



Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 06:40 PM EDT

PDB ID : 4V77 / pdb_00004v77
EMDB ID : EMD-2474
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post2b)
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on : 2013-10-14
Resolution : 17.00 Å(reported)
Based on initial models : 2WRI, 2HGP, 3I1O, 2K4C

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

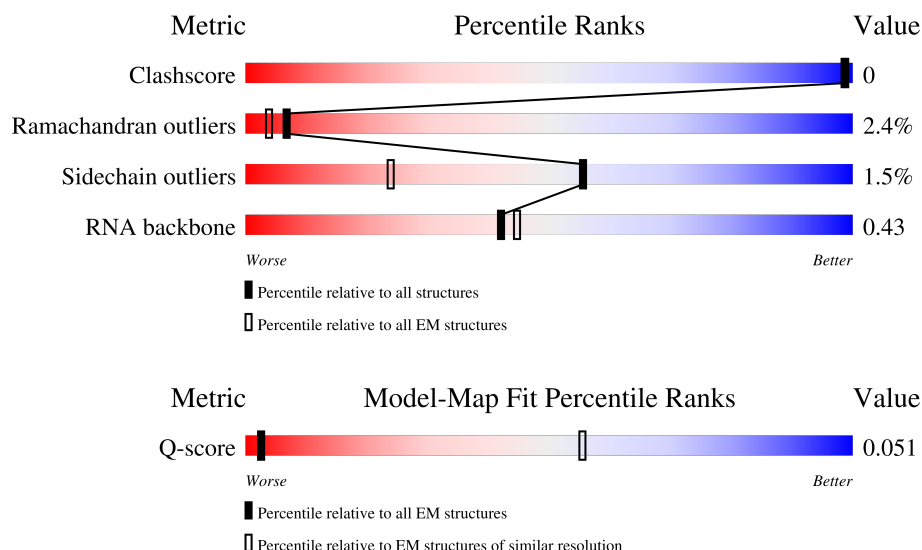
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	38 (16.50 - 17.50)

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

Mol	Chain	Length	Quality of chain
1	AB	220	22% 95% 5%
2	AC	208	36% 96% .
3	AD	206	33% 94% 5%

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Mol	Chain	Length	Quality of chain
4	AE	152	28% 95% 5% .
5	AF	101	38% 93% 7%
6	AG	152	50% 97% ..
7	AH	130	22% 97% ..
8	AI	128	32% 94% 6%
9	AJ	100	30% 93% 7%
10	AK	118	39% 94% . .
11	AL	124	48% 93% 6% .
12	AM	115	41% 94% . . .
13	AN	101	42% 95% . . .
14	AO	89	29% 93% . . .
15	AP	81	23% 98% .
16	AQ	82	44% 95% . . .
17	AR	57	53% 96% .
18	AS	81	38% 96% .
19	AT	86	44% 97% . .
20	AU	53	68% 89% 11%
21	AA	1533	12% 62% 31% 6% .
22	A1	76	20% 61% 36% .
23	A2	15	13% 33% 33% 27% 7%
24	A3	77	31% 58% 35% 5% .
25	BC	273	52% 95% 5%
26	BD	209	38% 93% 7%
27	BE	201	45% 95% 5%
28	BF	179	29% 91% 7% ..

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Mol	Chain	Length	Quality of chain
29	BG	177	29% 96% ..
30	BH	149	68% 97% .
31	BI	142	89% 99% .
32	BJ	142	24% 93% 7%
33	BK	123	46% 92% 8%
34	BL	144	33% 93% 5% ..
35	BM	136	26% 94% 6%
36	BN	121	29% 99% .
37	BO	117	19% 94% 5% .
38	BP	115	27% 93% 6% .
39	BQ	118	34% 97% ..
40	BR	103	36% 96% ..
41	BS	110	43% 97% .
42	BT	94	45% 90% 10%
43	BU	104	44% 89% 10% .
44	BV	94	33% 98% .
45	BW	80	45% 91% 9%
46	BX	79	59% 92% 5% .
47	BY	63	41% 98% .
48	BZ	59	47% 92% 7% .
49	B0	57	39% 93% ..
50	B1	52	40% 96% ..
51	B2	46	67% 96% .
52	B3	65	60% 88% 11% .
53	B4	38	37% 97% .

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Mol	Chain	Length	Quality of chain
54	BA	2903	18% 61% 32% 6%
55	BB	118	7% 72% 24%
56	B5	234	65% 92% 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		

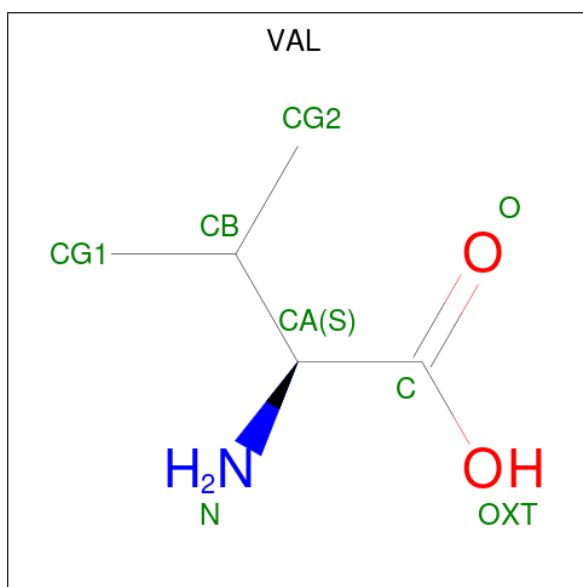
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

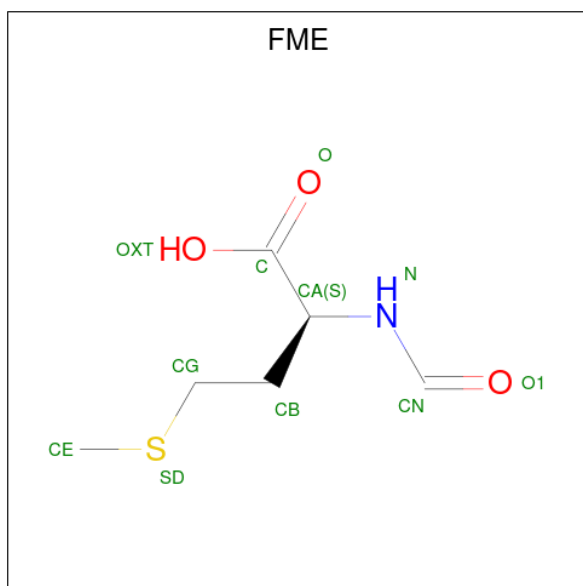
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- 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: $C_6H_{11}NO_3S$).

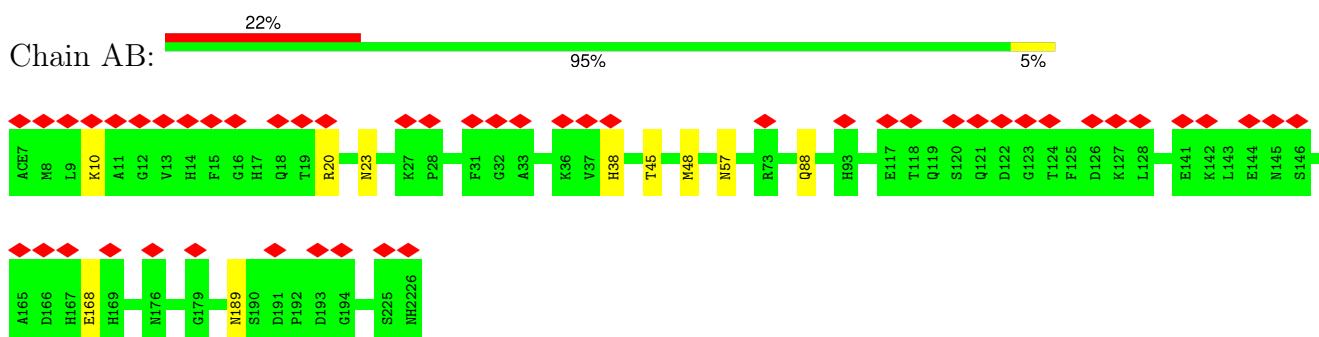


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

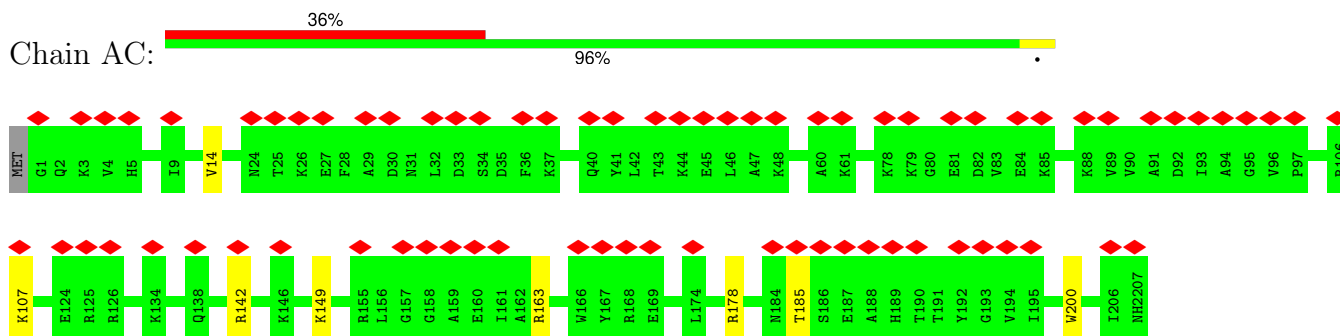
3 Residue-property plots

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

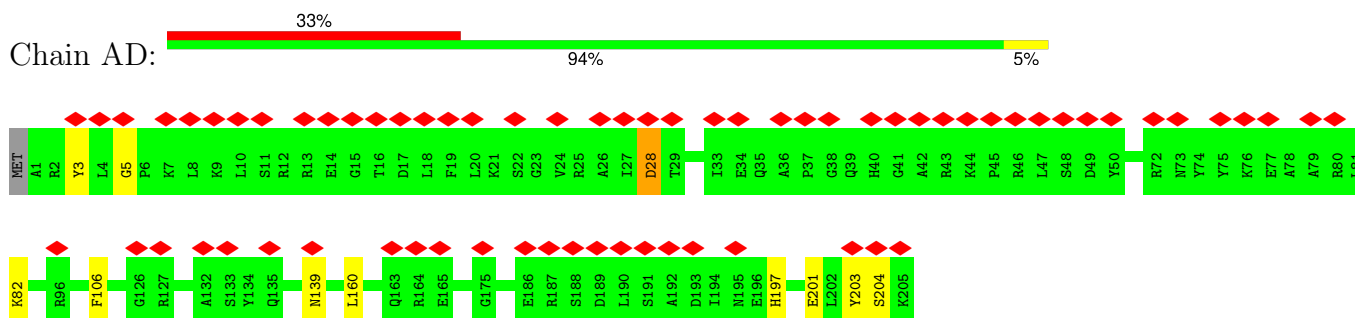
- Molecule 1: 30S ribosomal protein S2



- Molecule 2: 30S ribosomal protein S3

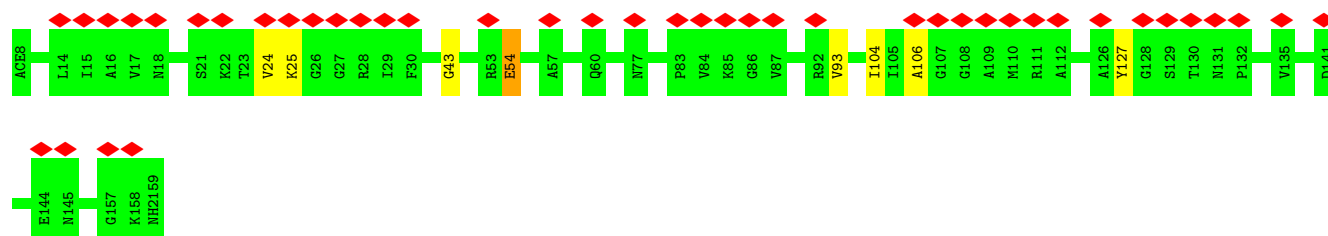


- Molecule 3: 30S ribosomal protein S4

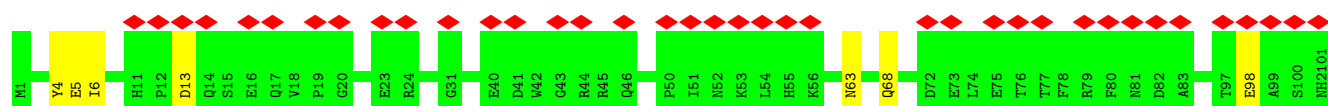
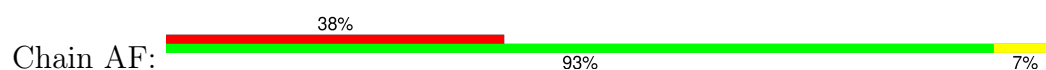


- Molecule 4: 30S ribosomal protein S5

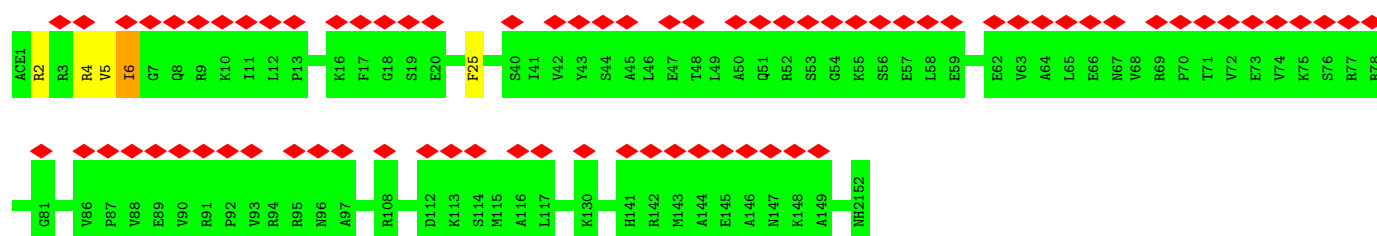




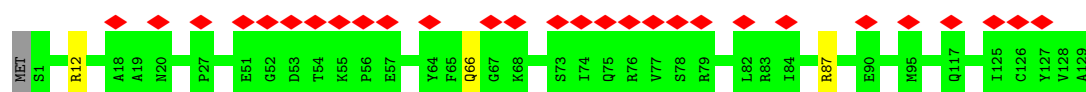
- Molecule 5: 30S ribosomal protein S6



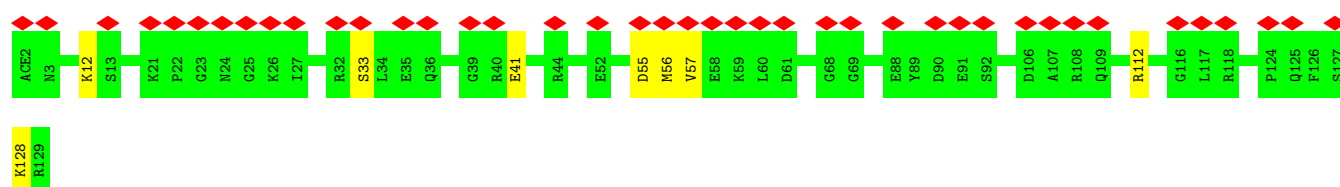
- Molecule 6: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S8

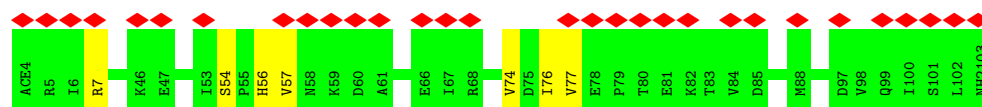


- Molecule 8: 30S ribosomal protein S9

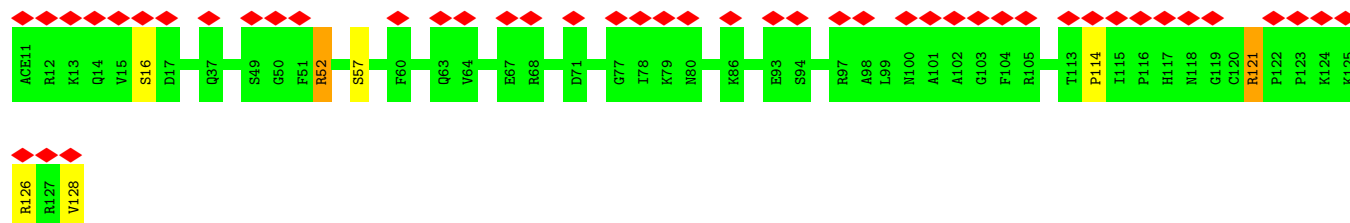
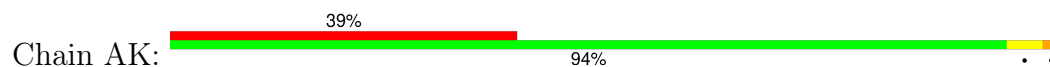


- Molecule 9: 30S ribosomal protein S10

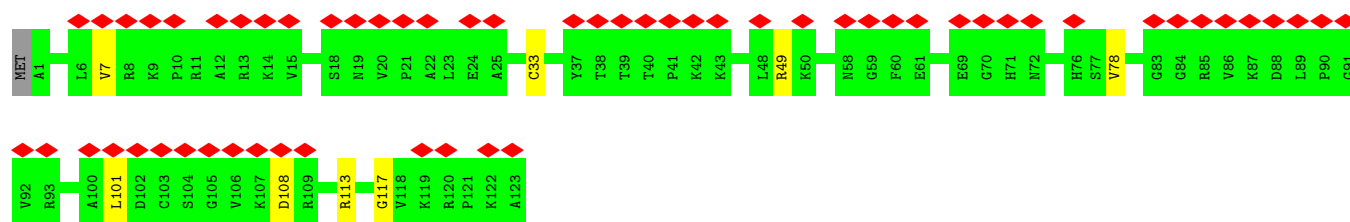




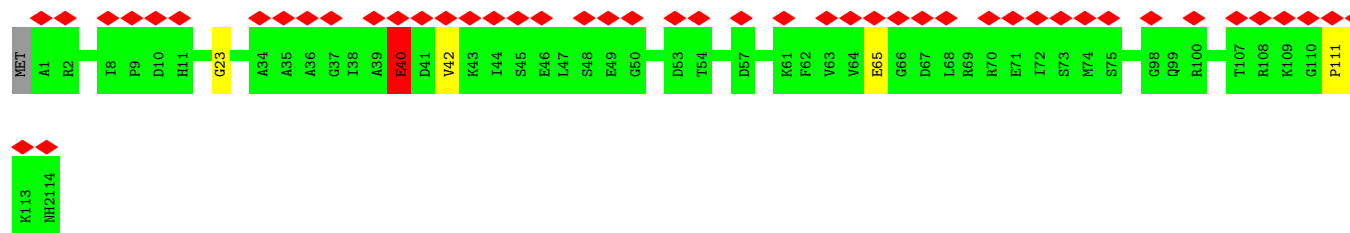
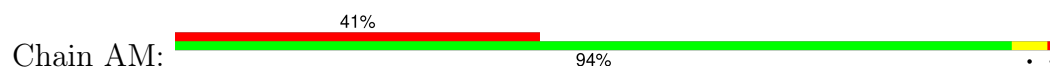
- Molecule 10: 30S ribosomal protein S11



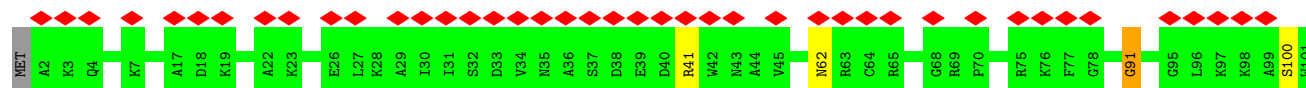
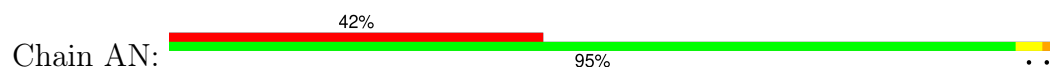
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13

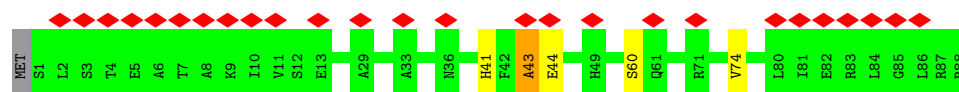


- Molecule 13: 30S ribosomal protein S14

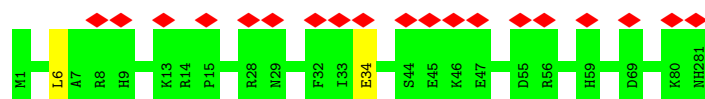


- Molecule 14: 30S ribosomal protein S15

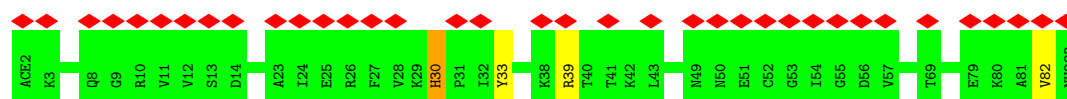




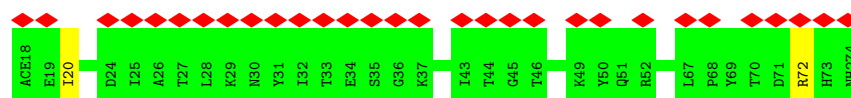
- Molecule 15: 30S ribosomal protein S16



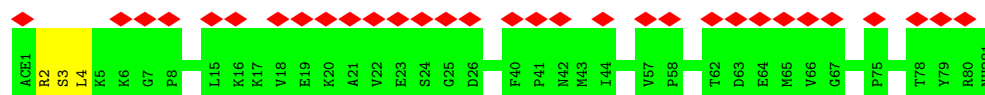
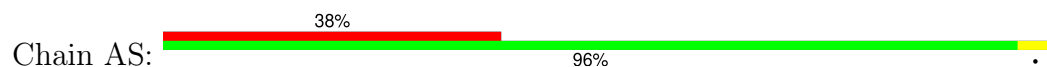
- Molecule 16: 30S ribosomal protein S17



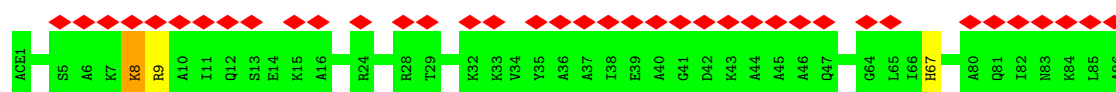
- Molecule 17: 30S ribosomal protein S18



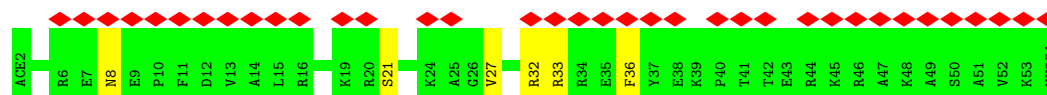
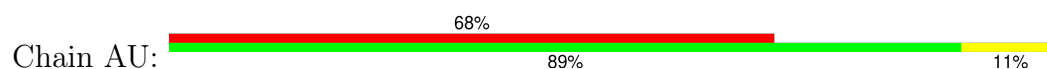
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20

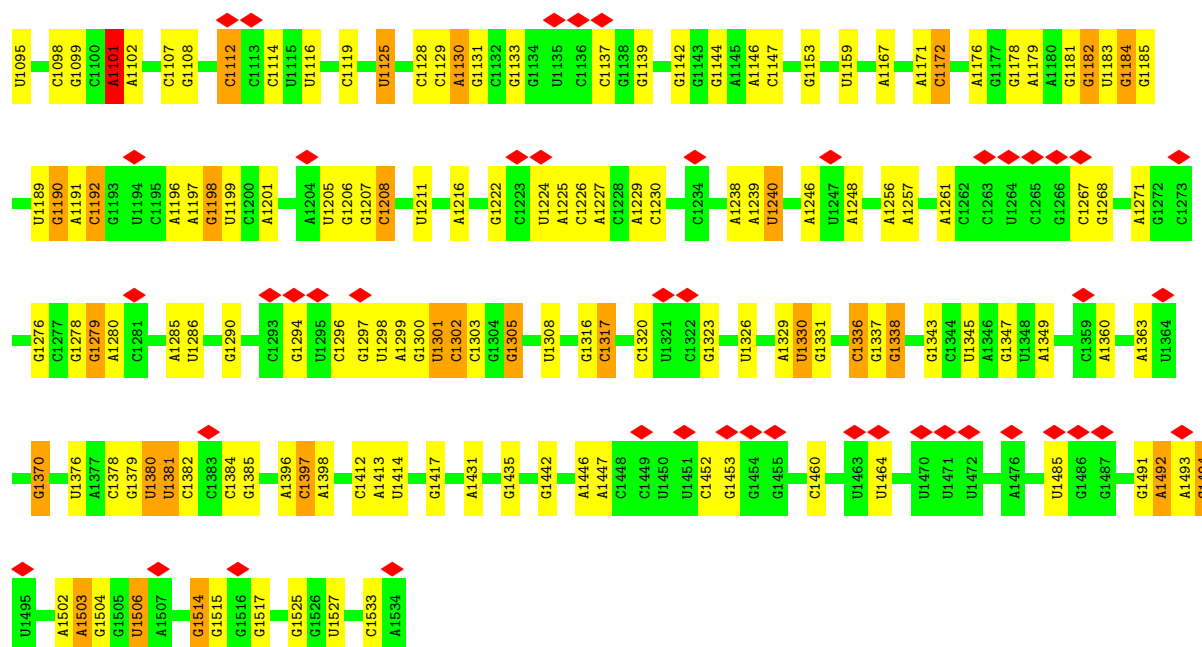


- Molecule 20: 30S ribosomal protein S21

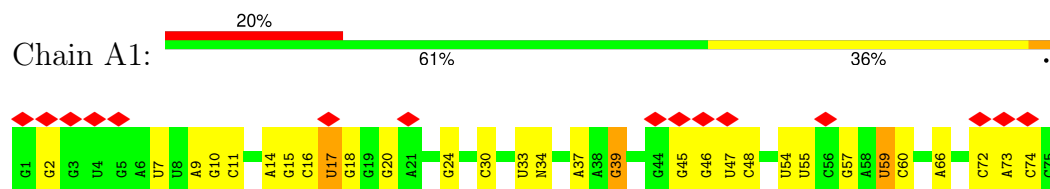


Chain AA:

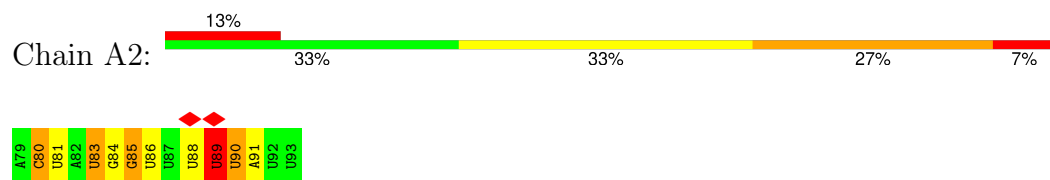




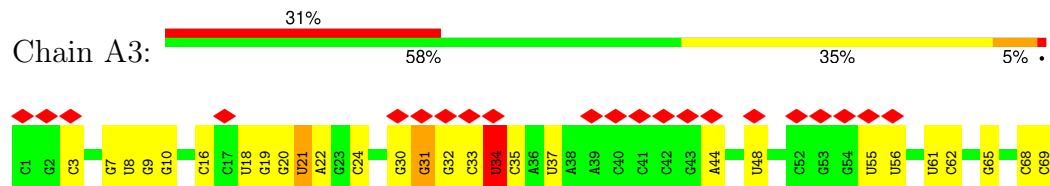
• Molecule 22: fMet-Val-tRNA-Val



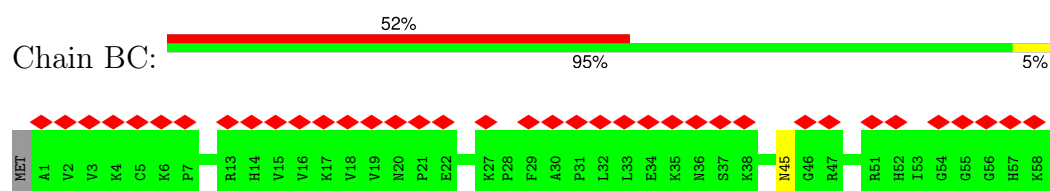
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

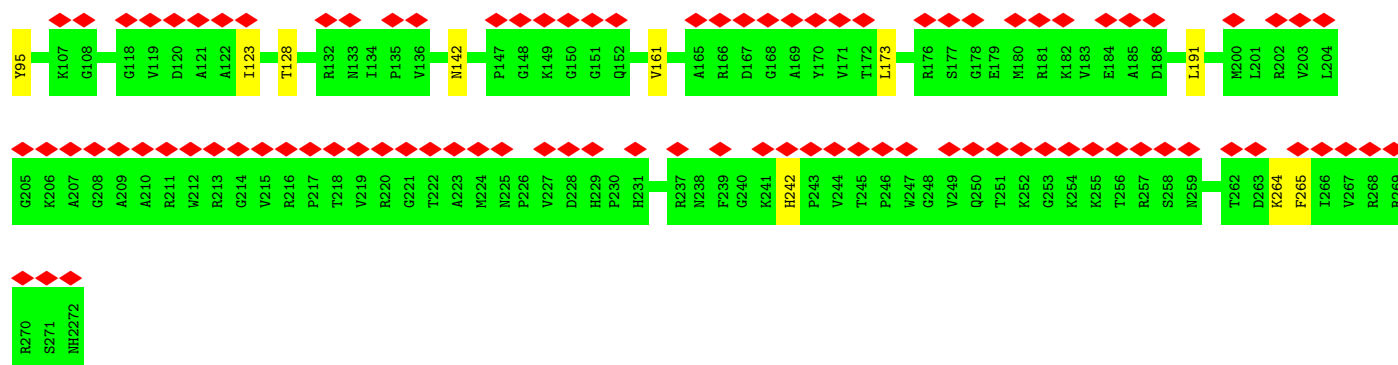


• Molecule 24: tRNA-fMet

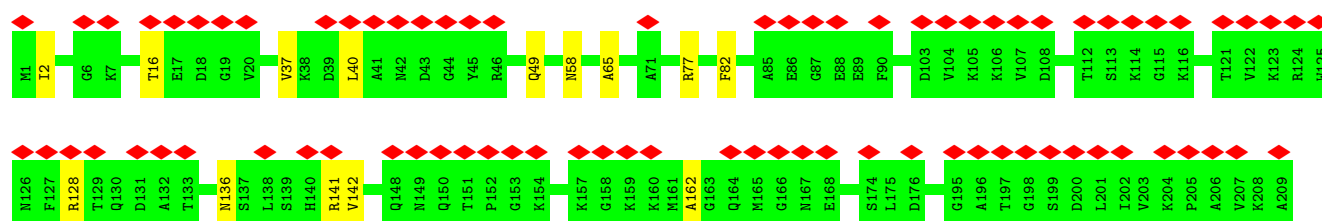
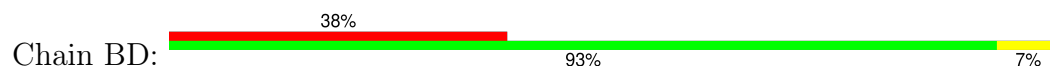


• Molecule 25: 50S ribosomal protein L2

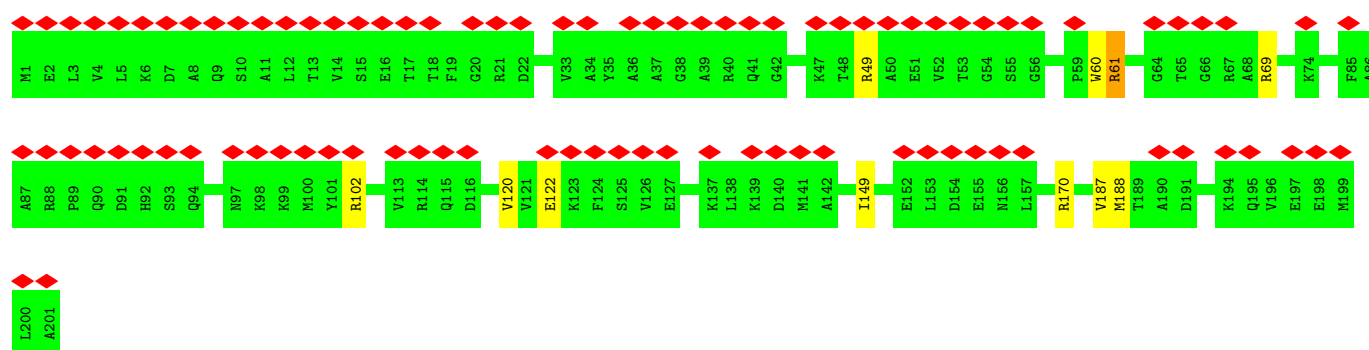




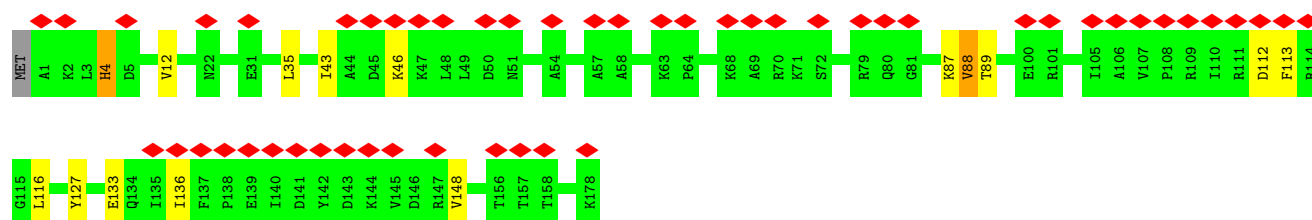
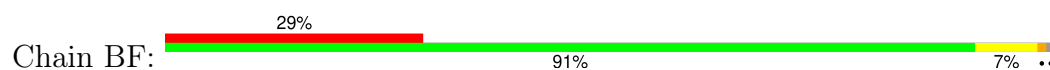
• Molecule 26: 50S ribosomal protein L3



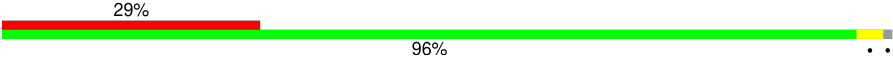
• Molecule 27: 50S ribosomal protein L4

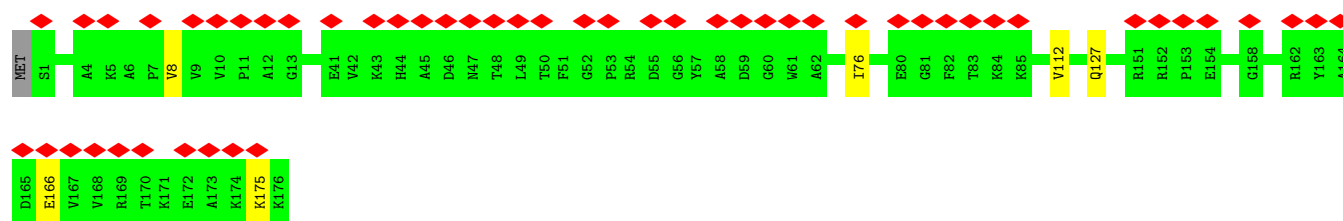


• Molecule 28: 50S ribosomal protein L5

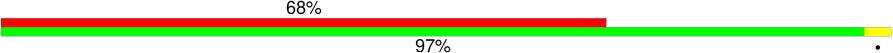


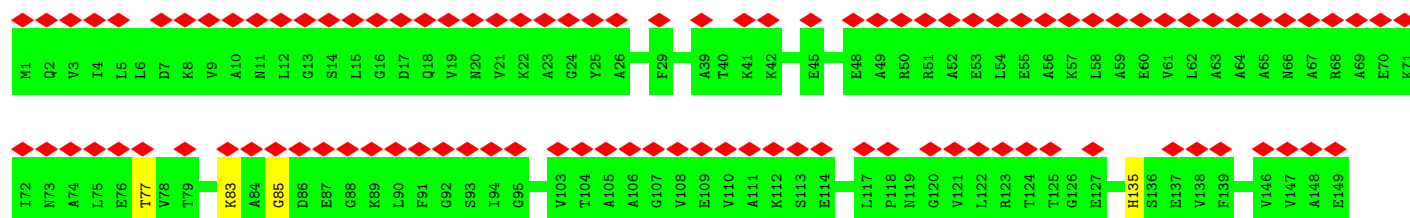
• Molecule 29: 50S ribosomal protein L6

Chain BG: 

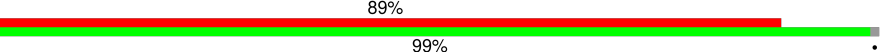


- Molecule 30: 50S ribosomal protein L9

Chain BH: 



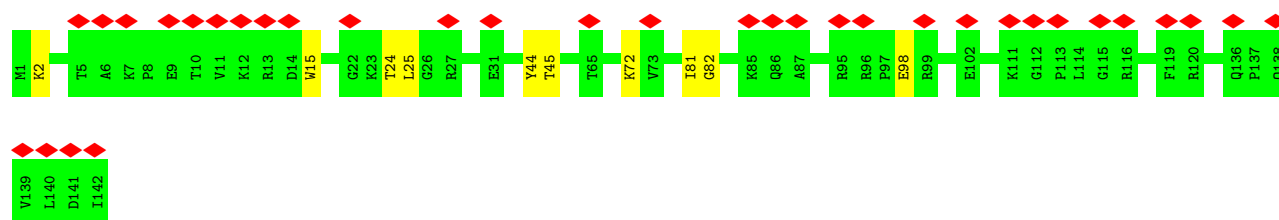
- Molecule 31: 50S ribosomal protein L11

Chain BI: 

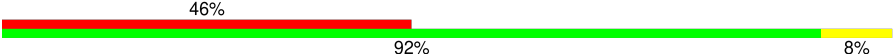


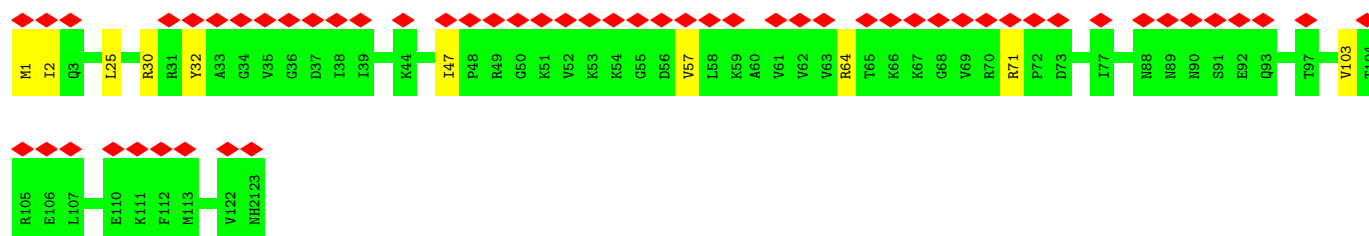
- Molecule 32: 50S ribosomal protein L13

Chain BJ: 

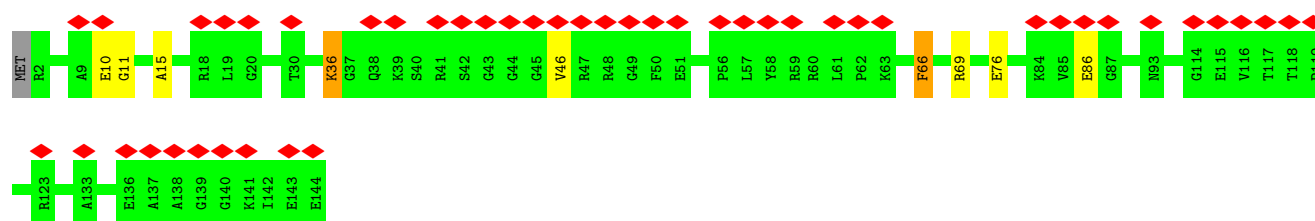


- Molecule 33: 50S ribosomal protein L14

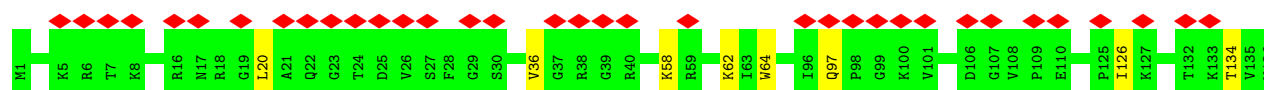
Chain BK: 



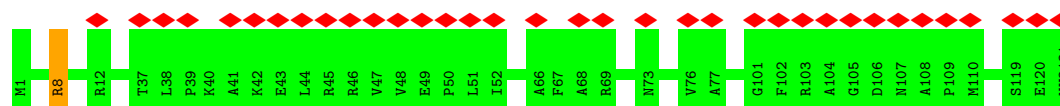
- Molecule 34: 50S ribosomal protein L15



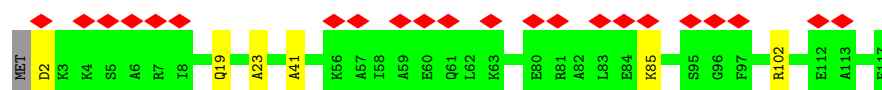
- Molecule 35: 50S ribosomal protein L16



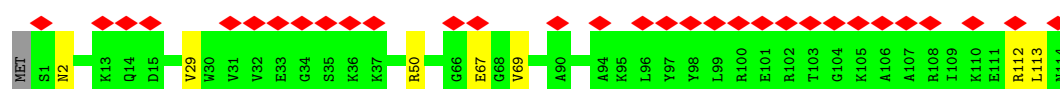
- Molecule 36: 50S ribosomal protein L17



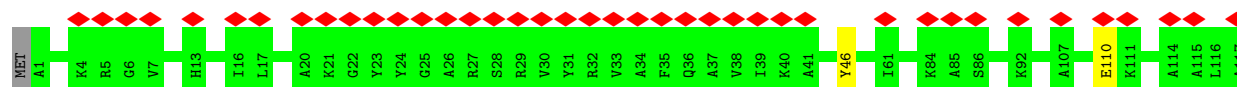
- Molecule 37: 50S ribosomal protein L18



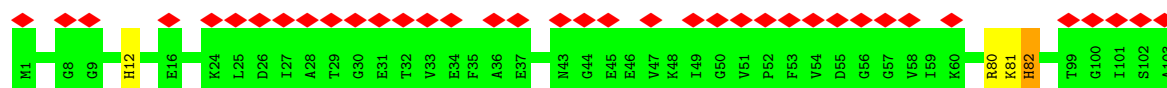
- Molecule 38: 50S ribosomal protein L19



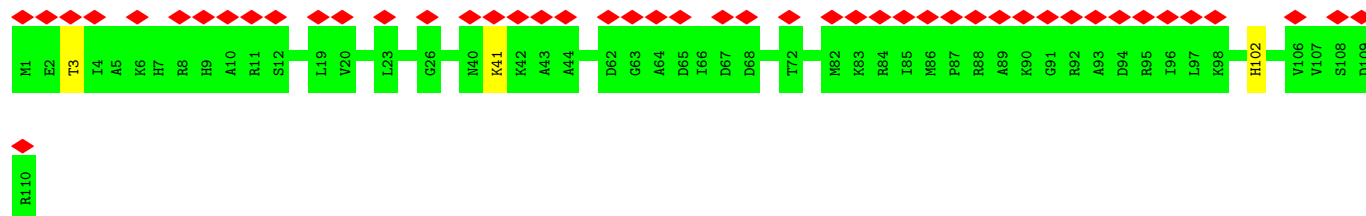
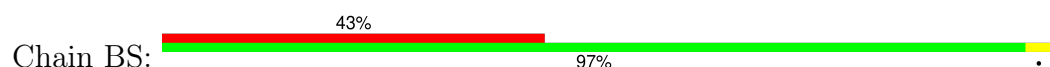
- Molecule 39: 50S ribosomal protein L20



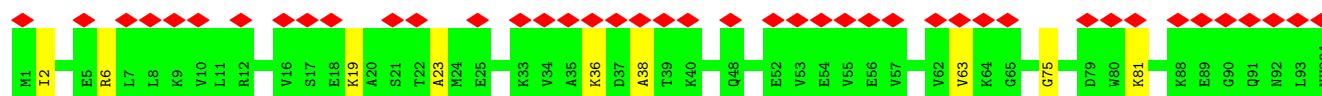
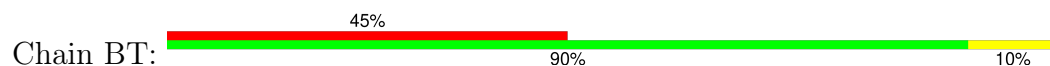
- Molecule 40: 50S ribosomal protein L21



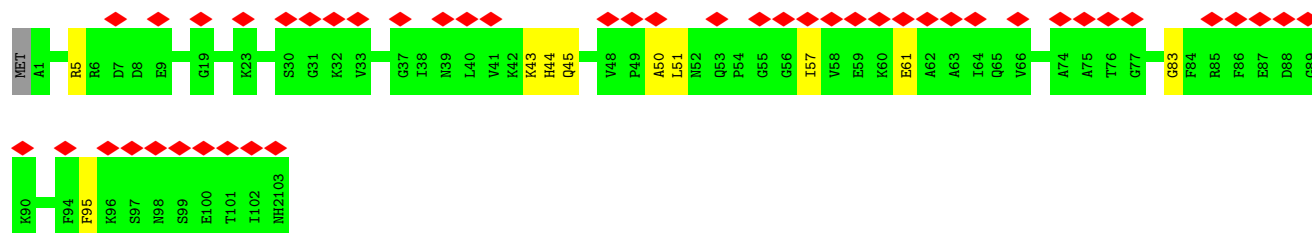
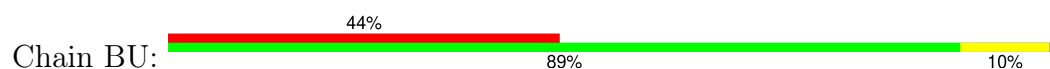
- Molecule 41: 50S ribosomal protein L22



- Molecule 42: 50S ribosomal protein L23

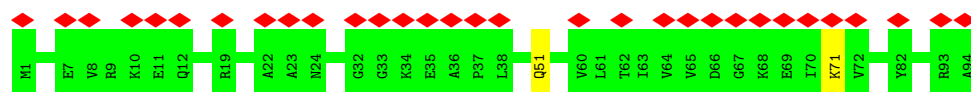


- Molecule 43: 50S ribosomal protein L24



- Molecule 44: 50S ribosomal protein L25

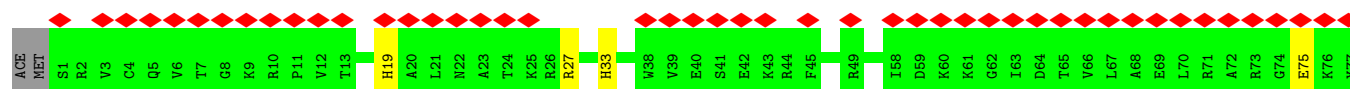




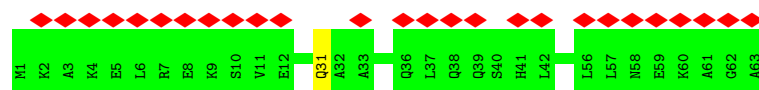
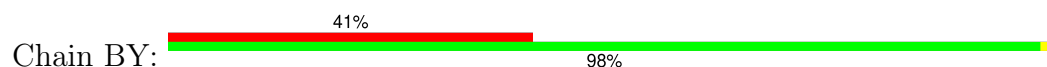
- Molecule 45: 50S ribosomal protein L27



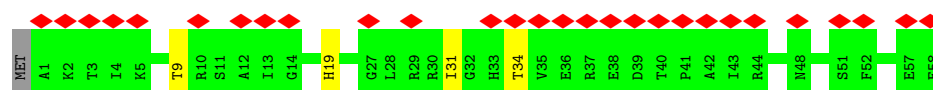
- Molecule 46: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L29



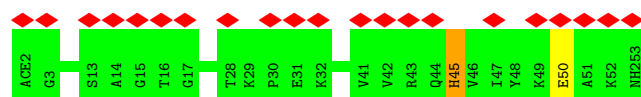
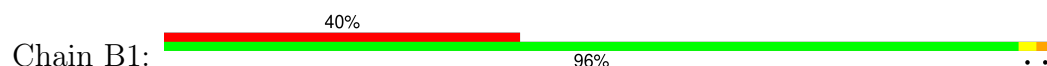
- Molecule 48: 50S ribosomal protein L30



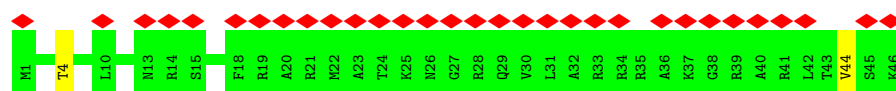
- Molecule 49: 50S ribosomal protein L32



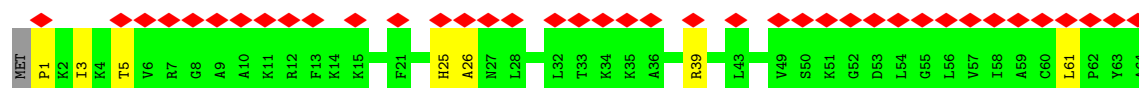
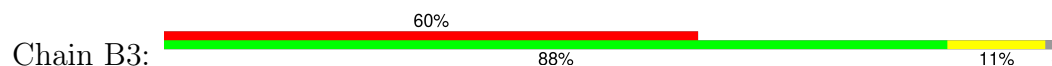
- Molecule 50: 50S ribosomal protein L33



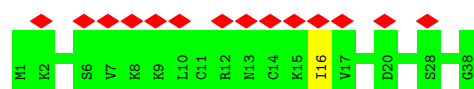
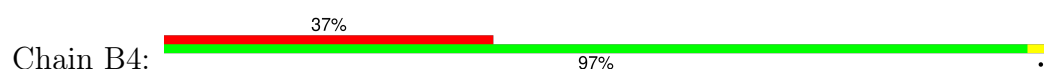
- Molecule 51: 50S ribosomal protein L34



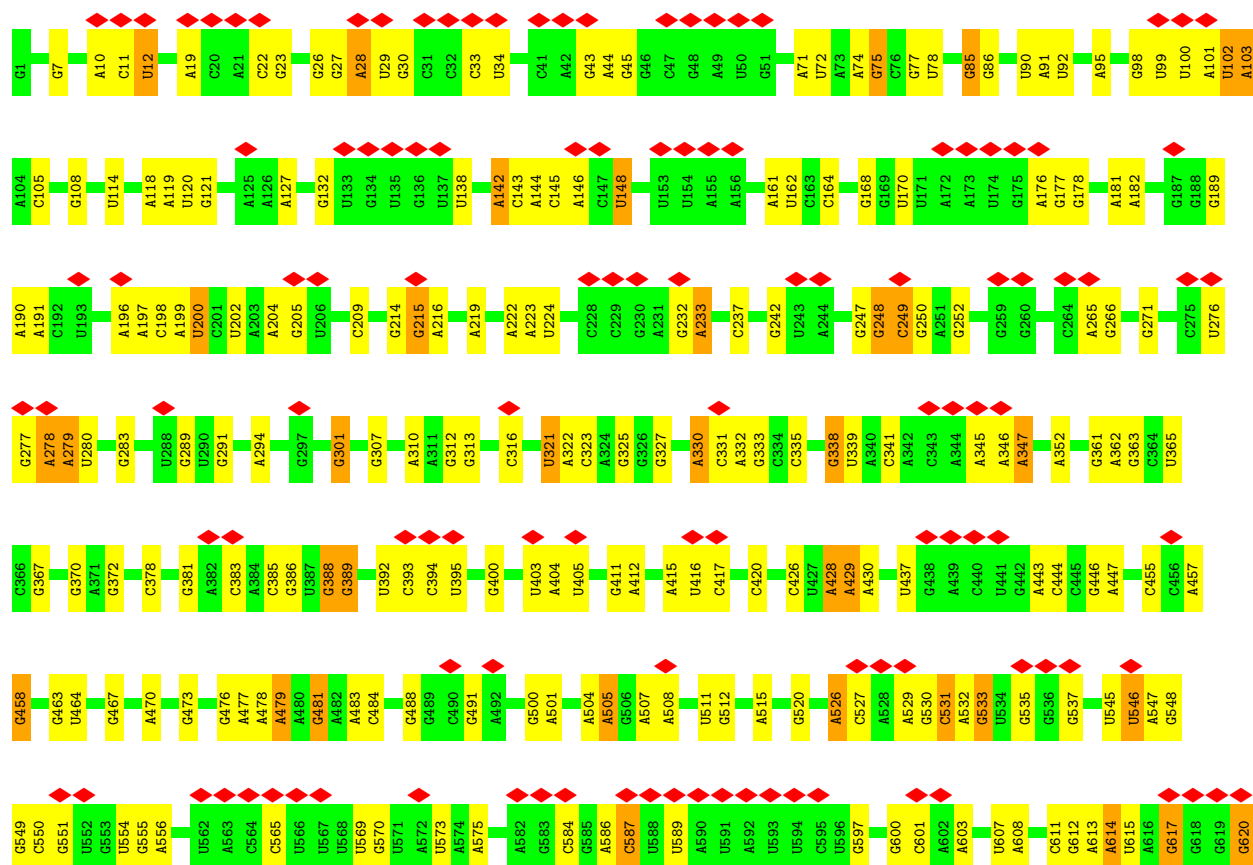
- Molecule 52: 50S ribosomal protein L35

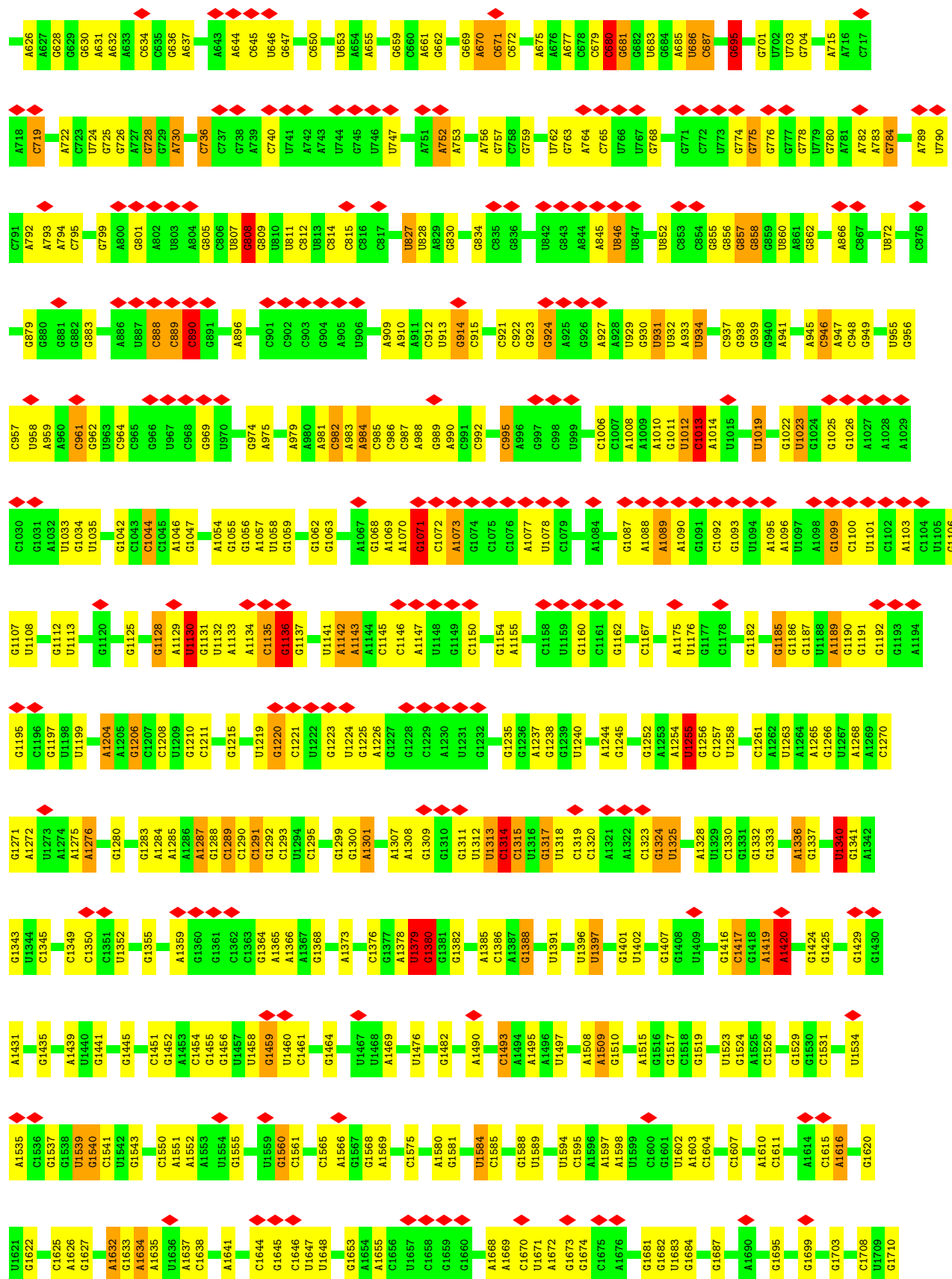


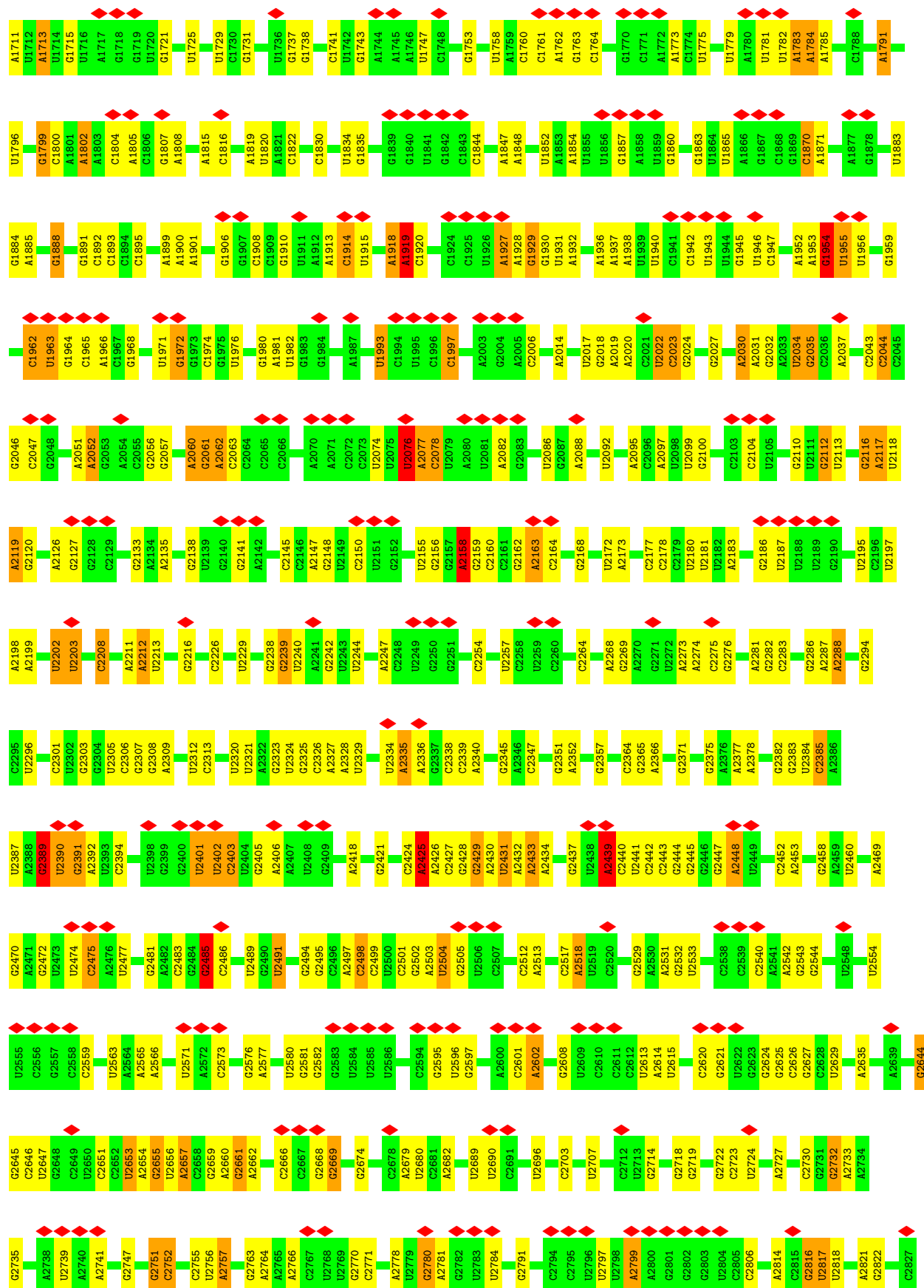
- Molecule 53: 50S ribosomal protein L36

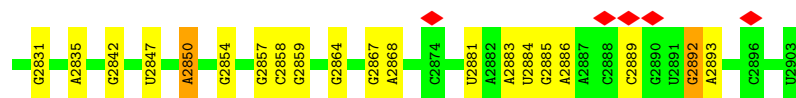


- Molecule 54: 23S ribosomal RNA

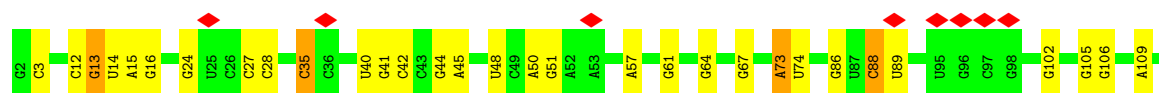
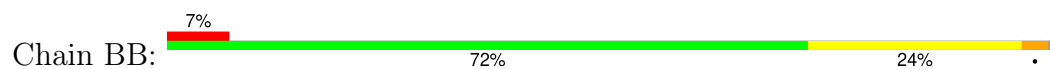




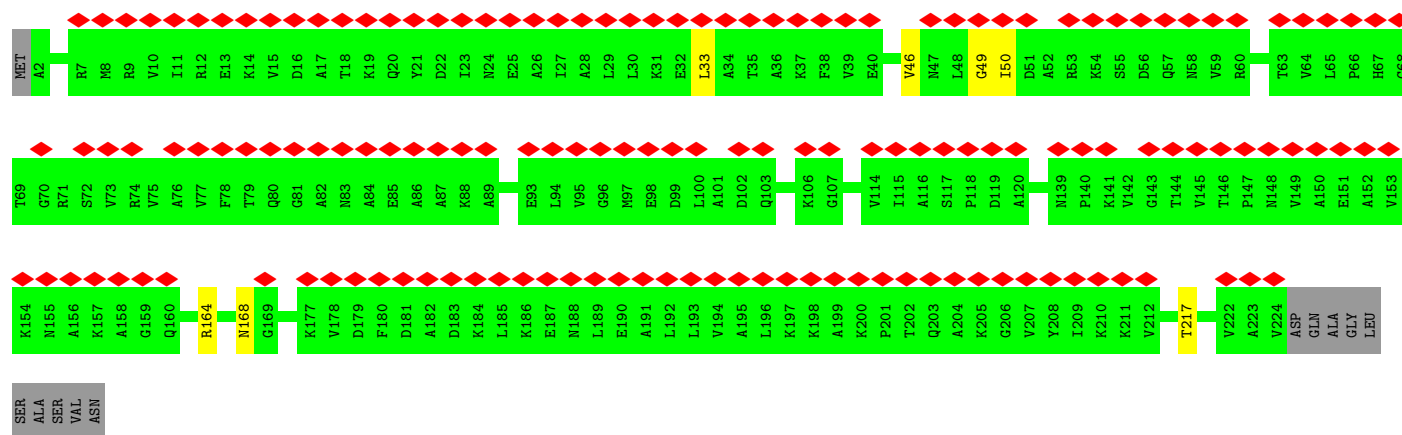




• Molecule 55: 5S ribosomal RNA



• Molecule 56: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3085	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	161000	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	181.278	Depositor
Minimum map value	-113.496	Depositor
Average map value	-0.658	Depositor
Map value standard deviation	18.679	Depositor
Recommended contour level	25	Depositor
Map size ($\text{\AA}$)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.8, 2.8, 2.8	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.96	0/1736	1.39	10/2340 (0.4%)
2	AC	0.93	0/1651	1.36	4/2225 (0.2%)
3	AD	0.96	0/1665	1.41	13/2227 (0.6%)
4	AE	0.92	0/1119	1.43	9/1506 (0.6%)
5	AF	0.98	0/835	1.43	0/1128
6	AG	0.98	0/1188	1.41	5/1593 (0.3%)
7	AH	0.91	0/989	1.31	2/1326 (0.2%)
8	AI	0.99	0/1035	1.45	6/1377 (0.4%)
9	AJ	0.99	0/797	1.38	5/1079 (0.5%)
10	AK	0.98	0/894	1.42	3/1207 (0.2%)
11	AL	0.98	0/969	1.44	3/1300 (0.2%)
12	AM	1.01	0/884	1.44	4/1181 (0.3%)
13	AN	1.01	0/817	1.47	4/1088 (0.4%)
14	AO	0.97	0/722	1.43	0/964
15	AP	0.95	0/648	1.38	0/870
16	AQ	0.95	0/658	1.36	1/883 (0.1%)
17	AR	0.99	0/463	1.36	0/623
18	AS	0.99	0/653	1.46	2/879 (0.2%)
19	AT	0.96	0/672	1.37	3/890 (0.3%)
20	AU	0.99	0/431	1.63	4/572 (0.7%)
21	AA	0.99	0/36759	1.15	55/57346 (0.1%)
22	A1	0.99	0/1668	1.13	2/2595 (0.1%)
23	A2	1.02	0/343	1.35	4/531 (0.8%)
24	A3	0.98	0/1722	1.16	3/2685 (0.1%)
25	BC	0.97	0/2121	1.48	1/2852 (0.0%)
26	BD	0.90	0/1586	1.47	6/2134 (0.3%)
27	BE	0.89	0/1571	1.44	2/2113 (0.1%)
28	BF	0.92	0/1444	1.44	4/1937 (0.2%)
29	BG	0.89	0/1343	1.44	4/1816 (0.2%)
30	BH	0.90	0/1122	1.46	3/1515 (0.2%)
31	BI	0.87	0/1046	1.39	0/1410
32	BJ	0.92	0/1152	1.51	5/1551 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BK	0.97	0/947	1.51	0/1268
34	BL	0.96	0/1054	1.56	0/1403
35	BM	0.92	0/1093	1.43	0/1460
36	BN	0.96	0/973	1.45	2/1301 (0.2%)
37	BO	0.94	0/902	1.48	3/1209 (0.2%)
38	BP	0.92	0/929	1.40	2/1242 (0.2%)
39	BQ	0.92	0/960	1.49	2/1278 (0.2%)
40	BR	0.90	0/829	1.46	3/1107 (0.3%)
41	BS	0.88	0/864	1.41	1/1156 (0.1%)
42	BT	0.88	0/744	1.51	1/994 (0.1%)
43	BU	0.90	0/787	1.47	2/1051 (0.2%)
44	BV	0.90	0/766	1.42	0/1025
45	BW	0.94	0/604	1.51	0/799
46	BX	0.95	0/635	1.49	2/848 (0.2%)
47	BY	0.87	0/510	1.42	1/677 (0.1%)
48	BZ	0.93	0/453	1.50	1/605 (0.2%)
49	B0	0.93	0/450	1.53	2/599 (0.3%)
50	B1	0.90	0/417	1.39	1/556 (0.2%)
51	B2	0.98	0/380	1.54	0/498
52	B3	0.94	0/513	1.52	3/676 (0.4%)
53	B4	0.94	0/303	1.46	0/397
54	BA	0.83	0/69796	1.15	125/108888 (0.1%)
55	BB	0.82	0/2800	1.13	2/4367 (0.0%)
56	B5	0.88	0/1673	1.45	3/2255 (0.1%)
All	All	0.90	0/160085	1.23	323/239402 (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
1	AB	0	1
2	AC	0	1
5	AF	0	1
10	AK	0	1
14	AO	0	1
21	AA	0	350
22	A1	0	16
23	A2	0	5
24	A3	0	17
26	BD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	BE	0	1
37	BO	0	1
54	BA	0	705
55	BB	0	21
All	All	0	1122

There are no bond length outliers.

All (323) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1379	U	O3'-P-O5'	-10.32	88.52	104.00
4	AE	24	VAL	CA-C-N	8.82	137.58	121.70
4	AE	24	VAL	C-N-CA	8.82	137.58	121.70
1	AB	10	LYS	CA-C-N	8.65	137.27	121.70
1	AB	10	LYS	C-N-CA	8.65	137.27	121.70
8	AI	128	LYS	CA-C-N	8.62	137.22	121.70
8	AI	128	LYS	C-N-CA	8.62	137.22	121.70
18	AS	3	SER	CA-C-N	8.15	136.36	121.70
18	AS	3	SER	C-N-CA	8.15	136.36	121.70
10	AK	52	ARG	NE-CZ-NH2	7.91	126.32	119.20
3	AD	204	SER	CA-C-N	7.62	135.42	121.70
3	AD	204	SER	C-N-CA	7.62	135.42	121.70
21	AA	872	A	C1'-O4'-C4'	-7.57	102.33	109.90
23	A2	85	G	C5'-C4'-C3'	-7.36	104.96	116.00
20	AU	8	ASN	CA-C-N	7.35	134.92	121.70
20	AU	8	ASN	C-N-CA	7.35	134.92	121.70
12	AM	111	PRO	CA-C-N	7.27	134.78	121.70
12	AM	111	PRO	C-N-CA	7.27	134.78	121.70
21	AA	1317	C	C1'-O4'-C4'	-7.12	102.78	109.90
21	AA	723	U	C1'-O4'-C4'	-6.98	102.92	109.90
28	BF	88	VAL	CA-C-N	6.97	130.72	120.90
28	BF	88	VAL	C-N-CA	6.97	130.72	120.90
32	BJ	24	THR	CA-C-N	6.96	134.24	121.70
32	BJ	24	THR	C-N-CA	6.96	134.24	121.70
54	BA	621	A	C5'-C4'-C3'	-6.89	105.66	116.00
13	AN	100	SER	CA-C-N	6.88	134.09	121.70
13	AN	100	SER	C-N-CA	6.88	134.09	121.70
54	BA	1634	A	C4'-C3'-O3'	6.76	119.54	109.40
54	BA	1142	A	C2'-C3'-O3'	6.67	119.51	109.50
54	BA	1314	C	N1-C1'-C2'	6.64	121.97	112.00
6	AG	6	ILE	CA-C-N	6.59	133.57	121.70
6	AG	6	ILE	C-N-CA	6.59	133.57	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AK	114	PRO	CA-C-N	6.56	133.51	121.70
10	AK	114	PRO	C-N-CA	6.56	133.51	121.70
21	AA	530	G	C1'-O4'-C4'	-6.55	103.15	109.70
21	AA	1229	A	C1'-O4'-C4'	-6.46	103.44	109.90
54	BA	808	G	C3'-C2'-O2'	6.41	120.31	110.70
1	AB	45	THR	CA-C-N	6.32	124.22	120.24
1	AB	45	THR	C-N-CA	6.32	124.22	120.24
11	AL	7	VAL	CA-C-N	6.31	133.06	121.70
11	AL	7	VAL	C-N-CA	6.31	133.06	121.70
54	BA	1927	A	O4'-C4'-C3'	6.30	110.30	104.00
26	BD	142	VAL	N-CA-C	6.30	114.36	109.19
54	BA	1189	A	C4'-C3'-C2'	-6.21	96.39	102.60
13	AN	91	GLY	CA-C-N	6.16	132.79	121.70
13	AN	91	GLY	C-N-CA	6.16	132.79	121.70
56	B5	49	GLY	CA-C-N	6.15	132.77	121.70
56	B5	49	GLY	C-N-CA	6.15	132.77	121.70
32	BJ	24	THR	O-C-N	-6.13	115.17	122.65
54	BA	1919	A	O4'-C1'-C2'	-6.13	101.47	107.60
40	BR	81	LYS	CA-C-N	6.11	133.22	121.54
40	BR	81	LYS	C-N-CA	6.11	133.22	121.54
54	BA	1962	C	O4'-C4'-C3'	6.09	110.09	104.00
54	BA	2485	G	C2'-C3'-O3'	6.08	122.82	113.70
4	AE	54	GLU	CA-C-N	6.03	126.22	120.43
4	AE	54	GLU	C-N-CA	6.03	126.22	120.43
54	BA	1019	U	O3'-P-O5'	6.00	113.00	104.00
21	AA	913	A	P-O3'-C3'	5.96	129.14	120.20
28	BF	4	HIS	CB-CG-CD2	-5.93	123.49	131.20
30	BH	85	GLY	CA-C-N	5.90	128.47	120.38
30	BH	85	GLY	C-N-CA	5.90	128.47	120.38
54	BA	1324	G	O4'-C4'-C3'	5.90	109.90	104.00
48	BZ	19	HIS	CB-CG-CD2	-5.90	123.53	131.20
54	BA	2657	A	O4'-C4'-C3'	5.90	109.90	104.00
29	BG	175	LYS	CA-C-N	5.89	132.30	121.70
29	BG	175	LYS	C-N-CA	5.89	132.30	121.70
54	BA	2646	C	N1-C1'-C2'	5.88	120.82	112.00
2	AC	107	LYS	CA-C-N	5.86	125.54	119.56
2	AC	107	LYS	C-N-CA	5.86	125.54	119.56
54	BA	2063	C	O4'-C4'-C3'	5.85	109.85	104.00
54	BA	2076	U	O4'-C1'-N1	5.85	116.97	108.20
54	BA	1352	U	O4'-C1'-N1	5.84	117.27	108.50
21	AA	1057	G	C5'-C4'-C3'	-5.84	107.24	116.00
54	BA	752	A	O4'-C1'-N9	5.83	116.95	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1270	C	O4'-C4'-C3'	5.83	109.83	104.00
54	BA	2425	A	C4'-C3'-O3'	5.83	118.14	109.40
54	BA	2158	A	O3'-P-O5'	-5.78	95.33	104.00
54	BA	1287	A	O4'-C4'-C3'	5.77	109.77	104.00
36	BN	8	ARG	CA-C-N	5.75	132.05	121.70
36	BN	8	ARG	C-N-CA	5.75	132.05	121.70
54	BA	636	G	O4'-C4'-C3'	5.73	109.73	104.00
21	AA	6	G	P-O3'-C3'	5.73	128.79	120.20
21	AA	1182	G	O4'-C4'-C3'	5.71	109.71	104.00
54	BA	614	A	C2'-C3'-O3'	5.69	118.03	109.50
54	BA	330	A	C2'-C3'-O3'	5.65	117.98	109.50
24	A3	22	A	C1'-O4'-C4'	-5.61	104.29	109.90
54	BA	1136	G	O4'-C4'-C3'	5.60	109.60	104.00
23	A2	83	U	O3'-P-O5'	-5.60	95.60	104.00
54	BA	2405	G	C2'-C3'-O3'	-5.60	105.30	113.70
54	BA	2859	G	O4'-C4'-C3'	5.58	109.58	104.00
55	BB	86	G	O3'-P-O5'	5.57	112.35	104.00
54	BA	1380	G	C5'-C4'-C3'	-5.56	107.66	116.00
21	AA	298	A	O4'-C4'-C3'	5.55	109.55	104.00
8	AI	56	MET	CA-C-N	5.54	131.95	121.97
8	AI	56	MET	C-N-CA	5.54	131.95	121.97
21	AA	494	G	O4'-C4'-C3'	5.54	109.54	104.00
54	BA	695	G	C4'-C3'-C2'	-5.54	97.06	102.60
54	BA	2031	A	C5'-C4'-C3'	-5.54	107.69	116.00
21	AA	896	C	O4'-C4'-C3'	5.53	109.53	104.00
16	AQ	30	HIS	CB-CG-CD2	-5.53	124.01	131.20
54	BA	1289	C	O4'-C4'-C3'	5.53	109.53	104.00
54	BA	1206	G	O4'-C4'-C3'	5.52	109.52	104.00
21	AA	306	A	O4'-C4'-C3'	5.52	109.52	104.00
54	BA	1607	C	O4'-C1'-N1	5.52	116.48	108.20
21	AA	560	A	O4'-C4'-C3'	5.52	109.52	104.00
50	B1	45	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	AB	23	ASN	CA-C-N	5.50	125.21	119.82
1	AB	23	ASN	C-N-CA	5.50	125.21	119.82
54	BA	2892	G	O4'-C4'-C3'	5.50	109.50	104.00
54	BA	2203	U	O4'-C4'-C3'	5.49	109.49	104.00
54	BA	1295	C	C4'-C3'-C2'	-5.49	97.11	102.60
54	BA	1263	U	O4'-C4'-C3'	5.48	109.48	104.00
6	AG	4	ARG	CA-C-N	5.48	131.84	121.97
6	AG	4	ARG	C-N-CA	5.48	131.84	121.97
54	BA	526	A	O4'-C1'-N9	5.48	116.72	108.50
54	BA	278	A	N9-C1'-C2'	5.48	120.22	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1781	U	O4'-C1'-N1	5.47	116.41	108.20
54	BA	2439	A	O4'-C1'-N9	5.47	116.41	108.20
54	BA	1099	G	O4'-C4'-C3'	5.47	109.47	104.00
21	AA	1101	A	P-O3'-C3'	5.47	128.40	120.20
43	BU	50	ALA	CA-C-N	5.47	131.98	121.54
43	BU	50	ALA	C-N-CA	5.47	131.98	121.54
2	AC	142	ARG	CA-C-N	5.46	128.62	120.31
2	AC	142	ARG	C-N-CA	5.46	128.62	120.31
21	AA	162	A	O4'-C4'-C3'	5.46	109.45	104.00
54	BA	1313	U	O4'-C4'-C3'	5.46	109.45	104.00
3	AD	106	PHE	CA-C-N	5.45	126.31	122.33
3	AD	106	PHE	C-N-CA	5.45	126.31	122.33
40	BR	12	HIS	CB-CG-CD2	-5.45	124.12	131.20
54	BA	458	G	O4'-C1'-N9	5.45	116.37	108.20
3	AD	203	TYR	CA-C-N	5.45	131.50	121.70
3	AD	203	TYR	C-N-CA	5.45	131.50	121.70
21	AA	476	U	P-O3'-C3'	5.44	128.36	120.20
21	AA	480	U	O4'-C4'-C3'	5.43	109.43	104.00
54	BA	987	C	O3'-P-O5'	5.43	112.15	104.00
54	BA	931	U	O4'-C1'-N1	5.42	116.34	108.20
54	BA	1805	A	C4'-C3'-C2'	-5.42	97.18	102.60
21	AA	952	U	C5'-C4'-C3'	-5.42	107.88	116.00
4	AE	104	ILE	CA-C-N	5.41	131.44	121.70
4	AE	104	ILE	C-N-CA	5.41	131.44	121.70
54	BA	670	A	C2'-C3'-O3'	5.41	117.61	109.50
54	BA	1954	G	O4'-C4'-C3'	5.41	109.41	104.00
21	AA	1296	C	O4'-C4'-C3'	5.40	109.40	104.00
21	AA	1065	U	C3'-C2'-C1'	5.40	106.70	101.30
21	AA	406	G	C5'-C4'-C3'	-5.39	107.91	116.00
54	BA	2655	G	O4'-C1'-N9	5.39	116.28	108.20
7	AH	66	GLN	OE1-CD-NE2	-5.39	117.21	122.60
54	BA	671	C	C2'-C3'-O3'	5.38	117.58	109.50
21	AA	776	G	O4'-C4'-C3'	5.38	109.38	104.00
54	BA	2335	A	O4'-C4'-C3'	5.38	109.38	104.00
49	B0	37	HIS	CB-CG-CD2	-5.37	124.22	131.20
23	A2	89	U	P-O3'-C3'	5.37	128.25	120.20
8	AI	41	GLU	CA-C-N	5.37	129.19	120.60
8	AI	41	GLU	C-N-CA	5.37	129.19	120.60
54	BA	2052	A	C5'-C4'-C3'	-5.37	107.95	116.00
54	BA	2239	G	O4'-C4'-C3'	5.37	109.36	104.00
21	AA	1197	A	O4'-C4'-C3'	5.36	109.36	104.00
21	AA	15	G	O4'-C4'-C3'	5.36	109.36	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1071	G	C3'-C2'-C1'	5.36	106.66	101.30
24	A3	62	C	O4'-C4'-C3'	5.35	109.35	104.00
20	AU	21	SER	CA-C-N	5.35	131.33	121.70
20	AU	21	SER	C-N-CA	5.35	131.33	121.70
21	AA	1208	C	C5'-C4'-C3'	-5.35	107.97	116.00
21	AA	1514	G	O3'-P-O5'	5.34	112.02	104.00
21	AA	117	G	O4'-C4'-C3'	5.34	109.34	104.00
54	BA	1899	A	O4'-C4'-C3'	5.33	109.33	104.00
21	AA	596	A	O4'-C4'-C3'	5.32	109.32	104.00
30	BH	135	HIS	CB-CG-CD2	-5.32	124.29	131.20
39	BQ	110	GLU	CA-C-N	5.31	127.40	120.28
39	BQ	110	GLU	C-N-CA	5.31	127.40	120.28
54	BA	2389	G	O4'-C4'-C3'	5.31	109.31	104.00
54	BA	2766	A	O4'-C4'-C3'	5.31	109.31	104.00
54	BA	1013	C	O4'-C4'-C3'	5.31	109.31	104.00
12	AM	40	GLU	CA-C-N	5.30	128.64	121.05
12	AM	40	GLU	C-N-CA	5.30	128.64	121.05
21	AA	476	U	C4'-C3'-O3'	5.30	120.95	113.00
54	BA	1417	C	C5'-C4'-C3'	-5.30	108.05	116.00
52	B3	1	PRO	CA-N-CD	-5.30	104.58	112.00
22	A1	10	G	O4'-C4'-C3'	5.29	109.29	104.00
21	AA	1492	A	O4'-C4'-C3'	5.28	109.28	104.00
54	BA	323	C	O4'-C1'-N1	5.28	116.12	108.20
54	BA	1783	A	O4'-C4'-C3'	5.28	109.28	104.00
54	BA	1135	C	O4'-C4'-C3'	5.28	109.28	104.00
54	BA	1551	A	O4'-C4'-C3'	5.28	109.28	104.00
54	BA	2724	U	O4'-C4'-C3'	5.27	109.27	104.00
9	AJ	76	ILE	CA-C-N	5.27	131.45	121.97
9	AJ	76	ILE	C-N-CA	5.27	131.45	121.97
21	AA	978	A	O4'-C4'-C3'	5.27	109.27	104.00
54	BA	1225	G	O4'-C4'-C3'	5.25	109.25	104.00
21	AA	1330	U	C5'-C4'-C3'	-5.25	108.13	116.00
54	BA	388	G	O4'-C4'-C3'	5.24	109.24	104.00
54	BA	1402	U	C4'-C3'-C2'	-5.24	97.36	102.60
56	B5	164	ARG	NE-CZ-NH2	5.24	123.92	119.20
21	AA	110	C	O4'-C4'-C3'	5.24	109.24	104.00
54	BA	2164	C	O4'-C4'-C3'	5.24	109.24	104.00
21	AA	844	G	O4'-C4'-C3'	5.24	109.24	104.00
54	BA	2757	A	C5'-C4'-C3'	-5.24	108.15	116.00
54	BA	2730	C	C4'-C3'-C2'	-5.23	97.37	102.60
21	AA	1184	G	O4'-C4'-C3'	5.23	109.23	104.00
25	BC	242	HIS	CB-CG-CD2	-5.22	124.41	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	39	G	C1'-O4'-C4'	-5.22	104.68	109.90
54	BA	565	C	C4'-C3'-C2'	-5.22	97.38	102.60
21	AA	366	A	O3'-P-O5'	-5.22	96.17	104.00
54	BA	828	U	N1-C1'-C2'	5.21	119.82	112.00
55	BB	113	C	C4'-C3'-C2'	-5.21	97.39	102.60
21	AA	1336	C	O4'-C4'-C3'	5.21	109.21	104.00
26	BD	128	ARG	NE-CZ-NH2	5.21	123.89	119.20
54	BA	1263	U	C3'-C2'-C1'	5.21	106.51	101.30
54	BA	1324	G	C3'-C2'-C1'	5.21	106.51	101.30
21	AA	1380	U	P-O3'-C3'	5.21	128.01	120.20
32	BJ	82	GLY	CA-C-N	5.21	124.92	119.92
32	BJ	82	GLY	C-N-CA	5.21	124.92	119.92
54	BA	1943	U	O4'-C1'-N1	5.21	116.01	108.20
54	BA	278	A	O4'-C1'-C2'	-5.20	102.40	107.60
9	AJ	7	ARG	NE-CZ-NH2	5.19	123.87	119.20
54	BA	312	G	O4'-C4'-C3'	5.19	109.19	104.00
46	BX	19	HIS	CB-CG-CD2	-5.19	124.45	131.20
21	AA	120	A	O4'-C4'-C3'	5.18	109.19	104.00
21	AA	276	G	O4'-C4'-C3'	5.18	109.18	104.00
54	BA	1204	A	O4'-C1'-N9	5.18	115.98	108.20
54	BA	1560	G	O4'-C4'-C3'	5.18	109.18	104.00
21	AA	900	A	O4'-C4'-C3'	5.18	109.18	104.00
54	BA	2755	C	O4'-C4'-C3'	5.18	109.18	104.00
54	BA	1632	A	O4'-C4'-C3'	5.18	109.18	104.00
54	BA	927	A	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	2329	U	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	1035	U	C4'-C3'-C2'	-5.17	97.43	102.60
3	AD	82	LYS	CA-C-N	5.17	124.88	119.92
3	AD	82	LYS	C-N-CA	5.17	124.88	119.92
21	AA	90	C	O4'-C4'-C3'	5.16	109.16	104.00
54	BA	1128	G	C1'-O4'-C4'	-5.16	104.54	109.70
54	BA	2195	U	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	1255	U	O3'-P-O5'	5.16	111.74	104.00
54	BA	1638	C	O4'-C4'-C3'	5.16	109.16	104.00
54	BA	1791	A	O4'-C4'-C3'	5.16	109.16	104.00
54	BA	2063	C	C3'-C2'-C1'	5.15	106.45	101.30
21	AA	998	C	O4'-C4'-C3'	5.15	109.15	104.00
54	BA	90	U	O3'-P-O5'	5.14	111.72	104.00
21	AA	549	C	O4'-C4'-C3'	5.14	109.14	104.00
54	BA	2202	U	C2'-C3'-O3'	-5.14	105.98	113.70
54	BA	2707	U	C4'-C3'-C2'	-5.14	97.46	102.60
41	BS	102	HIS	CB-CG-CD2	-5.13	124.53	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	B3	39	ARG	CA-C-N	5.13	127.47	120.54
52	B3	39	ARG	C-N-CA	5.13	127.47	120.54
54	BA	2387	U	O4'-C4'-C3'	5.13	109.13	104.00
9	AJ	54	SER	CA-C-N	5.13	125.20	119.87
9	AJ	54	SER	C-N-CA	5.13	125.20	119.87
54	BA	888	C	C1'-O4'-C4'	-5.13	104.57	109.70
54	BA	984	A	O4'-C4'-C3'	5.12	109.12	104.00
54	BA	1224	U	O4'-C4'-C3'	5.12	109.12	104.00
54	BA	1317	G	O4'-C4'-C3'	5.12	109.12	104.00
54	BA	1419	A	C2'-C3'-O3'	5.12	117.17	109.50
21	AA	1101	A	C2'-C3'-O3'	5.11	117.17	109.50
23	A2	85	G	C2'-C3'-O3'	5.11	121.37	113.70
49	B0	4	GLN	OE1-CD-NE2	-5.11	117.49	122.60
54	BA	501	A	O4'-C4'-C3'	5.11	109.11	104.00
54	BA	367	G	C4'-C3'-C2'	-5.11	97.49	102.60
54	BA	866	A	O4'-C4'-C3'	5.11	109.11	104.00
26	BD	65	ALA	CA-C-N	5.11	125.75	120.03
26	BD	65	ALA	C-N-CA	5.11	125.75	120.03
7	AH	87	ARG	NE-CZ-NH2	5.11	123.79	119.20
54	BA	964	C	C4'-C3'-C2'	-5.10	97.50	102.60
54	BA	2439	A	C1'-O4'-C4'	-5.10	104.60	109.70
54	BA	601	C	C4'-C3'-C2'	-5.10	97.50	102.60
54	BA	1799	G	C2'-C3'-O3'	5.10	117.15	109.50
4	AE	104	ILE	O-C-N	-5.09	116.21	122.57
54	BA	1195	G	C4'-C3'-C2'	-5.09	97.51	102.60
54	BA	1010	A	O4'-C4'-C3'	5.09	109.09	104.00
54	BA	1340	U	O4'-C1'-N1	5.09	116.13	108.50
54	BA	2597	G	O4'-C4'-C3'	5.08	109.08	104.00
29	BG	76	ILE	CA-C-N	5.08	125.73	119.99
29	BG	76	ILE	C-N-CA	5.08	125.73	119.99
54	BA	1420	A	O4'-C1'-N9	5.08	115.82	108.20
54	BA	429	A	O4'-C4'-C3'	5.08	109.08	104.00
21	AA	1181	G	C1'-O4'-C4'	-5.08	104.83	109.90
3	AD	5	GLY	CA-C-N	5.07	125.22	119.90
3	AD	5	GLY	C-N-CA	5.07	125.22	119.90
54	BA	2850	A	O4'-C4'-C3'	5.07	109.07	104.00
54	BA	1226	A	O4'-C4'-C3'	5.07	109.06	104.00
21	AA	603	U	O4'-C4'-C3'	5.06	109.06	104.00
54	BA	178	G	O3'-P-O5'	5.06	111.59	104.00
46	BX	33	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	AB	57	ASN	CA-C-N	5.06	127.37	120.54
1	AB	57	ASN	C-N-CA	5.06	127.37	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2116	G	O4'-C4'-C3'	5.06	109.06	104.00
42	BT	6	ARG	NE-CZ-NH2	5.06	123.75	119.20
4	AE	106	ALA	CA-C-N	5.05	124.90	120.10
4	AE	106	ALA	C-N-CA	5.05	124.90	120.10
37	BO	19	GLN	OE1-CD-NE2	-5.05	117.55	122.60
54	BA	857	G	C2'-C3'-O3'	-5.05	106.12	113.70
21	AA	575	G	P-O3'-C3'	5.04	127.77	120.20
26	BD	162	ALA	CA-C-N	5.04	125.13	120.34
26	BD	162	ALA	C-N-CA	5.04	125.13	120.34
19	AT	8	LYS	CA-C-N	5.04	131.16	121.54
19	AT	8	LYS	C-N-CA	5.04	131.16	121.54
37	BO	41	ALA	CA-C-N	5.04	124.76	119.82
37	BO	41	ALA	C-N-CA	5.04	124.76	119.82
3	AD	28	ASP	CA-C-N	5.03	131.16	121.54
3	AD	28	ASP	C-N-CA	5.03	131.16	121.54
24	A3	34	U	O4'-C4'-C3'	5.03	109.03	104.00
1	AB	48	MET	CA-C-N	5.03	126.98	120.44
1	AB	48	MET	C-N-CA	5.03	126.98	120.44
38	BP	50	ARG	CA-C-N	5.03	130.76	121.70
38	BP	50	ARG	C-N-CA	5.03	130.76	121.70
3	AD	197	HIS	CB-CG-CD2	-5.03	124.66	131.20
21	AA	194	C	O4'-C4'-C3'	5.03	109.03	104.00
21	AA	659	U	O4'-C4'-C3'	5.03	109.03	104.00
54	BA	2047	C	C4'-C3'-C2'	-5.02	97.58	102.60
54	BA	2653	U	C4'-C3'-O3'	5.02	120.53	113.00
19	AT	67	HIS	CB-CG-CD2	-5.02	124.67	131.20
54	BA	511	U	C2'-C3'-O3'	-5.02	106.17	113.70
54	BA	2364	C	C4'-C3'-C2'	-5.02	97.58	102.60
6	AG	2	ARG	NE-CZ-NH2	5.01	123.71	119.20
21	AA	573	A	O4'-C4'-C3'	5.01	109.01	104.00
21	AA	632	U	O4'-C4'-C3'	5.01	109.01	104.00
21	AA	859	G	O4'-C4'-C3'	5.01	109.01	104.00
54	BA	1597	A	C2'-C3'-O3'	-5.01	106.19	113.70
11	AL	49	ARG	NH1-CZ-NH2	-5.01	112.79	119.30
28	BF	89	THR	N-CA-C	5.01	117.30	110.24
27	BE	102	ARG	CA-C-N	5.01	125.50	119.94
27	BE	102	ARG	C-N-CA	5.01	125.50	119.94
21	AA	1370	G	C5'-C4'-C3'	-5.00	108.50	116.00
47	BY	31	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (1122) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	11	C	Sidechain
22	A1	14	A	Sidechain
22	A1	15	G	Sidechain
22	A1	17	U	Sidechain
22	A1	2	G	Sidechain
22	A1	24	G	Sidechain
22	A1	30	C	Sidechain
22	A1	33	U	Sidechain
22	A1	45	G	Sidechain
22	A1	57	G	Sidechain
22	A1	59	U	Sidechain
22	A1	60	C	Sidechain
22	A1	66	A	Sidechain
22	A1	72	C	Sidechain
22	A1	73	A	Sidechain
22	A1	9	A	Sidechain
23	A2	80	C	Sidechain
23	A2	83	U	Sidechain
23	A2	89	U	Sidechain
23	A2	90	U	Sidechain
23	A2	91	A	Sidechain
24	A3	16	C	Sidechain
24	A3	19	G	Sidechain
24	A3	20	G	Sidechain
24	A3	24	C	Sidechain
24	A3	3	C	Sidechain
24	A3	30	G	Sidechain
24	A3	31	G	Sidechain
24	A3	34	U	Sidechain
24	A3	37	U	Sidechain
24	A3	44	A	Sidechain
24	A3	61	U	Sidechain
24	A3	65	G	Sidechain
24	A3	68	C	Sidechain
24	A3	69	C	Sidechain
24	A3	7	G	Sidechain
24	A3	73	A	Sidechain
24	A3	77	A	Sidechain
21	AA	100	G	Sidechain
21	AA	1008	U	Sidechain
21	AA	1010	U	Sidechain
21	AA	1013	G	Sidechain
21	AA	1015	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	102	G	Sidechain
21	AA	1025	U	Sidechain
21	AA	1026	G	Sidechain
21	AA	1028	C	Sidechain
21	AA	1029	U	Sidechain
21	AA	1030	U	Sidechain
21	AA	1033	G	Sidechain
21	AA	1036	A	Sidechain
21	AA	1039	G	Sidechain
21	AA	1044	A	Sidechain
21	AA	1045	C	Sidechain
21	AA	1046	A	Sidechain
21	AA	1048	G	Sidechain
21	AA	1049	U	Sidechain
21	AA	106	C	Sidechain
21	AA	1060	U	Sidechain
21	AA	1061	G	Sidechain
21	AA	1073	U	Sidechain
21	AA	1077	G	Sidechain
21	AA	108	G	Sidechain
21	AA	1090	U	Sidechain
21	AA	1092	A	Sidechain
21	AA	1098	C	Sidechain
21	AA	1099	G	Sidechain
21	AA	1101	A	Sidechain
21	AA	1107	C	Sidechain
21	AA	1108	G	Sidechain
21	AA	111	G	Sidechain
21	AA	1112	C	Sidechain
21	AA	1114	C	Sidechain
21	AA	1116	U	Sidechain
21	AA	1119	C	Sidechain
21	AA	112	G	Sidechain
21	AA	1125	U	Sidechain
21	AA	1128	C	Sidechain
21	AA	1130	A	Sidechain
21	AA	1131	G	Sidechain
21	AA	1142	G	Sidechain
21	AA	1144	G	Sidechain
21	AA	1153	G	Sidechain
21	AA	1167	A	Sidechain
21	AA	1172	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1176	A	Sidechain
21	AA	1178	G	Sidechain
21	AA	1179	A	Sidechain
21	AA	118	U	Sidechain
21	AA	1190	G	Sidechain
21	AA	1192	C	Sidechain
21	AA	1198	G	Sidechain
21	AA	1199	U	Sidechain
21	AA	12	U	Sidechain
21	AA	1205	U	Sidechain
21	AA	1206	G	Sidechain
21	AA	1207	G	Sidechain
21	AA	1208	C	Sidechain
21	AA	1211	U	Sidechain
21	AA	1216	A	Sidechain
21	AA	1224	U	Sidechain
21	AA	1230	C	Sidechain
21	AA	1238	A	Sidechain
21	AA	1239	A	Sidechain
21	AA	1240	U	Sidechain
21	AA	1246	A	Sidechain
21	AA	1248	A	Sidechain
21	AA	1261	A	Sidechain
21	AA	1268	G	Sidechain
21	AA	1271	A	Sidechain
21	AA	1276	G	Sidechain
21	AA	1279	G	Sidechain
21	AA	129	A	Sidechain
21	AA	1290	G	Sidechain
21	AA	1294	G	Sidechain
21	AA	1297	G	Sidechain
21	AA	1301	U	Sidechain
21	AA	1302	C	Sidechain
21	AA	1305	G	Sidechain
21	AA	1308	U	Sidechain
21	AA	1316	G	Sidechain
21	AA	1317	C	Sidechain
21	AA	1326	U	Sidechain
21	AA	1329	A	Sidechain
21	AA	1330	U	Sidechain
21	AA	1338	G	Sidechain
21	AA	134	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1343	G	Sidechain
21	AA	1345	U	Sidechain
21	AA	1349	A	Sidechain
21	AA	1360	A	Sidechain
21	AA	1363	A	Sidechain
21	AA	137	U	Sidechain
21	AA	1370	G	Sidechain
21	AA	1376	U	Sidechain
21	AA	1378	C	Sidechain
21	AA	1381	U	Sidechain
21	AA	1382	C	Sidechain
21	AA	1384	C	Sidechain
21	AA	1385	G	Sidechain
21	AA	1397	C	Sidechain
21	AA	1398	A	Sidechain
21	AA	1412	C	Sidechain
21	AA	1413	A	Sidechain
21	AA	1414	U	Sidechain
21	AA	1417	G	Sidechain
21	AA	143	A	Sidechain
21	AA	1431	A	Sidechain
21	AA	1435	G	Sidechain
21	AA	1442	G	Sidechain
21	AA	1460	C	Sidechain
21	AA	1464	U	Sidechain
21	AA	147	G	Sidechain
21	AA	1485	U	Sidechain
21	AA	1494	G	Sidechain
21	AA	1502	A	Sidechain
21	AA	1503	A	Sidechain
21	AA	1506	U	Sidechain
21	AA	1514	G	Sidechain
21	AA	1515	G	Sidechain
21	AA	1517	G	Sidechain
21	AA	1525	G	Sidechain
21	AA	1527	U	Sidechain
21	AA	159	G	Sidechain
21	AA	161	A	Sidechain
21	AA	181	A	Sidechain
21	AA	182	A	Sidechain
21	AA	185	U	Sidechain
21	AA	187	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	197	A	Sidechain
21	AA	200	G	Sidechain
21	AA	204	G	Sidechain
21	AA	208	U	Sidechain
21	AA	210	C	Sidechain
21	AA	211	G	Sidechain
21	AA	212	G	Sidechain
21	AA	213	G	Sidechain
21	AA	221	C	Sidechain
21	AA	229	U	Sidechain
21	AA	236	A	Sidechain
21	AA	239	U	Sidechain
21	AA	243	A	Sidechain
21	AA	25	C	Sidechain
21	AA	252	U	Sidechain
21	AA	255	G	Sidechain
21	AA	258	G	Sidechain
21	AA	26	A	Sidechain
21	AA	260	G	Sidechain
21	AA	261	U	Sidechain
21	AA	264	C	Sidechain
21	AA	269	C	Sidechain
21	AA	27	G	Sidechain
21	AA	275	G	Sidechain
21	AA	279	A	Sidechain
21	AA	281	G	Sidechain
21	AA	284	C	Sidechain
21	AA	291	U	Sidechain
21	AA	294	U	Sidechain
21	AA	297	G	Sidechain
21	AA	299	G	Sidechain
21	AA	30	U	Sidechain
21	AA	31	G	Sidechain
21	AA	310	G	Sidechain
21	AA	315	A	Sidechain
21	AA	318	G	Sidechain
21	AA	32	A	Sidechain
21	AA	321	A	Sidechain
21	AA	323	U	Sidechain
21	AA	324	G	Sidechain
21	AA	326	G	Sidechain
21	AA	327	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	328	C	Sidechain
21	AA	336	A	Sidechain
21	AA	339	C	Sidechain
21	AA	341	C	Sidechain
21	AA	348	G	Sidechain
21	AA	351	G	Sidechain
21	AA	354	G	Sidechain
21	AA	356	A	Sidechain
21	AA	360	G	Sidechain
21	AA	362	G	Sidechain
21	AA	363	A	Sidechain
21	AA	367	U	Sidechain
21	AA	376	G	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	383	A	Sidechain
21	AA	387	U	Sidechain
21	AA	391	G	Sidechain
21	AA	395	C	Sidechain
21	AA	402	G	Sidechain
21	AA	404	G	Sidechain
21	AA	405	U	Sidechain
21	AA	408	A	Sidechain
21	AA	409	U	Sidechain
21	AA	414	A	Sidechain
21	AA	421	U	Sidechain
21	AA	423	G	Sidechain
21	AA	428	G	Sidechain
21	AA	429	U	Sidechain
21	AA	432	A	Sidechain
21	AA	433	G	Sidechain
21	AA	439	U	Sidechain
21	AA	44	A	Sidechain
21	AA	448	A	Sidechain
21	AA	453	G	Sidechain
21	AA	456	A	Sidechain
21	AA	457	G	Sidechain
21	AA	468	A	Sidechain
21	AA	471	U	Sidechain
21	AA	474	G	Sidechain
21	AA	475	C	Sidechain
21	AA	476	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	48	C	Sidechain
21	AA	480	U	Sidechain
21	AA	485	U	Sidechain
21	AA	492	C	Sidechain
21	AA	493	A	Sidechain
21	AA	494	G	Sidechain
21	AA	499	A	Sidechain
21	AA	5	U	Sidechain
21	AA	507	C	Sidechain
21	AA	51	A	Sidechain
21	AA	510	A	Sidechain
21	AA	515	G	Sidechain
21	AA	519	C	Sidechain
21	AA	525	C	Sidechain
21	AA	528	C	Sidechain
21	AA	529	G	Sidechain
21	AA	533	A	Sidechain
21	AA	537	G	Sidechain
21	AA	553	A	Sidechain
21	AA	557	G	Sidechain
21	AA	566	G	Sidechain
21	AA	573	A	Sidechain
21	AA	575	G	Sidechain
21	AA	577	G	Sidechain
21	AA	583	A	Sidechain
21	AA	592	G	Sidechain
21	AA	593	U	Sidechain
21	AA	6	G	Sidechain
21	AA	606	G	Sidechain
21	AA	612	C	Sidechain
21	AA	622	A	Sidechain
21	AA	624	C	Sidechain
21	AA	632	U	Sidechain
21	AA	641	U	Sidechain
21	AA	642	A	Sidechain
21	AA	651	C	Sidechain
21	AA	653	U	Sidechain
21	AA	663	A	Sidechain
21	AA	664	G	Sidechain
21	AA	68	G	Sidechain
21	AA	680	C	Sidechain
21	AA	682	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	686	U	Sidechain
21	AA	687	A	Sidechain
21	AA	688	G	Sidechain
21	AA	69	G	Sidechain
21	AA	694	A	Sidechain
21	AA	698	G	Sidechain
21	AA	702	A	Sidechain
21	AA	707	U	Sidechain
21	AA	708	C	Sidechain
21	AA	715	A	Sidechain
21	AA	721	G	Sidechain
21	AA	722	G	Sidechain
21	AA	724	G	Sidechain
21	AA	727	G	Sidechain
21	AA	73	C	Sidechain
21	AA	731	G	Sidechain
21	AA	733	G	Sidechain
21	AA	736	C	Sidechain
21	AA	737	C	Sidechain
21	AA	738	C	Sidechain
21	AA	739	C	Sidechain
21	AA	741	G	Sidechain
21	AA	742	G	Sidechain
21	AA	743	A	Sidechain
21	AA	752	G	Sidechain
21	AA	754	C	Sidechain
21	AA	76	G	Sidechain
21	AA	761	G	Sidechain
21	AA	775	G	Sidechain
21	AA	781	A	Sidechain
21	AA	788	U	Sidechain
21	AA	789	U	Sidechain
21	AA	79	G	Sidechain
21	AA	8	A	Sidechain
21	AA	800	G	Sidechain
21	AA	804	U	Sidechain
21	AA	809	G	Sidechain
21	AA	812	G	Sidechain
21	AA	817	C	Sidechain
21	AA	818	G	Sidechain
21	AA	819	A	Sidechain
21	AA	826	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	838	G	Sidechain
21	AA	840	C	Sidechain
21	AA	855	U	Sidechain
21	AA	859	G	Sidechain
21	AA	86	G	Sidechain
21	AA	864	A	Sidechain
21	AA	868	C	Sidechain
21	AA	869	G	Sidechain
21	AA	87	C	Sidechain
21	AA	871	U	Sidechain
21	AA	872	A	Sidechain
21	AA	873	A	Sidechain
21	AA	875	U	Sidechain
21	AA	882	C	Sidechain
21	AA	884	U	Sidechain
21	AA	886	G	Sidechain
21	AA	890	G	Sidechain
21	AA	891	U	Sidechain
21	AA	892	A	Sidechain
21	AA	898	G	Sidechain
21	AA	899	C	Sidechain
21	AA	905	U	Sidechain
21	AA	906	A	Sidechain
21	AA	91	U	Sidechain
21	AA	914	A	Sidechain
21	AA	915	A	Sidechain
21	AA	916	U	Sidechain
21	AA	919	A	Sidechain
21	AA	922	G	Sidechain
21	AA	925	G	Sidechain
21	AA	932	C	Sidechain
21	AA	933	G	Sidechain
21	AA	939	G	Sidechain
21	AA	941	G	Sidechain
21	AA	946	A	Sidechain
21	AA	948	C	Sidechain
21	AA	95	C	Sidechain
21	AA	953	G	Sidechain
21	AA	954	G	Sidechain
21	AA	955	U	Sidechain
21	AA	957	U	Sidechain
21	AA	958	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	962	C	Sidechain
21	AA	966	G	Sidechain
21	AA	973	G	Sidechain
21	AA	979	C	Sidechain
21	AA	980	C	Sidechain
21	AA	983	A	Sidechain
21	AA	987	G	Sidechain
21	AA	99	C	Sidechain
21	AA	995	C	Sidechain
1	AB	20	ARG	Sidechain
2	AC	178	ARG	Sidechain
5	AF	4	TYR	Sidechain
10	AK	121	ARG	Peptide
14	AO	43	ALA	Peptide
54	BA	10	A	Sidechain
54	BA	1006	C	Sidechain
54	BA	1012	U	Sidechain
54	BA	1013	C	Sidechain
54	BA	1019	U	Sidechain
54	BA	102	U	Sidechain
54	BA	1023	U	Sidechain
54	BA	103	A	Sidechain
54	BA	1034	G	Sidechain
54	BA	1042	G	Sidechain
54	BA	1044	C	Sidechain
54	BA	1046	A	Sidechain
54	BA	1047	G	Sidechain
54	BA	105	C	Sidechain
54	BA	1054	A	Sidechain
54	BA	1055	G	Sidechain
54	BA	1059	G	Sidechain
54	BA	1062	G	Sidechain
54	BA	1068	G	Sidechain
54	BA	1071	G	Sidechain
54	BA	1072	C	Sidechain
54	BA	1073	A	Sidechain
54	BA	1077	A	Sidechain
54	BA	108	G	Sidechain
54	BA	1089	A	Sidechain
54	BA	1092	C	Sidechain
54	BA	1093	G	Sidechain
54	BA	1099	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	11	C	Sidechain
54	BA	1101	U	Sidechain
54	BA	1103	A	Sidechain
54	BA	1106	G	Sidechain
54	BA	1107	G	Sidechain
54	BA	1108	U	Sidechain
54	BA	1113	U	Sidechain
54	BA	1125	G	Sidechain
54	BA	1130	U	Sidechain
54	BA	1136	G	Sidechain
54	BA	1137	G	Sidechain
54	BA	114	U	Sidechain
54	BA	1141	U	Sidechain
54	BA	1143	A	Sidechain
54	BA	1145	C	Sidechain
54	BA	1146	C	Sidechain
54	BA	1147	A	Sidechain
54	BA	1150	C	Sidechain
54	BA	1154	G	Sidechain
54	BA	1160	G	Sidechain
54	BA	1162	G	Sidechain
54	BA	1167	C	Sidechain
54	BA	1182	G	Sidechain
54	BA	1185	G	Sidechain
54	BA	1186	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	1190	G	Sidechain
54	BA	1191	G	Sidechain
54	BA	1192	G	Sidechain
54	BA	1197	G	Sidechain
54	BA	1199	U	Sidechain
54	BA	12	U	Sidechain
54	BA	1206	G	Sidechain
54	BA	1208	C	Sidechain
54	BA	1215	G	Sidechain
54	BA	1219	U	Sidechain
54	BA	1220	G	Sidechain
54	BA	1221	C	Sidechain
54	BA	1223	G	Sidechain
54	BA	1235	G	Sidechain
54	BA	1240	U	Sidechain
54	BA	1244	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1245	G	Sidechain
54	BA	1255	U	Sidechain
54	BA	1257	C	Sidechain
54	BA	1258	U	Sidechain
54	BA	1261	C	Sidechain
54	BA	1266	G	Sidechain
54	BA	1268	A	Sidechain
54	BA	127	A	Sidechain
54	BA	1275	A	Sidechain
54	BA	1276	A	Sidechain
54	BA	1280	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	1284	A	Sidechain
54	BA	1285	A	Sidechain
54	BA	1291	C	Sidechain
54	BA	1293	C	Sidechain
54	BA	1299	G	Sidechain
54	BA	1301	A	Sidechain
54	BA	1309	G	Sidechain
54	BA	1311	G	Sidechain
54	BA	1314	C	Sidechain
54	BA	1315	C	Sidechain
54	BA	1319	C	Sidechain
54	BA	132	G	Sidechain
54	BA	1320	C	Sidechain
54	BA	1323	C	Sidechain
54	BA	1325	U	Sidechain
54	BA	1328	A	Sidechain
54	BA	1330	C	Sidechain
54	BA	1332	G	Sidechain
54	BA	1333	G	Sidechain
54	BA	1336	A	Sidechain
54	BA	1337	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1343	G	Sidechain
54	BA	1355	G	Sidechain
54	BA	1359	A	Sidechain
54	BA	1364	G	Sidechain
54	BA	1365	A	Sidechain
54	BA	1366	A	Sidechain
54	BA	1368	G	Sidechain
54	BA	1373	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1376	C	Sidechain
54	BA	1378	A	Sidechain
54	BA	1379	U	Sidechain
54	BA	138	U	Sidechain
54	BA	1380	G	Sidechain
54	BA	1382	G	Sidechain
54	BA	1386	C	Sidechain
54	BA	1388	G	Sidechain
54	BA	1391	U	Sidechain
54	BA	1396	U	Sidechain
54	BA	1397	U	Sidechain
54	BA	1401	G	Sidechain
54	BA	1407	G	Sidechain
54	BA	142	A	Sidechain
54	BA	1420	A	Sidechain
54	BA	1424	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1431	A	Sidechain
54	BA	1435	G	Sidechain
54	BA	1439	A	Sidechain
54	BA	1441	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1452	G	Sidechain
54	BA	1454	C	Sidechain
54	BA	1455	G	Sidechain
54	BA	1456	G	Sidechain
54	BA	1459	G	Sidechain
54	BA	146	A	Sidechain
54	BA	1461	C	Sidechain
54	BA	1464	G	Sidechain
54	BA	1469	A	Sidechain
54	BA	1476	U	Sidechain
54	BA	148	U	Sidechain
54	BA	1493	C	Sidechain
54	BA	1495	A	Sidechain
54	BA	1497	U	Sidechain
54	BA	1509	A	Sidechain
54	BA	1515	A	Sidechain
54	BA	1517	G	Sidechain
54	BA	1519	G	Sidechain
54	BA	1526	C	Sidechain
54	BA	1529	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1531	C	Sidechain
54	BA	1534	U	Sidechain
54	BA	1539	U	Sidechain
54	BA	1540	G	Sidechain
54	BA	1541	C	Sidechain
54	BA	1543	G	Sidechain
54	BA	1550	C	Sidechain
54	BA	1552	A	Sidechain
54	BA	1555	G	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1565	C	Sidechain
54	BA	1575	C	Sidechain
54	BA	1580	A	Sidechain
54	BA	1581	G	Sidechain
54	BA	1584	U	Sidechain
54	BA	1585	C	Sidechain
54	BA	1588	G	Sidechain
54	BA	1589	U	Sidechain
54	BA	1594	U	Sidechain
54	BA	1595	C	Sidechain
54	BA	1602	U	Sidechain
54	BA	1603	A	Sidechain
54	BA	1604	C	Sidechain
54	BA	161	A	Sidechain
54	BA	1611	C	Sidechain
54	BA	1616	A	Sidechain
54	BA	162	U	Sidechain
54	BA	1620	G	Sidechain
54	BA	1626	A	Sidechain
54	BA	1632	A	Sidechain
54	BA	1633	G	Sidechain
54	BA	1637	A	Sidechain
54	BA	164	C	Sidechain
54	BA	1641	A	Sidechain
54	BA	1644	C	Sidechain
54	BA	1653	G	Sidechain
54	BA	1655	A	Sidechain
54	BA	1670	C	Sidechain
54	BA	1671	U	Sidechain
54	BA	1672	A	Sidechain
54	BA	1673	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	168	G	Sidechain
54	BA	1681	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1683	U	Sidechain
54	BA	1684	G	Sidechain
54	BA	1687	G	Sidechain
54	BA	1695	G	Sidechain
54	BA	1699	G	Sidechain
54	BA	170	U	Sidechain
54	BA	1708	C	Sidechain
54	BA	1710	G	Sidechain
54	BA	1711	A	Sidechain
54	BA	1713	A	Sidechain
54	BA	1721	G	Sidechain
54	BA	1725	U	Sidechain
54	BA	1731	G	Sidechain
54	BA	1741	C	Sidechain
54	BA	1743	G	Sidechain
54	BA	1747	U	Sidechain
54	BA	1753	G	Sidechain
54	BA	1758	U	Sidechain
54	BA	176	A	Sidechain
54	BA	1762	A	Sidechain
54	BA	1763	G	Sidechain
54	BA	177	G	Sidechain
54	BA	1775	U	Sidechain
54	BA	1782	U	Sidechain
54	BA	1784	A	Sidechain
54	BA	1785	A	Sidechain
54	BA	1796	U	Sidechain
54	BA	1802	A	Sidechain
54	BA	1804	C	Sidechain
54	BA	1807	G	Sidechain
54	BA	1819	A	Sidechain
54	BA	182	A	Sidechain
54	BA	1820	U	Sidechain
54	BA	1822	C	Sidechain
54	BA	1830	C	Sidechain
54	BA	1834	U	Sidechain
54	BA	1835	G	Sidechain
54	BA	1844	C	Sidechain
54	BA	1852	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1854	A	Sidechain
54	BA	1857	G	Sidechain
54	BA	1860	G	Sidechain
54	BA	1865	U	Sidechain
54	BA	1870	C	Sidechain
54	BA	1883	U	Sidechain
54	BA	1884	G	Sidechain
54	BA	1885	A	Sidechain
54	BA	1888	G	Sidechain
54	BA	189	G	Sidechain
54	BA	1891	G	Sidechain
54	BA	1892	C	Sidechain
54	BA	1893	C	Sidechain
54	BA	1895	C	Sidechain
54	BA	19	A	Sidechain
54	BA	190	A	Sidechain
54	BA	1908	C	Sidechain
54	BA	191	A	Sidechain
54	BA	1910	G	Sidechain
54	BA	1914	C	Sidechain
54	BA	1915	U	Sidechain
54	BA	1918	A	Sidechain
54	BA	1919	A	Sidechain
54	BA	1929	G	Sidechain
54	BA	1931	U	Sidechain
54	BA	1932	A	Sidechain
54	BA	1938	A	Sidechain
54	BA	1946	U	Sidechain
54	BA	1947	C	Sidechain
54	BA	1954	G	Sidechain
54	BA	1955	U	Sidechain
54	BA	1959	G	Sidechain
54	BA	1963	U	Sidechain
54	BA	1964	G	Sidechain
54	BA	1968	G	Sidechain
54	BA	197	A	Sidechain
54	BA	1972	G	Sidechain
54	BA	1974	C	Sidechain
54	BA	1976	U	Sidechain
54	BA	198	C	Sidechain
54	BA	1982	U	Sidechain
54	BA	1993	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1997	C	Sidechain
54	BA	200	U	Sidechain
54	BA	2006	C	Sidechain
54	BA	2014	A	Sidechain
54	BA	2017	U	Sidechain
54	BA	2018	G	Sidechain
54	BA	2019	A	Sidechain
54	BA	202	U	Sidechain
54	BA	2020	A	Sidechain
54	BA	2022	U	Sidechain
54	BA	2023	C	Sidechain
54	BA	2024	G	Sidechain
54	BA	2027	G	Sidechain
54	BA	2030	A	Sidechain
54	BA	2034	U	Sidechain
54	BA	2035	G	Sidechain
54	BA	2037	A	Sidechain
54	BA	2044	C	Sidechain
54	BA	2046	G	Sidechain
54	BA	2057	G	Sidechain
54	BA	2060	A	Sidechain
54	BA	2061	G	Sidechain
54	BA	2062	A	Sidechain
54	BA	2074	U	Sidechain
54	BA	2076	U	Sidechain
54	BA	2077	A	Sidechain
54	BA	2078	C	Sidechain
54	BA	2082	A	Sidechain
54	BA	2086	U	Sidechain
54	BA	2088	A	Sidechain
54	BA	209	C	Sidechain
54	BA	2095	A	Sidechain
54	BA	2097	A	Sidechain
54	BA	2099	U	Sidechain
54	BA	2100	G	Sidechain
54	BA	2104	C	Sidechain
54	BA	2112	G	Sidechain
54	BA	2117	A	Sidechain
54	BA	2119	A	Sidechain
54	BA	2120	G	Sidechain
54	BA	2133	G	Sidechain
54	BA	2135	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2138	G	Sidechain
54	BA	214	G	Sidechain
54	BA	2141	G	Sidechain
54	BA	2145	C	Sidechain
54	BA	2147	A	Sidechain
54	BA	2148	G	Sidechain
54	BA	215	G	Sidechain
54	BA	2150	C	Sidechain
54	BA	2156	G	Sidechain
54	BA	2158	A	Sidechain
54	BA	2163	A	Sidechain
54	BA	2168	G	Sidechain
54	BA	2178	C	Sidechain
54	BA	2180	U	Sidechain
54	BA	2183	A	Sidechain
54	BA	2186	G	Sidechain
54	BA	2187	U	Sidechain
54	BA	219	A	Sidechain
54	BA	2197	U	Sidechain
54	BA	22	C	Sidechain
54	BA	2202	U	Sidechain
54	BA	2208	C	Sidechain
54	BA	2212	A	Sidechain
54	BA	2213	U	Sidechain
54	BA	2216	G	Sidechain
54	BA	2226	C	Sidechain
54	BA	2229	U	Sidechain
54	BA	2240	U	Sidechain
54	BA	2242	G	Sidechain
54	BA	2244	U	Sidechain
54	BA	2247	A	Sidechain
54	BA	2254	C	Sidechain
54	BA	2257	U	Sidechain
54	BA	2264	C	Sidechain
54	BA	2268	A	Sidechain
54	BA	2273	A	Sidechain
54	BA	2275	C	Sidechain
54	BA	2281	A	Sidechain
54	BA	2282	G	Sidechain
54	BA	2288	A	Sidechain
54	BA	2294	G	Sidechain
54	BA	2296	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	23	G	Sidechain
54	BA	2301	C	Sidechain
54	BA	2303	G	Sidechain
54	BA	2305	U	Sidechain
54	BA	232	G	Sidechain
54	BA	2323	G	Sidechain
54	BA	2324	U	Sidechain
54	BA	2326	C	Sidechain
54	BA	2327	A	Sidechain
54	BA	2328	A	Sidechain
54	BA	233	A	Sidechain
54	BA	2336	A	Sidechain
54	BA	2338	C	Sidechain
54	BA	2340	A	Sidechain
54	BA	2352	A	Sidechain
54	BA	2357	G	Sidechain
54	BA	2365	G	Sidechain
54	BA	2366	A	Sidechain
54	BA	237	C	Sidechain
54	BA	2371	G	Sidechain
54	BA	2375	G	Sidechain
54	BA	2377	A	Sidechain
54	BA	2378	A	Sidechain
54	BA	2382	G	Sidechain
54	BA	2384	U	Sidechain
54	BA	2385	C	Sidechain
54	BA	2389	G	Sidechain
54	BA	2390	U	Sidechain
54	BA	2391	G	Sidechain
54	BA	2401	U	Sidechain
54	BA	2402	U	Sidechain
54	BA	2403	C	Sidechain
54	BA	2418	A	Sidechain
54	BA	2421	G	Sidechain
54	BA	2424	C	Sidechain
54	BA	2425	A	Sidechain
54	BA	2429	G	Sidechain
54	BA	2431	U	Sidechain
54	BA	2433	A	Sidechain
54	BA	2434	A	Sidechain
54	BA	2437	G	Sidechain
54	BA	2439	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2444	G	Sidechain
54	BA	2447	G	Sidechain
54	BA	2448	A	Sidechain
54	BA	2452	C	Sidechain
54	BA	2453	A	Sidechain
54	BA	2458	G	Sidechain
54	BA	2460	U	Sidechain
54	BA	2469	A	Sidechain
54	BA	247	G	Sidechain
54	BA	2472	G	Sidechain
54	BA	2475	C	Sidechain
54	BA	2477	U	Sidechain
54	BA	248	G	Sidechain
54	BA	2481	G	Sidechain
54	BA	2483	C	Sidechain
54	BA	2485	G	Sidechain
54	BA	2489	U	Sidechain
54	BA	249	C	Sidechain
54	BA	2491	U	Sidechain
54	BA	2494	G	Sidechain
54	BA	2495	G	Sidechain
54	BA	2497	A	Sidechain
54	BA	2498	C	Sidechain
54	BA	250	G	Sidechain
54	BA	2504	U	Sidechain
54	BA	2512	C	Sidechain
54	BA	2513	A	Sidechain
54	BA	2517	C	Sidechain
54	BA	2518	A	Sidechain
54	BA	2529	G	Sidechain
54	BA	2531	A	Sidechain
54	BA	2559	C	Sidechain
54	BA	2563	U	Sidechain
54	BA	2571	U	Sidechain
54	BA	2576	G	Sidechain
54	BA	2577	A	Sidechain
54	BA	2580	U	Sidechain
54	BA	2581	G	Sidechain
54	BA	2582	G	Sidechain
54	BA	2595	G	Sidechain
54	BA	2596	U	Sidechain
54	BA	26	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2601	C	Sidechain
54	BA	2602	A	Sidechain
54	BA	2608	G	Sidechain
54	BA	2615	U	Sidechain
54	BA	2620	C	Sidechain
54	BA	2621	G	Sidechain
54	BA	2624	G	Sidechain
54	BA	2625	G	Sidechain
54	BA	2626	C	Sidechain
54	BA	2627	G	Sidechain
54	BA	2635	A	Sidechain
54	BA	2644	G	Sidechain
54	BA	2645	G	Sidechain
54	BA	2647	U	Sidechain
54	BA	2651	C	Sidechain
54	BA	2653	U	Sidechain
54	BA	2656	U	Sidechain
54	BA	2657	A	Sidechain
54	BA	2659	G	Sidechain
54	BA	2661	G	Sidechain
54	BA	2662	A	Sidechain
54	BA	2669	G	Sidechain
54	BA	2674	G	Sidechain
54	BA	2679	A	Sidechain
54	BA	2680	U	Sidechain
54	BA	2682	A	Sidechain
54	BA	2696	U	Sidechain
54	BA	27	G	Sidechain
54	BA	2703	C	Sidechain
54	BA	271	G	Sidechain
54	BA	2718	G	Sidechain
54	BA	2719	G	Sidechain
54	BA	2722	G	Sidechain
54	BA	2723	C	Sidechain
54	BA	2727	A	Sidechain
54	BA	2732	G	Sidechain
54	BA	2735	G	Sidechain
54	BA	2741	A	Sidechain
54	BA	2747	G	Sidechain
54	BA	2751	G	Sidechain
54	BA	2752	C	Sidechain
54	BA	276	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2763	G	Sidechain
54	BA	277	G	Sidechain
54	BA	2770	G	Sidechain
54	BA	2771	C	Sidechain
54	BA	2780	G	Sidechain
54	BA	2781	A	Sidechain
54	BA	2784	U	Sidechain
54	BA	279	A	Sidechain
54	BA	2799	A	Sidechain
54	BA	28	A	Sidechain
54	BA	2806	C	Sidechain
54	BA	2814	A	Sidechain
54	BA	2816	G	Sidechain
54	BA	2817	U	Sidechain
54	BA	2818	U	Sidechain
54	BA	2822	G	Sidechain
54	BA	283	G	Sidechain
54	BA	2831	G	Sidechain
54	BA	2835	A	Sidechain
54	BA	2842	G	Sidechain
54	BA	2847	U	Sidechain
54	BA	2854	G	Sidechain
54	BA	2857	G	Sidechain
54	BA	2864	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	2881	U	Sidechain
54	BA	2883	A	Sidechain
54	BA	2885	G	Sidechain
54	BA	2889	C	Sidechain
54	BA	289	G	Sidechain
54	BA	291	G	Sidechain
54	BA	30	G	Sidechain
54	BA	301	G	Sidechain
54	BA	307	G	Sidechain
54	BA	310	A	Sidechain
54	BA	313	G	Sidechain
54	BA	316	C	Sidechain
54	BA	321	U	Sidechain
54	BA	325	G	Sidechain
54	BA	327	G	Sidechain
54	BA	33	C	Sidechain
54	BA	338	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	339	U	Sidechain
54	BA	341	C	Sidechain
54	BA	345	A	Sidechain
54	BA	347	A	Sidechain
54	BA	352	A	Sidechain
54	BA	361	G	Sidechain
54	BA	362	A	Sidechain
54	BA	363	G	Sidechain
54	BA	365	U	Sidechain
54	BA	372	G	Sidechain
54	BA	378	C	Sidechain
54	BA	381	G	Sidechain
54	BA	383	C	Sidechain
54	BA	385	C	Sidechain
54	BA	389	G	Sidechain
54	BA	392	U	Sidechain
54	BA	393	C	Sidechain
54	BA	394	C	Sidechain
54	BA	395	U	Sidechain
54	BA	400	G	Sidechain
54	BA	403	U	Sidechain
54	BA	404	A	Sidechain
54	BA	405	U	Sidechain
54	BA	415	A	Sidechain
54	BA	416	U	Sidechain
54	BA	417	C	Sidechain
54	BA	420	C	Sidechain
54	BA	426	C	Sidechain
54	BA	428	A	Sidechain
54	BA	43	G	Sidechain
54	BA	430	A	Sidechain
54	BA	437	U	Sidechain
54	BA	44	A	Sidechain
54	BA	444	C	Sidechain
54	BA	447	A	Sidechain
54	BA	458	G	Sidechain
54	BA	463	G	Sidechain
54	BA	464	U	Sidechain
54	BA	470	A	Sidechain
54	BA	473	G	Sidechain
54	BA	476	G	Sidechain
54	BA	479	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	481	G	Sidechain
54	BA	483	A	Sidechain
54	BA	484	C	Sidechain
54	BA	488	G	Sidechain
54	BA	491	G	Sidechain
54	BA	500	G	Sidechain
54	BA	505	A	Sidechain
54	BA	507	A	Sidechain
54	BA	515	A	Sidechain
54	BA	520	G	Sidechain
54	BA	526	A	Sidechain
54	BA	530	G	Sidechain
54	BA	531	C	Sidechain
54	BA	533	G	Sidechain
54	BA	535	G	Sidechain
54	BA	537	G	Sidechain
54	BA	545	U	Sidechain
54	BA	546	U	Sidechain
54	BA	547	A	Sidechain
54	BA	551	G	Sidechain
54	BA	554	U	Sidechain
54	BA	584	C	Sidechain
54	BA	586	A	Sidechain
54	BA	587	C	Sidechain
54	BA	597	G	Sidechain
54	BA	600	G	Sidechain
54	BA	607	U	Sidechain
54	BA	608	A	Sidechain
54	BA	611	C	Sidechain
54	BA	612	G	Sidechain
54	BA	617	G	Sidechain
54	BA	620	G	Sidechain
54	BA	621	A	Sidechain
54	BA	626	A	Sidechain
54	BA	628	G	Sidechain
54	BA	630	G	Sidechain
54	BA	644	A	Sidechain
54	BA	646	U	Sidechain
54	BA	647	G	Sidechain
54	BA	650	C	Sidechain
54	BA	655	A	Sidechain
54	BA	659	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	669	G	Sidechain
54	BA	677	A	Sidechain
54	BA	679	C	Sidechain
54	BA	680	C	Sidechain
54	BA	681	G	Sidechain
54	BA	683	U	Sidechain
54	BA	686	U	Sidechain
54	BA	687	C	Sidechain
54	BA	695	G	Sidechain
54	BA	7	G	Sidechain
54	BA	701	G	Sidechain
54	BA	703	U	Sidechain
54	BA	704	G	Sidechain
54	BA	715	A	Sidechain
54	BA	719	C	Sidechain
54	BA	722	A	Sidechain
54	BA	726	G	Sidechain
54	BA	728	G	Sidechain
54	BA	730	A	Sidechain
54	BA	736	C	Sidechain
54	BA	740	C	Sidechain
54	BA	75	G	Sidechain
54	BA	756	A	Sidechain
54	BA	757	G	Sidechain
54	BA	759	G	Sidechain
54	BA	765	C	Sidechain
54	BA	768	G	Sidechain
54	BA	774	G	Sidechain
54	BA	775	G	Sidechain
54	BA	778	G	Sidechain
54	BA	78	U	Sidechain
54	BA	780	G	Sidechain
54	BA	783	A	Sidechain
54	BA	784	G	Sidechain
54	BA	795	C	Sidechain
54	BA	799	G	Sidechain
54	BA	801	G	Sidechain
54	BA	807	U	Sidechain
54	BA	808	G	Sidechain
54	BA	811	U	Sidechain
54	BA	812	C	Sidechain
54	BA	827	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	830	G	Sidechain
54	BA	834	G	Sidechain
54	BA	845	A	Sidechain
54	BA	846	U	Sidechain
54	BA	85	G	Sidechain
54	BA	852	U	Sidechain
54	BA	856	G	Sidechain
54	BA	858	G	Sidechain
54	BA	860	U	Sidechain
54	BA	862	G	Sidechain
54	BA	872	U	Sidechain
54	BA	879	G	Sidechain
54	BA	883	G	Sidechain
54	BA	890	C	Sidechain
54	BA	909	A	Sidechain
54	BA	912	C	Sidechain
54	BA	913	U	Sidechain
54	BA	914	G	Sidechain
54	BA	921	C	Sidechain
54	BA	922	C	Sidechain
54	BA	923	G	Sidechain
54	BA	924	G	Sidechain
54	BA	929	U	Sidechain
54	BA	930	G	Sidechain
54	BA	934	U	Sidechain
54	BA	937	C	Sidechain
54	BA	938	G	Sidechain
54	BA	939	G	Sidechain
54	BA	945	A	Sidechain
54	BA	946	C	Sidechain
54	BA	947	A	Sidechain
54	BA	948	C	Sidechain
54	BA	949	G	Sidechain
54	BA	95	A	Sidechain
54	BA	955	U	Sidechain
54	BA	956	G	Sidechain
54	BA	961	C	Sidechain
54	BA	962	G	Sidechain
54	BA	969	G	Sidechain
54	BA	979	A	Sidechain
54	BA	982	C	Sidechain
54	BA	986	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	988	A	Sidechain
54	BA	989	G	Sidechain
54	BA	99	U	Sidechain
54	BA	990	A	Sidechain
54	BA	995	C	Sidechain
55	BB	102	G	Sidechain
55	BB	105	G	Sidechain
55	BB	106	G	Sidechain
55	BB	12	C	Sidechain
55	BB	13	G	Sidechain
55	BB	16	G	Sidechain
55	BB	24	G	Sidechain
55	BB	27	C	Sidechain
55	BB	28	C	Sidechain
55	BB	3	C	Sidechain
55	BB	35	C	Sidechain
55	BB	40	U	Sidechain
55	BB	41	G	Sidechain
55	BB	50	A	Sidechain
55	BB	51	G	Sidechain
55	BB	57	A	Sidechain
55	BB	61	G	Sidechain
55	BB	64	G	Sidechain
55	BB	67	G	Sidechain
55	BB	73	A	Sidechain
55	BB	88	C	Sidechain
26	BD	141	ARG	Sidechain
27	BE	49	ARG	Sidechain
37	BO	102	ARG	Sidechain

5.2 Too-close contacts

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	1	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	1	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16520	1	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	2	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	1	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	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	1	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	1	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	1	0
53	B4	302	0	343	0	0
54	BA	62317	0	31345	4	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99663	16	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BA:889:C:H1'	54:BA:890:C:C6	2.44	0.52
42:BT:19:LYS:HA	42:BT:23:ALA:HB3	1.92	0.52
27:BE:60:TRP:CG	27:BE:61:ARG:H	2.31	0.48
21:AA:577:G:H1'	21:AA:816:A:C4	2.49	0.47
2:AC:149:LYS:HE3	2:AC:200:TRP:CZ3	2.50	0.46
54:BA:680:C:H2'	54:BA:681:G:C8	2.52	0.44
52:B3:25:HIS:CG	52:B3:26:ALA:H	2.36	0.44
54:BA:1130:U:H2'	54:BA:1131:G:H2'	2.00	0.43
9:AJ:56:HIS:CG	9:AJ:57:VAL:H	2.36	0.43
12:AM:40:GLU:CD	12:AM:40:GLU:H	2.27	0.42
35:BM:62:LYS:HE3	35:BM:64:TRP:CZ2	2.54	0.42
25:BC:70:LYS:HE3	25:BC:95:TYR:CZ	2.54	0.42
54:BA:1737:G:H2'	54:BA:1738:G:C2	2.56	0.41
16:AQ:30:HIS:CE1	16:AQ:33:TYR:CD2	3.09	0.41
37:BO:85:LYS:HA	37:BO:85:LYS:HE2	2.03	0.41
25:BC:264:LYS:HE3	25:BC:265:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	202 (93%)	16 (7%)	0	100	100
2	AC	205/208 (99%)	190 (93%)	13 (6%)	2 (1%)	12	49
3	AD	203/206 (98%)	191 (94%)	10 (5%)	2 (1%)	12	49
4	AE	150/152 (99%)	135 (90%)	10 (7%)	5 (3%)	3	21
5	AF	99/101 (98%)	87 (88%)	8 (8%)	4 (4%)	2	18
6	AG	150/152 (99%)	134 (89%)	14 (9%)	2 (1%)	9	42
7	AH	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
8	AI	126/128 (98%)	119 (94%)	4 (3%)	3 (2%)	4	27
9	AJ	98/100 (98%)	93 (95%)	3 (3%)	2 (2%)	6	31
10	AK	116/118 (98%)	105 (90%)	8 (7%)	3 (3%)	4	25
11	AL	121/124 (98%)	106 (88%)	10 (8%)	5 (4%)	2	18
12	AM	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	2	20
13	AN	98/101 (97%)	88 (90%)	8 (8%)	2 (2%)	6	31
14	AO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	3	20
15	AP	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
16	AQ	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	4	26
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	6	34
18	AS	79/81 (98%)	69 (87%)	10 (13%)	0	100	100
19	AT	84/86 (98%)	72 (86%)	10 (12%)	2 (2%)	4	27
20	AU	51/53 (96%)	36 (71%)	11 (22%)	4 (8%)	1	10
25	BC	270/273 (99%)	244 (90%)	22 (8%)	4 (2%)	8	40
26	BD	207/209 (99%)	182 (88%)	19 (9%)	6 (3%)	3	23
27	BE	199/201 (99%)	185 (93%)	7 (4%)	7 (4%)	3	20
28	BF	176/179 (98%)	149 (85%)	16 (9%)	11 (6%)	1	13
29	BG	174/177 (98%)	154 (88%)	18 (10%)	2 (1%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BH	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	18	56
31	BI	139/142 (98%)	125 (90%)	14 (10%)	0	100	100
32	BJ	140/142 (99%)	125 (89%)	10 (7%)	5 (4%)	2	20
33	BK	121/123 (98%)	106 (88%)	9 (7%)	6 (5%)	1	16
34	BL	141/144 (98%)	118 (84%)	15 (11%)	8 (6%)	1	14
35	BM	134/136 (98%)	128 (96%)	2 (2%)	4 (3%)	3	23
36	BN	119/121 (98%)	105 (88%)	13 (11%)	1 (1%)	16	54
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	14	51
38	BP	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	2	20
39	BQ	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
40	BR	101/103 (98%)	88 (87%)	11 (11%)	2 (2%)	6	31
41	BS	108/110 (98%)	100 (93%)	6 (6%)	2 (2%)	6	32
42	BT	92/94 (98%)	75 (82%)	13 (14%)	4 (4%)	2	17
43	BU	101/104 (97%)	85 (84%)	9 (9%)	7 (7%)	1	11
44	BV	92/94 (98%)	88 (96%)	3 (3%)	1 (1%)	11	46
45	BW	78/80 (98%)	60 (77%)	13 (17%)	5 (6%)	1	12
46	BX	75/79 (95%)	67 (89%)	7 (9%)	1 (1%)	9	42
47	BY	61/63 (97%)	53 (87%)	8 (13%)	0	100	100
48	BZ	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	1	15
49	B0	54/57 (95%)	47 (87%)	6 (11%)	1 (2%)	6	32
50	B1	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	2	18
51	B2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	2	17
52	B3	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	7	38
53	B4	36/38 (95%)	28 (78%)	7 (19%)	1 (3%)	4	24
56	B5	221/234 (94%)	205 (93%)	13 (6%)	3 (1%)	9	40
All	All	5876/6008 (98%)	5257 (90%)	478 (8%)	141 (2%)	7	27

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	AG	5	VAL
11	AL	108	ASP
19	AT	9	ARG

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Mol	Chain	Res	Type
26	BD	2	ILE
27	BE	69	ARG
27	BE	170	ARG
28	BF	12	VAL
28	BF	46	LYS
29	BG	8	VAL
32	BJ	81	ILE
33	BK	103	VAL
34	BL	46	VAL
40	BR	82	HIS
42	BT	81	LYS
43	BU	57	ILE
43	BU	95	PHE
45	BW	70	VAL
45	BW	78	PHE
48	BZ	31	ILE
50	B1	50	GLU
52	B3	3	ILE
56	B5	50	ILE
2	AC	14	VAL
2	AC	163	ARG
4	AE	25	LYS
5	AF	6	ILE
5	AF	63	ASN
5	AF	98	GLU
6	AG	6	ILE
8	AI	12	LYS
9	AJ	77	VAL
13	AN	91	GLY
14	AO	43	ALA
14	AO	44	GLU
14	AO	74	VAL
20	AU	32	ARG
25	BC	142	ASN
25	BC	161	VAL
26	BD	37	VAL
26	BD	49	GLN
26	BD	82	PHE
27	BE	61	ARG
28	BF	87	LYS
28	BF	116	LEU
28	BF	136	ILE

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Mol	Chain	Res	Type
30	BH	83	LYS
32	BJ	2	LYS
33	BK	25	LEU
33	BK	32	TYR
34	BL	15	ALA
34	BL	36	LYS
35	BM	20	LEU
38	BP	113	LEU
41	BS	41	LYS
42	BT	63	VAL
43	BU	45	GLN
43	BU	83	GLY
4	AE	127	TYR
8	AI	55	ASP
10	AK	16	SER
10	AK	121	ARG
11	AL	117	GLY
12	AM	112	ARG
16	AQ	82	VAL
19	AT	8	LYS
20	AU	36	PHE
25	BC	191	LEU
26	BD	77	ARG
27	BE	120	VAL
27	BE	188	MET
28	BF	35	LEU
34	BL	11	GLY
35	BM	58	LYS
38	BP	2	ASN
38	BP	112	ARG
40	BR	80	ARG
42	BT	38	ALA
43	BU	43	LYS
43	BU	51	LEU
44	BV	71	LYS
45	BW	52	CYS
46	BX	27	ARG
48	BZ	34	THR
50	B1	45	HIS
56	B5	217	THR
3	AD	28	ASP
4	AE	43	GLY

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Mol	Chain	Res	Type
4	AE	54	GLU
5	AF	68	GLN
11	AL	33	CYS
11	AL	78	VAL
16	AQ	39	ARG
20	AU	33	ARG
26	BD	40	LEU
28	BF	113	PHE
29	BG	112	VAL
32	BJ	25	LEU
34	BL	10	GLU
34	BL	66	PHE
34	BL	69	ARG
34	BL	86	GLU
41	BS	3	THR
42	BT	75	GLY
43	BU	5	ARG
51	B2	4	THR
53	B4	16	ILE
3	AD	3	TYR
10	AK	126	ARG
12	AM	23	GLY
12	AM	65	GLU
13	AN	41	ARG
28	BF	4	HIS
33	BK	2	ILE
35	BM	134	THR
36	BN	8	ARG
37	BO	23	ALA
38	BP	69	VAL
45	BW	35	ILE
45	BW	74	LYS
56	B5	168	ASN
11	AL	101	LEU
28	BF	133	GLU
32	BJ	45	THR
32	BJ	72	LYS
48	BZ	9	THR
4	AE	93	VAL
17	AR	20	ILE
9	AJ	74	VAL
28	BF	148	VAL

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Mol	Chain	Res	Type
8	AI	57	VAL
25	BC	123	ILE
27	BE	187	VAL
28	BF	43	ILE
33	BK	47	ILE
51	B2	44	VAL
20	AU	27	VAL
27	BE	149	ILE
12	AM	42	VAL
33	BK	71	ARG
35	BM	36	VAL
49	B0	54	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	176 (98%)	4 (2%)	45	64
2	AC	170/171 (99%)	169 (99%)	1 (1%)	78	83
3	AD	172/173 (99%)	169 (98%)	3 (2%)	53	69
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	85 (98%)	2 (2%)	44	64
6	AG	123/123 (100%)	122 (99%)	1 (1%)	73	80
7	AH	104/105 (99%)	103 (99%)	1 (1%)	68	78
8	AI	105/105 (100%)	103 (98%)	2 (2%)	50	67
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	87 (97%)	3 (3%)	33	55
11	AL	103/104 (99%)	102 (99%)	1 (1%)	68	78
12	AM	91/92 (99%)	90 (99%)	1 (1%)	65	76
13	AN	83/84 (99%)	82 (99%)	1 (1%)	63	75
14	AO	76/77 (99%)	74 (97%)	2 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AP	65/65 (100%)	63 (97%)	2 (3%)	35	56
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	47 (98%)	1 (2%)	47	65
18	AS	70/70 (100%)	68 (97%)	2 (3%)	37	58
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	212 (98%)	4 (2%)	50	67
26	BD	164/164 (100%)	161 (98%)	3 (2%)	51	68
27	BE	165/165 (100%)	164 (99%)	1 (1%)	78	83
28	BF	149/150 (99%)	146 (98%)	3 (2%)	48	66
29	BG	137/138 (99%)	135 (98%)	2 (2%)	57	72
30	BH	114/114 (100%)	113 (99%)	1 (1%)	70	79
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	40	62
33	BK	103/103 (100%)	99 (96%)	4 (4%)	28	49
34	BL	102/103 (99%)	99 (97%)	3 (3%)	37	58
35	BM	109/109 (100%)	107 (98%)	2 (2%)	51	68
36	BN	100/100 (100%)	100 (100%)	0	100	100
37	BO	86/87 (99%)	85 (99%)	1 (1%)	63	75
38	BP	99/100 (99%)	97 (98%)	2 (2%)	48	66
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	65	76
40	BR	84/84 (100%)	83 (99%)	1 (1%)	63	75
41	BS	93/93 (100%)	93 (100%)	0	100	100
42	BT	80/80 (100%)	78 (98%)	2 (2%)	42	63
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%)	57 (97%)	2 (3%)	32	54
46	BX	67/68 (98%)	66 (98%)	1 (2%)	57	72
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	47	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	49 (96%)	2 (4%)	28	49
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	171 (99%)	2 (1%)	63	75
All	All	4842/4870 (99%)	4771 (98%)	71 (2%)	55	72

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	38	HIS
1	AB	88	GLN
1	AB	168	GLU
1	AB	189	ASN
2	AC	185	THR
3	AD	139	ASN
3	AD	160	LEU
3	AD	201	GLU
5	AF	5	GLU
5	AF	13	ASP
6	AG	25	PHE
7	AH	12	ARG
8	AI	33	SER
8	AI	112	ARG
10	AK	52	ARG
10	AK	57	SER
10	AK	128	VAL
11	AL	113	ARG
12	AM	40	GLU
13	AN	62	ASN
14	AO	41	HIS
14	AO	60	SER
15	AP	6	LEU
15	AP	34	GLU
17	AR	72	ARG
18	AS	2	ARG
18	AS	4	LEU
25	BC	45	ASN
25	BC	73	ILE
25	BC	128	THR

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Mol	Chain	Res	Type
25	BC	173	LEU
26	BD	16	THR
26	BD	58	ASN
26	BD	136	ASN
27	BE	122	GLU
28	BF	88	VAL
28	BF	112	ASP
28	BF	127	TYR
29	BG	127	GLN
29	BG	166	GLU
30	BH	77	THR
32	BJ	15	TRP
32	BJ	44	TYR
32	BJ	98	GLU
33	BK	1	MET
33	BK	30	ARG
33	BK	57	VAL
33	BK	64	ARG
34	BL	36	LYS
34	BL	66	PHE
34	BL	76	GLU
35	BM	97	GLN
35	BM	126	ILE
37	BO	2	ASP
38	BP	29	VAL
38	BP	67	GLU
39	BQ	46	TYR
40	BR	82	HIS
42	BT	2	ILE
42	BT	36	LYS
43	BU	44	HIS
43	BU	61	GLU
44	BV	51	GLN
45	BW	13	ARG
45	BW	23	LYS
46	BX	75	GLU
49	B0	37	HIS
52	B3	5	THR
52	B3	61	LEU
56	B5	33	LEU
56	B5	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54)

such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	108	GLN
1	AB	202	ASN
2	AC	40	GLN
2	AC	68	HIS
4	AE	18	ASN
4	AE	72	ASN
4	AE	76	ASN
4	AE	81	GLN
4	AE	88	HIS
4	AE	120	HIS
4	AE	145	ASN
5	AF	3	HIS
5	AF	94	HIS
7	AH	37	ASN
7	AH	117	GLN
8	AI	74	GLN
10	AK	118	ASN
11	AL	72	ASN
11	AL	95	HIS
15	AP	9	HIS
15	AP	29	ASN
15	AP	40	ASN
16	AQ	49	ASN
18	AS	42	ASN
19	AT	54	GLN
19	AT	67	HIS
25	BC	14	HIS
25	BC	44	ASN
25	BC	114	GLN
25	BC	116	GLN
25	BC	133	ASN
25	BC	199	HIS
26	BD	134	HIS
26	BD	148	GLN
27	BE	195	GLN
28	BF	134	GLN
32	BJ	76	HIS
33	BK	5	GLN
36	BN	11	ASN
36	BN	31	HIS
36	BN	107	ASN
38	BP	6	GLN

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Mol	Chain	Res	Type
38	BP	55	HIS
38	BP	74	GLN
38	BP	76	HIS
39	BQ	36	GLN
41	BS	31	GLN
45	BW	56	HIS
46	BX	15	ASN
46	BX	22	ASN
46	BX	33	HIS
47	BY	36	GLN
47	BY	39	GLN
47	BY	45	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	270 (17%)	90 (5%)
22	A1	75/76 (98%)	9 (12%)	2 (2%)
23	A2	14/15 (93%)	7 (50%)	2 (14%)
24	A3	76/77 (98%)	12 (15%)	5 (6%)
54	BA	2902/2903 (99%)	486 (16%)	137 (4%)
55	BB	116/118 (98%)	12 (10%)	3 (2%)
All	All	4713/4722 (99%)	796 (16%)	239 (5%)

All (796) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	32	A
21	AA	33	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	51	A
21	AA	69	G
21	AA	70	U
21	AA	84	U

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Mol	Chain	Res	Type
21	AA	85	U
21	AA	86	G
21	AA	96	U
21	AA	109	A
21	AA	110	C
21	AA	111	G
21	AA	120	A
21	AA	121	U
21	AA	122	G
21	AA	128	G
21	AA	129	A
21	AA	131	A
21	AA	133	U
21	AA	144	G
21	AA	153	C
21	AA	173	U
21	AA	174	A
21	AA	183	C
21	AA	187	G
21	AA	191	G
21	AA	198	G
21	AA	212	G
21	AA	213	G
21	AA	235	C
21	AA	240	G
21	AA	243	A
21	AA	244	U
21	AA	247	G
21	AA	250	A
21	AA	252	U
21	AA	266	G
21	AA	289	G
21	AA	299	G
21	AA	306	A
21	AA	307	C
21	AA	324	G
21	AA	328	C
21	AA	329	A
21	AA	330	C
21	AA	346	G
21	AA	347	G
21	AA	350	G

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Mol	Chain	Res	Type
21	AA	351	G
21	AA	352	C
21	AA	354	G
21	AA	356	A
21	AA	357	G
21	AA	358	U
21	AA	367	U
21	AA	372	C
21	AA	373	A
21	AA	381	C
21	AA	384	G
21	AA	388	G
21	AA	389	A
21	AA	397	A
21	AA	398	U
21	AA	406	G
21	AA	408	A
21	AA	409	U
21	AA	412	A
21	AA	413	G
21	AA	415	A
21	AA	424	G
21	AA	429	U
21	AA	461	A
21	AA	462	G
21	AA	465	A
21	AA	467	U
21	AA	468	A
21	AA	472	U
21	AA	476	U
21	AA	477	C
21	AA	480	U
21	AA	481	G
21	AA	482	A
21	AA	486	U
21	AA	509	A
21	AA	510	A
21	AA	511	C
21	AA	518	C
21	AA	527	G
21	AA	532	A
21	AA	533	A

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Mol	Chain	Res	Type
21	AA	547	A
21	AA	548	G
21	AA	550	G
21	AA	562	U
21	AA	567	G
21	AA	572	A
21	AA	573	A
21	AA	575	G
21	AA	576	C
21	AA	619	U
21	AA	625	U
21	AA	632	U
21	AA	633	G
21	AA	653	U
21	AA	654	G
21	AA	665	A
21	AA	676	A
21	AA	688	G
21	AA	693	G
21	AA	703	G
21	AA	704	A
21	AA	717	U
21	AA	718	A
21	AA	719	C
21	AA	720	C
21	AA	721	G
21	AA	724	G
21	AA	731	G
21	AA	732	C
21	AA	734	G
21	AA	755	G
21	AA	761	G
21	AA	762	U
21	AA	777	A
21	AA	778	G
21	AA	794	A
21	AA	827	U
21	AA	828	U
21	AA	841	C
21	AA	843	U
21	AA	846	G
21	AA	859	G

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Mol	Chain	Res	Type
21	AA	870	U
21	AA	882	C
21	AA	886	G
21	AA	887	G
21	AA	888	G
21	AA	889	A
21	AA	890	G
21	AA	891	U
21	AA	913	A
21	AA	914	A
21	AA	920	U
21	AA	926	G
21	AA	927	G
21	AA	934	C
21	AA	935	A
21	AA	945	G
21	AA	946	A
21	AA	958	A
21	AA	959	A
21	AA	960	U
21	AA	962	C
21	AA	963	G
21	AA	965	U
21	AA	966	G
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	972	C
21	AA	975	A
21	AA	977	A
21	AA	978	A
21	AA	979	C
21	AA	983	A
21	AA	984	C
21	AA	992	U
21	AA	993	G
21	AA	998	C
21	AA	999	C
21	AA	1004	A
21	AA	1015	G
21	AA	1026	G
21	AA	1030	U

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Mol	Chain	Res	Type
21	AA	1031	C
21	AA	1032	G
21	AA	1037	C
21	AA	1042	A
21	AA	1043	G
21	AA	1050	G
21	AA	1051	C
21	AA	1052	U
21	AA	1053	G
21	AA	1054	C
21	AA	1055	A
21	AA	1058	G
21	AA	1064	G
21	AA	1065	U
21	AA	1066	C
21	AA	1067	A
21	AA	1068	G
21	AA	1086	U
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1112	C
21	AA	1125	U
21	AA	1129	C
21	AA	1130	A
21	AA	1133	G
21	AA	1137	C
21	AA	1139	G
21	AA	1146	A
21	AA	1147	C
21	AA	1159	U
21	AA	1171	A
21	AA	1172	C
21	AA	1182	G
21	AA	1183	U
21	AA	1184	G
21	AA	1185	G
21	AA	1189	U
21	AA	1191	A
21	AA	1192	C
21	AA	1196	A

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Mol	Chain	Res	Type
21	AA	1198	G
21	AA	1201	A
21	AA	1222	G
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1240	U
21	AA	1256	A
21	AA	1257	A
21	AA	1267	C
21	AA	1278	G
21	AA	1279	G
21	AA	1280	A
21	AA	1285	A
21	AA	1286	U
21	AA	1298	U
21	AA	1299	A
21	AA	1300	G
21	AA	1301	U
21	AA	1302	C
21	AA	1303	C
21	AA	1305	G
21	AA	1320	C
21	AA	1323	G
21	AA	1331	G
21	AA	1336	C
21	AA	1337	G
21	AA	1338	G
21	AA	1347	G
21	AA	1379	G
21	AA	1380	U
21	AA	1381	U
21	AA	1396	A
21	AA	1397	C
21	AA	1446	A
21	AA	1447	A
21	AA	1452	C
21	AA	1453	G
21	AA	1491	G
21	AA	1492	A
21	AA	1493	A
21	AA	1494	G

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Mol	Chain	Res	Type
21	AA	1503	A
21	AA	1504	G
21	AA	1506	U
21	AA	1533	C
22	A1	16	C
22	A1	17	U
22	A1	18	G
22	A1	20	G
22	A1	39	G
22	A1	47	U
22	A1	48	C
22	A1	59	U
22	A1	74	C
23	A2	80	C
23	A2	81	U
23	A2	84	G
23	A2	86	U
23	A2	88	U
23	A2	89	U
23	A2	90	U
24	A3	9	G
24	A3	10	G
24	A3	18	U
24	A3	21	H2U
24	A3	31	G
24	A3	32	G
24	A3	34	U
24	A3	35	C
24	A3	48	U
24	A3	74	A
24	A3	76	C
24	A3	77	A
54	BA	12	U
54	BA	28	A
54	BA	29	U
54	BA	34	U
54	BA	45	G
54	BA	71	A
54	BA	72	U
54	BA	74	A
54	BA	75	G
54	BA	77	G

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Mol	Chain	Res	Type
54	BA	85	G
54	BA	86	G
54	BA	91	A
54	BA	92	U
54	BA	98	G
54	BA	100	U
54	BA	101	A
54	BA	102	U
54	BA	103	A
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	142	A
54	BA	143	C
54	BA	144	A
54	BA	145	C
54	BA	148	U
54	BA	181	A
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	223	A
54	BA	224	U
54	BA	233	A
54	BA	242	G
54	BA	248	G
54	BA	249	C
54	BA	252	G
54	BA	265	A
54	BA	266	G
54	BA	278	A
54	BA	279	A
54	BA	280	U
54	BA	294	A
54	BA	301	G
54	BA	321	U
54	BA	330	A

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Mol	Chain	Res	Type
54	BA	331	C
54	BA	332	A
54	BA	333	G
54	BA	335	C
54	BA	338	G
54	BA	346	A
54	BA	347	A
54	BA	370	G
54	BA	386	G
54	BA	388	G
54	BA	389	G
54	BA	411	G
54	BA	412	A
54	BA	428	A
54	BA	429	A
54	BA	443	A
54	BA	455	C
54	BA	457	A
54	BA	467	G
54	BA	477	A
54	BA	478	A
54	BA	479	A
54	BA	481	G
54	BA	504	A
54	BA	505	A
54	BA	508	A
54	BA	512	G
54	BA	527	C
54	BA	529	A
54	BA	531	C
54	BA	532	A
54	BA	533	G
54	BA	546	U
54	BA	548	G
54	BA	549	G
54	BA	550	C
54	BA	555	G
54	BA	556	A
54	BA	569	U
54	BA	570	G
54	BA	573	U
54	BA	575	A

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Mol	Chain	Res	Type
54	BA	587	C
54	BA	589	U
54	BA	603	A
54	BA	613	A
54	BA	614	A
54	BA	615	U
54	BA	617	G
54	BA	620	G
54	BA	631	A
54	BA	632	A
54	BA	634	C
54	BA	637	A
54	BA	653	U
54	BA	662	G
54	BA	671	C
54	BA	672	C
54	BA	675	A
54	BA	680	C
54	BA	686	U
54	BA	687	C
54	BA	695	G
54	BA	719	C
54	BA	724	U
54	BA	725	G
54	BA	728	G
54	BA	730	A
54	BA	736	C
54	BA	747	U
54	BA	752	A
54	BA	753	A
54	BA	762	U
54	BA	763	G
54	BA	764	A
54	BA	775	G
54	BA	776	G
54	BA	782	A
54	BA	784	G
54	BA	789	A
54	BA	790	U
54	BA	792	A
54	BA	793	A
54	BA	794	A

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Mol	Chain	Res	Type
54	BA	805	G
54	BA	809	G
54	BA	814	C
54	BA	815	C
54	BA	827	U
54	BA	846	U
54	BA	855	G
54	BA	857	G
54	BA	858	G
54	BA	888	C
54	BA	889	C
54	BA	890	C
54	BA	896	A
54	BA	910	A
54	BA	914	G
54	BA	915	C
54	BA	924	G
54	BA	931	U
54	BA	932	U
54	BA	933	A
54	BA	934	U
54	BA	941	A
54	BA	946	C
54	BA	957	C
54	BA	958	U
54	BA	959	A
54	BA	961	C
54	BA	974	G
54	BA	975	A
54	BA	982	C
54	BA	983	A
54	BA	984	A
54	BA	985	C
54	BA	995	C
54	BA	1008	A
54	BA	1011	G
54	BA	1012	U
54	BA	1013	C
54	BA	1014	A
54	BA	1022	G
54	BA	1023	U
54	BA	1025	G

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Mol	Chain	Res	Type
54	BA	1026	G
54	BA	1033	U
54	BA	1044	C
54	BA	1056	G
54	BA	1057	A
54	BA	1058	U
54	BA	1063	G
54	BA	1070	A
54	BA	1071	G
54	BA	1073	A
54	BA	1087	G
54	BA	1088	A
54	BA	1089	A
54	BA	1090	A
54	BA	1095	A
54	BA	1096	A
54	BA	1100	C
54	BA	1112	G
54	BA	1128	G
54	BA	1129	A
54	BA	1130	U
54	BA	1132	U
54	BA	1133	A
54	BA	1134	A
54	BA	1135	C
54	BA	1136	G
54	BA	1142	A
54	BA	1143	A
54	BA	1155	A
54	BA	1175	A
54	BA	1176	U
54	BA	1189	A
54	BA	1204	A
54	BA	1211	C
54	BA	1220	G
54	BA	1237	A
54	BA	1238	G
54	BA	1254	A
54	BA	1255	U
54	BA	1256	G
54	BA	1265	A
54	BA	1271	G

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Mol	Chain	Res	Type
54	BA	1272	A
54	BA	1276	A
54	BA	1287	A
54	BA	1288	G
54	BA	1289	C
54	BA	1290	C
54	BA	1291	C
54	BA	1292	G
54	BA	1300	G
54	BA	1301	A
54	BA	1307	A
54	BA	1308	A
54	BA	1312	U
54	BA	1313	U
54	BA	1314	C
54	BA	1315	C
54	BA	1317	G
54	BA	1318	U
54	BA	1324	G
54	BA	1325	U
54	BA	1336	A
54	BA	1341	G
54	BA	1345	C
54	BA	1349	C
54	BA	1350	C
54	BA	1379	U
54	BA	1380	G
54	BA	1388	G
54	BA	1397	U
54	BA	1416	G
54	BA	1417	C
54	BA	1420	A
54	BA	1429	G
54	BA	1458	U
54	BA	1459	G
54	BA	1460	U
54	BA	1482	G
54	BA	1490	A
54	BA	1493	C
54	BA	1508	A
54	BA	1509	A
54	BA	1510	G

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Mol	Chain	Res	Type
54	BA	1523	U
54	BA	1524	G
54	BA	1537	G
54	BA	1539	U
54	BA	1540	G
54	BA	1566	A
54	BA	1568	G
54	BA	1569	A
54	BA	1584	U
54	BA	1598	A
54	BA	1610	A
54	BA	1615	C
54	BA	1616	A
54	BA	1622	G
54	BA	1625	C
54	BA	1627	G
54	BA	1634	A
54	BA	1635	A
54	BA	1645	G
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1668	A
54	BA	1669	A
54	BA	1674	G
54	BA	1703	G
54	BA	1713	A
54	BA	1715	G
54	BA	1729	U
54	BA	1761	C
54	BA	1764	C
54	BA	1773	A
54	BA	1783	A
54	BA	1784	A
54	BA	1791	A
54	BA	1799	G
54	BA	1800	C
54	BA	1802	A
54	BA	1808	A
54	BA	1815	A
54	BA	1816	C
54	BA	1847	A

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Mol	Chain	Res	Type
54	BA	1848	A
54	BA	1870	C
54	BA	1871	A
54	BA	1888	G
54	BA	1900	A
54	BA	1901	A
54	BA	1906	G
54	BA	1913	A
54	BA	1914	C
54	BA	1918	A
54	BA	1919	A
54	BA	1920	C
54	BA	1927	A
54	BA	1928	A
54	BA	1929	G
54	BA	1930	G
54	BA	1937	A
54	BA	1940	U
54	BA	1942	C
54	BA	1953	A
54	BA	1954	G
54	BA	1955	U
54	BA	1956	U
54	BA	1962	C
54	BA	1963	U
54	BA	1965	C
54	BA	1966	A
54	BA	1971	U
54	BA	1972	G
54	BA	1980	G
54	BA	1981	A
54	BA	1993	U
54	BA	1997	C
54	BA	2022	U
54	BA	2023	C
54	BA	2030	A
54	BA	2032	G
54	BA	2034	U
54	BA	2043	C
54	BA	2044	C
54	BA	2051	A
54	BA	2052	A

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Mol	Chain	Res	Type
54	BA	2056	G
54	BA	2060	A
54	BA	2061	G
54	BA	2062	A
54	BA	2076	U
54	BA	2077	A
54	BA	2078	C
54	BA	2092	U
54	BA	2110	G
54	BA	2112	G
54	BA	2113	U
54	BA	2116	G
54	BA	2117	A
54	BA	2118	U
54	BA	2119	A
54	BA	2126	A
54	BA	2127	G
54	BA	2155	U
54	BA	2158	A
54	BA	2159	G
54	BA	2160	C
54	BA	2162	G
54	BA	2163	A
54	BA	2172	U
54	BA	2173	A
54	BA	2177	C
54	BA	2181	U
54	BA	2198	A
54	BA	2199	A
54	BA	2203	U
54	BA	2208	C
54	BA	2211	A
54	BA	2212	A
54	BA	2238	G
54	BA	2239	G
54	BA	2269	G
54	BA	2274	A
54	BA	2276	G
54	BA	2283	C
54	BA	2286	G
54	BA	2287	A
54	BA	2306	C

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Mol	Chain	Res	Type
54	BA	2307	G
54	BA	2308	G
54	BA	2309	A
54	BA	2312	U
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2334	U
54	BA	2335	A
54	BA	2339	C
54	BA	2345	G
54	BA	2347	C
54	BA	2383	G
54	BA	2385	C
54	BA	2390	U
54	BA	2391	G
54	BA	2392	A
54	BA	2394	C
54	BA	2401	U
54	BA	2402	U
54	BA	2403	C
54	BA	2406	A
54	BA	2425	A
54	BA	2426	A
54	BA	2427	C
54	BA	2428	G
54	BA	2429	G
54	BA	2430	A
54	BA	2431	U
54	BA	2432	A
54	BA	2433	A
54	BA	2439	A
54	BA	2440	C
54	BA	2441	U
54	BA	2442	C
54	BA	2443	C
54	BA	2445	G
54	BA	2448	A
54	BA	2470	G
54	BA	2474	U
54	BA	2475	C

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Mol	Chain	Res	Type
54	BA	2486	C
54	BA	2491	U
54	BA	2498	C
54	BA	2499	C
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2504	U
54	BA	2505	G
54	BA	2518	A
54	BA	2532	G
54	BA	2533	U
54	BA	2540	C
54	BA	2542	A
54	BA	2543	G
54	BA	2544	G
54	BA	2554	U
54	BA	2565	A
54	BA	2566	A
54	BA	2573	C
54	BA	2602	A
54	BA	2613	U
54	BA	2614	A
54	BA	2629	U
54	BA	2654	A
54	BA	2655	G
54	BA	2660	A
54	BA	2661	G
54	BA	2666	C
54	BA	2668	G
54	BA	2669	G
54	BA	2689	U
54	BA	2690	U
54	BA	2714	G
54	BA	2732	G
54	BA	2733	A
54	BA	2739	U
54	BA	2751	G
54	BA	2752	C
54	BA	2757	A
54	BA	2764	A
54	BA	2778	A

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Mol	Chain	Res	Type
54	BA	2780	G
54	BA	2791	G
54	BA	2797	U
54	BA	2799	A
54	BA	2816	G
54	BA	2817	U
54	BA	2821	A
54	BA	2850	A
54	BA	2858	C
54	BA	2867	G
54	BA	2884	U
54	BA	2886	A
54	BA	2892	G
54	BA	2893	A
55	BB	13	G
55	BB	14	U
55	BB	15	A
55	BB	35	C
55	BB	42	C
55	BB	44	G
55	BB	45	A
55	BB	48	U
55	BB	74	U
55	BB	88	C
55	BB	89	U
55	BB	109	A

All (239) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	13	U
21	AA	32	A
21	AA	49	U
21	AA	69	G
21	AA	110	C
21	AA	120	A
21	AA	128	G
21	AA	173	U
21	AA	212	G
21	AA	243	A

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Mol	Chain	Res	Type
21	AA	251	G
21	AA	306	A
21	AA	307	C
21	AA	327	A
21	AA	328	C
21	AA	346	G
21	AA	350	G
21	AA	351	G
21	AA	357	G
21	AA	372	C
21	AA	388	G
21	AA	408	A
21	AA	412	A
21	AA	421	U
21	AA	422	C
21	AA	461	A
21	AA	476	U
21	AA	480	U
21	AA	482	A
21	AA	494	G
21	AA	509	A
21	AA	530	G
21	AA	532	A
21	AA	573	A
21	AA	575	G
21	AA	577	G
21	AA	624	C
21	AA	632	U
21	AA	703	G
21	AA	717	U
21	AA	719	C
21	AA	722	G
21	AA	731	G
21	AA	761	G
21	AA	777	A
21	AA	787	A
21	AA	827	U
21	AA	869	G
21	AA	886	G
21	AA	888	G
21	AA	890	G
21	AA	913	A

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Mol	Chain	Res	Type
21	AA	945	G
21	AA	962	C
21	AA	965	U
21	AA	977	A
21	AA	978	A
21	AA	982	U
21	AA	983	A
21	AA	992	U
21	AA	998	C
21	AA	1030	U
21	AA	1042	A
21	AA	1050	G
21	AA	1054	C
21	AA	1065	U
21	AA	1066	C
21	AA	1086	U
21	AA	1101	A
21	AA	1129	C
21	AA	1139	G
21	AA	1146	A
21	AA	1159	U
21	AA	1171	A
21	AA	1182	G
21	AA	1184	G
21	AA	1190	G
21	AA	1191	A
21	AA	1225	A
21	AA	1278	G
21	AA	1279	G
21	AA	1298	U
21	AA	1299	A
21	AA	1336	C
21	AA	1380	U
21	AA	1396	A
21	AA	1452	C
21	AA	1492	A
22	A1	16	C
22	A1	47	U
23	A2	85	G
23	A2	89	U
24	A3	9	G
24	A3	31	G

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Mol	Chain	Res	Type
24	A3	34	U
24	A3	73	A
24	A3	76	C
54	BA	34	U
54	BA	71	A
54	BA	101	A
54	BA	142	A
54	BA	199	A
54	BA	215	G
54	BA	223	A
54	BA	278	A
54	BA	279	A
54	BA	322	A
54	BA	330	A
54	BA	388	G
54	BA	428	A
54	BA	446	G
54	BA	529	A
54	BA	531	C
54	BA	549	G
54	BA	555	G
54	BA	613	A
54	BA	631	A
54	BA	645	C
54	BA	661	A
54	BA	670	A
54	BA	685	A
54	BA	724	U
54	BA	752	A
54	BA	762	U
54	BA	776	G
54	BA	793	A
54	BA	805	G
54	BA	808	G
54	BA	888	C
54	BA	896	A
54	BA	914	G
54	BA	931	U
54	BA	933	A
54	BA	957	C
54	BA	981	A
54	BA	984	A

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Mol	Chain	Res	Type
54	BA	992	C
54	BA	1013	C
54	BA	1022	G
54	BA	1056	G
54	BA	1069	A
54	BA	1071	G
54	BA	1078	U
54	BA	1087	G
54	BA	1089	A
54	BA	1128	G
54	BA	1132	U
54	BA	1185	G
54	BA	1210	G
54	BA	1252	G
54	BA	1254	A
54	BA	1255	U
54	BA	1287	A
54	BA	1289	C
54	BA	1290	C
54	BA	1291	C
54	BA	1300	G
54	BA	1307	A
54	BA	1312	U
54	BA	1314	C
54	BA	1317	G
54	BA	1324	G
54	BA	1340	U
54	BA	1349	C
54	BA	1385	A
54	BA	1419	A
54	BA	1451	C
54	BA	1508	A
54	BA	1509	A
54	BA	1523	U
54	BA	1535	A
54	BA	1539	U
54	BA	1568	G
54	BA	1610	A
54	BA	1615	C
54	BA	1634	A
54	BA	1668	A
54	BA	1760	C

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Mol	Chain	Res	Type
54	BA	1779	U
54	BA	1783	A
54	BA	1799	G
54	BA	1863	G
54	BA	1918	A
54	BA	1919	A
54	BA	1927	A
54	BA	1929	G
54	BA	1936	A
54	BA	1945	G
54	BA	1952	A
54	BA	1954	G
54	BA	1955	U
54	BA	1962	C
54	BA	1980	G
54	BA	2022	U
54	BA	2032	G
54	BA	2035	G
54	BA	2043	C
54	BA	2062	A
54	BA	2076	U
54	BA	2077	A
54	BA	2116	G
54	BA	2117	A
54	BA	2126	A
54	BA	2162	G
54	BA	2198	A
54	BA	2212	A
54	BA	2286	G
54	BA	2288	A
54	BA	2306	C
54	BA	2308	G
54	BA	2351	G
54	BA	2389	G
54	BA	2391	G
54	BA	2401	U
54	BA	2425	A
54	BA	2427	C
54	BA	2430	A
54	BA	2431	U
54	BA	2439	A
54	BA	2442	C

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Mol	Chain	Res	Type
54	BA	2474	U
54	BA	2485	G
54	BA	2503	A
54	BA	2504	U
54	BA	2542	A
54	BA	2543	G
54	BA	2613	U
54	BA	2644	G
54	BA	2666	C
54	BA	2689	U
54	BA	2732	G
54	BA	2751	G
54	BA	2756	U
54	BA	2892	G
55	BB	14	U
55	BB	15	A
55	BB	73	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	PSU	A1	55	22	18,21,22	0.80	0	21,30,33	1.13	2 (9%)
24	H2U	A3	21	24	18,21,22	1.33	2 (11%)	19,30,33	1.46	3 (15%)
22	6MZ	A1	37	22	22,25,26	0.65	0	29,36,39	1.26	3 (10%)
24	4SU	A3	8	24	18,21,22	1.48	2 (11%)	25,30,33	0.88	1 (4%)
22	7MG	A1	46	22	23,26,27	4.06	3 (13%)	27,39,42	1.55	2 (7%)
22	5MU	A1	54	22	19,22,23	0.80	0	27,32,35	1.47	4 (14%)
22	CM0	A1	34	23,22	21,26,27	1.32	2 (9%)	26,37,40	0.93	0
24	5MU	A3	55	24	19,22,23	0.74	0	27,32,35	1.35	3 (11%)
22	4SU	A1	7	22	18,21,22	1.42	2 (11%)	25,30,33	0.97	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	OMC	A3	33	24	19,22,23	0.74	0	25,31,34	1.07	2 (8%)
24	PSU	A3	56	24	18,21,22	0.89	0	21,30,33	1.13	2 (9%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-19.05	1.33	1.45
24	A3	8	4SU	C5-C4	-5.22	1.36	1.42
22	A1	7	4SU	C5-C4	-5.10	1.36	1.42
22	A1	34	CM0	O5-C5	-4.84	1.25	1.36
24	A3	21	H2U	C4-N3	-3.54	1.31	1.37
24	A3	21	H2U	C2-N3	-3.38	1.32	1.38
22	A1	46	7MG	C8-N7	-2.34	1.31	1.42
22	A1	46	7MG	C5-N7	2.18	1.38	1.35
22	A1	34	CM0	O8-C8	-2.17	1.23	1.30
22	A1	7	4SU	C4-S4	-2.15	1.64	1.68
24	A3	8	4SU	C4-S4	-2.05	1.65	1.68

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	5.79	111.57	103.37
22	A1	37	6MZ	C9-N6-C6	4.40	126.93	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	21	H2U	N3-C2-N1	3.98	120.65	116.65
22	A1	54	5MU	C5M-C5-C6	-3.92	117.55	122.85
24	A3	55	5MU	C5M-C5-C6	-3.63	117.94	122.85
22	A1	54	5MU	C5M-C5-C4	3.01	122.00	118.78
22	A1	54	5MU	C6-C5-C4	2.95	120.45	118.02
24	A3	55	5MU	C6-C5-C4	2.80	120.33	118.02
22	A1	37	6MZ	C4-C5-C6	-2.79	114.46	116.78
22	A1	55	PSU	C6-C5-C4	2.77	120.05	118.17
24	A3	55	5MU	C5M-C5-C4	2.76	121.73	118.78
24	A3	33	OMC	O2-C2-N3	-2.74	118.02	122.33
24	A3	33	OMC	C2'-C1'-N1	-2.71	109.10	114.24
24	A3	8	4SU	C6-C5-C4	2.58	122.18	119.95
22	A1	37	6MZ	C6-C5-N7	2.47	135.12	132.43
24	A3	56	PSU	O4'-C1'-C2'	2.44	108.53	105.15
24	A3	56	PSU	C6-C5-C4	2.39	119.78	118.17
24	A3	21	H2U	O2-C2-N3	-2.37	117.11	121.49
24	A3	21	H2U	C5-C4-N3	2.33	119.17	116.69
22	A1	7	4SU	C6-C5-C4	2.29	121.94	119.95
22	A1	7	4SU	O4'-C4'-C3'	2.25	109.61	105.15
22	A1	55	PSU	O4'-C1'-C2'	2.20	108.20	105.15
22	A1	54	5MU	C5-C6-N1	-2.17	120.96	123.31
22	A1	46	7MG	C6-C5-C4	-2.05	118.80	122.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A3	56	PSU	O4'-C1'-C5-C6
22	A1	34	CM0	O5-C7-C8-O9
22	A1	34	CM0	O5-C7-C8-O8
24	A3	56	PSU	O4'-C1'-C5-C4
22	A1	34	CM0	C6-C5-O5-C7
22	A1	55	PSU	O4'-C1'-C5-C6
22	A1	37	6MZ	N1-C6-N6-C9
22	A1	37	6MZ	C5-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	FME	BA	3001	57	8,9,10	0.72	0	8,9,11	1.97	3 (37%)
57	VAL	A1	101	22,58	4,6,7	0.69	0	6,7,9	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	FME	BA	3001	57	-	0/7/9/11	-
57	VAL	A1	101	22,58	-	3/5/6/8	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	FME	CA-N-CN	3.70	128.52	122.82
58	BA	3001	FME	C-CA-N	3.00	115.29	109.50
58	BA	3001	FME	O-C-CA	-2.61	118.07	124.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

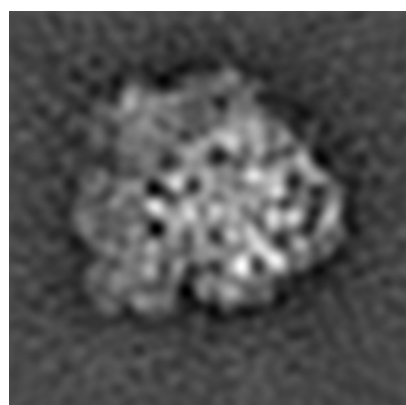
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2474. These allow visual inspection of the internal detail of the map and identification of artifacts.

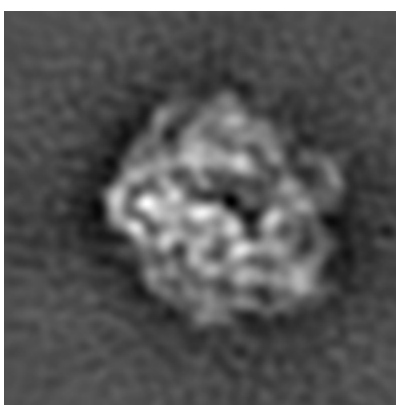
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

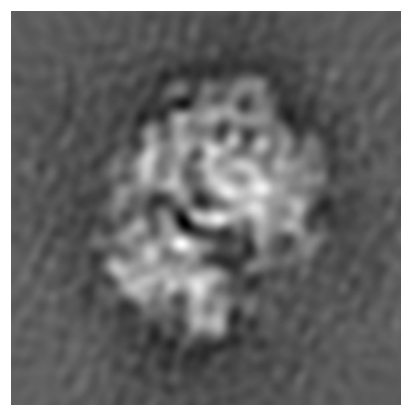
6.1.1 Primary map



X



Y

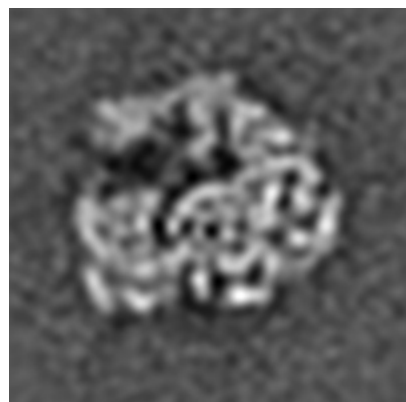


Z

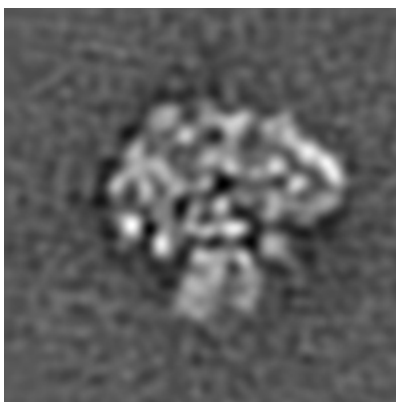
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

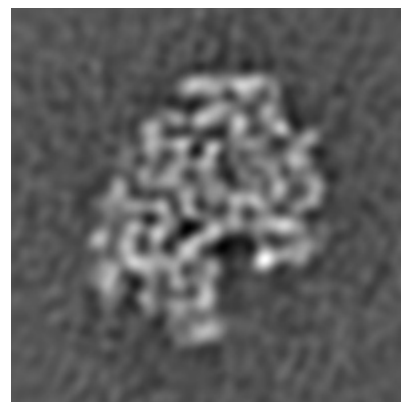
6.2.1 Primary map



X Index: 64



Y Index: 64

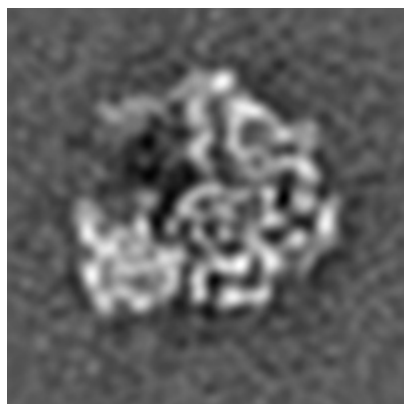


Z Index: 64

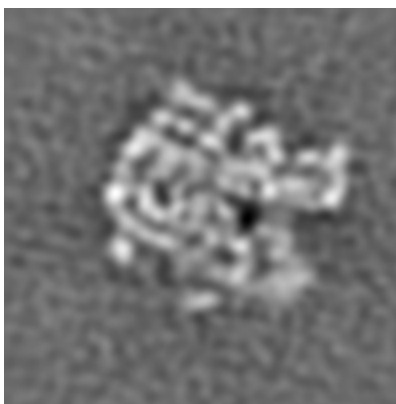
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 66



Y Index: 70

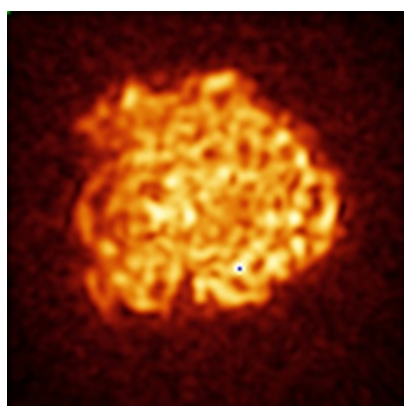


Z Index: 62

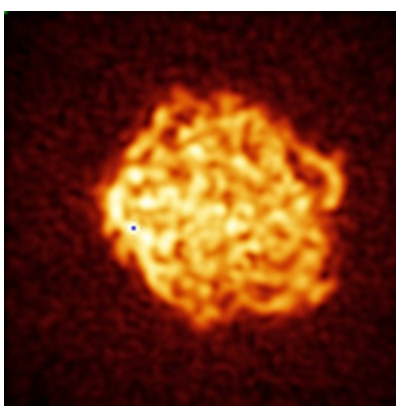
The images above show the largest variance slices of the map in three orthogonal directions.

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

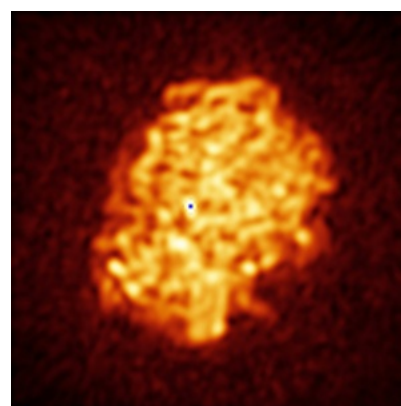
6.4.1 Primary map



X



Y

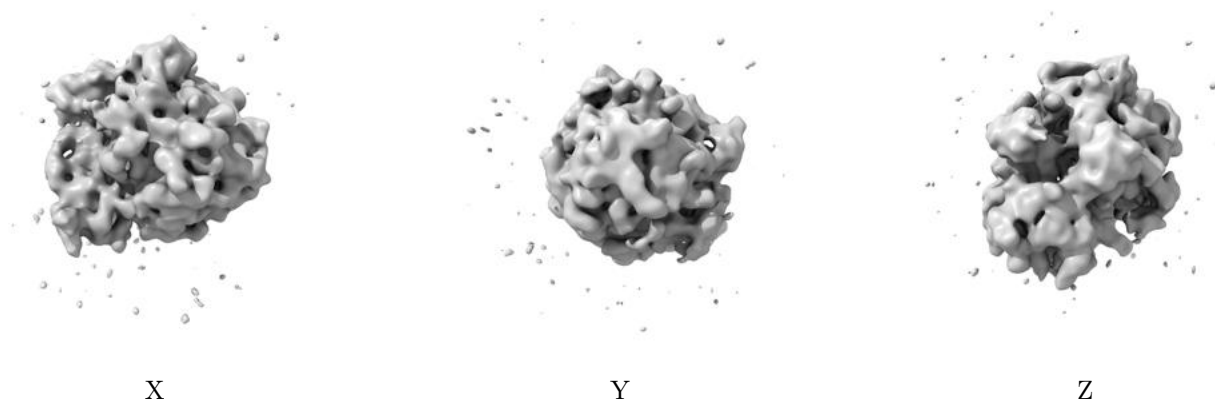


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

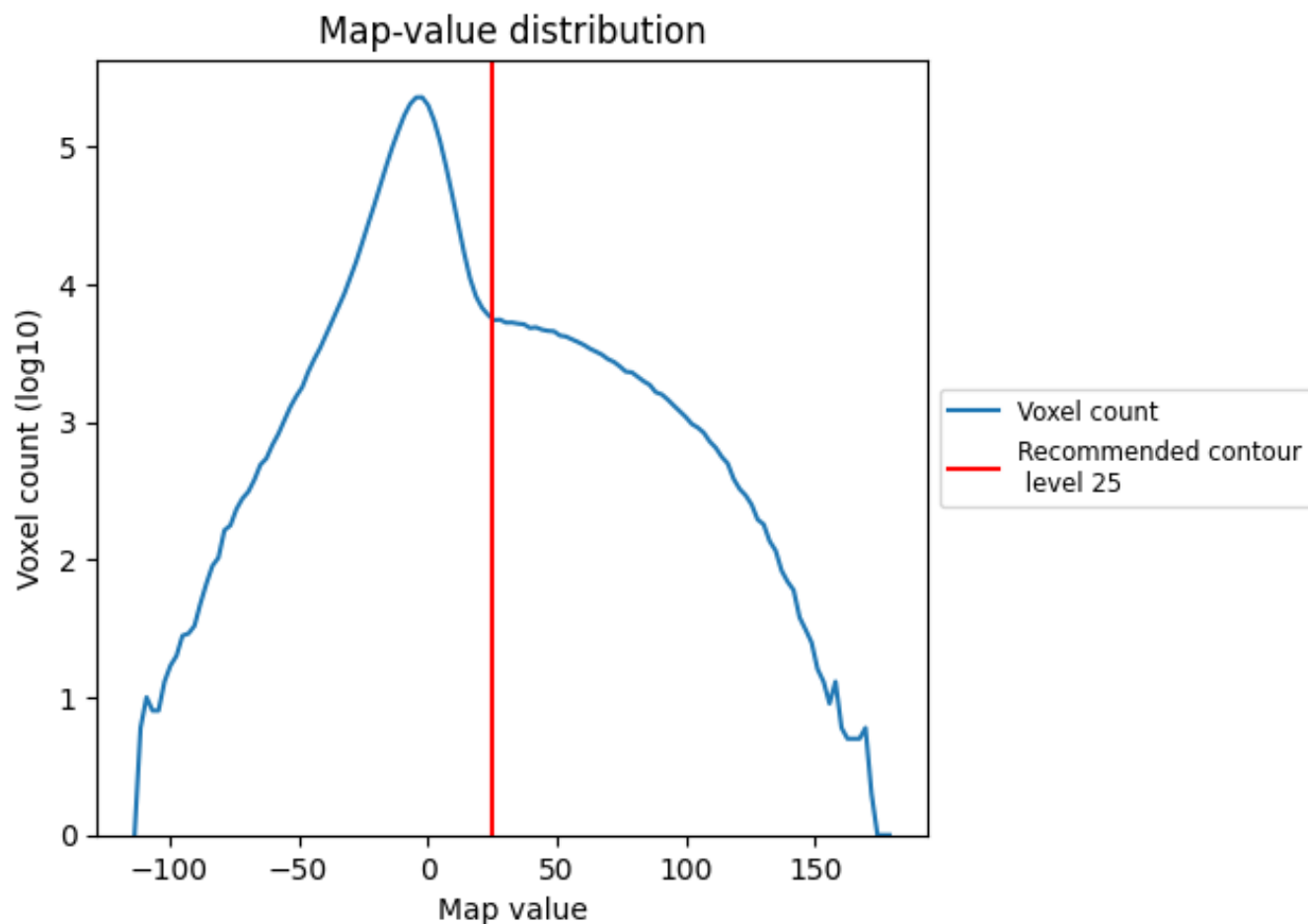
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

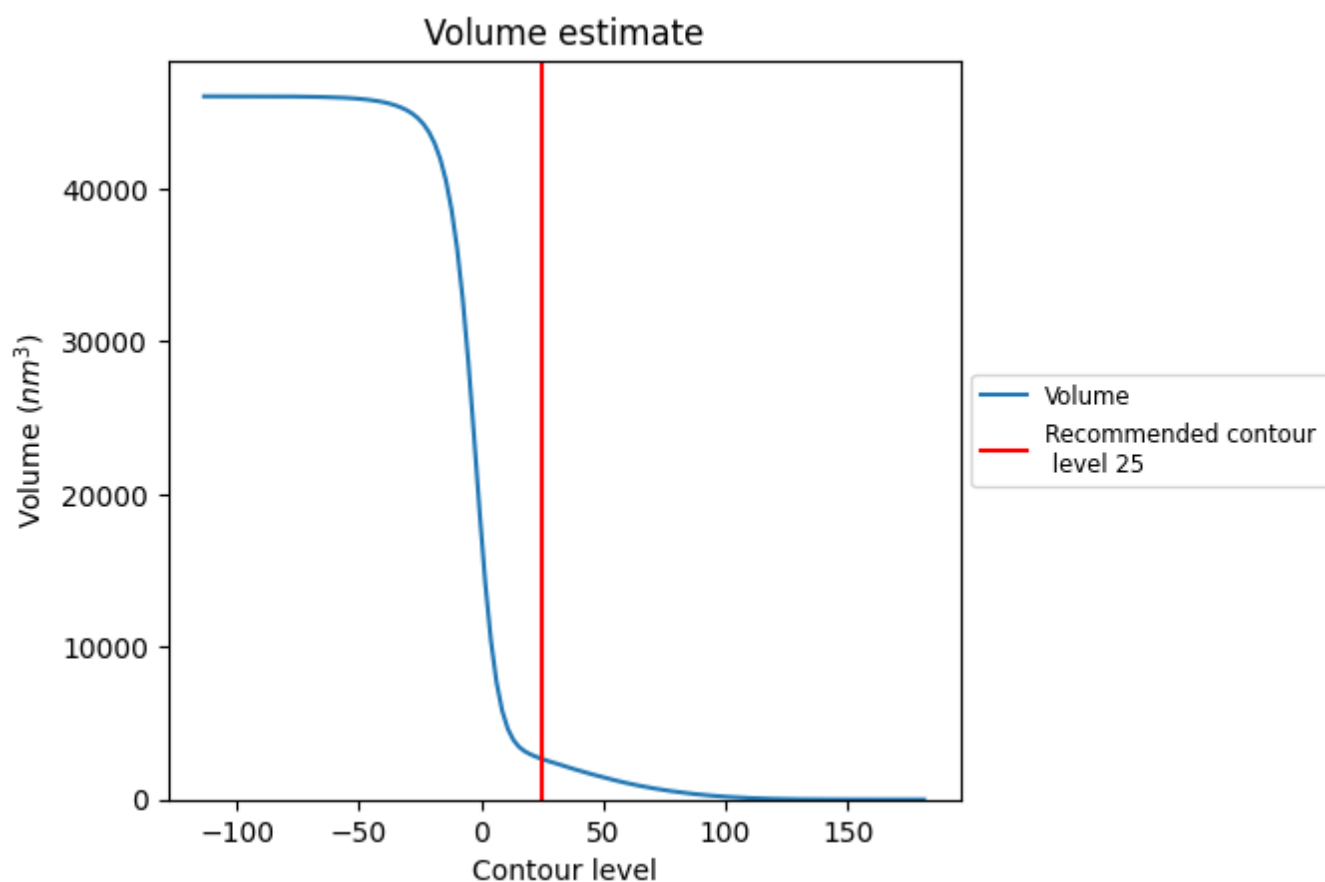
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

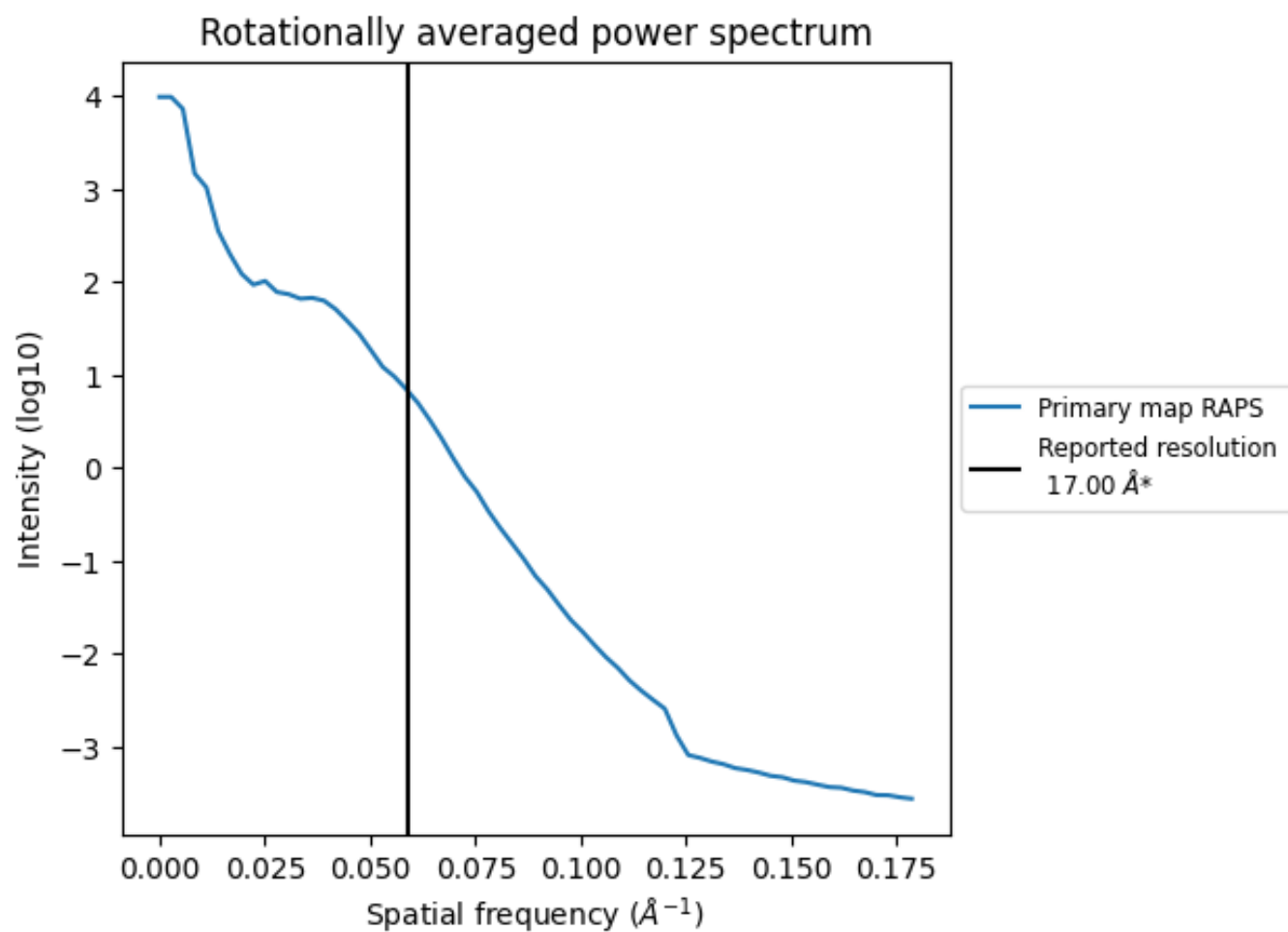
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2652 nm³; this corresponds to an approximate mass of 2396 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.059 $\text{\AA}^{-1}$

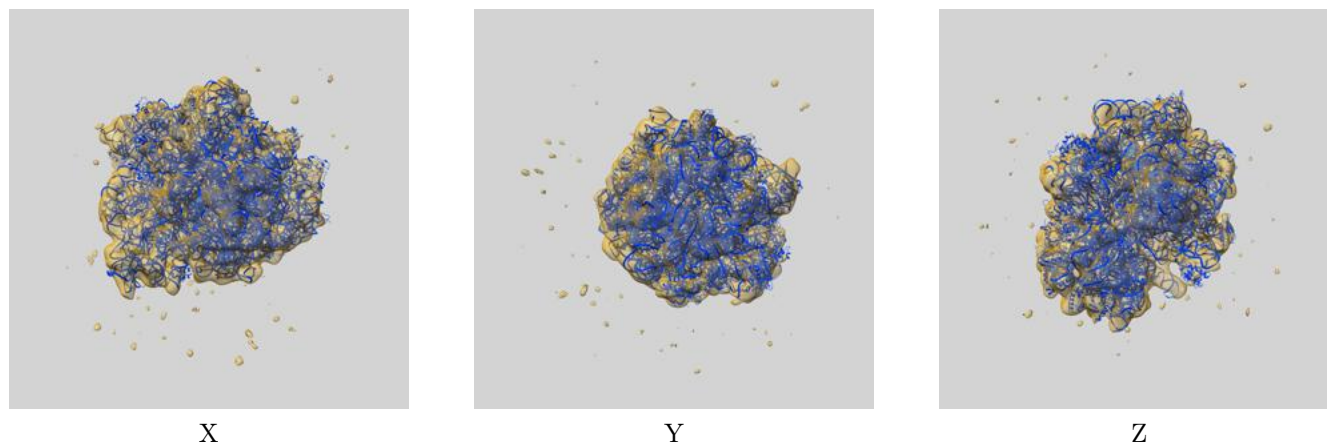
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2474 and PDB model 4V77. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



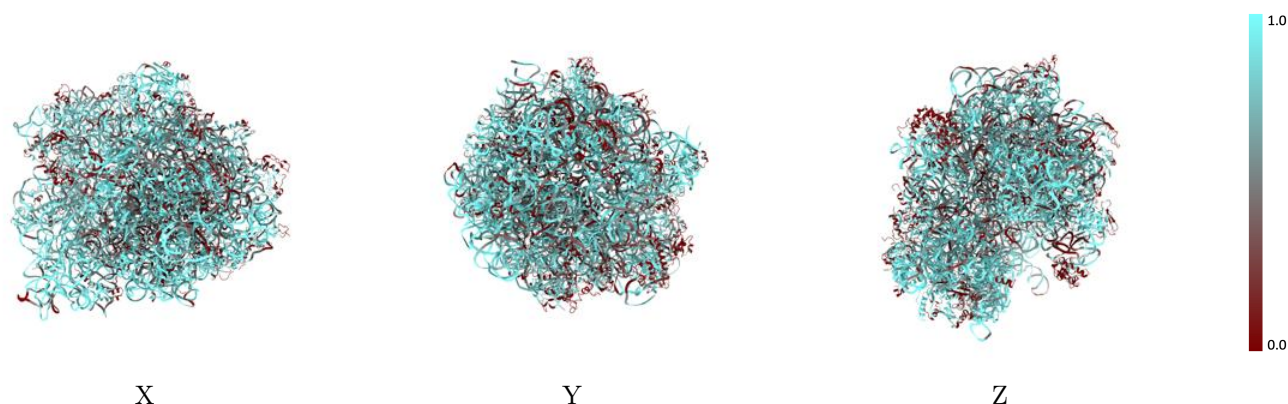
The images above show the 3D surface view of the map at the recommended contour level 25.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



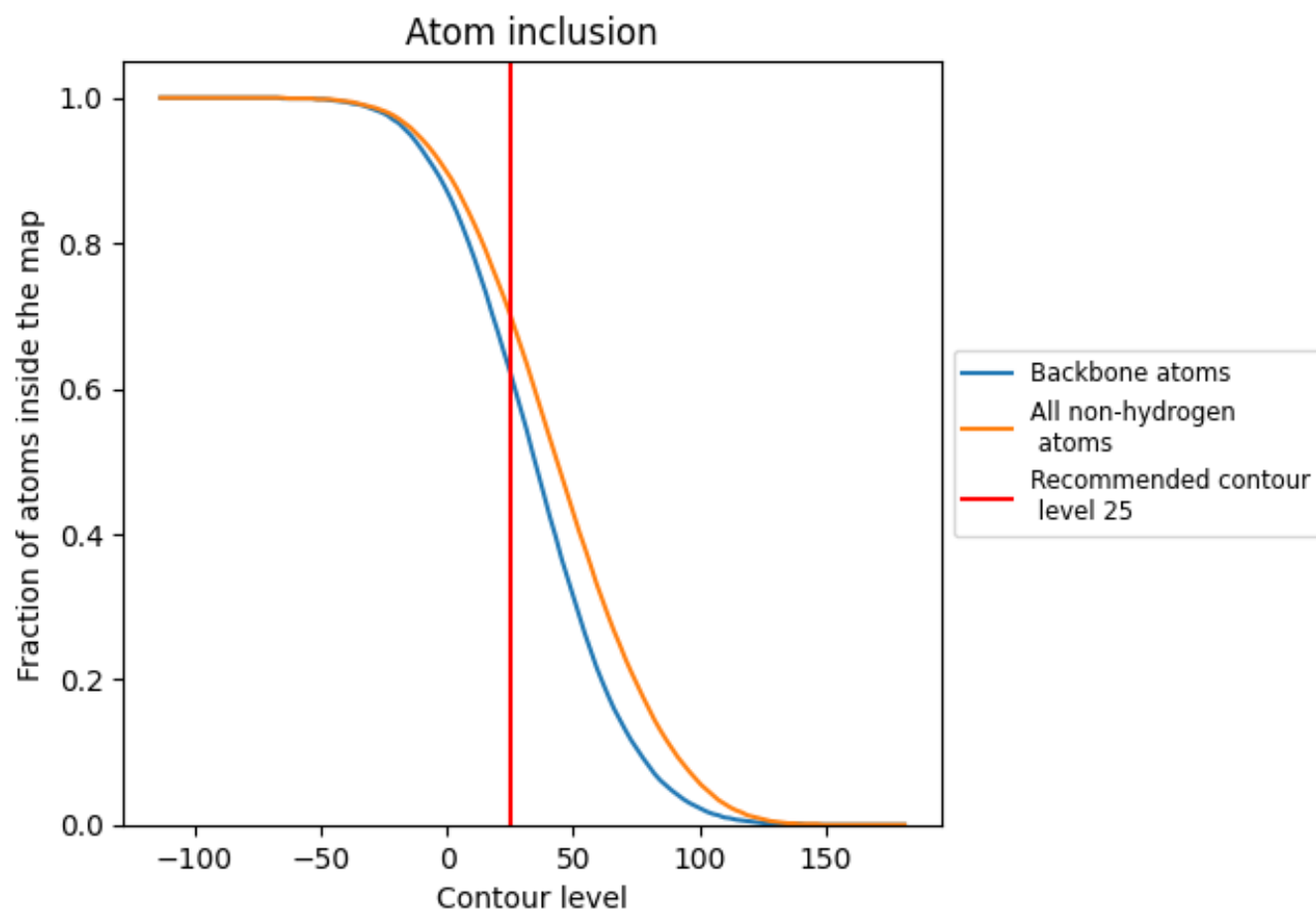
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.7020	 0.0510
A1	 0.6820	 0.0680
A2	 0.7440	 0.0280
A3	 0.6280	 0.0530
AA	 0.8010	 0.0680
AB	 0.7340	 0.0570
AC	 0.5910	 0.0360
AD	 0.6310	 0.0310
AE	 0.6600	 0.0460
AF	 0.5960	 0.0460
AG	 0.4900	 0.0510
AH	 0.7060	 0.0440
AI	 0.6120	 0.0210
AJ	 0.6670	 0.0170
AK	 0.5540	 0.0260
AL	 0.4650	 0.0100
AM	 0.5690	 0.0430
AN	 0.5300	 0.0330
AO	 0.6620	 0.0380
AP	 0.7410	 0.0380
AQ	 0.5290	 0.0380
AR	 0.4830	 0.0190
AS	 0.6120	 0.0230
AT	 0.5150	 0.0100
AU	 0.2710	 -0.0160
B0	 0.5840	 0.0160
B1	 0.6340	 0.0630
B2	 0.3320	 -0.0150
B3	 0.3850	 -0.0630
B4	 0.5890	 0.0060
B5	 0.2970	 0.0180
BA	 0.7470	 0.0580
BB	 0.8690	 0.0750
BC	 0.4370	 -0.0000
BD	 0.5920	 0.0220



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Chain	Atom inclusion	Q-score
BE	 0.5350	 0.0290
BF	 0.6730	 0.0450
BG	 0.6650	 0.0410
BH	 0.2920	 0.0370
BI	 0.1040	 0.0440
BJ	 0.7140	 0.0300
BK	 0.4850	 0.0160
BL	 0.6110	 0.0320
BM	 0.7200	 0.0300
BN	 0.6550	 0.0120
BO	 0.7550	 0.0270
BP	 0.6970	 0.0500
BQ	 0.6210	 -0.0020
BR	 0.6340	 0.0470
BS	 0.5320	 0.0040
BT	 0.5310	 0.0060
BU	 0.5290	 0.0040
BV	 0.6370	 0.0370
BW	 0.5220	 0.0220
BX	 0.3880	 0.0040
BY	 0.5410	 0.0280
BZ	 0.4900	 0.0450