



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 04:30 AM EDT

PDB ID : 4V75 / pdb_00004v75
EMDB ID : EMD-1721
Title : E. coli 70S-fMetVal-tRNAVal-tRNA^{fMet} complex in classic post-translocation state (post1)
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on : 2013-10-14
Resolution : 12.00 Å (reported)
Based on initial models : 3I1O, 2WRI, 2K4C, 2HGP

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

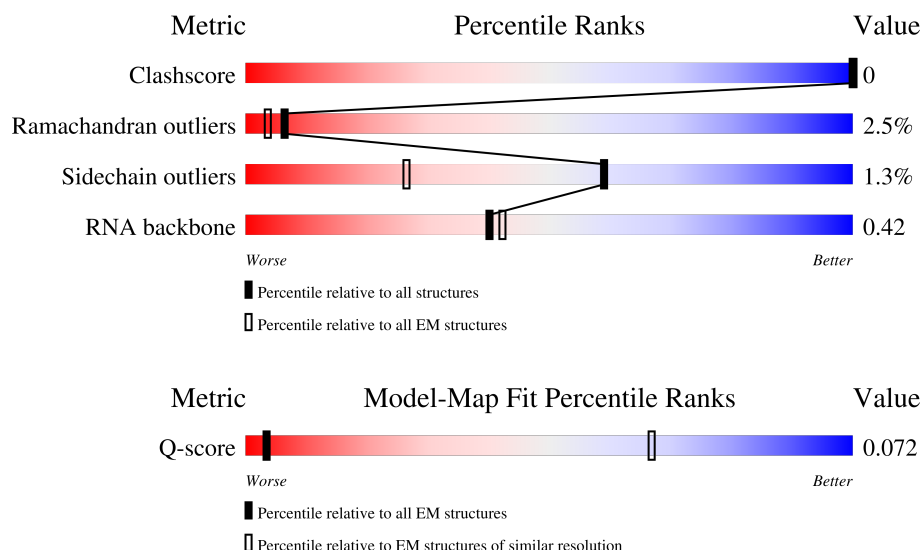
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 12.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	93 (11.50 - 12.50)

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

Mol	Chain	Length	Quality of chain
1	AB	220	34% 98%
2	AC	208	35% 98%
3	AD	206	35% 95%

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

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

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Mol	Chain	Length	Quality of chain
54	BA	2903	9% 62% 32% 6%
55	BB	118	17% 61% 29% 8% ••
56	B5	234	53% 94% • 5%

2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

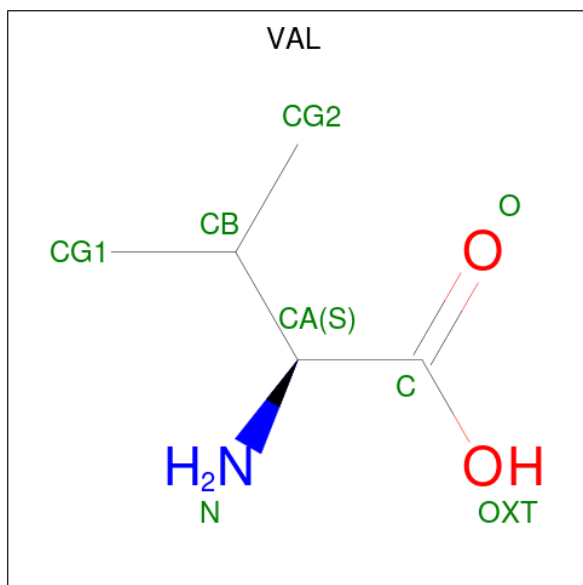
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

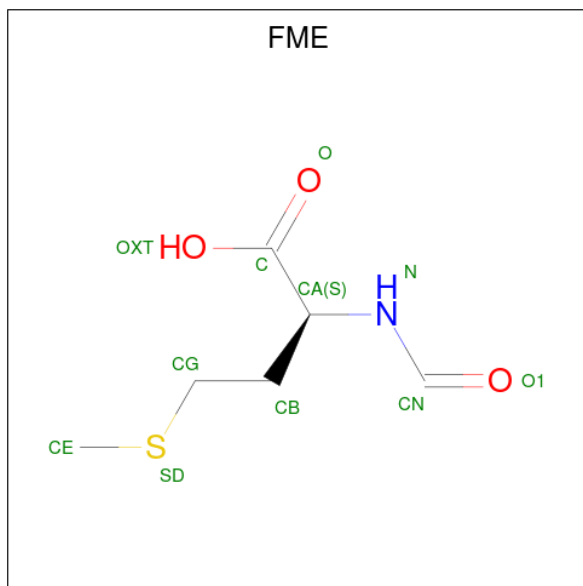
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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



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

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

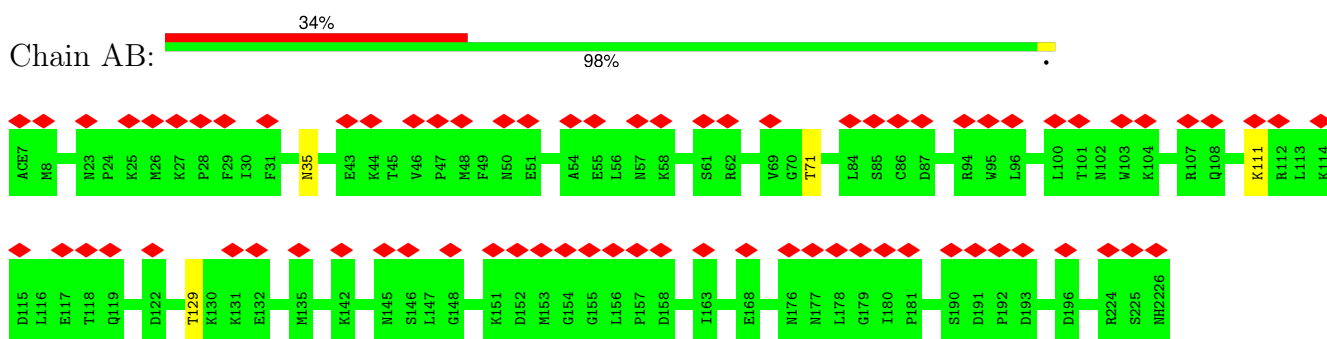


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

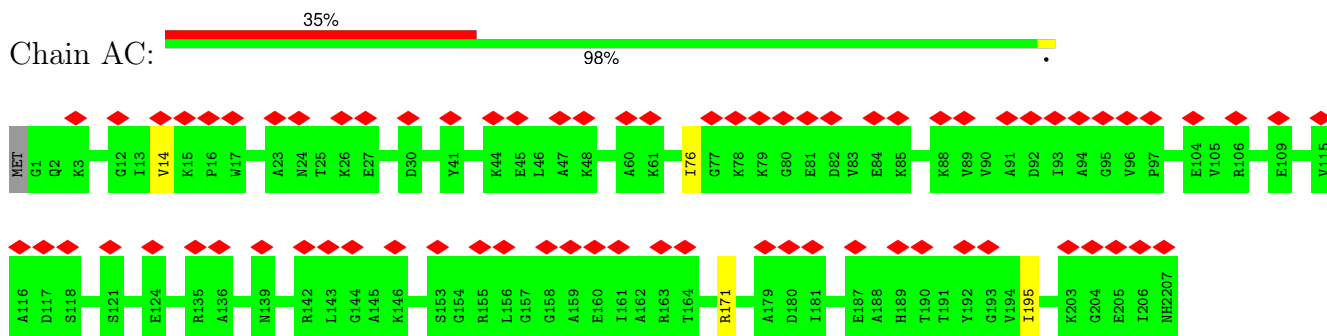
3 Residue-property plots

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

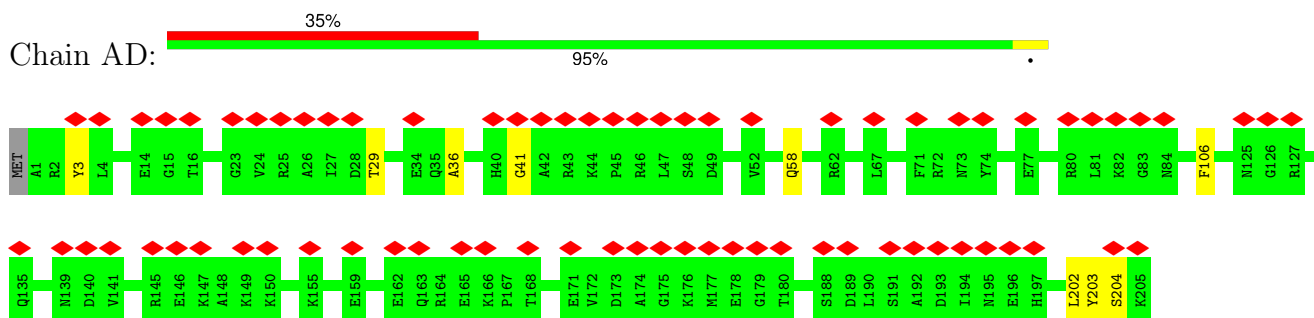
• Molecule 1: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S3

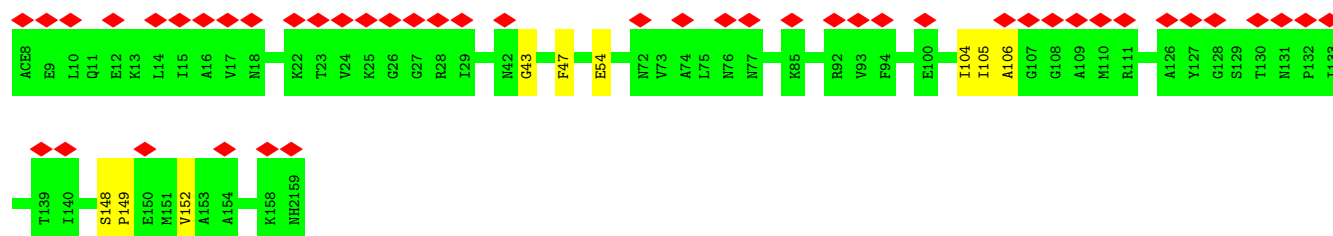


• Molecule 3: 30S ribosomal protein S4

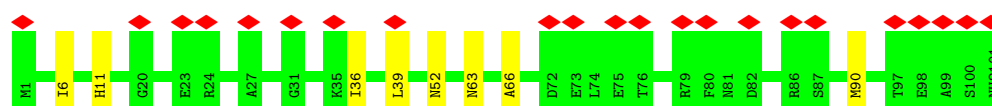
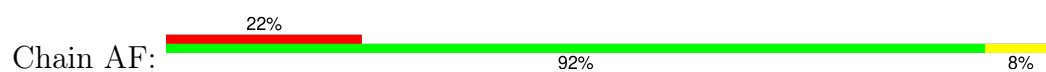


• Molecule 4: 30S ribosomal protein S5

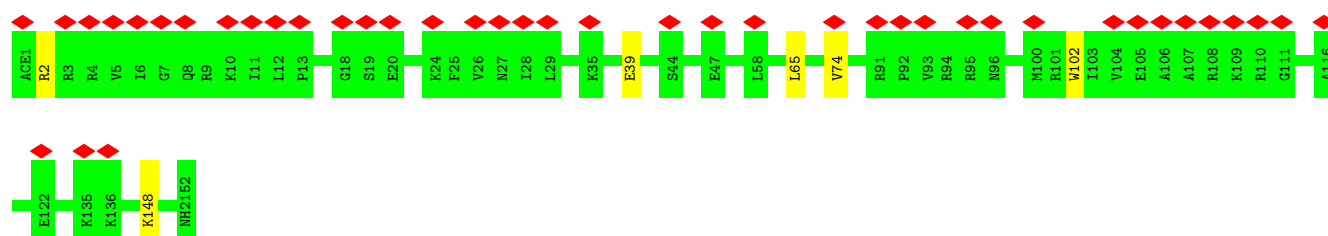




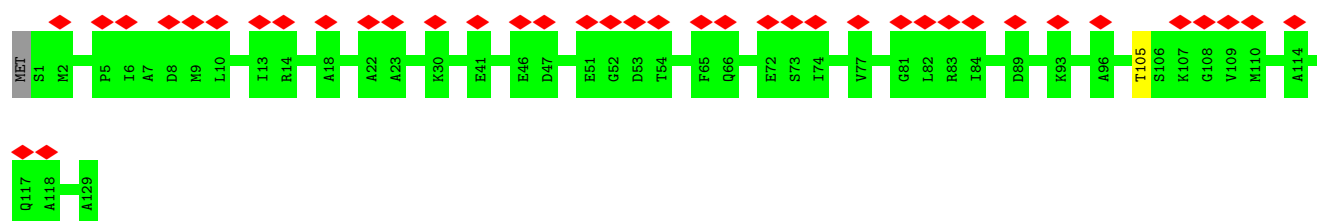
• Molecule 5: 30S ribosomal protein S6



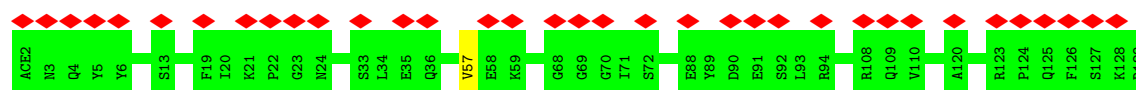
• Molecule 6: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S8

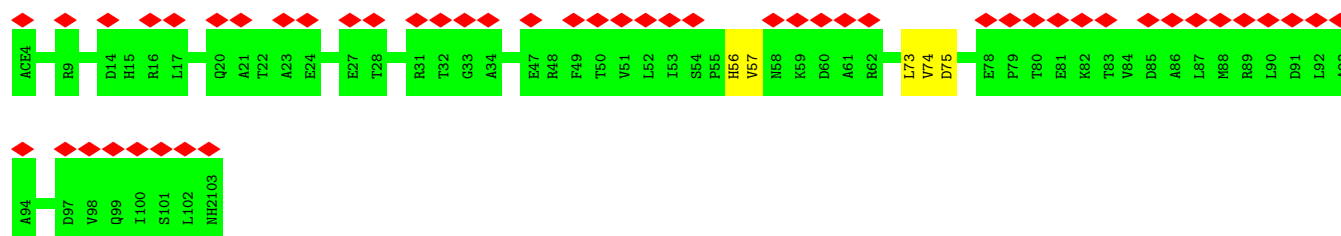


• Molecule 8: 30S ribosomal protein S9

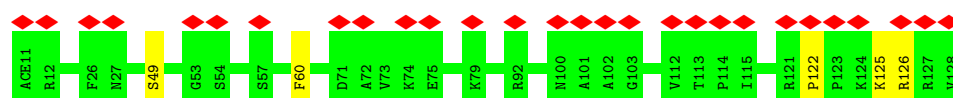


• Molecule 9: 30S ribosomal protein S10

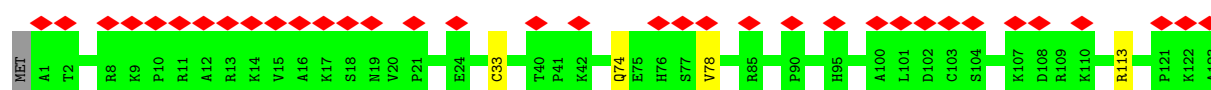




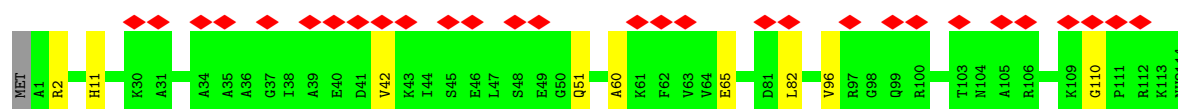
- Molecule 10: 30S ribosomal protein S11



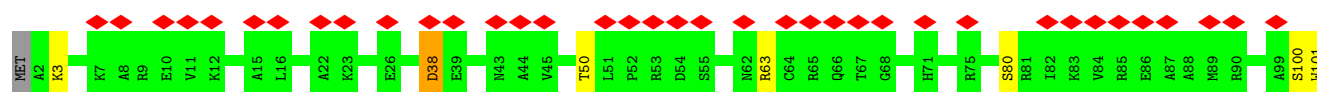
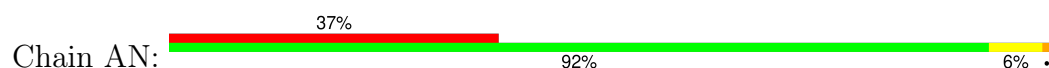
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S14

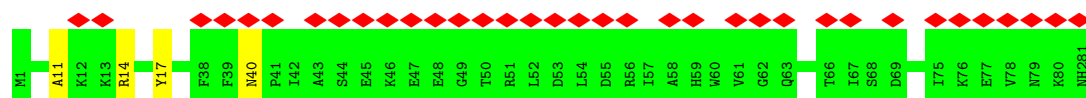


- Molecule 14: 30S ribosomal protein S15

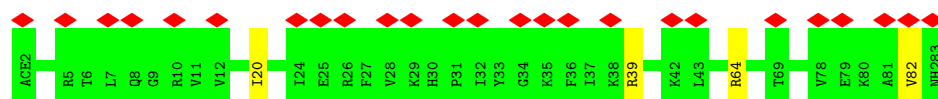


- Molecule 15: 30S ribosomal protein S16

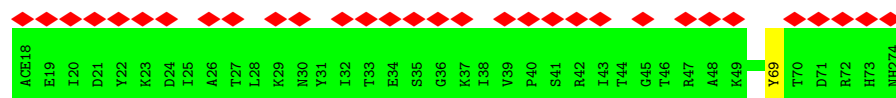




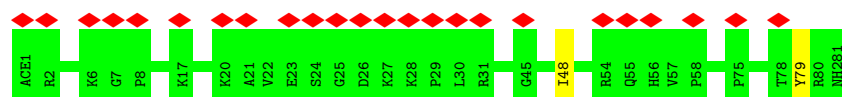
- Molecule 16: 30S ribosomal protein S17



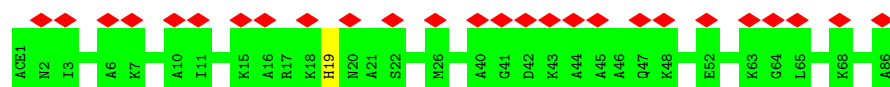
- Molecule 17: 30S ribosomal protein S18



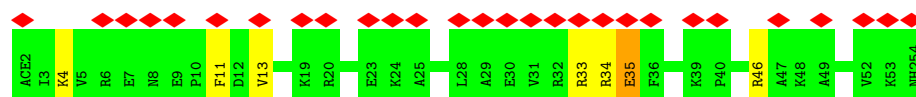
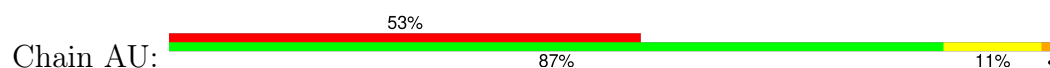
- Molecule 18: 30S ribosomal protein S19



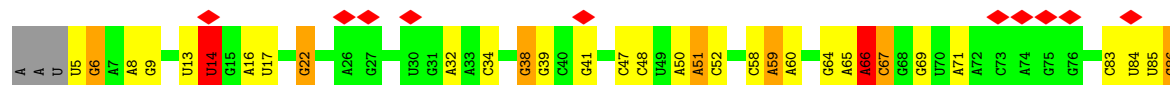
- Molecule 19: 30S ribosomal protein S20

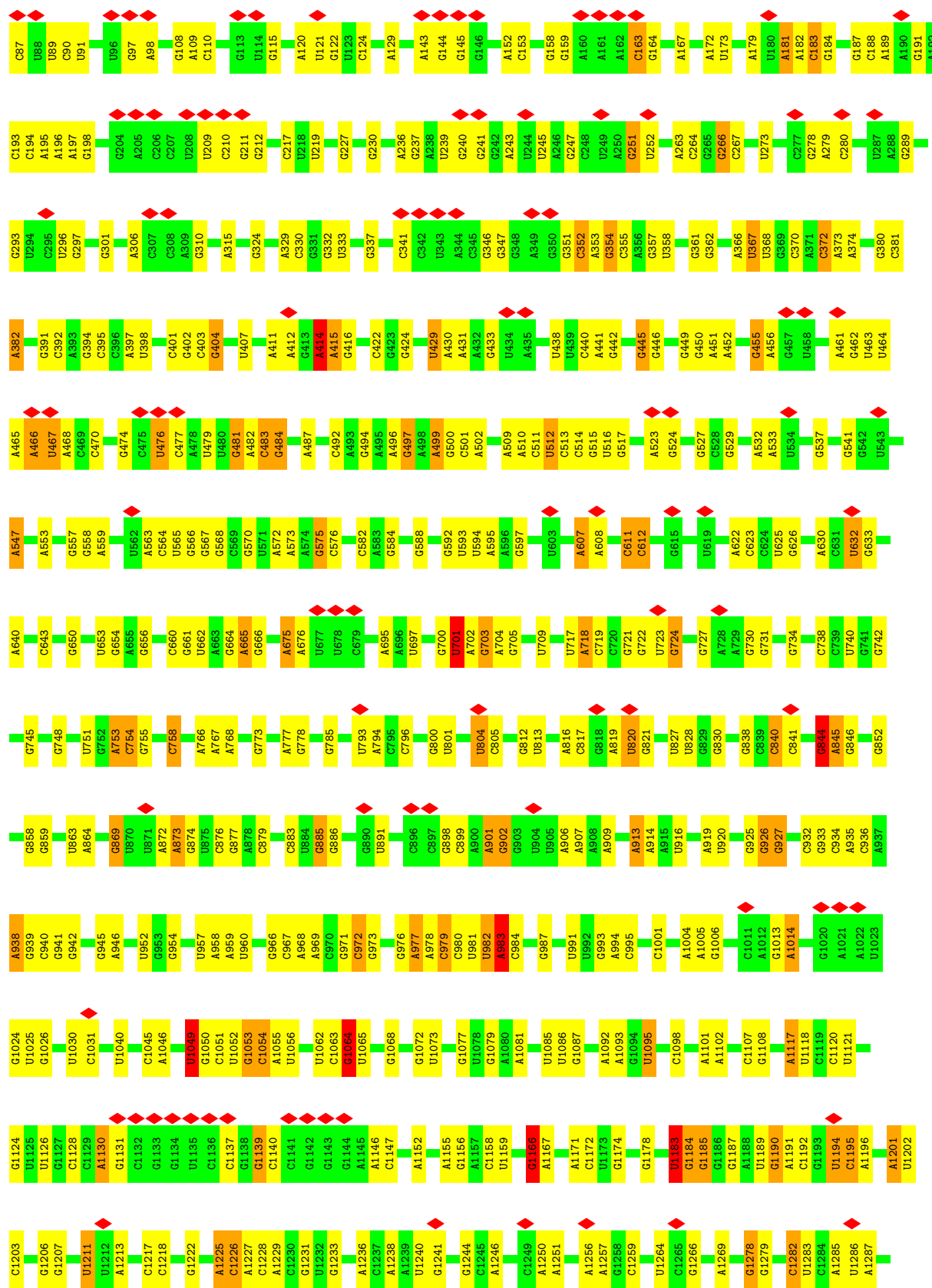


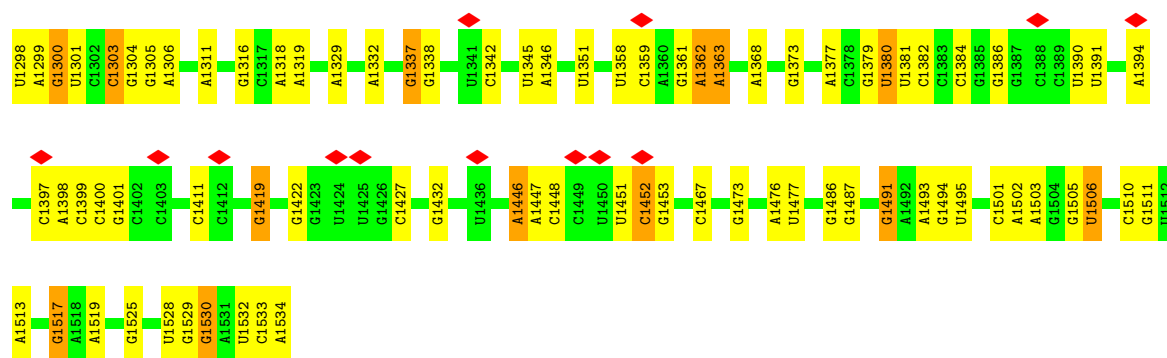
- Molecule 20: 30S ribosomal protein S21



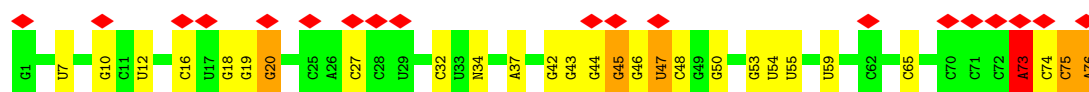
- Molecule 21: 16S ribosomal RNA



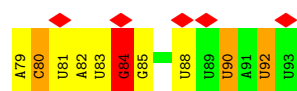




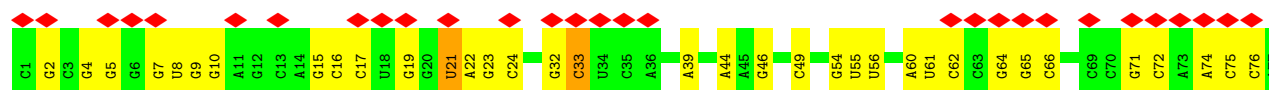
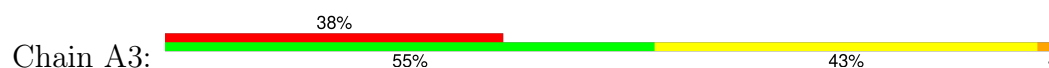
• Molecule 22: fMet-Val-tRNA-Val



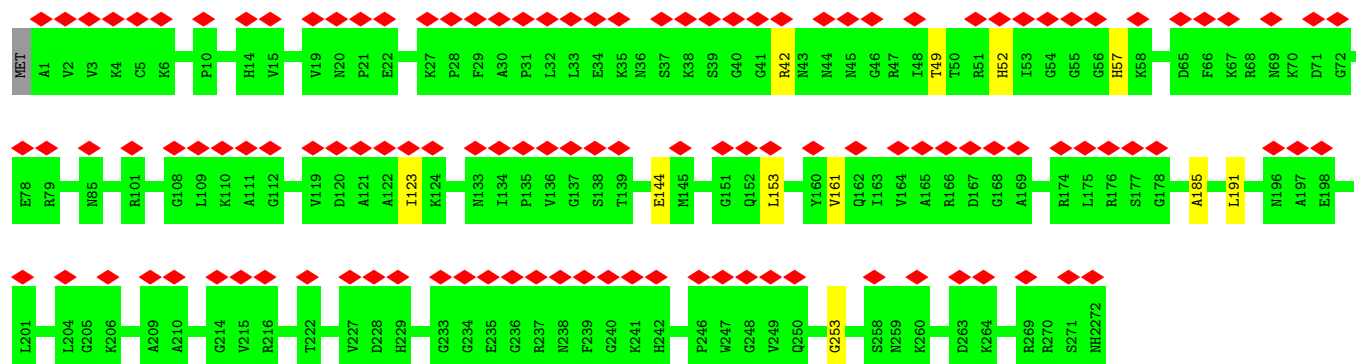
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'



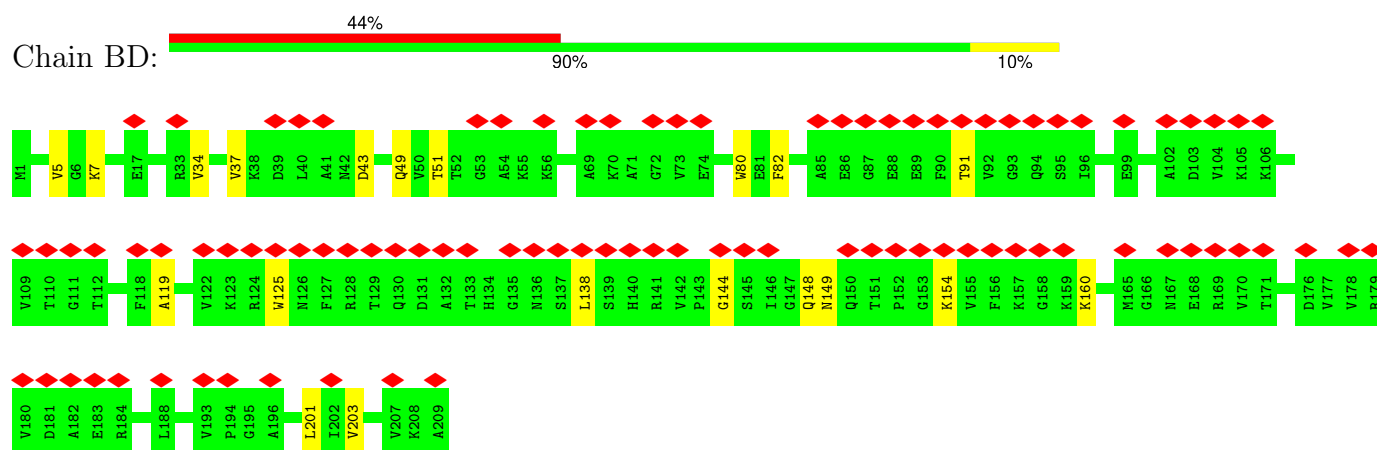
• Molecule 24: tRNA-fMet



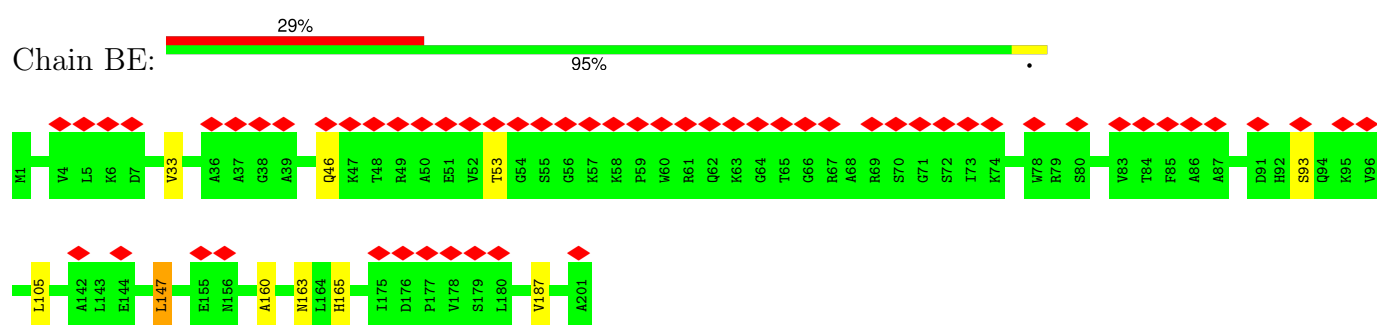
• Molecule 25: 50S ribosomal protein L2



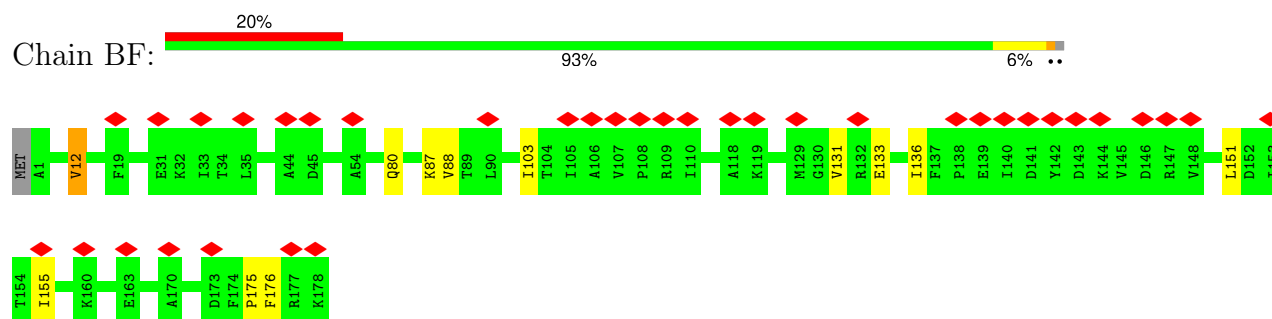
• Molecule 26: 50S ribosomal protein L3



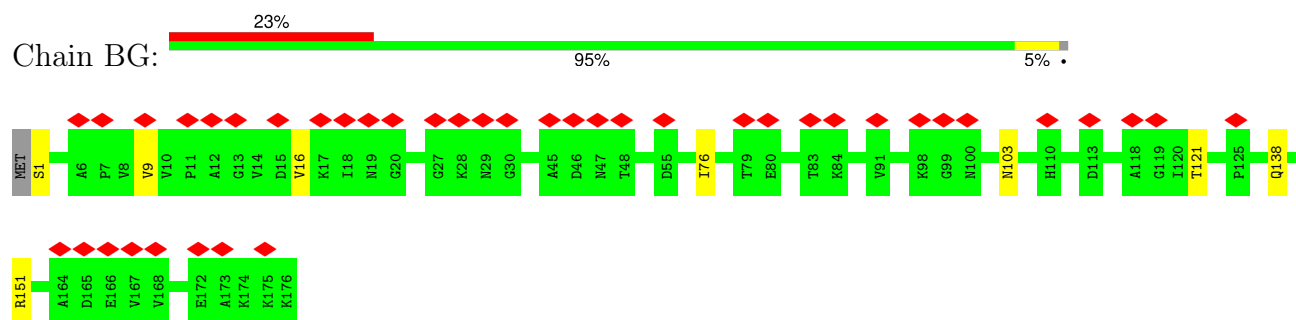
- Molecule 27: 50S ribosomal protein L4



- Molecule 28: 50S ribosomal protein L5

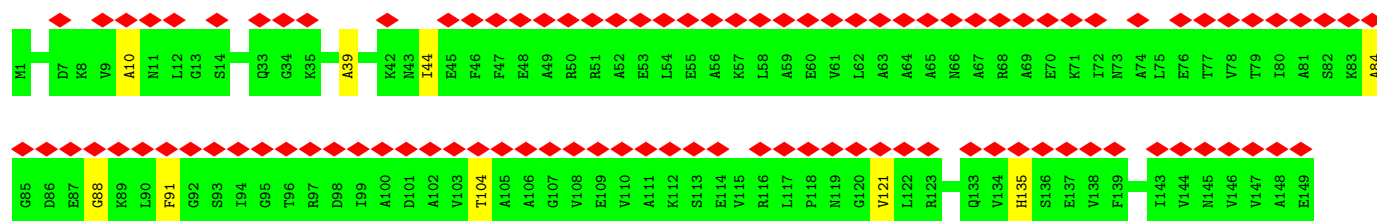


- Molecule 29: 50S ribosomal protein L6

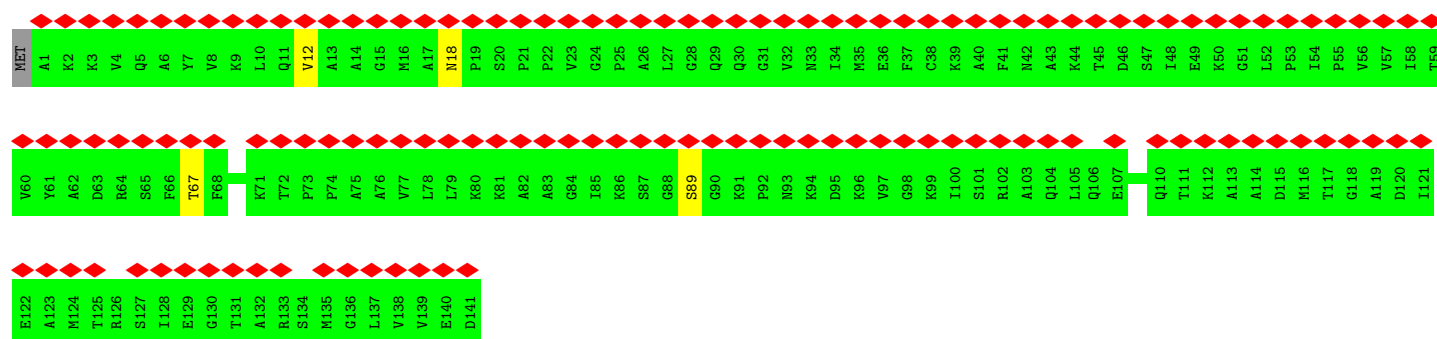


- Molecule 30: 50S ribosomal protein L9

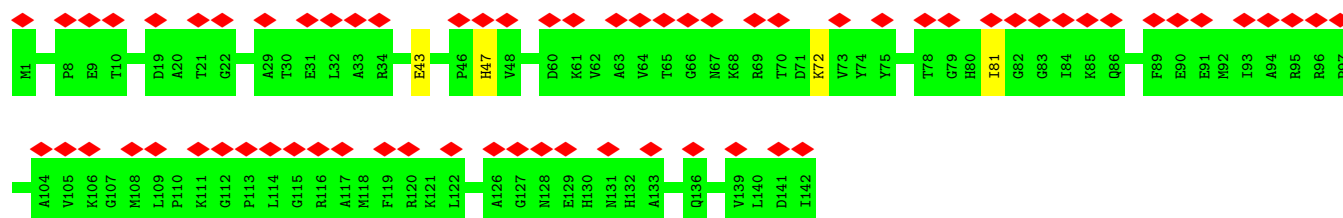




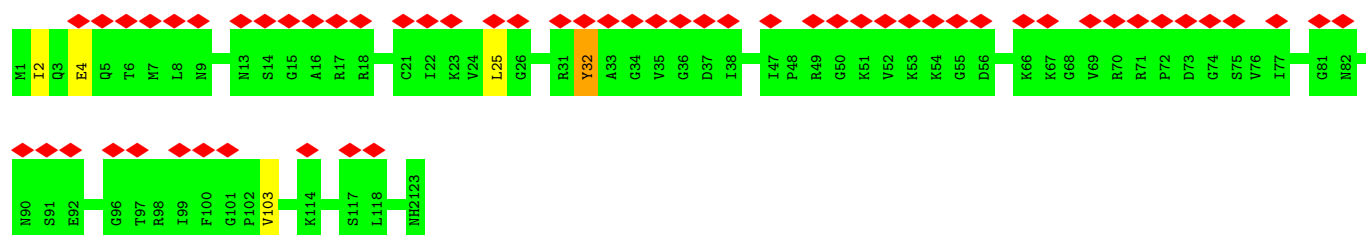
• Molecule 31: 50S ribosomal protein L11



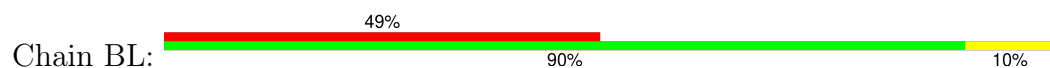
• Molecule 32: 50S ribosomal protein L13

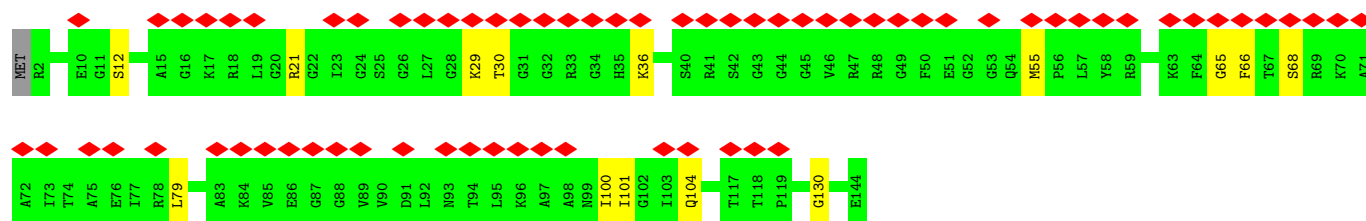


• Molecule 33: 50S ribosomal protein L14

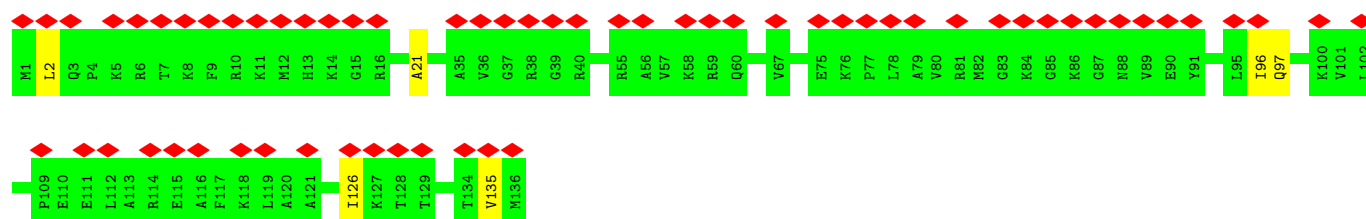


• Molecule 34: 50S ribosomal protein L15

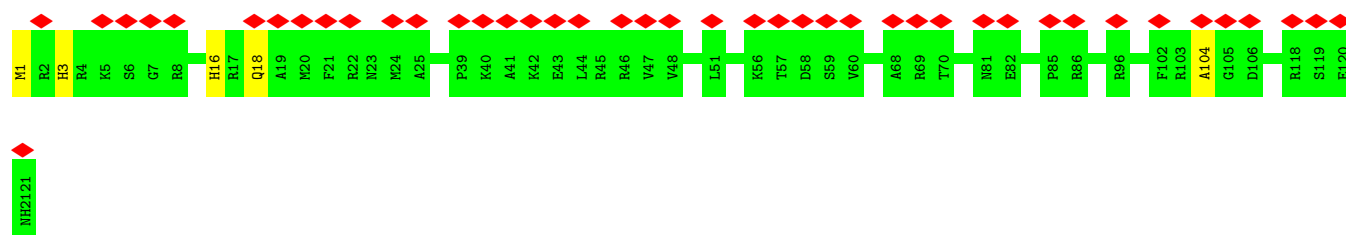




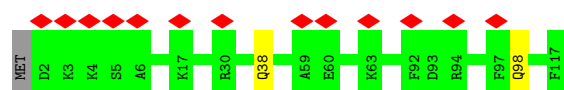
- Molecule 35: 50S ribosomal protein L16



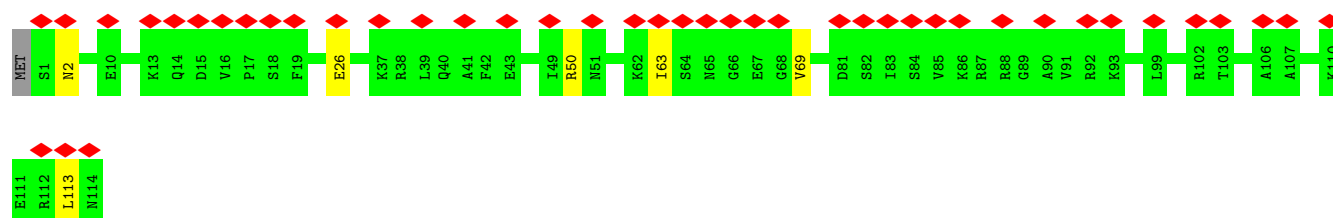
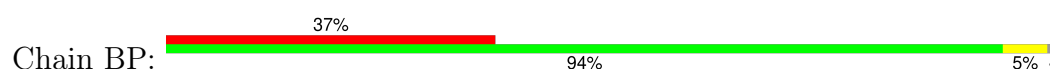
- Molecule 36: 50S ribosomal protein L17



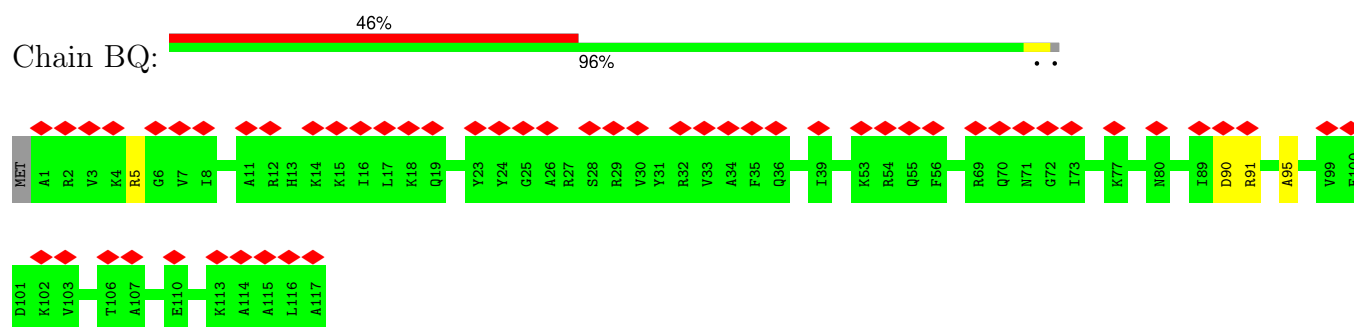
- Molecule 37: 50S ribosomal protein L18



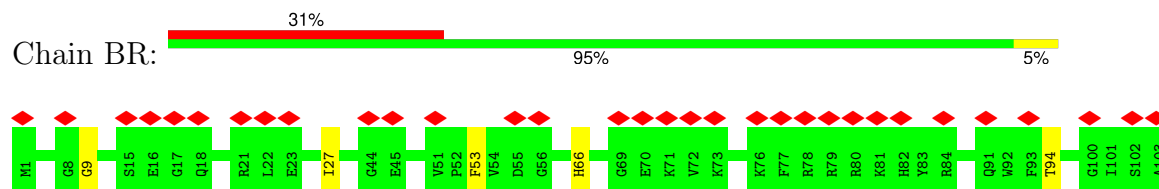
- Molecule 38: 50S ribosomal protein L19



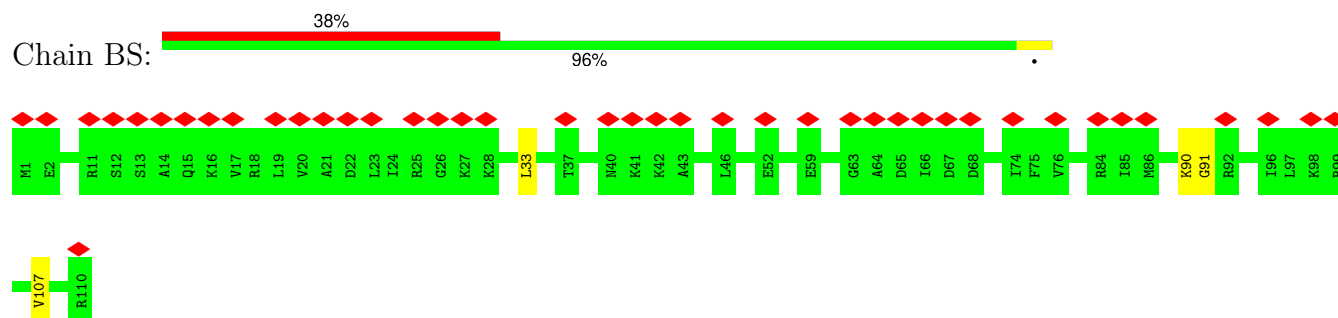
- Molecule 39: 50S ribosomal protein L20



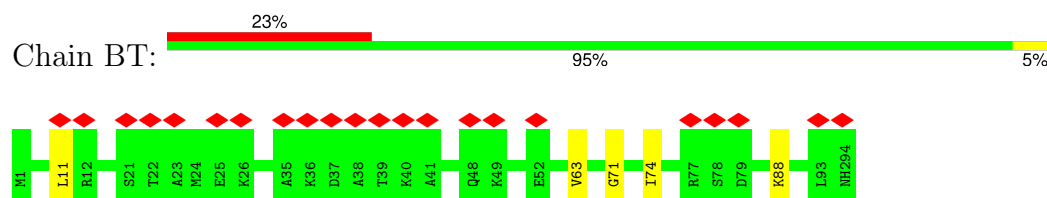
- Molecule 40: 50S ribosomal protein L21



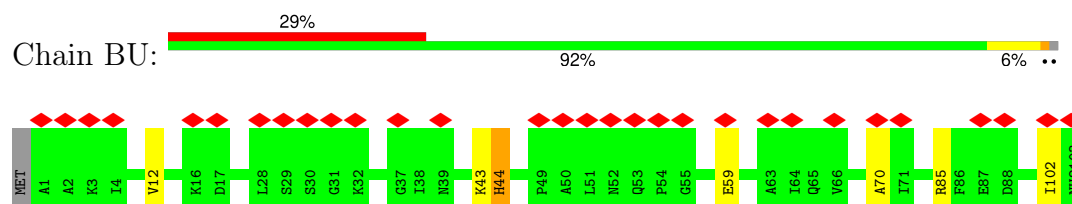
- Molecule 41: 50S ribosomal protein L22



- Molecule 42: 50S ribosomal protein L23

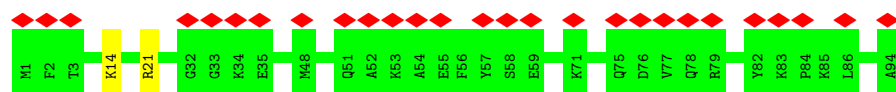


- Molecule 43: 50S ribosomal protein L24

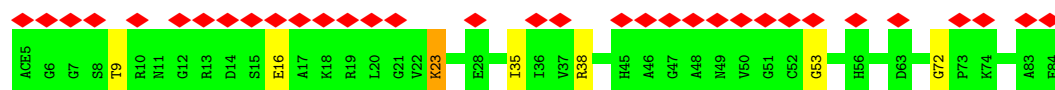
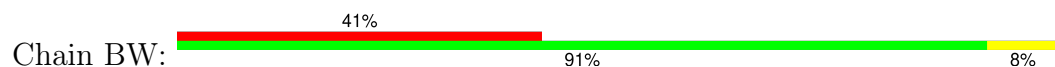


- Molecule 44: 50S ribosomal protein L25

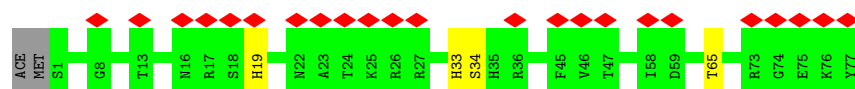




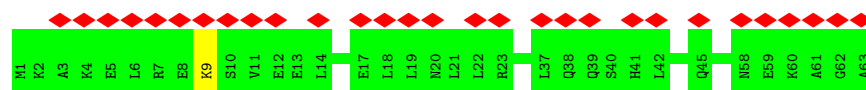
- Molecule 45: 50S ribosomal protein L27



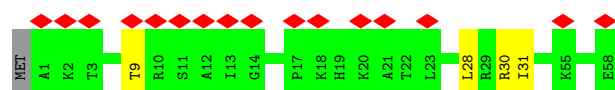
- Molecule 46: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L29



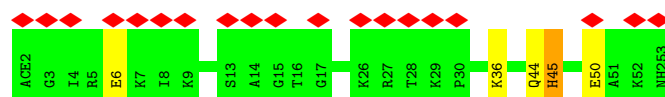
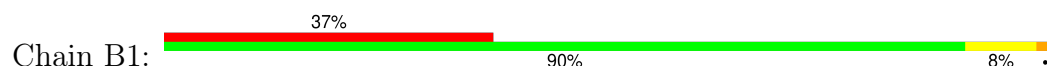
- Molecule 48: 50S ribosomal protein L30



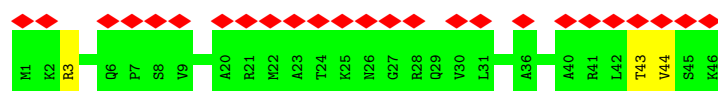
- Molecule 49: 50S ribosomal protein L32



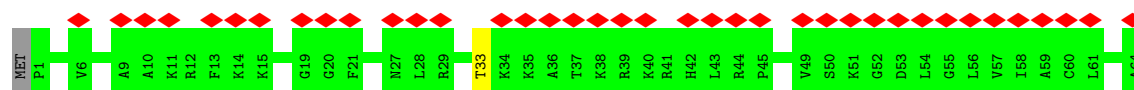
- Molecule 50: 50S ribosomal protein L33



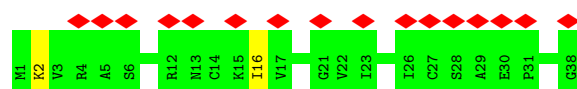
- Molecule 51: 50S ribosomal protein L34



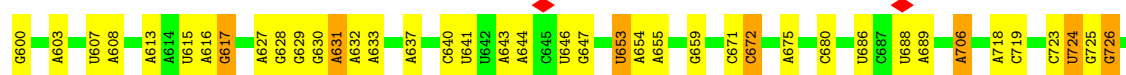
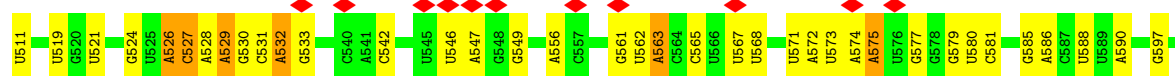
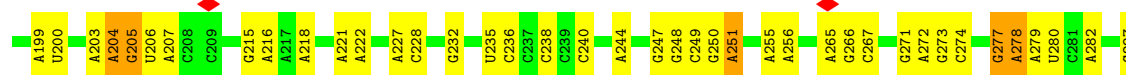
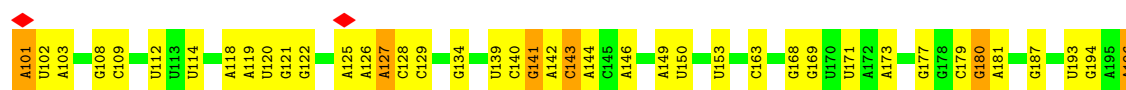
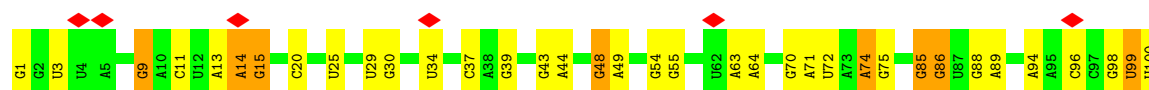
- Molecule 52: 50S ribosomal protein L35

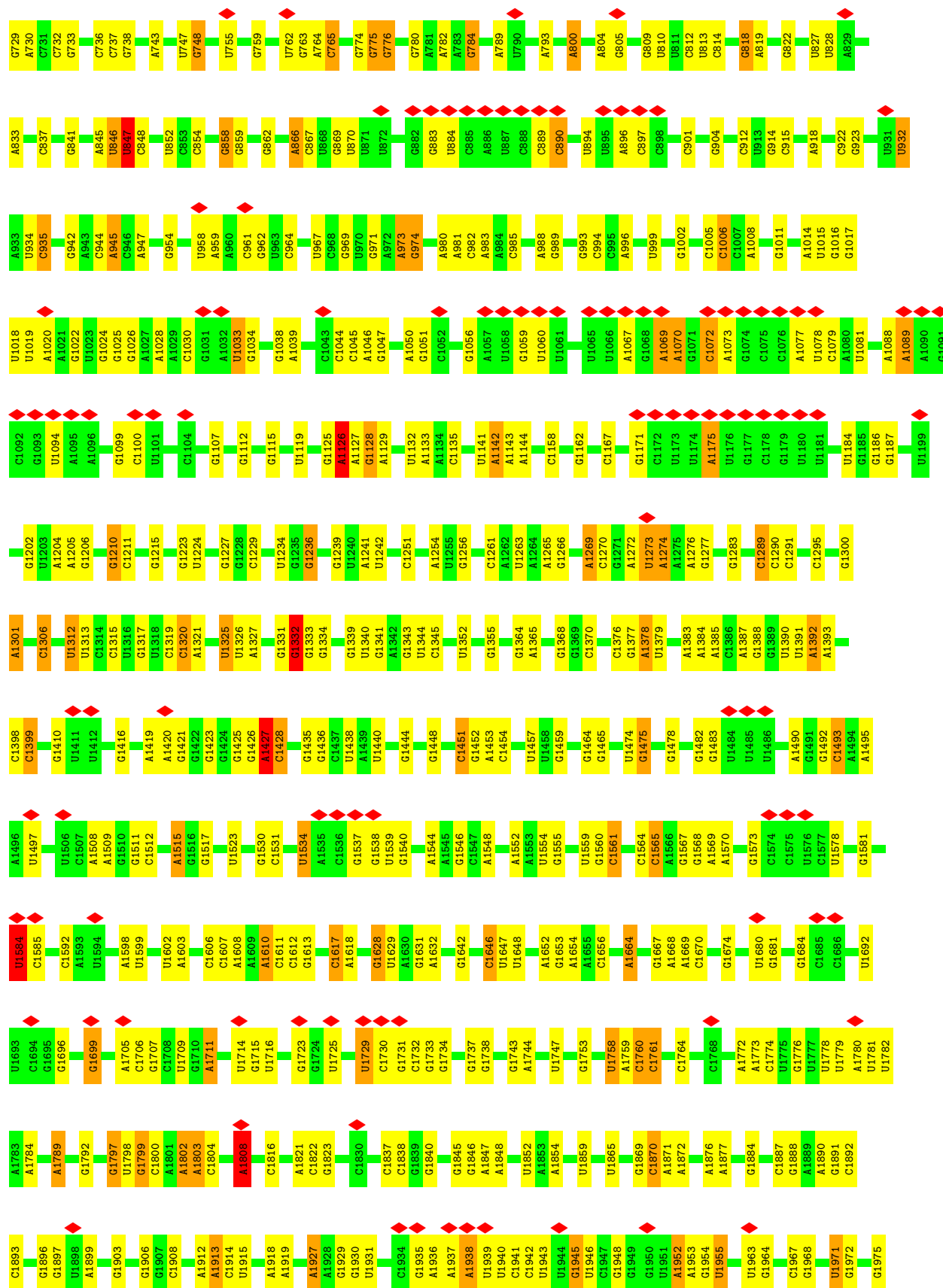


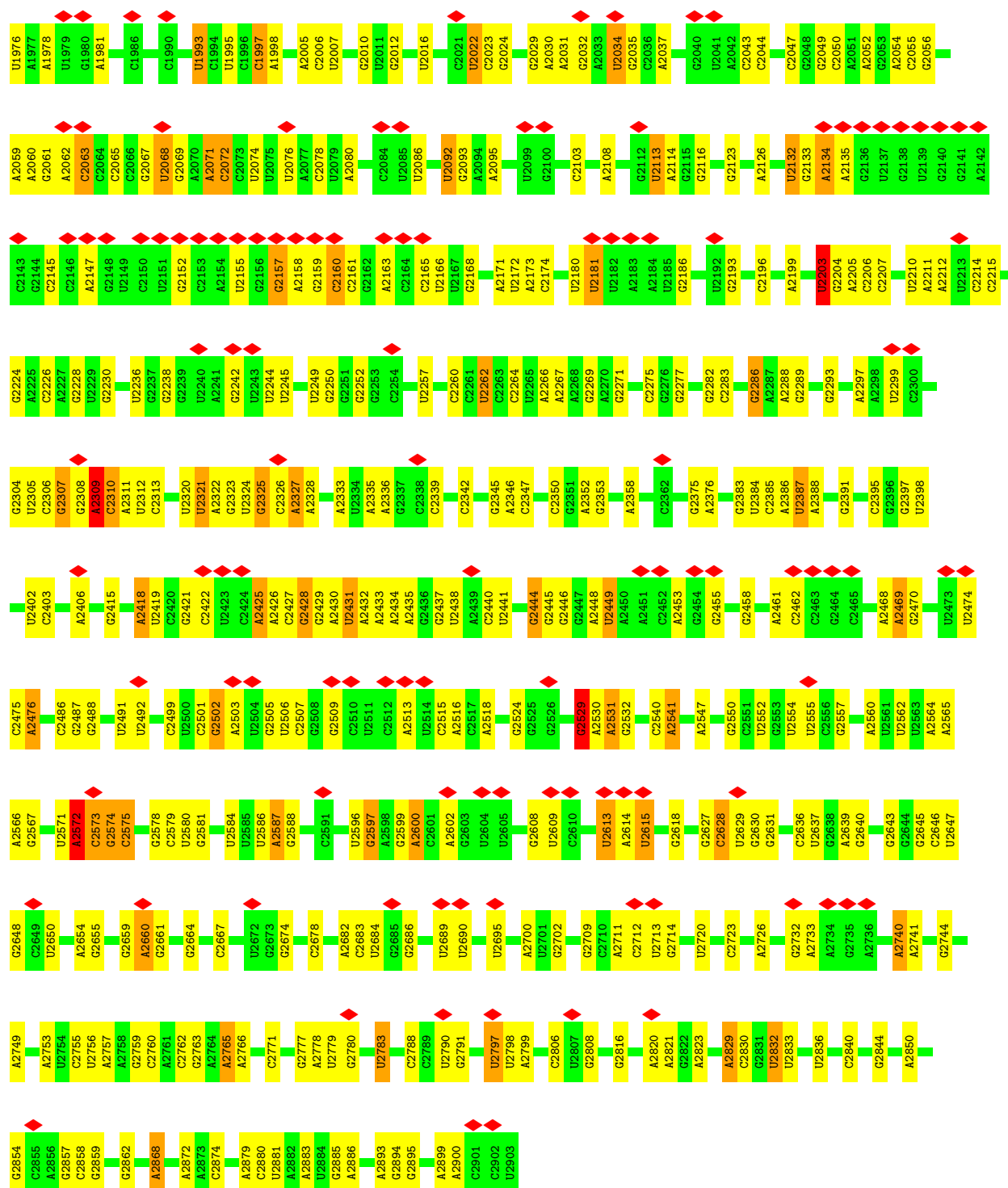
- Molecule 53: 50S ribosomal protein L36

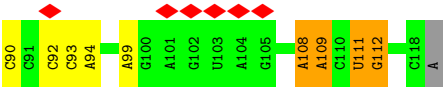


- Molecule 54: 23S ribosomal RNA

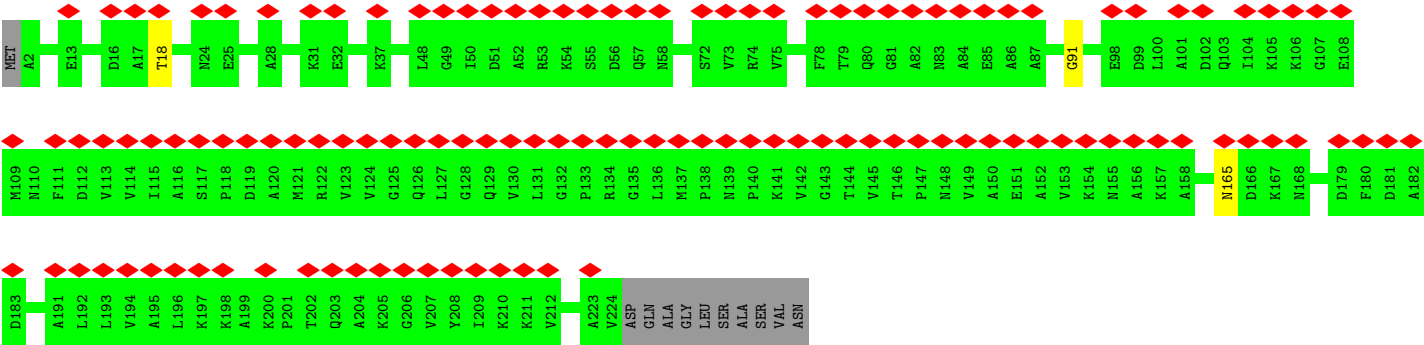








• Molecule 56: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13207	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	162740	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	202.135	Depositor
Minimum map value	-122.001	Depositor
Average map value	-1.093	Depositor
Map value standard deviation	20.632	Depositor
Recommended contour level	27	Depositor
Map size ($\text{\AA}$)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	2.8, 2.8, 2.8	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AB	0.93	0/1736	1.35	4/2340 (0.2%)
2	AC	0.93	0/1651	1.33	0/2225
3	AD	0.93	0/1665	1.35	4/2227 (0.2%)
4	AE	0.91	0/1119	1.44	9/1506 (0.6%)
5	AF	0.93	0/835	1.37	2/1128 (0.2%)
6	AG	0.95	0/1188	1.40	2/1593 (0.1%)
7	AH	0.91	0/989	1.34	0/1326
8	AI	0.97	0/1035	1.41	0/1377
9	AJ	0.95	0/797	1.36	4/1079 (0.4%)
10	AK	0.97	0/894	1.42	6/1207 (0.5%)
11	AL	0.96	0/969	1.41	2/1300 (0.2%)
12	AM	1.01	0/884	1.47	9/1181 (0.8%)
13	AN	1.00	0/817	1.46	6/1088 (0.6%)
14	AO	0.96	0/722	1.49	7/964 (0.7%)
15	AP	0.99	0/648	1.38	2/870 (0.2%)
16	AQ	0.91	0/658	1.36	0/883
17	AR	0.96	0/463	1.33	0/623
18	AS	0.95	0/653	1.36	0/879
19	AT	0.93	0/672	1.37	1/890 (0.1%)
20	AU	1.00	0/431	1.63	6/572 (1.0%)
21	AA	0.99	0/36759	1.15	58/57346 (0.1%)
22	A1	1.01	0/1668	1.17	5/2595 (0.2%)
23	A2	1.00	0/343	1.28	2/531 (0.4%)
24	A3	0.98	0/1722	1.16	3/2685 (0.1%)
25	BC	0.96	0/2121	1.52	1/2852 (0.0%)
26	BD	0.90	1/1586 (0.1%)	1.50	3/2134 (0.1%)
27	BE	0.86	0/1571	1.43	0/2113
28	BF	0.89	0/1444	1.47	1/1937 (0.1%)
29	BG	0.88	0/1343	1.48	3/1816 (0.2%)
30	BH	0.87	0/1122	1.46	4/1515 (0.3%)
31	BI	0.87	0/1046	1.39	0/1410
32	BJ	0.90	0/1152	1.44	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BK	0.93	0/947	1.47	0/1268
34	BL	0.94	0/1054	1.49	2/1403 (0.1%)
35	BM	0.91	0/1093	1.44	0/1460
36	BN	0.95	0/973	1.45	1/1301 (0.1%)
37	BO	0.91	0/902	1.42	1/1209 (0.1%)
38	BP	0.95	0/929	1.45	1/1242 (0.1%)
39	BQ	0.92	0/960	1.44	2/1278 (0.2%)
40	BR	0.90	0/829	1.44	1/1107 (0.1%)
41	BS	0.86	0/864	1.44	4/1156 (0.3%)
42	BT	0.83	0/744	1.48	4/994 (0.4%)
43	BU	0.89	0/787	1.52	1/1051 (0.1%)
44	BV	0.88	0/766	1.47	1/1025 (0.1%)
45	BW	0.90	0/604	1.56	4/799 (0.5%)
46	BX	0.92	0/635	1.49	3/848 (0.4%)
47	BY	0.87	0/510	1.42	0/677
48	BZ	0.96	0/453	1.51	0/605
49	B0	0.99	0/450	1.55	0/599
50	B1	0.94	0/417	1.51	2/556 (0.4%)
51	B2	0.97	0/380	1.55	1/498 (0.2%)
52	B3	0.96	0/513	1.48	0/676
53	B4	0.90	0/303	1.48	0/397
54	BA	0.83	0/69796	1.15	113/108888 (0.1%)
55	BB	0.84	0/2800	1.14	3/4367 (0.1%)
56	B5	0.86	0/1673	1.40	0/2255
All	All	0.90	1/160085 (0.0%)	1.23	288/239402 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AD	0	2
4	AE	0	1
21	AA	0	350
22	A1	0	14
23	A2	0	5
24	A3	0	16
25	BC	0	1
38	BP	0	1
54	BA	0	663
55	BB	0	31
All	All	0	1084

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BD	148	GLN	CA-C	5.34	1.55	1.52

All (288) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BD	148	GLN	CA-C-N	9.44	138.70	121.70
26	BD	148	GLN	C-N-CA	9.44	138.70	121.70
4	AE	149	PRO	CA-C-N	8.16	136.38	121.70
4	AE	149	PRO	C-N-CA	8.16	136.38	121.70
54	BA	1610	A	O4'-C1'-N9	7.33	119.20	108.20
54	BA	2740	A	O4'-C1'-N9	7.22	119.33	108.50
20	AU	35	GLU	CA-C-N	7.21	134.68	121.70
20	AU	35	GLU	C-N-CA	7.21	134.68	121.70
54	BA	2636	C	C5'-C4'-C3'	-7.20	105.21	116.00
54	BA	1451	C	C2'-C3'-O3'	7.18	120.26	109.50
54	BA	1954	G	O4'-C4'-C3'	6.86	110.86	104.00
44	BV	21	ARG	NE-CZ-NH2	6.77	125.29	119.20
54	BA	1451	C	C4'-C3'-O3'	6.73	119.49	109.40
21	AA	210	C	O4'-C4'-C3'	6.72	110.72	104.00
54	BA	1312	U	C2'-C3'-O3'	6.68	119.52	109.50
10	AK	125	LYS	CA-C-N	6.68	133.72	121.70
10	AK	125	LYS	C-N-CA	6.68	133.72	121.70
22	A1	73	A	C5'-C4'-C3'	-6.59	105.31	115.20
54	BA	1584	U	O4'-C1'-N1	6.59	118.38	108.50
21	AA	1049	U	C5'-C4'-C3'	-6.54	105.39	115.20
13	AN	100	SER	CA-C-N	6.53	133.46	121.70
13	AN	100	SER	C-N-CA	6.53	133.46	121.70
54	BA	2740	A	C1'-O4'-C4'	-6.49	103.41	109.90
4	AE	104	ILE	CA-C-N	6.43	133.28	121.70
4	AE	104	ILE	C-N-CA	6.43	133.28	121.70
54	BA	127	A	O4'-C4'-C3'	6.43	110.43	104.00
54	BA	280	U	O4'-C1'-N1	6.43	118.14	108.50
54	BA	1038	G	C5'-C4'-C3'	-6.35	106.48	116.00
54	BA	323	C	O4'-C1'-N1	6.35	117.72	108.20
54	BA	2072	C	C4'-C3'-C2'	-6.32	96.28	102.60
54	BA	2425	A	C4'-C3'-O3'	6.28	118.83	109.40
54	BA	1606	C	O4'-C1'-N1	6.27	117.90	108.50
36	BN	16	HIS	CB-CG-CD2	-6.26	123.06	131.20
54	BA	2428	G	C2'-C3'-O3'	6.21	118.81	109.50
20	AU	33	ARG	NE-CZ-NH2	6.17	124.76	119.20
21	AA	1049	U	C1'-O4'-C4'	-6.15	103.55	109.70
21	AA	1183	U	C1'-O4'-C4'	-6.10	103.80	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AE	152	VAL	CA-C-N	6.08	132.64	121.70
4	AE	152	VAL	C-N-CA	6.08	132.64	121.70
21	AA	793	U	C1'-O4'-C4'	-6.08	103.82	109.90
54	BA	2613	U	C2'-C3'-O3'	6.06	118.59	109.50
46	BX	19	HIS	CA-C-N	6.03	132.56	121.70
46	BX	19	HIS	C-N-CA	6.03	132.56	121.70
41	BS	90	LYS	CA-C-N	6.01	132.51	121.70
41	BS	90	LYS	C-N-CA	6.01	132.51	121.70
54	BA	1799	G	C2'-C3'-O3'	5.96	118.43	109.50
22	A1	73	A	O4'-C1'-N9	5.96	117.13	108.20
54	BA	2740	A	O4'-C4'-C3'	-5.95	98.05	104.00
26	BD	148	GLN	O-C-N	-5.95	115.35	120.71
13	AN	50	THR	CA-C-N	5.95	127.52	120.09
13	AN	50	THR	C-N-CA	5.95	127.52	120.09
54	BA	1729	U	O4'-C1'-N1	5.94	117.11	108.20
54	BA	971	G	C4'-C3'-C2'	-5.92	96.68	102.60
54	BA	99	U	O4'-C1'-N1	5.91	117.37	108.50
9	AJ	73	LEU	CA-C-N	5.88	132.56	121.97
9	AJ	73	LEU	C-N-CA	5.88	132.56	121.97
21	AA	1337	G	C5'-C4'-C3'	-5.88	107.18	116.00
54	BA	2572	A	O4'-C1'-N9	5.80	116.90	108.20
54	BA	2740	A	C5'-C4'-O4'	5.79	118.48	109.80
54	BA	1870	C	O4'-C1'-N1	5.76	116.84	108.20
1	AB	35	ASN	CA-C-N	5.76	131.59	122.61
1	AB	35	ASN	C-N-CA	5.76	131.59	122.61
21	AA	455	G	O4'-C4'-C3'	5.71	109.71	104.00
54	BA	2573	C	O4'-C1'-N1	5.69	116.74	108.20
54	BA	1699	G	O4'-C1'-N9	5.69	116.73	108.20
21	AA	38	G	O3'-P-O5'	-5.67	95.49	104.00
51	B2	3	ARG	NE-CZ-NH2	5.67	124.30	119.20
21	AA	22	G	O4'-C4'-C3'	5.66	109.66	104.00
21	AA	1201	A	P-O3'-C3'	5.66	128.69	120.20
21	AA	509	A	O4'-C4'-C3'	5.65	109.65	104.00
54	BA	1427	A	C2'-C3'-O3'	5.64	117.96	109.50
54	BA	2702	G	O4'-C4'-C3'	5.63	109.63	104.00
21	AA	675	A	P-O3'-C3'	5.63	128.64	120.20
54	BA	2586	U	O4'-C4'-C3'	5.63	109.63	104.00
54	BA	1899	A	O4'-C4'-C3'	5.62	109.62	104.00
39	BQ	95	ALA	CA-C-N	5.61	128.57	120.38
39	BQ	95	ALA	C-N-CA	5.61	128.57	120.38
21	AA	570	G	O4'-C4'-C3'	5.60	109.60	104.00
54	BA	271	G	C2'-C3'-O3'	5.58	117.88	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BH	91	PHE	CA-C-N	5.58	125.28	119.92
30	BH	91	PHE	C-N-CA	5.58	125.28	119.92
21	AA	1533	C	O4'-C4'-C3'	5.58	109.58	104.00
21	AA	983	A	O4'-C4'-C3'	5.58	109.58	104.00
21	AA	382	A	O4'-C4'-C3'	5.57	109.57	104.00
38	BP	69	VAL	N-CA-C	5.57	116.12	110.05
21	AA	1194	U	O4'-C4'-C3'	5.57	109.57	104.00
21	AA	1166	G	O4'-C4'-C3'	5.56	109.56	104.00
1	AB	111	LYS	CA-C-N	5.55	127.72	120.28
1	AB	111	LYS	C-N-CA	5.55	127.72	120.28
3	AD	58	GLN	CA-C-N	5.55	129.14	120.82
3	AD	58	GLN	C-N-CA	5.55	129.14	120.82
46	BX	33	HIS	CB-CG-CD2	-5.55	123.99	131.20
54	BA	2277	G	O4'-C4'-C3'	5.55	109.55	104.00
23	A2	90	U	C5'-C4'-C3'	-5.54	107.69	116.00
21	AA	1318	A	O4'-C4'-C3'	5.54	109.54	104.00
54	BA	1876	A	O4'-C1'-C2'	-5.53	102.07	107.60
21	AA	588	G	O4'-C4'-C3'	5.53	109.53	104.00
54	BA	251	A	C4'-C3'-C2'	-5.52	97.08	102.60
54	BA	1938	A	O4'-C1'-N9	5.51	116.47	108.20
54	BA	2541	A	O4'-C4'-C3'	5.49	109.49	104.00
14	AO	49	HIS	CB-CG-CD2	-5.49	124.07	131.20
21	AA	1014	A	O4'-C4'-C3'	5.49	109.49	104.00
21	AA	1211	U	O4'-C4'-C3'	5.49	109.48	104.00
54	BA	1758	U	O4'-C1'-N1	5.49	116.43	108.20
20	AU	46	ARG	NE-CZ-NH2	5.48	124.13	119.20
54	BA	1339	G	C2'-C3'-O3'	-5.47	105.49	113.70
54	BA	1295	C	C4'-C3'-C2'	-5.47	97.13	102.60
54	BA	1269	A	O4'-C4'-C3'	5.47	109.47	104.00
55	BB	89	U	O4'-C1'-N1	5.46	116.39	108.20
21	AA	1184	G	O4'-C4'-C3'	5.45	109.45	104.00
12	AM	60	ALA	CA-C-N	5.44	131.50	121.70
12	AM	60	ALA	C-N-CA	5.44	131.50	121.70
21	AA	445	G	O4'-C4'-C3'	5.44	109.44	104.00
21	AA	966	G	O4'-C4'-C3'	5.44	109.44	104.00
9	AJ	56	HIS	CA-C-N	5.43	131.75	121.97
9	AJ	56	HIS	C-N-CA	5.43	131.75	121.97
54	BA	1236	G	O4'-C4'-C3'	5.43	109.43	104.00
54	BA	1377	G	C2'-C3'-O3'	-5.43	105.56	113.70
54	BA	1332	G	O4'-C1'-N9	5.42	116.33	108.20
54	BA	1610	A	C1'-O4'-C4'	-5.42	104.28	109.70
21	AA	816	A	C5'-C4'-C3'	-5.41	107.88	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1352	U	O4'-C1'-N1	5.41	116.61	108.50
12	AM	82	LEU	CA-C-N	5.40	125.23	120.10
12	AM	82	LEU	C-N-CA	5.40	125.23	120.10
54	BA	203	A	C2'-C3'-O3'	-5.39	105.61	113.70
54	BA	527	C	C2'-C3'-O3'	5.39	117.58	109.50
22	A1	73	A	C1'-O4'-C4'	-5.37	104.33	109.70
21	AA	189	A	O4'-C4'-C3'	5.37	109.37	104.00
21	AA	172	A	O4'-C4'-C3'	5.36	109.36	104.00
21	AA	1117	A	O4'-C4'-C3'	5.35	109.35	104.00
21	AA	703	G	O4'-C4'-C3'	5.35	109.35	104.00
34	BL	100	ILE	CA-C-N	5.35	131.60	121.97
34	BL	100	ILE	C-N-CA	5.35	131.60	121.97
21	AA	414	A	O4'-C4'-C3'	5.34	109.34	104.00
40	BR	66	HIS	CB-CG-CD2	-5.34	124.25	131.20
15	AP	14	ARG	CA-C-N	5.34	125.54	120.31
15	AP	14	ARG	C-N-CA	5.34	125.54	120.31
54	BA	337	C	C4'-C3'-C2'	-5.33	97.27	102.60
54	BA	108	G	O4'-C4'-C3'	5.33	109.33	104.00
54	BA	2395	C	C4'-C3'-C2'	-5.33	97.27	102.60
21	AA	483	C	O4'-C4'-C3'	5.32	109.32	104.00
54	BA	386	G	C4'-C3'-O3'	5.32	120.98	113.00
54	BA	2615	U	O4'-C4'-C3'	5.32	109.32	104.00
37	BO	98	GLN	OE1-CD-NE2	-5.31	117.29	122.60
54	BA	1564	C	C2'-C3'-O3'	-5.31	105.73	113.70
50	B1	45	HIS	CB-CG-CD2	-5.31	124.30	131.20
54	BA	1332	G	C3'-C2'-C1'	5.31	106.81	101.50
29	BG	138	GLN	OE1-CD-NE2	-5.31	117.29	122.60
14	AO	22	GLY	CA-C-N	5.30	128.34	120.17
14	AO	22	GLY	C-N-CA	5.30	128.34	120.17
54	BA	1289	C	C3'-C2'-C1'	5.30	106.60	101.30
12	AM	51	GLN	OE1-CD-NE2	-5.30	117.30	122.60
21	AA	597	G	C5'-C4'-C3'	-5.29	108.06	116.00
23	A2	84	G	O4'-C4'-C3'	5.29	109.29	104.00
54	BA	1427	A	P-O3'-C3'	5.29	128.14	120.20
3	AD	106	PHE	CA-C-N	5.29	125.25	121.65
3	AD	106	PHE	C-N-CA	5.29	125.25	121.65
54	BA	323	C	C1'-O4'-C4'	-5.29	104.41	109.70
21	AA	1501	C	O4'-C4'-C3'	5.27	109.27	104.00
54	BA	2628	C	O4'-C1'-N1	5.27	116.41	108.50
21	AA	14	U	O4'-C4'-C3'	5.27	109.27	104.00
54	BA	86	G	C1'-O4'-C4'	-5.26	104.64	109.90
54	BA	1451	C	O4'-C1'-N1	5.26	116.10	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1927	A	O4'-C4'-C3'	5.26	109.26	104.00
54	BA	2350	C	C4'-C3'-C2'	-5.26	97.34	102.60
21	AA	1064	G	P-O3'-C3'	5.25	128.08	120.20
4	AE	149	PRO	N-CA-CB	5.25	108.76	103.25
54	BA	2529	G	O4'-C4'-C3'	5.25	109.25	104.00
22	A1	75	C	C2'-C3'-O3'	-5.24	105.83	113.70
54	BA	2309	A	O4'-C1'-N9	5.23	116.35	108.50
24	A3	2	G	O4'-C4'-C3'	5.23	109.23	104.00
21	AA	476	U	P-O3'-C3'	5.22	128.04	120.20
54	BA	1808	A	O4'-C1'-N9	5.22	116.04	108.20
21	AA	718	A	O4'-C4'-C3'	5.22	109.22	104.00
54	BA	1822	C	C4'-C3'-C2'	-5.22	97.38	102.60
54	BA	2757	A	C5'-C4'-C3'	-5.22	108.17	116.00
5	AF	66	ALA	N-CA-C	5.21	112.71	108.07
54	BA	2755	C	O4'-C4'-C3'	5.21	109.21	104.00
41	BS	91	GLY	CA-C-N	5.20	131.06	121.70
41	BS	91	GLY	C-N-CA	5.20	131.06	121.70
42	BT	71	GLY	CA-C-N	5.20	131.06	121.70
42	BT	71	GLY	C-N-CA	5.20	131.06	121.70
55	BB	86	G	C5'-C4'-C3'	-5.20	108.20	116.00
55	BB	42	C	C5'-C4'-C3'	-5.20	108.20	116.00
14	AO	43	ALA	CA-C-N	5.19	131.04	121.70
14	AO	43	ALA	C-N-CA	5.19	131.04	121.70
21	AA	840	C	O4'-C4'-C3'	5.19	109.19	104.00
42	BT	74	ILE	CA-C-N	5.18	126.59	121.57
42	BT	74	ILE	C-N-CA	5.18	126.59	121.57
54	BA	2386	A	O4'-C4'-C3'	5.17	109.17	104.00
54	BA	2092	U	O4'-C1'-N1	5.17	115.96	108.20
54	BA	1126	A	C4'-C3'-O3'	5.17	117.16	109.40
6	AG	39	GLU	CA-C-N	5.17	127.92	120.38
6	AG	39	GLU	C-N-CA	5.17	127.92	120.38
50	B1	44	GLN	OE1-CD-NE2	-5.16	117.44	122.60
54	BA	465	G	O4'-C4'-C3'	5.16	109.16	104.00
54	BA	2342	C	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	1789	A	O4'-C4'-C3'	5.16	109.16	104.00
22	A1	45	G	O4'-C4'-C3'	5.16	109.16	104.00
54	BA	1393	A	O4'-C4'-C3'	5.15	109.15	104.00
21	AA	496	A	C1'-O4'-C4'	-5.15	104.75	109.90
54	BA	737	C	C4'-C3'-C2'	-5.14	97.46	102.60
54	BA	1378	A	O3'-P-O5'	-5.14	96.29	104.00
54	BA	2531	A	O4'-C1'-C2'	-5.14	102.46	107.60
45	BW	72	GLY	CA-C-N	5.13	125.06	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BW	72	GLY	C-N-CA	5.13	125.06	119.78
54	BA	1797	G	O4'-C4'-C3'	5.13	109.13	104.00
43	BU	44	HIS	CB-CG-CD2	-5.13	124.53	131.20
54	BA	3	U	C4'-C3'-C2'	-5.12	97.47	102.60
21	AA	701	U	C2'-C3'-O3'	5.12	117.19	109.50
54	BA	308	G	O4'-C4'-C3'	5.12	109.12	104.00
54	BA	2203	U	O4'-C4'-C3'	5.12	109.12	104.00
13	AN	80	SER	CA-C-N	5.12	128.50	120.82
13	AN	80	SER	C-N-CA	5.12	128.50	120.82
54	BA	2667	C	O4'-C4'-C3'	5.12	109.12	104.00
54	BA	1392	A	O4'-C4'-C3'	5.12	109.12	104.00
54	BA	144	A	C4'-C3'-O3'	5.11	117.07	109.40
12	AM	110	GLY	CA-C-N	5.11	125.38	119.92
12	AM	110	GLY	C-N-CA	5.11	125.38	119.92
21	AA	1337	G	O3'-P-O5'	-5.10	96.35	104.00
21	AA	1006	G	O4'-C4'-C3'	5.10	109.10	104.00
21	AA	575	G	P-O3'-C3'	5.10	127.84	120.20
54	BA	2067	G	C2'-C3'-O3'	-5.09	106.06	113.70
28	BF	131	VAL	N-CA-C	5.09	115.86	110.72
30	BH	84	ALA	CA-C-N	5.09	126.29	121.46
30	BH	84	ALA	C-N-CA	5.09	126.29	121.46
10	AK	122	PRO	CA-C-N	5.08	125.16	119.87
10	AK	122	PRO	C-N-CA	5.08	125.16	119.87
54	BA	2783	U	O4'-C4'-C3'	5.08	109.08	104.00
54	BA	1846	G	O4'-C4'-C3'	5.08	109.08	104.00
4	AE	104	ILE	O-C-N	-5.08	116.22	122.57
21	AA	979	C	C5'-C4'-C3'	-5.08	108.38	116.00
21	AA	901	A	O4'-C4'-C3'	5.07	109.07	104.00
10	AK	126	ARG	CA-C-N	5.07	130.83	121.70
10	AK	126	ARG	C-N-CA	5.07	130.83	121.70
29	BG	76	ILE	CA-C-N	5.07	125.61	119.98
29	BG	76	ILE	C-N-CA	5.07	125.61	119.98
54	BA	55	G	C4'-C3'-C2'	-5.06	97.54	102.60
54	BA	1664	A	O4'-C4'-C3'	5.06	109.06	104.00
54	BA	2307	G	O4'-C1'-N9	5.06	115.79	108.20
21	AA	1130	A	C5'-C4'-C3'	-5.06	108.41	116.00
4	AE	149	PRO	O-C-N	-5.06	115.81	122.64
54	BA	2244	U	O4'-C4'-C3'	5.06	109.06	104.00
12	AM	11	HIS	CB-CG-CD2	-5.05	124.63	131.20
21	AA	66	A	C5'-C4'-C3'	-5.05	108.42	116.00
54	BA	37	C	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	2438	U	O4'-C4'-C3'	5.05	109.05	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AF	11	HIS	CB-CG-CD2	-5.05	124.63	131.20
21	AA	1452	C	P-O3'-C3'	5.05	127.78	120.20
19	AT	19	HIS	CB-CG-CD2	-5.05	124.64	131.20
54	BA	2428	G	C4'-C3'-O3'	5.05	116.97	109.40
21	AA	734	G	O4'-C4'-C3'	5.04	109.04	104.00
54	BA	277	G	O4'-C1'-N9	5.04	115.76	108.20
54	BA	527	C	P-O3'-C3'	5.04	127.76	120.20
54	BA	725	G	C2'-C3'-O3'	-5.04	106.14	113.70
54	BA	1128	G	C1'-O4'-C4'	-5.04	104.66	109.70
54	BA	2600	A	C1'-O4'-C4'	-5.03	104.87	109.90
21	AA	913	A	P-O3'-C3'	5.03	127.75	120.20
21	AA	59	A	C5'-C4'-C3'	-5.03	108.45	116.00
54	BA	2108	A	O4'-C4'-C3'	5.03	109.03	104.00
54	BA	947	A	C4'-C3'-C2'	-5.03	97.57	102.60
21	AA	404	G	O4'-C4'-C3'	5.03	109.03	104.00
54	BA	1301	A	O4'-C1'-C2'	-5.02	100.78	105.80
21	AA	607	A	O4'-C4'-C3'	5.02	109.02	104.00
12	AM	2	ARG	NE-CZ-NH2	5.02	123.72	119.20
11	AL	74	GLN	CA-C-N	5.02	128.00	120.87
11	AL	74	GLN	C-N-CA	5.02	128.00	120.87
21	AA	982	U	P-O3'-C3'	5.02	127.73	120.20
21	AA	1092	A	O4'-C4'-C3'	5.02	109.02	104.00
24	A3	15	G	O4'-C4'-C3'	5.02	109.02	104.00
24	A3	75	C	O4'-C4'-C3'	5.02	109.02	104.00
21	AA	844	G	O4'-C4'-C3'	5.02	109.02	104.00
25	BC	52	HIS	CB-CG-CD2	-5.02	124.68	131.20
54	BA	363	G	O4'-C4'-C3'	5.02	109.02	104.00
14	AO	34	GLN	OE1-CD-NE2	-5.01	117.59	122.60
54	BA	1603	A	O4'-C4'-C3'	5.01	109.02	104.00
54	BA	2327	A	O4'-C4'-C3'	5.01	109.01	104.00
54	BA	2515	C	C4'-C3'-C2'	-5.01	97.58	102.60
54	BA	1534	U	O4'-C1'-N1	5.01	115.72	108.20
54	BA	706	A	C5'-C4'-C3'	-5.01	108.48	116.00
14	AO	37	HIS	CB-CG-CD2	-5.01	124.69	131.20
20	AU	11	PHE	CA-C-N	5.01	130.72	121.70
20	AU	11	PHE	C-N-CA	5.01	130.72	121.70
54	BA	847	U	O4'-C1'-N1	5.01	116.01	108.50
21	AA	827	U	O4'-C4'-C3'	5.01	109.01	104.00
45	BW	9	THR	CA-C-N	5.00	131.09	121.54
45	BW	9	THR	C-N-CA	5.00	131.09	121.54
54	BA	2531	A	N9-C1'-C2'	5.00	119.50	112.00

There are no chirality outliers.

All (1084) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	12	U	Sidechain
22	A1	20	G	Sidechain
22	A1	27	C	Sidechain
22	A1	32	C	Sidechain
22	A1	42	G	Sidechain
22	A1	43	G	Sidechain
22	A1	44	G	Sidechain
22	A1	45	G	Sidechain
22	A1	47	U	Sidechain
22	A1	50	G	Sidechain
22	A1	53	G	Sidechain
22	A1	65	C	Sidechain
22	A1	73	A	Sidechain
22	A1	76	A	Sidechain
23	A2	79	A	Sidechain
23	A2	80	C	Sidechain
23	A2	84	G	Sidechain
23	A2	90	U	Sidechain
23	A2	92	U	Sidechain
24	A3	16	C	Sidechain
24	A3	23	G	Sidechain
24	A3	24	C	Sidechain
24	A3	39	A	Sidechain
24	A3	4	G	Sidechain
24	A3	44	A	Sidechain
24	A3	46	G	Sidechain
24	A3	54	G	Sidechain
24	A3	60	A	Sidechain
24	A3	61	U	Sidechain
24	A3	64	G	Sidechain
24	A3	65	G	Sidechain
24	A3	66	C	Sidechain
24	A3	7	G	Sidechain
24	A3	74	A	Sidechain
24	A3	76	C	Sidechain
21	AA	1001	C	Sidechain
21	AA	1005	A	Sidechain
21	AA	1013	G	Sidechain
21	AA	1014	A	Sidechain
21	AA	1024	G	Sidechain
21	AA	1025	U	Sidechain
21	AA	1040	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1049	U	Sidechain
21	AA	1051	C	Sidechain
21	AA	1052	U	Sidechain
21	AA	1053	G	Sidechain
21	AA	1054	C	Sidechain
21	AA	1055	A	Sidechain
21	AA	1062	U	Sidechain
21	AA	1064	G	Sidechain
21	AA	1072	G	Sidechain
21	AA	1073	U	Sidechain
21	AA	1077	G	Sidechain
21	AA	1079	G	Sidechain
21	AA	108	G	Sidechain
21	AA	1081	A	Sidechain
21	AA	1085	U	Sidechain
21	AA	1086	U	Sidechain
21	AA	1087	G	Sidechain
21	AA	1093	A	Sidechain
21	AA	1095	U	Sidechain
21	AA	1098	C	Sidechain
21	AA	1107	C	Sidechain
21	AA	1108	G	Sidechain
21	AA	1118	U	Sidechain
21	AA	1120	C	Sidechain
21	AA	1121	U	Sidechain
21	AA	1124	G	Sidechain
21	AA	1126	U	Sidechain
21	AA	1128	C	Sidechain
21	AA	1131	G	Sidechain
21	AA	1139	G	Sidechain
21	AA	115	G	Sidechain
21	AA	1155	A	Sidechain
21	AA	1156	G	Sidechain
21	AA	1158	C	Sidechain
21	AA	1159	U	Sidechain
21	AA	1166	G	Sidechain
21	AA	1174	G	Sidechain
21	AA	1178	G	Sidechain
21	AA	1183	U	Sidechain
21	AA	1185	G	Sidechain
21	AA	1187	G	Sidechain
21	AA	1190	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1192	C	Sidechain
21	AA	1195	C	Sidechain
21	AA	1203	C	Sidechain
21	AA	1206	G	Sidechain
21	AA	1207	G	Sidechain
21	AA	121	U	Sidechain
21	AA	1211	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1222	G	Sidechain
21	AA	1225	A	Sidechain
21	AA	1226	C	Sidechain
21	AA	1228	C	Sidechain
21	AA	1231	G	Sidechain
21	AA	1236	A	Sidechain
21	AA	124	C	Sidechain
21	AA	1244	G	Sidechain
21	AA	1246	A	Sidechain
21	AA	1250	A	Sidechain
21	AA	1259	C	Sidechain
21	AA	1264	U	Sidechain
21	AA	1266	G	Sidechain
21	AA	1269	A	Sidechain
21	AA	1278	G	Sidechain
21	AA	1282	C	Sidechain
21	AA	1283	U	Sidechain
21	AA	1287	A	Sidechain
21	AA	129	A	Sidechain
21	AA	1300	G	Sidechain
21	AA	1303	C	Sidechain
21	AA	1304	G	Sidechain
21	AA	1306	A	Sidechain
21	AA	1311	A	Sidechain
21	AA	1316	G	Sidechain
21	AA	1319	A	Sidechain
21	AA	1329	A	Sidechain
21	AA	1332	A	Sidechain
21	AA	1342	C	Sidechain
21	AA	1345	U	Sidechain
21	AA	1351	U	Sidechain
21	AA	1358	U	Sidechain
21	AA	1359	C	Sidechain
21	AA	1361	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1362	A	Sidechain
21	AA	1363	A	Sidechain
21	AA	1368	A	Sidechain
21	AA	1373	G	Sidechain
21	AA	1377	A	Sidechain
21	AA	1380	U	Sidechain
21	AA	1384	C	Sidechain
21	AA	1386	G	Sidechain
21	AA	1390	U	Sidechain
21	AA	1391	U	Sidechain
21	AA	14	U	Sidechain
21	AA	1411	C	Sidechain
21	AA	1419	G	Sidechain
21	AA	1422	G	Sidechain
21	AA	1427	C	Sidechain
21	AA	143	A	Sidechain
21	AA	144	G	Sidechain
21	AA	1446	A	Sidechain
21	AA	145	G	Sidechain
21	AA	1451	U	Sidechain
21	AA	1467	C	Sidechain
21	AA	1473	G	Sidechain
21	AA	1486	G	Sidechain
21	AA	1487	G	Sidechain
21	AA	1491	G	Sidechain
21	AA	1495	U	Sidechain
21	AA	1502	A	Sidechain
21	AA	1506	U	Sidechain
21	AA	1510	C	Sidechain
21	AA	1513	A	Sidechain
21	AA	1517	G	Sidechain
21	AA	1519	A	Sidechain
21	AA	152	A	Sidechain
21	AA	1525	G	Sidechain
21	AA	1528	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1530	G	Sidechain
21	AA	1532	U	Sidechain
21	AA	158	G	Sidechain
21	AA	159	G	Sidechain
21	AA	163	C	Sidechain
21	AA	164	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	167	A	Sidechain
21	AA	173	U	Sidechain
21	AA	179	A	Sidechain
21	AA	181	A	Sidechain
21	AA	183	C	Sidechain
21	AA	187	G	Sidechain
21	AA	188	C	Sidechain
21	AA	193	C	Sidechain
21	AA	196	A	Sidechain
21	AA	197	A	Sidechain
21	AA	209	U	Sidechain
21	AA	217	C	Sidechain
21	AA	219	U	Sidechain
21	AA	227	G	Sidechain
21	AA	230	G	Sidechain
21	AA	236	A	Sidechain
21	AA	239	U	Sidechain
21	AA	241	G	Sidechain
21	AA	243	A	Sidechain
21	AA	251	G	Sidechain
21	AA	263	A	Sidechain
21	AA	264	C	Sidechain
21	AA	266	G	Sidechain
21	AA	273	U	Sidechain
21	AA	278	G	Sidechain
21	AA	293	G	Sidechain
21	AA	296	U	Sidechain
21	AA	297	G	Sidechain
21	AA	301	G	Sidechain
21	AA	310	G	Sidechain
21	AA	315	A	Sidechain
21	AA	324	G	Sidechain
21	AA	333	U	Sidechain
21	AA	337	G	Sidechain
21	AA	34	C	Sidechain
21	AA	341	C	Sidechain
21	AA	352	C	Sidechain
21	AA	353	A	Sidechain
21	AA	354	G	Sidechain
21	AA	355	C	Sidechain
21	AA	362	G	Sidechain
21	AA	367	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	370	C	Sidechain
21	AA	372	C	Sidechain
21	AA	374	A	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	382	A	Sidechain
21	AA	391	G	Sidechain
21	AA	394	G	Sidechain
21	AA	395	C	Sidechain
21	AA	401	C	Sidechain
21	AA	402	G	Sidechain
21	AA	403	C	Sidechain
21	AA	404	G	Sidechain
21	AA	407	U	Sidechain
21	AA	41	G	Sidechain
21	AA	414	A	Sidechain
21	AA	415	A	Sidechain
21	AA	416	G	Sidechain
21	AA	429	U	Sidechain
21	AA	430	A	Sidechain
21	AA	431	A	Sidechain
21	AA	433	G	Sidechain
21	AA	438	U	Sidechain
21	AA	440	C	Sidechain
21	AA	441	A	Sidechain
21	AA	442	G	Sidechain
21	AA	445	G	Sidechain
21	AA	449	G	Sidechain
21	AA	450	G	Sidechain
21	AA	466	A	Sidechain
21	AA	467	U	Sidechain
21	AA	470	C	Sidechain
21	AA	474	G	Sidechain
21	AA	479	U	Sidechain
21	AA	481	G	Sidechain
21	AA	484	G	Sidechain
21	AA	487	A	Sidechain
21	AA	492	C	Sidechain
21	AA	494	G	Sidechain
21	AA	497	G	Sidechain
21	AA	499	A	Sidechain
21	AA	502	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	51	A	Sidechain
21	AA	512	U	Sidechain
21	AA	513	C	Sidechain
21	AA	515	G	Sidechain
21	AA	516	U	Sidechain
21	AA	517	G	Sidechain
21	AA	523	A	Sidechain
21	AA	524	G	Sidechain
21	AA	529	G	Sidechain
21	AA	533	A	Sidechain
21	AA	537	G	Sidechain
21	AA	541	G	Sidechain
21	AA	547	A	Sidechain
21	AA	553	A	Sidechain
21	AA	557	G	Sidechain
21	AA	558	G	Sidechain
21	AA	563	A	Sidechain
21	AA	566	G	Sidechain
21	AA	568	G	Sidechain
21	AA	58	C	Sidechain
21	AA	582	C	Sidechain
21	AA	584	G	Sidechain
21	AA	592	G	Sidechain
21	AA	593	U	Sidechain
21	AA	594	U	Sidechain
21	AA	595	A	Sidechain
21	AA	6	G	Sidechain
21	AA	611	C	Sidechain
21	AA	612	C	Sidechain
21	AA	622	A	Sidechain
21	AA	623	C	Sidechain
21	AA	625	U	Sidechain
21	AA	626	G	Sidechain
21	AA	632	U	Sidechain
21	AA	633	G	Sidechain
21	AA	640	A	Sidechain
21	AA	643	C	Sidechain
21	AA	65	A	Sidechain
21	AA	650	G	Sidechain
21	AA	653	U	Sidechain
21	AA	654	G	Sidechain
21	AA	656	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	66	A	Sidechain
21	AA	660	C	Sidechain
21	AA	661	G	Sidechain
21	AA	662	U	Sidechain
21	AA	664	G	Sidechain
21	AA	665	A	Sidechain
21	AA	67	C	Sidechain
21	AA	69	G	Sidechain
21	AA	695	A	Sidechain
21	AA	697	U	Sidechain
21	AA	701	U	Sidechain
21	AA	709	U	Sidechain
21	AA	71	A	Sidechain
21	AA	717	U	Sidechain
21	AA	724	G	Sidechain
21	AA	727	G	Sidechain
21	AA	738	C	Sidechain
21	AA	740	U	Sidechain
21	AA	742	G	Sidechain
21	AA	745	G	Sidechain
21	AA	748	G	Sidechain
21	AA	751	U	Sidechain
21	AA	753	A	Sidechain
21	AA	754	C	Sidechain
21	AA	758	C	Sidechain
21	AA	766	A	Sidechain
21	AA	768	A	Sidechain
21	AA	773	G	Sidechain
21	AA	778	G	Sidechain
21	AA	785	G	Sidechain
21	AA	796	C	Sidechain
21	AA	800	G	Sidechain
21	AA	801	U	Sidechain
21	AA	804	U	Sidechain
21	AA	805	C	Sidechain
21	AA	813	U	Sidechain
21	AA	820	U	Sidechain
21	AA	830	G	Sidechain
21	AA	838	G	Sidechain
21	AA	844	G	Sidechain
21	AA	845	A	Sidechain
21	AA	852	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	858	G	Sidechain
21	AA	859	G	Sidechain
21	AA	86	G	Sidechain
21	AA	863	U	Sidechain
21	AA	864	A	Sidechain
21	AA	869	G	Sidechain
21	AA	873	A	Sidechain
21	AA	874	G	Sidechain
21	AA	877	G	Sidechain
21	AA	879	C	Sidechain
21	AA	883	C	Sidechain
21	AA	885	G	Sidechain
21	AA	886	G	Sidechain
21	AA	89	U	Sidechain
21	AA	891	U	Sidechain
21	AA	898	G	Sidechain
21	AA	90	C	Sidechain
21	AA	901	A	Sidechain
21	AA	902	G	Sidechain
21	AA	906	A	Sidechain
21	AA	907	A	Sidechain
21	AA	909	A	Sidechain
21	AA	91	U	Sidechain
21	AA	916	U	Sidechain
21	AA	919	A	Sidechain
21	AA	925	G	Sidechain
21	AA	926	G	Sidechain
21	AA	927	G	Sidechain
21	AA	932	C	Sidechain
21	AA	933	G	Sidechain
21	AA	938	A	Sidechain
21	AA	940	C	Sidechain
21	AA	941	G	Sidechain
21	AA	942	G	Sidechain
21	AA	946	A	Sidechain
21	AA	952	U	Sidechain
21	AA	954	G	Sidechain
21	AA	957	U	Sidechain
21	AA	967	C	Sidechain
21	AA	97	G	Sidechain
21	AA	972	C	Sidechain
21	AA	973	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	976	G	Sidechain
21	AA	977	A	Sidechain
21	AA	98	A	Sidechain
21	AA	983	A	Sidechain
21	AA	987	G	Sidechain
21	AA	991	U	Sidechain
21	AA	994	A	Sidechain
3	AD	3	TYR	Sidechain
3	AD	36	ALA	Peptide
4	AE	148	SER	Peptide
54	BA	1	G	Sidechain
54	BA	1002	G	Sidechain
54	BA	1006	C	Sidechain
54	BA	1008	A	Sidechain
54	BA	101	A	Sidechain
54	BA	1014	A	Sidechain
54	BA	1015	U	Sidechain
54	BA	1016	G	Sidechain
54	BA	1017	G	Sidechain
54	BA	1018	U	Sidechain
54	BA	1019	U	Sidechain
54	BA	1020	A	Sidechain
54	BA	1028	A	Sidechain
54	BA	1030	C	Sidechain
54	BA	1033	U	Sidechain
54	BA	1039	A	Sidechain
54	BA	1044	C	Sidechain
54	BA	1045	C	Sidechain
54	BA	1050	A	Sidechain
54	BA	1051	G	Sidechain
54	BA	1056	G	Sidechain
54	BA	1059	G	Sidechain
54	BA	1069	A	Sidechain
54	BA	1070	A	Sidechain
54	BA	1072	C	Sidechain
54	BA	1077	A	Sidechain
54	BA	1079	C	Sidechain
54	BA	1081	U	Sidechain
54	BA	1089	A	Sidechain
54	BA	109	C	Sidechain
54	BA	1099	G	Sidechain
54	BA	11	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1100	C	Sidechain
54	BA	1107	G	Sidechain
54	BA	1115	G	Sidechain
54	BA	1119	U	Sidechain
54	BA	1125	G	Sidechain
54	BA	1126	A	Sidechain
54	BA	114	U	Sidechain
54	BA	1142	A	Sidechain
54	BA	1144	A	Sidechain
54	BA	1158	C	Sidechain
54	BA	1162	G	Sidechain
54	BA	1167	C	Sidechain
54	BA	1171	G	Sidechain
54	BA	1175	A	Sidechain
54	BA	1184	U	Sidechain
54	BA	1186	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	1202	G	Sidechain
54	BA	1210	G	Sidechain
54	BA	1215	G	Sidechain
54	BA	1223	G	Sidechain
54	BA	1224	U	Sidechain
54	BA	1227	G	Sidechain
54	BA	1229	C	Sidechain
54	BA	1234	U	Sidechain
54	BA	1236	G	Sidechain
54	BA	1239	G	Sidechain
54	BA	1251	C	Sidechain
54	BA	1261	C	Sidechain
54	BA	1263	U	Sidechain
54	BA	1265	A	Sidechain
54	BA	1269	A	Sidechain
54	BA	1270	C	Sidechain
54	BA	1273	U	Sidechain
54	BA	1274	A	Sidechain
54	BA	1277	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	129	C	Sidechain
54	BA	1291	C	Sidechain
54	BA	1306	C	Sidechain
54	BA	1315	C	Sidechain
54	BA	1319	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1320	C	Sidechain
54	BA	1325	U	Sidechain
54	BA	1326	U	Sidechain
54	BA	1327	A	Sidechain
54	BA	1331	G	Sidechain
54	BA	1332	G	Sidechain
54	BA	1333	G	Sidechain
54	BA	1334	G	Sidechain
54	BA	134	G	Sidechain
54	BA	1343	G	Sidechain
54	BA	1344	U	Sidechain
54	BA	1355	G	Sidechain
54	BA	1364	G	Sidechain
54	BA	1368	G	Sidechain
54	BA	1370	C	Sidechain
54	BA	1376	C	Sidechain
54	BA	1387	A	Sidechain
54	BA	1390	U	Sidechain
54	BA	1391	U	Sidechain
54	BA	1392	A	Sidechain
54	BA	1398	C	Sidechain
54	BA	1399	C	Sidechain
54	BA	14	A	Sidechain
54	BA	141	G	Sidechain
54	BA	1410	G	Sidechain
54	BA	1419	A	Sidechain
54	BA	142	A	Sidechain
54	BA	1423	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1426	G	Sidechain
54	BA	1427	A	Sidechain
54	BA	1428	C	Sidechain
54	BA	143	C	Sidechain
54	BA	1436	G	Sidechain
54	BA	1438	U	Sidechain
54	BA	1440	U	Sidechain
54	BA	1444	G	Sidechain
54	BA	1448	G	Sidechain
54	BA	1457	U	Sidechain
54	BA	146	A	Sidechain
54	BA	1464	G	Sidechain
54	BA	1465	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1474	U	Sidechain
54	BA	1475	G	Sidechain
54	BA	1478	G	Sidechain
54	BA	1483	G	Sidechain
54	BA	1492	G	Sidechain
54	BA	1493	C	Sidechain
54	BA	1495	A	Sidechain
54	BA	15	G	Sidechain
54	BA	150	U	Sidechain
54	BA	1509	A	Sidechain
54	BA	1515	A	Sidechain
54	BA	1517	G	Sidechain
54	BA	153	U	Sidechain
54	BA	1530	G	Sidechain
54	BA	1531	C	Sidechain
54	BA	1534	U	Sidechain
54	BA	1540	G	Sidechain
54	BA	1544	A	Sidechain
54	BA	1546	G	Sidechain
54	BA	1548	A	Sidechain
54	BA	1552	A	Sidechain
54	BA	1554	U	Sidechain
54	BA	1555	G	Sidechain
54	BA	1559	U	Sidechain
54	BA	1561	C	Sidechain
54	BA	1565	C	Sidechain
54	BA	1567	G	Sidechain
54	BA	1569	A	Sidechain
54	BA	1573	G	Sidechain
54	BA	1581	G	Sidechain
54	BA	1584	U	Sidechain
54	BA	1585	C	Sidechain
54	BA	1592	C	Sidechain
54	BA	1598	A	Sidechain
54	BA	1602	U	Sidechain
54	BA	1612	C	Sidechain
54	BA	1613	G	Sidechain
54	BA	1617	C	Sidechain
54	BA	1628	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1642	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1646	C	Sidechain
54	BA	1652	A	Sidechain
54	BA	1653	G	Sidechain
54	BA	1656	C	Sidechain
54	BA	1664	A	Sidechain
54	BA	1667	G	Sidechain
54	BA	168	G	Sidechain
54	BA	1680	U	Sidechain
54	BA	1681	G	Sidechain
54	BA	1684	G	Sidechain
54	BA	169	G	Sidechain
54	BA	1692	U	Sidechain
54	BA	1696	G	Sidechain
54	BA	1699	G	Sidechain
54	BA	1705	A	Sidechain
54	BA	1706	C	Sidechain
54	BA	1707	G	Sidechain
54	BA	1709	U	Sidechain
54	BA	171	U	Sidechain
54	BA	1711	A	Sidechain
54	BA	1714	U	Sidechain
54	BA	1716	U	Sidechain
54	BA	1723	G	Sidechain
54	BA	1725	U	Sidechain
54	BA	1729	U	Sidechain
54	BA	173	A	Sidechain
54	BA	1737	G	Sidechain
54	BA	1738	G	Sidechain
54	BA	1743	G	Sidechain
54	BA	1744	A	Sidechain
54	BA	1747	U	Sidechain
54	BA	1753	G	Sidechain
54	BA	1759	A	Sidechain
54	BA	177	G	Sidechain
54	BA	1772	A	Sidechain
54	BA	1774	C	Sidechain
54	BA	1778	U	Sidechain
54	BA	1779	U	Sidechain
54	BA	1789	A	Sidechain
54	BA	179	C	Sidechain
54	BA	1792	G	Sidechain
54	BA	1797	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1798	U	Sidechain
54	BA	180	G	Sidechain
54	BA	1802	A	Sidechain
54	BA	1803	A	Sidechain
54	BA	1804	C	Sidechain
54	BA	1808	A	Sidechain
54	BA	1821	A	Sidechain
54	BA	1823	G	Sidechain
54	BA	1837	C	Sidechain
54	BA	1838	C	Sidechain
54	BA	1840	G	Sidechain
54	BA	1845	G	Sidechain
54	BA	1852	U	Sidechain
54	BA	1854	A	Sidechain
54	BA	1859	U	Sidechain
54	BA	1865	U	Sidechain
54	BA	1869	G	Sidechain
54	BA	187	G	Sidechain
54	BA	1884	G	Sidechain
54	BA	1887	C	Sidechain
54	BA	1890	A	Sidechain
54	BA	1891	G	Sidechain
54	BA	1892	C	Sidechain
54	BA	1893	C	Sidechain
54	BA	1896	G	Sidechain
54	BA	1897	G	Sidechain
54	BA	1903	G	Sidechain
54	BA	1908	C	Sidechain
54	BA	1912	A	Sidechain
54	BA	1913	A	Sidechain
54	BA	1915	U	Sidechain
54	BA	1918	A	Sidechain
54	BA	1919	A	Sidechain
54	BA	1927	A	Sidechain
54	BA	193	U	Sidechain
54	BA	1935	G	Sidechain
54	BA	1938	A	Sidechain
54	BA	194	G	Sidechain
54	BA	1941	C	Sidechain
54	BA	1942	C	Sidechain
54	BA	1945	G	Sidechain
54	BA	1946	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1948	G	Sidechain
54	BA	1952	A	Sidechain
54	BA	1955	U	Sidechain
54	BA	196	A	Sidechain
54	BA	1964	G	Sidechain
54	BA	1967	C	Sidechain
54	BA	1968	G	Sidechain
54	BA	1971	U	Sidechain
54	BA	1975	G	Sidechain
54	BA	1976	U	Sidechain
54	BA	1978	A	Sidechain
54	BA	1993	U	Sidechain
54	BA	1995	U	Sidechain
54	BA	1997	C	Sidechain
54	BA	1998	A	Sidechain
54	BA	200	U	Sidechain
54	BA	2005	A	Sidechain
54	BA	2006	C	Sidechain
54	BA	2007	U	Sidechain
54	BA	2010	G	Sidechain
54	BA	2012	G	Sidechain
54	BA	2016	U	Sidechain
54	BA	2022	U	Sidechain
54	BA	2024	G	Sidechain
54	BA	2029	G	Sidechain
54	BA	2034	U	Sidechain
54	BA	2037	A	Sidechain
54	BA	204	A	Sidechain
54	BA	2044	C	Sidechain
54	BA	2047	C	Sidechain
54	BA	2049	G	Sidechain
54	BA	205	G	Sidechain
54	BA	2050	C	Sidechain
54	BA	2052	A	Sidechain
54	BA	2054	A	Sidechain
54	BA	2056	G	Sidechain
54	BA	206	U	Sidechain
54	BA	2063	C	Sidechain
54	BA	2065	C	Sidechain
54	BA	2068	U	Sidechain
54	BA	207	A	Sidechain
54	BA	2071	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2074	U	Sidechain
54	BA	2076	U	Sidechain
54	BA	2078	C	Sidechain
54	BA	2080	A	Sidechain
54	BA	2086	U	Sidechain
54	BA	2093	G	Sidechain
54	BA	2095	A	Sidechain
54	BA	2103	C	Sidechain
54	BA	2113	U	Sidechain
54	BA	2116	G	Sidechain
54	BA	2123	G	Sidechain
54	BA	2132	U	Sidechain
54	BA	2134	A	Sidechain
54	BA	2147	A	Sidechain
54	BA	215	G	Sidechain
54	BA	2152	G	Sidechain
54	BA	2157	G	Sidechain
54	BA	2158	A	Sidechain
54	BA	2160	C	Sidechain
54	BA	2161	C	Sidechain
54	BA	2163	A	Sidechain
54	BA	2165	C	Sidechain
54	BA	2166	U	Sidechain
54	BA	2168	G	Sidechain
54	BA	218	A	Sidechain
54	BA	2181	U	Sidechain
54	BA	2186	G	Sidechain
54	BA	2193	G	Sidechain
54	BA	2196	C	Sidechain
54	BA	2203	U	Sidechain
54	BA	2205	A	Sidechain
54	BA	2207	C	Sidechain
54	BA	221	A	Sidechain
54	BA	2210	U	Sidechain
54	BA	2212	A	Sidechain
54	BA	2215	C	Sidechain
54	BA	2224	G	Sidechain
54	BA	2226	C	Sidechain
54	BA	2228	G	Sidechain
54	BA	2230	G	Sidechain
54	BA	2236	U	Sidechain
54	BA	2242	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2249	U	Sidechain
54	BA	2250	G	Sidechain
54	BA	2252	G	Sidechain
54	BA	2257	U	Sidechain
54	BA	2260	C	Sidechain
54	BA	2262	U	Sidechain
54	BA	2264	C	Sidechain
54	BA	227	A	Sidechain
54	BA	2271	G	Sidechain
54	BA	2282	G	Sidechain
54	BA	2286	G	Sidechain
54	BA	2293	G	Sidechain
54	BA	2297	A	Sidechain
54	BA	2299	U	Sidechain
54	BA	2304	G	Sidechain
54	BA	2306	C	Sidechain
54	BA	2309	A	Sidechain
54	BA	2310	C	Sidechain
54	BA	232	G	Sidechain
54	BA	2321	U	Sidechain
54	BA	2323	G	Sidechain
54	BA	2324	U	Sidechain
54	BA	2325	G	Sidechain
54	BA	2327	A	Sidechain
54	BA	2328	A	Sidechain
54	BA	2336	A	Sidechain
54	BA	235	U	Sidechain
54	BA	2352	A	Sidechain
54	BA	2358	A	Sidechain
54	BA	236	C	Sidechain
54	BA	2375	G	Sidechain
54	BA	2376	A	Sidechain
54	BA	238	C	Sidechain
54	BA	2384	U	Sidechain
54	BA	2387	U	Sidechain
54	BA	2391	G	Sidechain
54	BA	2397	G	Sidechain
54	BA	2398	U	Sidechain
54	BA	240	C	Sidechain
54	BA	2415	G	Sidechain
54	BA	2418	A	Sidechain
54	BA	2421	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2422	C	Sidechain
54	BA	2431	U	Sidechain
54	BA	2432	A	Sidechain
54	BA	2437	G	Sidechain
54	BA	244	A	Sidechain
54	BA	2440	C	Sidechain
54	BA	2444	G	Sidechain
54	BA	2445	G	Sidechain
54	BA	2446	G	Sidechain
54	BA	2449	U	Sidechain
54	BA	2453	A	Sidechain
54	BA	2455	G	Sidechain
54	BA	2458	G	Sidechain
54	BA	2461	A	Sidechain
54	BA	2462	C	Sidechain
54	BA	2468	A	Sidechain
54	BA	2469	A	Sidechain
54	BA	247	G	Sidechain
54	BA	2474	U	Sidechain
54	BA	2475	C	Sidechain
54	BA	2476	A	Sidechain
54	BA	2486	C	Sidechain
54	BA	2487	G	Sidechain
54	BA	2488	G	Sidechain
54	BA	2499	C	Sidechain
54	BA	25	U	Sidechain
54	BA	250	G	Sidechain
54	BA	2502	G	Sidechain
54	BA	2506	U	Sidechain
54	BA	2507	C	Sidechain
54	BA	2509	G	Sidechain
54	BA	251	A	Sidechain
54	BA	2513	A	Sidechain
54	BA	2516	A	Sidechain
54	BA	2524	G	Sidechain
54	BA	2529	G	Sidechain
54	BA	2530	A	Sidechain
54	BA	2541	A	Sidechain
54	BA	2550	G	Sidechain
54	BA	2552	U	Sidechain
54	BA	2557	G	Sidechain
54	BA	2560	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2562	U	Sidechain
54	BA	2572	A	Sidechain
54	BA	2574	G	Sidechain
54	BA	2575	C	Sidechain
54	BA	2579	C	Sidechain
54	BA	2580	U	Sidechain
54	BA	2587	A	Sidechain
54	BA	2588	G	Sidechain
54	BA	2597	G	Sidechain
54	BA	2602	A	Sidechain
54	BA	2608	G	Sidechain
54	BA	2609	U	Sidechain
54	BA	2618	G	Sidechain
54	BA	2627	G	Sidechain
54	BA	2628	C	Sidechain
54	BA	2630	G	Sidechain
54	BA	2631	G	Sidechain
54	BA	2637	U	Sidechain
54	BA	2639	A	Sidechain
54	BA	2640	G	Sidechain
54	BA	2643	G	Sidechain
54	BA	2647	U	Sidechain
54	BA	2648	G	Sidechain
54	BA	2650	U	Sidechain
54	BA	2654	A	Sidechain
54	BA	2659	G	Sidechain
54	BA	2660	A	Sidechain
54	BA	2661	G	Sidechain
54	BA	2664	G	Sidechain
54	BA	267	C	Sidechain
54	BA	2678	C	Sidechain
54	BA	2682	A	Sidechain
54	BA	2683	C	Sidechain
54	BA	2686	G	Sidechain
54	BA	2695	U	Sidechain
54	BA	2700	A	Sidechain
54	BA	2711	A	Sidechain
54	BA	2713	U	Sidechain
54	BA	2720	U	Sidechain
54	BA	2723	C	Sidechain
54	BA	273	G	Sidechain
54	BA	274	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2753	A	Sidechain
54	BA	2756	U	Sidechain
54	BA	2759	G	Sidechain
54	BA	2760	C	Sidechain
54	BA	2762	C	Sidechain
54	BA	2763	G	Sidechain
54	BA	2765	A	Sidechain
54	BA	277	G	Sidechain
54	BA	2771	C	Sidechain
54	BA	2777	G	Sidechain
54	BA	278	A	Sidechain
54	BA	2780	G	Sidechain
54	BA	2783	U	Sidechain
54	BA	2788	C	Sidechain
54	BA	2797	U	Sidechain
54	BA	2798	U	Sidechain
54	BA	2799	A	Sidechain
54	BA	2806	C	Sidechain
54	BA	2816	G	Sidechain
54	BA	282	A	Sidechain
54	BA	2829	A	Sidechain
54	BA	2832	U	Sidechain
54	BA	2836	U	Sidechain
54	BA	2840	C	Sidechain
54	BA	2844	G	Sidechain
54	BA	2854	G	Sidechain
54	BA	2857	G	Sidechain
54	BA	2862	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	287	G	Sidechain
54	BA	2872	A	Sidechain
54	BA	2874	C	Sidechain
54	BA	2883	A	Sidechain
54	BA	2885	G	Sidechain
54	BA	2893	A	Sidechain
54	BA	2899	A	Sidechain
54	BA	29	U	Sidechain
54	BA	2900	A	Sidechain
54	BA	291	G	Sidechain
54	BA	293	U	Sidechain
54	BA	30	G	Sidechain
54	BA	304	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	307	G	Sidechain
54	BA	308	G	Sidechain
54	BA	310	A	Sidechain
54	BA	313	G	Sidechain
54	BA	314	C	Sidechain
54	BA	316	C	Sidechain
54	BA	319	G	Sidechain
54	BA	327	G	Sidechain
54	BA	328	U	Sidechain
54	BA	344	A	Sidechain
54	BA	352	A	Sidechain
54	BA	354	A	Sidechain
54	BA	360	U	Sidechain
54	BA	361	G	Sidechain
54	BA	364	C	Sidechain
54	BA	365	U	Sidechain
54	BA	370	G	Sidechain
54	BA	374	A	Sidechain
54	BA	385	C	Sidechain
54	BA	389	G	Sidechain
54	BA	392	U	Sidechain
54	BA	395	U	Sidechain
54	BA	417	C	Sidechain
54	BA	418	C	Sidechain
54	BA	426	C	Sidechain
54	BA	429	A	Sidechain
54	BA	43	G	Sidechain
54	BA	44	A	Sidechain
54	BA	441	U	Sidechain
54	BA	443	A	Sidechain
54	BA	449	A	Sidechain
54	BA	452	G	Sidechain
54	BA	462	C	Sidechain
54	BA	463	G	Sidechain
54	BA	464	U	Sidechain
54	BA	475	C	Sidechain
54	BA	477	A	Sidechain
54	BA	479	A	Sidechain
54	BA	48	G	Sidechain
54	BA	487	C	Sidechain
54	BA	488	G	Sidechain
54	BA	49	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	494	G	Sidechain
54	BA	500	G	Sidechain
54	BA	501	A	Sidechain
54	BA	502	A	Sidechain
54	BA	506	G	Sidechain
54	BA	511	U	Sidechain
54	BA	519	U	Sidechain
54	BA	521	U	Sidechain
54	BA	524	G	Sidechain
54	BA	526	A	Sidechain
54	BA	529	A	Sidechain
54	BA	532	A	Sidechain
54	BA	54	G	Sidechain
54	BA	542	C	Sidechain
54	BA	556	A	Sidechain
54	BA	561	G	Sidechain
54	BA	563	A	Sidechain
54	BA	565	C	Sidechain
54	BA	567	U	Sidechain
54	BA	568	U	Sidechain
54	BA	571	U	Sidechain
54	BA	572	A	Sidechain
54	BA	575	A	Sidechain
54	BA	577	G	Sidechain
54	BA	579	G	Sidechain
54	BA	580	U	Sidechain
54	BA	581	C	Sidechain
54	BA	585	G	Sidechain
54	BA	586	A	Sidechain
54	BA	597	G	Sidechain
54	BA	600	G	Sidechain
54	BA	608	A	Sidechain
54	BA	617	G	Sidechain
54	BA	628	G	Sidechain
54	BA	629	G	Sidechain
54	BA	63	A	Sidechain
54	BA	630	G	Sidechain
54	BA	631	A	Sidechain
54	BA	633	A	Sidechain
54	BA	64	A	Sidechain
54	BA	640	C	Sidechain
54	BA	641	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	646	U	Sidechain
54	BA	647	G	Sidechain
54	BA	653	U	Sidechain
54	BA	659	G	Sidechain
54	BA	671	C	Sidechain
54	BA	672	C	Sidechain
54	BA	675	A	Sidechain
54	BA	680	C	Sidechain
54	BA	688	U	Sidechain
54	BA	689	A	Sidechain
54	BA	70	G	Sidechain
54	BA	706	A	Sidechain
54	BA	718	A	Sidechain
54	BA	723	C	Sidechain
54	BA	724	U	Sidechain
54	BA	726	G	Sidechain
54	BA	729	G	Sidechain
54	BA	732	C	Sidechain
54	BA	733	G	Sidechain
54	BA	738	G	Sidechain
54	BA	74	A	Sidechain
54	BA	748	G	Sidechain
54	BA	755	U	Sidechain
54	BA	759	G	Sidechain
54	BA	765	C	Sidechain
54	BA	774	G	Sidechain
54	BA	775	G	Sidechain
54	BA	776	G	Sidechain
54	BA	780	G	Sidechain
54	BA	784	G	Sidechain
54	BA	789	A	Sidechain
54	BA	800	A	Sidechain
54	BA	804	A	Sidechain
54	BA	809	G	Sidechain
54	BA	810	U	Sidechain
54	BA	813	U	Sidechain
54	BA	818	G	Sidechain
54	BA	822	G	Sidechain
54	BA	828	U	Sidechain
54	BA	833	A	Sidechain
54	BA	837	C	Sidechain
54	BA	841	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	845	A	Sidechain
54	BA	846	U	Sidechain
54	BA	847	U	Sidechain
54	BA	848	C	Sidechain
54	BA	85	G	Sidechain
54	BA	854	C	Sidechain
54	BA	858	G	Sidechain
54	BA	862	G	Sidechain
54	BA	866	A	Sidechain
54	BA	869	G	Sidechain
54	BA	870	U	Sidechain
54	BA	883	G	Sidechain
54	BA	884	U	Sidechain
54	BA	89	A	Sidechain
54	BA	890	C	Sidechain
54	BA	894	U	Sidechain
54	BA	9	G	Sidechain
54	BA	901	C	Sidechain
54	BA	904	G	Sidechain
54	BA	912	C	Sidechain
54	BA	918	A	Sidechain
54	BA	922	C	Sidechain
54	BA	923	G	Sidechain
54	BA	932	U	Sidechain
54	BA	935	C	Sidechain
54	BA	94	A	Sidechain
54	BA	942	G	Sidechain
54	BA	944	C	Sidechain
54	BA	945	A	Sidechain
54	BA	954	G	Sidechain
54	BA	959	A	Sidechain
54	BA	96	C	Sidechain
54	BA	964	C	Sidechain
54	BA	967	U	Sidechain
54	BA	969	G	Sidechain
54	BA	973	A	Sidechain
54	BA	974	G	Sidechain
54	BA	982	C	Sidechain
54	BA	988	A	Sidechain
54	BA	989	G	Sidechain
54	BA	99	U	Sidechain
54	BA	993	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	999	U	Sidechain
55	BB	10	G	Sidechain
55	BB	108	A	Sidechain
55	BB	109	A	Sidechain
55	BB	111	U	Sidechain
55	BB	112	G	Sidechain
55	BB	18	G	Sidechain
55	BB	23	G	Sidechain
55	BB	24	G	Sidechain
55	BB	27	C	Sidechain
55	BB	3	C	Sidechain
55	BB	30	C	Sidechain
55	BB	31	C	Sidechain
55	BB	32	U	Sidechain
55	BB	40	U	Sidechain
55	BB	41	G	Sidechain
55	BB	42	C	Sidechain
55	BB	43	C	Sidechain
55	BB	48	U	Sidechain
55	BB	49	C	Sidechain
55	BB	57	A	Sidechain
55	BB	58	A	Sidechain
55	BB	6	G	Sidechain
55	BB	60	C	Sidechain
55	BB	66	A	Sidechain
55	BB	75	G	Sidechain
55	BB	84	G	Sidechain
55	BB	88	C	Sidechain
55	BB	92	C	Sidechain
55	BB	93	C	Sidechain
55	BB	94	A	Sidechain
55	BB	99	A	Sidechain
25	BC	42	ARG	Sidechain
38	BP	113	LEU	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	1	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	1	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	1	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16522	4	0
22	A1	1627	0	832	0	0
23	A2	309	0	156	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	1	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	1	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	0
49	B0	444	0	461	1	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31339	2	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	99657	10	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 (10) 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)
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.76	0.51
21:AA:730:G:C5	21:AA:731:G:H1'	2.48	0.48
6:AG:148:LYS:HE3	10:AK:60:PHE:CZ	2.48	0.47
26:BD:125:TRP:CE3	26:BD:160:LYS:HE3	2.48	0.47
29:BG:1:SER:HA	54:BA:2749:A:OP1	2.18	0.43
54:BA:1760:C:H5''	54:BA:1761:C:C5	2.55	0.42
21:AA:22:G:H4'	21:AA:885:G:C8	2.55	0.42
21:AA:1063:C:H2'	21:AA:1064:G:C8	2.55	0.42
49:B0:30:ASP:CG	49:B0:31:LYS:H	2.27	0.41
14:AO:50:HIS:CD2	21:AA:666:G:H21	2.38	0.41

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%)	15 (7%)	1 (0%)	24	63
2	AC	205/208 (99%)	190 (93%)	12 (6%)	3 (2%)	8	40
3	AD	203/206 (98%)	189 (93%)	10 (5%)	4 (2%)	6	31
4	AE	150/152 (99%)	135 (90%)	11 (7%)	4 (3%)	4	25
5	AF	99/101 (98%)	90 (91%)	4 (4%)	5 (5%)	1	15
6	AG	150/152 (99%)	130 (87%)	18 (12%)	2 (1%)	9	42
7	AH	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
8	AI	126/128 (98%)	114 (90%)	11 (9%)	1 (1%)	16	54
9	AJ	98/100 (98%)	92 (94%)	3 (3%)	3 (3%)	3	22
10	AK	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14	51
11	AL	121/124 (98%)	108 (89%)	11 (9%)	2 (2%)	7	36
12	AM	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	6	34
13	AN	98/101 (97%)	90 (92%)	6 (6%)	2 (2%)	6	31
14	AO	86/89 (97%)	76 (88%)	7 (8%)	3 (4%)	3	20
15	AP	79/81 (98%)	65 (82%)	11 (14%)	3 (4%)	2	19
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%)	73 (92%)	5 (6%)	1 (1%)	9	42
19	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	AU	51/53 (96%)	36 (71%)	12 (24%)	3 (6%)	1	13
25	BC	270/273 (99%)	241 (89%)	22 (8%)	7 (3%)	4	25
26	BD	207/209 (99%)	172 (83%)	20 (10%)	15 (7%)	1	11
27	BE	199/201 (99%)	179 (90%)	17 (8%)	3 (2%)	8	40
28	BF	176/179 (98%)	142 (81%)	25 (14%)	9 (5%)	1	15
29	BG	174/177 (98%)	156 (90%)	15 (9%)	3 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BH	147/149 (99%)	128 (87%)	14 (10%)	5 (3%)	3	21
31	BI	139/142 (98%)	128 (92%)	9 (6%)	2 (1%)	9	40
32	BJ	140/142 (99%)	128 (91%)	10 (7%)	2 (1%)	9	40
33	BK	121/123 (98%)	102 (84%)	15 (12%)	4 (3%)	3	21
34	BL	141/144 (98%)	111 (79%)	19 (14%)	11 (8%)	1	10
35	BM	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	5	29
36	BN	119/121 (98%)	108 (91%)	9 (8%)	2 (2%)	7	36
37	BO	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
38	BP	112/115 (97%)	99 (88%)	10 (9%)	3 (3%)	4	25
39	BQ	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	4	25
40	BR	101/103 (98%)	92 (91%)	7 (7%)	2 (2%)	6	31
41	BS	108/110 (98%)	95 (88%)	13 (12%)	0	100	100
42	BT	92/94 (98%)	77 (84%)	12 (13%)	3 (3%)	3	21
43	BU	101/104 (97%)	83 (82%)	12 (12%)	6 (6%)	1	13
44	BV	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	11	46
45	BW	78/80 (98%)	64 (82%)	10 (13%)	4 (5%)	1	15
46	BX	75/79 (95%)	66 (88%)	8 (11%)	1 (1%)	9	42
47	BY	61/63 (97%)	54 (88%)	6 (10%)	1 (2%)	7	38
48	BZ	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	1	15
49	B0	54/57 (95%)	47 (87%)	7 (13%)	0	100	100
50	B1	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1	9
51	B2	44/46 (96%)	38 (86%)	5 (11%)	1 (2%)	5	28
52	B3	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
53	B4	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	1	14
56	B5	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	24	63
All	All	5876/6008 (98%)	5234 (89%)	497 (8%)	145 (2%)	6	26

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	AH	105	THR
9	AJ	74	VAL
12	AM	65	GLU

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Mol	Chain	Res	Type
14	AO	45	HIS
16	AQ	39	ARG
25	BC	191	LEU
26	BD	51	THR
33	BK	103	VAL
34	BL	21	ARG
34	BL	101	ILE
35	BM	135	VAL
38	BP	63	ILE
43	BU	43	LYS
43	BU	70	ALA
44	BV	14	LYS
48	BZ	31	ILE
50	B1	36	LYS
2	AC	171	ARG
2	AC	195	ILE
4	AE	105	ILE
5	AF	63	ASN
5	AF	90	MET
8	AI	57	VAL
9	AJ	57	VAL
9	AJ	75	ASP
12	AM	42	VAL
13	AN	63	ARG
15	AP	11	ALA
25	BC	161	VAL
26	BD	80	TRP
26	BD	203	VAL
28	BF	133	GLU
28	BF	176	PHE
29	BG	9	VAL
29	BG	151	ARG
31	BI	12	VAL
32	BJ	81	ILE
38	BP	2	ASN
38	BP	26	GLU
39	BQ	90	ASP
42	BT	11	LEU
43	BU	12	VAL
43	BU	85	ARG
43	BU	102	ILE
46	BX	34	SER

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Mol	Chain	Res	Type
53	B4	16	ILE
3	AD	29	THR
5	AF	36	ILE
5	AF	39	LEU
6	AG	2	ARG
10	AK	49	SER
11	AL	33	CYS
14	AO	43	ALA
15	AP	17	TYR
17	AR	69	TYR
20	AU	34	ARG
20	AU	35	GLU
26	BD	7	LYS
26	BD	49	GLN
26	BD	82	PHE
26	BD	149	ASN
28	BF	87	LYS
28	BF	136	ILE
29	BG	16	VAL
30	BH	104	THR
33	BK	2	ILE
34	BL	29	LYS
36	BN	3	HIS
39	BQ	5	ARG
39	BQ	91	ARG
40	BR	9	GLY
40	BR	53	PHE
42	BT	63	VAL
42	BT	88	LYS
43	BU	59	GLU
45	BW	53	GLY
47	BY	9	LYS
56	B5	91	GLY
3	AD	204	SER
4	AE	43	GLY
4	AE	106	ALA
20	AU	4	LYS
25	BC	153	LEU
26	BD	34	VAL
26	BD	144	GLY
26	BD	201	LEU
27	BE	147	LEU

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Mol	Chain	Res	Type
30	BH	10	ALA
30	BH	39	ALA
33	BK	32	TYR
34	BL	30	THR
34	BL	68	SER
35	BM	2	LEU
35	BM	21	ALA
36	BN	104	ALA
45	BW	23	LYS
45	BW	38	ARG
48	BZ	9	THR
48	BZ	30	ARG
50	B1	6	GLU
51	B2	44	VAL
1	AB	129	THR
2	AC	14	VAL
3	AD	203	TYR
5	AF	6	ILE
11	AL	78	VAL
13	AN	38	ASP
15	AP	40	ASN
18	AS	79	TYR
25	BC	144	GLU
26	BD	43	ASP
26	BD	119	ALA
27	BE	165	HIS
28	BF	155	ILE
30	BH	88	GLY
30	BH	121	VAL
32	BJ	72	LYS
33	BK	25	LEU
34	BL	36	LYS
34	BL	66	PHE
53	B4	2	LYS
4	AE	54	GLU
6	AG	74	VAL
14	AO	18	ALA
25	BC	185	ALA
26	BD	37	VAL
26	BD	138	LEU
27	BE	160	ALA
34	BL	12	SER

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Mol	Chain	Res	Type
34	BL	55	MET
45	BW	16	GLU
50	B1	45	HIS
50	B1	50	GLU
3	AD	41	GLY
25	BC	123	ILE
26	BD	5	VAL
31	BI	18	ASN
34	BL	130	GLY
16	AQ	82	VAL
28	BF	12	VAL
28	BF	88	VAL
25	BC	253	GLY
28	BF	103	ILE
34	BL	65	GLY
28	BF	175	PRO

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%)	179 (99%)	1 (1%)	78	83
2	AC	170/171 (99%)	169 (99%)	1 (1%)	78	83
3	AD	172/173 (99%)	171 (99%)	1 (1%)	78	83
4	AE	113/113 (100%)	112 (99%)	1 (1%)	70	79
5	AF	87/87 (100%)	86 (99%)	1 (1%)	65	76
6	AG	123/123 (100%)	121 (98%)	2 (2%)	55	70
7	AH	104/105 (99%)	104 (100%)	0	100	100
8	AI	105/105 (100%)	105 (100%)	0	100	100
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	102 (99%)	1 (1%)	68	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AM	91/92 (99%)	90 (99%)	1 (1%)	65	76
13	AN	83/84 (99%)	80 (96%)	3 (4%)	31	52
14	AO	76/77 (99%)	75 (99%)	1 (1%)	61	74
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	39	61
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	69 (99%)	1 (1%)	59	72
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	43 (98%)	1 (2%)	44	64
25	BC	216/217 (100%)	214 (99%)	2 (1%)	70	79
26	BD	164/164 (100%)	162 (99%)	2 (1%)	63	75
27	BE	165/165 (100%)	157 (95%)	8 (5%)	23	44
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%)	112 (98%)	2 (2%)	51	68
31	BI	109/110 (99%)	107 (98%)	2 (2%)	51	68
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	53	69
33	BK	103/103 (100%)	101 (98%)	2 (2%)	50	67
34	BL	102/103 (99%)	100 (98%)	2 (2%)	48	66
35	BM	109/109 (100%)	106 (97%)	3 (3%)	38	60
36	BN	100/100 (100%)	98 (98%)	2 (2%)	48	66
37	BO	86/87 (99%)	85 (99%)	1 (1%)	63	75
38	BP	99/100 (99%)	98 (99%)	1 (1%)	68	78
39	BQ	89/90 (99%)	89 (100%)	0	100	100
40	BR	84/84 (100%)	82 (98%)	2 (2%)	43	64
41	BS	93/93 (100%)	91 (98%)	2 (2%)	45	64
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	82 (99%)	1 (1%)	63	75
44	BV	78/78 (100%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	57 (97%)	2 (3%)	32	54
46	BX	67/68 (98%)	66 (98%)	1 (2%)	57	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	47 (100%)	0	100	100
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	37 (97%)	1 (3%)	40	62
52	B3	51/52 (98%)	50 (98%)	1 (2%)	48	66
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%)	4779 (99%)	63 (1%)	59	74

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

Mol	Chain	Res	Type
1	AB	71	THR
2	AC	76	ILE
3	AD	202	LEU
4	AE	47	PHE
5	AF	52	ASN
6	AG	65	LEU
6	AG	102	TRP
11	AL	113	ARG
12	AM	96	VAL
13	AN	3	LYS
13	AN	38	ASP
13	AN	101	TRP
14	AO	49	HIS
16	AQ	20	ILE
16	AQ	64	ARG
18	AS	48	ILE
20	AU	13	VAL
25	BC	49	THR
25	BC	57	HIS
26	BD	91	THR
26	BD	154	LYS
27	BE	33	VAL
27	BE	46	GLN
27	BE	53	THR
27	BE	93	SER
27	BE	105	LEU

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Mol	Chain	Res	Type
27	BE	147	LEU
27	BE	163	ASN
27	BE	187	VAL
28	BF	12	VAL
28	BF	80	GLN
28	BF	151	LEU
29	BG	103	ASN
29	BG	121	THR
30	BH	44	ILE
30	BH	135	HIS
31	BI	67	THR
31	BI	89	SER
32	BJ	43	GLU
32	BJ	47	HIS
33	BK	4	GLU
33	BK	32	TYR
34	BL	79	LEU
34	BL	104	GLN
35	BM	96	ILE
35	BM	97	GLN
35	BM	126	ILE
36	BN	1	MET
36	BN	18	GLN
37	BO	38	GLN
38	BP	50	ARG
40	BR	27	ILE
40	BR	94	THR
41	BS	33	LEU
41	BS	107	VAL
43	BU	44	HIS
45	BW	23	LYS
45	BW	35	ILE
46	BX	65	THR
51	B2	43	THR
52	B3	33	THR
56	B5	18	THR
56	B5	165	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	17	HIS

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Mol	Chain	Res	Type
1	AB	57	ASN
1	AB	88	GLN
2	AC	2	GLN
2	AC	5	HIS
2	AC	24	ASN
3	AD	39	GLN
3	AD	40	HIS
4	AE	120	HIS
5	AF	14	GLN
5	AF	17	GLN
5	AF	94	HIS
6	AG	27	ASN
6	AG	67	ASN
6	AG	96	ASN
6	AG	129	ASN
7	AH	37	ASN
8	AI	49	GLN
9	AJ	64	GLN
9	AJ	70	HIS
10	AK	23	HIS
10	AK	80	ASN
13	AN	4	GLN
15	AP	63	GLN
15	AP	79	ASN
16	AQ	44	HIS
19	AT	54	GLN
25	BC	24	HIS
25	BC	59	GLN
26	BD	32	ASN
26	BD	49	GLN
26	BD	67	HIS
26	BD	164	GLN
27	BE	29	HIS
27	BE	156	ASN
28	BF	4	HIS
28	BF	80	GLN
29	BG	63	GLN
29	BG	114	HIS
29	BG	127	GLN
30	BH	2	GLN
30	BH	18	GLN
30	BH	33	GLN

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Mol	Chain	Res	Type
30	BH	119	ASN
31	BI	18	ASN
33	BK	5	GLN
34	BL	38	GLN
35	BM	3	GLN
35	BM	13	HIS
37	BO	19	GLN
37	BO	116	GLN
39	BQ	36	GLN
39	BQ	55	GLN
40	BR	18	GLN
40	BR	86	GLN
41	BS	9	HIS
42	BT	48	GLN
42	BT	70	HIS
43	BU	53	GLN
43	BU	65	GLN
44	BV	88	HIS
45	BW	11	ASN
47	BY	15	ASN
47	BY	38	GLN
49	B0	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	273 (17%)	84 (5%)
22	A1	75/76 (98%)	11 (14%)	4 (5%)
23	A2	14/15 (93%)	8 (57%)	2 (14%)
24	A3	76/77 (98%)	13 (17%)	2 (2%)
54	BA	2902/2903 (99%)	480 (16%)	119 (4%)
55	BB	117/118 (99%)	21 (17%)	6 (5%)
All	All	4714/4722 (99%)	806 (17%)	217 (4%)

All (806) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	8	A
21	AA	9	G
21	AA	13	U

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Mol	Chain	Res	Type
21	AA	14	U
21	AA	16	A
21	AA	17	U
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	50	A
21	AA	51	A
21	AA	52	C
21	AA	59	A
21	AA	60	A
21	AA	66	A
21	AA	67	C
21	AA	83	C
21	AA	84	U
21	AA	85	U
21	AA	86	G
21	AA	87	C
21	AA	109	A
21	AA	110	C
21	AA	120	A
21	AA	122	G
21	AA	163	C
21	AA	182	A
21	AA	183	C
21	AA	184	G
21	AA	191	G
21	AA	194	C
21	AA	195	A
21	AA	198	G
21	AA	211	G
21	AA	212	G
21	AA	237	G
21	AA	240	G
21	AA	245	U
21	AA	247	G
21	AA	251	G
21	AA	252	U
21	AA	266	G
21	AA	267	C
21	AA	280	C

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Mol	Chain	Res	Type
21	AA	289	G
21	AA	306	A
21	AA	329	A
21	AA	330	C
21	AA	332	G
21	AA	346	G
21	AA	347	G
21	AA	351	G
21	AA	352	C
21	AA	354	G
21	AA	357	G
21	AA	358	U
21	AA	361	G
21	AA	366	A
21	AA	367	U
21	AA	368	U
21	AA	372	C
21	AA	373	A
21	AA	381	C
21	AA	392	C
21	AA	397	A
21	AA	398	U
21	AA	411	A
21	AA	412	A
21	AA	414	A
21	AA	415	A
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	446	G
21	AA	452	A
21	AA	455	G
21	AA	456	A
21	AA	461	A
21	AA	462	G
21	AA	463	U
21	AA	464	U
21	AA	465	A
21	AA	466	A
21	AA	467	U
21	AA	468	A
21	AA	476	U

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Mol	Chain	Res	Type
21	AA	477	C
21	AA	481	G
21	AA	482	A
21	AA	483	C
21	AA	484	G
21	AA	497	G
21	AA	500	G
21	AA	501	C
21	AA	510	A
21	AA	511	C
21	AA	512	U
21	AA	514	C
21	AA	527	G
21	AA	532	A
21	AA	547	A
21	AA	559	A
21	AA	564	C
21	AA	565	U
21	AA	567	G
21	AA	572	A
21	AA	573	A
21	AA	576	C
21	AA	607	A
21	AA	608	A
21	AA	611	C
21	AA	612	C
21	AA	632	U
21	AA	665	A
21	AA	675	A
21	AA	676	A
21	AA	700	G
21	AA	701	U
21	AA	702	A
21	AA	703	G
21	AA	704	A
21	AA	705	G
21	AA	718	A
21	AA	719	C
21	AA	721	G
21	AA	722	G
21	AA	723	U
21	AA	724	G

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Mol	Chain	Res	Type
21	AA	753	A
21	AA	754	C
21	AA	755	G
21	AA	767	A
21	AA	777	A
21	AA	794	A
21	AA	812	G
21	AA	817	C
21	AA	819	A
21	AA	820	U
21	AA	821	G
21	AA	828	U
21	AA	840	C
21	AA	841	C
21	AA	844	G
21	AA	845	A
21	AA	846	G
21	AA	869	G
21	AA	872	A
21	AA	873	A
21	AA	876	C
21	AA	899	C
21	AA	902	G
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	936	C
21	AA	938	A
21	AA	939	G
21	AA	945	G
21	AA	958	A
21	AA	959	A
21	AA	960	U
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	972	C
21	AA	977	A
21	AA	978	A

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Mol	Chain	Res	Type
21	AA	979	C
21	AA	981	U
21	AA	983	A
21	AA	984	C
21	AA	993	G
21	AA	995	C
21	AA	1004	A
21	AA	1026	G
21	AA	1030	U
21	AA	1031	C
21	AA	1045	C
21	AA	1046	A
21	AA	1049	U
21	AA	1050	G
21	AA	1053	G
21	AA	1054	C
21	AA	1056	U
21	AA	1064	G
21	AA	1065	U
21	AA	1068	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1130	A
21	AA	1137	C
21	AA	1139	G
21	AA	1140	C
21	AA	1146	A
21	AA	1147	C
21	AA	1152	A
21	AA	1167	A
21	AA	1171	A
21	AA	1172	C
21	AA	1183	U
21	AA	1184	G
21	AA	1185	G
21	AA	1189	U
21	AA	1191	A
21	AA	1194	U
21	AA	1195	C
21	AA	1196	A
21	AA	1201	A

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Mol	Chain	Res	Type
21	AA	1202	U
21	AA	1218	C
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1229	A
21	AA	1233	G
21	AA	1238	A
21	AA	1240	U
21	AA	1241	G
21	AA	1251	A
21	AA	1256	A
21	AA	1257	A
21	AA	1278	G
21	AA	1279	G
21	AA	1282	C
21	AA	1285	A
21	AA	1286	U
21	AA	1298	U
21	AA	1299	A
21	AA	1300	G
21	AA	1301	U
21	AA	1303	C
21	AA	1305	G
21	AA	1337	G
21	AA	1338	G
21	AA	1346	A
21	AA	1362	A
21	AA	1363	A
21	AA	1379	G
21	AA	1380	U
21	AA	1381	U
21	AA	1382	C
21	AA	1394	A
21	AA	1397	C
21	AA	1398	A
21	AA	1399	C
21	AA	1400	C
21	AA	1401	G
21	AA	1419	G
21	AA	1432	G
21	AA	1446	A

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Mol	Chain	Res	Type
21	AA	1447	A
21	AA	1448	C
21	AA	1452	C
21	AA	1453	G
21	AA	1476	A
21	AA	1477	U
21	AA	1491	G
21	AA	1493	A
21	AA	1494	G
21	AA	1503	A
21	AA	1505	G
21	AA	1506	U
21	AA	1511	G
21	AA	1517	G
21	AA	1529	G
21	AA	1530	G
21	AA	1534	A
22	A1	10	G
22	A1	16	C
22	A1	18	G
22	A1	19	G
22	A1	20	G
22	A1	47	U
22	A1	48	C
22	A1	59	U
22	A1	73	A
22	A1	74	C
22	A1	76	A
23	A2	80	C
23	A2	81	U
23	A2	82	A
23	A2	83	U
23	A2	84	G
23	A2	85	G
23	A2	88	U
23	A2	92	U
24	A3	5	G
24	A3	9	G
24	A3	10	G
24	A3	17	C
24	A3	19	G
24	A3	21	H2U

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Mol	Chain	Res	Type
24	A3	22	A
24	A3	32	G
24	A3	33	OMC
24	A3	49	C
24	A3	62	C
24	A3	71	G
24	A3	72	C
54	BA	9	G
54	BA	13	A
54	BA	15	G
54	BA	20	C
54	BA	34	U
54	BA	39	G
54	BA	71	A
54	BA	72	U
54	BA	74	A
54	BA	75	G
54	BA	85	G
54	BA	86	G
54	BA	88	G
54	BA	98	G
54	BA	100	U
54	BA	101	A
54	BA	102	U
54	BA	103	A
54	BA	112	U
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	125	A
54	BA	126	A
54	BA	127	A
54	BA	128	C
54	BA	139	U
54	BA	140	C
54	BA	141	G
54	BA	143	C
54	BA	149	A
54	BA	163	C
54	BA	180	G
54	BA	181	A

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Mol	Chain	Res	Type
54	BA	196	A
54	BA	204	A
54	BA	205	G
54	BA	216	A
54	BA	222	A
54	BA	228	C
54	BA	248	G
54	BA	249	C
54	BA	255	A
54	BA	256	A
54	BA	265	A
54	BA	266	G
54	BA	272	A
54	BA	278	A
54	BA	279	A
54	BA	294	A
54	BA	299	A
54	BA	302	C
54	BA	316	C
54	BA	327	G
54	BA	330	A
54	BA	346	A
54	BA	370	G
54	BA	386	G
54	BA	387	U
54	BA	388	G
54	BA	389	G
54	BA	390	U
54	BA	404	A
54	BA	405	U
54	BA	411	G
54	BA	428	A
54	BA	451	U
54	BA	455	C
54	BA	457	A
54	BA	475	C
54	BA	482	A
54	BA	503	A
54	BA	504	A
54	BA	505	A
54	BA	506	G
54	BA	508	A

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Mol	Chain	Res	Type
54	BA	526	A
54	BA	528	A
54	BA	529	A
54	BA	530	G
54	BA	531	C
54	BA	532	A
54	BA	533	G
54	BA	546	U
54	BA	549	G
54	BA	562	U
54	BA	563	A
54	BA	573	U
54	BA	574	A
54	BA	575	A
54	BA	588	U
54	BA	590	A
54	BA	603	A
54	BA	607	U
54	BA	613	A
54	BA	615	U
54	BA	616	A
54	BA	617	G
54	BA	627	A
54	BA	631	A
54	BA	632	A
54	BA	637	A
54	BA	643	A
54	BA	644	A
54	BA	653	U
54	BA	654	A
54	BA	655	A
54	BA	672	C
54	BA	686	U
54	BA	719	C
54	BA	724	U
54	BA	726	G
54	BA	730	A
54	BA	736	C
54	BA	743	A
54	BA	747	U
54	BA	762	U
54	BA	763	G

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Mol	Chain	Res	Type
54	BA	764	A
54	BA	765	C
54	BA	775	G
54	BA	776	G
54	BA	782	A
54	BA	784	G
54	BA	793	A
54	BA	800	A
54	BA	805	G
54	BA	812	C
54	BA	814	C
54	BA	819	A
54	BA	827	U
54	BA	846	U
54	BA	847	U
54	BA	852	U
54	BA	858	G
54	BA	859	G
54	BA	866	A
54	BA	867	C
54	BA	889	C
54	BA	890	C
54	BA	896	A
54	BA	897	C
54	BA	914	G
54	BA	915	C
54	BA	932	U
54	BA	934	U
54	BA	935	C
54	BA	945	A
54	BA	958	U
54	BA	961	C
54	BA	962	G
54	BA	973	A
54	BA	974	G
54	BA	980	A
54	BA	981	A
54	BA	983	A
54	BA	985	C
54	BA	994	C
54	BA	996	A
54	BA	1005	C

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Mol	Chain	Res	Type
54	BA	1006	C
54	BA	1011	G
54	BA	1022	G
54	BA	1024	G
54	BA	1025	G
54	BA	1026	G
54	BA	1033	U
54	BA	1034	G
54	BA	1046	A
54	BA	1047	G
54	BA	1060	U
54	BA	1067	A
54	BA	1069	A
54	BA	1070	A
54	BA	1072	C
54	BA	1073	A
54	BA	1078	U
54	BA	1088	A
54	BA	1089	A
54	BA	1094	U
54	BA	1112	G
54	BA	1127	A
54	BA	1128	G
54	BA	1129	A
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1142	A
54	BA	1143	A
54	BA	1175	A
54	BA	1204	A
54	BA	1205	A
54	BA	1206	G
54	BA	1211	C
54	BA	1241	A
54	BA	1242	U
54	BA	1254	A
54	BA	1256	G
54	BA	1266	G
54	BA	1272	A
54	BA	1273	U
54	BA	1274	A

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Mol	Chain	Res	Type
54	BA	1276	A
54	BA	1289	C
54	BA	1290	C
54	BA	1300	G
54	BA	1301	A
54	BA	1306	C
54	BA	1313	U
54	BA	1317	G
54	BA	1320	C
54	BA	1321	A
54	BA	1325	U
54	BA	1332	G
54	BA	1340	U
54	BA	1341	G
54	BA	1345	C
54	BA	1365	A
54	BA	1378	A
54	BA	1379	U
54	BA	1383	A
54	BA	1384	A
54	BA	1388	G
54	BA	1399	C
54	BA	1416	G
54	BA	1420	A
54	BA	1421	G
54	BA	1427	A
54	BA	1428	C
54	BA	1435	G
54	BA	1452	G
54	BA	1453	A
54	BA	1454	C
54	BA	1459	G
54	BA	1475	G
54	BA	1482	G
54	BA	1493	C
54	BA	1497	U
54	BA	1508	A
54	BA	1511	G
54	BA	1515	A
54	BA	1523	U
54	BA	1538	G
54	BA	1539	U

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Mol	Chain	Res	Type
54	BA	1560	G
54	BA	1561	C
54	BA	1565	C
54	BA	1568	G
54	BA	1570	A
54	BA	1578	U
54	BA	1584	U
54	BA	1599	U
54	BA	1608	A
54	BA	1610	A
54	BA	1611	C
54	BA	1617	C
54	BA	1618	A
54	BA	1628	G
54	BA	1629	U
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1654	A
54	BA	1668	A
54	BA	1669	A
54	BA	1670	C
54	BA	1674	G
54	BA	1711	A
54	BA	1715	G
54	BA	1730	C
54	BA	1731	G
54	BA	1732	C
54	BA	1733	G
54	BA	1734	G
54	BA	1758	U
54	BA	1760	C
54	BA	1761	C
54	BA	1764	C
54	BA	1773	A
54	BA	1776	G
54	BA	1780	A
54	BA	1781	U
54	BA	1782	U
54	BA	1784	A
54	BA	1799	G
54	BA	1800	C

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Mol	Chain	Res	Type
54	BA	1802	A
54	BA	1803	A
54	BA	1808	A
54	BA	1816	C
54	BA	1848	A
54	BA	1870	C
54	BA	1871	A
54	BA	1872	A
54	BA	1877	A
54	BA	1888	G
54	BA	1906	G
54	BA	1913	A
54	BA	1914	C
54	BA	1929	G
54	BA	1930	G
54	BA	1931	U
54	BA	1937	A
54	BA	1940	U
54	BA	1943	U
54	BA	1945	G
54	BA	1953	A
54	BA	1955	U
54	BA	1963	U
54	BA	1971	U
54	BA	1972	G
54	BA	1993	U
54	BA	1997	C
54	BA	2022	U
54	BA	2023	C
54	BA	2030	A
54	BA	2031	A
54	BA	2032	G
54	BA	2034	U
54	BA	2035	G
54	BA	2043	C
54	BA	2055	C
54	BA	2059	A
54	BA	2060	A
54	BA	2061	G
54	BA	2062	A
54	BA	2063	C
54	BA	2068	U

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Mol	Chain	Res	Type
54	BA	2069	G
54	BA	2071	A
54	BA	2072	C
54	BA	2092	U
54	BA	2113	U
54	BA	2114	A
54	BA	2126	A
54	BA	2132	U
54	BA	2133	G
54	BA	2134	A
54	BA	2135	A
54	BA	2155	U
54	BA	2157	G
54	BA	2159	G
54	BA	2160	C
54	BA	2172	U
54	BA	2173	A
54	BA	2174	C
54	BA	2181	U
54	BA	2199	A
54	BA	2203	U
54	BA	2204	G
54	BA	2206	C
54	BA	2211	A
54	BA	2214	C
54	BA	2238	G
54	BA	2245	U
54	BA	2262	U
54	BA	2266	A
54	BA	2267	A
54	BA	2269	G
54	BA	2275	C
54	BA	2283	C
54	BA	2288	A
54	BA	2289	G
54	BA	2305	U
54	BA	2307	G
54	BA	2308	G
54	BA	2309	A
54	BA	2310	C
54	BA	2311	A
54	BA	2312	U

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Mol	Chain	Res	Type
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2322	A
54	BA	2325	G
54	BA	2326	C
54	BA	2333	A
54	BA	2335	A
54	BA	2339	C
54	BA	2345	G
54	BA	2346	A
54	BA	2347	C
54	BA	2353	G
54	BA	2383	G
54	BA	2385	C
54	BA	2387	U
54	BA	2388	A
54	BA	2403	C
54	BA	2406	A
54	BA	2419	U
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	2434	A
54	BA	2435	A
54	BA	2441	U
54	BA	2444	G
54	BA	2448	A
54	BA	2449	U
54	BA	2469	A
54	BA	2470	G
54	BA	2476	A
54	BA	2491	U
54	BA	2492	U
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2505	G

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Mol	Chain	Res	Type
54	BA	2518	A
54	BA	2529	G
54	BA	2531	A
54	BA	2532	G
54	BA	2540	C
54	BA	2547	A
54	BA	2554	U
54	BA	2555	U
54	BA	2564	A
54	BA	2565	A
54	BA	2566	A
54	BA	2567	G
54	BA	2572	A
54	BA	2573	C
54	BA	2574	G
54	BA	2578	G
54	BA	2581	G
54	BA	2584	U
54	BA	2587	A
54	BA	2596	U
54	BA	2597	G
54	BA	2599	G
54	BA	2600	A
54	BA	2613	U
54	BA	2614	A
54	BA	2615	U
54	BA	2629	U
54	BA	2645	G
54	BA	2646	C
54	BA	2655	G
54	BA	2660	A
54	BA	2674	G
54	BA	2684	U
54	BA	2689	U
54	BA	2690	U
54	BA	2709	G
54	BA	2714	G
54	BA	2726	A
54	BA	2732	G
54	BA	2733	A
54	BA	2740	A
54	BA	2741	A

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Mol	Chain	Res	Type
54	BA	2744	G
54	BA	2765	A
54	BA	2766	A
54	BA	2778	A
54	BA	2779	U
54	BA	2791	G
54	BA	2797	U
54	BA	2808	G
54	BA	2820	A
54	BA	2821	A
54	BA	2823	A
54	BA	2829	A
54	BA	2830	C
54	BA	2832	U
54	BA	2833	U
54	BA	2850	A
54	BA	2858	C
54	BA	2859	G
54	BA	2868	A
54	BA	2879	A
54	BA	2880	C
54	BA	2881	U
54	BA	2886	A
54	BA	2894	G
54	BA	2895	G
55	BB	3	C
55	BB	4	C
55	BB	5	U
55	BB	13	G
55	BB	14	U
55	BB	15	A
55	BB	16	G
55	BB	25	U
55	BB	35	C
55	BB	42	C
55	BB	44	G
55	BB	57	A
55	BB	58	A
55	BB	66	A
55	BB	73	A
55	BB	88	C
55	BB	89	U

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Mol	Chain	Res	Type
55	BB	90	C
55	BB	108	A
55	BB	109	A
55	BB	112	G

All (217) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	13	U
21	AA	16	A
21	AA	50	A
21	AA	51	A
21	AA	59	A
21	AA	64	G
21	AA	66	A
21	AA	84	U
21	AA	109	A
21	AA	181	A
21	AA	251	G
21	AA	266	G
21	AA	279	A
21	AA	346	G
21	AA	351	G
21	AA	357	G
21	AA	372	C
21	AA	412	A
21	AA	451	A
21	AA	455	G
21	AA	461	A
21	AA	465	A
21	AA	467	U
21	AA	476	U
21	AA	481	G
21	AA	483	C
21	AA	499	A
21	AA	500	G
21	AA	510	A
21	AA	559	A
21	AA	573	A
21	AA	575	G
21	AA	607	A

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Mol	Chain	Res	Type
21	AA	611	C
21	AA	630	A
21	AA	675	A
21	AA	701	U
21	AA	703	G
21	AA	704	A
21	AA	718	A
21	AA	721	G
21	AA	753	A
21	AA	755	G
21	AA	758	C
21	AA	804	U
21	AA	819	A
21	AA	840	C
21	AA	844	G
21	AA	872	A
21	AA	913	A
21	AA	938	A
21	AA	958	A
21	AA	959	A
21	AA	980	C
21	AA	982	U
21	AA	983	A
21	AA	1049	U
21	AA	1053	G
21	AA	1064	G
21	AA	1101	A
21	AA	1117	A
21	AA	1146	A
21	AA	1166	G
21	AA	1171	A
21	AA	1184	G
21	AA	1190	G
21	AA	1194	U
21	AA	1195	C
21	AA	1201	A
21	AA	1217	C
21	AA	1225	A
21	AA	1233	G
21	AA	1298	U
21	AA	1337	G
21	AA	1380	U

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Mol	Chain	Res	Type
21	AA	1397	C
21	AA	1399	C
21	AA	1446	A
21	AA	1447	A
21	AA	1452	C
21	AA	1476	A
21	AA	1493	A
21	AA	1529	G
22	A1	10	G
22	A1	18	G
22	A1	47	U
22	A1	75	C
23	A2	80	C
23	A2	84	G
24	A3	21	H2U
24	A3	71	G
54	BA	14	A
54	BA	34	U
54	BA	48	G
54	BA	71	A
54	BA	102	U
54	BA	118	A
54	BA	119	A
54	BA	125	A
54	BA	127	A
54	BA	180	G
54	BA	196	A
54	BA	199	A
54	BA	255	A
54	BA	278	A
54	BA	323	C
54	BA	386	G
54	BA	387	U
54	BA	388	G
54	BA	503	A
54	BA	505	A
54	BA	527	C
54	BA	547	A
54	BA	573	U
54	BA	615	U
54	BA	631	A
54	BA	643	A

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Mol	Chain	Res	Type
54	BA	748	G
54	BA	762	U
54	BA	764	A
54	BA	818	G
54	BA	827	U
54	BA	846	U
54	BA	896	A
54	BA	934	U
54	BA	958	U
54	BA	1005	C
54	BA	1033	U
54	BA	1088	A
54	BA	1126	A
54	BA	1128	G
54	BA	1141	U
54	BA	1142	A
54	BA	1204	A
54	BA	1205	A
54	BA	1210	G
54	BA	1273	U
54	BA	1289	C
54	BA	1300	G
54	BA	1301	A
54	BA	1312	U
54	BA	1320	C
54	BA	1383	A
54	BA	1385	A
54	BA	1420	A
54	BA	1427	A
54	BA	1451	C
54	BA	1453	A
54	BA	1490	A
54	BA	1512	C
54	BA	1537	G
54	BA	1560	G
54	BA	1607	C
54	BA	1610	A
54	BA	1617	C
54	BA	1628	G
54	BA	1647	U
54	BA	1668	A
54	BA	1730	C

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Mol	Chain	Res	Type
54	BA	1732	C
54	BA	1760	C
54	BA	1780	A
54	BA	1799	G
54	BA	1802	A
54	BA	1847	A
54	BA	1871	A
54	BA	1930	G
54	BA	1936	A
54	BA	1939	U
54	BA	1952	A
54	BA	1955	U
54	BA	1981	A
54	BA	2034	U
54	BA	2060	A
54	BA	2062	A
54	BA	2071	A
54	BA	2113	U
54	BA	2132	U
54	BA	2133	G
54	BA	2145	C
54	BA	2171	A
54	BA	2172	U
54	BA	2180	U
54	BA	2286	G
54	BA	2288	A
54	BA	2321	U
54	BA	2325	G
54	BA	2345	G
54	BA	2402	U
54	BA	2418	A
54	BA	2425	A
54	BA	2427	C
54	BA	2428	G
54	BA	2429	G
54	BA	2433	A
54	BA	2503	A
54	BA	2531	A
54	BA	2564	A
54	BA	2571	U
54	BA	2573	C
54	BA	2575	C

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Mol	Chain	Res	Type
54	BA	2596	U
54	BA	2712	C
54	BA	2732	G
54	BA	2740	A
54	BA	2778	A
54	BA	2790	U
54	BA	2829	A
54	BA	2832	U
54	BA	2858	C
55	BB	2	G
55	BB	4	C
55	BB	14	U
55	BB	15	A
55	BB	57	A
55	BB	111	U

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	0.79	0	21,30,33	1.15	2 (9%)
24	H2U	A3	21	24	18,21,22	1.29	2 (11%)	19,30,33	1.45	4 (21%)
22	CM0	A1	34	22,23	21,26,27	1.30	2 (9%)	26,37,40	1.53	2 (7%)
24	4SU	A3	8	24	18,21,22	1.50	2 (11%)	25,30,33	0.90	1 (4%)
24	5MU	A3	55	24	19,22,23	0.67	0	27,32,35	1.51	5 (18%)
22	4SU	A1	7	22	18,21,22	1.47	2 (11%)	25,30,33	0.96	1 (4%)
22	5MU	A1	54	22	19,22,23	0.72	0	27,32,35	1.32	3 (11%)
22	6MZ	A1	37	22	22,25,26	0.71	0	29,36,39	1.13	2 (6%)
22	7MG	A1	46	22	23,26,27	4.10	3 (13%)	27,39,42	1.42	1 (3%)
24	PSU	A3	56	24	18,21,22	0.85	0	21,30,33	1.34	2 (9%)
24	OMC	A3	33	24	19,22,23	0.69	0	25,31,34	1.06	2 (8%)

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	-	2/7/25/26	0/2/2/2
24	H2U	A3	21	24	-	1/7/38/39	0/2/2/2
22	CM0	A1	34	22,23	-	2/12/30/31	0/2/2/2
24	4SU	A3	8	24	-	0/7/25/26	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
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
22	6MZ	A1	37	22	-	0/9/27/28	0/3/3/3
22	7MG	A1	46	22	-	0/7/37/38	0/3/3/3
24	PSU	A3	56	24	-	1/7/25/26	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	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	-19.23	1.33	1.45
22	A1	7	4SU	C5-C4	-5.22	1.36	1.42
24	A3	8	4SU	C5-C4	-5.15	1.36	1.42
22	A1	34	CM0	O5-C5	-4.54	1.26	1.36
24	A3	21	H2U	C2-N3	-3.35	1.32	1.38
24	A3	21	H2U	C4-N3	-3.20	1.32	1.37
22	A1	46	7MG	C8-N7	-2.47	1.30	1.42
24	A3	8	4SU	C4-S4	-2.36	1.64	1.68
22	A1	7	4SU	C4-S4	-2.16	1.64	1.68
22	A1	46	7MG	C5-N7	2.07	1.38	1.35
22	A1	34	CM0	O8-C8	-2.03	1.24	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	5.85	111.65	103.37
22	A1	34	CM0	C7-O5-C5	5.32	124.26	117.48
24	A3	56	PSU	C6-C5-C4	3.84	120.76	118.17
22	A1	37	6MZ	C9-N6-C6	3.65	126.23	122.85
22	A1	54	5MU	C5M-C5-C6	-3.62	117.95	122.85
24	A3	55	5MU	C5M-C5-C6	-3.60	117.97	122.85
24	A3	55	5MU	C6-C5-C4	3.45	120.86	118.02
24	A3	21	H2U	N3-C2-N1	3.11	119.77	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	33	OMC	O2-C2-N3	-3.06	117.50	122.33
22	A1	54	5MU	C5M-C5-C4	2.81	121.78	118.78
24	A3	21	H2U	C5-C4-N3	2.75	119.61	116.69
24	A3	56	PSU	O4'-C1'-C2'	2.74	108.94	105.15
22	A1	54	5MU	C6-C5-C4	2.72	120.26	118.02
22	A1	7	4SU	C6-C5-C4	2.54	122.15	119.95
24	A3	55	5MU	O4-C4-C5	2.43	127.69	124.92
24	A3	55	5MU	C5-C6-N1	-2.36	120.75	123.31
22	A1	37	6MZ	C4-C5-C6	-2.36	114.82	116.78
24	A3	21	H2U	O4'-C4'-C3'	2.33	109.77	105.15
24	A3	8	4SU	C6-C5-C4	2.28	121.92	119.95
24	A3	33	OMC	C2'-C1'-N1	-2.27	109.93	114.24
24	A3	55	5MU	C5M-C5-C4	2.23	121.17	118.78
22	A1	55	PSU	C6-C5-C4	2.23	119.68	118.17
22	A1	34	CM0	O2-C2-N3	-2.03	117.74	121.49
22	A1	55	PSU	O4'-C1'-C2'	2.03	107.95	105.15
24	A3	21	H2U	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	55	PSU	C2'-C1'-C5-C4
24	A3	21	H2U	C4'-C5'-O5'-P
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9
22	A1	55	PSU	O4'-C1'-C5-C4
24	A3	56	PSU	O4'-C1'-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
57	VAL	A1	101	22,58	4,6,7	0.77	0	6,7,9	0.65	0
58	FME	BA	3001	57	8,9,10	0.67	0	8,9,11	1.46	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	VAL	A1	101	22,58	-	0/5/6/8	-
58	FME	BA	3001	57	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	FME	O-C-CA	-2.48	118.39	124.77
58	BA	3001	FME	C-CA-N	2.38	114.08	109.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

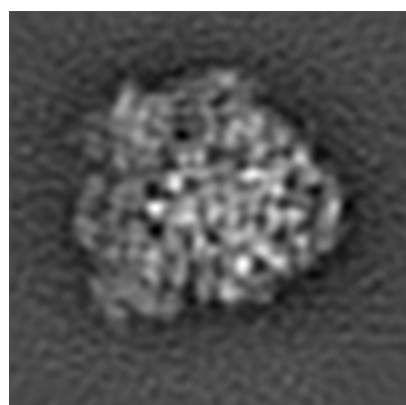
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1721. These allow visual inspection of the internal detail of the map and identification of artifacts.

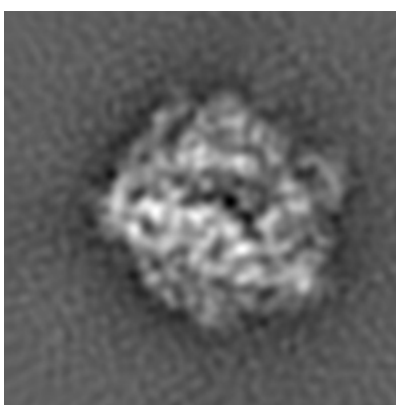
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

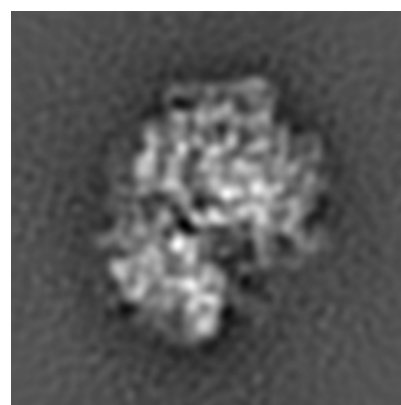
6.1.1 Primary map



X



Y

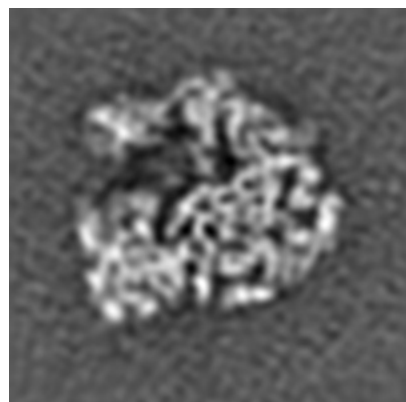


Z

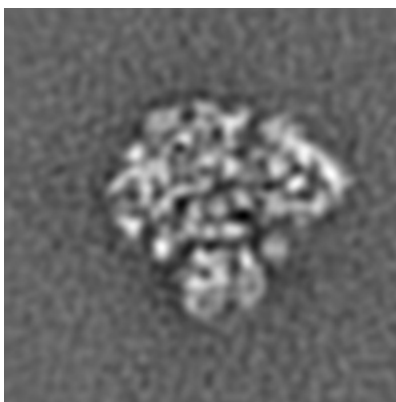
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

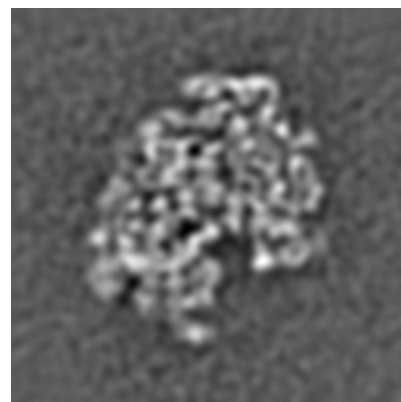
6.2.1 Primary map



X Index: 64



Y Index: 64

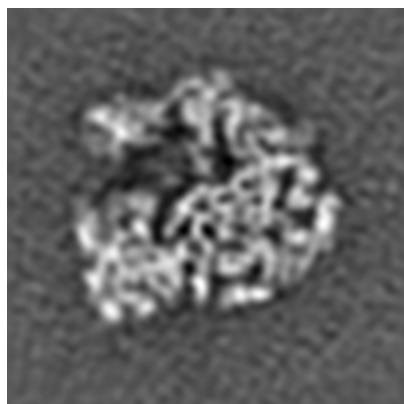


Z Index: 64

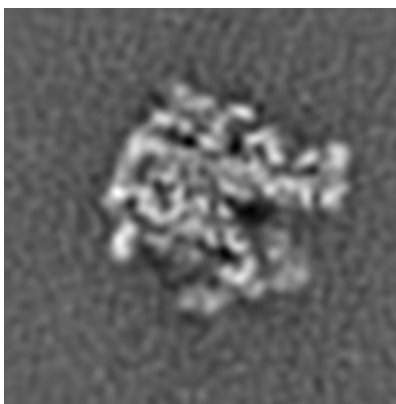
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

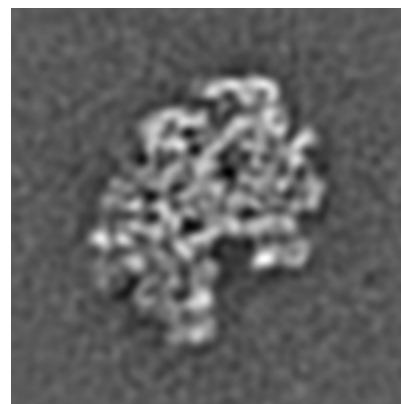
6.3.1 Primary map



X Index: 64



Y Index: 69

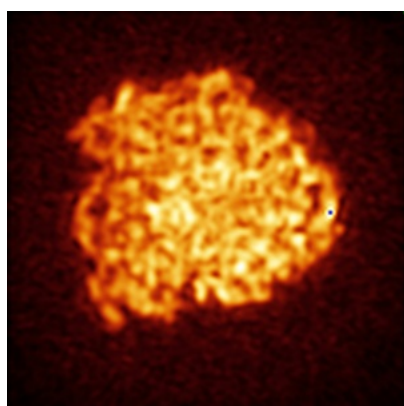


Z Index: 62

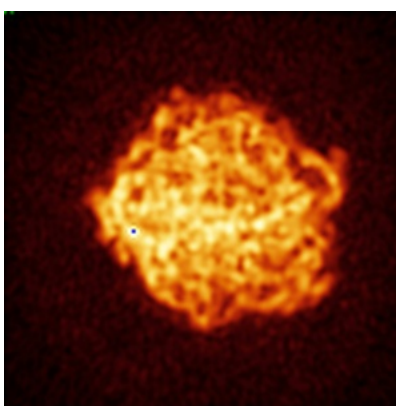
The images above show the largest variance slices of the map in three orthogonal directions.

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

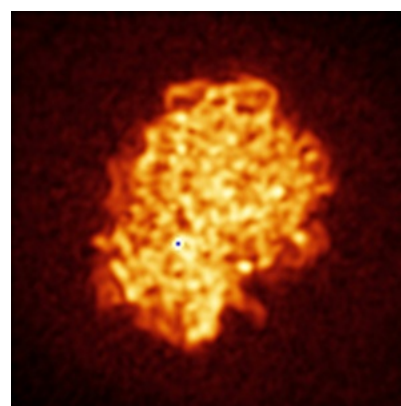
6.4.1 Primary map



X



Y

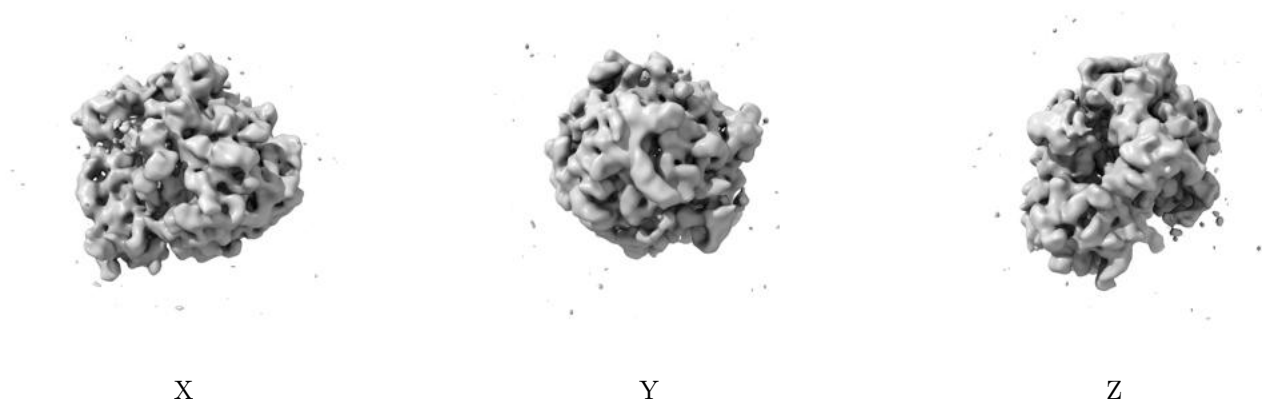


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 27.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

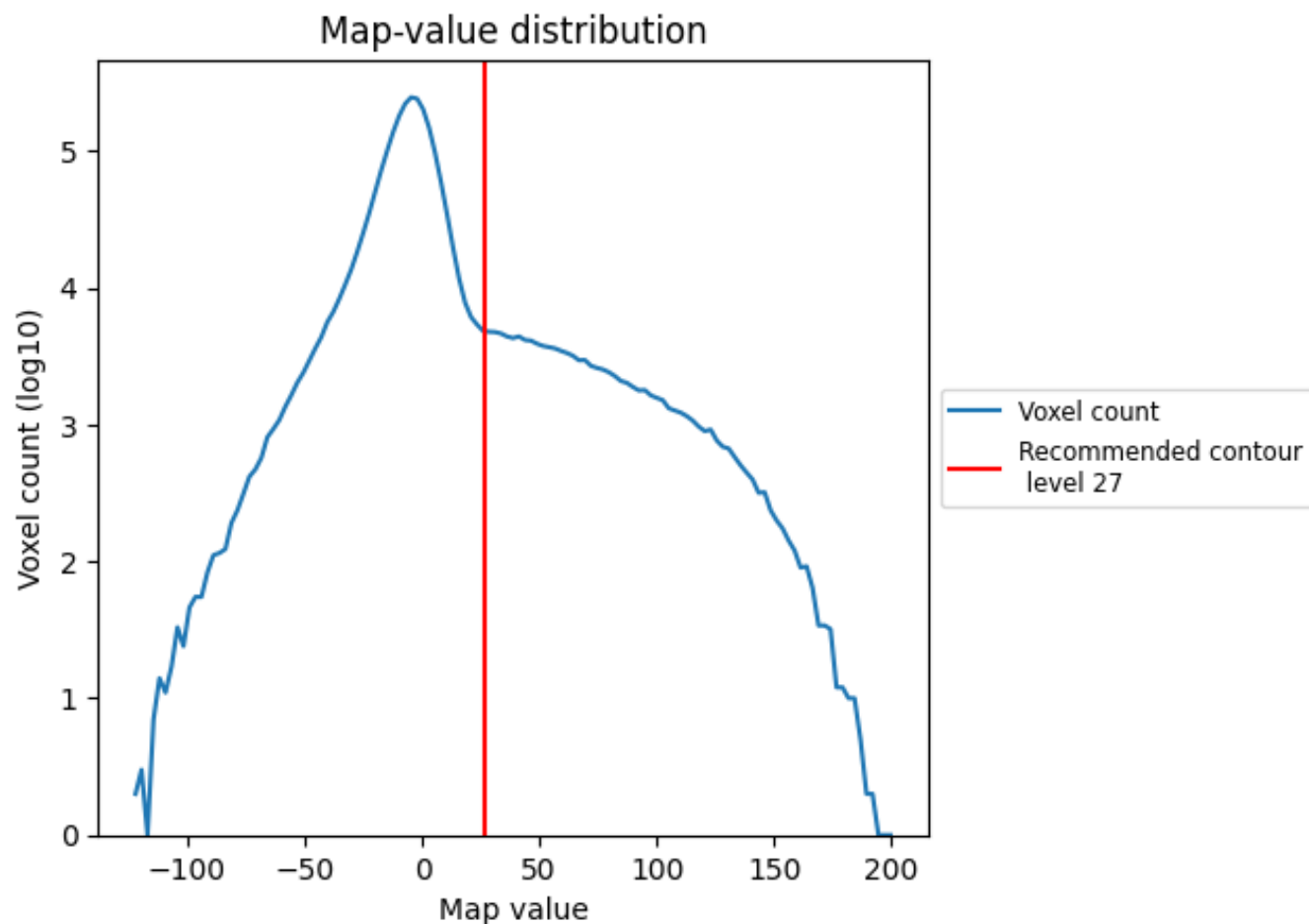
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

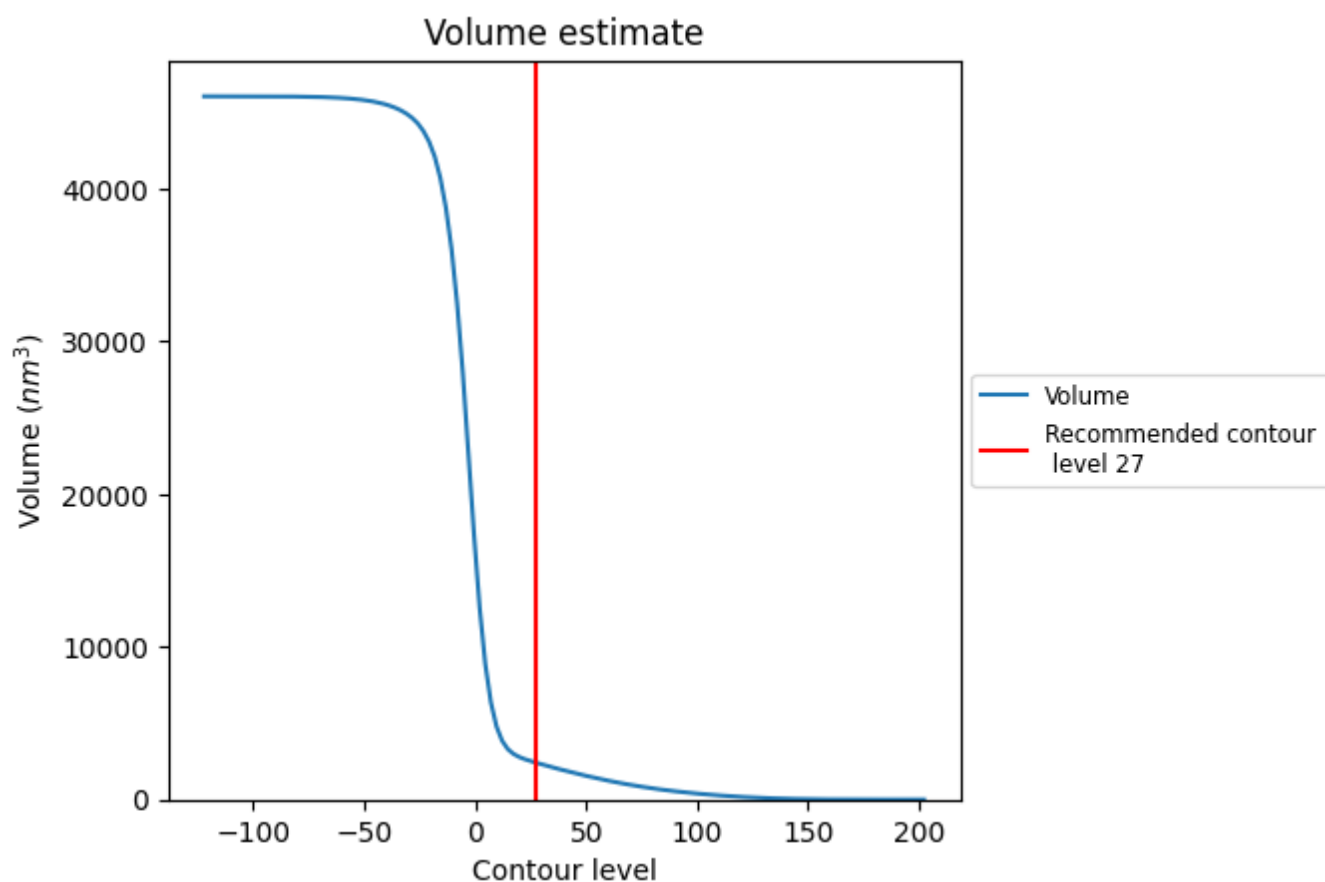
This section contains the results of statistical analysis of the map.

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.

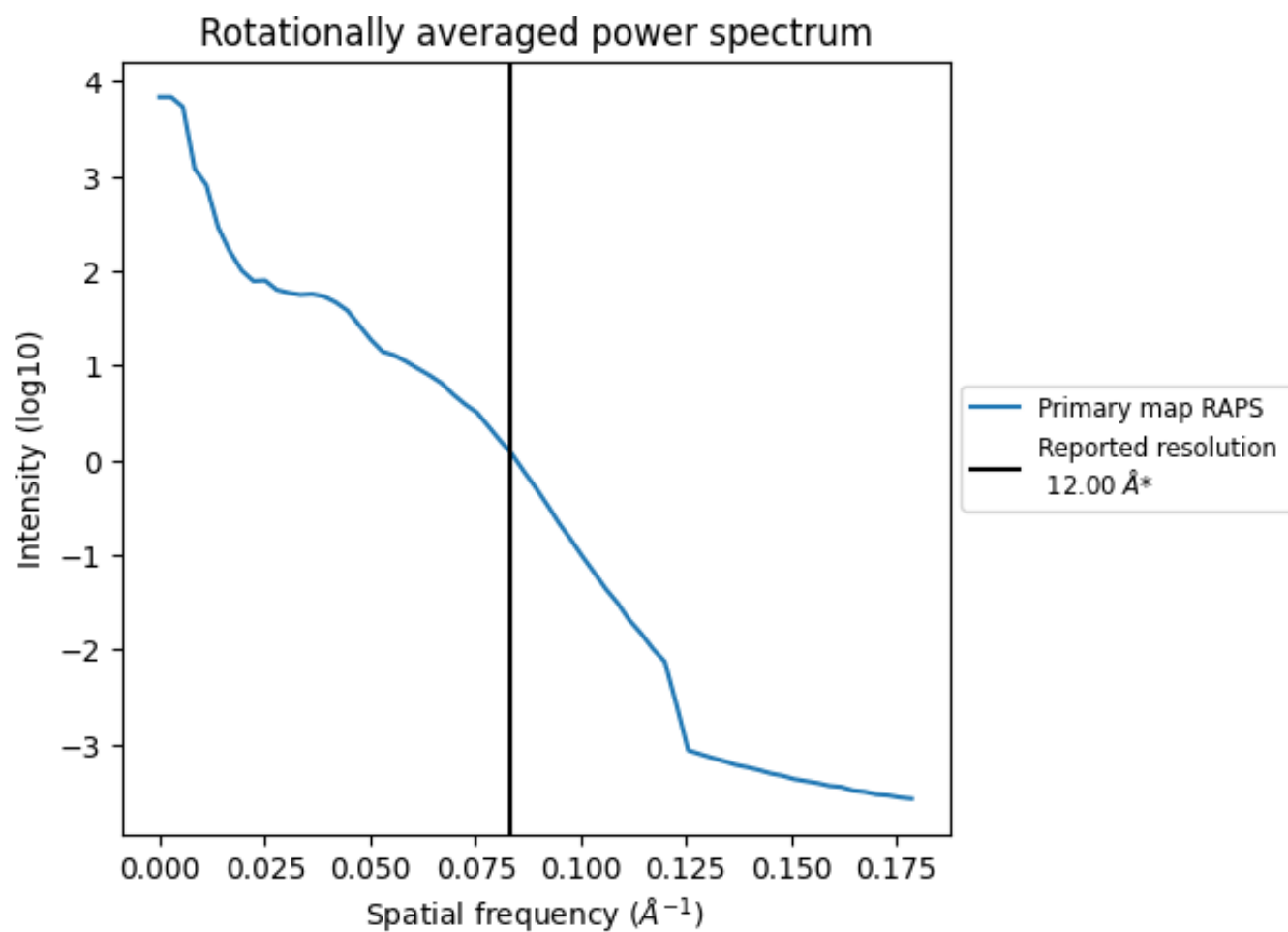
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2432 nm³; this corresponds to an approximate mass of 2196 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.083 Å⁻¹

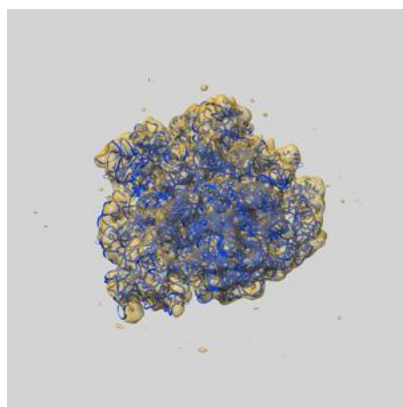
8 Fourier-Shell correlation

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

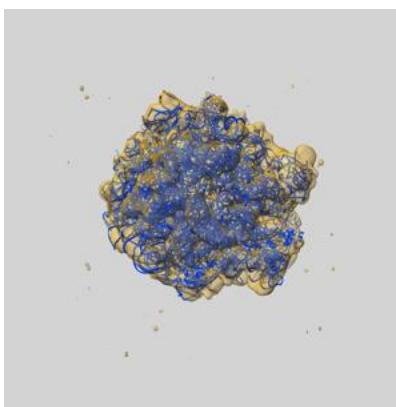
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1721 and PDB model 4V75. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

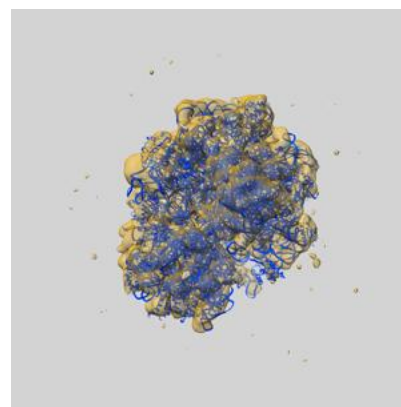
9.1 Map-model overlay [i](#)



X



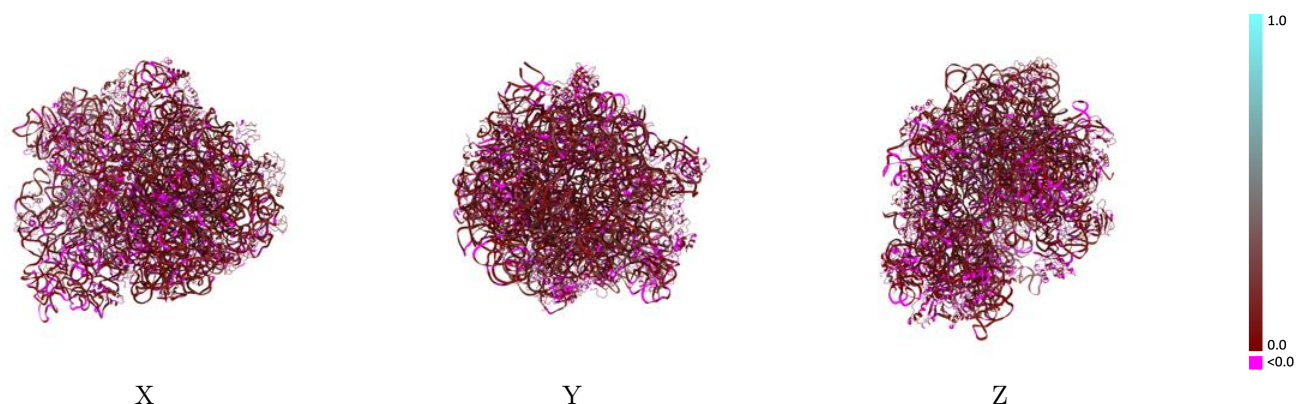
Y



Z

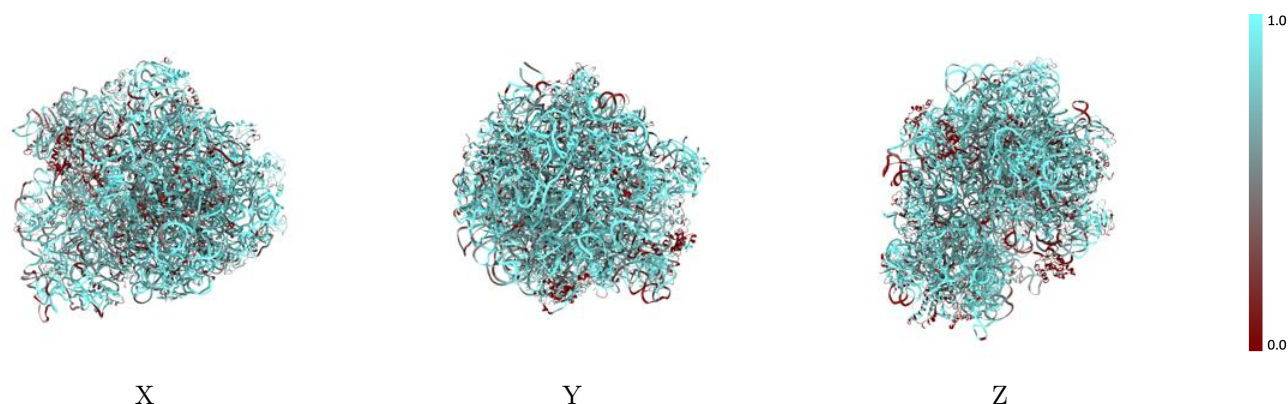
The images above show the 3D surface view of the map at the recommended contour level 27.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



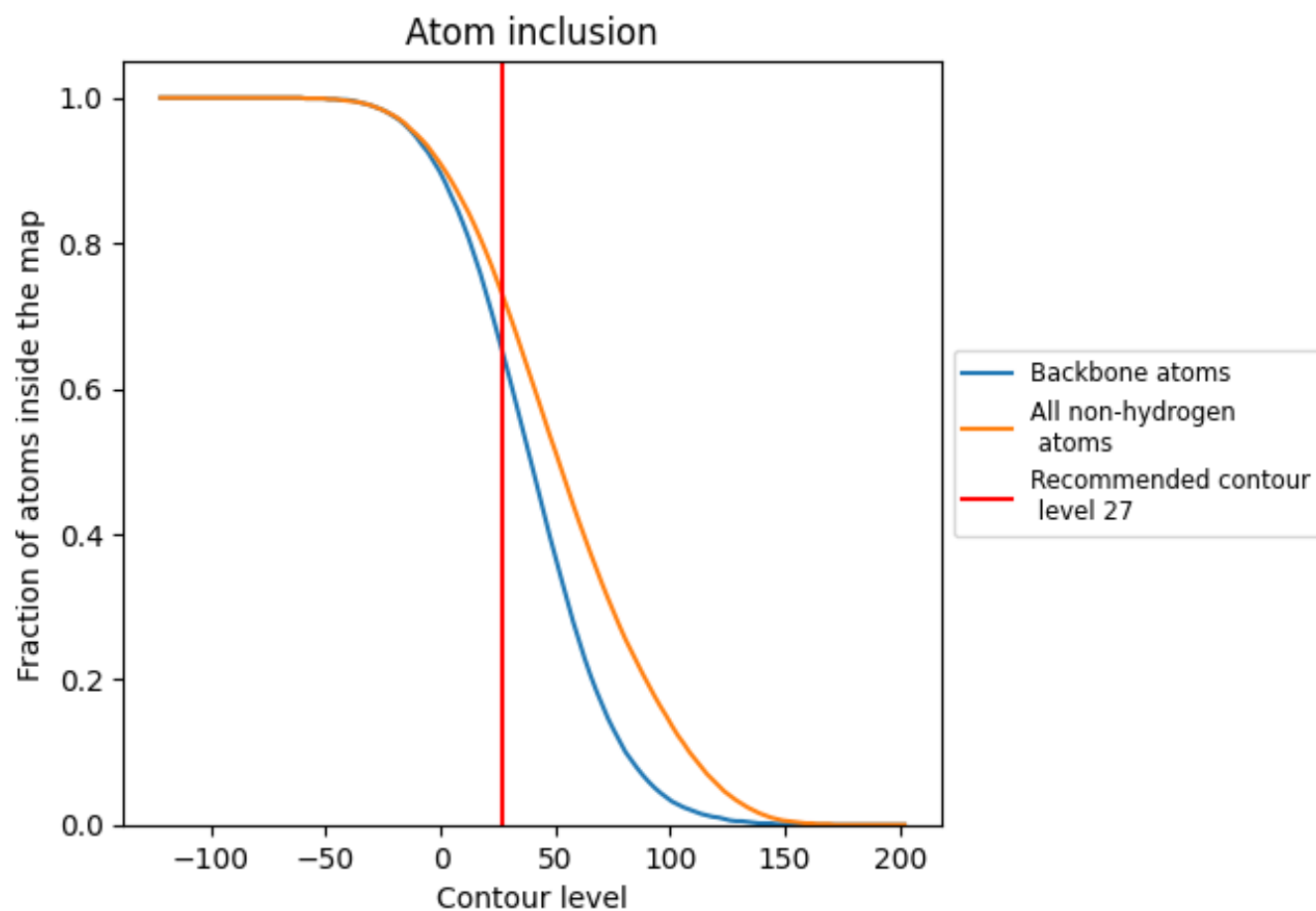
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (27).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 73% 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 (27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.0720
A1	 0.6500	 0.0960
A2	 0.5920	 0.0590
A3	 0.5400	 0.0610
AA	 0.8090	 0.0810
AB	 0.6030	 0.0610
AC	 0.6120	 0.0470
AD	 0.6200	 0.0320
AE	 0.6310	 0.0690
AF	 0.7180	 0.0780
AG	 0.6480	 0.0570
AH	 0.6450	 0.0510
AI	 0.6830	 0.0270
AJ	 0.5100	 0.0090
AK	 0.7170	 0.0570
AL	 0.6500	 0.0410
AM	 0.7100	 0.0720
AN	 0.5930	 0.0150
AO	 0.6670	 0.0410
AP	 0.5400	 0.0440
AQ	 0.6410	 0.0680
AR	 0.4510	 0.0160
AS	 0.6150	 0.0200
AT	 0.6700	 0.0090
AU	 0.4250	 -0.0020
B0	 0.6190	 0.0430
B1	 0.5790	 0.0530
B2	 0.4250	 0.0420
B3	 0.3810	 0.0100
B4	 0.5410	 -0.0020
B5	 0.4320	 0.0320
BA	 0.8020	 0.0900
BB	 0.7530	 0.0550
BC	 0.4990	 0.0430
BD	 0.5140	 0.0360



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Chain	Atom inclusion	Q-score
BE	 0.6760	 0.0610
BF	 0.7380	 0.0580
BG	 0.7370	 0.0770
BH	 0.3010	 0.0310
BI	 0.0490	 0.0220
BJ	 0.5080	 0.0280
BK	 0.4790	 0.0490
BL	 0.4660	 -0.0000
BM	 0.5120	 0.0410
BN	 0.5860	 0.0350
BO	 0.8200	 0.0410
BP	 0.5440	 0.0400
BQ	 0.4980	 0.0270
BR	 0.6460	 0.0530
BS	 0.5710	 0.0500
BT	 0.7040	 0.0490
BU	 0.6440	 0.0440
BV	 0.6520	 0.0560
BW	 0.5740	 0.0240
BX	 0.6420	 0.0430
BY	 0.5150	 0.0330
BZ	 0.6770	 0.0460