



Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 08:25 PM EDT

PDB ID : 4V72 / pdb_00004v72
EMDB ID : EMD-1719
Title : E. coli 70S-fMetVal-tRNAVal-tRNA^fMet complex in hybrid pre-translocation state (pre4)
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 : 13.00 Å (reported)
Based on initial models : 2WRI, 2K4C, 2HGP, 3I1O

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

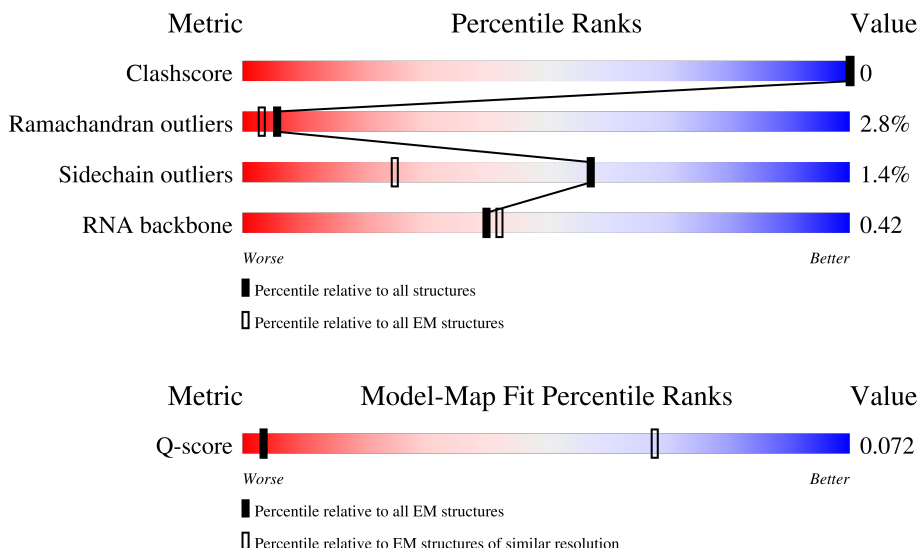
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 13.00 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	65 (12.50 - 13.50)

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	
2	AC	208	
3	AD	206	

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Mol	Chain	Length	Quality of chain
4	AE	152	28% 95% 5% .
5	AF	101	14% 90% 10%
6	AG	152	22% 93% 5% .
7	AH	130	32% 96% . .
8	AI	128	27% 96% . .
9	AJ	100	33% 94% 5% .
10	AK	118	34% 97% .
11	AL	124	38% 98% . .
12	AM	115	38% 93% 5% . .
13	AN	101	40% 97% . .
14	AO	89	17% 97% . . .
15	AP	81	44% 99% .
16	AQ	82	26% 96% .
17	AR	57	30% 96% .
18	AS	81	21% 95% . .
19	AT	86	29% 98% .
20	AU	53	57% 89% 11%
21	AA	1533	6% 61% 31% 7%
22	A1	76	34% 63% 32% 5%
23	A2	15	40% 47% 20% 27% 7%
24	A3	77	10% 52% 35% 13%
25	BC	273	47% 92% 7%
26	BD	209	44% 94% 6%
27	BE	201	32% 96% .
28	BF	179	22% 93% 6% . .

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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	7% 61% 33% 6%
55	BB	118	7% 63% 32% • •
56	B5	234	48% 94% • 5%

2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

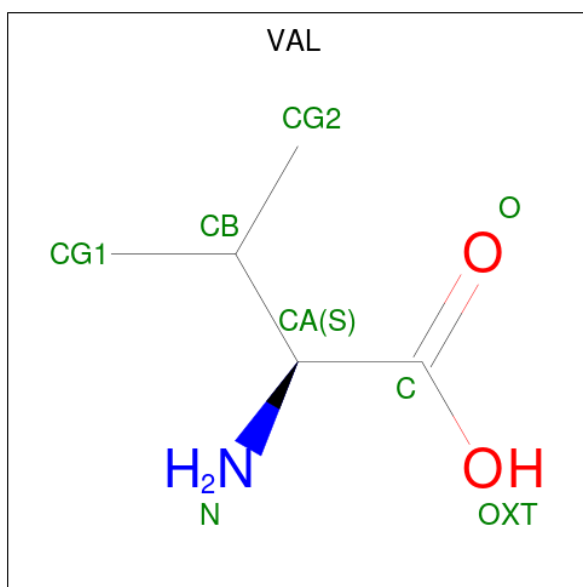
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

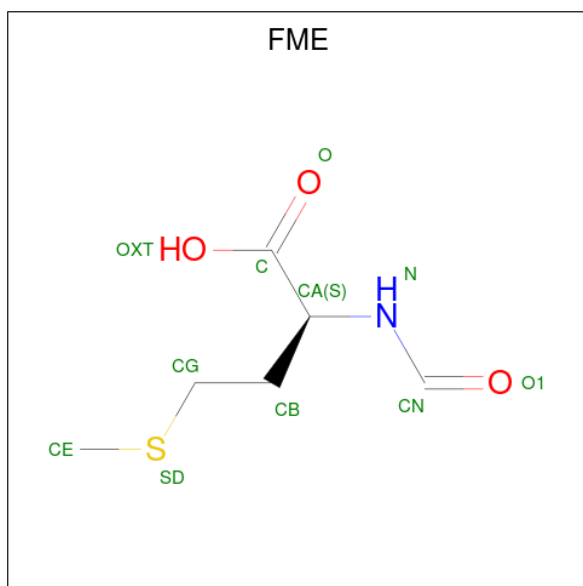
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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



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

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

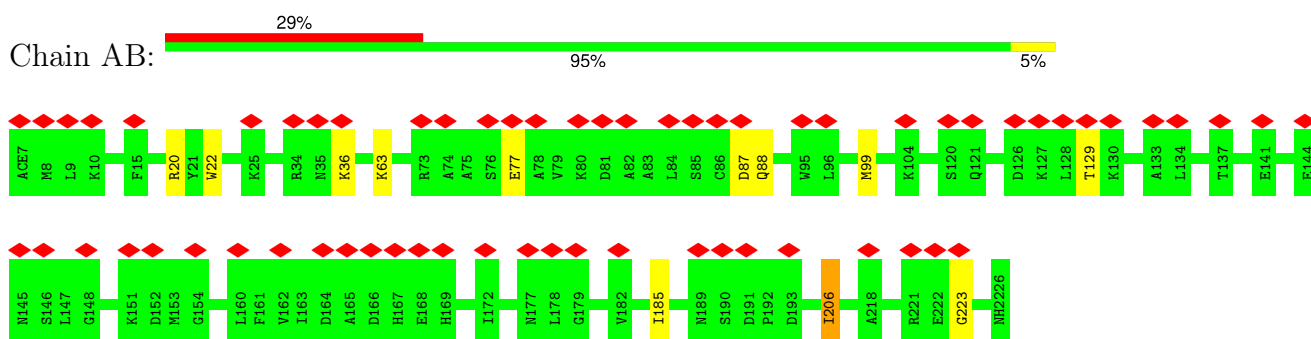


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

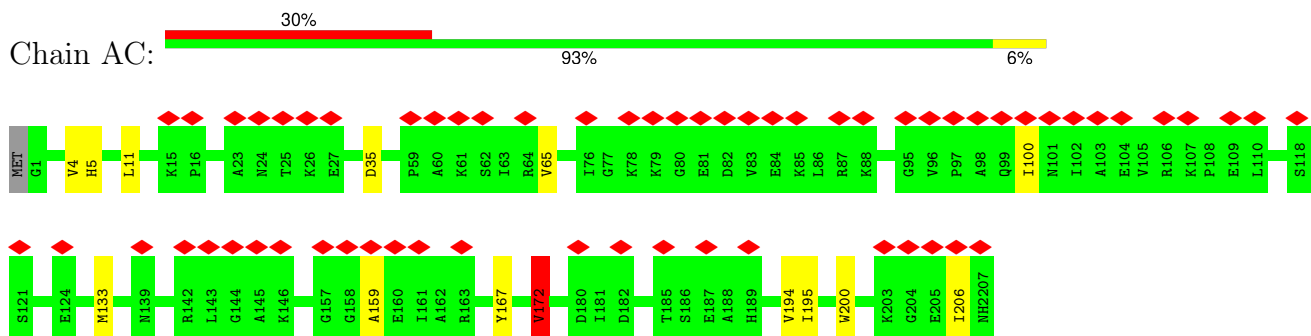
3 Residue-property plots

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

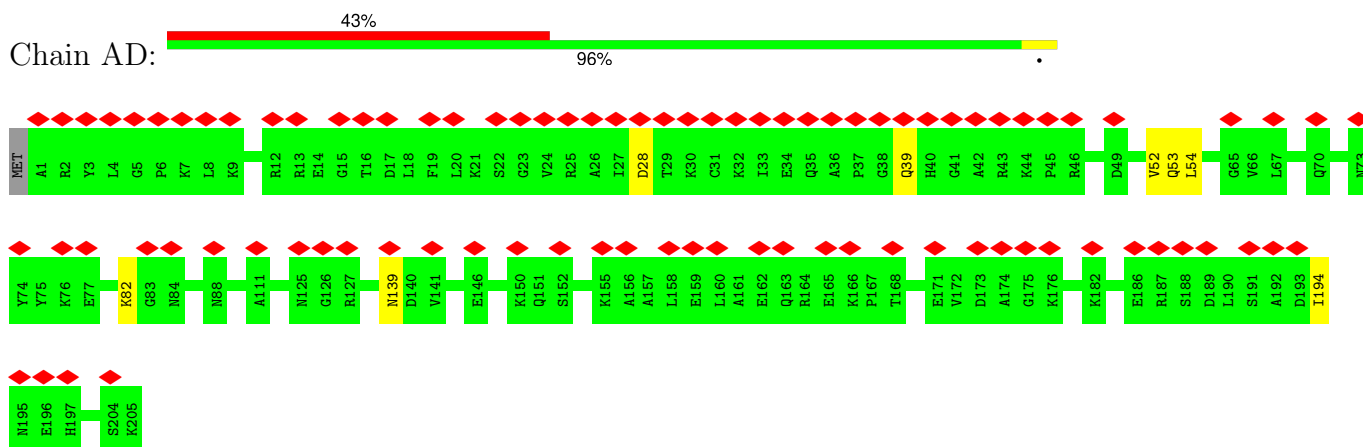
• Molecule 1: 30S ribosomal protein S2



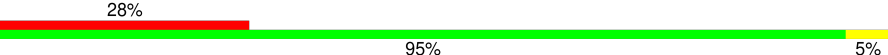
• Molecule 2: 30S ribosomal protein S3

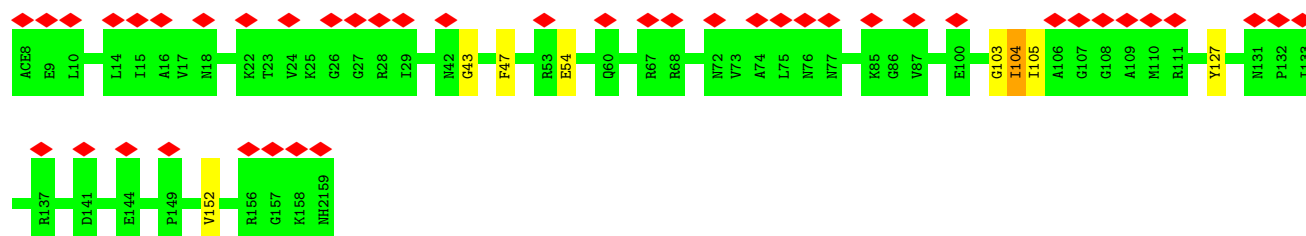


• Molecule 3: 30S ribosomal protein S4



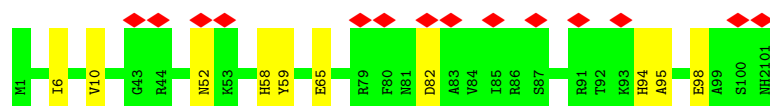
- Molecule 4: 30S ribosomal protein S5

Chain AE: 

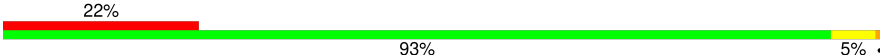


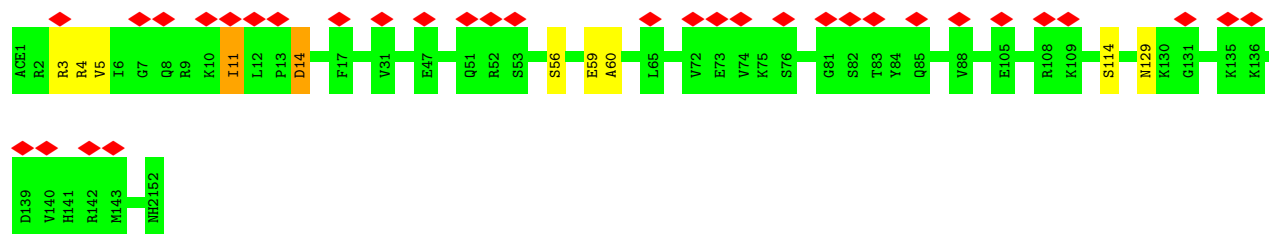
- Molecule 5: 30S ribosomal protein S6

Chain AF: 



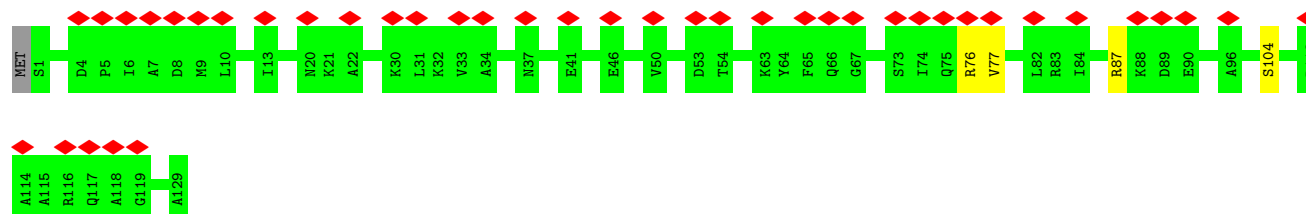
- Molecule 6: 30S ribosomal protein S7

Chain AG: 

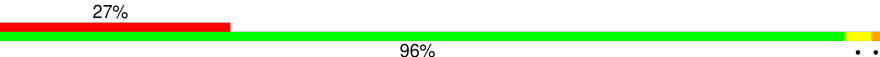


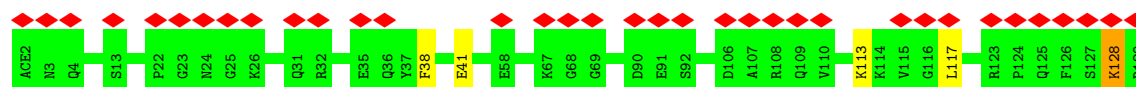
- Molecule 7: 30S ribosomal protein S8

Chain AH: 

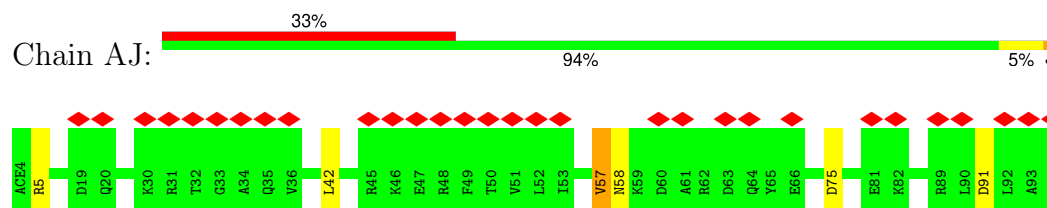


- Molecule 8: 30S ribosomal protein S9

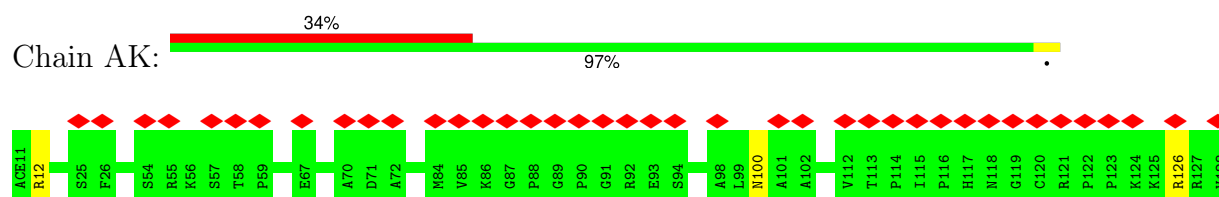
Chain AI: 



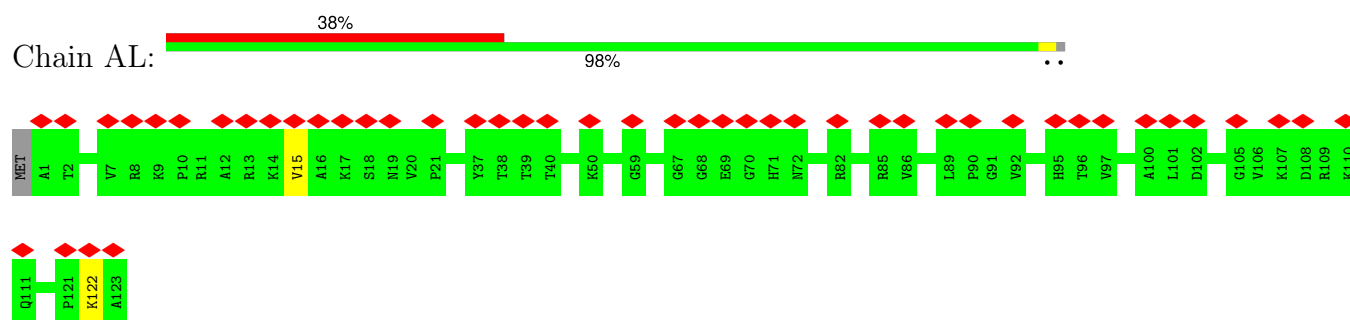
- Molecule 9: 30S ribosomal protein S10



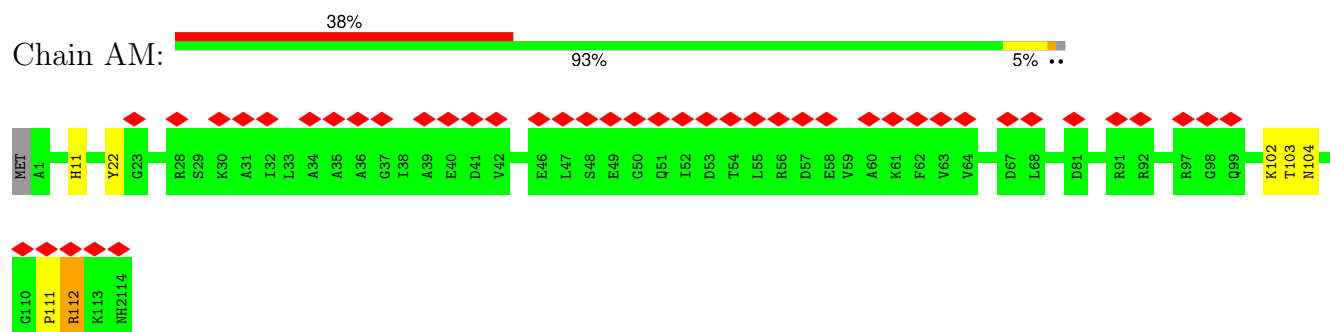
- Molecule 10: 30S ribosomal protein S11



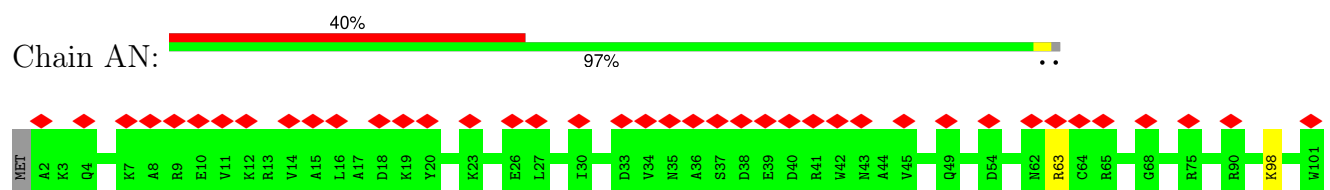
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13

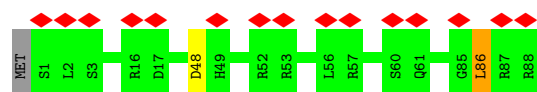


- Molecule 13: 30S ribosomal protein S14

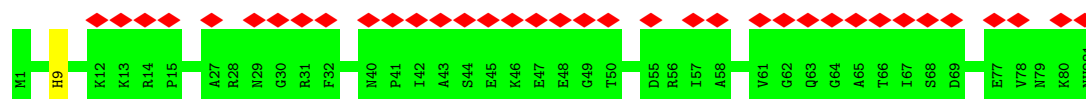


- Molecule 14: 30S ribosomal protein S15

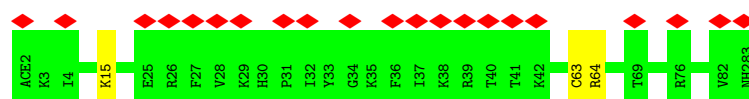




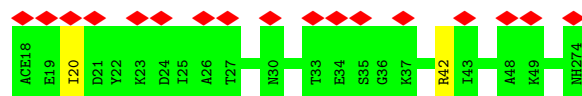
- Molecule 15: 30S ribosomal protein S16



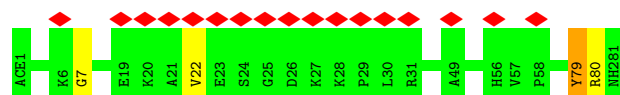
- Molecule 16: 30S ribosomal protein S17



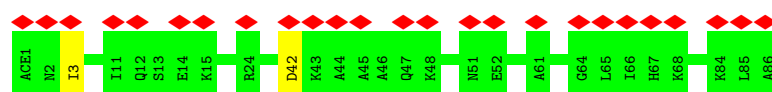
- Molecule 17: 30S ribosomal protein S18



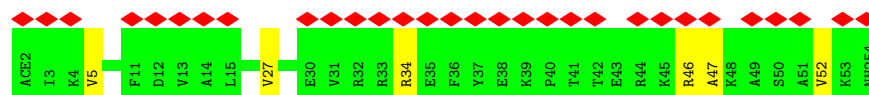
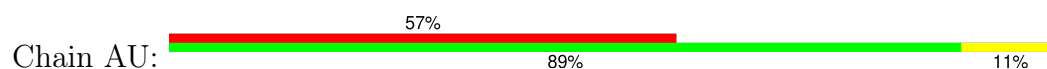
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20

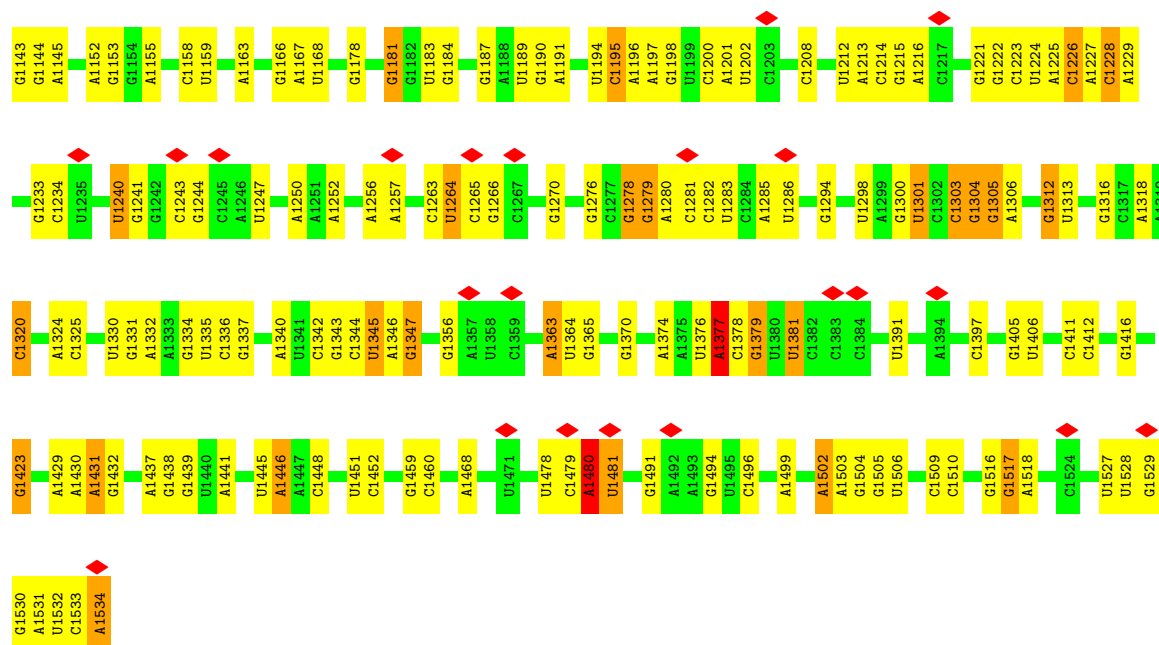


- Molecule 20: 30S ribosomal protein S21

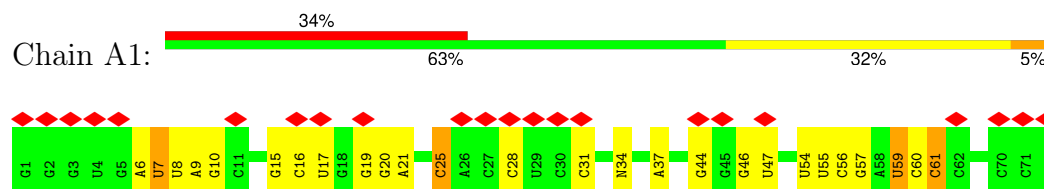


Chain AA:

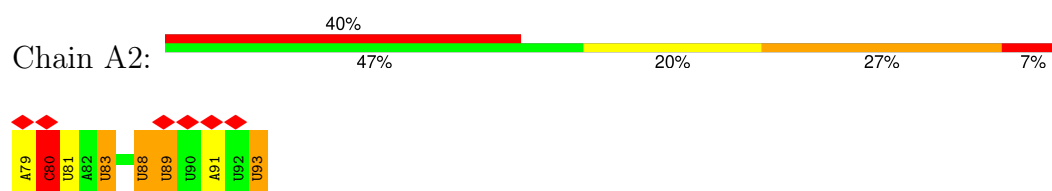




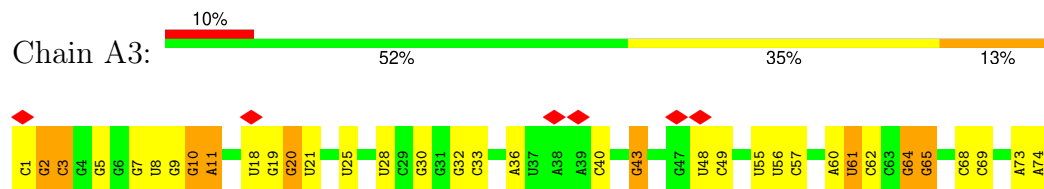
• Molecule 22: fMet-Val-tRNA-Val



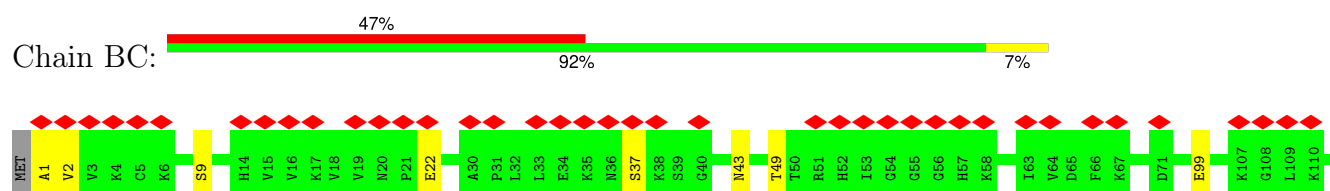
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

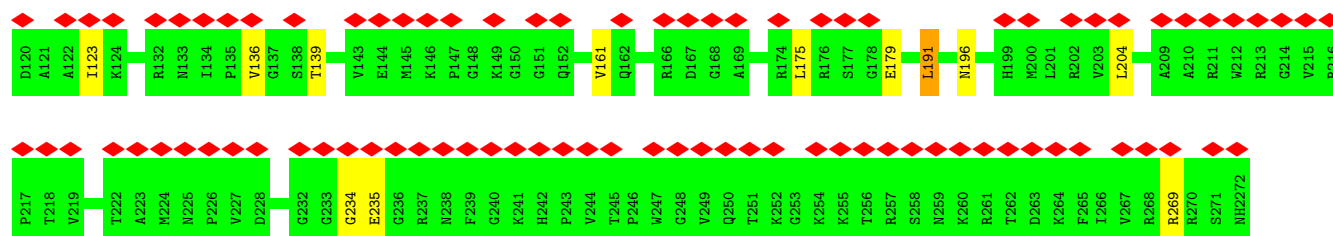


• Molecule 24: tRNA-fMet

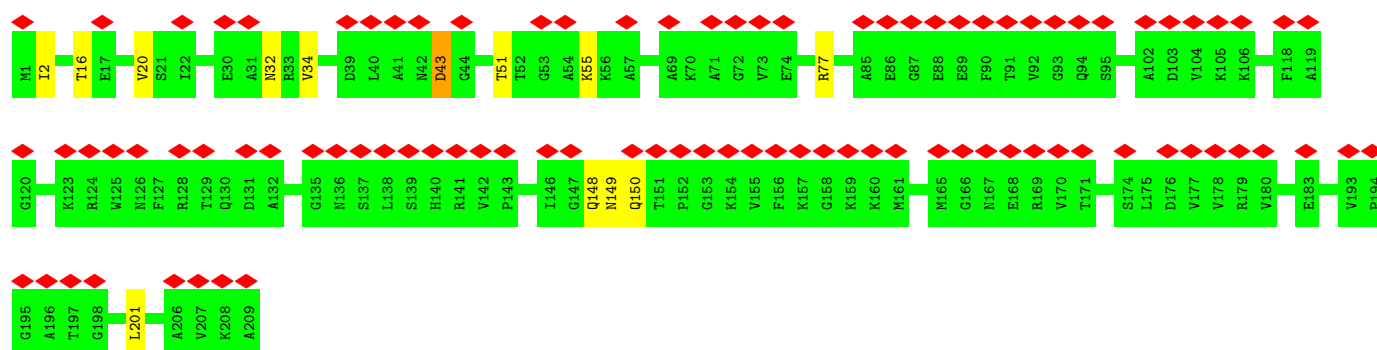


• Molecule 25: 50S ribosomal protein L2

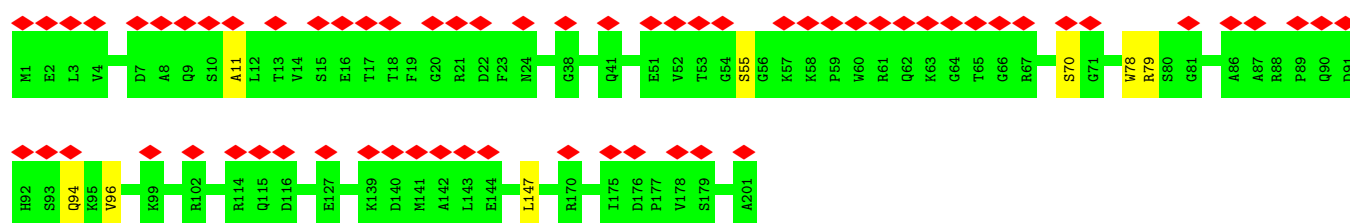




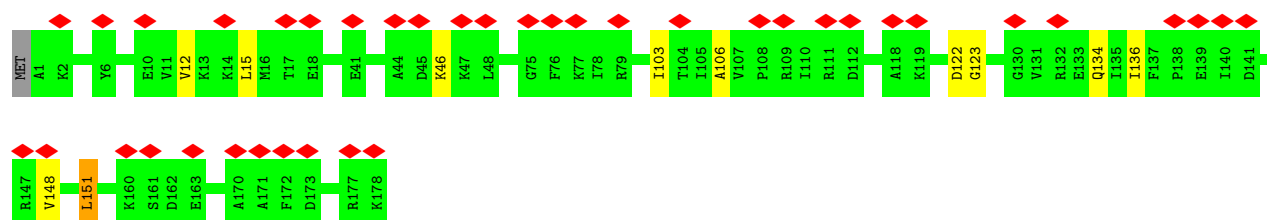
• Molecule 26: 50S ribosomal protein L3



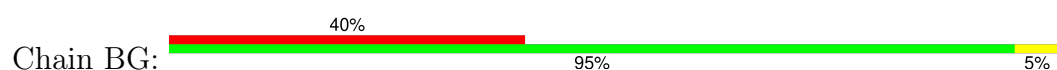
• Molecule 27: 50S ribosomal protein L4

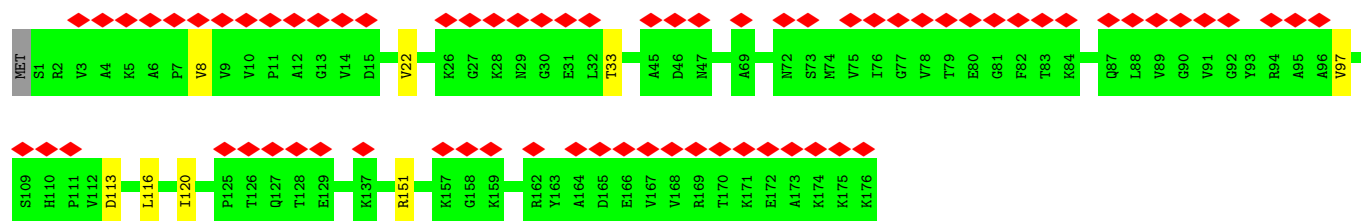


• Molecule 28: 50S ribosomal protein L5

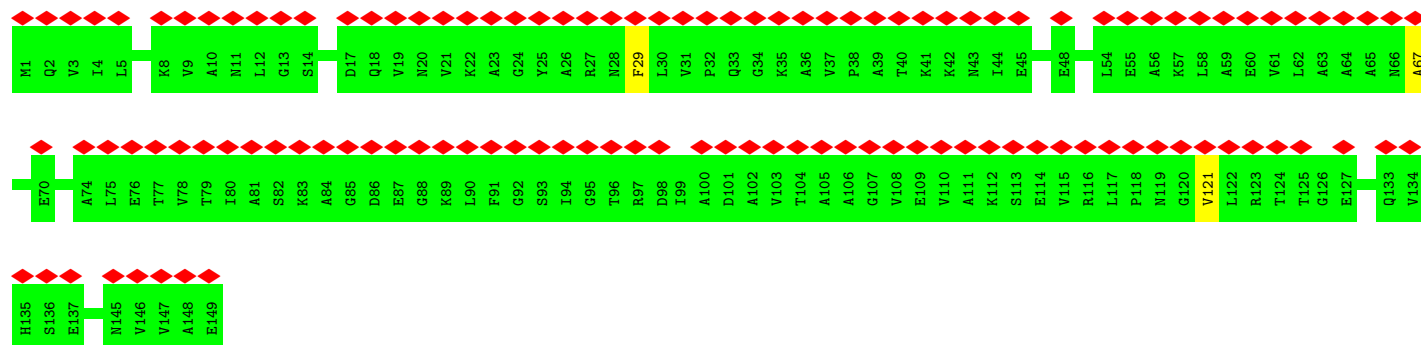
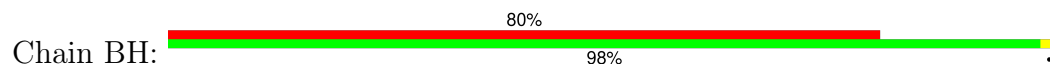


• Molecule 29: 50S ribosomal protein L6

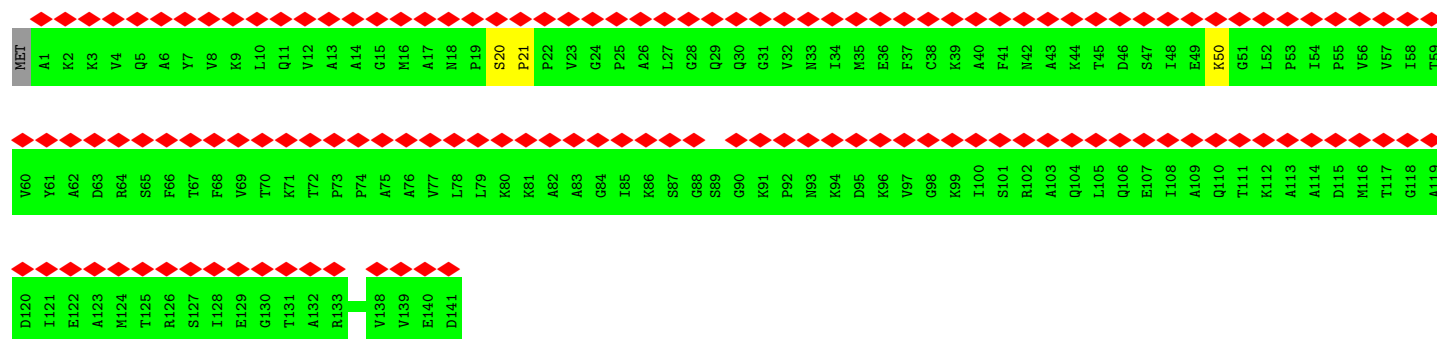




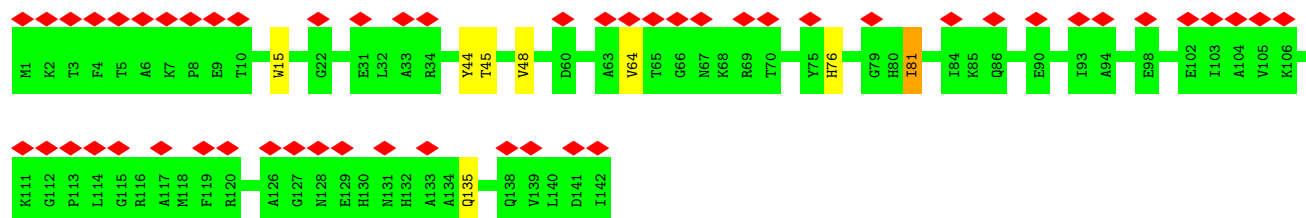
• Molecule 30: 50S ribosomal protein L9



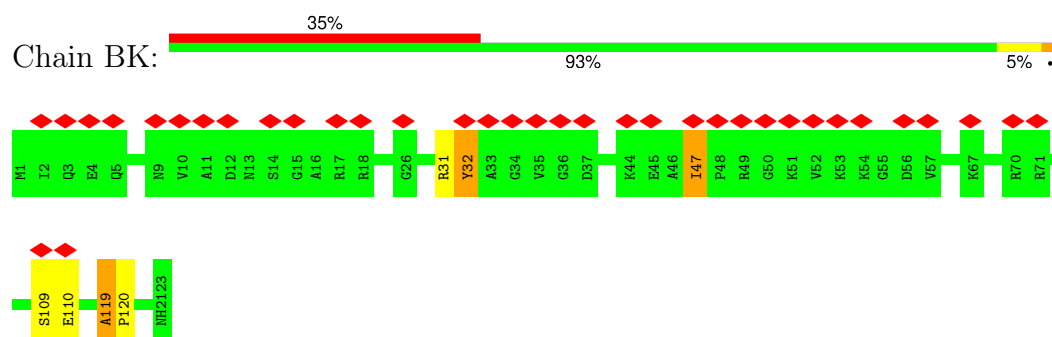
• Molecule 31: 50S ribosomal protein L11



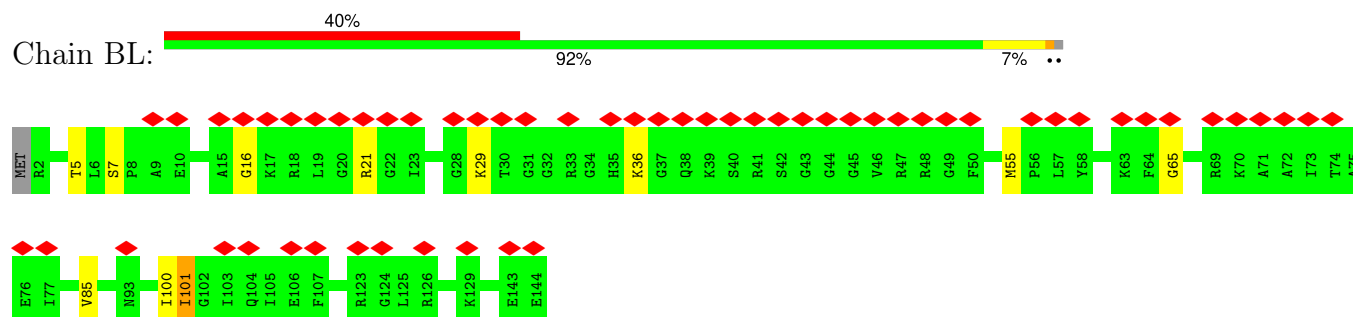
• Molecule 32: 50S ribosomal protein L13



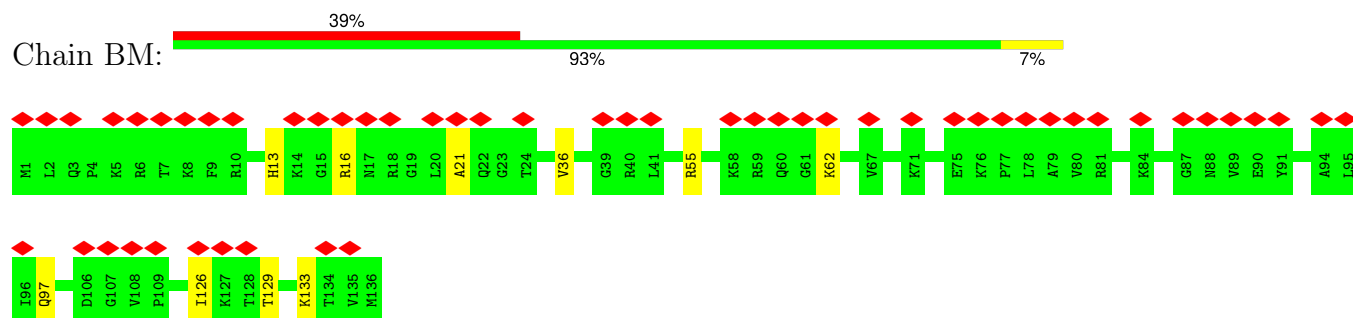
• Molecule 33: 50S ribosomal protein L14



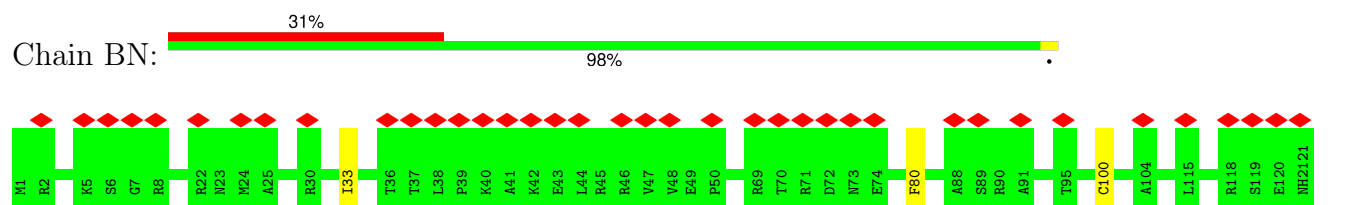
- Molecule 34: 50S ribosomal protein L15



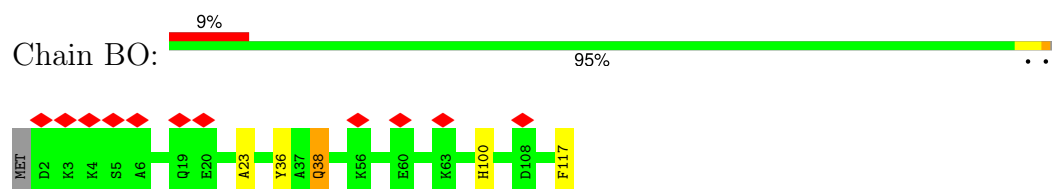
- Molecule 35: 50S ribosomal protein L16



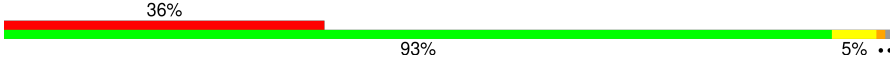
- Molecule 36: 50S ribosomal protein L17

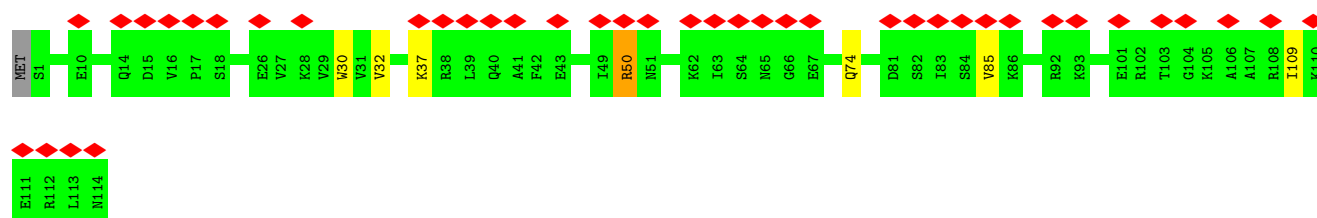


- Molecule 37: 50S ribosomal protein L18

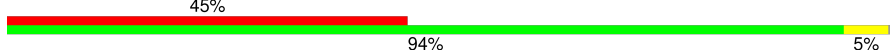


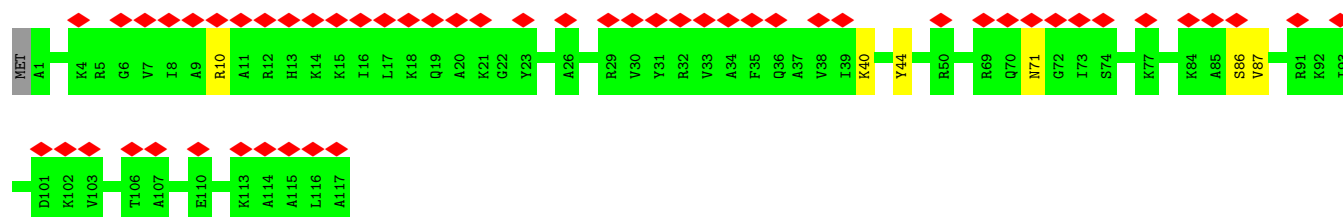
- Molecule 38: 50S ribosomal protein L19

Chain BP: 

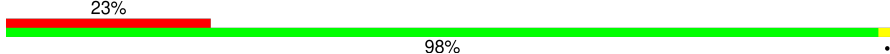


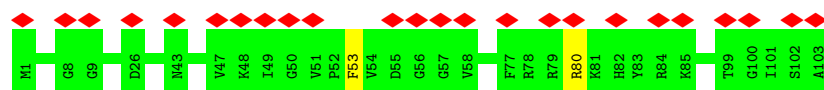
- Molecule 39: 50S ribosomal protein L20

Chain BQ: 

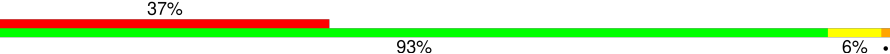


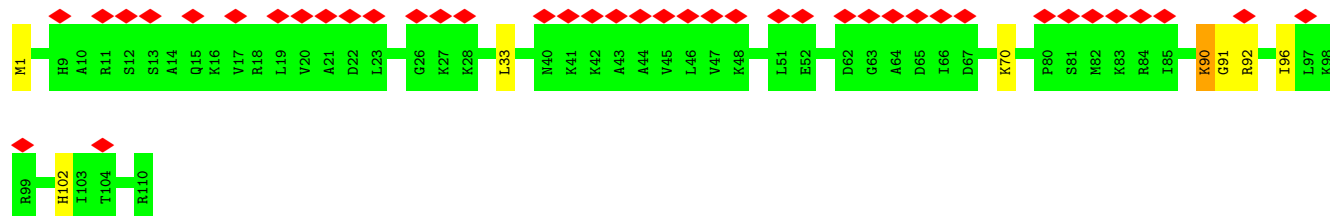
- Molecule 40: 50S ribosomal protein L21

Chain BR: 

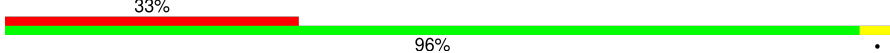


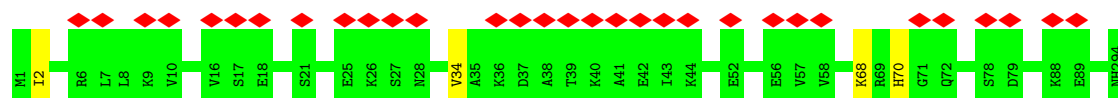
- Molecule 41: 50S ribosomal protein L22

Chain BS: 

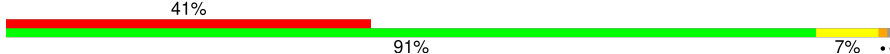


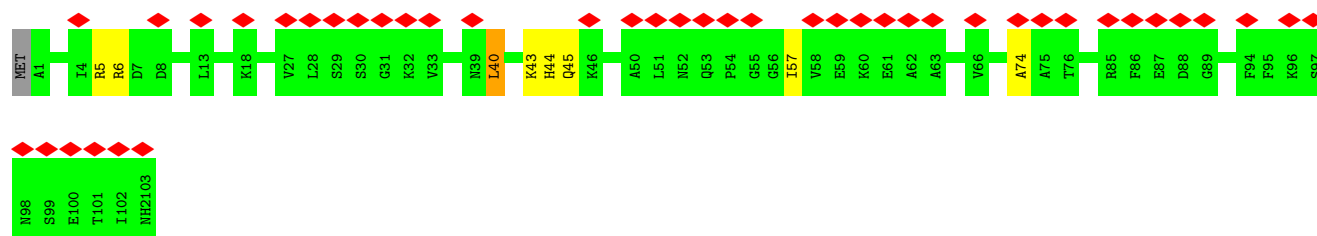
- Molecule 42: 50S ribosomal protein L23

Chain BT: 

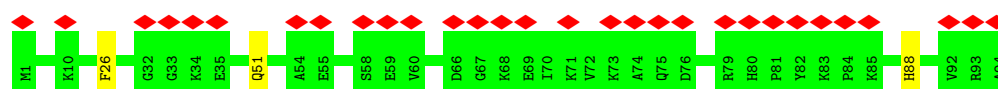


- Molecule 43: 50S ribosomal protein L24

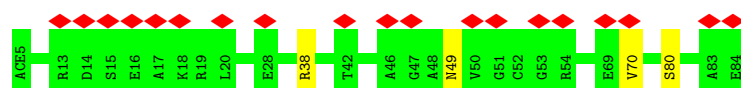
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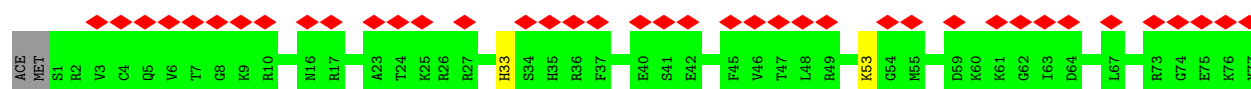
- Molecule 44: 50S ribosomal protein L25



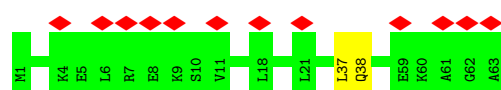
- Molecule 45: 50S ribosomal protein L27



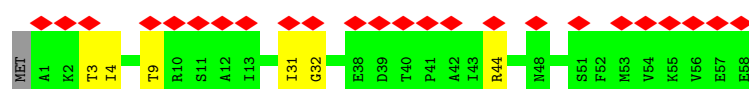
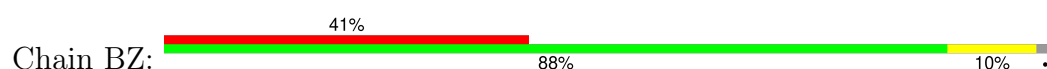
- Molecule 46: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L29

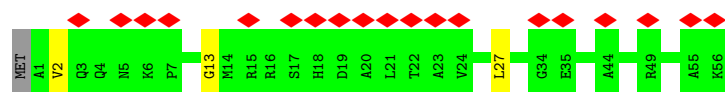


- Molecule 48: 50S ribosomal protein L30

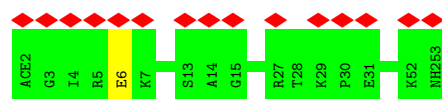


- Molecule 49: 50S ribosomal protein L32

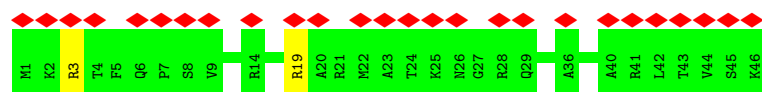




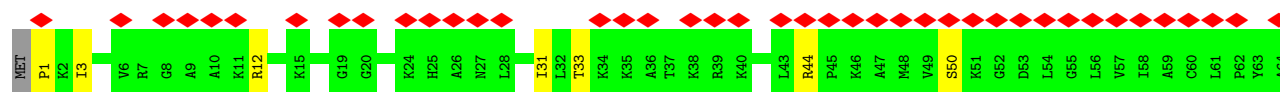
- Molecule 50: 50S ribosomal protein L33



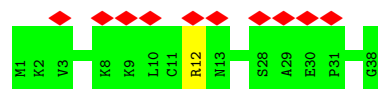
- Molecule 51: 50S ribosomal protein L34



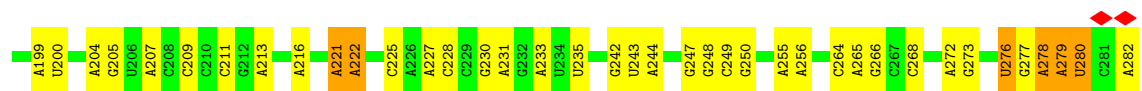
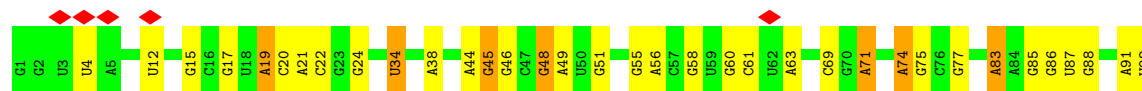
- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36

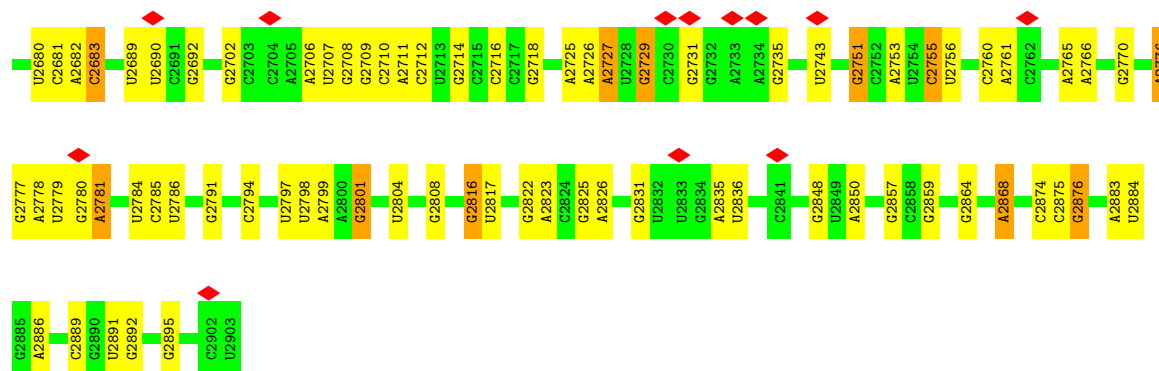


- Molecule 54: 23S ribosomal RNA

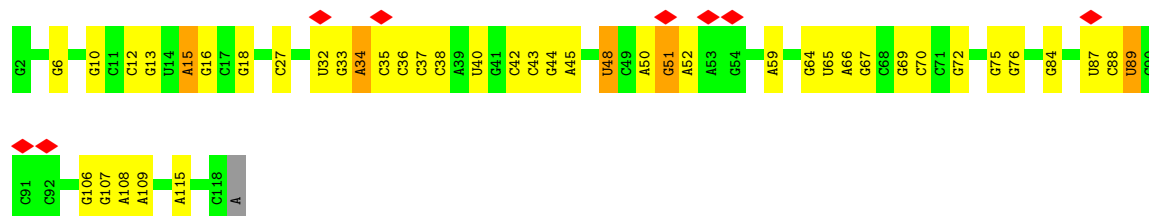




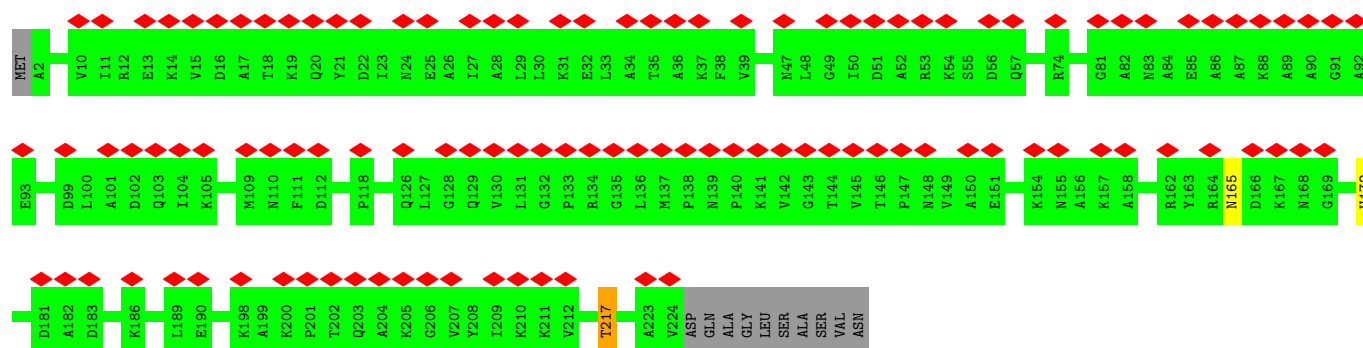
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• Molecule 55: 5S ribosomal RNA



• Molecule 56: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8375	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	194.626	Depositor
Minimum map value	-114.806	Depositor
Average map value	-0.932	Depositor
Map value standard deviation	20.010	Depositor
Recommended contour level	26	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: 4SU, OMC, PSU, 5MU, CM0, ACE, 7MG, H2U, 6MZ, NH2, 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	0.96	0/1736	1.39	7/2340 (0.3%)
2	AC	0.97	0/1651	1.38	4/2225 (0.2%)
3	AD	0.98	0/1665	1.42	5/2227 (0.2%)
4	AE	0.95	0/1119	1.39	4/1506 (0.3%)
5	AF	0.96	0/835	1.47	2/1128 (0.2%)
6	AG	0.96	0/1188	1.44	4/1593 (0.3%)
7	AH	0.93	0/989	1.32	1/1326 (0.1%)
8	AI	0.99	0/1035	1.43	4/1377 (0.3%)
9	AJ	0.97	0/797	1.41	2/1079 (0.2%)
10	AK	0.99	0/894	1.41	3/1207 (0.2%)
11	AL	1.02	0/969	1.42	2/1300 (0.2%)
12	AM	1.02	0/884	1.51	6/1181 (0.5%)
13	AN	1.00	0/817	1.38	0/1088
14	AO	0.97	0/722	1.39	0/964
15	AP	0.99	0/648	1.35	0/870
16	AQ	0.96	1/658 (0.2%)	1.48	3/883 (0.3%)
17	AR	0.99	0/463	1.34	1/623 (0.2%)
18	AS	1.00	0/653	1.48	5/879 (0.6%)
19	AT	0.93	0/672	1.40	0/890
20	AU	0.99	0/431	1.57	4/572 (0.7%)
21	AA	0.98	0/36759	1.16	58/57346 (0.1%)
22	A1	0.99	0/1668	1.14	0/2595
23	A2	1.03	0/343	1.31	3/531 (0.6%)
24	A3	1.00	0/1722	1.16	5/2685 (0.2%)
25	BC	0.99	0/2121	1.56	8/2852 (0.3%)
26	BD	0.91	0/1586	1.48	3/2134 (0.1%)
27	BE	0.88	0/1571	1.43	0/2113
28	BF	0.90	0/1444	1.40	2/1937 (0.1%)
29	BG	0.89	0/1343	1.45	0/1816
30	BH	0.88	0/1122	1.43	0/1515
31	BI	0.91	0/1046	1.43	1/1410 (0.1%)
32	BJ	0.96	0/1152	1.51	5/1551 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BK	0.95	0/947	1.43	3/1268 (0.2%)
34	BL	0.97	0/1054	1.53	4/1403 (0.3%)
35	BM	0.94	0/1093	1.51	2/1460 (0.1%)
36	BN	0.96	0/973	1.47	2/1301 (0.2%)
37	BO	0.94	0/902	1.44	2/1209 (0.2%)
38	BP	0.95	0/929	1.45	1/1242 (0.1%)
39	BQ	0.96	0/960	1.49	0/1278
40	BR	0.91	0/829	1.46	0/1107
41	BS	0.89	0/864	1.45	5/1156 (0.4%)
42	BT	0.86	0/744	1.44	2/994 (0.2%)
43	BU	0.93	0/787	1.57	2/1051 (0.2%)
44	BV	0.93	0/766	1.49	2/1025 (0.2%)
45	BW	0.96	0/604	1.56	0/799
46	BX	0.96	0/635	1.45	3/848 (0.4%)
47	BY	0.91	0/510	1.49	1/677 (0.1%)
48	BZ	0.95	0/453	1.53	2/605 (0.3%)
49	B0	0.99	0/450	1.51	0/599
50	B1	0.89	0/417	1.43	0/556
51	B2	0.99	0/380	1.53	1/498 (0.2%)
52	B3	1.01	0/513	1.51	1/676 (0.1%)
53	B4	0.96	0/303	1.49	1/397 (0.3%)
54	BA	0.83	0/69796	1.14	112/108888 (0.1%)
55	BB	0.83	0/2800	1.13	0/4367
56	B5	0.89	0/1673	1.41	1/2255 (0.0%)
All	All	0.91	1/160085 (0.0%)	1.23	289/239402 (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
2	AC	0	1
6	AG	0	1
7	AH	0	1
21	AA	0	369
22	A1	0	10
23	A2	0	4
24	A3	0	19
37	BO	0	1
52	B3	0	1
54	BA	0	715

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	28
All	All	0	1150

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	AQ	63	CYS	CA-C	6.04	1.56	1.53

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AQ	63	CYS	CA-C-N	10.20	140.06	121.70
16	AQ	63	CYS	C-N-CA	10.20	140.06	121.70
1	AB	206	ILE	CA-C-N	10.17	140.01	121.70
1	AB	206	ILE	C-N-CA	10.17	140.01	121.70
12	AM	102	LYS	CA-C-N	9.58	138.94	121.70
12	AM	102	LYS	C-N-CA	9.58	138.94	121.70
16	AQ	63	CYS	O-C-N	-9.47	113.79	121.65
21	AA	576	C	C1'-O4'-C4'	-9.24	100.45	109.70
18	AS	79	TYR	CA-C-N	8.85	137.63	121.70
18	AS	79	TYR	C-N-CA	8.85	137.63	121.70
6	AG	4	ARG	CA-C-N	8.69	137.34	121.70
6	AG	4	ARG	C-N-CA	8.69	137.34	121.70
54	BA	670	A	C2'-C3'-O3'	8.04	121.56	109.50
3	AD	52	VAL	CA-C-N	8.01	136.12	121.70
3	AD	52	VAL	C-N-CA	8.01	136.12	121.70
21	AA	38	G	O3'-P-O5'	-7.09	93.36	104.00
21	AA	1480	A	P-O3'-C3'	6.85	130.48	120.20
10	AK	126	ARG	NE-CZ-NH2	6.80	125.32	119.20
54	BA	573	U	C2'-C3'-O3'	6.78	119.67	109.50
12	AM	111	PRO	CA-C-N	6.71	133.79	121.70
12	AM	111	PRO	C-N-CA	6.71	133.79	121.70
21	AA	130	A	C5'-C4'-C3'	-6.66	105.21	115.20
20	AU	52	VAL	CA-C-N	6.63	133.64	121.70
20	AU	52	VAL	C-N-CA	6.63	133.64	121.70
54	BA	2282	G	C4'-C3'-O3'	6.59	122.89	113.00
54	BA	2116	G	O4'-C4'-C3'	6.57	110.56	104.00
21	AA	872	A	C1'-O4'-C4'	-6.55	103.35	109.90
8	AI	128	LYS	CA-C-N	6.50	133.41	121.70
8	AI	128	LYS	C-N-CA	6.50	133.41	121.70
35	BM	55	ARG	NE-CZ-NH2	6.40	124.96	119.20
54	BA	989	G	C4'-C3'-O3'	6.38	122.57	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BJ	44	TYR	CA-C-N	6.36	133.15	121.70
32	BJ	44	TYR	C-N-CA	6.36	133.15	121.70
36	BN	100	CYS	CA-C-N	6.29	126.08	120.10
36	BN	100	CYS	C-N-CA	6.29	126.08	120.10
4	AE	104	ILE	CA-C-N	6.27	132.99	121.70
4	AE	104	ILE	C-N-CA	6.27	132.99	121.70
1	AB	206	ILE	O-C-N	-6.26	114.74	122.57
54	BA	2428	G	O4'-C4'-C3'	6.22	110.22	104.00
54	BA	114	U	O4'-C4'-C3'	6.21	110.21	104.00
2	AC	172	VAL	CA-C-N	6.18	127.57	119.84
2	AC	172	VAL	C-N-CA	6.18	127.57	119.84
54	BA	1682	G	O4'-C4'-C3'	6.12	110.12	104.00
54	BA	1236	G	O4'-C4'-C3'	6.12	110.12	104.00
54	BA	2112	G	O4'-C1'-N9	6.09	117.63	108.50
54	BA	225	C	C4'-C3'-C2'	-6.08	96.52	102.60
54	BA	2776	A	P-O3'-C3'	6.03	129.25	120.20
54	BA	1256	G	O4'-C4'-C3'	6.03	110.03	104.00
54	BA	147	C	C1'-O4'-C4'	-5.99	103.91	109.90
54	BA	2272	U	O4'-C4'-C3'	5.97	109.97	104.00
10	AK	126	ARG	CA-C-N	5.94	132.39	121.70
10	AK	126	ARG	C-N-CA	5.94	132.39	121.70
25	BC	269	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	AB	20	ARG	CA-C-N	5.91	132.34	121.70
1	AB	20	ARG	C-N-CA	5.91	132.34	121.70
25	BC	234	GLY	CA-C-N	5.91	132.34	121.70
25	BC	234	GLY	C-N-CA	5.91	132.34	121.70
54	BA	1383	A	C2'-C3'-O3'	5.91	118.36	109.50
41	BS	91	GLY	CA-C-N	5.90	132.32	121.70
41	BS	91	GLY	C-N-CA	5.90	132.32	121.70
21	AA	793	U	C1'-O4'-C4'	-5.87	104.03	109.90
24	A3	64	G	O4'-C4'-C3'	5.87	109.87	104.00
18	AS	7	GLY	CA-C-N	5.86	126.32	120.52
18	AS	7	GLY	C-N-CA	5.86	126.32	120.52
8	AI	113	LYS	CA-C-N	5.86	132.24	121.70
8	AI	113	LYS	C-N-CA	5.86	132.24	121.70
51	B2	3	ARG	NE-CZ-NH2	5.85	124.46	119.20
54	BA	48	G	C5'-C4'-C3'	-5.82	107.27	116.00
43	BU	44	HIS	CB-CG-CD2	-5.81	123.64	131.20
7	AH	87	ARG	NE-CZ-NH2	5.79	124.41	119.20
9	AJ	91	ASP	CA-C-N	5.79	132.12	121.70
9	AJ	91	ASP	C-N-CA	5.79	132.12	121.70
54	BA	2755	C	O4'-C4'-C3'	5.78	109.78	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BC	1	ALA	CA-C-N	5.77	132.09	121.70
25	BC	1	ALA	C-N-CA	5.77	132.09	121.70
20	AU	46	ARG	CA-C-N	5.75	132.06	121.70
20	AU	46	ARG	C-N-CA	5.75	132.06	121.70
54	BA	2425	A	C4'-C3'-O3'	5.75	118.03	109.40
21	AA	869	G	O4'-C4'-C3'	5.75	109.75	104.00
54	BA	2164	C	O4'-C4'-C3'	5.75	109.75	104.00
21	AA	268	U	O4'-C4'-C3'	5.74	109.74	104.00
25	BC	9	SER	N-CA-C	5.73	113.38	108.22
21	AA	1345	U	O4'-C4'-C3'	5.71	109.71	104.00
54	BA	422	A	O4'-C4'-C3'	5.71	109.71	104.00
54	BA	800	A	C4'-C3'-O3'	-5.71	100.84	109.40
54	BA	547	A	O4'-C1'-N9	5.70	116.75	108.20
54	BA	1312	U	C2'-C3'-O3'	5.70	118.05	109.50
54	BA	1438	U	N1-C1'-C2'	5.69	120.54	112.00
2	AC	5	HIS	CA-C-N	5.69	125.40	119.82
2	AC	5	HIS	C-N-CA	5.69	125.40	119.82
54	BA	826	U	O4'-C4'-C3'	5.68	109.68	104.00
54	BA	1150	C	C4'-C3'-C2'	-5.67	96.93	102.60
54	BA	1309	G	C4'-C3'-C2'	-5.67	96.93	102.60
21	AA	659	U	O4'-C4'-C3'	5.66	109.66	104.00
21	AA	587	G	O4'-C4'-C3'	5.66	109.66	104.00
54	BA	635	C	C4'-C3'-C2'	-5.66	96.94	102.60
11	AL	122	LYS	CA-C-N	5.65	131.88	121.70
11	AL	122	LYS	C-N-CA	5.65	131.88	121.70
54	BA	19	A	C2'-C3'-O3'	-5.65	105.22	113.70
54	BA	1439	A	O4'-C1'-N9	5.65	116.97	108.50
21	AA	164	G	C1'-O4'-C4'	-5.64	104.06	109.70
28	BF	106	ALA	CA-C-N	5.63	123.79	120.24
28	BF	106	ALA	C-N-CA	5.63	123.79	120.24
21	AA	1216	A	O4'-C4'-C3'	5.63	109.63	104.00
54	BA	975	A	C4'-C3'-C2'	-5.63	96.97	102.60
54	BA	2531	A	O4'-C4'-C3'	5.63	109.63	104.00
44	BV	26	PHE	N-CA-C	5.63	113.28	108.22
54	BA	2249	U	C2'-C3'-O3'	5.62	117.93	109.50
54	BA	738	G	O4'-C4'-C3'	5.62	109.61	104.00
54	BA	330	A	C1'-O4'-C4'	-5.61	104.09	109.70
21	AA	1377	A	O4'-C4'-C3'	5.61	109.61	104.00
54	BA	1128	G	C1'-O4'-C4'	-5.61	104.09	109.70
54	BA	2692	G	C4'-C3'-C2'	-5.60	97.00	102.60
54	BA	2389	G	O4'-C4'-C3'	5.60	109.60	104.00
44	BV	88	HIS	CB-CG-CD2	-5.59	123.93	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BC	43	ASN	CA-C-N	5.58	128.03	120.38
25	BC	43	ASN	C-N-CA	5.58	128.03	120.38
21	AA	530	G	C1'-O4'-C4'	-5.58	104.33	109.90
54	BA	2660	A	O4'-C1'-N9	5.57	116.85	108.50
54	BA	527	C	C5'-C4'-C3'	-5.57	107.65	116.00
21	AA	505	G	O4'-C4'-C3'	5.55	109.56	104.00
31	BI	21	PRO	N-CA-C	5.55	117.48	110.70
21	AA	179	A	O4'-C4'-C3'	5.55	109.55	104.00
24	A3	2	G	O4'-C4'-C3'	5.53	109.53	104.00
54	BA	1300	G	C2'-C3'-O3'	5.53	117.79	109.50
34	BL	100	ILE	CA-C-N	5.52	131.90	121.97
34	BL	100	ILE	C-N-CA	5.52	131.90	121.97
54	BA	2581	G	O4'-C1'-N9	5.52	116.47	108.20
21	AA	707	U	O4'-C4'-C3'	5.51	109.51	104.00
54	BA	2423	U	O4'-C1'-N1	5.49	116.43	108.20
54	BA	38	A	C4'-C3'-C2'	-5.47	97.13	102.60
21	AA	312	C	O4'-C4'-C3'	5.45	109.45	104.00
21	AA	334	C	O4'-C4'-C3'	5.45	109.45	104.00
41	BS	90	LYS	CA-C-N	5.45	131.50	121.70
41	BS	90	LYS	C-N-CA	5.45	131.50	121.70
54	BA	2308	G	C4'-C3'-O3'	-5.44	101.24	109.40
54	BA	990	A	C1'-O4'-C4'	-5.44	104.46	109.90
53	B4	12	ARG	NE-CZ-NH2	5.43	124.09	119.20
21	AA	66	A	C5'-C4'-C3'	-5.42	107.86	116.00
54	BA	21	A	O4'-C4'-C3'	5.42	109.42	104.00
54	BA	2716	C	C4'-C3'-C2'	-5.40	97.20	102.60
17	AR	42	ARG	NE-CZ-NH2	5.40	124.06	119.20
54	BA	1125	G	O4'-C4'-C3'	5.40	109.40	104.00
4	AE	47	PHE	CA-C-N	5.40	125.32	121.65
4	AE	47	PHE	C-N-CA	5.40	125.32	121.65
21	AA	942	G	C5'-C4'-O4'	5.39	117.89	109.80
54	BA	2503	A	C4'-C3'-O3'	5.39	121.09	113.00
21	AA	1195	C	O4'-C4'-C3'	5.39	109.39	104.00
54	BA	1126	A	C2'-C3'-O3'	5.39	117.58	109.50
21	AA	1344	C	O3'-P-O5'	5.38	112.08	104.00
21	AA	1347	G	C4'-C3'-C2'	-5.38	97.22	102.60
54	BA	1090	A	O4'-C1'-C2'	-5.38	102.22	107.60
54	BA	2492	U	O4'-C1'-C2'	-5.37	102.23	107.60
21	AA	1494	G	O4'-C4'-C3'	5.37	109.37	104.00
32	BJ	135	GLN	CA-C-N	5.37	131.36	121.70
32	BJ	135	GLN	C-N-CA	5.37	131.36	121.70
54	BA	1263	U	O4'-C4'-C3'	5.37	109.36	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2266	A	C2'-C3'-O3'	5.37	117.55	109.50
54	BA	2554	U	C5'-C4'-C3'	-5.37	107.95	116.00
54	BA	291	G	C5'-C4'-C3'	-5.36	107.96	116.00
54	BA	1175	A	C1'-O4'-C4'	-5.34	104.56	109.90
54	BA	946	C	O4'-C1'-N1	5.34	116.51	108.50
48	BZ	44	ARG	CA-C-N	5.34	131.31	121.70
48	BZ	44	ARG	C-N-CA	5.34	131.31	121.70
54	BA	1822	C	C4'-C3'-C2'	-5.33	97.27	102.60
54	BA	235	U	O4'-C4'-C3'	5.32	109.31	104.00
54	BA	1758	U	O4'-C1'-N1	5.31	116.16	108.20
54	BA	1211	C	O4'-C1'-N1	5.30	116.15	108.20
33	BK	109	SER	N-CA-C	5.29	117.13	111.36
24	A3	43	G	C1'-O4'-C4'	-5.29	104.61	109.90
23	A2	80	C	O3'-P-O5'	5.29	111.93	104.00
21	AA	279	A	O4'-C4'-C3'	5.29	109.29	104.00
42	BT	68	LYS	CA-C-N	5.29	129.43	121.40
42	BT	68	LYS	C-N-CA	5.29	129.43	121.40
47	BY	38	GLN	OE1-CD-NE2	-5.29	117.31	122.60
54	BA	1664	A	O4'-C4'-C3'	5.29	109.28	104.00
21	AA	258	G	C5'-C4'-C3'	-5.28	108.08	116.00
23	A2	83	U	C5'-C4'-C3'	-5.28	108.08	116.00
21	AA	524	G	O4'-C4'-C3'	5.26	109.26	104.00
41	BS	102	HIS	CB-CG-CD2	-5.26	124.37	131.20
54	BA	705	A	C4'-C3'-C2'	-5.26	97.34	102.60
54	BA	1737	G	O4'-C4'-C3'	5.25	109.25	104.00
21	AA	354	G	C5'-C4'-C3'	-5.25	108.13	116.00
37	BO	38	GLN	OE1-CD-NE2	-5.24	117.36	122.60
54	BA	22	C	O4'-C4'-C3'	5.23	109.23	104.00
35	BM	13	HIS	CB-CG-CD2	-5.23	124.40	131.20
38	BP	50	ARG	N-CA-C	5.23	118.80	111.90
37	BO	100	HIS	CB-CG-CD2	-5.23	124.41	131.20
54	BA	839	U	O4'-C4'-C3'	5.23	109.23	104.00
54	BA	337	C	C4'-C3'-C2'	-5.22	97.38	102.60
1	AB	223	GLY	CA-C-N	5.22	131.09	121.70
1	AB	223	GLY	C-N-CA	5.22	131.09	121.70
21	AA	6	G	C1'-O4'-C4'	-5.21	104.69	109.90
54	BA	670	A	P-O3'-C3'	5.20	128.00	120.20
21	AA	254	G	O4'-C4'-C3'	5.20	109.20	104.00
54	BA	1185	G	O4'-C4'-C3'	5.20	109.20	104.00
52	B3	1	PRO	CA-N-CD	-5.19	104.73	112.00
21	AA	606	G	O4'-C4'-C3'	5.19	109.19	104.00
54	BA	2776	A	C2'-C3'-O3'	5.19	117.28	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	656	G	C5'-C4'-C3'	-5.19	108.22	116.00
21	AA	1304	G	O4'-C4'-C3'	5.18	109.18	104.00
21	AA	289	G	O4'-C4'-C3'	5.18	109.18	104.00
21	AA	776	G	O4'-C4'-C3'	5.18	109.18	104.00
21	AA	383	A	O4'-C4'-C3'	5.18	109.18	104.00
21	AA	1330	U	O4'-C4'-C3'	5.17	109.17	104.00
21	AA	693	G	O4'-C4'-C3'	5.17	109.17	104.00
24	A3	2	G	C3'-C2'-C1'	5.17	106.47	101.30
54	BA	2743	U	C5'-C4'-C3'	-5.17	108.25	116.00
54	BA	845	A	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	1352	U	C5'-C4'-C3'	-5.16	108.26	116.00
21	AA	497	G	O4'-C4'-C3'	5.16	109.16	104.00
54	BA	2347	C	C5'-C4'-C3'	-5.16	108.26	116.00
54	BA	2036	C	C3'-C2'-C1'	5.15	106.45	101.30
26	BD	149	ASN	CA-C-N	5.15	131.37	121.54
26	BD	149	ASN	C-N-CA	5.15	131.37	121.54
21	AA	1480	A	C4'-C3'-O3'	5.14	120.72	113.00
54	BA	2502	G	O4'-C4'-C3'	5.14	109.14	104.00
54	BA	2776	A	C4'-C3'-O3'	5.14	117.11	109.40
3	AD	52	VAL	O-C-N	-5.14	116.15	122.57
3	AD	53	GLN	CA-C-N	5.14	131.35	121.54
3	AD	53	GLN	C-N-CA	5.14	131.35	121.54
21	AA	1279	G	O4'-C4'-C3'	5.14	109.14	104.00
54	BA	573	U	P-O3'-C3'	5.14	127.91	120.20
54	BA	1009	A	O4'-C4'-C3'	5.14	109.14	104.00
54	BA	2169	A	O4'-C1'-N9	5.13	116.20	108.50
21	AA	414	A	O4'-C4'-C3'	5.13	109.13	104.00
21	AA	980	C	O3'-P-O5'	5.13	111.70	104.00
54	BA	815	C	C5'-C4'-C3'	-5.13	108.31	116.00
54	BA	938	G	O3'-P-O5'	5.13	111.69	104.00
54	BA	2642	G	C4'-C3'-C2'	-5.12	97.47	102.60
54	BA	2016	U	O4'-C4'-C3'	5.12	109.12	104.00
34	BL	101	ILE	N-CA-C	5.12	119.99	109.34
54	BA	2509	G	O4'-C4'-C3'	5.12	109.12	104.00
21	AA	978	A	O4'-C4'-C3'	5.11	109.11	104.00
54	BA	333	G	O4'-C4'-C3'	5.11	109.11	104.00
34	BL	7	SER	N-CA-C	5.10	112.61	108.07
21	AA	1117	A	O4'-C4'-C3'	5.10	109.10	104.00
46	BX	33	HIS	CB-CG-CD2	-5.10	124.57	131.20
21	AA	1318	A	O4'-C4'-C3'	5.10	109.10	104.00
46	BX	53	LYS	CA-C-N	5.10	125.50	119.94
46	BX	53	LYS	C-N-CA	5.10	125.50	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1365	G	O4'-C4'-C3'	5.09	109.09	104.00
21	AA	1363	A	C5'-C4'-C3'	-5.09	108.36	116.00
54	BA	1291	C	C2'-C3'-O3'	5.09	117.13	109.50
21	AA	199	A	O4'-C4'-C3'	5.08	109.08	104.00
54	BA	794	A	O4'-C4'-C3'	5.08	109.08	104.00
54	BA	2104	C	O4'-C1'-N1	5.08	116.13	108.50
54	BA	2598	A	O4'-C4'-C3'	5.08	109.08	104.00
6	AG	14	ASP	CA-C-N	5.08	124.77	119.64
6	AG	14	ASP	C-N-CA	5.08	124.77	119.64
54	BA	2725	A	O4'-C4'-C3'	5.07	109.07	104.00
21	AA	1116	U	O4'-C4'-C3'	5.07	109.07	104.00
21	AA	313	A	O4'-C4'-C3'	5.07	109.07	104.00
54	BA	280	U	O4'-C1'-N1	5.07	116.11	108.50
56	B5	172	HIS	CB-CG-CD2	-5.07	124.62	131.20
54	BA	1922	G	C4'-C3'-C2'	-5.06	97.54	102.60
54	BA	1126	A	P-O3'-C3'	5.06	127.79	120.20
21	AA	285	C	O4'-C4'-C3'	5.06	109.06	104.00
24	A3	36	A	O4'-C4'-C3'	5.06	109.06	104.00
54	BA	1807	G	O4'-C4'-C3'	5.06	109.06	104.00
26	BD	32	ASN	OD1-CG-ND2	-5.06	117.54	122.60
32	BJ	76	HIS	CB-CG-CD2	-5.05	124.64	131.20
54	BA	1263	U	C3'-C2'-C1'	5.05	106.35	101.30
33	BK	31	ARG	CA-C-N	5.04	131.17	121.54
33	BK	31	ARG	C-N-CA	5.04	131.17	121.54
18	AS	79	TYR	O-C-N	-5.04	115.89	122.59
21	AA	1055	A	O4'-C4'-C3'	5.04	109.04	104.00
54	BA	2543	G	O4'-C4'-C3'	5.03	109.03	104.00
5	AF	58	HIS	CA-C-N	5.02	131.14	121.54
5	AF	58	HIS	C-N-CA	5.02	131.14	121.54
12	AM	112	ARG	CA-C-N	5.02	130.74	121.70
12	AM	112	ARG	C-N-CA	5.02	130.74	121.70
21	AA	161	A	O4'-C4'-C3'	5.02	109.02	104.00
54	BA	2214	C	O4'-C4'-C3'	5.02	109.02	104.00
54	BA	328	U	O4'-C4'-C3'	5.02	109.02	104.00
54	BA	344	A	O4'-C4'-C3'	5.02	109.02	104.00
54	BA	492	A	C4'-C3'-C2'	-5.01	97.58	102.60
54	BA	2503	A	P-O3'-C3'	5.01	127.72	120.20
21	AA	55	A	P-O3'-C3'	5.01	127.72	120.20
43	BU	6	ARG	NE-CZ-NH2	5.01	123.71	119.20
23	A2	93	U	C1'-O4'-C4'	-5.01	104.69	109.70
54	BA	1773	A	C5'-C4'-C3'	-5.01	108.49	116.00
54	BA	1979	U	C4'-C3'-C2'	-5.01	97.59	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	83	C	O4'-C4'-C3'	5.00	109.00	104.00
54	BA	1313	U	O4'-C4'-C3'	5.00	109.00	104.00
54	BA	1535	A	O4'-C1'-N9	5.00	115.71	108.20
21	AA	381	C	C5'-C4'-C3'	-5.00	107.70	115.20
54	BA	99	U	O4'-C1'-N1	5.00	116.00	108.50
54	BA	121	G	C3'-C2'-C1'	5.00	106.30	101.30

There are no chirality outliers.

All (1150) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	15	G	Sidechain
22	A1	20	G	Sidechain
22	A1	25	C	Sidechain
22	A1	28	C	Sidechain
22	A1	31	C	Sidechain
22	A1	44	G	Sidechain
22	A1	59	U	Sidechain
22	A1	6	A	Sidechain
22	A1	61	C	Sidechain
22	A1	9	A	Sidechain
23	A2	80	C	Sidechain
23	A2	83	U	Sidechain
23	A2	88	U	Sidechain
23	A2	89	U	Sidechain
24	A3	1	C	Sidechain
24	A3	10	G	Sidechain
24	A3	11	A	Sidechain
24	A3	19	G	Sidechain
24	A3	20	G	Sidechain
24	A3	28	U	Sidechain
24	A3	3	C	Sidechain
24	A3	30	G	Sidechain
24	A3	32	G	Sidechain
24	A3	5	G	Sidechain
24	A3	57	C	Sidechain
24	A3	60	A	Sidechain
24	A3	61	U	Sidechain
24	A3	65	G	Sidechain
24	A3	68	C	Sidechain
24	A3	69	C	Sidechain
24	A3	7	G	Sidechain

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Mol	Chain	Res	Type	Group
24	A3	75	C	Sidechain
24	A3	9	G	Sidechain
21	AA	1000	A	Sidechain
21	AA	1002	G	Sidechain
21	AA	1003	G	Sidechain
21	AA	1013	G	Sidechain
21	AA	1016	A	Sidechain
21	AA	1020	G	Sidechain
21	AA	1027	C	Sidechain
21	AA	1028	C	Sidechain
21	AA	1035	A	Sidechain
21	AA	1044	A	Sidechain
21	AA	1046	A	Sidechain
21	AA	1049	U	Sidechain
21	AA	1050	G	Sidechain
21	AA	1055	A	Sidechain
21	AA	1060	U	Sidechain
21	AA	1061	G	Sidechain
21	AA	1075	U	Sidechain
21	AA	1078	U	Sidechain
21	AA	1084	G	Sidechain
21	AA	1090	U	Sidechain
21	AA	1092	A	Sidechain
21	AA	1094	G	Sidechain
21	AA	1095	U	Sidechain
21	AA	11	G	Sidechain
21	AA	1101	A	Sidechain
21	AA	111	G	Sidechain
21	AA	1110	A	Sidechain
21	AA	1111	A	Sidechain
21	AA	1112	C	Sidechain
21	AA	1121	U	Sidechain
21	AA	1123	U	Sidechain
21	AA	113	G	Sidechain
21	AA	1130	A	Sidechain
21	AA	1131	G	Sidechain
21	AA	1132	C	Sidechain
21	AA	1144	G	Sidechain
21	AA	1145	A	Sidechain
21	AA	115	G	Sidechain
21	AA	1155	A	Sidechain
21	AA	1158	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1163	A	Sidechain
21	AA	1166	G	Sidechain
21	AA	117	G	Sidechain
21	AA	1178	G	Sidechain
21	AA	1181	G	Sidechain
21	AA	1187	G	Sidechain
21	AA	1194	U	Sidechain
21	AA	1198	G	Sidechain
21	AA	1208	C	Sidechain
21	AA	1214	C	Sidechain
21	AA	1221	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1223	C	Sidechain
21	AA	1226	C	Sidechain
21	AA	1228	C	Sidechain
21	AA	123	U	Sidechain
21	AA	1233	G	Sidechain
21	AA	1234	C	Sidechain
21	AA	1240	U	Sidechain
21	AA	1241	G	Sidechain
21	AA	1243	C	Sidechain
21	AA	1244	G	Sidechain
21	AA	1247	U	Sidechain
21	AA	1250	A	Sidechain
21	AA	1252	A	Sidechain
21	AA	1263	C	Sidechain
21	AA	1264	U	Sidechain
21	AA	1266	G	Sidechain
21	AA	1270	G	Sidechain
21	AA	1276	G	Sidechain
21	AA	1278	G	Sidechain
21	AA	128	G	Sidechain
21	AA	1281	C	Sidechain
21	AA	1283	U	Sidechain
21	AA	1294	G	Sidechain
21	AA	1298	U	Sidechain
21	AA	1301	U	Sidechain
21	AA	1303	C	Sidechain
21	AA	1305	G	Sidechain
21	AA	1312	G	Sidechain
21	AA	1313	U	Sidechain
21	AA	1316	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1320	C	Sidechain
21	AA	1331	G	Sidechain
21	AA	1332	A	Sidechain
21	AA	1334	G	Sidechain
21	AA	1340	A	Sidechain
21	AA	1345	U	Sidechain
21	AA	1356	G	Sidechain
21	AA	1363	A	Sidechain
21	AA	1364	U	Sidechain
21	AA	137	U	Sidechain
21	AA	1370	G	Sidechain
21	AA	1374	A	Sidechain
21	AA	1376	U	Sidechain
21	AA	1377	A	Sidechain
21	AA	1379	G	Sidechain
21	AA	138	G	Sidechain
21	AA	1381	U	Sidechain
21	AA	1391	U	Sidechain
21	AA	1397	C	Sidechain
21	AA	14	U	Sidechain
21	AA	1405	G	Sidechain
21	AA	1406	U	Sidechain
21	AA	1412	C	Sidechain
21	AA	1416	G	Sidechain
21	AA	142	G	Sidechain
21	AA	1423	G	Sidechain
21	AA	1431	A	Sidechain
21	AA	1437	A	Sidechain
21	AA	1438	G	Sidechain
21	AA	1439	G	Sidechain
21	AA	1441	A	Sidechain
21	AA	1445	U	Sidechain
21	AA	1446	A	Sidechain
21	AA	1448	C	Sidechain
21	AA	145	G	Sidechain
21	AA	1478	U	Sidechain
21	AA	1479	C	Sidechain
21	AA	1480	A	Sidechain
21	AA	1481	U	Sidechain
21	AA	1491	G	Sidechain
21	AA	1496	C	Sidechain
21	AA	1502	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1509	C	Sidechain
21	AA	1510	C	Sidechain
21	AA	1517	G	Sidechain
21	AA	1518	A	Sidechain
21	AA	152	A	Sidechain
21	AA	1527	U	Sidechain
21	AA	1528	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1531	A	Sidechain
21	AA	1532	U	Sidechain
21	AA	1534	A	Sidechain
21	AA	155	A	Sidechain
21	AA	158	G	Sidechain
21	AA	159	G	Sidechain
21	AA	161	A	Sidechain
21	AA	164	G	Sidechain
21	AA	167	A	Sidechain
21	AA	173	U	Sidechain
21	AA	180	U	Sidechain
21	AA	185	U	Sidechain
21	AA	187	G	Sidechain
21	AA	189	A	Sidechain
21	AA	19	A	Sidechain
21	AA	190	A	Sidechain
21	AA	191	G	Sidechain
21	AA	195	A	Sidechain
21	AA	197	A	Sidechain
21	AA	203	G	Sidechain
21	AA	205	A	Sidechain
21	AA	207	C	Sidechain
21	AA	208	U	Sidechain
21	AA	212	G	Sidechain
21	AA	22	G	Sidechain
21	AA	222	C	Sidechain
21	AA	224	U	Sidechain
21	AA	226	G	Sidechain
21	AA	228	A	Sidechain
21	AA	236	A	Sidechain
21	AA	237	G	Sidechain
21	AA	238	A	Sidechain
21	AA	240	G	Sidechain
21	AA	241	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	242	G	Sidechain
21	AA	244	U	Sidechain
21	AA	250	A	Sidechain
21	AA	251	G	Sidechain
21	AA	254	G	Sidechain
21	AA	257	G	Sidechain
21	AA	26	A	Sidechain
21	AA	274	A	Sidechain
21	AA	278	G	Sidechain
21	AA	281	G	Sidechain
21	AA	285	C	Sidechain
21	AA	295	C	Sidechain
21	AA	297	G	Sidechain
21	AA	298	A	Sidechain
21	AA	308	C	Sidechain
21	AA	320	A	Sidechain
21	AA	321	A	Sidechain
21	AA	324	G	Sidechain
21	AA	326	G	Sidechain
21	AA	331	G	Sidechain
21	AA	339	C	Sidechain
21	AA	345	C	Sidechain
21	AA	35	G	Sidechain
21	AA	353	A	Sidechain
21	AA	355	C	Sidechain
21	AA	356	A	Sidechain
21	AA	362	G	Sidechain
21	AA	372	C	Sidechain
21	AA	377	G	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	381	C	Sidechain
21	AA	383	A	Sidechain
21	AA	390	U	Sidechain
21	AA	391	G	Sidechain
21	AA	401	C	Sidechain
21	AA	405	U	Sidechain
21	AA	409	U	Sidechain
21	AA	413	G	Sidechain
21	AA	414	A	Sidechain
21	AA	42	G	Sidechain
21	AA	425	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	429	U	Sidechain
21	AA	43	C	Sidechain
21	AA	434	U	Sidechain
21	AA	439	U	Sidechain
21	AA	448	A	Sidechain
21	AA	45	G	Sidechain
21	AA	464	U	Sidechain
21	AA	466	A	Sidechain
21	AA	467	U	Sidechain
21	AA	473	U	Sidechain
21	AA	475	C	Sidechain
21	AA	479	U	Sidechain
21	AA	48	C	Sidechain
21	AA	481	G	Sidechain
21	AA	485	U	Sidechain
21	AA	487	A	Sidechain
21	AA	490	C	Sidechain
21	AA	496	A	Sidechain
21	AA	497	G	Sidechain
21	AA	499	A	Sidechain
21	AA	50	A	Sidechain
21	AA	505	G	Sidechain
21	AA	506	G	Sidechain
21	AA	508	U	Sidechain
21	AA	509	A	Sidechain
21	AA	51	A	Sidechain
21	AA	517	G	Sidechain
21	AA	518	C	Sidechain
21	AA	520	A	Sidechain
21	AA	525	C	Sidechain
21	AA	529	G	Sidechain
21	AA	530	G	Sidechain
21	AA	539	A	Sidechain
21	AA	540	G	Sidechain
21	AA	542	G	Sidechain
21	AA	548	G	Sidechain
21	AA	550	G	Sidechain
21	AA	552	U	Sidechain
21	AA	554	A	Sidechain
21	AA	562	U	Sidechain
21	AA	569	C	Sidechain
21	AA	57	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	570	G	Sidechain
21	AA	577	G	Sidechain
21	AA	580	C	Sidechain
21	AA	585	G	Sidechain
21	AA	591	U	Sidechain
21	AA	592	G	Sidechain
21	AA	6	G	Sidechain
21	AA	60	A	Sidechain
21	AA	602	A	Sidechain
21	AA	605	U	Sidechain
21	AA	608	A	Sidechain
21	AA	612	C	Sidechain
21	AA	618	C	Sidechain
21	AA	620	C	Sidechain
21	AA	626	G	Sidechain
21	AA	633	G	Sidechain
21	AA	635	A	Sidechain
21	AA	642	A	Sidechain
21	AA	646	G	Sidechain
21	AA	65	A	Sidechain
21	AA	654	G	Sidechain
21	AA	659	U	Sidechain
21	AA	664	G	Sidechain
21	AA	666	G	Sidechain
21	AA	676	A	Sidechain
21	AA	685	G	Sidechain
21	AA	69	G	Sidechain
21	AA	690	G	Sidechain
21	AA	691	G	Sidechain
21	AA	694	A	Sidechain
21	AA	7	A	Sidechain
21	AA	704	A	Sidechain
21	AA	707	U	Sidechain
21	AA	711	G	Sidechain
21	AA	714	G	Sidechain
21	AA	718	A	Sidechain
21	AA	719	C	Sidechain
21	AA	720	C	Sidechain
21	AA	722	G	Sidechain
21	AA	727	G	Sidechain
21	AA	735	C	Sidechain
21	AA	737	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	739	C	Sidechain
21	AA	740	U	Sidechain
21	AA	741	G	Sidechain
21	AA	752	G	Sidechain
21	AA	753	A	Sidechain
21	AA	755	G	Sidechain
21	AA	76	G	Sidechain
21	AA	760	G	Sidechain
21	AA	765	G	Sidechain
21	AA	775	G	Sidechain
21	AA	776	G	Sidechain
21	AA	778	G	Sidechain
21	AA	781	A	Sidechain
21	AA	783	C	Sidechain
21	AA	785	G	Sidechain
21	AA	802	A	Sidechain
21	AA	807	A	Sidechain
21	AA	81	A	Sidechain
21	AA	812	G	Sidechain
21	AA	813	U	Sidechain
21	AA	82	G	Sidechain
21	AA	823	C	Sidechain
21	AA	827	U	Sidechain
21	AA	828	U	Sidechain
21	AA	83	C	Sidechain
21	AA	841	C	Sidechain
21	AA	843	U	Sidechain
21	AA	844	G	Sidechain
21	AA	845	A	Sidechain
21	AA	849	G	Sidechain
21	AA	854	U	Sidechain
21	AA	861	G	Sidechain
21	AA	863	U	Sidechain
21	AA	868	C	Sidechain
21	AA	87	C	Sidechain
21	AA	871	U	Sidechain
21	AA	873	A	Sidechain
21	AA	880	C	Sidechain
21	AA	883	C	Sidechain
21	AA	885	G	Sidechain
21	AA	888	G	Sidechain
21	AA	891	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	898	G	Sidechain
21	AA	90	C	Sidechain
21	AA	903	G	Sidechain
21	AA	909	A	Sidechain
21	AA	91	U	Sidechain
21	AA	917	G	Sidechain
21	AA	922	G	Sidechain
21	AA	925	G	Sidechain
21	AA	926	G	Sidechain
21	AA	928	G	Sidechain
21	AA	929	G	Sidechain
21	AA	932	C	Sidechain
21	AA	933	G	Sidechain
21	AA	935	A	Sidechain
21	AA	936	C	Sidechain
21	AA	94	G	Sidechain
21	AA	941	G	Sidechain
21	AA	944	G	Sidechain
21	AA	945	G	Sidechain
21	AA	946	A	Sidechain
21	AA	962	C	Sidechain
21	AA	963	G	Sidechain
21	AA	964	A	Sidechain
21	AA	965	U	Sidechain
21	AA	971	G	Sidechain
21	AA	973	G	Sidechain
21	AA	98	A	Sidechain
21	AA	987	G	Sidechain
21	AA	988	G	Sidechain
21	AA	989	U	Sidechain
21	AA	99	C	Sidechain
21	AA	993	G	Sidechain
21	AA	994	A	Sidechain
21	AA	995	C	Sidechain
21	AA	998	C	Sidechain
2	AC	172	VAL	Peptide
6	AG	3	ARG	Sidechain
7	AH	76	ARG	Sidechain
52	B3	12	ARG	Sidechain
54	BA	1000	A	Sidechain
54	BA	1007	C	Sidechain
54	BA	1016	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1023	U	Sidechain
54	BA	1025	G	Sidechain
54	BA	1027	A	Sidechain
54	BA	1033	U	Sidechain
54	BA	1040	A	Sidechain
54	BA	1051	G	Sidechain
54	BA	1053	C	Sidechain
54	BA	1056	G	Sidechain
54	BA	1063	G	Sidechain
54	BA	1066	U	Sidechain
54	BA	1074	G	Sidechain
54	BA	1080	A	Sidechain
54	BA	1081	U	Sidechain
54	BA	1083	U	Sidechain
54	BA	1093	G	Sidechain
54	BA	1094	U	Sidechain
54	BA	1096	A	Sidechain
54	BA	1097	U	Sidechain
54	BA	1103	A	Sidechain
54	BA	1106	G	Sidechain
54	BA	1107	G	Sidechain
54	BA	1109	C	Sidechain
54	BA	111	A	Sidechain
54	BA	1115	G	Sidechain
54	BA	112	U	Sidechain
54	BA	1124	G	Sidechain
54	BA	1126	A	Sidechain
54	BA	1136	G	Sidechain
54	BA	1137	G	Sidechain
54	BA	1138	G	Sidechain
54	BA	1139	G	Sidechain
54	BA	114	U	Sidechain
54	BA	1146	C	Sidechain
54	BA	1147	A	Sidechain
54	BA	1151	A	Sidechain
54	BA	1153	C	Sidechain
54	BA	1160	G	Sidechain
54	BA	1164	C	Sidechain
54	BA	1169	A	Sidechain
54	BA	1171	G	Sidechain
54	BA	119	A	Sidechain
54	BA	1198	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1199	U	Sidechain
54	BA	1209	U	Sidechain
54	BA	1211	C	Sidechain
54	BA	1219	U	Sidechain
54	BA	1221	C	Sidechain
54	BA	1223	G	Sidechain
54	BA	1224	U	Sidechain
54	BA	1226	A	Sidechain
54	BA	1229	C	Sidechain
54	BA	123	G	Sidechain
54	BA	1237	A	Sidechain
54	BA	1238	G	Sidechain
54	BA	1241	A	Sidechain
54	BA	1242	U	Sidechain
54	BA	1245	G	Sidechain
54	BA	1248	G	Sidechain
54	BA	1252	G	Sidechain
54	BA	1253	A	Sidechain
54	BA	1257	C	Sidechain
54	BA	1259	G	Sidechain
54	BA	1261	C	Sidechain
54	BA	1263	U	Sidechain
54	BA	1268	A	Sidechain
54	BA	1272	A	Sidechain
54	BA	1275	A	Sidechain
54	BA	1277	G	Sidechain
54	BA	1281	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	1291	C	Sidechain
54	BA	1292	G	Sidechain
54	BA	1294	U	Sidechain
54	BA	1296	G	Sidechain
54	BA	1299	G	Sidechain
54	BA	130	C	Sidechain
54	BA	1312	U	Sidechain
54	BA	132	G	Sidechain
54	BA	1322	A	Sidechain
54	BA	1323	C	Sidechain
54	BA	1324	G	Sidechain
54	BA	1328	A	Sidechain
54	BA	1336	A	Sidechain
54	BA	1338	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	134	G	Sidechain
54	BA	1341	G	Sidechain
54	BA	1343	G	Sidechain
54	BA	1348	C	Sidechain
54	BA	1349	C	Sidechain
54	BA	1352	U	Sidechain
54	BA	1353	A	Sidechain
54	BA	1356	G	Sidechain
54	BA	1362	C	Sidechain
54	BA	1365	A	Sidechain
54	BA	1368	G	Sidechain
54	BA	1372	U	Sidechain
54	BA	1384	A	Sidechain
54	BA	1386	C	Sidechain
54	BA	1387	A	Sidechain
54	BA	1389	G	Sidechain
54	BA	1392	A	Sidechain
54	BA	1398	C	Sidechain
54	BA	1399	C	Sidechain
54	BA	141	G	Sidechain
54	BA	1418	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1427	A	Sidechain
54	BA	1431	A	Sidechain
54	BA	1434	A	Sidechain
54	BA	1437	C	Sidechain
54	BA	1439	A	Sidechain
54	BA	144	A	Sidechain
54	BA	1440	U	Sidechain
54	BA	1441	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1450	G	Sidechain
54	BA	1451	C	Sidechain
54	BA	1453	A	Sidechain
54	BA	1455	G	Sidechain
54	BA	1456	G	Sidechain
54	BA	1458	U	Sidechain
54	BA	1459	G	Sidechain
54	BA	146	A	Sidechain
54	BA	1461	C	Sidechain
54	BA	1465	G	Sidechain
54	BA	1471	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1476	U	Sidechain
54	BA	1477	A	Sidechain
54	BA	1478	G	Sidechain
54	BA	1483	G	Sidechain
54	BA	1488	C	Sidechain
54	BA	1492	G	Sidechain
54	BA	1494	A	Sidechain
54	BA	1495	A	Sidechain
54	BA	1498	C	Sidechain
54	BA	1508	A	Sidechain
54	BA	1523	U	Sidechain
54	BA	1530	G	Sidechain
54	BA	1534	U	Sidechain
54	BA	1535	A	Sidechain
54	BA	1538	G	Sidechain
54	BA	1540	G	Sidechain
54	BA	1546	G	Sidechain
54	BA	1550	C	Sidechain
54	BA	1552	A	Sidechain
54	BA	1553	A	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1562	U	Sidechain
54	BA	1567	G	Sidechain
54	BA	1572	A	Sidechain
54	BA	1573	G	Sidechain
54	BA	1577	C	Sidechain
54	BA	1579	A	Sidechain
54	BA	1580	A	Sidechain
54	BA	1581	G	Sidechain
54	BA	1585	C	Sidechain
54	BA	1593	A	Sidechain
54	BA	1595	C	Sidechain
54	BA	1601	G	Sidechain
54	BA	1608	A	Sidechain
54	BA	1614	A	Sidechain
54	BA	1618	A	Sidechain
54	BA	162	U	Sidechain
54	BA	1620	G	Sidechain
54	BA	1624	U	Sidechain
54	BA	1626	A	Sidechain
54	BA	1628	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1636	U	Sidechain
54	BA	1637	A	Sidechain
54	BA	1641	A	Sidechain
54	BA	1642	G	Sidechain
54	BA	1646	C	Sidechain
54	BA	1647	U	Sidechain
54	BA	1651	G	Sidechain
54	BA	1652	A	Sidechain
54	BA	1653	G	Sidechain
54	BA	1655	A	Sidechain
54	BA	1656	C	Sidechain
54	BA	1657	U	Sidechain
54	BA	1665	A	Sidechain
54	BA	1666	G	Sidechain
54	BA	1667	G	Sidechain
54	BA	1671	U	Sidechain
54	BA	1674	G	Sidechain
54	BA	168	G	Sidechain
54	BA	1680	U	Sidechain
54	BA	1683	U	Sidechain
54	BA	1685	C	Sidechain
54	BA	1693	U	Sidechain
54	BA	1698	A	Sidechain
54	BA	17	G	Sidechain
54	BA	1705	A	Sidechain
54	BA	1706	C	Sidechain
54	BA	1707	G	Sidechain
54	BA	1709	U	Sidechain
54	BA	1713	A	Sidechain
54	BA	1716	U	Sidechain
54	BA	1726	C	Sidechain
54	BA	1728	C	Sidechain
54	BA	1730	C	Sidechain
54	BA	1732	C	Sidechain
54	BA	1738	G	Sidechain
54	BA	1740	G	Sidechain
54	BA	1744	A	Sidechain
54	BA	1750	G	Sidechain
54	BA	1753	G	Sidechain
54	BA	1757	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	176	A	Sidechain
54	BA	1763	G	Sidechain
54	BA	1769	U	Sidechain
54	BA	177	G	Sidechain
54	BA	1773	A	Sidechain
54	BA	1774	C	Sidechain
54	BA	1775	U	Sidechain
54	BA	1782	U	Sidechain
54	BA	1784	A	Sidechain
54	BA	1788	C	Sidechain
54	BA	1790	C	Sidechain
54	BA	1791	A	Sidechain
54	BA	1795	C	Sidechain
54	BA	1797	G	Sidechain
54	BA	180	G	Sidechain
54	BA	1802	A	Sidechain
54	BA	1804	C	Sidechain
54	BA	1805	A	Sidechain
54	BA	1807	G	Sidechain
54	BA	181	A	Sidechain
54	BA	1814	G	Sidechain
54	BA	1816	C	Sidechain
54	BA	1821	A	Sidechain
54	BA	1828	G	Sidechain
54	BA	1831	G	Sidechain
54	BA	1832	C	Sidechain
54	BA	1837	C	Sidechain
54	BA	1839	G	Sidechain
54	BA	1842	G	Sidechain
54	BA	1844	C	Sidechain
54	BA	1847	A	Sidechain
54	BA	1849	G	Sidechain
54	BA	1855	U	Sidechain
54	BA	1860	G	Sidechain
54	BA	1861	G	Sidechain
54	BA	1869	G	Sidechain
54	BA	1881	C	Sidechain
54	BA	1883	U	Sidechain
54	BA	1884	G	Sidechain
54	BA	189	G	Sidechain
54	BA	19	A	Sidechain
54	BA	190	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1906	G	Sidechain
54	BA	1910	G	Sidechain
54	BA	1916	A	Sidechain
54	BA	1927	A	Sidechain
54	BA	1931	U	Sidechain
54	BA	1932	A	Sidechain
54	BA	1933	G	Sidechain
54	BA	1937	A	Sidechain
54	BA	194	G	Sidechain
54	BA	1942	C	Sidechain
54	BA	1950	G	Sidechain
54	BA	1954	G	Sidechain
54	BA	1956	U	Sidechain
54	BA	1958	C	Sidechain
54	BA	1959	G	Sidechain
54	BA	196	A	Sidechain
54	BA	1960	A	Sidechain
54	BA	1969	A	Sidechain
54	BA	1972	G	Sidechain
54	BA	1974	C	Sidechain
54	BA	1979	U	Sidechain
54	BA	2006	C	Sidechain
54	BA	2009	A	Sidechain
54	BA	2014	A	Sidechain
54	BA	2018	G	Sidechain
54	BA	2028	U	Sidechain
54	BA	2029	G	Sidechain
54	BA	2032	G	Sidechain
54	BA	2034	U	Sidechain
54	BA	2035	G	Sidechain
54	BA	2043	C	Sidechain
54	BA	205	G	Sidechain
54	BA	2058	A	Sidechain
54	BA	2063	C	Sidechain
54	BA	2067	G	Sidechain
54	BA	207	A	Sidechain
54	BA	2070	A	Sidechain
54	BA	2086	U	Sidechain
54	BA	2089	C	Sidechain
54	BA	209	C	Sidechain
54	BA	2090	A	Sidechain
54	BA	2091	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2093	G	Sidechain
54	BA	2098	U	Sidechain
54	BA	2106	U	Sidechain
54	BA	2107	G	Sidechain
54	BA	2108	A	Sidechain
54	BA	211	C	Sidechain
54	BA	2112	G	Sidechain
54	BA	2113	U	Sidechain
54	BA	2115	G	Sidechain
54	BA	2120	G	Sidechain
54	BA	2127	G	Sidechain
54	BA	2129	C	Sidechain
54	BA	213	A	Sidechain
54	BA	2132	U	Sidechain
54	BA	2133	G	Sidechain
54	BA	2134	A	Sidechain
54	BA	2137	U	Sidechain
54	BA	2138	G	Sidechain
54	BA	2141	G	Sidechain
54	BA	2143	C	Sidechain
54	BA	2145	C	Sidechain
54	BA	2148	G	Sidechain
54	BA	2149	U	Sidechain
54	BA	2153	C	Sidechain
54	BA	2157	G	Sidechain
54	BA	2159	G	Sidechain
54	BA	2160	C	Sidechain
54	BA	2168	G	Sidechain
54	BA	2180	U	Sidechain
54	BA	2182	U	Sidechain
54	BA	2186	G	Sidechain
54	BA	2189	U	Sidechain
54	BA	2192	U	Sidechain
54	BA	2194	U	Sidechain
54	BA	2200	C	Sidechain
54	BA	2204	G	Sidechain
54	BA	2208	C	Sidechain
54	BA	221	A	Sidechain
54	BA	2211	A	Sidechain
54	BA	2215	C	Sidechain
54	BA	222	A	Sidechain
54	BA	2228	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2230	G	Sidechain
54	BA	2237	G	Sidechain
54	BA	2243	U	Sidechain
54	BA	2246	G	Sidechain
54	BA	2247	A	Sidechain
54	BA	2259	U	Sidechain
54	BA	2260	C	Sidechain
54	BA	2265	U	Sidechain
54	BA	2266	A	Sidechain
54	BA	227	A	Sidechain
54	BA	2282	G	Sidechain
54	BA	2289	G	Sidechain
54	BA	2293	G	Sidechain
54	BA	2296	U	Sidechain
54	BA	2300	C	Sidechain
54	BA	2301	C	Sidechain
54	BA	2305	U	Sidechain
54	BA	231	A	Sidechain
54	BA	2311	A	Sidechain
54	BA	2318	G	Sidechain
54	BA	2325	G	Sidechain
54	BA	2326	C	Sidechain
54	BA	2327	A	Sidechain
54	BA	2331	G	Sidechain
54	BA	2336	A	Sidechain
54	BA	2338	C	Sidechain
54	BA	2342	C	Sidechain
54	BA	2349	G	Sidechain
54	BA	2357	G	Sidechain
54	BA	2358	A	Sidechain
54	BA	2363	G	Sidechain
54	BA	2367	G	Sidechain
54	BA	2375	G	Sidechain
54	BA	2386	A	Sidechain
54	BA	2390	U	Sidechain
54	BA	2391	G	Sidechain
54	BA	2394	C	Sidechain
54	BA	2395	C	Sidechain
54	BA	24	G	Sidechain
54	BA	2402	U	Sidechain
54	BA	2408	U	Sidechain
54	BA	2415	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2428	G	Sidechain
54	BA	243	U	Sidechain
54	BA	244	A	Sidechain
54	BA	2444	G	Sidechain
54	BA	2447	G	Sidechain
54	BA	2448	A	Sidechain
54	BA	2454	G	Sidechain
54	BA	2458	G	Sidechain
54	BA	2460	U	Sidechain
54	BA	247	G	Sidechain
54	BA	2472	G	Sidechain
54	BA	2473	U	Sidechain
54	BA	2474	U	Sidechain
54	BA	2475	C	Sidechain
54	BA	2476	A	Sidechain
54	BA	2477	U	Sidechain
54	BA	2488	G	Sidechain
54	BA	2489	U	Sidechain
54	BA	249	C	Sidechain
54	BA	2491	U	Sidechain
54	BA	2494	G	Sidechain
54	BA	2496	C	Sidechain
54	BA	250	G	Sidechain
54	BA	2500	U	Sidechain
54	BA	2501	C	Sidechain
54	BA	2502	G	Sidechain
54	BA	2505	G	Sidechain
54	BA	2506	U	Sidechain
54	BA	2507	C	Sidechain
54	BA	2516	A	Sidechain
54	BA	2517	C	Sidechain
54	BA	2521	C	Sidechain
54	BA	2529	G	Sidechain
54	BA	2536	G	Sidechain
54	BA	2538	C	Sidechain
54	BA	2540	C	Sidechain
54	BA	2549	G	Sidechain
54	BA	2552	U	Sidechain
54	BA	2553	G	Sidechain
54	BA	2564	A	Sidechain
54	BA	2565	A	Sidechain
54	BA	2566	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2581	G	Sidechain
54	BA	2584	U	Sidechain
54	BA	2586	U	Sidechain
54	BA	2589	A	Sidechain
54	BA	2595	G	Sidechain
54	BA	2600	A	Sidechain
54	BA	2608	G	Sidechain
54	BA	2609	U	Sidechain
54	BA	2618	G	Sidechain
54	BA	2622	U	Sidechain
54	BA	2624	G	Sidechain
54	BA	2628	C	Sidechain
54	BA	2633	G	Sidechain
54	BA	2637	U	Sidechain
54	BA	264	C	Sidechain
54	BA	2645	G	Sidechain
54	BA	2649	C	Sidechain
54	BA	265	A	Sidechain
54	BA	2651	C	Sidechain
54	BA	2655	G	Sidechain
54	BA	2656	U	Sidechain
54	BA	2659	G	Sidechain
54	BA	2664	G	Sidechain
54	BA	2665	A	Sidechain
54	BA	2667	C	Sidechain
54	BA	2669	G	Sidechain
54	BA	2670	A	Sidechain
54	BA	2674	G	Sidechain
54	BA	2677	G	Sidechain
54	BA	268	C	Sidechain
54	BA	2680	U	Sidechain
54	BA	2681	C	Sidechain
54	BA	2682	A	Sidechain
54	BA	2683	C	Sidechain
54	BA	2702	G	Sidechain
54	BA	2706	A	Sidechain
54	BA	2710	C	Sidechain
54	BA	2711	A	Sidechain
54	BA	2712	C	Sidechain
54	BA	2714	G	Sidechain
54	BA	2727	A	Sidechain
54	BA	2729	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2731	G	Sidechain
54	BA	2735	G	Sidechain
54	BA	2751	G	Sidechain
54	BA	2753	A	Sidechain
54	BA	2756	U	Sidechain
54	BA	276	U	Sidechain
54	BA	2760	C	Sidechain
54	BA	2770	G	Sidechain
54	BA	278	A	Sidechain
54	BA	2781	A	Sidechain
54	BA	2784	U	Sidechain
54	BA	2785	C	Sidechain
54	BA	2786	U	Sidechain
54	BA	279	A	Sidechain
54	BA	2794	C	Sidechain
54	BA	2801	G	Sidechain
54	BA	2804	U	Sidechain
54	BA	2808	G	Sidechain
54	BA	2816	G	Sidechain
54	BA	2817	U	Sidechain
54	BA	282	A	Sidechain
54	BA	2822	G	Sidechain
54	BA	2825	G	Sidechain
54	BA	2831	G	Sidechain
54	BA	2835	A	Sidechain
54	BA	2836	U	Sidechain
54	BA	2848	G	Sidechain
54	BA	2857	G	Sidechain
54	BA	2859	G	Sidechain
54	BA	2864	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	2874	C	Sidechain
54	BA	2875	C	Sidechain
54	BA	2876	G	Sidechain
54	BA	2883	A	Sidechain
54	BA	2886	A	Sidechain
54	BA	2889	C	Sidechain
54	BA	2891	U	Sidechain
54	BA	2892	G	Sidechain
54	BA	296	U	Sidechain
54	BA	298	G	Sidechain
54	BA	303	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	304	U	Sidechain
54	BA	307	G	Sidechain
54	BA	308	G	Sidechain
54	BA	311	A	Sidechain
54	BA	313	G	Sidechain
54	BA	314	C	Sidechain
54	BA	318	C	Sidechain
54	BA	319	G	Sidechain
54	BA	323	C	Sidechain
54	BA	331	C	Sidechain
54	BA	332	A	Sidechain
54	BA	333	G	Sidechain
54	BA	34	U	Sidechain
54	BA	341	C	Sidechain
54	BA	354	A	Sidechain
54	BA	360	U	Sidechain
54	BA	363	G	Sidechain
54	BA	364	C	Sidechain
54	BA	365	U	Sidechain
54	BA	372	G	Sidechain
54	BA	379	G	Sidechain
54	BA	381	G	Sidechain
54	BA	387	U	Sidechain
54	BA	392	U	Sidechain
54	BA	394	C	Sidechain
54	BA	395	U	Sidechain
54	BA	4	U	Sidechain
54	BA	401	A	Sidechain
54	BA	406	G	Sidechain
54	BA	418	C	Sidechain
54	BA	419	U	Sidechain
54	BA	422	A	Sidechain
54	BA	423	A	Sidechain
54	BA	424	G	Sidechain
54	BA	434	U	Sidechain
54	BA	439	A	Sidechain
54	BA	44	A	Sidechain
54	BA	440	C	Sidechain
54	BA	446	G	Sidechain
54	BA	45	G	Sidechain
54	BA	450	G	Sidechain
54	BA	452	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	455	C	Sidechain
54	BA	456	C	Sidechain
54	BA	458	G	Sidechain
54	BA	46	G	Sidechain
54	BA	460	A	Sidechain
54	BA	464	U	Sidechain
54	BA	472	A	Sidechain
54	BA	473	G	Sidechain
54	BA	474	G	Sidechain
54	BA	476	G	Sidechain
54	BA	479	A	Sidechain
54	BA	48	G	Sidechain
54	BA	481	G	Sidechain
54	BA	482	A	Sidechain
54	BA	488	G	Sidechain
54	BA	49	A	Sidechain
54	BA	491	G	Sidechain
54	BA	495	G	Sidechain
54	BA	500	G	Sidechain
54	BA	501	A	Sidechain
54	BA	505	A	Sidechain
54	BA	506	G	Sidechain
54	BA	509	C	Sidechain
54	BA	51	G	Sidechain
54	BA	518	G	Sidechain
54	BA	525	U	Sidechain
54	BA	528	A	Sidechain
54	BA	529	A	Sidechain
54	BA	537	G	Sidechain
54	BA	541	A	Sidechain
54	BA	548	G	Sidechain
54	BA	55	G	Sidechain
54	BA	552	U	Sidechain
54	BA	556	A	Sidechain
54	BA	558	U	Sidechain
54	BA	56	A	Sidechain
54	BA	561	G	Sidechain
54	BA	567	U	Sidechain
54	BA	568	U	Sidechain
54	BA	570	G	Sidechain
54	BA	575	A	Sidechain
54	BA	577	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	58	G	Sidechain
54	BA	581	C	Sidechain
54	BA	585	G	Sidechain
54	BA	588	U	Sidechain
54	BA	594	U	Sidechain
54	BA	606	U	Sidechain
54	BA	607	U	Sidechain
54	BA	608	A	Sidechain
54	BA	611	C	Sidechain
54	BA	612	G	Sidechain
54	BA	617	G	Sidechain
54	BA	623	C	Sidechain
54	BA	63	A	Sidechain
54	BA	630	G	Sidechain
54	BA	631	A	Sidechain
54	BA	636	G	Sidechain
54	BA	640	C	Sidechain
54	BA	641	U	Sidechain
54	BA	642	U	Sidechain
54	BA	647	G	Sidechain
54	BA	650	C	Sidechain
54	BA	653	U	Sidechain
54	BA	655	A	Sidechain
54	BA	656	G	Sidechain
54	BA	669	G	Sidechain
54	BA	670	A	Sidechain
54	BA	671	C	Sidechain
54	BA	674	G	Sidechain
54	BA	679	C	Sidechain
54	BA	682	G	Sidechain
54	BA	683	U	Sidechain
54	BA	686	U	Sidechain
54	BA	687	C	Sidechain
54	BA	69	C	Sidechain
54	BA	690	G	Sidechain
54	BA	698	C	Sidechain
54	BA	700	G	Sidechain
54	BA	703	U	Sidechain
54	BA	707	G	Sidechain
54	BA	71	A	Sidechain
54	BA	710	U	Sidechain
54	BA	714	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	721	A	Sidechain
54	BA	724	U	Sidechain
54	BA	726	G	Sidechain
54	BA	727	A	Sidechain
54	BA	728	G	Sidechain
54	BA	729	G	Sidechain
54	BA	732	C	Sidechain
54	BA	74	A	Sidechain
54	BA	742	A	Sidechain
54	BA	744	U	Sidechain
54	BA	748	G	Sidechain
54	BA	759	G	Sidechain
54	BA	768	G	Sidechain
54	BA	77	G	Sidechain
54	BA	772	C	Sidechain
54	BA	775	G	Sidechain
54	BA	777	G	Sidechain
54	BA	779	U	Sidechain
54	BA	792	A	Sidechain
54	BA	795	C	Sidechain
54	BA	800	A	Sidechain
54	BA	802	A	Sidechain
54	BA	809	G	Sidechain
54	BA	811	U	Sidechain
54	BA	820	A	Sidechain
54	BA	823	C	Sidechain
54	BA	827	U	Sidechain
54	BA	828	U	Sidechain
54	BA	83	A	Sidechain
54	BA	833	A	Sidechain
54	BA	834	G	Sidechain
54	BA	837	C	Sidechain
54	BA	845	A	Sidechain
54	BA	846	U	Sidechain
54	BA	847	U	Sidechain
54	BA	85	G	Sidechain
54	BA	852	U	Sidechain
54	BA	858	G	Sidechain
54	BA	859	G	Sidechain
54	BA	86	G	Sidechain
54	BA	864	G	Sidechain
54	BA	868	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	869	G	Sidechain
54	BA	87	U	Sidechain
54	BA	871	U	Sidechain
54	BA	874	G	Sidechain
54	BA	875	G	Sidechain
54	BA	877	A	Sidechain
54	BA	884	U	Sidechain
54	BA	886	A	Sidechain
54	BA	892	A	Sidechain
54	BA	896	A	Sidechain
54	BA	900	A	Sidechain
54	BA	909	A	Sidechain
54	BA	910	A	Sidechain
54	BA	912	C	Sidechain
54	BA	914	G	Sidechain
54	BA	92	U	Sidechain
54	BA	923	G	Sidechain
54	BA	930	G	Sidechain
54	BA	934	U	Sidechain
54	BA	936	A	Sidechain
54	BA	94	A	Sidechain
54	BA	942	G	Sidechain
54	BA	945	A	Sidechain
54	BA	947	A	Sidechain
54	BA	949	G	Sidechain
54	BA	95	A	Sidechain
54	BA	950	G	Sidechain
54	BA	954	G	Sidechain
54	BA	956	G	Sidechain
54	BA	958	U	Sidechain
54	BA	962	G	Sidechain
54	BA	964	C	Sidechain
54	BA	972	A	Sidechain
54	BA	974	G	Sidechain
54	BA	975	A	Sidechain
54	BA	985	C	Sidechain
54	BA	986	C	Sidechain
54	BA	989	G	Sidechain
54	BA	993	G	Sidechain
54	BA	994	C	Sidechain
55	BB	10	G	Sidechain
55	BB	106	G	Sidechain

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Mol	Chain	Res	Type	Group
55	BB	115	A	Sidechain
55	BB	15	A	Sidechain
55	BB	18	G	Sidechain
55	BB	27	C	Sidechain
55	BB	32	U	Sidechain
55	BB	33	G	Sidechain
55	BB	34	A	Sidechain
55	BB	37	C	Sidechain
55	BB	38	C	Sidechain
55	BB	40	U	Sidechain
55	BB	43	C	Sidechain
55	BB	48	U	Sidechain
55	BB	50	A	Sidechain
55	BB	51	G	Sidechain
55	BB	59	A	Sidechain
55	BB	6	G	Sidechain
55	BB	64	G	Sidechain
55	BB	65	U	Sidechain
55	BB	69	G	Sidechain
55	BB	70	C	Sidechain
55	BB	72	G	Sidechain
55	BB	75	G	Sidechain
55	BB	76	G	Sidechain
55	BB	84	G	Sidechain
55	BB	87	U	Sidechain
55	BB	89	U	Sidechain
37	BO	36	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	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	2	0
6	AG	1178	0	1234	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	1	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16520	2	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	1	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	1	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	2	0
39	BQ	947	0	1022	1	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31345	1	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99663	11	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 (11) 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)
28:BF:151:LEU:HD13	28:BF:151:LEU:H	1.75	0.51
9:AJ:57:VAL:HG23	9:AJ:58:ASN:H	1.77	0.50
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.30	0.50
21:AA:565:U:H2'	21:AA:566:G:C8	2.48	0.47
21:AA:940:C:H2'	21:AA:941:G:C8	2.50	0.46
39:BQ:40:LYS:HE3	39:BQ:44:TYR:CZ	2.51	0.45
33:BK:119:ALA:H	33:BK:120:PRO:CD	2.32	0.43
38:BP:30:TRP:CD2	38:BP:37:LYS:HE2	2.53	0.43
54:BA:1256:G:H2'	54:BA:1257:C:C6	2.54	0.42
5:AF:94:HIS:CG	5:AF:95:ALA:N	2.89	0.41
38:BP:30:TRP:CE2	38:BP:37:LYS:HE2	2.55	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	198 (91%)	16 (7%)	4 (2%)	6	34
2	AC	205/208 (99%)	188 (92%)	8 (4%)	9 (4%)	2	17
3	AD	203/206 (98%)	182 (90%)	18 (9%)	3 (2%)	8	40
4	AE	150/152 (99%)	136 (91%)	8 (5%)	6 (4%)	2	18
5	AF	99/101 (98%)	84 (85%)	9 (9%)	6 (6%)	1	13
6	AG	150/152 (99%)	130 (87%)	14 (9%)	6 (4%)	2	18
7	AH	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	16	54
8	AI	126/128 (98%)	115 (91%)	9 (7%)	2 (2%)	7	38
9	AJ	98/100 (98%)	92 (94%)	2 (2%)	4 (4%)	2	18
10	AK	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	14	51
11	AL	121/124 (98%)	107 (88%)	13 (11%)	1 (1%)	16	54
12	AM	112/115 (97%)	98 (88%)	9 (8%)	5 (4%)	2	17
13	AN	98/101 (97%)	87 (89%)	10 (10%)	1 (1%)	12	49
14	AO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	44
15	AP	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	9	42
16	AQ	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	4	26
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	6	34
18	AS	79/81 (98%)	67 (85%)	9 (11%)	3 (4%)	2	19
19	AT	84/86 (98%)	78 (93%)	4 (5%)	2 (2%)	4	27
20	AU	51/53 (96%)	33 (65%)	14 (28%)	4 (8%)	1	10
25	BC	270/273 (99%)	237 (88%)	25 (9%)	8 (3%)	3	23
26	BD	207/209 (99%)	181 (87%)	17 (8%)	9 (4%)	2	17
27	BE	199/201 (99%)	180 (90%)	12 (6%)	7 (4%)	3	20
28	BF	176/179 (98%)	161 (92%)	8 (4%)	7 (4%)	2	18
29	BG	174/177 (98%)	158 (91%)	11 (6%)	5 (3%)	3	23
30	BH	147/149 (99%)	129 (88%)	15 (10%)	3 (2%)	6	31
31	BI	139/142 (98%)	132 (95%)	7 (5%)	0	100	100
32	BJ	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	2	20
33	BK	121/123 (98%)	103 (85%)	12 (10%)	6 (5%)	1	16
34	BL	141/144 (98%)	122 (86%)	10 (7%)	9 (6%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BM	134/136 (98%)	121 (90%)	8 (6%)	5 (4%)	2	20
36	BN	119/121 (98%)	101 (85%)	17 (14%)	1 (1%)	16	54
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	14	51
38	BP	112/115 (97%)	99 (88%)	10 (9%)	3 (3%)	4	25
39	BQ	115/118 (98%)	105 (91%)	7 (6%)	3 (3%)	4	25
40	BR	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	6	31
41	BS	108/110 (98%)	96 (89%)	8 (7%)	4 (4%)	2	20
42	BT	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	5	29
43	BU	101/104 (97%)	79 (78%)	16 (16%)	6 (6%)	1	13
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	64 (82%)	12 (15%)	2 (3%)	4	25
46	BX	75/79 (95%)	69 (92%)	6 (8%)	0	100	100
47	BY	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	7	38
48	BZ	56/59 (95%)	47 (84%)	4 (7%)	5 (9%)	0	8
49	B0	54/57 (95%)	50 (93%)	2 (4%)	2 (4%)	2	20
50	B1	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	6	31
51	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
52	B3	62/65 (95%)	50 (81%)	8 (13%)	4 (6%)	1	12
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	205 (93%)	15 (7%)	1 (0%)	24	63
All	All	5876/6008 (98%)	5258 (90%)	453 (8%)	165 (3%)	6	24

All (165) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	206	ILE
2	AC	4	VAL
3	AD	54	LEU
4	AE	105	ILE
5	AF	59	TYR
6	AG	11	ILE
13	AN	63	ARG
18	AS	22	VAL
18	AS	79	TYR
26	BD	2	ILE

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Mol	Chain	Res	Type
26	BD	51	THR
26	BD	77	ARG
26	BD	150	GLN
27	BE	70	SER
27	BE	79	ARG
28	BF	12	VAL
28	BF	103	ILE
30	BH	121	VAL
33	BK	32	TYR
33	BK	119	ALA
34	BL	21	ARG
34	BL	101	ILE
35	BM	36	VAL
42	BT	70	HIS
43	BU	57	ILE
1	AB	87	ASP
5	AF	10	VAL
6	AG	5	VAL
6	AG	56	SER
6	AG	129	ASN
7	AH	77	VAL
8	AI	117	LEU
9	AJ	75	ASP
12	AM	11	HIS
12	AM	22	TYR
19	AT	3	ILE
20	AU	34	ARG
25	BC	136	VAL
26	BD	34	VAL
27	BE	94	GLN
27	BE	147	LEU
28	BF	136	ILE
30	BH	29	PHE
30	BH	67	ALA
34	BL	29	LYS
38	BP	32	VAL
38	BP	109	ILE
39	BQ	86	SER
39	BQ	87	VAL
40	BR	80	ARG
43	BU	43	LYS
48	BZ	3	THR

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Mol	Chain	Res	Type
48	BZ	4	ILE
48	BZ	31	ILE
49	B0	13	GLY
52	B3	3	ILE
2	AC	159	ALA
2	AC	195	ILE
4	AE	103	GLY
5	AF	65	GLU
6	AG	60	ALA
6	AG	114	SER
8	AI	128	LYS
16	AQ	64	ARG
19	AT	42	ASP
25	BC	37	SER
25	BC	123	ILE
25	BC	191	LEU
25	BC	235	GLU
26	BD	20	VAL
26	BD	201	LEU
27	BE	11	ALA
28	BF	46	LYS
29	BG	22	VAL
29	BG	113	ASP
32	BJ	15	TRP
34	BL	16	GLY
34	BL	65	GLY
35	BM	21	ALA
38	BP	74	GLN
41	BS	90	LYS
43	BU	45	GLN
45	BW	38	ARG
50	B1	6	GLU
1	AB	36	LYS
2	AC	65	VAL
2	AC	100	ILE
3	AD	28	ASP
4	AE	54	GLU
4	AE	104	ILE
4	AE	127	TYR
5	AF	82	ASP
5	AF	98	GLU
9	AJ	5	ARG

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Mol	Chain	Res	Type
9	AJ	57	VAL
10	AK	12	ARG
11	AL	15	VAL
12	AM	104	ASN
12	AM	112	ARG
14	AO	86	LEU
15	AP	9	HIS
20	AU	47	ALA
25	BC	196	ASN
26	BD	55	LYS
27	BE	55	SER
27	BE	96	VAL
29	BG	8	VAL
29	BG	151	ARG
32	BJ	81	ILE
33	BK	103	VAL
33	BK	110	GLU
34	BL	36	LYS
35	BM	62	LYS
35	BM	133	LYS
37	BO	23	ALA
39	BQ	10	ARG
40	BR	53	PHE
43	BU	74	ALA
48	BZ	9	THR
52	B3	31	ILE
2	AC	167	TYR
5	AF	6	ILE
12	AM	103	THR
18	AS	80	ARG
25	BC	99	GLU
26	BD	43	ASP
28	BF	122	ASP
28	BF	148	VAL
32	BJ	45	THR
32	BJ	64	VAL
36	BN	80	PHE
41	BS	33	LEU
41	BS	92	ARG
42	BT	2	ILE
43	BU	5	ARG
43	BU	40	LEU

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Mol	Chain	Res	Type
47	BY	37	LEU
49	B0	27	LEU
52	B3	50	SER
56	B5	217	THR
3	AD	82	LYS
16	AQ	15	LYS
17	AR	20	ILE
34	BL	5	THR
34	BL	85	VAL
45	BW	70	VAL
4	AE	43	GLY
20	AU	27	VAL
33	BK	93	GLN
34	BL	55	MET
41	BS	96	ILE
48	BZ	32	GLY
1	AB	185	ILE
2	AC	172	VAL
2	AC	194	VAL
9	AJ	42	LEU
25	BC	2	VAL
32	BJ	48	VAL
2	AC	206	ILE
20	AU	5	VAL
28	BF	123	GLY
33	BK	47	ILE
29	BG	116	LEU
35	BM	126	ILE
52	B3	44	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AB	180/180 (100%)	174 (97%)	6 (3%)	33 55
2	AC	170/171 (99%)	166 (98%)	4 (2%)	43 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	172/173 (99%)	169 (98%)	3 (2%)	53	69
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%)	120 (98%)	3 (2%)	43	64
7	AH	104/105 (99%)	103 (99%)	1 (1%)	68	78
8	AI	105/105 (100%)	103 (98%)	2 (2%)	50	67
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	89 (99%)	1 (1%)	65	76
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	82 (99%)	1 (1%)	63	75
14	AO	76/77 (99%)	74 (97%)	2 (3%)	40	62
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	208 (96%)	8 (4%)	30	51
26	BD	164/164 (100%)	161 (98%)	3 (2%)	51	68
27	BE	165/165 (100%)	164 (99%)	1 (1%)	78	83
28	BF	149/150 (99%)	146 (98%)	3 (2%)	48	66
29	BG	137/138 (99%)	134 (98%)	3 (2%)	45	64
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	107 (98%)	2 (2%)	51	68
32	BJ	116/116 (100%)	115 (99%)	1 (1%)	70	79
33	BK	103/103 (100%)	101 (98%)	2 (2%)	50	67
34	BL	102/103 (99%)	102 (100%)	0	100	100
35	BM	109/109 (100%)	106 (97%)	3 (3%)	38	60
36	BN	100/100 (100%)	99 (99%)	1 (1%)	68	78
37	BO	86/87 (99%)	84 (98%)	2 (2%)	44	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BP	99/100 (99%)	97 (98%)	2 (2%)	48	66
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	65	76
40	BR	84/84 (100%)	84 (100%)	0	100	100
41	BS	93/93 (100%)	91 (98%)	2 (2%)	45	64
42	BT	80/80 (100%)	79 (99%)	1 (1%)	61	74
43	BU	83/84 (99%)	82 (99%)	1 (1%)	63	75
44	BV	78/78 (100%)	77 (99%)	1 (1%)	61	74
45	BW	59/59 (100%)	57 (97%)	2 (3%)	32	54
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	47	65
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	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%)	4773 (99%)	69 (1%)	57	72

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	22	TRP
1	AB	63	LYS
1	AB	77	GLU
1	AB	88	GLN
1	AB	99	MET
1	AB	129	THR
2	AC	11	LEU
2	AC	35	ASP
2	AC	133	MET
2	AC	200	TRP
3	AD	39	GLN
3	AD	139	ASN
3	AD	194	ILE
4	AE	152	VAL

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Mol	Chain	Res	Type
5	AF	52	ASN
6	AG	11	ILE
6	AG	14	ASP
6	AG	59	GLU
7	AH	104	SER
8	AI	38	PHE
8	AI	41	GLU
10	AK	100	ASN
13	AN	98	LYS
14	AO	48	ASP
14	AO	86	LEU
25	BC	22	GLU
25	BC	49	THR
25	BC	139	THR
25	BC	161	VAL
25	BC	175	LEU
25	BC	179	GLU
25	BC	191	LEU
25	BC	204	LEU
26	BD	16	THR
26	BD	43	ASP
26	BD	148	GLN
27	BE	78	TRP
28	BF	15	LEU
28	BF	134	GLN
28	BF	151	LEU
29	BG	33	THR
29	BG	97	VAL
29	BG	120	ILE
31	BI	20	SER
31	BI	50	LYS
32	BJ	81	ILE
33	BK	32	TYR
33	BK	47	ILE
35	BM	16	ARG
35	BM	97	GLN
35	BM	129	THR
36	BN	33	ILE
37	BO	38	GLN
37	BO	117	PHE
38	BP	50	ARG
38	BP	85	VAL

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Mol	Chain	Res	Type
39	BQ	71	ASN
41	BS	1	MET
41	BS	70	LYS
42	BT	34	VAL
43	BU	40	LEU
44	BV	51	GLN
45	BW	49	ASN
45	BW	80	SER
49	B0	2	VAL
51	B2	19	ARG
52	B3	33	THR
56	B5	165	ASN
56	B5	217	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	177	ASN
2	AC	2	GLN
3	AD	39	GLN
3	AD	135	GLN
4	AE	11	GLN
4	AE	72	ASN
5	AF	14	GLN
6	AG	51	GLN
7	AH	20	ASN
9	AJ	70	HIS
10	AK	80	ASN
10	AK	100	ASN
11	AL	19	ASN
12	AM	7	ASN
14	AO	49	HIS
14	AO	79	GLN
15	AP	18	GLN
16	AQ	8	GLN
16	AQ	44	HIS
17	AR	53	GLN
18	AS	51	HIS
19	AT	51	ASN
19	AT	54	GLN
19	AT	60	GLN
19	AT	67	HIS

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Mol	Chain	Res	Type
19	AT	83	ASN
25	BC	59	GLN
25	BC	85	ASN
25	BC	133	ASN
25	BC	196	ASN
26	BD	49	GLN
26	BD	130	GLN
26	BD	140	HIS
28	BF	51	ASN
30	BH	2	GLN
30	BH	18	GLN
30	BH	66	ASN
30	BH	119	ASN
30	BH	145	ASN
31	BI	110	GLN
35	BM	97	GLN
36	BN	3	HIS
36	BN	16	HIS
37	BO	29	HIS
37	BO	104	GLN
41	BS	31	GLN
41	BS	57	ASN
42	BT	72	GLN
44	BV	80	HIS
44	BV	87	GLN
45	BW	39	GLN
47	BY	36	GLN
47	BY	39	GLN
48	BZ	8	GLN
49	B0	5	ASN
49	B0	18	HIS
49	B0	37	HIS
51	B2	13	ASN
51	B2	26	ASN
53	B4	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	268 (17%)	86 (5%)
22	A1	75/76 (98%)	15 (20%)	5 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	A2	15/15 (100%)	5 (33%)	4 (26%)
24	A3	76/77 (98%)	19 (25%)	6 (7%)
54	BA	2902/2903 (99%)	485 (16%)	117 (4%)
55	BB	116/118 (98%)	18 (15%)	4 (3%)
All	All	4713/4722 (99%)	810 (17%)	222 (4%)

All (810) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	27	G
21	AA	28	A
21	AA	32	A
21	AA	35	G
21	AA	36	C
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	49	U
21	AA	50	A
21	AA	51	A
21	AA	55	A
21	AA	56	U
21	AA	61	G
21	AA	66	A
21	AA	67	C
21	AA	69	G
21	AA	70	U
21	AA	86	G
21	AA	87	C
21	AA	95	C
21	AA	108	G
21	AA	109	A
21	AA	120	A
21	AA	124	C
21	AA	130	A
21	AA	131	A
21	AA	144	G
21	AA	159	G
21	AA	164	G
21	AA	165	G
21	AA	180	U

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Mol	Chain	Res	Type
21	AA	183	C
21	AA	190	A
21	AA	191	G
21	AA	198	G
21	AA	211	G
21	AA	214	C
21	AA	227	G
21	AA	228	A
21	AA	240	G
21	AA	244	U
21	AA	247	G
21	AA	251	G
21	AA	252	U
21	AA	258	G
21	AA	259	G
21	AA	266	G
21	AA	268	U
21	AA	269	C
21	AA	282	A
21	AA	289	G
21	AA	290	C
21	AA	305	G
21	AA	306	A
21	AA	308	C
21	AA	316	C
21	AA	328	C
21	AA	329	A
21	AA	345	C
21	AA	352	C
21	AA	353	A
21	AA	354	G
21	AA	367	U
21	AA	368	U
21	AA	369	G
21	AA	372	C
21	AA	373	A
21	AA	381	C
21	AA	382	A
21	AA	383	A
21	AA	392	C
21	AA	397	A
21	AA	406	G

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Mol	Chain	Res	Type
21	AA	412	A
21	AA	413	G
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	462	G
21	AA	463	U
21	AA	465	A
21	AA	466	A
21	AA	468	A
21	AA	493	A
21	AA	499	A
21	AA	505	G
21	AA	506	G
21	AA	511	C
21	AA	518	C
21	AA	519	C
21	AA	520	A
21	AA	524	G
21	AA	525	C
21	AA	527	G
21	AA	532	A
21	AA	547	A
21	AA	559	A
21	AA	560	A
21	AA	561	U
21	AA	563	A
21	AA	564	C
21	AA	565	U
21	AA	570	G
21	AA	571	U
21	AA	573	A
21	AA	576	C
21	AA	589	U
21	AA	607	A
21	AA	608	A
21	AA	615	G
21	AA	632	U
21	AA	633	G
21	AA	653	U
21	AA	659	U
21	AA	660	C

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Mol	Chain	Res	Type
21	AA	665	A
21	AA	687	A
21	AA	700	G
21	AA	704	A
21	AA	705	G
21	AA	755	G
21	AA	761	G
21	AA	762	U
21	AA	764	C
21	AA	765	G
21	AA	777	A
21	AA	778	G
21	AA	779	C
21	AA	794	A
21	AA	812	G
21	AA	816	A
21	AA	828	U
21	AA	841	C
21	AA	842	U
21	AA	843	U
21	AA	844	G
21	AA	845	A
21	AA	846	G
21	AA	913	A
21	AA	914	A
21	AA	926	G
21	AA	927	G
21	AA	932	C
21	AA	933	G
21	AA	934	C
21	AA	935	A
21	AA	939	G
21	AA	942	G
21	AA	944	G
21	AA	959	A
21	AA	960	U
21	AA	961	U
21	AA	966	G
21	AA	968	A
21	AA	971	G
21	AA	976	G
21	AA	977	A

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Mol	Chain	Res	Type
21	AA	980	C
21	AA	981	U
21	AA	991	U
21	AA	993	G
21	AA	996	A
21	AA	1003	G
21	AA	1004	A
21	AA	1006	G
21	AA	1025	U
21	AA	1026	G
21	AA	1029	U
21	AA	1030	U
21	AA	1032	G
21	AA	1033	G
21	AA	1053	G
21	AA	1054	C
21	AA	1065	U
21	AA	1081	A
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1112	C
21	AA	1113	C
21	AA	1124	G
21	AA	1125	U
21	AA	1130	A
21	AA	1137	C
21	AA	1139	G
21	AA	1143	G
21	AA	1152	A
21	AA	1153	G
21	AA	1159	U
21	AA	1167	A
21	AA	1168	U
21	AA	1183	U
21	AA	1184	G
21	AA	1189	U
21	AA	1190	G
21	AA	1191	A
21	AA	1195	C
21	AA	1196	A

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Mol	Chain	Res	Type
21	AA	1197	A
21	AA	1200	C
21	AA	1201	A
21	AA	1202	U
21	AA	1212	U
21	AA	1213	A
21	AA	1215	G
21	AA	1224	U
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1228	C
21	AA	1229	A
21	AA	1240	U
21	AA	1256	A
21	AA	1257	A
21	AA	1264	U
21	AA	1265	C
21	AA	1279	G
21	AA	1280	A
21	AA	1282	C
21	AA	1285	A
21	AA	1286	U
21	AA	1300	G
21	AA	1301	U
21	AA	1303	C
21	AA	1304	G
21	AA	1305	G
21	AA	1306	A
21	AA	1312	G
21	AA	1320	C
21	AA	1324	A
21	AA	1325	C
21	AA	1335	U
21	AA	1336	C
21	AA	1337	G
21	AA	1342	C
21	AA	1343	G
21	AA	1346	A
21	AA	1347	G
21	AA	1378	C
21	AA	1379	G

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Mol	Chain	Res	Type
21	AA	1381	U
21	AA	1423	G
21	AA	1429	A
21	AA	1430	A
21	AA	1431	A
21	AA	1432	G
21	AA	1446	A
21	AA	1451	U
21	AA	1452	C
21	AA	1459	G
21	AA	1460	C
21	AA	1468	A
21	AA	1481	U
21	AA	1499	A
21	AA	1502	A
21	AA	1503	A
21	AA	1504	G
21	AA	1505	G
21	AA	1506	U
21	AA	1516	G
21	AA	1517	G
21	AA	1529	G
21	AA	1530	G
21	AA	1533	C
21	AA	1534	A
22	A1	7	4SU
22	A1	8	U
22	A1	16	C
22	A1	17	U
22	A1	19	G
22	A1	21	A
22	A1	25	C
22	A1	47	U
22	A1	56	C
22	A1	57	G
22	A1	59	U
22	A1	60	C
22	A1	61	C
22	A1	75	C
22	A1	76	A
23	A2	80	C
23	A2	81	U

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Mol	Chain	Res	Type
23	A2	89	U
23	A2	91	A
23	A2	93	U
24	A3	2	G
24	A3	3	C
24	A3	10	G
24	A3	11	A
24	A3	18	U
24	A3	20	G
24	A3	25	U
24	A3	40	C
24	A3	43	G
24	A3	48	U
24	A3	49	C
24	A3	61	U
24	A3	62	C
24	A3	64	G
24	A3	65	G
24	A3	73	A
24	A3	74	A
24	A3	75	C
24	A3	77	A
54	BA	12	U
54	BA	20	C
54	BA	34	U
54	BA	45	G
54	BA	60	G
54	BA	61	C
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	83	A
54	BA	88	G
54	BA	91	A
54	BA	100	U
54	BA	101	A
54	BA	102	U
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G

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Mol	Chain	Res	Type
54	BA	125	A
54	BA	126	A
54	BA	138	U
54	BA	139	U
54	BA	147	C
54	BA	163	C
54	BA	164	C
54	BA	181	A
54	BA	196	A
54	BA	199	A
54	BA	200	U
54	BA	204	A
54	BA	216	A
54	BA	222	A
54	BA	230	G
54	BA	233	A
54	BA	242	G
54	BA	248	G
54	BA	255	A
54	BA	256	A
54	BA	266	G
54	BA	272	A
54	BA	273	G
54	BA	276	U
54	BA	277	G
54	BA	278	A
54	BA	279	A
54	BA	280	U
54	BA	294	A
54	BA	302	C
54	BA	316	C
54	BA	321	U
54	BA	322	A
54	BA	323	C
54	BA	324	A
54	BA	330	A
54	BA	332	A
54	BA	333	G
54	BA	334	C
54	BA	346	A
54	BA	370	G
54	BA	372	G

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Mol	Chain	Res	Type
54	BA	373	U
54	BA	374	A
54	BA	386	G
54	BA	390	U
54	BA	396	G
54	BA	411	G
54	BA	412	A
54	BA	413	C
54	BA	428	A
54	BA	429	A
54	BA	451	U
54	BA	452	G
54	BA	453	A
54	BA	454	A
54	BA	455	C
54	BA	457	A
54	BA	470	A
54	BA	471	A
54	BA	475	C
54	BA	482	A
54	BA	483	A
54	BA	484	C
54	BA	501	A
54	BA	502	A
54	BA	504	A
54	BA	505	A
54	BA	509	C
54	BA	510	C
54	BA	520	G
54	BA	527	C
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	547	A
54	BA	548	G
54	BA	562	U
54	BA	563	A
54	BA	569	U
54	BA	573	U

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Mol	Chain	Res	Type
54	BA	574	A
54	BA	590	A
54	BA	603	A
54	BA	615	U
54	BA	637	A
54	BA	644	A
54	BA	653	U
54	BA	654	A
54	BA	655	A
54	BA	670	A
54	BA	671	C
54	BA	672	C
54	BA	685	A
54	BA	686	U
54	BA	723	C
54	BA	728	G
54	BA	730	A
54	BA	745	G
54	BA	747	U
54	BA	748	G
54	BA	750	A
54	BA	751	A
54	BA	752	A
54	BA	758	C
54	BA	764	A
54	BA	775	G
54	BA	776	G
54	BA	782	A
54	BA	785	G
54	BA	789	A
54	BA	790	U
54	BA	791	C
54	BA	792	A
54	BA	801	G
54	BA	804	A
54	BA	805	G
54	BA	811	U
54	BA	812	C
54	BA	824	U
54	BA	827	U
54	BA	846	U
54	BA	869	G

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Mol	Chain	Res	Type
54	BA	889	C
54	BA	890	C
54	BA	891	G
54	BA	897	C
54	BA	908	C
54	BA	910	A
54	BA	915	C
54	BA	932	U
54	BA	933	A
54	BA	941	A
54	BA	945	A
54	BA	946	C
54	BA	947	A
54	BA	951	C
54	BA	961	C
54	BA	962	G
54	BA	974	G
54	BA	975	A
54	BA	977	G
54	BA	983	A
54	BA	990	A
54	BA	1012	U
54	BA	1013	C
54	BA	1017	G
54	BA	1022	G
54	BA	1026	G
54	BA	1028	A
54	BA	1033	U
54	BA	1034	G
54	BA	1044	C
54	BA	1045	C
54	BA	1046	A
54	BA	1055	G
54	BA	1063	G
54	BA	1070	A
54	BA	1071	G
54	BA	1072	C
54	BA	1073	A
54	BA	1076	C
54	BA	1088	A
54	BA	1089	A
54	BA	1090	A

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Mol	Chain	Res	Type
54	BA	1091	G
54	BA	1096	A
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	1148	U
54	BA	1157	G
54	BA	1158	C
54	BA	1176	U
54	BA	1177	G
54	BA	1189	A
54	BA	1204	A
54	BA	1210	G
54	BA	1211	C
54	BA	1220	G
54	BA	1224	U
54	BA	1230	A
54	BA	1236	G
54	BA	1237	A
54	BA	1253	A
54	BA	1266	G
54	BA	1271	G
54	BA	1272	A
54	BA	1273	U
54	BA	1276	A
54	BA	1292	G
54	BA	1300	G
54	BA	1301	A
54	BA	1302	A
54	BA	1303	G
54	BA	1313	U
54	BA	1314	C
54	BA	1332	G
54	BA	1341	G
54	BA	1348	C
54	BA	1365	A
54	BA	1366	A

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Mol	Chain	Res	Type
54	BA	1368	G
54	BA	1378	A
54	BA	1379	U
54	BA	1383	A
54	BA	1384	A
54	BA	1385	A
54	BA	1396	U
54	BA	1397	U
54	BA	1398	C
54	BA	1416	G
54	BA	1417	C
54	BA	1419	A
54	BA	1420	A
54	BA	1421	G
54	BA	1427	A
54	BA	1439	A
54	BA	1440	U
54	BA	1451	C
54	BA	1452	G
54	BA	1455	G
54	BA	1458	U
54	BA	1476	U
54	BA	1477	A
54	BA	1482	G
54	BA	1490	A
54	BA	1491	G
54	BA	1497	U
54	BA	1508	A
54	BA	1511	G
54	BA	1538	G
54	BA	1539	U
54	BA	1540	G
54	BA	1541	C
54	BA	1566	A
54	BA	1569	A
54	BA	1578	U
54	BA	1585	C
54	BA	1598	A
54	BA	1602	U
54	BA	1603	A
54	BA	1608	A
54	BA	1616	A

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Mol	Chain	Res	Type
54	BA	1618	A
54	BA	1622	G
54	BA	1625	C
54	BA	1626	A
54	BA	1639	C
54	BA	1646	C
54	BA	1648	U
54	BA	1664	A
54	BA	1665	A
54	BA	1669	A
54	BA	1670	C
54	BA	1674	G
54	BA	1701	A
54	BA	1713	A
54	BA	1714	U
54	BA	1715	G
54	BA	1730	C
54	BA	1731	G
54	BA	1733	G
54	BA	1739	A
54	BA	1745	A
54	BA	1758	U
54	BA	1764	C
54	BA	1773	A
54	BA	1776	G
54	BA	1786	A
54	BA	1787	A
54	BA	1788	C
54	BA	1800	C
54	BA	1801	A
54	BA	1808	A
54	BA	1816	C
54	BA	1821	A
54	BA	1829	A
54	BA	1848	A
54	BA	1900	A
54	BA	1901	A
54	BA	1906	G
54	BA	1913	A
54	BA	1914	C
54	BA	1920	C
54	BA	1931	U

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Mol	Chain	Res	Type
54	BA	1936	A
54	BA	1937	A
54	BA	1940	U
54	BA	1941	C
54	BA	1942	C
54	BA	1943	U
54	BA	1953	A
54	BA	1965	C
54	BA	1966	A
54	BA	1967	C
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1981	A
54	BA	1991	U
54	BA	1993	U
54	BA	1997	C
54	BA	2020	A
54	BA	2021	C
54	BA	2022	U
54	BA	2023	C
54	BA	2030	A
54	BA	2031	A
54	BA	2032	G
54	BA	2033	A
54	BA	2034	U
54	BA	2037	A
54	BA	2043	C
54	BA	2053	G
54	BA	2055	C
54	BA	2061	G
54	BA	2069	G
54	BA	2077	A
54	BA	2092	U
54	BA	2111	U
54	BA	2113	U
54	BA	2116	G
54	BA	2117	A
54	BA	2119	A
54	BA	2127	G
54	BA	2133	G
54	BA	2138	G

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Mol	Chain	Res	Type
54	BA	2159	G
54	BA	2160	C
54	BA	2164	C
54	BA	2165	C
54	BA	2173	A
54	BA	2174	C
54	BA	2181	U
54	BA	2198	A
54	BA	2203	U
54	BA	2204	G
54	BA	2211	A
54	BA	2212	A
54	BA	2213	U
54	BA	2225	A
54	BA	2238	G
54	BA	2250	G
54	BA	2251	G
54	BA	2267	A
54	BA	2269	G
54	BA	2270	A
54	BA	2275	C
54	BA	2283	C
54	BA	2286	G
54	BA	2287	A
54	BA	2296	U
54	BA	2297	A
54	BA	2305	U
54	BA	2309	A
54	BA	2310	C
54	BA	2311	A
54	BA	2312	U
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2332	C
54	BA	2333	A
54	BA	2334	U
54	BA	2335	A
54	BA	2339	C
54	BA	2345	G
54	BA	2346	A

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Mol	Chain	Res	Type
54	BA	2347	C
54	BA	2353	G
54	BA	2383	G
54	BA	2385	C
54	BA	2386	A
54	BA	2389	G
54	BA	2390	U
54	BA	2391	G
54	BA	2392	A
54	BA	2402	U
54	BA	2403	C
54	BA	2406	A
54	BA	2423	U
54	BA	2426	A
54	BA	2428	G
54	BA	2429	G
54	BA	2430	A
54	BA	2431	U
54	BA	2432	A
54	BA	2441	U
54	BA	2447	G
54	BA	2448	A
54	BA	2449	U
54	BA	2469	A
54	BA	2491	U
54	BA	2496	C
54	BA	2499	C
54	BA	2502	G
54	BA	2503	A
54	BA	2504	U
54	BA	2505	G
54	BA	2506	U
54	BA	2518	A
54	BA	2520	C
54	BA	2540	C
54	BA	2548	U
54	BA	2554	U
54	BA	2564	A
54	BA	2565	A
54	BA	2566	A
54	BA	2567	G
54	BA	2573	C

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Mol	Chain	Res	Type
54	BA	2576	G
54	BA	2578	G
54	BA	2596	U
54	BA	2602	A
54	BA	2603	G
54	BA	2609	U
54	BA	2610	C
54	BA	2613	U
54	BA	2615	U
54	BA	2616	C
54	BA	2645	G
54	BA	2646	C
54	BA	2655	G
54	BA	2669	G
54	BA	2683	C
54	BA	2689	U
54	BA	2690	U
54	BA	2707	U
54	BA	2709	G
54	BA	2718	G
54	BA	2726	A
54	BA	2727	A
54	BA	2729	G
54	BA	2751	G
54	BA	2755	C
54	BA	2761	A
54	BA	2765	A
54	BA	2766	A
54	BA	2777	G
54	BA	2778	A
54	BA	2779	U
54	BA	2780	G
54	BA	2781	A
54	BA	2791	G
54	BA	2797	U
54	BA	2798	U
54	BA	2799	A
54	BA	2801	G
54	BA	2816	G
54	BA	2823	A
54	BA	2850	A
54	BA	2868	A

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Mol	Chain	Res	Type
54	BA	2876	G
54	BA	2884	U
54	BA	2895	G
55	BB	13	G
55	BB	15	A
55	BB	16	G
55	BB	34	A
55	BB	35	C
55	BB	36	C
55	BB	42	C
55	BB	44	G
55	BB	45	A
55	BB	48	U
55	BB	51	G
55	BB	52	A
55	BB	67	G
55	BB	88	C
55	BB	89	U
55	BB	107	G
55	BB	108	A
55	BB	109	A

All (222) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	54	C
21	AA	55	A
21	AA	60	A
21	AA	66	A
21	AA	69	G
21	AA	70	U
21	AA	86	G
21	AA	164	G
21	AA	190	A
21	AA	227	G
21	AA	251	G
21	AA	258	G
21	AA	268	U
21	AA	289	G
21	AA	305	G
21	AA	327	A
21	AA	328	C

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Mol	Chain	Res	Type
21	AA	352	C
21	AA	354	G
21	AA	368	U
21	AA	382	A
21	AA	406	G
21	AA	461	A
21	AA	465	A
21	AA	505	G
21	AA	518	C
21	AA	519	C
21	AA	524	G
21	AA	563	A
21	AA	570	G
21	AA	575	G
21	AA	576	C
21	AA	607	A
21	AA	641	U
21	AA	659	U
21	AA	704	A
21	AA	761	G
21	AA	764	C
21	AA	778	G
21	AA	815	A
21	AA	827	U
21	AA	841	C
21	AA	843	U
21	AA	913	A
21	AA	932	C
21	AA	933	G
21	AA	959	A
21	AA	960	U
21	AA	978	A
21	AA	980	C
21	AA	991	U
21	AA	1003	G
21	AA	1025	U
21	AA	1029	U
21	AA	1032	G
21	AA	1053	G
21	AA	1101	A
21	AA	1112	C
21	AA	1124	G

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Mol	Chain	Res	Type
21	AA	1129	C
21	AA	1152	A
21	AA	1181	G
21	AA	1183	U
21	AA	1190	G
21	AA	1195	C
21	AA	1200	C
21	AA	1201	A
21	AA	1215	G
21	AA	1225	A
21	AA	1227	A
21	AA	1278	G
21	AA	1279	G
21	AA	1303	C
21	AA	1305	G
21	AA	1324	A
21	AA	1335	U
21	AA	1336	C
21	AA	1342	C
21	AA	1377	A
21	AA	1411	C
21	AA	1429	A
21	AA	1431	A
21	AA	1451	U
21	AA	1459	G
21	AA	1480	A
21	AA	1529	G
22	A1	7	4SU
22	A1	10	G
22	A1	56	C
22	A1	60	C
22	A1	75	C
23	A2	79	A
23	A2	80	C
23	A2	88	U
23	A2	91	A
24	A3	2	G
24	A3	10	G
24	A3	43	G
24	A3	61	U
24	A3	64	G
24	A3	73	A

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Mol	Chain	Res	Type
54	BA	15	G
54	BA	60	G
54	BA	91	A
54	BA	118	A
54	BA	121	G
54	BA	125	A
54	BA	138	U
54	BA	162	U
54	BA	163	C
54	BA	199	A
54	BA	221	A
54	BA	228	C
54	BA	255	A
54	BA	272	A
54	BA	276	U
54	BA	321	U
54	BA	330	A
54	BA	333	G
54	BA	372	G
54	BA	446	G
54	BA	452	G
54	BA	470	A
54	BA	482	A
54	BA	503	A
54	BA	509	C
54	BA	529	A
54	BA	530	G
54	BA	546	U
54	BA	547	A
54	BA	571	U
54	BA	573	U
54	BA	644	A
54	BA	653	U
54	BA	670	A
54	BA	750	A
54	BA	776	G
54	BA	791	C
54	BA	811	U
54	BA	889	C
54	BA	932	U
54	BA	945	A
54	BA	974	G

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Mol	Chain	Res	Type
54	BA	989	G
54	BA	1045	C
54	BA	1070	A
54	BA	1090	A
54	BA	1095	A
54	BA	1126	A
54	BA	1127	A
54	BA	1128	G
54	BA	1157	G
54	BA	1175	A
54	BA	1210	G
54	BA	1236	G
54	BA	1288	G
54	BA	1300	G
54	BA	1312	U
54	BA	1313	U
54	BA	1367	A
54	BA	1383	A
54	BA	1397	U
54	BA	1419	A
54	BA	1451	C
54	BA	1490	A
54	BA	1537	G
54	BA	1618	A
54	BA	1625	C
54	BA	1647	U
54	BA	1664	A
54	BA	1668	A
54	BA	1713	A
54	BA	1730	C
54	BA	1786	A
54	BA	1787	A
54	BA	1820	U
54	BA	1929	G
54	BA	1936	A
54	BA	1938	A
54	BA	1940	U
54	BA	1943	U
54	BA	1945	G
54	BA	2016	U
54	BA	2020	A
54	BA	2030	A

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Mol	Chain	Res	Type
54	BA	2033	A
54	BA	2163	A
54	BA	2164	C
54	BA	2250	G
54	BA	2266	A
54	BA	2282	G
54	BA	2286	G
54	BA	2296	U
54	BA	2312	U
54	BA	2332	C
54	BA	2385	C
54	BA	2389	G
54	BA	2391	G
54	BA	2425	A
54	BA	2428	G
54	BA	2430	A
54	BA	2447	G
54	BA	2495	G
54	BA	2503	A
54	BA	2505	G
54	BA	2564	A
54	BA	2565	A
54	BA	2602	A
54	BA	2612	C
54	BA	2615	U
54	BA	2645	G
54	BA	2689	U
54	BA	2708	G
54	BA	2726	A
54	BA	2776	A
54	BA	2777	G
54	BA	2780	G
54	BA	2826	A
55	BB	12	C
55	BB	51	G
55	BB	66	A
55	BB	107	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	CM0	A1	34	22,23	21,26,27	1.30	2 (9%)	26,37,40	1.36	3 (11%)
22	6MZ	A1	37	22	22,25,26	0.68	0	29,36,39	1.13	3 (10%)
22	4SU	A1	7	22	18,21,22	1.41	2 (11%)	25,30,33	1.08	3 (12%)
24	OMC	A3	33	24	19,22,23	0.68	0	25,31,34	1.12	1 (4%)
24	PSU	A3	56	24	18,21,22	0.82	0	21,30,33	1.10	2 (9%)
24	5MU	A3	55	24	19,22,23	0.71	0	27,32,35	1.33	3 (11%)
22	PSU	A1	55	22	18,21,22	0.82	0	21,30,33	1.36	3 (14%)
24	H2U	A3	21	24	18,21,22	1.36	2 (11%)	19,30,33	1.23	3 (15%)
22	5MU	A1	54	22	19,22,23	0.68	0	27,32,35	1.21	2 (7%)
22	7MG	A1	46	22	23,26,27	4.09	2 (8%)	27,39,42	1.51	2 (7%)
24	4SU	A3	8	24	18,21,22	1.49	1 (5%)	25,30,33	0.83	1 (4%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-19.21	1.33	1.45
24	A3	8	4SU	C5-C4	-5.26	1.36	1.42
22	A1	7	4SU	C5-C4	-5.02	1.36	1.42
22	A1	34	CM0	O5-C5	-4.72	1.25	1.36
24	A3	21	H2U	C2-N3	-3.46	1.31	1.38
24	A3	21	H2U	C4-N3	-3.26	1.32	1.37
22	A1	46	7MG	C8-N7	-2.38	1.30	1.42
22	A1	34	CM0	O8-C8	-2.20	1.23	1.30
22	A1	7	4SU	C4-S4	-2.11	1.65	1.68

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	6.08	111.97	103.37
22	A1	34	CM0	C7-O5-C5	4.47	123.17	117.48
22	A1	55	PSU	C6-C5-C4	3.73	120.69	118.17
22	A1	37	6MZ	C9-N6-C6	3.47	126.07	122.85
24	A3	33	OMC	O2-C2-N3	-3.45	116.89	122.33
24	A3	55	5MU	C5M-C5-C6	-3.34	118.34	122.85
24	A3	55	5MU	C6-C5-C4	3.07	120.55	118.02
22	A1	54	5MU	C6-C5-C4	3.06	120.54	118.02
22	A1	54	5MU	C5M-C5-C6	-2.85	119.00	122.85
24	A3	21	H2U	N3-C2-N1	2.83	119.49	116.65
22	A1	37	6MZ	C4-C5-C6	-2.68	114.55	116.78
22	A1	55	PSU	O4'-C1'-C2'	2.66	108.83	105.15
24	A3	21	H2U	C5-C4-N3	2.64	119.49	116.69
22	A1	7	4SU	C6-C5-C4	2.58	122.18	119.95
22	A1	7	4SU	O4'-C4'-C3'	2.37	109.86	105.15
24	A3	21	H2U	O2-C2-N3	-2.37	117.11	121.49
22	A1	37	6MZ	C6-C5-N7	2.28	134.92	132.43
22	A1	7	4SU	C3'-C2'-C1'	2.23	105.68	101.46
22	A1	55	PSU	N1-C2-N3	2.20	117.49	115.17
24	A3	55	5MU	C5M-C5-C4	2.19	121.12	118.78
24	A3	8	4SU	C6-C5-C4	2.10	121.77	119.95
22	A1	34	CM0	O8-C8-O9	-2.09	117.96	123.33
22	A1	46	7MG	C6-C5-C4	-2.07	118.75	122.40
24	A3	56	PSU	O4'-C1'-C2'	2.04	107.98	105.15
24	A3	56	PSU	C6-C5-C4	2.04	119.55	118.17
22	A1	34	CM0	N3-C2-N1	2.00	117.50	114.89

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A3	56	PSU	O4'-C1'-C5-C4
24	A3	56	PSU	O4'-C1'-C5-C6
22	A1	34	CM0	O5-C7-C8-O9
22	A1	34	CM0	O5-C7-C8-O8
22	A1	55	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	1.82	1 (16%)
58	FME	BA	3001	57	8,9,10	0.67	0	8,9,11	1.24	1 (12%)

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	-	1/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
57	A1	101	VAL	O-C-CA	-4.11	114.21	124.77
58	BA	3001	FME	C-CA-N	2.48	114.28	109.50

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

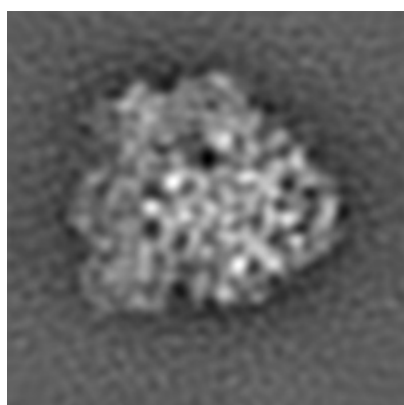
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1719. These allow visual inspection of the internal detail of the map and identification of artifacts.

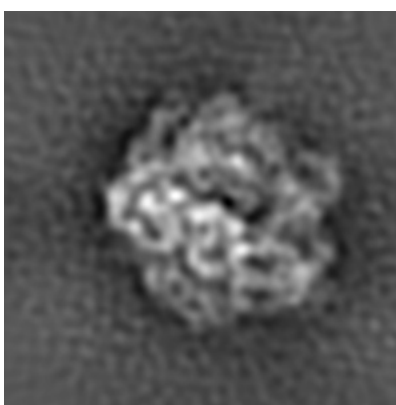
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

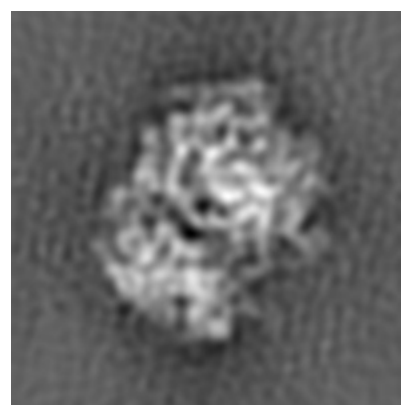
6.1.1 Primary map



X



Y

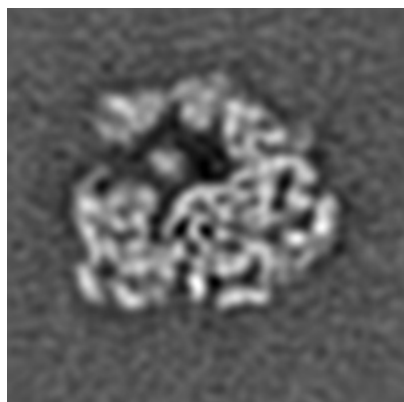


Z

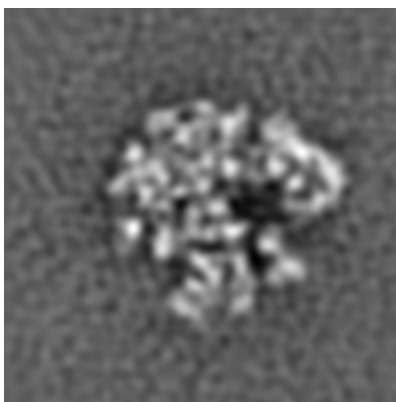
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

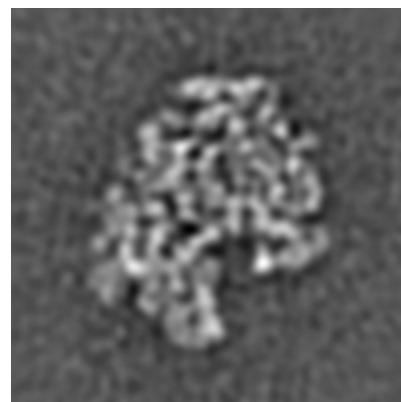
6.2.1 Primary map



X Index: 64



Y Index: 64

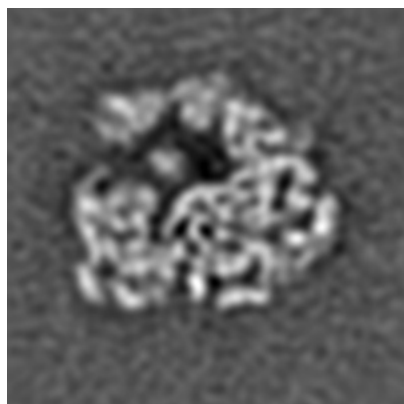


Z Index: 64

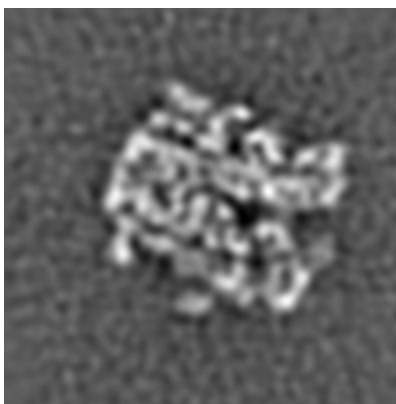
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

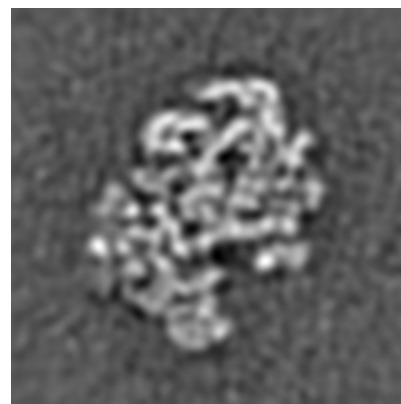
6.3.1 Primary map



X Index: 64



Y Index: 69

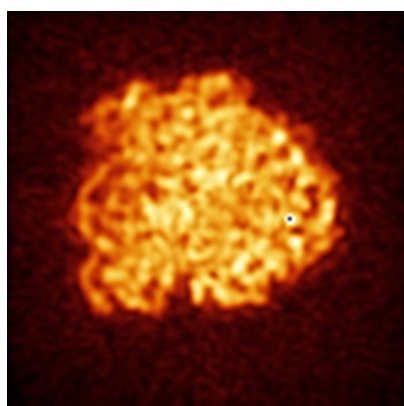


Z Index: 61

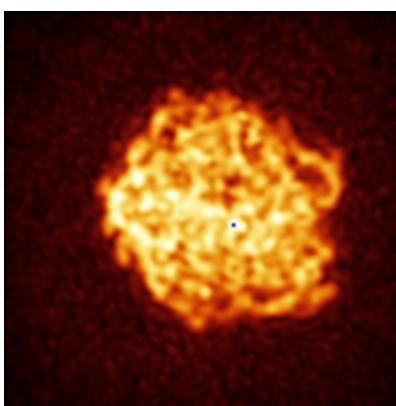
The images above show the largest variance slices of the map in three orthogonal directions.

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

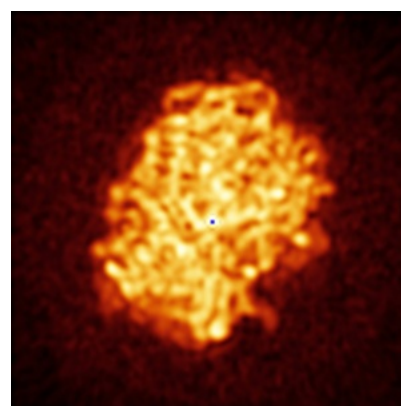
6.4.1 Primary map



X



Y

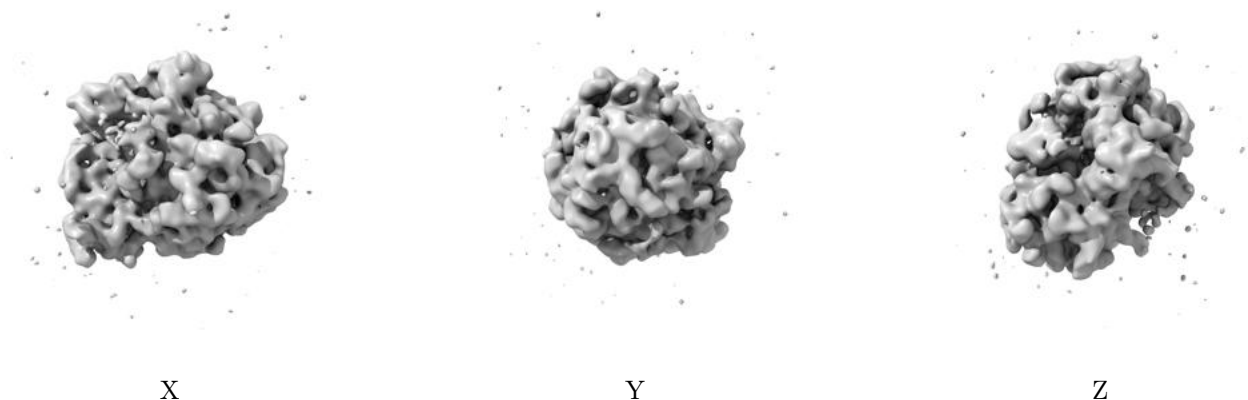


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 26.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

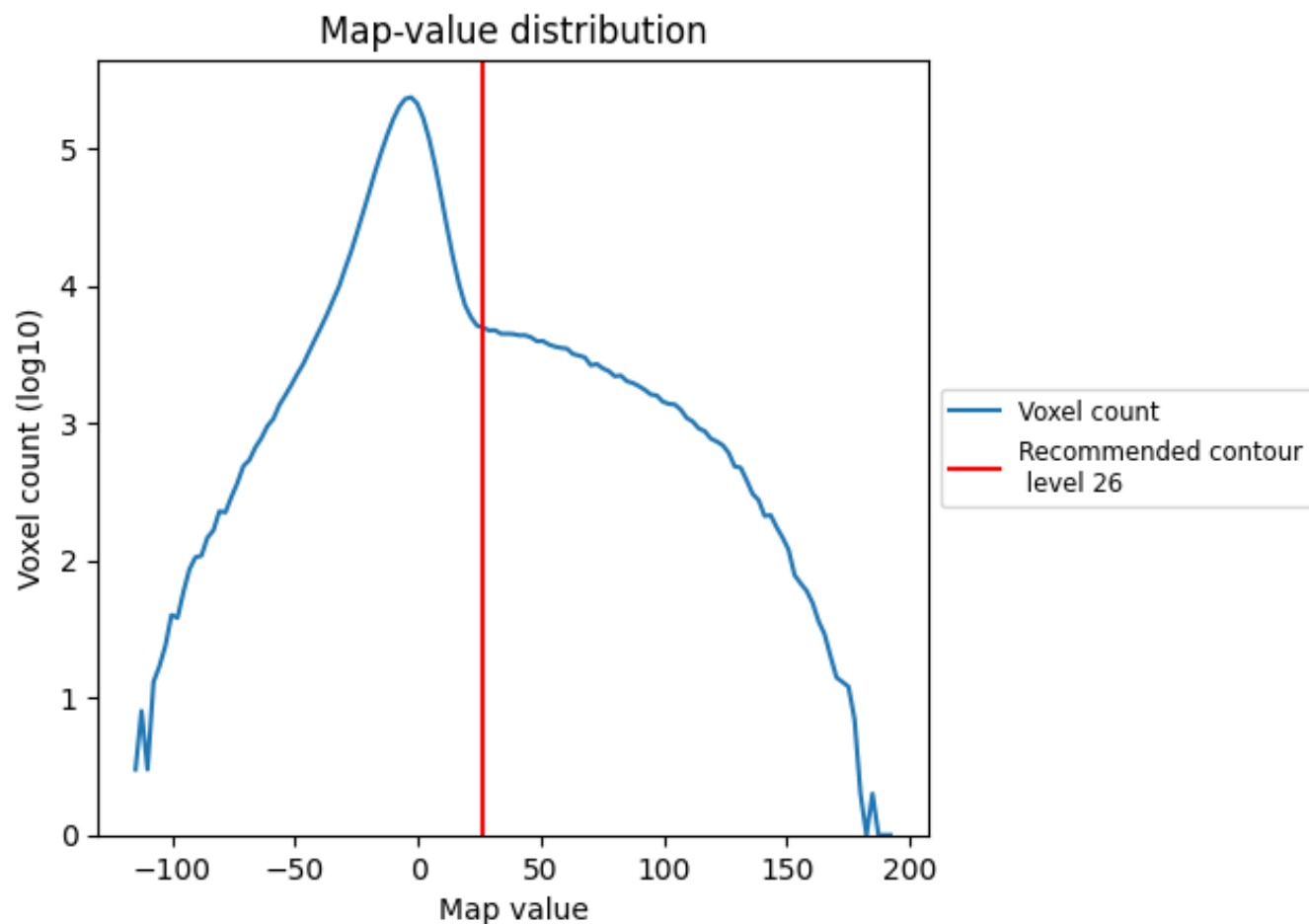
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

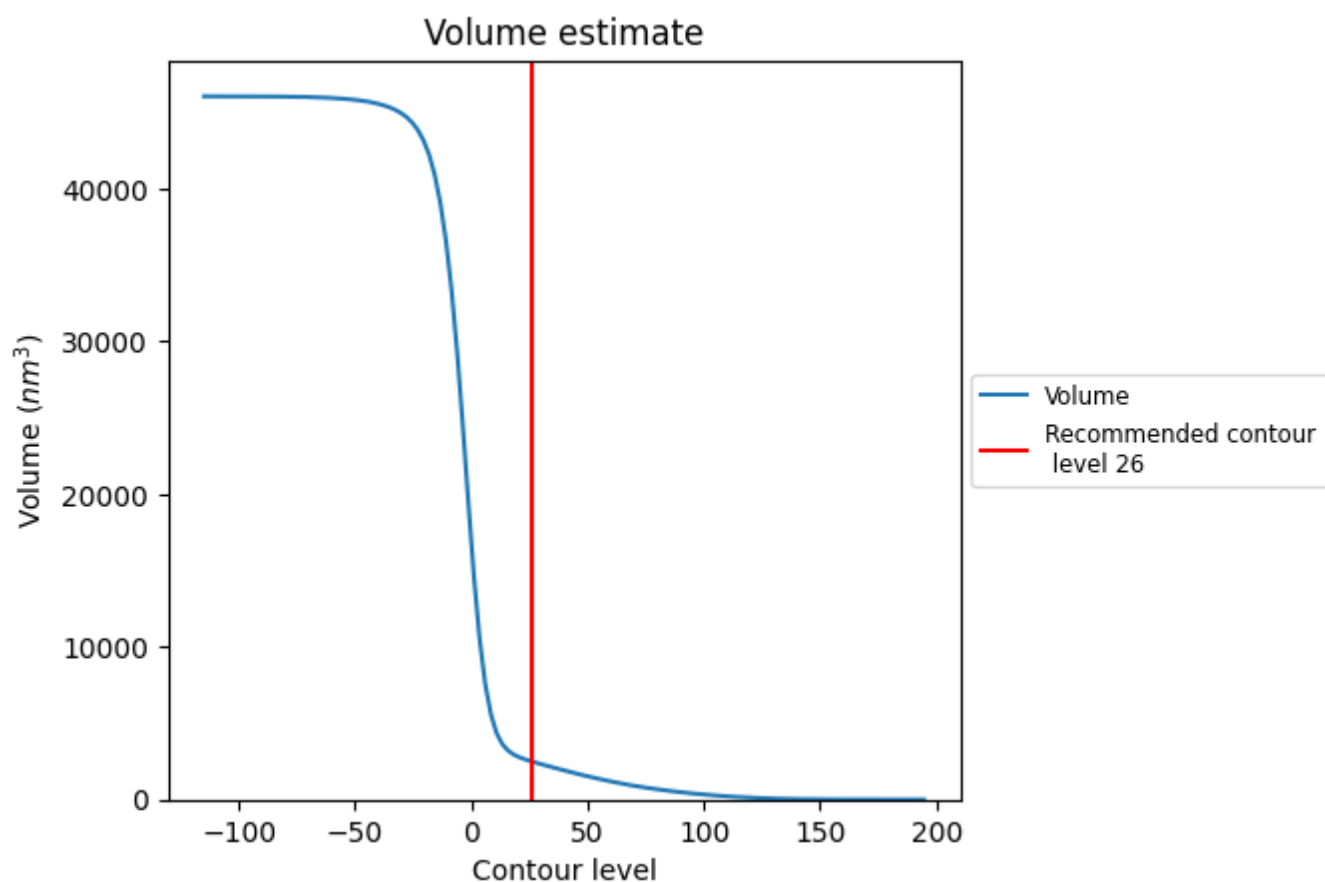
This section contains the results of statistical analysis of the map.

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.

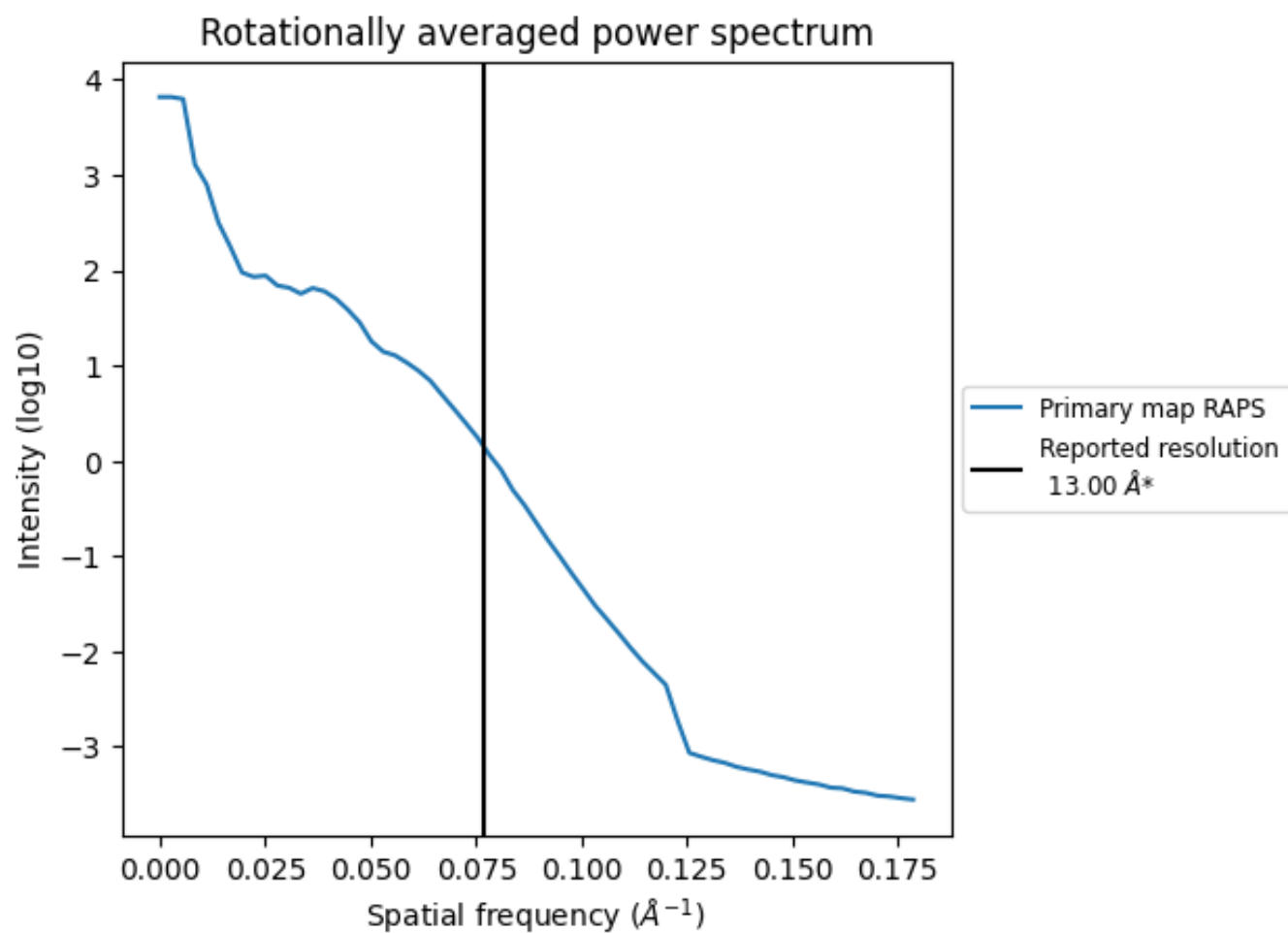
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2493 nm³; this corresponds to an approximate mass of 2252 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 0.077 $\text{\AA}^{-1}$

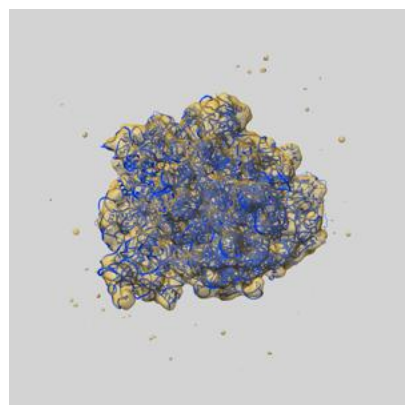
8 Fourier-Shell correlation

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

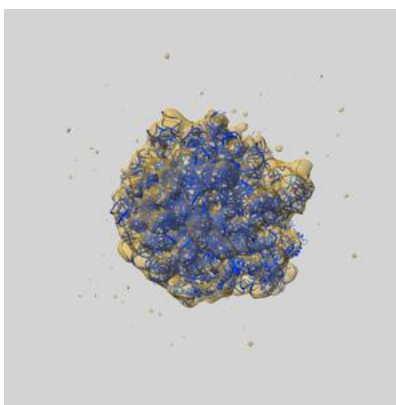
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1719 and PDB model 4V72. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

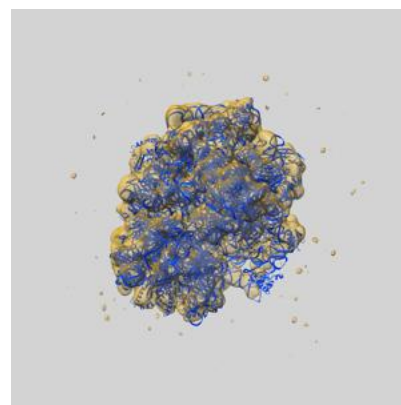
9.1 Map-model overlay [i](#)



X



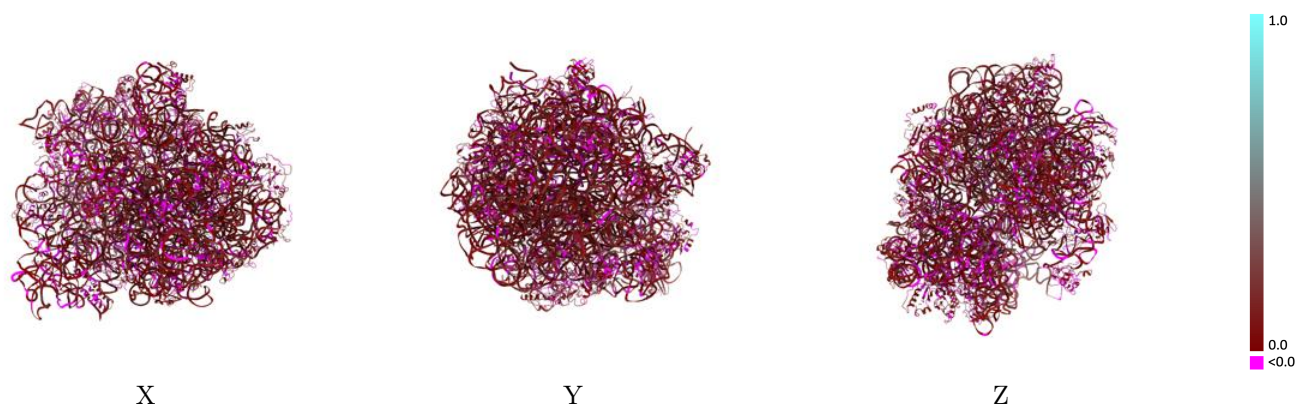
Y



Z

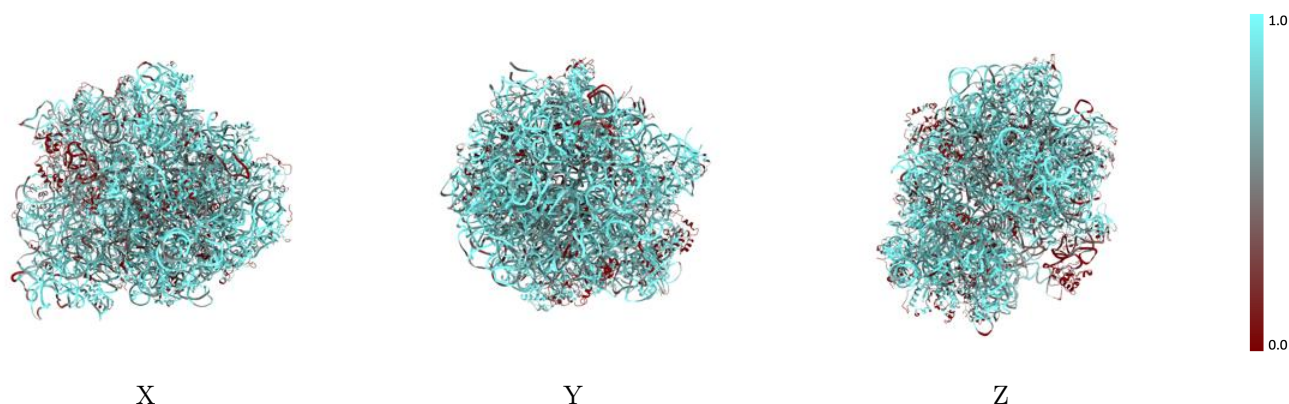
The images above show the 3D surface view of the map at the recommended contour level 26.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



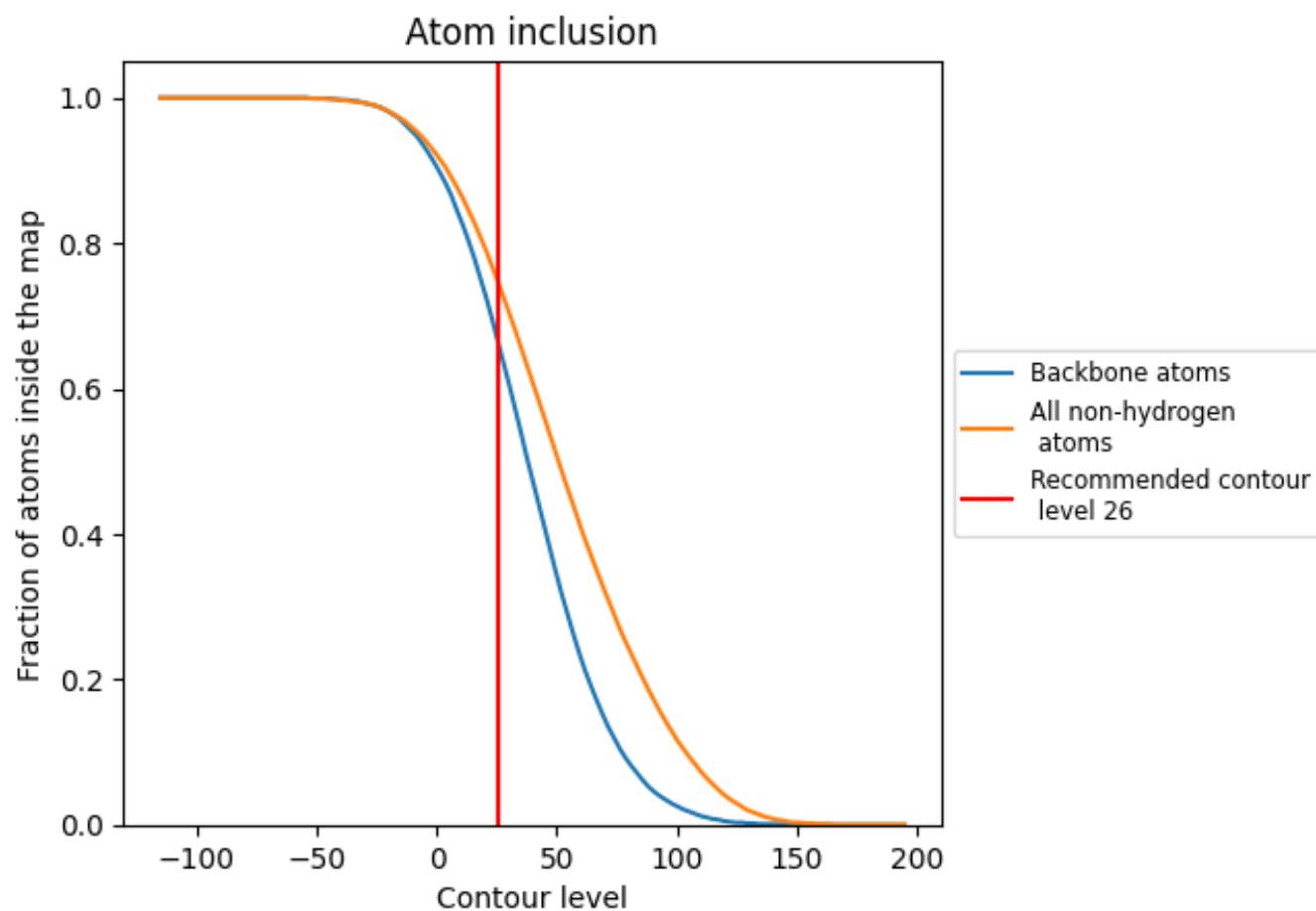
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (26).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 74% 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 (26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.0720
A1	 0.5900	 0.0670
A2	 0.5790	 0.0370
A3	 0.7360	 0.0960
AA	 0.8330	 0.0830
AB	 0.6480	 0.0790
AC	 0.6660	 0.0570
AD	 0.5620	 0.0410
AE	 0.6770	 0.0650
AF	 0.8080	 0.0820
AG	 0.7020	 0.0440
AH	 0.6150	 0.0490
AI	 0.6990	 0.0370
AJ	 0.6320	 0.0230
AK	 0.6220	 0.0360
AL	 0.5580	 0.0380
AM	 0.5750	 0.0250
AN	 0.5580	 0.0390
AO	 0.7460	 0.0500
AP	 0.5490	 0.0060
AQ	 0.6850	 0.0690
AR	 0.6860	 0.0420
AS	 0.7710	 0.0290
AT	 0.6640	 0.0250
AU	 0.3940	 -0.0080
B0	 0.6220	 0.0360
B1	 0.6810	 0.0480
B2	 0.3720	 0.0240
B3	 0.3320	 -0.0140
B4	 0.6440	 0.0190
B5	 0.4540	 0.0460
BA	 0.8100	 0.0890
BB	 0.8630	 0.0810
BC	 0.4930	 0.0310
BD	 0.5310	 0.0370



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Chain	Atom inclusion	Q-score
BE	 0.6160	 0.0380
BF	 0.7380	 0.0570
BG	 0.5690	 0.0360
BH	 0.2130	 0.0390
BI	 0.0290	 0.0230
BJ	 0.5760	 0.0310
BK	 0.5640	 0.0400
BL	 0.5720	 0.0130
BM	 0.5190	 0.0400
BN	 0.6150	 0.0260
BO	 0.8580	 0.0500
BP	 0.5770	 0.0500
BQ	 0.5120	 0.0270
BR	 0.7130	 0.0580
BS	 0.5730	 0.0520
BT	 0.6360	 0.0350
BU	 0.5640	 0.0190
BV	 0.6640	 0.0480
BW	 0.6860	 0.0440
BX	 0.4230	 0.0510
BY	 0.7450	 0.0880
BZ	 0.5450	 0.0230