



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:27 pm GMT

PDB ID : 4V70  
EMDB ID: : EMD-1718  
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate pre-translocation state (pre3)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 17.00 Å(reported)  
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

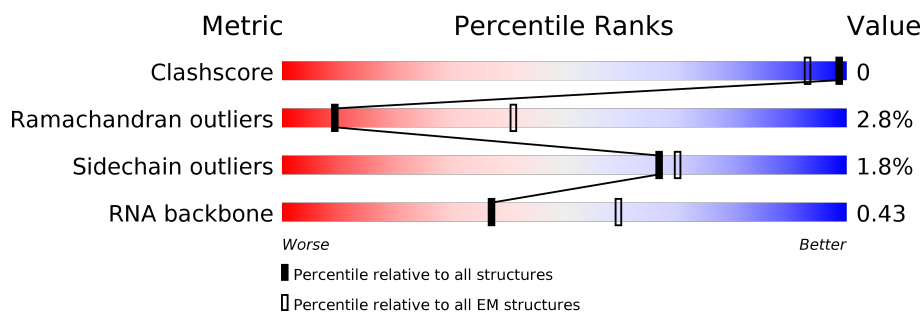
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 17.00 Å.

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















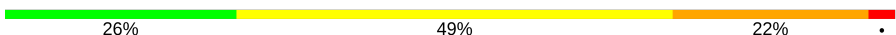


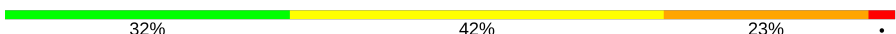









Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AB	220	93% 7%
2	AC	208	87% 13%
3	AD	206	89% 10%
4	AE	152	94% 6%
5	AF	101	85% 15%
6	AG	152	88% 11% .
7	AH	130	92% 8% .
8	AI	128	85% 13% .

















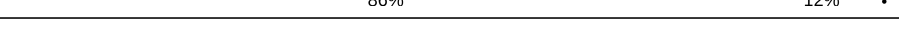

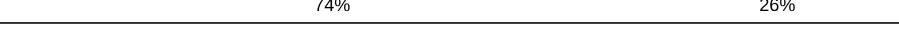


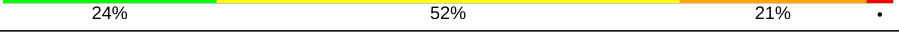
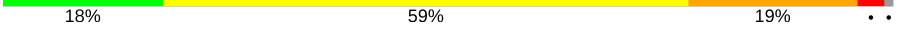
*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	AJ	100	 85% 14% .
10	AK	118	 92% 8%
11	AL	124	 86% 12% ..
12	AM	115	 82% 17% .
13	AN	101	 85% 12% ..
14	AO	89	 89% 10% .
15	AP	81	 89% 10% .
16	AQ	82	 89% 11%
17	AR	57	 89% 11%
18	AS	81	 89% 11%
19	AT	86	 87% 13%
20	AU	53	 75% 25%
21	AA	1533	 26% 49% 22% .
22	A1	76	 33% 47% 16% .
23	A2	15	 27% 33% 27% 13%
24	A3	77	 32% 42% 23% .
25	BC	273	 87% 12%
26	BD	209	 87% 12% .
27	BE	201	 92% 8%
28	BF	179	 89% 11% .
29	BG	177	 93% 6% ..
30	BH	149	 93% 7%
31	BI	142	 94% 6% .
32	BJ	142	 89% 11% .
33	BK	123	 89% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	BL	144	 86% 13% .
35	BM	136	 89% 10% .
36	BN	121	 83% 17%
37	BO	117	 87% 12% .
38	BP	115	 86% 12% ..
39	BQ	118	 84% 14% ..
40	BR	103	 91% 9%
41	BS	110	 89% 10% .
42	BT	94	 89% 11%
43	BU	104	 85% 13% ...
44	BV	94	 91% 9%
45	BW	80	 83% 16% .
46	BX	79	 77% 13% 8% .
47	BY	63	 92% 5% .
48	BZ	59	 90% 8% .
49	B0	57	 86% 12% .
50	B1	52	 87% 13%
51	B2	46	 74% 26%
52	B3	65	 86% 11% ..
53	B4	38	 89% 11%
54	BA	2903	 24% 52% 21% .
55	BB	118	 18% 59% 19% ..
56	B5	234	 88% 7% 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

*Continued on next page...*



*Continued from previous page...*

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		

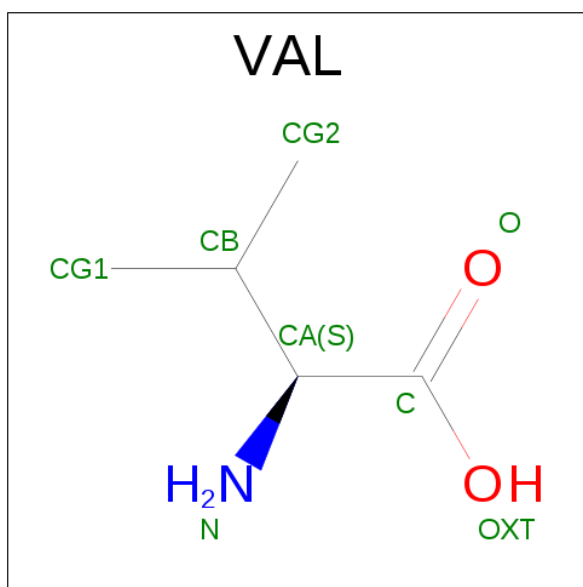
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

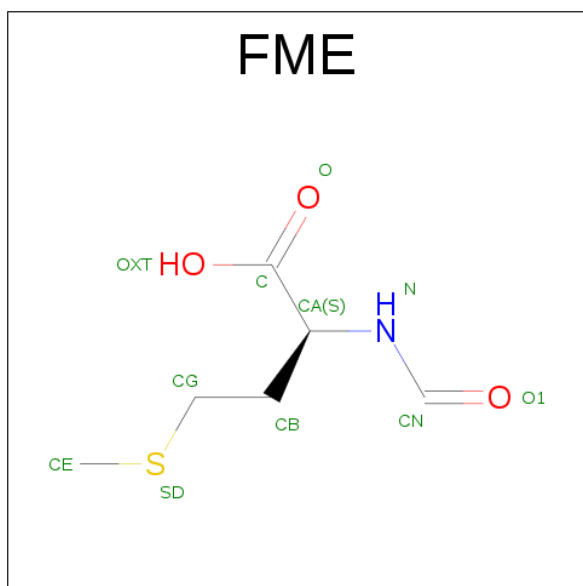
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



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

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



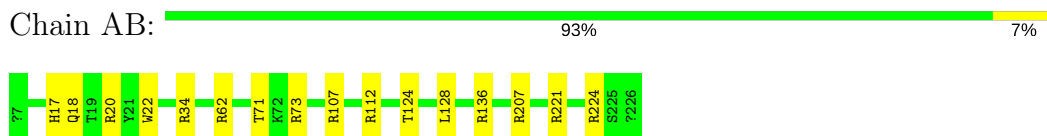
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



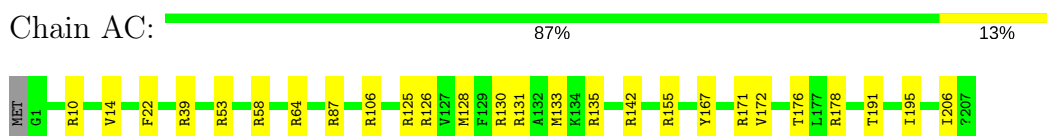
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

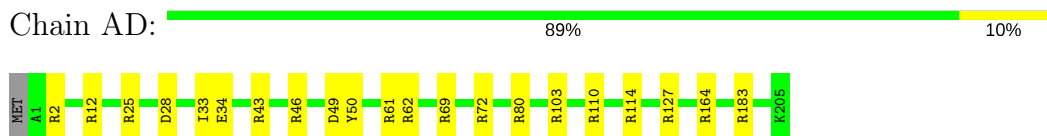
- Molecule 1: 30S ribosomal protein S2



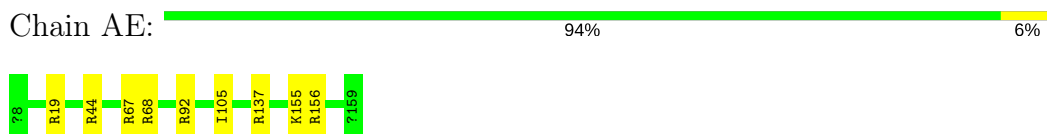
- Molecule 2: 30S ribosomal protein S3



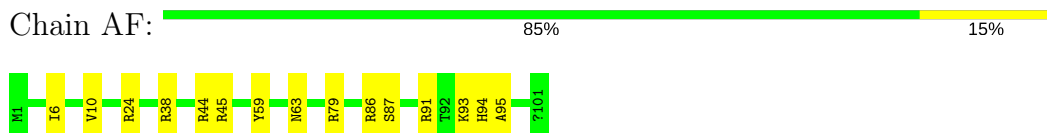
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





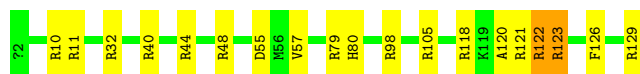
- Molecule 7: 30S ribosomal protein S8

Chain AH: 92% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 85% 13%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 85% 14%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 92% 8%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 86% 12%



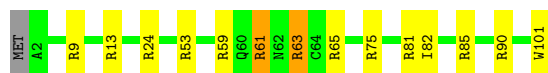
- Molecule 12: 30S ribosomal protein S13

Chain AM: 82% 17%

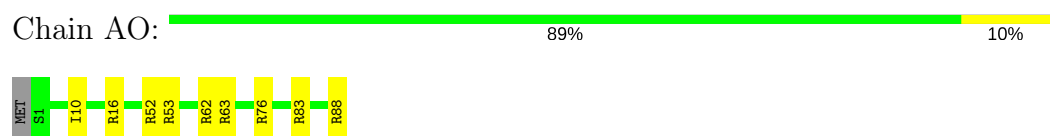


- Molecule 13: 30S ribosomal protein S14

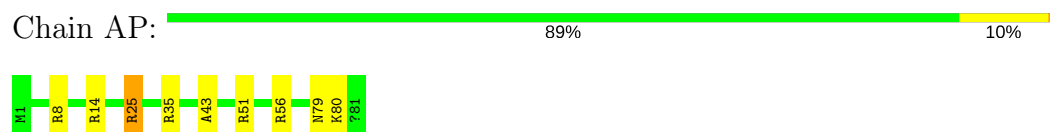
Chain AN: 85% 12%



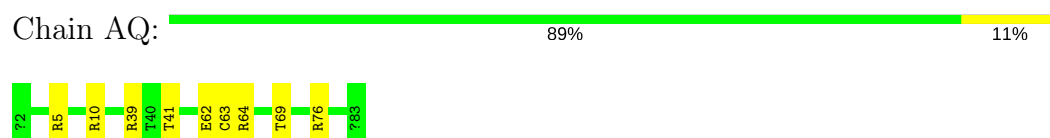
- Molecule 14: 30S ribosomal protein S15



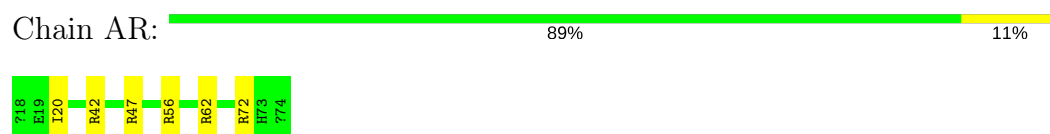
- Molecule 15: 30S ribosomal protein S16



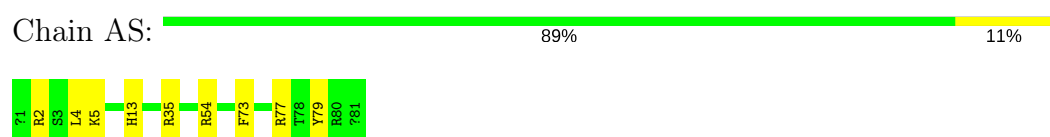
- Molecule 16: 30S ribosomal protein S17



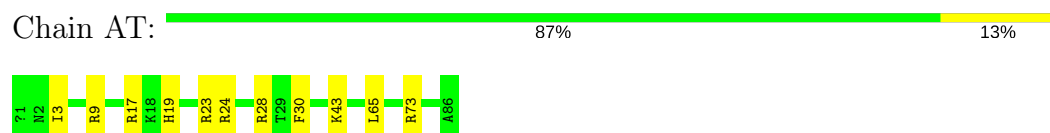
- Molecule 17: 30S ribosomal protein S18



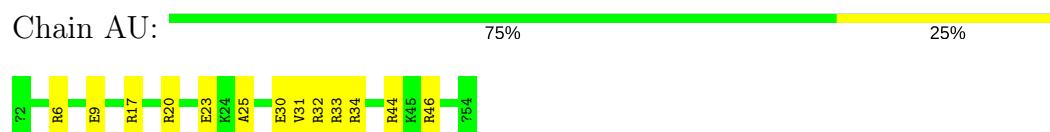
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



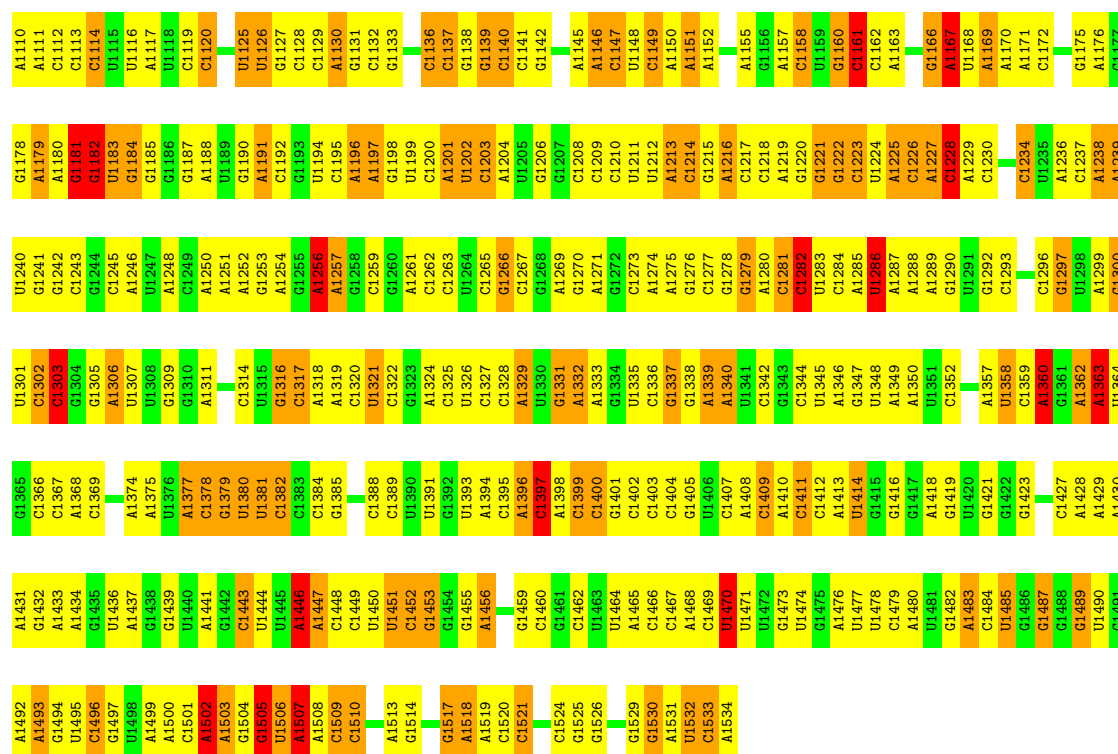
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA

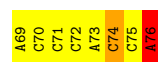


A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---



### • Molecule 22: fMet-Val-tRNA-Val

Chain A1: 33% 47% 16%



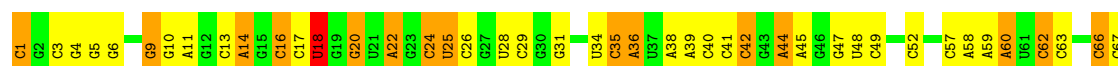
### • Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'

Chain A2: 27% 33% 27% 13%

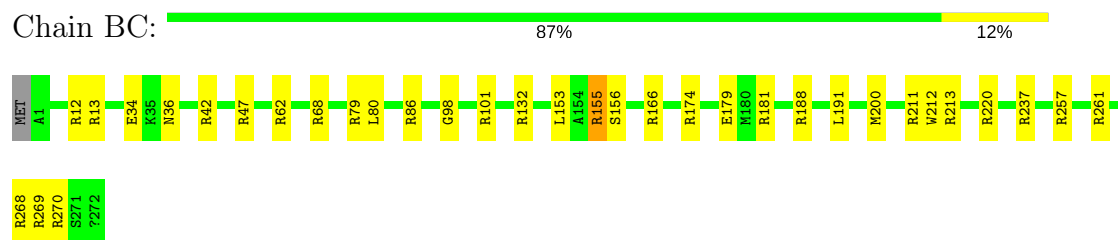


### • Molecule 24: tRNA-fMet

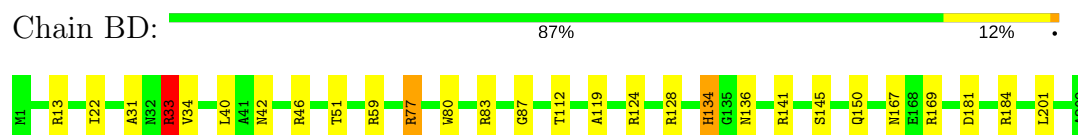
Chain A3: 32% 42% 23%



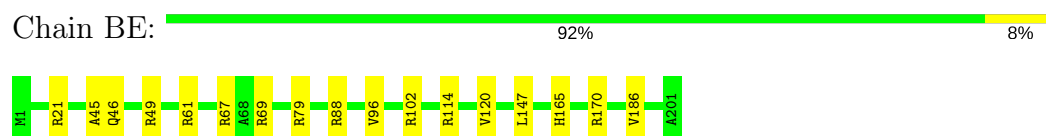
### • Molecule 25: 50S ribosomal protein L2



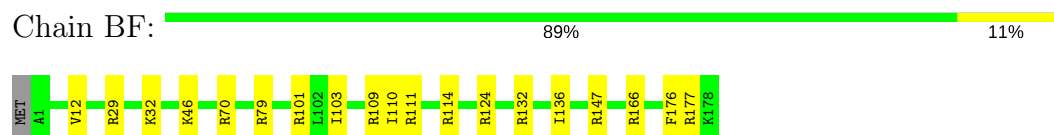
- Molecule 26: 50S ribosomal protein L3



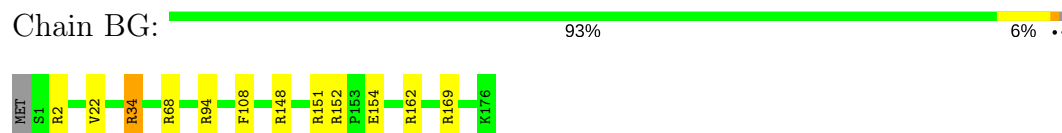
- Molecule 27: 50S ribosomal protein L4



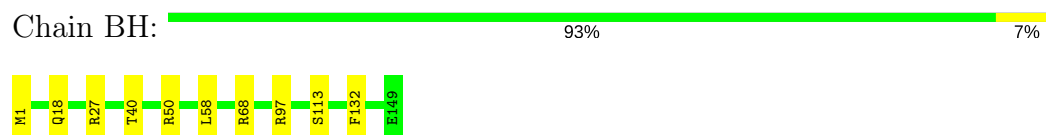
- Molecule 28: 50S ribosomal protein L5



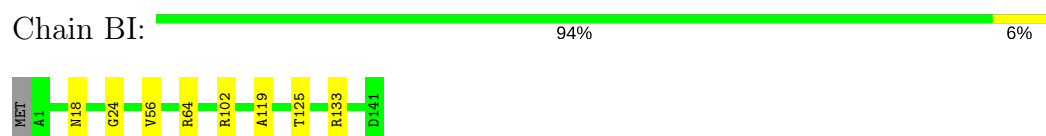
- Molecule 29: 50S ribosomal protein L6




- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L11



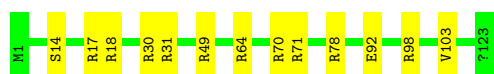
- Molecule 32: 50S ribosomal protein L13

Chain BJ:  89% 11%




- Molecule 33: 50S ribosomal protein L14

Chain BK:  89% 11%



- Molecule 34: 50S ribosomal protein L15

Chain BL:  86% 13%




- Molecule 35: 50S ribosomal protein L16

Chain BM:  89% 10%




- Molecule 36: 50S ribosomal protein L17

Chain BN:  83% 17%




- Molecule 37: 50S ribosomal protein L18

Chain BO:  87% 12%




- Molecule 38: 50S ribosomal protein L19

Chain BP:  86% 12%



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  84% 14%



- Molecule 40: 50S ribosomal protein L21

Chain BR: 91% 9%



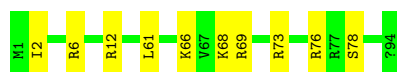
- Molecule 41: 50S ribosomal protein L22

Chain BS: 89% 10%



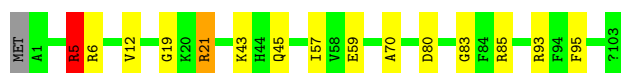
- Molecule 42: 50S ribosomal protein L23

Chain BT: 89% 11%



- Molecule 43: 50S ribosomal protein L24

Chain BU: 85% 13%



- Molecule 44: 50S ribosomal protein L25

Chain BV: 91% 9%



- Molecule 45: 50S ribosomal protein L27

Chain BW: 83% 16%



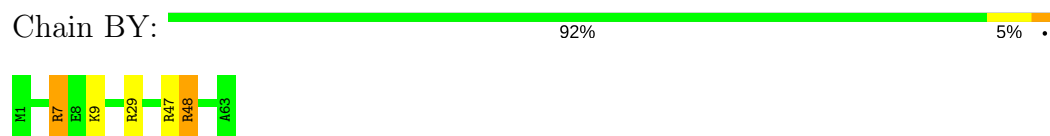
- Molecule 46: 50S ribosomal protein L28

Chain BX: 77% 13% 8%

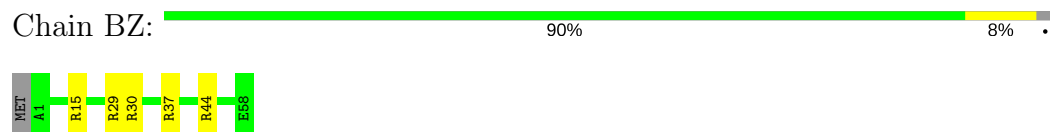




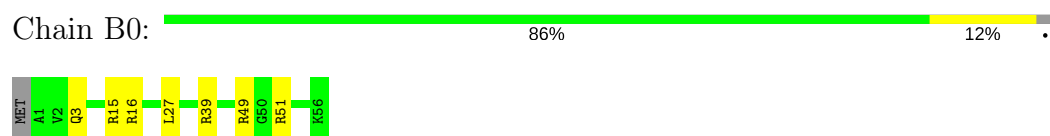
- Molecule 47: 50S ribosomal protein L29



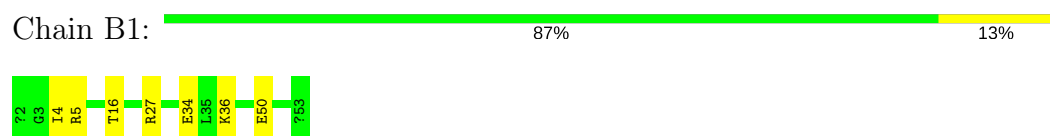
- Molecule 48: 50S ribosomal protein L30



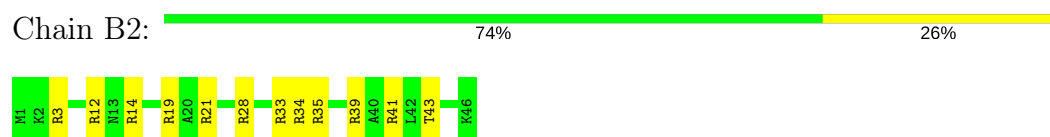
- Molecule 49: 50S ribosomal protein L32



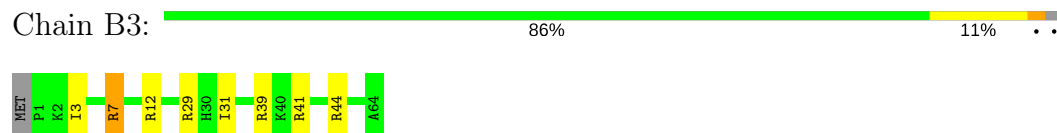
- Molecule 50: 50S ribosomal protein L33



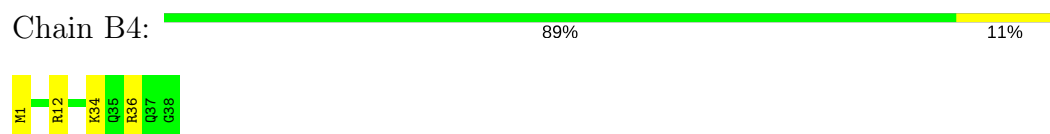
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36



- Molecule 54: 23S ribosomal RNA

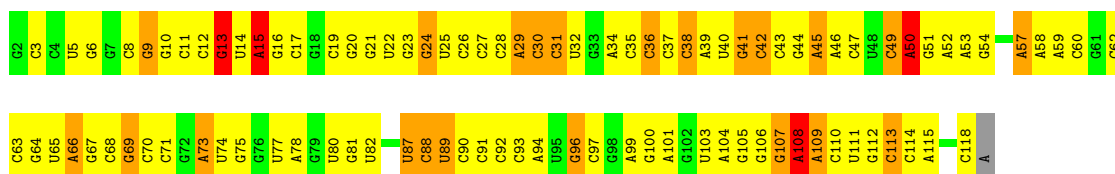


A1032	A1033	A1034	U1035	A1039	A1040	A1041	G1042	C1043	C1044	C1045	A1046	G1047	A1048	C1049	A1050	G1051	C1052	C1053	A1054	G1055	G1056	A1057	U1058	U1061	G1062	G1063	C1064	A1067	G1068	A1069	A1070	G1071	C1072	A1073	G1074	C1075	C1076	A1077	U1078	C1079	A1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	A1089	A1090	G1091	C1092	G1093	U1094	A1095																																																																																																																																																																																																																																																																			
A972	A973	G974	U975	G976	G977	G978	A979	A980	A981	C982	A983	A984	C985	C986	C987	G988	A989	C990	C991	C992	G993	C994	C995	A996	G997	C998	U999	G1000	A1001	G1002	G1003	U1004	C1005	C1006	C1007	A1008	A1009	A1010	C1010	U1011	U1012	C1013	A1014	U1015	U1018	U1019	U1083	A1084	A1085	A1086	G1087	A1088	A1089	A1090	G1091	C1092	G1093	U1094	A1095																																																																																																																																																																																																																																																																
U846	U847	C848	A849	U850	U851	U852	C853	C854	C855	C856	C857	A858	C859	U860	A861	C862	A863	C864	C865	A866	C867	U868	C869	U870	U871	U872	C873	C874	C875	C876	A877	U878	A879	C880	C881	C882	C883	U884	C885	A886	U887	C888	C889	C890	C891	A892	C893	U894	U895	A896	C897	C898	A899	A900	C901	C902	C903	G904	A905	U906																																																																																																																																																																																																																																																															
G907	C908	A909	A910	A911	C912	U913	C914	C915	G916	A917	A918	C919	A920	C921	C922	G923	G924	A925	G926	A927	A928	U929	U930	U931	U932	A933	U934	C935	A936	C937	A941	G942	A943	C944	A945	C946	A947	C948	G949	U950	U951	C952	G953	G954	C955	A956	C957	A958	A959	C960	G961	G962	A963	A964	C965	U966	C967	C968																																																																																																																																																																																																																																																																	
G784	G785	C786	C787	A788	A789	U790	C791	A792	A793	A794	C795	C796	G797	A800	C801	A802	U803	A804	C805	C806	U807	U810	U811	C812	U813	C814	C815	C816	C817	G818	A819	A820	A821	C822	C823	U824	A825	U826	U827	U828	A829	C830	C831	U832	U833	A834	C835	G836	C837	C838	U839	C840	G841	U842	G843	A844	A845																																																																																																																																																																																																																																																																		
C717	A718	C719	U720	A721	A722	C723	U724	G725	A726	A727	C728	G729	A730	C731	C732	G733	A735	C736	C737	G738	A739	C740	U741	A742	A743	U744	G745	U746	U747	G748	A749	A750	A751	A752	A753	U754	U755	A756	G757	C758	G759	G760	A761	U762	G763	A764	C765	C772	U773	G774	G775	G776	G780	A781	A782	A783																																																																																																																																																																																																																																																																			
U652	U653	A654	A655	U656	U657	C660	A661	U665	A666	U667	A668	C669	A670	C671	C672	C673	C674	A675	A676	A677	C678	C679	C680	U683	G684	G685	A686	C687	U688	U689	A690	C691	C692	C693	C694	C695	A696	A697	C698	A699	G700	C701	U702	U703	G704	A705	A706	U707	U710	G711	G712	G713	U714	A715	A716																																																																																																																																																																																																																																																																				
U525	A526	C527	A528	U529	A530	G531	A532	C533	U537	A538	A539	A540	A541	C542	G543	C544	U545	U546	A547	A548	A549	C550	G551	A552	G553	U554	G555	C556	C557	A558	G559	C560	U561	U562	U563	U564	G565	C566	C567	U568	A569	A570	U571	A572	U573	A574	A575	U576	G577	A578	G579	A580	U581	A582	C583	C584	G585	A586	C587																																																																																																																																																																																																																																																																
U588	U589	A590	U591	A592	U593	U594	C595	U596	G597	U598	A599	G600	C601	A602	G603	U606	U607	A608	A609	C610	C611	C612	A613	A614	U615	A616	G617	A618	A619	C620	A621	C622	C623	C624	C625	A626	A627	G628	C629	C630	A631	A632	C633	C634	U635	C636	U637	U638	U639	C640	U641	U642	U643	A644	C645	C646	C650	G651																																																																																																																																																																																																																																																																	
U852	U853	A854	A855	U856	U857	C860	A861	U865	A866	U867	A868	C869	A870	C871	C872	C873	C874	A875	A876	A877	C878	C879	C880	U883	G884	G885	A886	C887	U888	U889	A890	C891	C892	C893	C894	C895	A896	A897	C898	A899	G900	C901	U902	U903	A904	A905	U906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031																																																																																																																																															
U459	A460	C461	G462	C463	U464	A465	A466	C467	C468	A469	A470	A471	A472	C475	C476	A477	A478	A479	A480	A481	A482	A483	A484	C485	C486	C487	C490	C491	A492	C493	A494	A495	A496	A497	C498	U499	G500	A501	A502	A503	A504	U505	G506	A507	A508	C509	A510	A511	A512	A513	U514	A515	A516	C517	A518	A519	C520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	C532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716																																																														
C394	U395	G396	U397	C398	U399	A400	A401	A402	U403	A404	U405	A412	C413	C414	A415	C417	C418	A419	A420	A421	A422	A423	A424	C425	G426	A427	A428	A429	A430	A431	A432	C433	U434	C435	C436	U437	G438	A439	A440	U441	A442	A443	A444	A445	U446	A447	U448	A449	G450	U451	C452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716
U328	U329	A330	C331	A332	C333	C334	C335	C336	C337	G338	U339	A340	C341	A342	C343	A344	A345	A346	A347	A348	U349	A352	C353	A354	C357	U360	G361	A362	C363	C364	U365	C366	G367	A368	U369	C370	A371	C372	U373	A374	C378	A382	C383	A384	C385	C386	U387	U390	A391	C392	C393	U394	U395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562</																																																																																															






Chain BB:  18% 59% 19% 4%



- Molecule 56: 50S ribosomal protein L1

Chain B5:



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	2648	Depositor
Resolution determination method	FSC at 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	4k CCD camera (TVIPS)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	AB	0.74	0/1736	1.04	11/2340 (0.5%)
10	AK	0.77	0/894	1.18	9/1207 (0.7%)
11	AL	0.78	0/969	1.23	14/1300 (1.1%)
12	AM	0.77	0/884	1.30	16/1181 (1.4%)
13	AN	0.80	0/817	1.35	12/1088 (1.1%)
14	AO	0.74	0/722	1.20	9/964 (0.9%)
15	AP	0.80	0/648	1.15	5/870 (0.6%)
16	AQ	0.72	0/658	1.10	7/883 (0.8%)
17	AR	0.82	0/463	1.18	5/623 (0.8%)
18	AS	0.78	0/653	1.12	6/879 (0.7%)
19	AT	0.71	0/672	1.18	8/890 (0.9%)
2	AC	0.75	0/1651	1.19	17/2225 (0.8%)
20	AU	0.86	0/431	1.59	9/572 (1.6%)
21	AA	1.52	0/36759	2.22	1943/57346 (3.4%)
22	A1	1.54	0/1668	2.18	94/2595 (3.6%)
23	A2	1.50	0/343	2.20	15/531 (2.8%)
24	A3	1.51	0/1722	2.19	80/2685 (3.0%)
25	BC	0.76	0/2121	1.28	25/2852 (0.9%)
26	BD	0.71	0/1586	1.19	12/2134 (0.6%)
27	BE	0.70	0/1571	1.14	9/2113 (0.4%)
28	BF	0.77	0/1444	1.16	12/1937 (0.6%)
29	BG	0.72	0/1343	1.14	9/1816 (0.5%)
3	AD	0.80	0/1665	1.19	16/2227 (0.7%)
30	BH	0.70	0/1122	1.11	5/1515 (0.3%)
31	BI	0.69	0/1046	1.08	4/1410 (0.3%)
32	BJ	0.76	0/1152	1.12	6/1551 (0.4%)
33	BK	0.73	0/947	1.20	10/1268 (0.8%)
34	BL	0.75	0/1054	1.29	14/1403 (1.0%)
35	BM	0.78	0/1093	1.23	12/1460 (0.8%)
36	BN	0.79	0/973	1.35	16/1301 (1.2%)
37	BO	0.76	0/902	1.29	15/1209 (1.2%)
38	BP	0.76	0/929	1.27	9/1242 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.80	0/960	1.30	15/1278 (1.2%)
4	AE	0.73	0/1119	1.04	7/1506 (0.5%)
40	BR	0.75	0/829	1.12	6/1107 (0.5%)
41	BS	0.68	0/864	1.19	11/1156 (1.0%)
42	BT	0.68	0/744	1.17	5/994 (0.5%)
43	BU	0.73	0/787	1.15	7/1051 (0.7%)
44	BV	0.74	0/766	1.17	6/1025 (0.6%)
45	BW	0.78	0/604	1.34	10/799 (1.3%)
46	BX	0.78	0/635	1.35	10/848 (1.2%)
47	BY	0.71	0/510	1.22	5/677 (0.7%)
48	BZ	0.72	0/453	1.27	5/605 (0.8%)
49	B0	0.74	0/450	1.22	5/599 (0.8%)
5	AF	0.76	0/835	1.17	8/1128 (0.7%)
50	B1	0.76	0/417	1.09	2/556 (0.4%)
51	B2	0.82	0/380	1.56	13/498 (2.6%)
52	B3	0.75	0/513	1.26	8/676 (1.2%)
53	B4	0.68	0/303	1.13	2/397 (0.5%)
54	BA	1.40	1/69796 (0.0%)	2.21	4048/108888 (3.7%)
55	BB	1.41	0/2800	2.18	153/4367 (3.5%)
56	B5	0.68	0/1673	1.13	11/2255 (0.5%)
6	AG	0.77	0/1188	1.19	13/1593 (0.8%)
7	AH	0.71	0/989	1.03	8/1326 (0.6%)
8	AI	0.83	0/1035	1.33	19/1377 (1.4%)
9	AJ	0.75	0/797	1.24	12/1079 (1.1%)
All	All	1.28	1/160085 (0.0%)	1.99	6823/239402 (2.9%)

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
10	AK	0	1
2	AC	0	1
21	AA	0	365
22	A1	0	13
23	A2	0	5
24	A3	0	17
25	BC	0	1
43	BU	0	1
54	BA	0	636
55	BB	0	20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
8	AI	0	1
9	AJ	0	1
All	All	0	1062

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	945	A	N3-C4	5.58	1.38	1.34

The worst 5 of 6823 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	330	A	O4'-C1'-N9	12.97	118.58	108.20
54	BA	2270	A	N1-C6-N6	-12.77	110.94	118.60
54	BA	900	A	N1-C6-N6	-12.68	110.99	118.60
54	BA	1069	A	N1-C6-N6	-12.45	111.13	118.60
54	BA	1616	A	N1-C6-N6	-12.33	111.20	118.60

There are no chirality outliers.

5 of 1062 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	5	U	Sidechain
2	AC	172	VAL	Peptide
8	AI	123	ARG	Peptide
9	AJ	37	ARG	Sidechain
10	AK	115	ILE	Peptide

## 5.2 Too-close contacts

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

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AF	818	0	808	1	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	1	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	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	16522	0	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	1	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	1	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	1	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	1	0
54	BA	62317	0	31345	6	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	1	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99665	12	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.

The worst 5 of 12 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)
35:BM:126:ILE:HD13	35:BM:126:ILE:H	1.74	0.53
54:BA:2105:U:HO2'	56:B5:2:ALA:N	2.13	0.46
24:A3:24:C:H2'	24:A3:25:U:C6	2.53	0.43
54:BA:2352:A:C5	54:BA:2353:G:H1'	2.53	0.43
54:BA:480:A:H3'	54:BA:481:G:C5'	2.48	0.43

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%)	17 (8%)	3 (1%)	13	54
2	AC	205/208 (99%)	185 (90%)	15 (7%)	5 (2%)	7	42
3	AD	203/206 (98%)	189 (93%)	11 (5%)	3 (2%)	12	53
4	AE	150/152 (99%)	137 (91%)	12 (8%)	1 (1%)	25	68
5	AF	99/101 (98%)	83 (84%)	10 (10%)	6 (6%)	2	22
6	AG	150/152 (99%)	134 (89%)	11 (7%)	5 (3%)	4	35
7	AH	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	22	67
8	AI	126/128 (98%)	109 (86%)	12 (10%)	5 (4%)	3	31
9	AJ	98/100 (98%)	91 (93%)	4 (4%)	3 (3%)	5	37
10	AK	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
11	AL	121/124 (98%)	107 (88%)	10 (8%)	4 (3%)	4	35
12	AM	112/115 (97%)	98 (88%)	11 (10%)	3 (3%)	6	40
13	AN	98/101 (97%)	84 (86%)	13 (13%)	1 (1%)	18	61
14	AO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	15	57
15	AP	79/81 (98%)	69 (87%)	6 (8%)	4 (5%)	2	26
16	AQ	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	14	56
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	10	49
18	AS	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	14	56
19	AT	84/86 (98%)	78 (93%)	3 (4%)	3 (4%)	4	33
20	AU	51/53 (96%)	40 (78%)	7 (14%)	4 (8%)	1	18
25	BC	270/273 (99%)	242 (90%)	25 (9%)	3 (1%)	17	60
26	BD	207/209 (99%)	176 (85%)	16 (8%)	15 (7%)	1	19
27	BE	199/201 (99%)	174 (87%)	17 (8%)	8 (4%)	3	31
28	BF	176/179 (98%)	158 (90%)	11 (6%)	7 (4%)	3	31
29	BG	174/177 (98%)	148 (85%)	24 (14%)	2 (1%)	17	60
30	BH	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
31	BI	139/142 (98%)	121 (87%)	14 (10%)	4 (3%)	5	38
32	BJ	140/142 (99%)	127 (91%)	8 (6%)	5 (4%)	4	33
33	BK	121/123 (98%)	106 (88%)	12 (10%)	3 (2%)	6	41
34	BL	141/144 (98%)	125 (89%)	10 (7%)	6 (4%)	3	29
35	BM	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	8	44
36	BN	119/121 (98%)	105 (88%)	10 (8%)	4 (3%)	4	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	105 (92%)	8 (7%)	1 (1%)	20	63
38	BP	112/115 (97%)	97 (87%)	11 (10%)	4 (4%)	4	33
39	BQ	115/118 (98%)	103 (90%)	8 (7%)	4 (4%)	4	34
40	BR	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	5	37
41	BS	108/110 (98%)	101 (94%)	5 (5%)	2 (2%)	9	47
42	BT	92/94 (98%)	81 (88%)	7 (8%)	4 (4%)	3	29
43	BU	101/104 (97%)	87 (86%)	5 (5%)	9 (9%)	1	15
44	BV	92/94 (98%)	88 (96%)	3 (3%)	1 (1%)	17	60
45	BW	78/80 (98%)	58 (74%)	17 (22%)	3 (4%)	4	32
46	BX	75/79 (95%)	62 (83%)	8 (11%)	5 (7%)	1	21
47	BY	61/63 (97%)	55 (90%)	3 (5%)	3 (5%)	2	27
48	BZ	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
49	B0	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	9	47
50	B1	50/52 (96%)	46 (92%)	1 (2%)	3 (6%)	2	23
51	B2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	B3	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	5	36
53	B4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
56	B5	221/234 (94%)	206 (93%)	12 (5%)	3 (1%)	13	54
All	All	5876/6008 (98%)	5263 (90%)	450 (8%)	163 (3%)	9	39

5 of 163 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	206	ILE
6	AG	11	ILE
9	AJ	75	ASP
11	AL	43	LYS

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	176 (98%)	4 (2%)	57	79
2	AC	170/171 (99%)	167 (98%)	3 (2%)	64	84
3	AD	172/173 (99%)	169 (98%)	3 (2%)	66	84
4	AE	113/113 (100%)	112 (99%)	1 (1%)	82	91
5	AF	87/87 (100%)	87 (100%)	0	100	100
6	AG	123/123 (100%)	122 (99%)	1 (1%)	85	92
7	AH	104/105 (99%)	102 (98%)	2 (2%)	62	82
8	AI	105/105 (100%)	104 (99%)	1 (1%)	80	90
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	102 (99%)	1 (1%)	80	90
12	AM	91/92 (99%)	90 (99%)	1 (1%)	78	89
13	AN	83/84 (99%)	80 (96%)	3 (4%)	40	68
14	AO	76/77 (99%)	76 (100%)	0	100	100
15	AP	65/65 (100%)	64 (98%)	1 (2%)	70	85
16	AQ	74/74 (100%)	71 (96%)	3 (4%)	35	65
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	67 (96%)	3 (4%)	33	64
19	AT	65/65 (100%)	63 (97%)	2 (3%)	45	71
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	208 (96%)	8 (4%)	39	68
26	BD	164/164 (100%)	159 (97%)	5 (3%)	46	72
27	BE	165/165 (100%)	165 (100%)	0	100	100
28	BF	149/150 (99%)	149 (100%)	0	100	100
29	BG	137/138 (99%)	135 (98%)	2 (2%)	70	85
30	BH	114/114 (100%)	108 (95%)	6 (5%)	26	59
31	BI	109/110 (99%)	108 (99%)	1 (1%)	82	91
32	BJ	116/116 (100%)	110 (95%)	6 (5%)	27	59
33	BK	103/103 (100%)	103 (100%)	0	100	100
34	BL	102/103 (99%)	102 (100%)	0	100	100
35	BM	109/109 (100%)	107 (98%)	2 (2%)	64	84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	99 (99%)	1 (1%)	80	90
37	BO	86/87 (99%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	96 (97%)	3 (3%)	46	72
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	78	89
40	BR	84/84 (100%)	84 (100%)	0	100	100
41	BS	93/93 (100%)	92 (99%)	1 (1%)	78	89
42	BT	80/80 (100%)	79 (99%)	1 (1%)	73	87
43	BU	83/84 (99%)	80 (96%)	3 (4%)	40	68
44	BV	78/78 (100%)	77 (99%)	1 (1%)	73	87
45	BW	59/59 (100%)	56 (95%)	3 (5%)	28	60
46	BX	67/68 (98%)	60 (90%)	7 (10%)	8	32
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%)	59	80
50	B1	45/45 (100%)	43 (96%)	2 (4%)	33	63
51	B2	38/38 (100%)	37 (97%)	1 (3%)	51	75
52	B3	51/52 (98%)	50 (98%)	1 (2%)	60	82
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	171 (99%)	2 (1%)	75	88
All	All	4842/4870 (99%)	4755 (98%)	87 (2%)	67	84

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	BD	134	HIS
30	BH	113	SER
49	B0	3	GLN
26	BD	136	ASN
30	BH	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	AF	58	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	271 (17%)	0
22	A1	73/76 (96%)	11 (15%)	0
23	A2	14/15 (93%)	6 (42%)	0
24	A3	76/77 (98%)	13 (17%)	0
54	BA	2902/2903 (99%)	460 (15%)	0
55	BB	116/118 (98%)	21 (18%)	0
All	All	4710/4722 (99%)	782 (16%)	0

5 of 782 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	17	U

There are no RNA pucker outliers to report.

## 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	16,26,27	1.76	3 (18%)	14,37,40	3.38	3 (21%)
22	6MZ	A1	37	22	18,25,26	0.97	1 (5%)	16,36,39	1.88	3 (18%)
22	7MG	A1	46	22	20,26,27	2.19	4 (20%)	22,39,42	1.90	2 (9%)
22	5MU	A1	54	22	14,22,23	1.21	1 (7%)	16,32,35	4.02	2 (12%)
22	PSU	A1	55	22	16,21,22	1.23	2 (12%)	20,30,33	5.29	7 (35%)
22	4SU	A1	7	22	14,21,22	1.10	0	15,30,33	2.79	4 (26%)
24	H2U	A3	21	24	17,21,22	1.44	2 (11%)	21,30,33	1.26	4 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	OMC	A3	33	24	15,22,23	1.13	0	19,31,34	0.89	1 (5%)
24	5MU	A3	55	24	14,22,23	1.04	1 (7%)	16,32,35	3.82	2 (12%)
24	PSU	A3	56	24	16,21,22	1.19	2 (12%)	20,30,33	5.58	8 (40%)
24	4SU	A3	8	24	14,21,22	1.14	1 (7%)	15,30,33	2.84	2 (13%)

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

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.02	1.33	1.45
22	A1	34	CM0	O5-C5	-5.35	1.26	1.37
24	A3	21	H2U	C4-N3	-3.45	1.32	1.37
24	A3	21	H2U	C2-N3	-3.41	1.31	1.38
22	A1	46	7MG	C8-N7	-2.82	1.30	1.43

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	56	PSU	N1-C2-N3	-16.19	116.75	128.40
22	A1	55	PSU	N1-C2-N3	-15.36	117.35	128.40
24	A3	56	PSU	C5-C4-N3	-12.76	114.96	125.43
22	A1	55	PSU	C5-C4-N3	-12.26	115.37	125.43
22	A1	54	5MU	C5-C4-N3	-9.70	114.55	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	58,22	6,6,7	0.98	0	6,7,9	1.60	1 (16%)
58	FME	BA	3001	57	9,9,10	1.32	1 (11%)	7,9,11	1.08	0

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	3001	FME	CA-C	3.44	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
57	A1	101	VAL	O-C-CA	-3.44	117.12	125.15

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.