G	Sidechain
54	BA	1700	A	Sidechain
54	BA	1704	C	Sidechain
54	BA	1705	A	Sidechain
54	BA	1707	G	Sidechain
54	BA	1710	G	Sidechain
54	BA	1718	G	Sidechain
54	BA	1719	G	Sidechain
54	BA	1720	U	Sidechain
54	BA	1721	G	Sidechain
54	BA	1724	G	Sidechain
54	BA	1733	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1735	A	Sidechain
54	BA	1744	A	Sidechain
54	BA	1750	G	Sidechain
54	BA	1753	G	Sidechain
54	BA	1755	A	Sidechain
54	BA	1759	A	Sidechain
54	BA	1760	C	Sidechain
54	BA	1762	A	Sidechain
54	BA	1769	U	Sidechain
54	BA	177	G	Sidechain
54	BA	1780	A	Sidechain
54	BA	1787	A	Sidechain
54	BA	1790	C	Sidechain
54	BA	1796	U	Sidechain
54	BA	18	U	Sidechain
54	BA	180	G	Sidechain
54	BA	1806	C	Sidechain
54	BA	181	A	Sidechain
54	BA	182	A	Sidechain
54	BA	1820	U	Sidechain
54	BA	1827	U	Sidechain
54	BA	1830	C	Sidechain
54	BA	1831	G	Sidechain
54	BA	1840	G	Sidechain
54	BA	1841	U	Sidechain
54	BA	1842	G	Sidechain
54	BA	1845	G	Sidechain
54	BA	1852	U	Sidechain
54	BA	1855	U	Sidechain
54	BA	1859	U	Sidechain
54	BA	1864	U	Sidechain
54	BA	1869	G	Sidechain
54	BA	1876	A	Sidechain
54	BA	188	G	Sidechain
54	BA	1880	U	Sidechain
54	BA	1883	U	Sidechain
54	BA	1884	G	Sidechain
54	BA	1887	C	Sidechain
54	BA	1899	A	Sidechain
54	BA	190	A	Sidechain
54	BA	1902	C	Sidechain
54	BA	1904	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1907	G	Sidechain
54	BA	1909	C	Sidechain
54	BA	1920	C	Sidechain
54	BA	1922	G	Sidechain
54	BA	1931	U	Sidechain
54	BA	1932	A	Sidechain
54	BA	1936	A	Sidechain
54	BA	1938	A	Sidechain
54	BA	1949	G	Sidechain
54	BA	1952	A	Sidechain
54	BA	1957	C	Sidechain
54	BA	1958	C	Sidechain
54	BA	1959	G	Sidechain
54	BA	196	A	Sidechain
54	BA	1960	A	Sidechain
54	BA	1964	G	Sidechain
54	BA	1965	C	Sidechain
54	BA	1969	A	Sidechain
54	BA	1981	A	Sidechain
54	BA	1982	U	Sidechain
54	BA	1993	U	Sidechain
54	BA	200	U	Sidechain
54	BA	2007	U	Sidechain
54	BA	2008	C	Sidechain
54	BA	2013	A	Sidechain
54	BA	2015	A	Sidechain
54	BA	2016	U	Sidechain
54	BA	2018	G	Sidechain
54	BA	2022	U	Sidechain
54	BA	2023	C	Sidechain
54	BA	2025	C	Sidechain
54	BA	2028	U	Sidechain
54	BA	2029	G	Sidechain
54	BA	2036	C	Sidechain
54	BA	2037	A	Sidechain
54	BA	204	A	Sidechain
54	BA	2040	G	Sidechain
54	BA	2042	A	Sidechain
54	BA	2049	G	Sidechain
54	BA	2052	A	Sidechain
54	BA	2055	C	Sidechain
54	BA	206	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2060	A	Sidechain
54	BA	2062	A	Sidechain
54	BA	2064	C	Sidechain
54	BA	2065	C	Sidechain
54	BA	2066	C	Sidechain
54	BA	2070	A	Sidechain
54	BA	2077	A	Sidechain
54	BA	2078	C	Sidechain
54	BA	2083	G	Sidechain
54	BA	2086	U	Sidechain
54	BA	2087	G	Sidechain
54	BA	209	C	Sidechain
54	BA	2090	A	Sidechain
54	BA	2091	C	Sidechain
54	BA	2092	U	Sidechain
54	BA	2098	U	Sidechain
54	BA	2099	U	Sidechain
54	BA	2102	G	Sidechain
54	BA	2104	C	Sidechain
54	BA	2112	G	Sidechain
54	BA	2114	A	Sidechain
54	BA	212	G	Sidechain
54	BA	2121	G	Sidechain
54	BA	2124	G	Sidechain
54	BA	2125	G	Sidechain
54	BA	2130	U	Sidechain
54	BA	2133	G	Sidechain
54	BA	2137	U	Sidechain
54	BA	2141	G	Sidechain
54	BA	2149	U	Sidechain
54	BA	2155	U	Sidechain
54	BA	2157	G	Sidechain
54	BA	2173	A	Sidechain
54	BA	2179	C	Sidechain
54	BA	218	A	Sidechain
54	BA	2186	G	Sidechain
54	BA	2197	U	Sidechain
54	BA	2198	A	Sidechain
54	BA	2204	G	Sidechain
54	BA	2207	C	Sidechain
54	BA	2211	A	Sidechain
54	BA	2214	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2216	G	Sidechain
54	BA	2218	G	Sidechain
54	BA	2225	A	Sidechain
54	BA	2226	C	Sidechain
54	BA	2230	G	Sidechain
54	BA	2232	C	Sidechain
54	BA	2238	G	Sidechain
54	BA	2241	A	Sidechain
54	BA	2243	U	Sidechain
54	BA	2252	G	Sidechain
54	BA	2254	C	Sidechain
54	BA	2259	U	Sidechain
54	BA	226	A	Sidechain
54	BA	2260	C	Sidechain
54	BA	2269	G	Sidechain
54	BA	2271	G	Sidechain
54	BA	2273	A	Sidechain
54	BA	2274	A	Sidechain
54	BA	2282	G	Sidechain
54	BA	2283	C	Sidechain
54	BA	2286	G	Sidechain
54	BA	229	C	Sidechain
54	BA	2295	C	Sidechain
54	BA	230	G	Sidechain
54	BA	2300	C	Sidechain
54	BA	2306	C	Sidechain
54	BA	2307	G	Sidechain
54	BA	2308	G	Sidechain
54	BA	231	A	Sidechain
54	BA	2311	A	Sidechain
54	BA	2318	G	Sidechain
54	BA	2320	U	Sidechain
54	BA	2323	G	Sidechain
54	BA	2326	C	Sidechain
54	BA	2328	A	Sidechain
54	BA	2337	G	Sidechain
54	BA	234	U	Sidechain
54	BA	2341	G	Sidechain
54	BA	2342	C	Sidechain
54	BA	2349	G	Sidechain
54	BA	235	U	Sidechain
54	BA	2357	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2365	G	Sidechain
54	BA	2366	A	Sidechain
54	BA	2367	G	Sidechain
54	BA	2368	C	Sidechain
54	BA	2369	A	Sidechain
54	BA	2372	U	Sidechain
54	BA	2375	G	Sidechain
54	BA	238	C	Sidechain
54	BA	2387	U	Sidechain
54	BA	239	C	Sidechain
54	BA	2392	A	Sidechain
54	BA	2399	G	Sidechain
54	BA	24	G	Sidechain
54	BA	2400	G	Sidechain
54	BA	2409	G	Sidechain
54	BA	2410	G	Sidechain
54	BA	2411	A	Sidechain
54	BA	2413	G	Sidechain
54	BA	2418	A	Sidechain
54	BA	2420	C	Sidechain
54	BA	2421	G	Sidechain
54	BA	2426	A	Sidechain
54	BA	2427	C	Sidechain
54	BA	2428	G	Sidechain
54	BA	2430	A	Sidechain
54	BA	2432	A	Sidechain
54	BA	2434	A	Sidechain
54	BA	2436	G	Sidechain
54	BA	2437	G	Sidechain
54	BA	2440	C	Sidechain
54	BA	2443	C	Sidechain
54	BA	2446	G	Sidechain
54	BA	2454	G	Sidechain
54	BA	2460	U	Sidechain
54	BA	2462	C	Sidechain
54	BA	2466	C	Sidechain
54	BA	2473	U	Sidechain
54	BA	2475	C	Sidechain
54	BA	2478	A	Sidechain
54	BA	2485	G	Sidechain
54	BA	249	C	Sidechain
54	BA	2491	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2492	U	Sidechain
54	BA	2496	C	Sidechain
54	BA	2497	A	Sidechain
54	BA	2507	C	Sidechain
54	BA	2517	C	Sidechain
54	BA	2521	C	Sidechain
54	BA	2529	G	Sidechain
54	BA	2530	A	Sidechain
54	BA	2534	A	Sidechain
54	BA	2538	C	Sidechain
54	BA	2539	C	Sidechain
54	BA	2544	G	Sidechain
54	BA	2545	G	Sidechain
54	BA	2549	G	Sidechain
54	BA	2550	G	Sidechain
54	BA	2551	C	Sidechain
54	BA	2552	U	Sidechain
54	BA	2559	C	Sidechain
54	BA	256	A	Sidechain
54	BA	2560	A	Sidechain
54	BA	2564	A	Sidechain
54	BA	2565	A	Sidechain
54	BA	2571	U	Sidechain
54	BA	2572	A	Sidechain
54	BA	2575	C	Sidechain
54	BA	2576	G	Sidechain
54	BA	2579	C	Sidechain
54	BA	2580	U	Sidechain
54	BA	2581	G	Sidechain
54	BA	2585	U	Sidechain
54	BA	2587	A	Sidechain
54	BA	2595	G	Sidechain
54	BA	26	G	Sidechain
54	BA	2601	C	Sidechain
54	BA	2605	U	Sidechain
54	BA	2608	G	Sidechain
54	BA	2609	U	Sidechain
54	BA	2611	C	Sidechain
54	BA	2613	U	Sidechain
54	BA	2614	A	Sidechain
54	BA	262	A	Sidechain
54	BA	2623	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2626	C	Sidechain
54	BA	2631	G	Sidechain
54	BA	2638	G	Sidechain
54	BA	264	C	Sidechain
54	BA	2654	A	Sidechain
54	BA	2658	C	Sidechain
54	BA	2659	G	Sidechain
54	BA	266	G	Sidechain
54	BA	2661	G	Sidechain
54	BA	2663	G	Sidechain
54	BA	2670	A	Sidechain
54	BA	2683	C	Sidechain
54	BA	2686	G	Sidechain
54	BA	2689	U	Sidechain
54	BA	2690	U	Sidechain
54	BA	2694	G	Sidechain
54	BA	2696	U	Sidechain
54	BA	2701	U	Sidechain
54	BA	2710	C	Sidechain
54	BA	2712	C	Sidechain
54	BA	272	A	Sidechain
54	BA	2721	A	Sidechain
54	BA	2727	A	Sidechain
54	BA	2728	U	Sidechain
54	BA	2729	G	Sidechain
54	BA	273	G	Sidechain
54	BA	2732	G	Sidechain
54	BA	274	C	Sidechain
54	BA	2740	A	Sidechain
54	BA	2745	C	Sidechain
54	BA	2747	G	Sidechain
54	BA	2751	G	Sidechain
54	BA	2755	C	Sidechain
54	BA	2756	U	Sidechain
54	BA	276	U	Sidechain
54	BA	2777	G	Sidechain
54	BA	2779	U	Sidechain
54	BA	2781	A	Sidechain
54	BA	2783	U	Sidechain
54	BA	2785	C	Sidechain
54	BA	2786	U	Sidechain
54	BA	2799	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2808	G	Sidechain
54	BA	281	C	Sidechain
54	BA	2815	C	Sidechain
54	BA	2817	U	Sidechain
54	BA	2819	G	Sidechain
54	BA	2825	G	Sidechain
54	BA	2827	C	Sidechain
54	BA	2831	G	Sidechain
54	BA	2832	U	Sidechain
54	BA	2833	U	Sidechain
54	BA	2836	U	Sidechain
54	BA	2853	C	Sidechain
54	BA	2856	A	Sidechain
54	BA	2859	G	Sidechain
54	BA	2860	A	Sidechain
54	BA	2862	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	287	G	Sidechain
54	BA	2873	A	Sidechain
54	BA	2877	G	Sidechain
54	BA	2878	U	Sidechain
54	BA	2879	A	Sidechain
54	BA	288	U	Sidechain
54	BA	2883	A	Sidechain
54	BA	2888	C	Sidechain
54	BA	2889	C	Sidechain
54	BA	2891	U	Sidechain
54	BA	2893	A	Sidechain
54	BA	2895	G	Sidechain
54	BA	2896	C	Sidechain
54	BA	291	G	Sidechain
54	BA	297	G	Sidechain
54	BA	301	G	Sidechain
54	BA	307	G	Sidechain
54	BA	308	G	Sidechain
54	BA	310	A	Sidechain
54	BA	311	A	Sidechain
54	BA	313	G	Sidechain
54	BA	317	G	Sidechain
54	BA	319	G	Sidechain
54	BA	322	A	Sidechain
54	BA	33	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	333	G	Sidechain
54	BA	334	C	Sidechain
54	BA	342	A	Sidechain
54	BA	346	A	Sidechain
54	BA	350	G	Sidechain
54	BA	359	G	Sidechain
54	BA	360	U	Sidechain
54	BA	370	G	Sidechain
54	BA	372	G	Sidechain
54	BA	375	G	Sidechain
54	BA	383	C	Sidechain
54	BA	384	A	Sidechain
54	BA	389	G	Sidechain
54	BA	395	U	Sidechain
54	BA	401	A	Sidechain
54	BA	405	U	Sidechain
54	BA	411	G	Sidechain
54	BA	412	A	Sidechain
54	BA	416	U	Sidechain
54	BA	417	C	Sidechain
54	BA	418	C	Sidechain
54	BA	419	U	Sidechain
54	BA	42	A	Sidechain
54	BA	420	C	Sidechain
54	BA	43	G	Sidechain
54	BA	436	C	Sidechain
54	BA	446	G	Sidechain
54	BA	448	U	Sidechain
54	BA	452	G	Sidechain
54	BA	454	A	Sidechain
54	BA	457	A	Sidechain
54	BA	463	G	Sidechain
54	BA	464	U	Sidechain
54	BA	471	A	Sidechain
54	BA	474	G	Sidechain
54	BA	476	G	Sidechain
54	BA	479	A	Sidechain
54	BA	481	G	Sidechain
54	BA	484	C	Sidechain
54	BA	485	C	Sidechain
54	BA	486	C	Sidechain
54	BA	487	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	489	G	Sidechain
54	BA	49	A	Sidechain
54	BA	490	C	Sidechain
54	BA	496	G	Sidechain
54	BA	498	G	Sidechain
54	BA	50	U	Sidechain
54	BA	500	G	Sidechain
54	BA	503	A	Sidechain
54	BA	505	A	Sidechain
54	BA	506	G	Sidechain
54	BA	509	C	Sidechain
54	BA	521	U	Sidechain
54	BA	522	A	Sidechain
54	BA	528	A	Sidechain
54	BA	530	G	Sidechain
54	BA	541	A	Sidechain
54	BA	544	C	Sidechain
54	BA	546	U	Sidechain
54	BA	550	C	Sidechain
54	BA	551	G	Sidechain
54	BA	555	G	Sidechain
54	BA	556	A	Sidechain
54	BA	559	G	Sidechain
54	BA	56	A	Sidechain
54	BA	562	U	Sidechain
54	BA	572	A	Sidechain
54	BA	575	A	Sidechain
54	BA	577	G	Sidechain
54	BA	58	G	Sidechain
54	BA	582	A	Sidechain
54	BA	585	G	Sidechain
54	BA	592	A	Sidechain
54	BA	595	C	Sidechain
54	BA	597	G	Sidechain
54	BA	608	A	Sidechain
54	BA	611	C	Sidechain
54	BA	615	U	Sidechain
54	BA	617	G	Sidechain
54	BA	62	U	Sidechain
54	BA	621	A	Sidechain
54	BA	63	A	Sidechain
54	BA	630	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	648	G	Sidechain
54	BA	654	A	Sidechain
54	BA	666	A	Sidechain
54	BA	671	C	Sidechain
54	BA	679	C	Sidechain
54	BA	680	C	Sidechain
54	BA	682	G	Sidechain
54	BA	683	U	Sidechain
54	BA	685	A	Sidechain
54	BA	686	U	Sidechain
54	BA	689	A	Sidechain
54	BA	690	G	Sidechain
54	BA	691	C	Sidechain
54	BA	697	G	Sidechain
54	BA	70	G	Sidechain
54	BA	700	G	Sidechain
54	BA	704	G	Sidechain
54	BA	710	U	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	719	C	Sidechain
54	BA	724	U	Sidechain
54	BA	726	G	Sidechain
54	BA	730	A	Sidechain
54	BA	733	G	Sidechain
54	BA	739	A	Sidechain
54	BA	753	A	Sidechain
54	BA	754	U	Sidechain
54	BA	76	C	Sidechain
54	BA	763	G	Sidechain
54	BA	791	C	Sidechain
54	BA	792	A	Sidechain
54	BA	795	C	Sidechain
54	BA	800	A	Sidechain
54	BA	802	A	Sidechain
54	BA	810	U	Sidechain
54	BA	811	U	Sidechain
54	BA	812	C	Sidechain
54	BA	813	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	821	A	Sidechain
54	BA	828	U	Sidechain
54	BA	829	A	Sidechain
54	BA	835	C	Sidechain
54	BA	839	U	Sidechain
54	BA	84	A	Sidechain
54	BA	85	G	Sidechain
54	BA	850	U	Sidechain
54	BA	852	U	Sidechain
54	BA	853	C	Sidechain
54	BA	854	C	Sidechain
54	BA	857	G	Sidechain
54	BA	858	G	Sidechain
54	BA	866	A	Sidechain
54	BA	871	U	Sidechain
54	BA	890	C	Sidechain
54	BA	893	C	Sidechain
54	BA	894	U	Sidechain
54	BA	895	U	Sidechain
54	BA	896	A	Sidechain
54	BA	905	A	Sidechain
54	BA	907	G	Sidechain
54	BA	910	A	Sidechain
54	BA	912	C	Sidechain
54	BA	913	U	Sidechain
54	BA	914	G	Sidechain
54	BA	915	C	Sidechain
54	BA	92	U	Sidechain
54	BA	925	A	Sidechain
54	BA	932	U	Sidechain
54	BA	934	U	Sidechain
54	BA	936	A	Sidechain
54	BA	944	C	Sidechain
54	BA	949	G	Sidechain
54	BA	95	A	Sidechain
54	BA	956	G	Sidechain
54	BA	957	C	Sidechain
54	BA	959	A	Sidechain
54	BA	97	C	Sidechain
54	BA	979	A	Sidechain
54	BA	982	C	Sidechain
54	BA	984	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	986	C	Sidechain
54	BA	989	G	Sidechain
54	BA	990	A	Sidechain
54	BA	996	A	Sidechain
54	BA	998	C	Sidechain
55	BB	107	G	Sidechain
55	BB	109	A	Sidechain
55	BB	115	A	Sidechain
55	BB	117	G	Sidechain
55	BB	12	C	Sidechain
55	BB	13	G	Sidechain
55	BB	14	U	Sidechain
55	BB	27	C	Sidechain
55	BB	29	A	Sidechain
55	BB	31	C	Sidechain
55	BB	32	U	Sidechain
55	BB	33	G	Sidechain
55	BB	39	A	Sidechain
55	BB	40	U	Sidechain
55	BB	42	C	Sidechain
55	BB	48	U	Sidechain
55	BB	5	U	Sidechain
55	BB	50	A	Sidechain
55	BB	51	G	Sidechain
55	BB	54	G	Sidechain
55	BB	57	A	Sidechain
55	BB	68	C	Sidechain
55	BB	7	G	Sidechain
55	BB	73	A	Sidechain
55	BB	86	G	Sidechain
55	BB	87	U	Sidechain
55	BB	9	G	Sidechain
55	BB	90	C	Sidechain
55	BB	96	G	Sidechain
36	BN	4	ARG	Sidechain
37	BO	30	ARG	Peptide
38	BP	112	ARG	Sidechain
38	BP	38	ARG	Sidechain
46	BX	18	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	3	0
2	AC	1625	0	1699	1	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	0	0
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	0	0
19	AT	668	0	718	1	0
20	AU	429	0	453	0	0
21	AA	32828	0	16514	4	0
22	A1	1627	0	830	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	1	0
27	BE	1552	0	1619	1	0
28	BF	1420	0	1460	1	0
29	BG	1323	0	1374	2	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	1	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	1	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
43	BU	780	0	834	1	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	1	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	1	0
50	B1	413	0	444	2	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31323	8	0
55	BB	2504	0	1271	2	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	99633	29	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 (29) 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)
2:AC:4:VAL:HG22	2:AC:5:HIS:H	1.60	0.65
1:AB:103:TRP:CZ2	1:AB:104:LYS:HE3	2.47	0.49
21:AA:483:C:H2'	21:AA:484:G:C8	2.49	0.48
54:BA:866:A:C8	54:BA:914:G:C8	3.02	0.47
50:B1:18:HIS:CG	50:B1:19:PHE:H	2.32	0.47
43:BU:3:LYS:HE3	43:BU:84:PHE:CZ	2.50	0.46
50:B1:36:LYS:HE2	50:B1:45:HIS:CG	2.50	0.46
29:BG:85:LYS:HE3	29:BG:163:TYR:CE2	2.51	0.46
55:BB:115:A:H2'	55:BB:116:G:C8	2.52	0.45
26:BD:175:LEU:H	26:BD:175:LEU:HD23	1.80	0.45
21:AA:715:A:H2'	21:AA:716:A:C8	2.53	0.44
40:BR:10:LYS:HE3	54:BA:994:C:H4'	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BT:33:LYS:HE2	42:BT:80:TRP:CZ3	2.53	0.44
49:B0:38:LEU:H	49:B0:41:HIS:CD2	2.36	0.44
54:BA:250:G:H2'	54:BA:251:A:C8	2.53	0.43
28:BF:3:LEU:C	28:BF:3:LEU:HD13	2.44	0.43
1:AB:84:LEU:H	1:AB:84:LEU:HD23	1.85	0.42
21:AA:1001:C:H2'	21:AA:1002:G:C8	2.54	0.42
31:BI:102:ARG:HE	31:BI:129:GLU:CD	2.28	0.42
54:BA:1960:A:H2'	54:BA:1961:C:C6	2.55	0.42
19:AT:19:HIS:CE1	21:AA:1447:A:H1'	2.55	0.41
54:BA:77:G:H2'	54:BA:78:U:C6	2.56	0.41
27:BE:78:TRP:CG	27:BE:79:ARG:H	2.38	0.41
29:BG:44:HIS:HD1	29:BG:46:ASP:H	1.68	0.41
46:BX:61:LYS:HE3	54:BA:372:G:H5'	2.01	0.41
54:BA:2243:U:H2'	54:BA:2244:U:C6	2.56	0.41
54:BA:1241:A:C2	54:BA:1242:U:H1'	2.56	0.41
1:AB:103:TRP:CH2	1:AB:104:LYS:HE3	2.56	0.40
35:BM:38:ARG:HH22	55:BB:90:C:P	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	195 (89%)	20 (9%)	3 (1%)	9	40
2	AC	205/208 (99%)	194 (95%)	7 (3%)	4 (2%)	6	31
3	AD	203/206 (98%)	189 (93%)	10 (5%)	4 (2%)	6	31
4	AE	150/152 (99%)	136 (91%)	10 (7%)	4 (3%)	4	25
5	AF	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	3	23
6	AG	150/152 (99%)	131 (87%)	15 (10%)	4 (3%)	4	25
7	AH	127/130 (98%)	122 (96%)	3 (2%)	2 (2%)	7	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AI	126/128 (98%)	118 (94%)	5 (4%)	3 (2%)	4	27
9	AJ	98/100 (98%)	88 (90%)	6 (6%)	4 (4%)	2	18
10	AK	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14	51
11	AL	121/124 (98%)	107 (88%)	9 (7%)	5 (4%)	2	18
12	AM	112/115 (97%)	97 (87%)	12 (11%)	3 (3%)	4	25
13	AN	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	3	22
14	AO	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
15	AP	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
16	AQ	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	9	42
17	AR	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
18	AS	79/81 (98%)	68 (86%)	9 (11%)	2 (2%)	4	26
19	AT	84/86 (98%)	77 (92%)	6 (7%)	1 (1%)	10	44
20	AU	51/53 (96%)	35 (69%)	13 (26%)	3 (6%)	1	13
25	BC	270/273 (99%)	244 (90%)	18 (7%)	8 (3%)	3	23
26	BD	207/209 (99%)	187 (90%)	12 (6%)	8 (4%)	2	19
27	BE	199/201 (99%)	177 (89%)	11 (6%)	11 (6%)	1	15
28	BF	176/179 (98%)	145 (82%)	24 (14%)	7 (4%)	2	18
29	BG	174/177 (98%)	157 (90%)	14 (8%)	3 (2%)	7	36
30	BH	147/149 (99%)	132 (90%)	12 (8%)	3 (2%)	6	31
31	BI	139/142 (98%)	126 (91%)	10 (7%)	3 (2%)	5	29
32	BJ	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
33	BK	121/123 (98%)	108 (89%)	9 (7%)	4 (3%)	3	21
34	BL	141/144 (98%)	112 (79%)	19 (14%)	10 (7%)	1	11
35	BM	134/136 (98%)	123 (92%)	7 (5%)	4 (3%)	3	23
36	BN	119/121 (98%)	104 (87%)	14 (12%)	1 (1%)	16	54
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	14	51
38	BP	112/115 (97%)	98 (88%)	11 (10%)	3 (3%)	4	25
39	BQ	115/118 (98%)	106 (92%)	6 (5%)	3 (3%)	4	25
40	BR	101/103 (98%)	90 (89%)	8 (8%)	3 (3%)	3	23
41	BS	108/110 (98%)	96 (89%)	12 (11%)	0	100	100
42	BT	92/94 (98%)	70 (76%)	15 (16%)	7 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BU	101/104 (97%)	85 (84%)	10 (10%)	6 (6%)	1	13
44	BV	92/94 (98%)	86 (94%)	4 (4%)	2 (2%)	5	29
45	BW	78/80 (98%)	59 (76%)	14 (18%)	5 (6%)	1	12
46	BX	75/79 (95%)	64 (85%)	6 (8%)	5 (7%)	1	12
47	BY	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
48	BZ	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	2	20
49	B0	54/57 (95%)	49 (91%)	3 (6%)	2 (4%)	2	20
50	B1	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	6	31
51	B2	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5	28
52	B3	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	7	38
53	B4	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	4	24
56	B5	221/234 (94%)	205 (93%)	14 (6%)	2 (1%)	14	51
All	All	5876/6008 (98%)	5257 (90%)	462 (8%)	157 (3%)	6	25

All (157) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	4	VAL
3	AD	47	LEU
4	AE	105	ILE
4	AE	149	PRO
5	AF	61	LEU
6	AG	103	ILE
9	AJ	57	VAL
9	AJ	74	VAL
19	AT	4	LYS
26	BD	2	ILE
28	BF	73	VAL
34	BL	5	THR
34	BL	29	LYS
34	BL	101	ILE
38	BP	26	GLU
42	BT	40	LYS
42	BT	63	VAL
43	BU	40	LEU
49	B0	2	VAL
51	B2	44	VAL
53	B4	16	ILE

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Mol	Chain	Res	Type
1	AB	36	LYS
4	AE	24	VAL
5	AF	6	ILE
8	AI	126	PHE
9	AJ	77	VAL
11	AL	15	VAL
12	AM	42	VAL
13	AN	99	ALA
16	AQ	69	THR
20	AU	5	VAL
20	AU	37	TYR
25	BC	64	VAL
26	BD	75	ALA
26	BD	77	ARG
26	BD	119	ALA
26	BD	138	LEU
27	BE	43	THR
27	BE	55	SER
27	BE	70	SER
27	BE	149	ILE
27	BE	166	LYS
28	BF	12	VAL
29	BG	8	VAL
34	BL	30	THR
34	BL	32	GLY
34	BL	36	LYS
35	BM	134	THR
42	BT	70	HIS
42	BT	78	SER
43	BU	12	VAL
43	BU	96	LYS
45	BW	16	GLU
45	BW	74	LYS
46	BX	5	GLN
46	BX	33	HIS
1	AB	208	ALA
2	AC	195	ILE
3	AD	203	TYR
4	AE	25	LYS
6	AG	4	ARG
8	AI	39	GLY
11	AL	78	VAL

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Mol	Chain	Res	Type
11	AL	112	ALA
20	AU	32	ARG
25	BC	89	ASN
25	BC	153	LEU
25	BC	189	ALA
27	BE	147	LEU
27	BE	165	HIS
28	BF	176	PHE
29	BG	174	LYS
31	BI	18	ASN
33	BK	71	ARG
35	BM	36	VAL
39	BQ	91	ARG
40	BR	53	PHE
40	BR	86	GLN
40	BR	87	GLN
42	BT	66	LYS
45	BW	23	LYS
46	BX	52	ALA
46	BX	75	GLU
48	BZ	30	ARG
50	B1	6	GLU
2	AC	14	VAL
3	AD	28	ASP
3	AD	187	ARG
5	AF	92	THR
7	AH	2	MET
7	AH	69	ALA
8	AI	128	LYS
11	AL	33	CYS
18	AS	23	GLU
25	BC	144	GLU
26	BD	76	GLY
27	BE	160	ALA
28	BF	103	ILE
30	BH	75	LEU
30	BH	121	VAL
31	BI	93	ASN
33	BK	25	LEU
33	BK	103	VAL
35	BM	82	MET
36	BN	47	VAL

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Mol	Chain	Res	Type
39	BQ	86	SER
42	BT	61	LEU
42	BT	81	LYS
43	BU	19	GLY
46	BX	27	ARG
49	B0	5	ASN
56	B5	13	GLU
1	AB	18	GLN
10	AK	118	ASN
13	AN	38	ASP
18	AS	79	TYR
25	BC	123	ILE
25	BC	191	LEU
26	BD	112	THR
28	BF	119	LYS
29	BG	9	VAL
31	BI	13	ALA
33	BK	16	ALA
34	BL	55	MET
34	BL	66	PHE
34	BL	69	ARG
35	BM	20	LEU
39	BQ	21	LYS
43	BU	5	ARG
43	BU	16	LYS
44	BV	26	PHE
45	BW	44	PHE
6	AG	80	GLY
6	AG	133	ALA
12	AM	23	GLY
13	AN	39	GLU
27	BE	61	ARG
27	BE	71	GLY
28	BF	126	ASN
28	BF	175	PRO
34	BL	33	ARG
38	BP	112	ARG
48	BZ	9	THR
25	BC	63	ILE
30	BH	61	VAL
45	BW	26	GLY
2	AC	206	ILE

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Mol	Chain	Res	Type
11	AL	84	GLY
38	BP	63	ILE
12	AM	6	ILE
27	BE	148	ILE
37	BO	42	PRO
44	BV	83	LYS
26	BD	73	VAL
56	B5	91	GLY
9	AJ	42	LEU
52	B3	44	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	177 (98%)	3 (2%)	53	69
2	AC	170/171 (99%)	168 (99%)	2 (1%)	63	75
3	AD	172/173 (99%)	170 (99%)	2 (1%)	63	75
4	AE	113/113 (100%)	111 (98%)	2 (2%)	51	68
5	AF	87/87 (100%)	87 (100%)	0	100	100
6	AG	123/123 (100%)	120 (98%)	3 (2%)	43	64
7	AH	104/105 (99%)	104 (100%)	0	100	100
8	AI	105/105 (100%)	104 (99%)	1 (1%)	68	78
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	44	64
10	AK	90/90 (100%)	89 (99%)	1 (1%)	65	76
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	82 (99%)	1 (1%)	63	75
14	AO	76/77 (99%)	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	43 (98%)	1 (2%)	44	64
25	BC	216/217 (100%)	213 (99%)	3 (1%)	59	72
26	BD	164/164 (100%)	163 (99%)	1 (1%)	78	83
27	BE	165/165 (100%)	160 (97%)	5 (3%)	36	57
28	BF	149/150 (99%)	148 (99%)	1 (1%)	76	81
29	BG	137/138 (99%)	134 (98%)	3 (2%)	45	64
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	108 (99%)	1 (1%)	70	79
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	53	69
33	BK	103/103 (100%)	101 (98%)	2 (2%)	50	67
34	BL	102/103 (99%)	98 (96%)	4 (4%)	28	49
35	BM	109/109 (100%)	107 (98%)	2 (2%)	51	68
36	BN	100/100 (100%)	99 (99%)	1 (1%)	68	78
37	BO	86/87 (99%)	83 (96%)	3 (4%)	32	53
38	BP	99/100 (99%)	98 (99%)	1 (1%)	68	78
39	BQ	89/90 (99%)	89 (100%)	0	100	100
40	BR	84/84 (100%)	84 (100%)	0	100	100
41	BS	93/93 (100%)	91 (98%)	2 (2%)	45	64
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	43	64
44	BV	78/78 (100%)	77 (99%)	1 (1%)	61	74
45	BW	59/59 (100%)	58 (98%)	1 (2%)	53	69
46	BX	67/68 (98%)	65 (97%)	2 (3%)	36	57
47	BY	55/55 (100%)	54 (98%)	1 (2%)	51	68
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%)	44 (98%)	1 (2%)	45	64
51	B2	38/38 (100%)	37 (97%)	1 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	B3	51/52 (98%)	50 (98%)	1 (2%)	48	66
53	B4	34/34 (100%)	32 (94%)	2 (6%)	18	39
56	B5	173/181 (96%)	172 (99%)	1 (1%)	78	83
All	All	4842/4870 (99%)	4779 (99%)	63 (1%)	59	74

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	71	THR
1	AB	103	TRP
1	AB	219	THR
2	AC	19	SER
2	AC	128	MET
3	AD	162	GLU
3	AD	196	GLU
4	AE	35	LEU
4	AE	119	VAL
6	AG	3	ARG
6	AG	57	GLU
6	AG	138	GLU
8	AI	56	MET
9	AJ	32	THR
9	AJ	75	ASP
10	AK	76	TYR
13	AN	73	PHE
20	AU	3	ILE
25	BC	62	ARG
25	BC	191	LEU
25	BC	238	ASN
26	BD	151	THR
27	BE	43	THR
27	BE	70	SER
27	BE	73	ILE
27	BE	77	ILE
27	BE	145	ASP
28	BF	143	ASP
29	BG	25	ILE
29	BG	46	ASP
29	BG	71	LEU
31	BI	54	ILE
32	BJ	14	ASP

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Mol	Chain	Res	Type
32	BJ	50	THR
33	BK	37	ASP
33	BK	105	ARG
34	BL	82	LEU
34	BL	86	GLU
34	BL	103	ILE
34	BL	109	LYS
35	BM	12	MET
35	BM	84	LYS
36	BN	97	ILE
37	BO	12	THR
37	BO	94	ARG
37	BO	100	HIS
38	BP	30	TRP
41	BS	57	ASN
41	BS	68	ASP
43	BU	5	ARG
43	BU	44	HIS
44	BV	80	HIS
45	BW	14	ASP
46	BX	24	THR
46	BX	37	PHE
47	BY	55	THR
49	B0	41	HIS
50	B1	42	VAL
51	B2	2	LYS
52	B3	1	PRO
53	B4	16	ILE
53	B4	36	ARG
56	B5	165	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	177	ASN
1	AB	189	ASN
2	AC	31	ASN
2	AC	99	GLN
3	AD	53	GLN
3	AD	163	GLN
4	AE	42	ASN
4	AE	121	ASN

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Mol	Chain	Res	Type
4	AE	134	ASN
5	AF	46	GLN
5	AF	58	HIS
6	AG	121	ASN
10	AK	21	HIS
10	AK	63	GLN
10	AK	80	ASN
11	AL	95	HIS
12	AM	7	ASN
12	AM	104	ASN
14	AO	34	GLN
14	AO	49	HIS
14	AO	50	HIS
17	AR	51	GLN
18	AS	56	HIS
19	AT	19	HIS
25	BC	24	HIS
25	BC	57	HIS
25	BC	114	GLN
25	BC	199	HIS
26	BD	58	ASN
26	BD	94	GLN
26	BD	126	ASN
26	BD	173	GLN
27	BE	62	GLN
28	BF	4	HIS
29	BG	47	ASN
29	BG	127	GLN
30	BH	20	ASN
30	BH	28	ASN
30	BH	33	GLN
37	BO	38	GLN
37	BO	116	GLN
38	BP	2	ASN
38	BP	11	GLN
41	BS	9	HIS
42	BT	48	GLN
43	BU	65	GLN
43	BU	68	ASN
44	BV	51	GLN
45	BW	11	ASN
47	BY	20	ASN

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Mol	Chain	Res	Type
47	BY	45	GLN
47	BY	58	ASN
50	B1	44	GLN
53	B4	35	GLN
56	B5	83	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	290 (18%)	92 (6%)
22	A1	75/76 (98%)	9 (12%)	4 (5%)
23	A2	14/15 (93%)	9 (64%)	2 (14%)
24	A3	76/77 (98%)	19 (25%)	6 (7%)
54	BA	2902/2903 (99%)	486 (16%)	127 (4%)
55	BB	116/118 (98%)	16 (13%)	4 (3%)
All	All	4713/4722 (99%)	829 (17%)	235 (4%)

All (829) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	25	C
21	AA	30	U
21	AA	31	G
21	AA	32	A
21	AA	39	G
21	AA	43	C
21	AA	47	C
21	AA	48	C
21	AA	50	A
21	AA	51	A
21	AA	54	C
21	AA	55	A
21	AA	58	C
21	AA	59	A
21	AA	64	G

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Mol	Chain	Res	Type
21	AA	65	A
21	AA	83	C
21	AA	85	U
21	AA	86	G
21	AA	87	C
21	AA	95	C
21	AA	98	A
21	AA	109	A
21	AA	110	C
21	AA	111	G
21	AA	120	A
21	AA	121	U
21	AA	125	U
21	AA	163	C
21	AA	173	U
21	AA	182	A
21	AA	189	A
21	AA	191	G
21	AA	198	G
21	AA	209	U
21	AA	212	G
21	AA	213	G
21	AA	235	C
21	AA	237	G
21	AA	240	G
21	AA	244	U
21	AA	247	G
21	AA	250	A
21	AA	251	G
21	AA	252	U
21	AA	266	G
21	AA	267	C
21	AA	289	G
21	AA	299	G
21	AA	306	A
21	AA	315	A
21	AA	316	C
21	AA	328	C
21	AA	347	G
21	AA	351	G
21	AA	352	C
21	AA	354	G

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Mol	Chain	Res	Type
21	AA	355	C
21	AA	367	U
21	AA	369	G
21	AA	372	C
21	AA	381	C
21	AA	384	G
21	AA	389	A
21	AA	397	A
21	AA	398	U
21	AA	406	G
21	AA	412	A
21	AA	415	A
21	AA	420	U
21	AA	421	U
21	AA	424	G
21	AA	429	U
21	AA	461	A
21	AA	462	G
21	AA	466	A
21	AA	467	U
21	AA	478	A
21	AA	479	U
21	AA	482	A
21	AA	483	C
21	AA	484	G
21	AA	485	U
21	AA	486	U
21	AA	505	G
21	AA	511	C
21	AA	518	C
21	AA	519	C
21	AA	527	G
21	AA	532	A
21	AA	533	A
21	AA	547	A
21	AA	559	A
21	AA	560	A
21	AA	564	C
21	AA	565	U
21	AA	566	G
21	AA	567	G
21	AA	569	C

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Mol	Chain	Res	Type
21	AA	570	G
21	AA	571	U
21	AA	572	A
21	AA	575	G
21	AA	576	C
21	AA	577	G
21	AA	598	U
21	AA	611	C
21	AA	612	C
21	AA	622	A
21	AA	628	G
21	AA	633	G
21	AA	641	U
21	AA	642	A
21	AA	643	C
21	AA	649	A
21	AA	665	A
21	AA	674	G
21	AA	675	A
21	AA	685	G
21	AA	688	G
21	AA	700	G
21	AA	702	A
21	AA	718	A
21	AA	719	C
21	AA	729	A
21	AA	751	U
21	AA	752	G
21	AA	755	G
21	AA	756	C
21	AA	767	A
21	AA	777	A
21	AA	778	G
21	AA	779	C
21	AA	787	A
21	AA	793	U
21	AA	794	A
21	AA	803	G
21	AA	812	G
21	AA	817	C
21	AA	819	A
21	AA	820	U

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Mol	Chain	Res	Type
21	AA	821	G
21	AA	828	U
21	AA	842	U
21	AA	843	U
21	AA	846	G
21	AA	867	G
21	AA	873	A
21	AA	884	U
21	AA	885	G
21	AA	889	A
21	AA	907	A
21	AA	908	A
21	AA	914	A
21	AA	920	U
21	AA	927	G
21	AA	934	C
21	AA	940	C
21	AA	941	G
21	AA	948	C
21	AA	960	U
21	AA	961	U
21	AA	966	G
21	AA	968	A
21	AA	969	A
21	AA	974	A
21	AA	975	A
21	AA	976	G
21	AA	977	A
21	AA	978	A
21	AA	979	C
21	AA	981	U
21	AA	982	U
21	AA	983	A
21	AA	984	C
21	AA	990	C
21	AA	991	U
21	AA	992	U
21	AA	993	G
21	AA	995	C
21	AA	996	A
21	AA	1004	A
21	AA	1017	U

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Mol	Chain	Res	Type
21	AA	1025	U
21	AA	1026	G
21	AA	1030	U
21	AA	1032	G
21	AA	1037	C
21	AA	1050	G
21	AA	1051	C
21	AA	1054	C
21	AA	1055	A
21	AA	1056	U
21	AA	1065	U
21	AA	1073	U
21	AA	1094	G
21	AA	1101	A
21	AA	1102	A
21	AA	1123	U
21	AA	1124	G
21	AA	1125	U
21	AA	1126	U
21	AA	1129	C
21	AA	1130	A
21	AA	1136	C
21	AA	1139	G
21	AA	1140	C
21	AA	1182	G
21	AA	1189	U
21	AA	1191	A
21	AA	1195	C
21	AA	1196	A
21	AA	1202	U
21	AA	1203	C
21	AA	1204	A
21	AA	1211	U
21	AA	1212	U
21	AA	1217	C
21	AA	1222	G
21	AA	1227	A
21	AA	1233	G
21	AA	1234	C
21	AA	1238	A
21	AA	1256	A
21	AA	1258	G

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Mol	Chain	Res	Type
21	AA	1268	G
21	AA	1274	A
21	AA	1280	A
21	AA	1281	C
21	AA	1285	A
21	AA	1286	U
21	AA	1298	U
21	AA	1299	A
21	AA	1300	G
21	AA	1302	C
21	AA	1303	C
21	AA	1308	U
21	AA	1312	G
21	AA	1317	C
21	AA	1318	A
21	AA	1319	A
21	AA	1330	U
21	AA	1331	G
21	AA	1335	U
21	AA	1336	C
21	AA	1338	G
21	AA	1340	A
21	AA	1345	U
21	AA	1358	U
21	AA	1359	C
21	AA	1363	A
21	AA	1364	U
21	AA	1365	G
21	AA	1374	A
21	AA	1375	A
21	AA	1378	C
21	AA	1382	C
21	AA	1384	C
21	AA	1385	G
21	AA	1394	A
21	AA	1397	C
21	AA	1398	A
21	AA	1400	C
21	AA	1401	G
21	AA	1414	U
21	AA	1445	U
21	AA	1446	A

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Mol	Chain	Res	Type
21	AA	1447	A
21	AA	1448	C
21	AA	1451	U
21	AA	1452	C
21	AA	1453	G
21	AA	1469	C
21	AA	1492	A
21	AA	1493	A
21	AA	1494	G
21	AA	1502	A
21	AA	1503	A
21	AA	1506	U
21	AA	1507	A
21	AA	1520	C
21	AA	1529	G
21	AA	1530	G
21	AA	1534	A
22	A1	16	C
22	A1	18	G
22	A1	20	G
22	A1	46	7MG
22	A1	47	U
22	A1	48	C
22	A1	49	G
22	A1	75	C
22	A1	76	A
23	A2	81	U
23	A2	82	A
23	A2	83	U
23	A2	84	G
23	A2	86	U
23	A2	87	U
23	A2	88	U
23	A2	92	U
23	A2	93	U
24	A3	16	C
24	A3	17	C
24	A3	18	U
24	A3	19	G
24	A3	20	G
24	A3	21	H2U
24	A3	22	A

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Mol	Chain	Res	Type
24	A3	26	C
24	A3	32	G
24	A3	33	OMC
24	A3	48	U
24	A3	49	C
24	A3	61	U
24	A3	62	C
24	A3	72	C
24	A3	73	A
24	A3	75	C
24	A3	76	C
24	A3	77	A
54	BA	15	G
54	BA	33	C
54	BA	34	U
54	BA	35	G
54	BA	45	G
54	BA	46	G
54	BA	50	U
54	BA	51	G
54	BA	62	U
54	BA	71	A
54	BA	72	U
54	BA	74	A
54	BA	75	G
54	BA	83	A
54	BA	84	A
54	BA	85	G
54	BA	101	A
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	126	A
54	BA	128	C
54	BA	142	A
54	BA	143	C
54	BA	144	A
54	BA	145	C
54	BA	146	A
54	BA	147	C

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Mol	Chain	Res	Type
54	BA	161	A
54	BA	163	C
54	BA	164	C
54	BA	196	A
54	BA	199	A
54	BA	200	U
54	BA	204	A
54	BA	205	G
54	BA	216	A
54	BA	222	A
54	BA	245	G
54	BA	248	G
54	BA	249	C
54	BA	272	A
54	BA	273	G
54	BA	277	G
54	BA	278	A
54	BA	281	C
54	BA	294	A
54	BA	295	G
54	BA	300	A
54	BA	301	G
54	BA	302	C
54	BA	316	C
54	BA	323	C
54	BA	324	A
54	BA	330	A
54	BA	331	C
54	BA	332	A
54	BA	335	C
54	BA	346	A
54	BA	347	A
54	BA	370	G
54	BA	374	A
54	BA	376	G
54	BA	377	G
54	BA	383	C
54	BA	386	G
54	BA	387	U
54	BA	388	G
54	BA	404	A
54	BA	405	U

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Mol	Chain	Res	Type
54	BA	411	G
54	BA	428	A
54	BA	435	C
54	BA	451	U
54	BA	453	A
54	BA	454	A
54	BA	457	A
54	BA	473	G
54	BA	478	A
54	BA	479	A
54	BA	484	C
54	BA	490	C
54	BA	491	G
54	BA	504	A
54	BA	505	A
54	BA	508	A
54	BA	510	C
54	BA	512	G
54	BA	527	C
54	BA	528	A
54	BA	531	C
54	BA	546	U
54	BA	547	A
54	BA	548	G
54	BA	549	G
54	BA	556	A
54	BA	562	U
54	BA	573	U
54	BA	575	A
54	BA	586	A
54	BA	603	A
54	BA	613	A
54	BA	614	A
54	BA	615	U
54	BA	616	A
54	BA	617	G
54	BA	627	A
54	BA	628	G
54	BA	631	A
54	BA	632	A
54	BA	637	A
54	BA	644	A

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Mol	Chain	Res	Type
54	BA	645	C
54	BA	646	U
54	BA	647	G
54	BA	653	U
54	BA	654	A
54	BA	671	C
54	BA	672	C
54	BA	686	U
54	BA	716	A
54	BA	719	C
54	BA	724	U
54	BA	727	A
54	BA	728	G
54	BA	730	A
54	BA	745	G
54	BA	747	U
54	BA	748	G
54	BA	750	A
54	BA	751	A
54	BA	764	A
54	BA	775	G
54	BA	776	G
54	BA	782	A
54	BA	784	G
54	BA	785	G
54	BA	789	A
54	BA	791	C
54	BA	800	A
54	BA	805	G
54	BA	821	A
54	BA	822	G
54	BA	827	U
54	BA	830	G
54	BA	846	U
54	BA	860	U
54	BA	866	A
54	BA	867	C
54	BA	888	C
54	BA	889	C
54	BA	890	C
54	BA	893	C
54	BA	897	C

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Mol	Chain	Res	Type
54	BA	905	A
54	BA	910	A
54	BA	914	G
54	BA	915	C
54	BA	933	A
54	BA	934	U
54	BA	943	A
54	BA	945	A
54	BA	958	U
54	BA	961	C
54	BA	974	G
54	BA	981	A
54	BA	982	C
54	BA	983	A
54	BA	987	C
54	BA	990	A
54	BA	996	A
54	BA	1005	C
54	BA	1006	C
54	BA	1011	G
54	BA	1012	U
54	BA	1013	C
54	BA	1024	G
54	BA	1025	G
54	BA	1026	G
54	BA	1057	A
54	BA	1058	U
54	BA	1070	A
54	BA	1071	G
54	BA	1073	A
54	BA	1076	C
54	BA	1079	C
54	BA	1088	A
54	BA	1089	A
54	BA	1093	G
54	BA	1094	U
54	BA	1095	A
54	BA	1096	A
54	BA	1097	U
54	BA	1112	G
54	BA	1127	A
54	BA	1128	G

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Mol	Chain	Res	Type
54	BA	1130	U
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1139	G
54	BA	1142	A
54	BA	1155	A
54	BA	1156	A
54	BA	1186	G
54	BA	1204	A
54	BA	1205	A
54	BA	1206	G
54	BA	1211	C
54	BA	1237	A
54	BA	1238	G
54	BA	1242	U
54	BA	1243	C
54	BA	1251	C
54	BA	1252	G
54	BA	1253	A
54	BA	1255	U
54	BA	1256	G
54	BA	1263	U
54	BA	1271	G
54	BA	1273	U
54	BA	1274	A
54	BA	1275	A
54	BA	1276	A
54	BA	1287	A
54	BA	1288	G
54	BA	1289	C
54	BA	1290	C
54	BA	1292	G
54	BA	1301	A
54	BA	1304	A
54	BA	1311	G
54	BA	1312	U
54	BA	1313	U
54	BA	1314	C
54	BA	1320	C
54	BA	1321	A
54	BA	1324	G

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Mol	Chain	Res	Type
54	BA	1325	U
54	BA	1332	G
54	BA	1334	G
54	BA	1341	G
54	BA	1360	G
54	BA	1365	A
54	BA	1368	G
54	BA	1379	U
54	BA	1383	A
54	BA	1385	A
54	BA	1388	G
54	BA	1397	U
54	BA	1398	C
54	BA	1416	G
54	BA	1427	A
54	BA	1428	C
54	BA	1435	G
54	BA	1440	U
54	BA	1452	G
54	BA	1454	C
54	BA	1455	G
54	BA	1458	U
54	BA	1460	U
54	BA	1475	G
54	BA	1482	G
54	BA	1486	U
54	BA	1493	C
54	BA	1508	A
54	BA	1523	U
54	BA	1536	C
54	BA	1538	G
54	BA	1560	G
54	BA	1566	A
54	BA	1567	G
54	BA	1569	A
54	BA	1585	C
54	BA	1598	A
54	BA	1607	C
54	BA	1608	A
54	BA	1614	A
54	BA	1616	A
54	BA	1618	A

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Mol	Chain	Res	Type
54	BA	1619	G
54	BA	1622	G
54	BA	1629	U
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1665	A
54	BA	1670	C
54	BA	1674	G
54	BA	1696	G
54	BA	1707	G
54	BA	1711	A
54	BA	1712	U
54	BA	1717	A
54	BA	1730	C
54	BA	1738	G
54	BA	1739	A
54	BA	1764	C
54	BA	1773	A
54	BA	1775	U
54	BA	1782	U
54	BA	1784	A
54	BA	1790	C
54	BA	1800	C
54	BA	1801	A
54	BA	1808	A
54	BA	1811	G
54	BA	1815	A
54	BA	1817	G
54	BA	1821	A
54	BA	1828	G
54	BA	1829	A
54	BA	1847	A
54	BA	1870	C
54	BA	1871	A
54	BA	1903	G
54	BA	1906	G
54	BA	1913	A
54	BA	1914	C
54	BA	1919	A
54	BA	1937	A
54	BA	1938	A

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Mol	Chain	Res	Type
54	BA	1939	U
54	BA	1940	U
54	BA	1945	G
54	BA	1946	U
54	BA	1955	U
54	BA	1963	U
54	BA	1965	C
54	BA	1969	A
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1981	A
54	BA	1982	U
54	BA	1993	U
54	BA	1997	C
54	BA	2006	C
54	BA	2021	C
54	BA	2023	C
54	BA	2030	A
54	BA	2031	A
54	BA	2032	G
54	BA	2033	A
54	BA	2034	U
54	BA	2035	G
54	BA	2043	C
54	BA	2049	G
54	BA	2052	A
54	BA	2055	C
54	BA	2060	A
54	BA	2061	G
54	BA	2076	U
54	BA	2077	A
54	BA	2092	U
54	BA	2112	G
54	BA	2113	U
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	2155	U

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Mol	Chain	Res	Type
54	BA	2156	G
54	BA	2157	G
54	BA	2159	G
54	BA	2160	C
54	BA	2172	U
54	BA	2173	A
54	BA	2174	C
54	BA	2194	U
54	BA	2198	A
54	BA	2203	U
54	BA	2208	C
54	BA	2211	A
54	BA	2212	A
54	BA	2213	U
54	BA	2225	A
54	BA	2232	C
54	BA	2233	U
54	BA	2237	G
54	BA	2238	G
54	BA	2239	G
54	BA	2245	U
54	BA	2250	G
54	BA	2259	U
54	BA	2262	U
54	BA	2283	C
54	BA	2307	G
54	BA	2308	G
54	BA	2309	A
54	BA	2310	C
54	BA	2320	U
54	BA	2325	G
54	BA	2333	A
54	BA	2334	U
54	BA	2335	A
54	BA	2339	C
54	BA	2345	G
54	BA	2346	A
54	BA	2347	C
54	BA	2353	G
54	BA	2383	G
54	BA	2385	C
54	BA	2403	C

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Mol	Chain	Res	Type
54	BA	2407	A
54	BA	2418	A
54	BA	2422	C
54	BA	2423	U
54	BA	2424	C
54	BA	2425	A
54	BA	2426	A
54	BA	2427	C
54	BA	2428	G
54	BA	2430	A
54	BA	2439	A
54	BA	2441	U
54	BA	2446	G
54	BA	2447	G
54	BA	2448	A
54	BA	2449	U
54	BA	2476	A
54	BA	2491	U
54	BA	2492	U
54	BA	2494	G
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2505	G
54	BA	2507	C
54	BA	2533	U
54	BA	2539	C
54	BA	2542	A
54	BA	2543	G
54	BA	2554	U
54	BA	2566	A
54	BA	2567	G
54	BA	2573	C
54	BA	2575	C
54	BA	2576	G
54	BA	2585	U
54	BA	2586	U
54	BA	2602	A
54	BA	2603	G
54	BA	2609	U
54	BA	2610	C
54	BA	2614	A

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Mol	Chain	Res	Type
54	BA	2629	U
54	BA	2637	U
54	BA	2640	G
54	BA	2645	G
54	BA	2646	C
54	BA	2656	U
54	BA	2660	A
54	BA	2661	G
54	BA	2665	A
54	BA	2668	G
54	BA	2669	G
54	BA	2684	U
54	BA	2689	U
54	BA	2690	U
54	BA	2712	C
54	BA	2726	A
54	BA	2746	U
54	BA	2756	U
54	BA	2765	A
54	BA	2766	A
54	BA	2778	A
54	BA	2782	G
54	BA	2783	U
54	BA	2797	U
54	BA	2798	U
54	BA	2799	A
54	BA	2800	A
54	BA	2817	U
54	BA	2823	A
54	BA	2850	A
54	BA	2858	C
54	BA	2859	G
54	BA	2868	A
54	BA	2884	U
54	BA	2886	A
54	BA	2895	G
55	BB	6	G
55	BB	7	G
55	BB	14	U
55	BB	15	A
55	BB	25	U
55	BB	36	C

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Mol	Chain	Res	Type
55	BB	42	C
55	BB	45	A
55	BB	48	U
55	BB	51	G
55	BB	67	G
55	BB	86	G
55	BB	88	C
55	BB	89	U
55	BB	90	C
55	BB	109	A

All (235) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	13	U
21	AA	30	U
21	AA	54	C
21	AA	64	G
21	AA	85	U
21	AA	110	C
21	AA	120	A
21	AA	130	A
21	AA	208	U
21	AA	236	A
21	AA	250	A
21	AA	251	G
21	AA	266	G
21	AA	315	A
21	AA	345	C
21	AA	354	G
21	AA	369	G
21	AA	420	U
21	AA	429	U
21	AA	461	A
21	AA	465	A
21	AA	466	A
21	AA	478	A
21	AA	482	A
21	AA	485	U

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Mol	Chain	Res	Type
21	AA	505	G
21	AA	518	C
21	AA	532	A
21	AA	570	G
21	AA	575	G
21	AA	576	C
21	AA	611	C
21	AA	641	U
21	AA	642	A
21	AA	674	G
21	AA	701	U
21	AA	718	A
21	AA	719	C
21	AA	725	G
21	AA	751	U
21	AA	755	G
21	AA	778	G
21	AA	820	U
21	AA	872	A
21	AA	884	U
21	AA	907	A
21	AA	919	A
21	AA	934	C
21	AA	960	U
21	AA	974	A
21	AA	977	A
21	AA	982	U
21	AA	983	A
21	AA	991	U
21	AA	1025	U
21	AA	1050	G
21	AA	1054	C
21	AA	1065	U
21	AA	1094	G
21	AA	1101	A
21	AA	1123	U
21	AA	1125	U
21	AA	1129	C
21	AA	1137	C
21	AA	1139	G
21	AA	1190	G
21	AA	1195	C

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Mol	Chain	Res	Type
21	AA	1201	A
21	AA	1203	C
21	AA	1211	U
21	AA	1226	C
21	AA	1233	G
21	AA	1257	A
21	AA	1280	A
21	AA	1298	U
21	AA	1302	C
21	AA	1330	U
21	AA	1335	U
21	AA	1358	U
21	AA	1374	A
21	AA	1377	A
21	AA	1382	C
21	AA	1384	C
21	AA	1397	C
21	AA	1399	C
21	AA	1445	U
21	AA	1452	C
21	AA	1492	A
21	AA	1504	G
22	A1	46	7MG
22	A1	48	C
22	A1	74	C
22	A1	75	C
23	A2	83	U
23	A2	86	U
24	A3	17	C
24	A3	19	G
24	A3	48	U
24	A3	61	U
24	A3	72	C
24	A3	75	C
54	BA	33	C
54	BA	34	U
54	BA	49	A
54	BA	70	G
54	BA	74	A
54	BA	83	A
54	BA	118	A
54	BA	143	C

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Mol	Chain	Res	Type
54	BA	163	C
54	BA	177	G
54	BA	196	A
54	BA	199	A
54	BA	265	A
54	BA	272	A
54	BA	301	G
54	BA	323	C
54	BA	330	A
54	BA	332	A
54	BA	346	A
54	BA	376	G
54	BA	382	A
54	BA	387	U
54	BA	457	A
54	BA	481	G
54	BA	490	C
54	BA	497	A
54	BA	527	C
54	BA	531	C
54	BA	547	A
54	BA	548	G
54	BA	574	A
54	BA	627	A
54	BA	631	A
54	BA	645	C
54	BA	670	A
54	BA	747	U
54	BA	750	A
54	BA	821	A
54	BA	892	A
54	BA	909	A
54	BA	914	G
54	BA	933	A
54	BA	981	A
54	BA	1057	A
54	BA	1070	A
54	BA	1093	G
54	BA	1096	A
54	BA	1126	A
54	BA	1205	A
54	BA	1209	U

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Mol	Chain	Res	Type
54	BA	1210	G
54	BA	1242	U
54	BA	1272	A
54	BA	1275	A
54	BA	1286	A
54	BA	1289	C
54	BA	1313	U
54	BA	1320	C
54	BA	1324	G
54	BA	1378	A
54	BA	1397	U
54	BA	1420	A
54	BA	1427	A
54	BA	1451	C
54	BA	1485	U
54	BA	1559	U
54	BA	1566	A
54	BA	1606	C
54	BA	1609	A
54	BA	1616	A
54	BA	1646	C
54	BA	1647	U
54	BA	1664	A
54	BA	1699	G
54	BA	1706	C
54	BA	1738	G
54	BA	1789	A
54	BA	1799	G
54	BA	1800	C
54	BA	1828	G
54	BA	1912	A
54	BA	1913	A
54	BA	1930	G
54	BA	1936	A
54	BA	1938	A
54	BA	1939	U
54	BA	1944	U
54	BA	1945	G
54	BA	1981	A
54	BA	2015	A
54	BA	2032	G
54	BA	2033	A

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Mol	Chain	Res	Type
54	BA	2034	U
54	BA	2048	G
54	BA	2060	A
54	BA	2117	A
54	BA	2126	A
54	BA	2155	U
54	BA	2172	U
54	BA	2197	U
54	BA	2198	A
54	BA	2211	A
54	BA	2225	A
54	BA	2232	C
54	BA	2237	G
54	BA	2238	G
54	BA	2258	C
54	BA	2286	G
54	BA	2307	G
54	BA	2345	G
54	BA	2422	C
54	BA	2423	U
54	BA	2425	A
54	BA	2429	G
54	BA	2430	A
54	BA	2489	U
54	BA	2501	C
54	BA	2542	A
54	BA	2566	A
54	BA	2585	U
54	BA	2602	A
54	BA	2636	C
54	BA	2646	C
54	BA	2690	U
54	BA	2782	G
54	BA	2797	U
54	BA	2885	G
55	BB	6	G
55	BB	14	U
55	BB	57	A
55	BB	88	C

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	5MU	A1	54	22	19,22,23	0.79	0	27,32,35	1.25	3 (11%)
24	PSU	A3	56	24	18,21,22	0.85	0	21,30,33	1.27	2 (9%)
24	H2U	A3	21	24	18,21,22	1.41	2 (11%)	19,30,33	1.51	3 (15%)
22	4SU	A1	7	22	18,21,22	1.47	2 (11%)	25,30,33	0.85	0
22	6MZ	A1	37	22	22,25,26	0.69	0	29,36,39	1.26	3 (10%)
22	PSU	A1	55	22	18,21,22	0.81	0	21,30,33	1.12	3 (14%)
22	CM0	A1	34	22	21,26,27	1.27	2 (9%)	26,37,40	1.43	3 (11%)
24	5MU	A3	55	24	19,22,23	0.73	0	27,32,35	1.33	4 (14%)
24	4SU	A3	8	24	18,21,22	1.42	1 (5%)	25,30,33	0.90	1 (4%)
24	OMC	A3	33	24	19,22,23	0.75	0	25,31,34	1.06	1 (4%)
22	7MG	A1	46	22	23,26,27	3.98	2 (8%)	27,39,42	1.58	2 (7%)

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	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
24	PSU	A3	56	24	-	2/7/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2
22	6MZ	A1	37	22	-	2/9/27/28	0/3/3/3
22	PSU	A1	55	22	-	1/7/25/26	0/2/2/2
22	CM0	A1	34	22	-	2/12/30/31	0/2/2/2
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	4/7/25/26	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-18.65	1.33	1.45
24	A3	8	4SU	C5-C4	-5.15	1.36	1.42
22	A1	7	4SU	C5-C4	-5.10	1.36	1.42
22	A1	34	CM0	O5-C5	-4.57	1.26	1.36
24	A3	21	H2U	C4-N3	-3.74	1.31	1.37
24	A3	21	H2U	C2-N3	-3.69	1.31	1.38
22	A1	7	4SU	C4-S4	-2.50	1.64	1.68
22	A1	46	7MG	C8-N7	-2.33	1.31	1.42
22	A1	34	CM0	O8-C8	-2.10	1.23	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	5.93	111.77	103.37
22	A1	34	CM0	C7-O5-C5	4.92	123.75	117.48
24	A3	21	H2U	N3-C2-N1	4.29	120.96	116.65
22	A1	37	6MZ	C9-N6-C6	3.88	126.45	122.85
24	A3	55	5MU	C5M-C5-C6	-3.44	118.20	122.85
24	A3	33	OMC	O2-C2-N3	-3.37	117.02	122.33
22	A1	54	5MU	C5M-C5-C6	-3.16	118.58	122.85
24	A3	55	5MU	C6-C5-C4	2.87	120.39	118.02
22	A1	37	6MZ	C4-C5-C6	-2.75	114.49	116.78
22	A1	37	6MZ	C6-C5-N7	2.65	135.32	132.43
22	A1	54	5MU	C6-C5-C4	2.65	120.20	118.02
24	A3	56	PSU	C6-C5-C4	2.59	119.92	118.17
24	A3	8	4SU	C6-C5-C4	2.58	122.19	119.95
22	A1	55	PSU	C6-C5-C4	2.55	119.90	118.17
24	A3	55	5MU	C5M-C5-C4	2.47	121.41	118.78
24	A3	56	PSU	O4'-C1'-C2'	2.38	108.45	105.15
24	A3	21	H2U	O2-C2-N3	-2.35	117.16	121.49
22	A1	34	CM0	O8-C8-O9	-2.28	117.47	123.33
22	A1	54	5MU	C5M-C5-C4	2.28	121.21	118.78
22	A1	55	PSU	O4'-C1'-C2'	2.24	108.26	105.15
22	A1	55	PSU	N1-C2-N3	2.17	117.45	115.17
22	A1	46	7MG	C4'-O4'-C1'	-2.12	104.78	109.47
24	A3	55	5MU	C5-C6-N1	-2.12	121.02	123.31
22	A1	34	CM0	O4'-C4'-C3'	2.04	109.20	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	21	H2U	O4'-C4'-C3'	2.00	109.13	105.15

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	37	6MZ	C5-C6-N6-C9
22	A1	37	6MZ	N1-C6-N6-C9
22	A1	46	7MG	C2'-C1'-N9-C8
24	A3	56	PSU	O4'-C1'-C5-C4
24	A3	56	PSU	O4'-C1'-C5-C6
22	A1	34	CM0	C6-C5-O5-C7
22	A1	34	CM0	C4-C5-O5-C7
24	A3	8	4SU	C2'-C1'-N1-C6
24	A3	8	4SU	O4'-C1'-N1-C6
24	A3	8	4SU	O4'-C1'-N1-C2
22	A1	55	PSU	O4'-C1'-C5-C6
24	A3	8	4SU	C2'-C1'-N1-C2

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	0.60	0	8,9,11	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	VAL	A1	101	22,58	4,6,7	0.82	0	6,7,9	0.93	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	22,58	-	1/5/6/8	-

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	-2.09	119.41	124.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

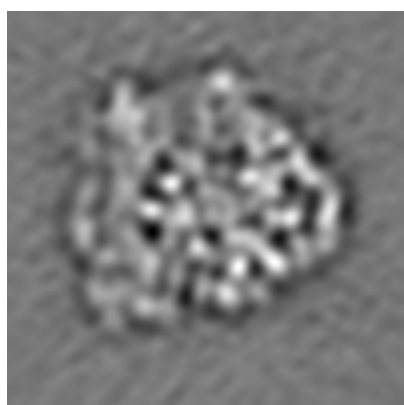
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1723. These allow visual inspection of the internal detail of the map and identification of artifacts.

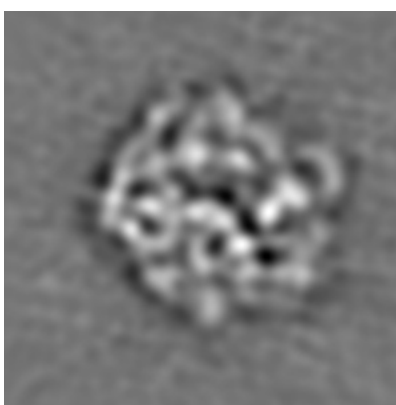
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

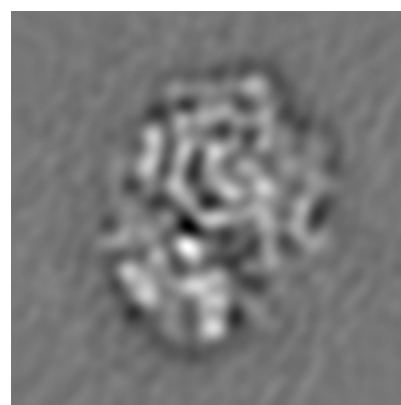
6.1.1 Primary map



X



Y



Z

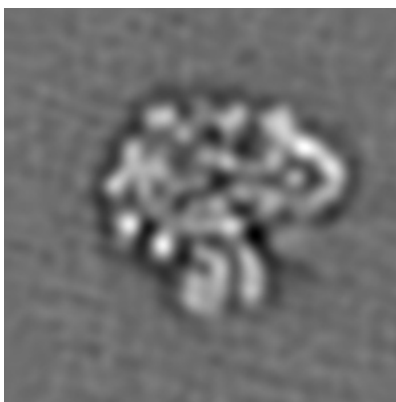
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

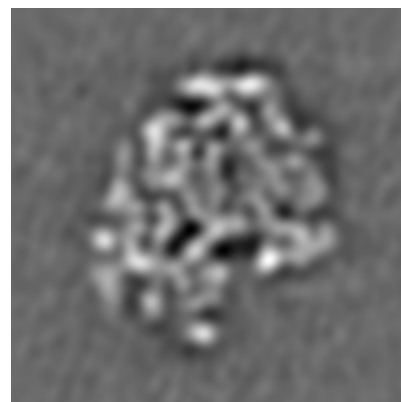
6.2.1 Primary map



X Index: 64



Y Index: 64



Z Index: 64

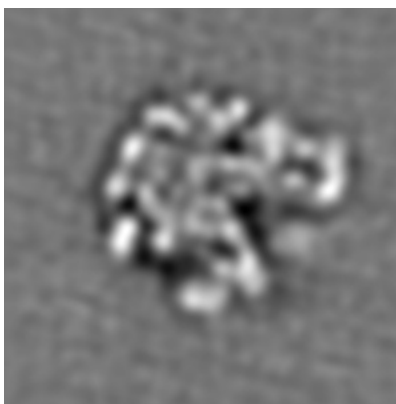
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 64



Y Index: 67

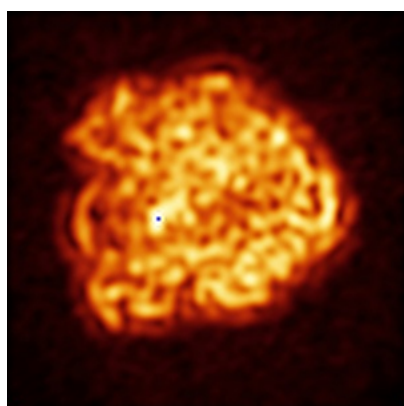


Z Index: 61

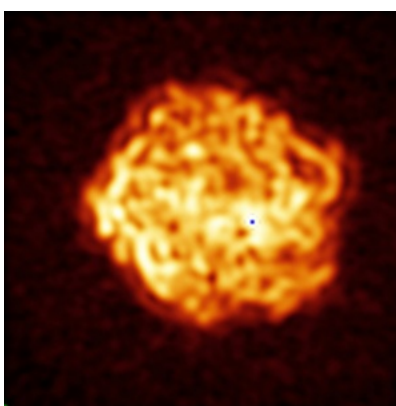
The images above show the largest variance slices of the map in three orthogonal directions.

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

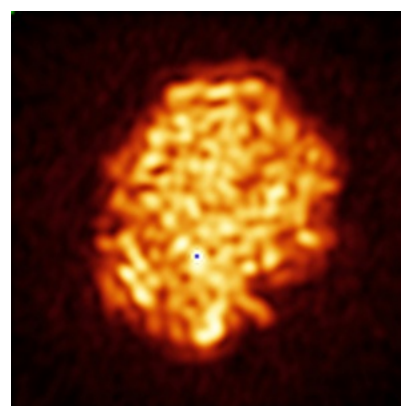
6.4.1 Primary map



X



Y

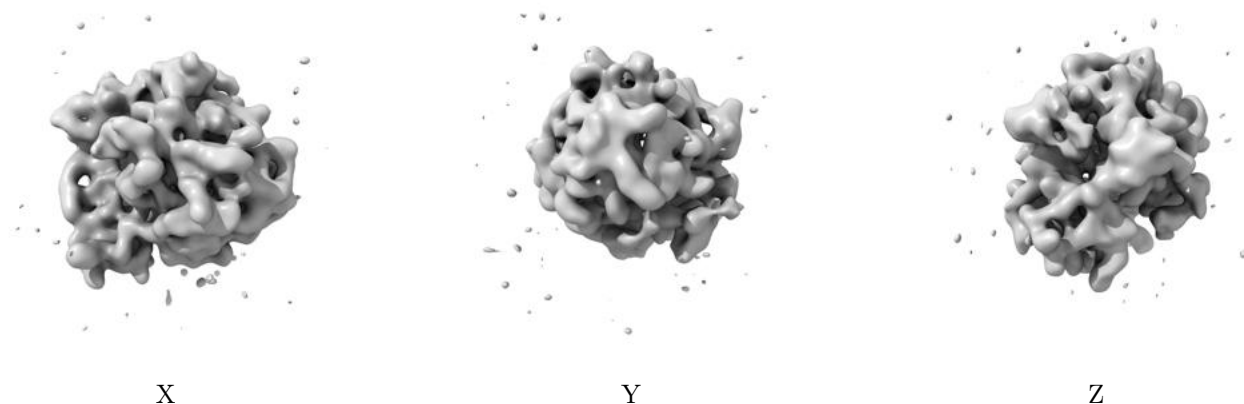


Z

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

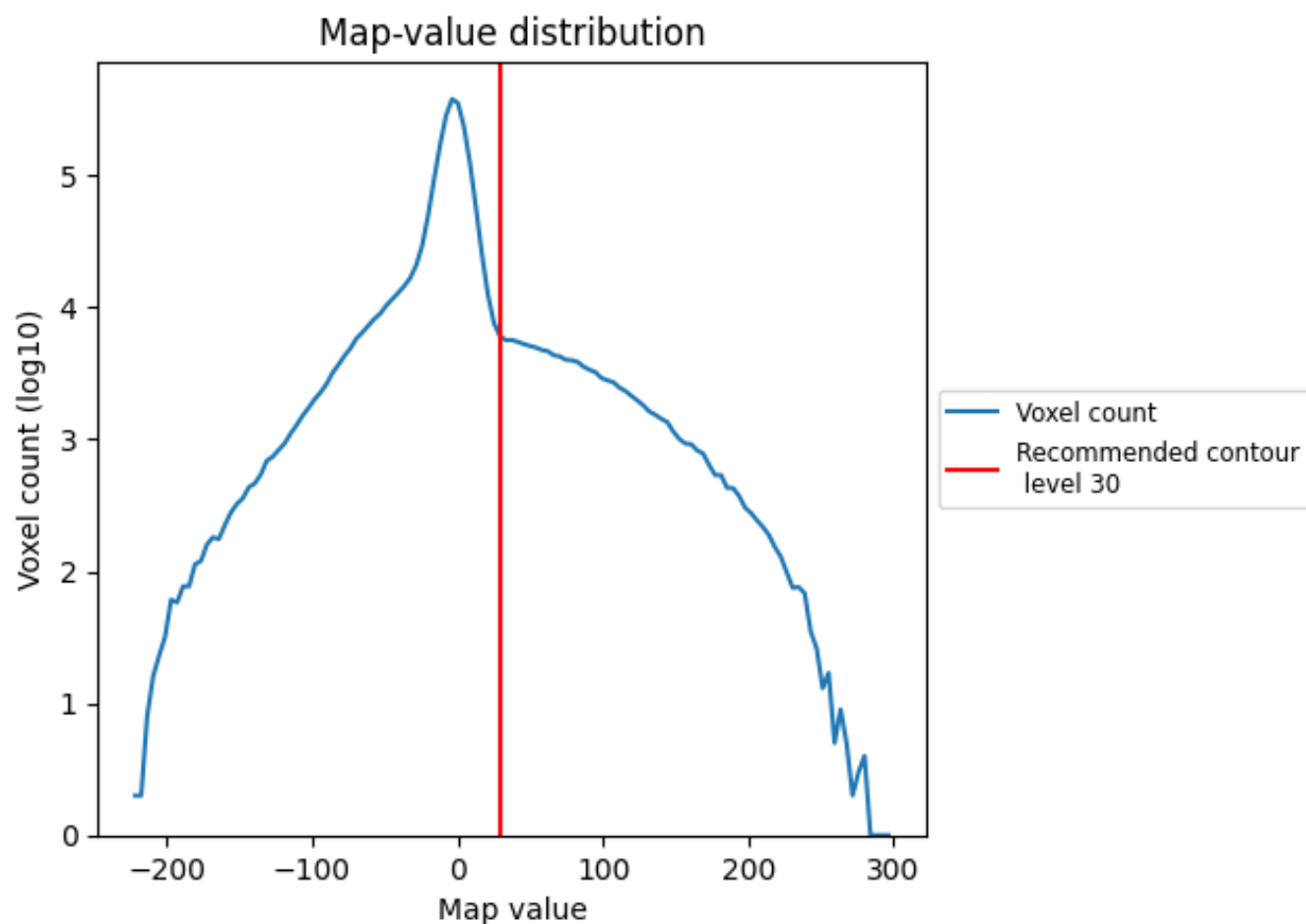
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

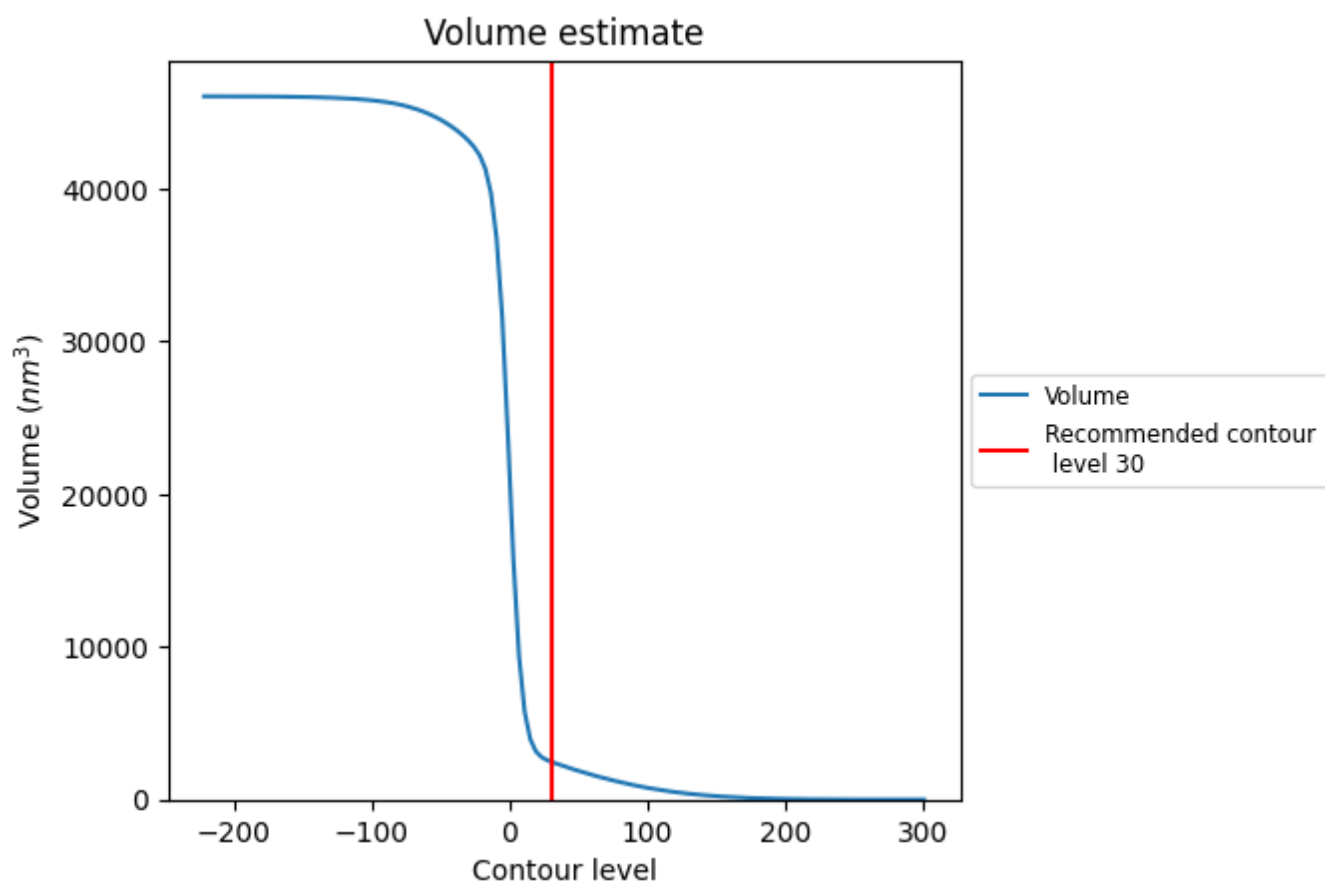
This section contains the results of statistical analysis of the map.

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.

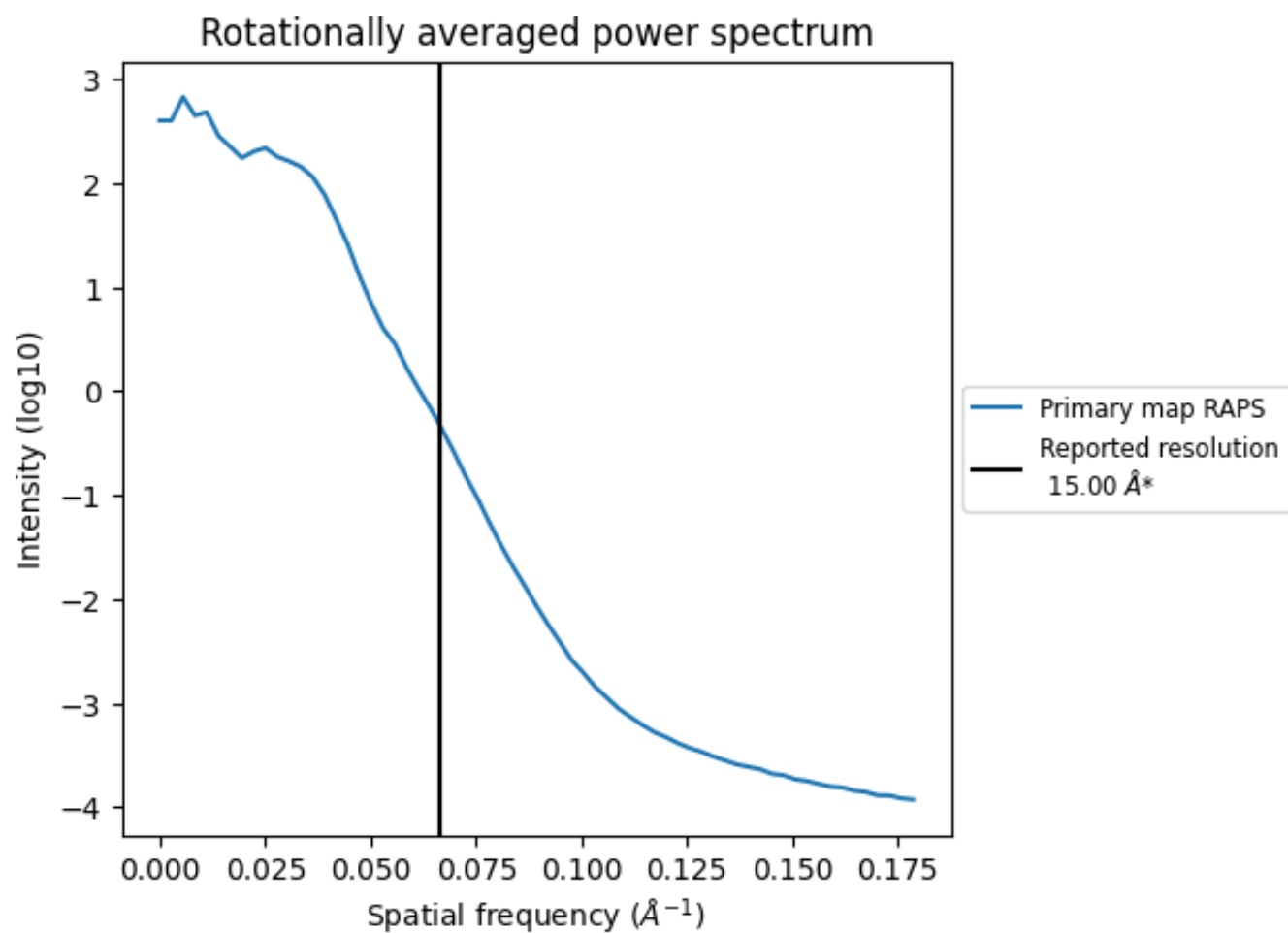
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2478 nm³; this corresponds to an approximate mass of 2238 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.067 Å⁻¹

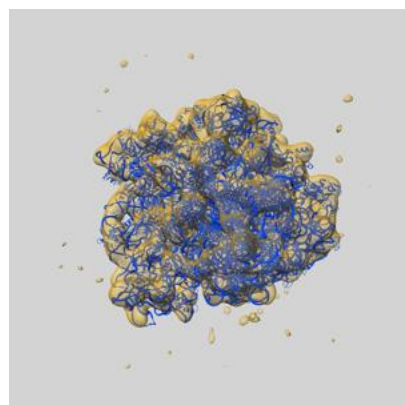
8 Fourier-Shell correlation

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

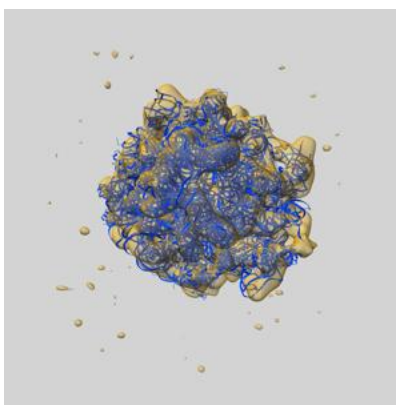
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1723 and PDB model 4V79. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

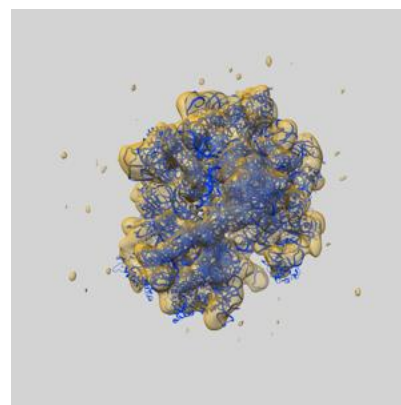
9.1 Map-model overlay [i](#)



X



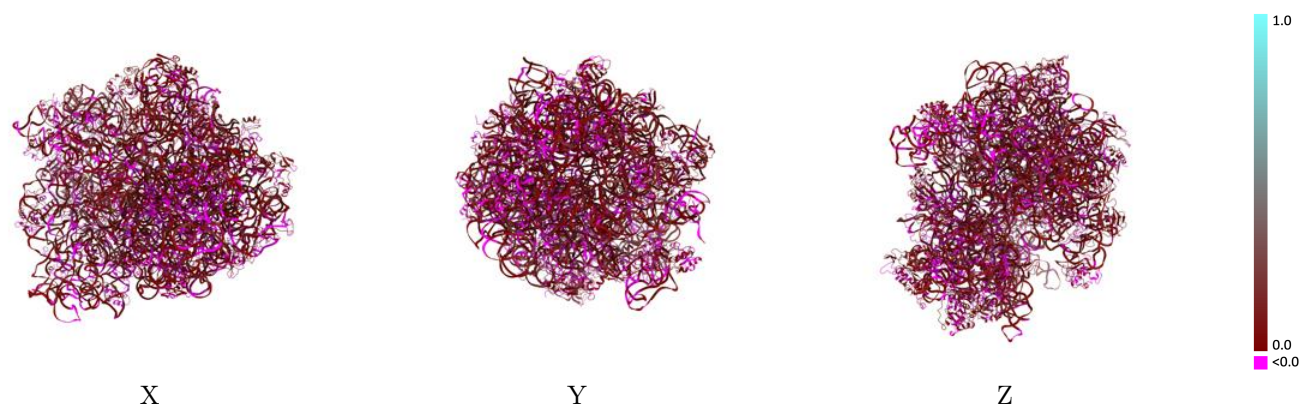
Y



Z

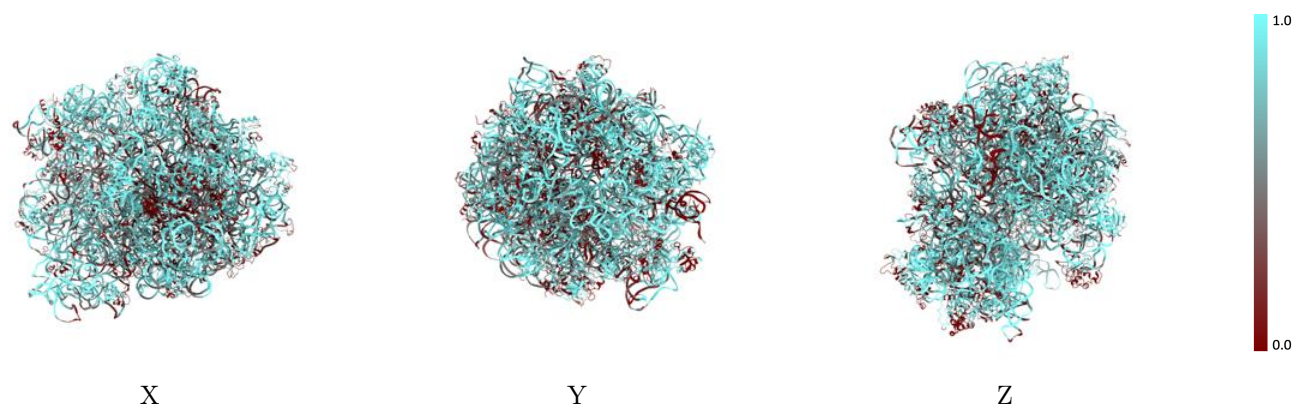
The images above show the 3D surface view of the map at the recommended contour level 30.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



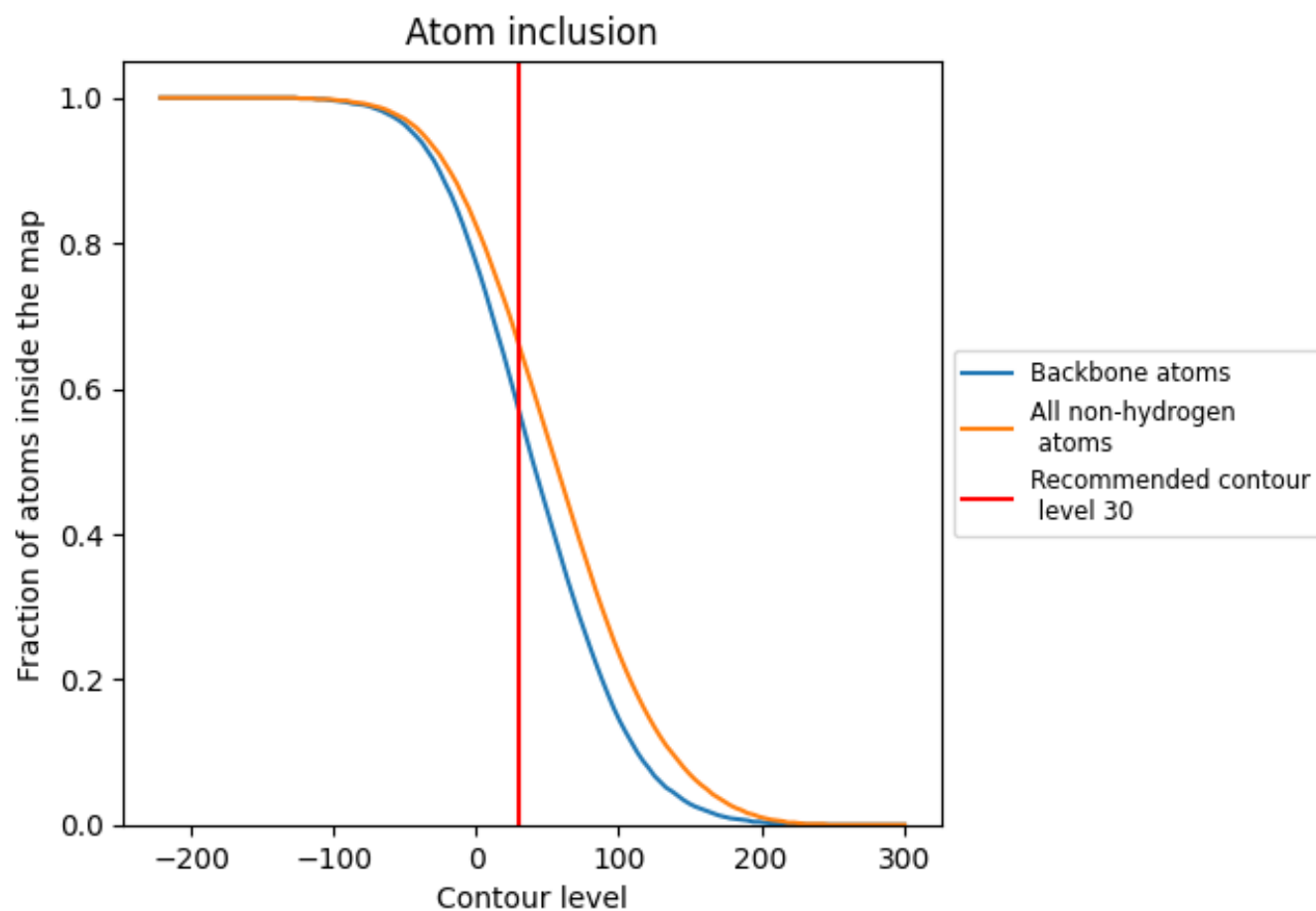
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (30).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 66% 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 (30) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6600	 0.0510
A1	 0.6390	 0.0700
A2	 0.3530	 0.0140
A3	 0.3100	 0.0220
AA	 0.7540	 0.0640
AB	 0.5600	 0.0370
AC	 0.4330	 0.0460
AD	 0.4990	 0.0150
AE	 0.6490	 0.0500
AF	 0.6020	 0.0540
AG	 0.5550	 0.0380
AH	 0.7620	 0.0410
AI	 0.6320	 0.0260
AJ	 0.4460	 -0.0010
AK	 0.5720	 0.0360
AL	 0.5360	 0.0320
AM	 0.8200	 0.0600
AN	 0.5120	 0.0180
AO	 0.7220	 0.0420
AP	 0.4120	 0.0210
AQ	 0.5890	 0.0180
AR	 0.5400	 0.0130
AS	 0.8860	 0.0580
AT	 0.6590	 0.0080
AU	 0.4720	 0.0090
B0	 0.4930	 0.0210
B1	 0.4930	 0.0570
B2	 0.1490	 -0.0430
B3	 0.1390	 -0.0670
B4	 0.7190	 0.0120
B5	 0.4080	 0.0120
BA	 0.7190	 0.0640
BB	 0.8690	 0.0840
BC	 0.3550	 0.0030
BD	 0.4160	 0.0090



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Chain	Atom inclusion	Q-score
BE	 0.6150	 0.0340
BF	 0.6990	 0.0520
BG	 0.7890	 0.0630
BH	 0.3890	 0.0370
BI	 0.1500	 0.0110
BJ	 0.3860	 0.0160
BK	 0.5130	 0.0370
BL	 0.4180	 -0.0250
BM	 0.3790	 0.0090
BN	 0.5290	 0.0030
BO	 0.7150	 0.0200
BP	 0.2840	 -0.0030
BQ	 0.4920	 0.0010
BR	 0.6290	 0.0370
BS	 0.3970	 0.0130
BT	 0.4870	 0.0250
BU	 0.5380	 0.0280
BV	 0.7820	 0.0540
BW	 0.4260	 0.0220
BX	 0.1300	 -0.0330
BY	 0.4330	 0.0270
BZ	 0.5560	 0.0370