



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:57 PM BST

PDB ID : 4V4X  
Title : Crystal structure of the 70S *Thermus thermophilus* ribosome showing how the 16S 3'-end mimicks mRNA E and P codons.  
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.  
Deposited on : 2006-06-27  
Resolution : 5.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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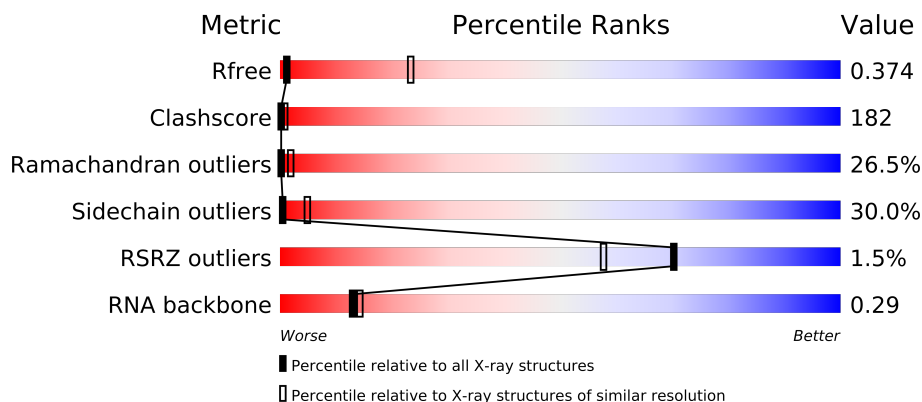
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance



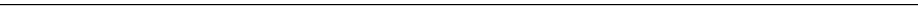


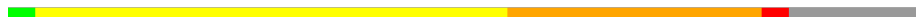


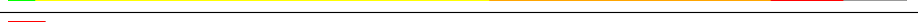

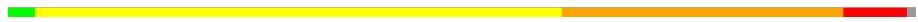

The reported resolution of this entry is 5.00 Å.

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1052 (6.50-3.50)
Clashscore	79885	1327 (6.50-3.50)
Ramachandran outliers	78287	1242 (6.50-3.50)
Sidechain outliers	78261	1221 (6.50-3.50)
RSRZ outliers	66119	1051 (6.50-3.50)
RNA backbone	1838	1037 (7.00-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1522	
2	AC	77	
3	AD	76	
4	AE	256	
5	AF	239	
6	AG	209	
7	AH	162	
8	AI	101	
9	AJ	156	
10	AK	138	
11	AL	128	
12	AM	105	

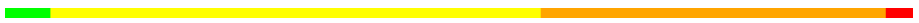
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Mol	Chain	Length	Quality of chain
13	AN	129	
14	AO	132	
15	AP	126	
16	AQ	61	
17	AR	89	
18	AS	88	
19	AT	105	
20	AU	88	
21	AV	93	
22	AW	106	
23	AX	27	
24	BA	2916	
25	BB	123	
26	BC	229	
27	BD	276	
28	BE	206	
29	BF	210	
30	BG	182	
31	BH	180	
32	BK	148	
33	BL	147	
34	BM	140	
35	BN	122	
36	BO	150	
37	BP	141	
38	BQ	118	
39	BR	112	
40	BS	146	
41	BT	118	
42	BU	101	
43	BV	113	
44	BW	96	
45	BX	110	
46	BY	206	
47	BZ	85	
48	B1	67	
49	B2	60	
50	B3	71	
51	B4	60	
52	B5	54	
53	B6	49	
54	B7	65	

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Mol	Chain	Length	Quality of chain
55	B8	37	 A horizontal bar chart representing the quality of chain B8. The bar is divided into four segments: a short green segment at the beginning, followed by a long yellow segment, then a medium orange segment, and a very short red segment at the end.

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 149044 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1515	Total	C	N	O	P	0	0	0
			32554	14490	6022	10527	1515			

- Molecule 2 is a RNA chain called tRNA fMET (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	76	Total	C	N	O	P	0	0	0
			1624	723	295	530	76			

- Molecule 3 is a RNA chain called tRNA PHE (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 16 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	73	Total	C	N	O		0	0	0
			597	380	118	99				

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 23 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	AX	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2889	Total	C	N	O	P	0	0	0
			62218	27691	11629	20009	2889			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	496	G	-	INSERTION	GB 48268

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	123	Total	C	N	O	P	0	0	0
			2641	1175	488	855	123			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	INSERTION	GB 48271
BB	120	U	-	INSERTION	GB 48271

- Molecule 26 is a protein called 50S ribosomal protein L1.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BC	228	Total	C	N	O	S	0	0	0
			1742	1102	318	319	3			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	272	Total	C	N	O	S	0	0	0
			2124	1339	424	358	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	206	Total	C	N	O	S	0	0	0
			1578	997	302	273	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	208	Total	C	N	O	S	0	0	0
			1625	1034	303	286	2			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	182	Total	C	N	O	S	0	0	0
			1482	947	269	261	5			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1328	844	248	235	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	148	Total	C	N	O	S	0	0	0
			1155	737	205	212	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	138	Total	C	N	O	S	0	0	0
			1025	654	181	185	5			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BM	139	Total	C	N	O	S	0	0	0
			1113	717	207	186	3			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	145	Total	C	N	O	S	0	0	0
			1106	688	226	190	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BP	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BQ	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BR	110	Total	C	N	O	0	0	0
			877	553	175	149			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BS	117	Total	C	N	O	S	0	0	0
			976	614	197	164	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BV	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BW	94	Total	C	N	O	0	0	0
			742	483	133	126			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BX	110	Total	C	N	O	S	0	0	0
			844	539	158	141	6			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BY	180	Total	C	N	O	S	0	0	0
			1435	916	256	260	3			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BZ	85	Total	C	N	O	S	0	0	0
			670	415	141	112	2			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	67	Total	C	N	O	S	0	0	0
			567	350	116	99	2			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	59	Total	C	N	O	S	0	0	0
			469	298	90	81				

- Molecule 50 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	57	Total	C	N	O	S	0	0	0
			445	279	87	74	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	49	Total	C	N	O	S	0	0	0
			426	265	87	70	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	64	Total	C	N	O	S	0	0	0
			515	331	102	79	3			

- Molecule 55 is a protein called 50S ribosomal protein L36.

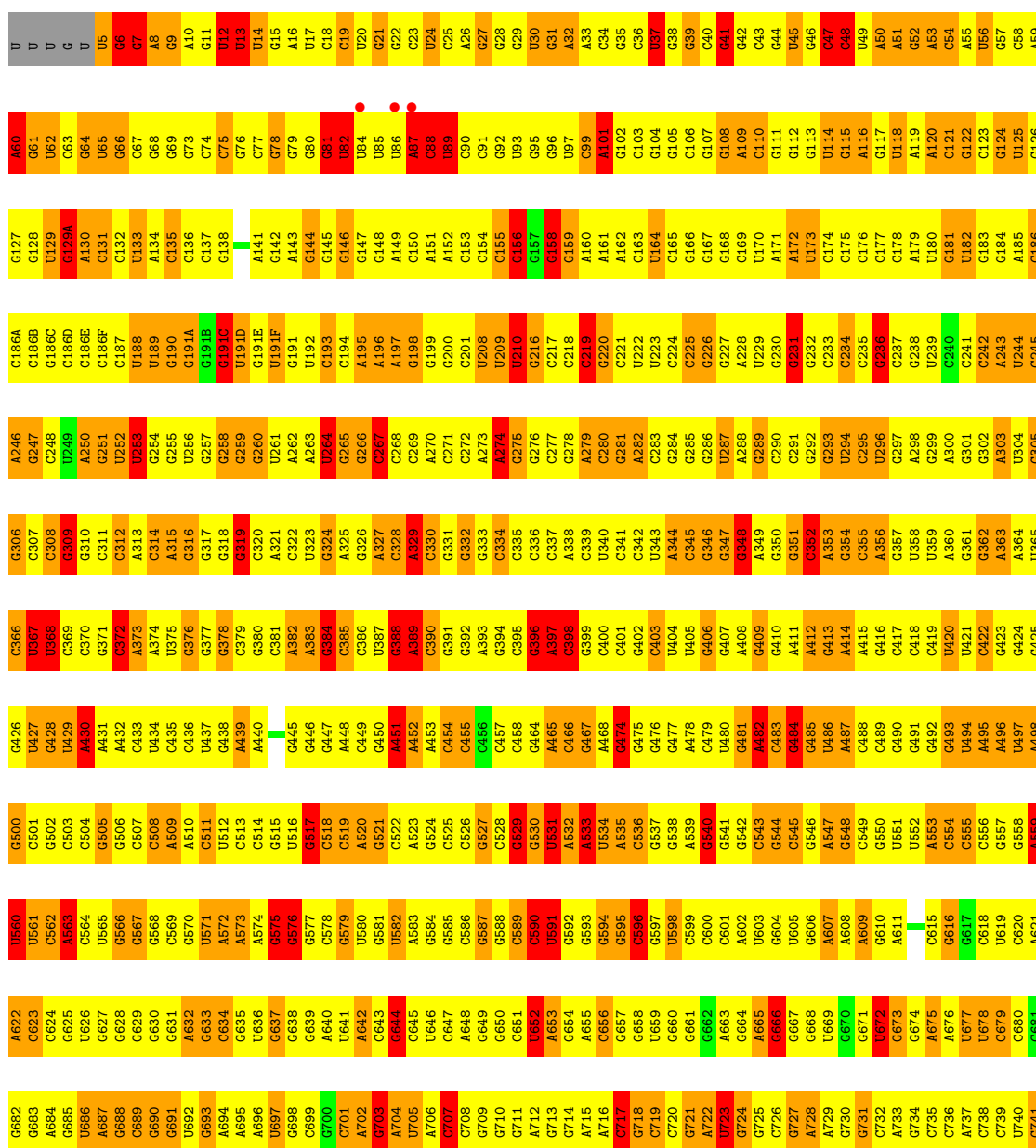
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: 16S rRNA

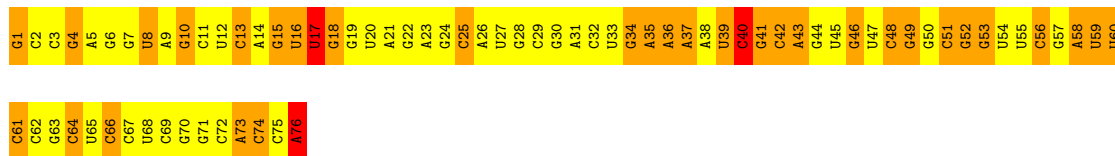
Chain AA: 





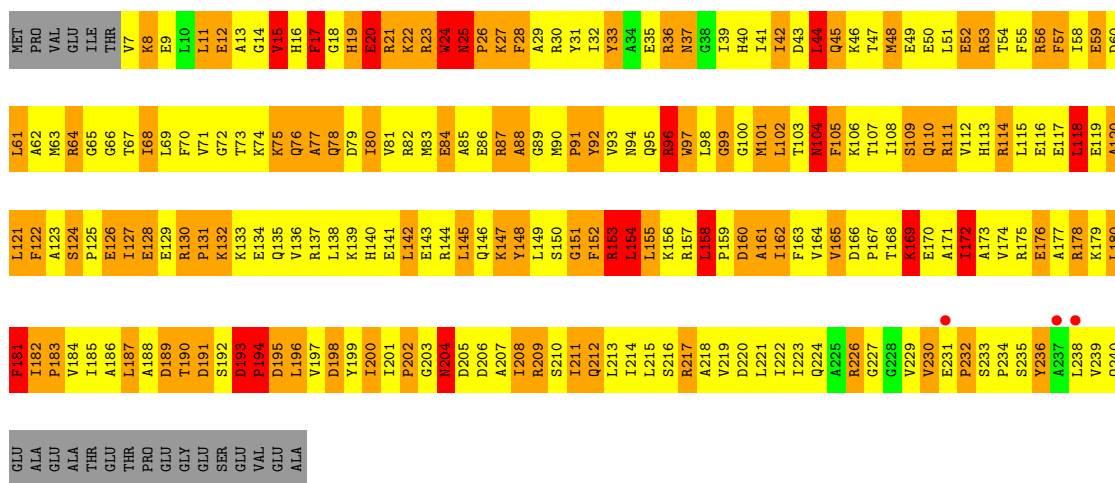
- Molecule 3: tRNA PHE (unmodified bases)

Chain AD:



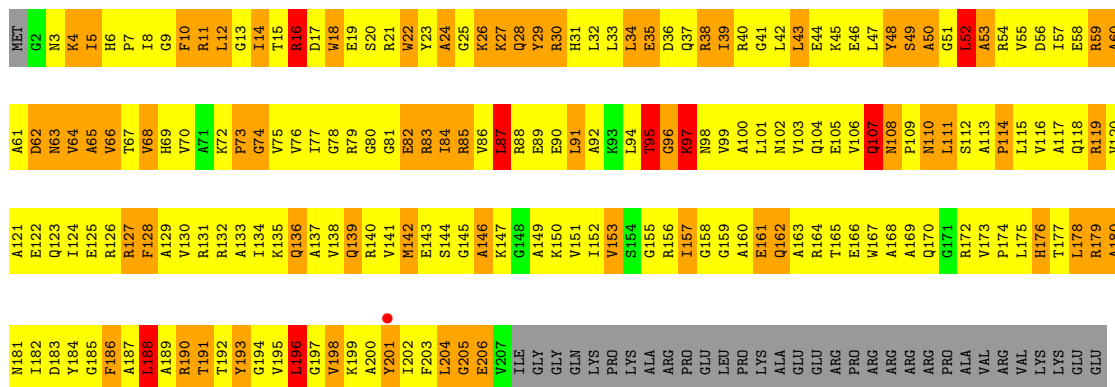
- Molecule 4: 30S ribosomal protein S2

Chain AE:



- Molecule 5: 30S ribosomal protein S3

Chain AF:



- Molecule 6: 30S ribosomal protein S4

Chain AG:





K61 Q62 K63 K64 R65 R66 R67 R68 R69 R70 R71 R72 R73 R74 R75 R76 R77 R78 R79 R80 R81 R82 R83 R84 R85 R86 R87 R88 R89 R90 R91 R92 R93 R94 R95 R96 R97 R98 R99 R100 R101 R102 R103 R104 R105 R106 R107 R108 R109 R110 R111 R112 R113 R114 R115 R116 R117 R118 R119 R120

V121 R122 H123 H124 H125 H126 H127 H128 H129 H130 H131 H132 H133 H134 H135 H136 H137 H138 H139 H140 H141 H142 H143 H144 H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 H156 H157 H158 H159 H160 H161 H162 H163 H164 H165 H166 H167 H168 H169 H170 H171 H172 H173 H174 H175 H176 H177 H178 H179 H180

H181 K182 R183 K184 F185 F186 R187 R188 R189 R190 R191 R192 R193 R194 R195 R196 R197 R198 R199 R200 R201 R202 R203 R204 R205 R206 R207 R208 R209

### • Molecule 7: 30S ribosomal protein S5

Chain AH:

MET PRO GLU D5 D6 D7 D8 D9 D10 D11 D12 D13 D14 D15 D16 D17 D18 D19 D20 D21 D22 D23 D24 D25 D26 D27 D28 D29 D30 D31 D32 D33 D34 D35 D36 D37 D38 D39 D40 D41 D42 D43 D44 D45 D46 D47 D48 D49 D50 D51 D52 D53 D54 D55 D56 D57 D58 D59 D60

Y61 A62 R63 R64 R65 R66 R67 R68 R69 R70 R71 R72 R73 R74 R75 R76 R77 R78 R79 R80 R81 R82 R83 R84 R85 R86 R87 R88 R89 R90 R91 R92 R93 R94 R95 R96 R97 R98 R99 R100 R101 R102 R103 R104 R105 R106 R107 R108 R109 R110 R111 R112 R113 R114 R115 R116 R117 R118 R119 R120

K121 E122 L123 G124 S125 R126 R127 R128 R129 R130 R131 R132 R133 R134 R135 R136 R137 R138 R139 R140 R141 R142 R143 R144 R145 R146 R147 R148 R149 R150 R151 R152 R153 R154 R155 R156 R157 R158 R159 R160 R161 R162 R163 R164 R165 R166 R167 R168 R169 R170 R171 R172 R173 R174 R175 R176 R177 R178 R179 R180 R181 R182 R183 R184 R185 R186 R187 R188 R189 R190 R191 R192 R193 R194 R195 R196 R197 R198 R199 R200 R201 R202 R203 R204 R205 R206 R207 R208 R209 R210 R211 R212 R213 R214 R215 R216 R217 R218 R219 R220 R221 R222 R223 R224 R225 R226 R227 R228 R229 R230 R231 R232 R233 R234 R235 R236 R237 R238 R239 R240 R241 R242 R243 R244 R245 R246 R247 R248 R249 R250 R251 R252 R253 R254 R255 R256 R257 R258 R259 R260

### • Molecule 8: 30S ribosomal protein S6

Chain AI:

K1 A2 R3 R4 R5 R6 R7 R8 R9 R10 R11 R12 R13 R14 R15 R16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 R39 R40 R41 R42 R43 R44 R45 R46 R47 R48 R49 R50 R51 R52 R53 R54 R55 R56 R57 R58 R59 R60

L61 W62 Q63 Q64 R65 R66 R67 R68 R69 R70 R71 R72 R73 R74 R75 R76 R77 R78 R79 R80 R81 R82 R83 R84 R85 R86 R87 R88 R89 R90 R91 R92 R93 R94 R95 R96 R97 R98 R99 R100 R101 R102 R103 R104 R105 R106 R107 R108 R109 R110 R111 R112 R113 R114 R115 R116 R117 R118 R119 R120

### • Molecule 9: 30S ribosomal protein S7

Chain AJ:

MET A2 R3 R4 R5 R6 R7 R8 R9 R10 R11 R12 R13 R14 R15 R16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 R39 R40 R41 R42 R43 R44 R45 R46 R47 R48 R49 R50 R51 R52 R53 R54 R55 R56 R57 R58 R59 R60

V61 F62 K63 K64 A65 A66 A67 A68 A69 A70 A71 A72 A73 A74 A75 A76 A77 A78 A79 A80 A81 A82 A83 A84 A85 A86 A87 A88 A89 A90 A91 A92 A93 A94 A95 A96 A97 A98 A99 R100 R101 R102 R103 R104 R105 R106 R107 R108 R109 R110 R111 R112 R113 R114 R115 R116 R117 R118 R119 R120

A121 H122 E123 L124 M125 M126 A127 A128 A129 A130 K131 K132 K133 K134 K135 K136 K137 K138 K139 K140 K141 K142 K143 K144 K145 K146 K147 K148 K149 K150 K151 K152 K153 K154 K155 K156 K157 K158 K159 K160 K161 K162 K163 K164 K165 K166 K167 K168 K169 K170 K171 K172 K173 K174 K175 K176 K177 K178 K179 K180 K181 K182 K183 K184 K185 K186 K187 K188 K189 K190 K191 K192 K193 K194 K195 K196 K197 K198 K199 K200 K201 K202 K203 K204 K205 K206 K207 K208 K209 K210 K211 K212 K213 K214 K215 K216 K217 K218 K219 K220 K221 K222 K223 K224 K225 K226 K227 K228 K229 K230 K231 K232 K233 K234 K235 K236 K237 K238 K239 K240 K241 K242 K243 K244 K245 K246 K247 K248 K249 K250 K251 K252 K253 K254 K255 K256 K257 K258 K259 K260

### • Molecule 10: 30S ribosomal protein S8

Chain AK:

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V61 Y62 L63 K64 R65 R66 R67 R68 R69 R70 R71 R72 R73 R74 R75 R76 R77 R78 R79 R80 R81 R82 R83 R84 R85 R86 R87 R88 R89 R90 R91 R92 R93 R94 R95 R96 R97 R98 R99 R100 R101 R102 R103 R104 R105 R106 R107 R108 R109 R110 R111 R112 R113 R114 R115 R116 R117 R118 R119 R120



- Molecule 11: 30S ribosomal protein S9

Chain AL:



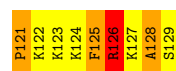
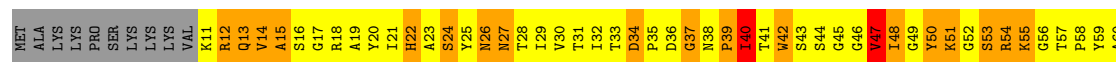
- Molecule 12: 30S ribosomal protein S10

Chain AM:



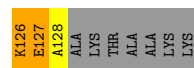
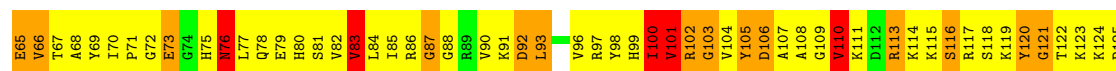
- Molecule 13: 30S ribosomal protein S11

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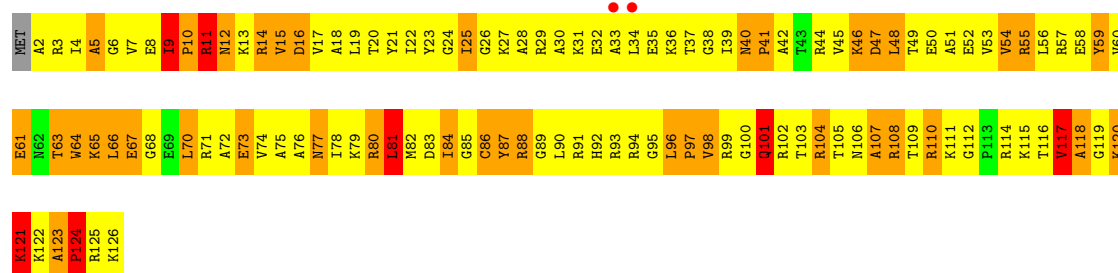


- Molecule 14: 30S ribosomal protein S12

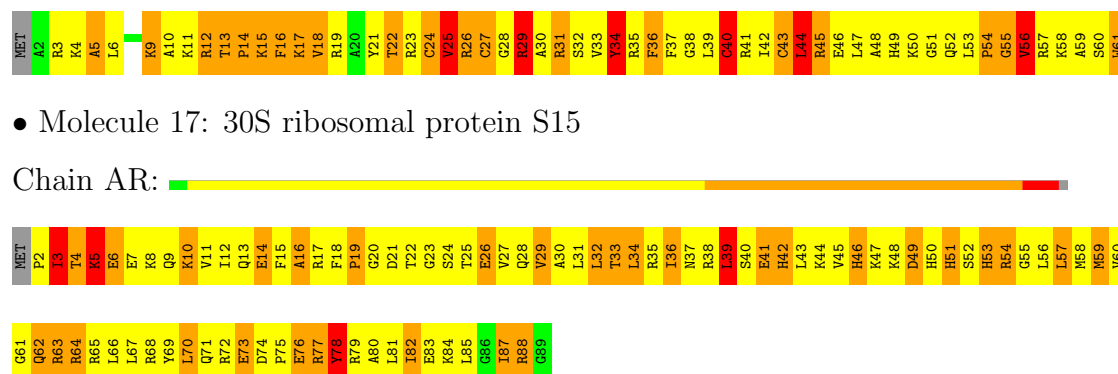
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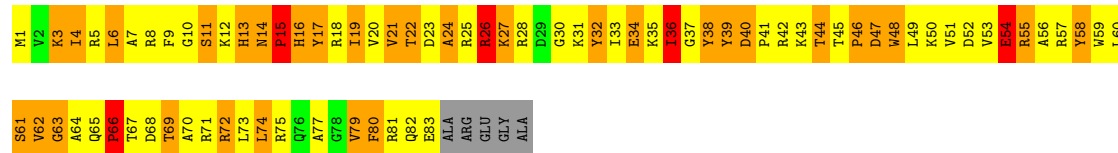
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Chain AP: 

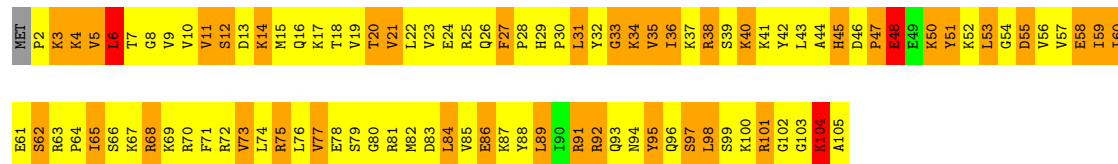
- Molecule 16: 30S ribosomal protein S14

Chain AQ: 

- Molecule 17: 30S ribosomal protein S15

Chain AR: 

- Molecule 18: 30S ribosomal protein S16

Chain AS: 

- Molecule 19: 30S ribosomal protein S17

Chain AT: 

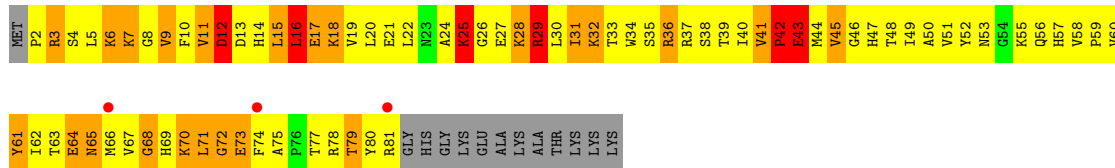
- Molecule 20: 30S ribosomal protein S18

Chain AU: 



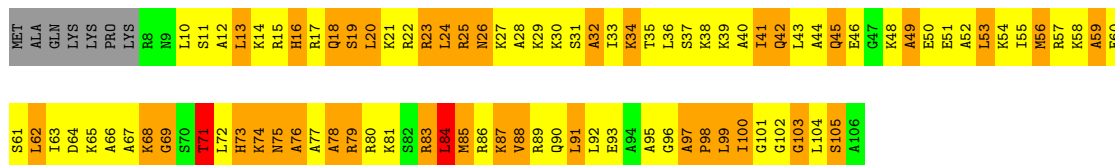
- Molecule 21: 30S ribosomal protein S19

Chain AV:



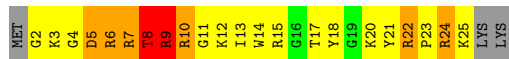
- Molecule 22: 30S ribosomal protein S20

Chain AW:



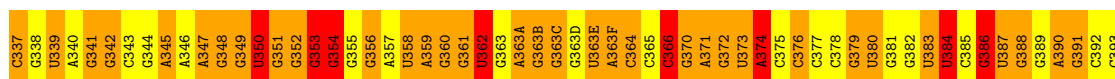
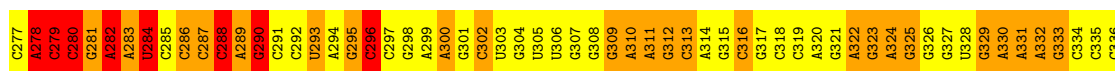
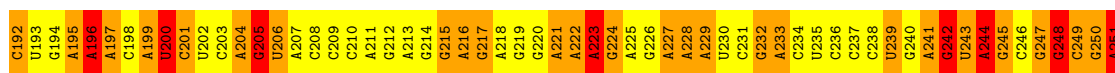
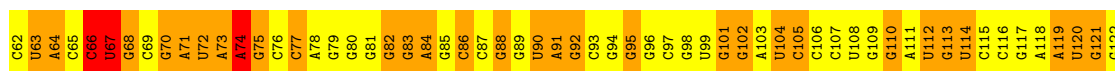
- Molecule 23: 30S ribosomal protein Thx

Chain AX:



- Molecule 24: 23S ribosomal RNA

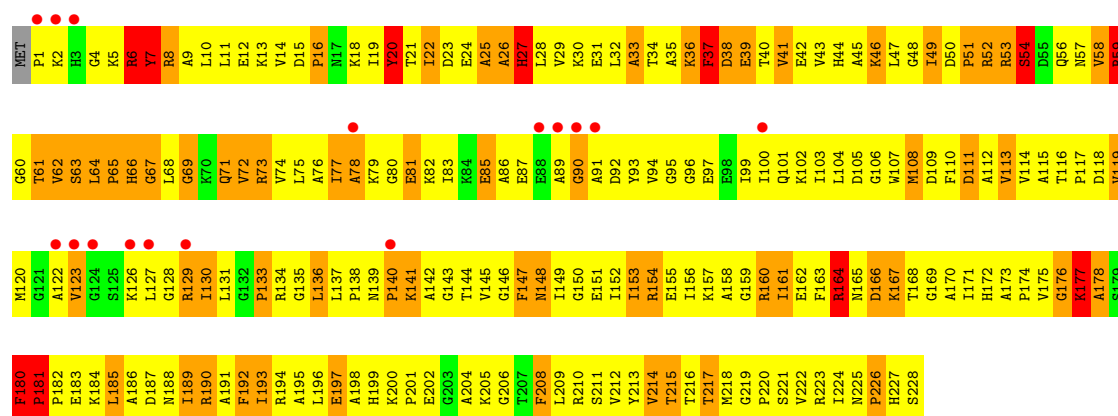
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G1277	G1217	A1156	A1096	G1036	G976	C916	G855	G795	A735	G675	A637	A579	C517	C455	G396
A1278	G1218	G1157	U1097	G1037	G977	A917	G856	G796	C736	A676	G638	C580	G518	A457	G397
G1279	G1219	C1158	A1098	U1038	G978	A918	C857	G797	C737	A677	U639	C581	U519	G458	G398
G1280	A1220	U1159	G1099	G1039	G979	G919	U858	G798	G738	C578	C640	G582	G520	U459	G399
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G1282	C1222	G1161	U1101	C1041	A981	G921	U860	A800	U740	G680	G642	C584	G522	C461	A401
G1283	C1223	G1162	C1102	G1042	C982	U922	A861	A802	G741	G681	A643	G585	C523	C462	A402
G1284	G1224	G1163	A1103	C1043	A983	G923	G862	A803	G742	G682	A644	A586	U524	G463	U403
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A1287	A1227	C1166	G1106	A1046	C986	A926	C865	G805	G745	A685	G647	C589	C527	G466	A406
G1228	G1228	U1167	U1107	G1047	G987	G928	U866	C806	U746	G686	G648	A590	A528	G467	G407
G1289	G1229	G1168	G1108	A1048	A988	G929	C867	U807	U747	C587	G649	C591	A529	G468	G408
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G1293	G1233	G1173	C1112	C1052	C992	A933	U871	U811	A751	C691	A	C595	A533	A472	A412
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G1296	G1236	G1176	G1115	G1055	C995	G936	G874	C814	C754	U694	C	G598	A536	U475	C415
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A1301	A1241	C1181	G1120	G1060	A1000	A941	G879	A819	G759	A699	C	A603	C542	A480	C419
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G1311	C1251	G1191	U1130	A1070	A1010	G951	C889	A829	G769	U709	C	G612	G552	G491	A429
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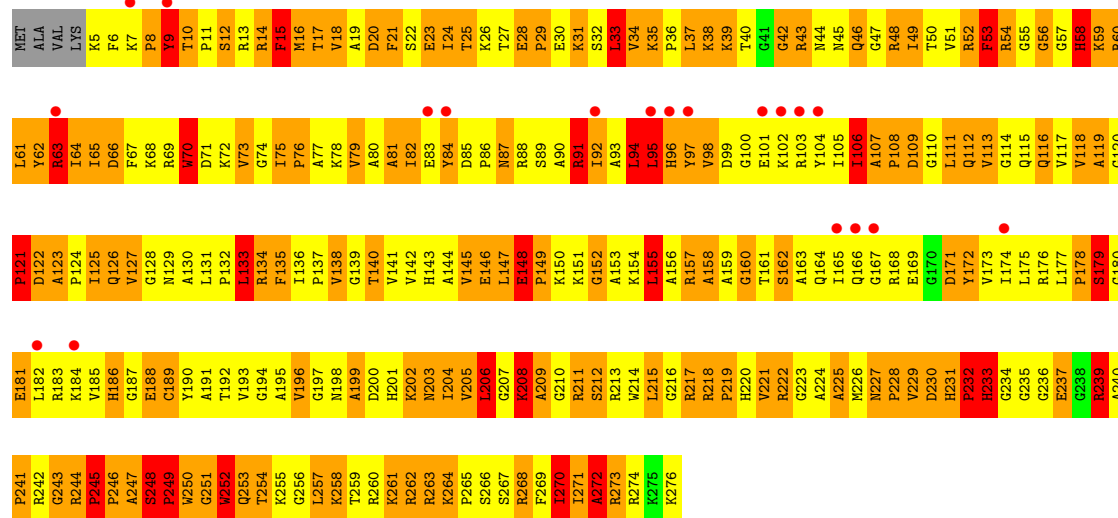
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G2242	U2172	G2112	G2052	G1992	A1932	G1863	C1803	C1741	C1667	A1608	C1547	G1488	G1428	G1368
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G2246	A2176	G2116	G2056	C1996	A1936	A1871	G1807	G1747	U1671	C1612	C1551	G1492	C1432	U1372
A2247	C2177	U2117	A2057	G1997	U1937	A1872	U1808	G1748	C1672	G1613	G1552	C1493	U1433	A1373
C2248	C2178	A2118	A2058	G1998	A1938	G1878	A1809	A1749	U1673	A1614	A1553	A1494	A1434	G1374
U2249	C2179	A2119	A2059	C1999	U1939	C1879	A1810	G1750	G1674	C1615	A1554	A1495	G1435	C1375
G2250	U2180	G2120	A2060	U1940	U1940	C1880	G1811	C1751	C1675	A1616	G1555	A1496	G1436	C1376
G2251	G2181	G2121	G2061	A2001	C1941	C1881	A1812	G1752	A1676	C1617	C1556	U1497	C1437	G1377
C2252	G2182	U2122	A2062	G2002	C1942	C1882	G1813	G1753	A1677	C1618	C1557	C1498	U1438	A1378
G2253	C2183	G2123	C2063	G2003	U1943	G1883	G1814	C1754	G1678	G1619	A1558	C1499	A1439	A1379
C2254	G2184	C2124	C2064	G2004	U1944	A1884	A1815	A1755	U1679	G1620	G1559	C1500	G1440	G1380
G2255	C2185	G2125	C2065	A2005	G1945	A1885	G1816	G1756	U1680	U1621	G1560	C1501	G1441	G1381
G2256	G2186	A2126	C2066	C2006	U1946	C1886	G1817	U1757	G1681	G1622	G1561	C1502	G1442	G1382
U2257	G2187	G2127	G2067	C2007	U1947	C1887	U1818	G1758	G1682	G1623	A1562	U1503	G1443	C1383
C2258	C2188	C2128	U2068	C2008	G1948	G1888	A1819	A1759	C1683	G1624	G1563	C1504	G1444	A1384
G2259	U2189	C2129	G2069	G2009	G1949	A1889	U1820	A1760	C1684	C1625	C1564	C1505	A1444A	G1385
C2260	U2190	G2130	G2070	U1950	A1890	A1890	A1821	C1761	C1685	G1626	C1565	C1506	C1445	G1386
C2261	G2191	C2131	A2071	U1951	U1951	G1891	G1822	A1762	C1686	G1627	A1566	A1507	C1446	C1387
U2262	G2192	U2132	G2072	A1952	C1892	C1892	G1763	G1763	C1687	G1628	A1567	A1508	G1447	G1388
C2263	G2193	C2073	A2013	A1953	C1893	G1894	G1824	G1764	U1688	U1629	G1568	C1509	G1448	G1389
C2264	A2194	A2134	U2074	G1954	C1894	C1894	A1825	G1765	A1689	G1630	A1569	A1510	A1449	U1390
U2265	C2195	U2075	U2075	U1955	U1955	C1895	G1826	U1766	A1690	C1630A	A1570	A1511	G1449A	U1391
A2266	C2196	U2076	U2076	U1956	U1956	G1896	G1827	C1767	C1691	A1631	A1571	A1512	G1450	A1392
G2267	U2197	C2137	A2077	C1957	U1957	G1897	G1828	U1768	C1692	C1632	A1572	C1513	C1451	A1393
A2268	A2198	C2138	C2078	C1958	C1958	U1898	A1829	G1769	U1693	G1633	U1573	U1514	A1453	U1394

Chain BC:



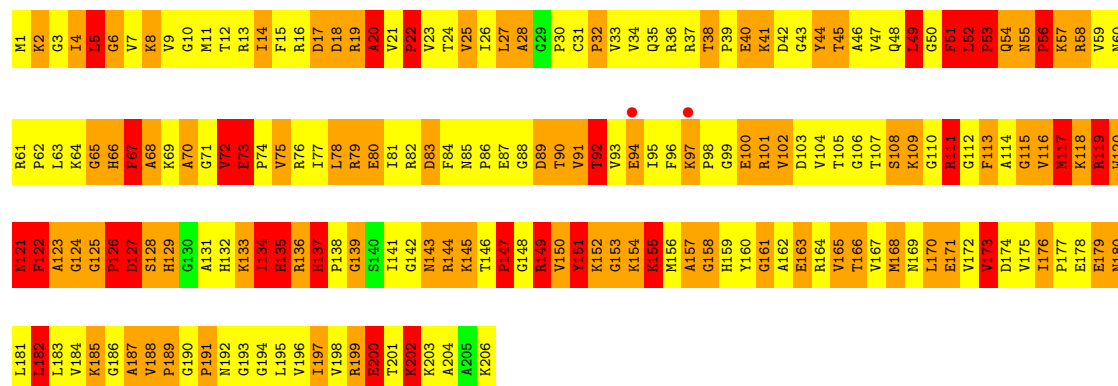
• Molecule 27: 50S ribosomal protein L2

Chain BD:



• Molecule 28: 50S ribosomal protein L3

Chain BE:



• Molecule 29: 50S ribosomal protein L4

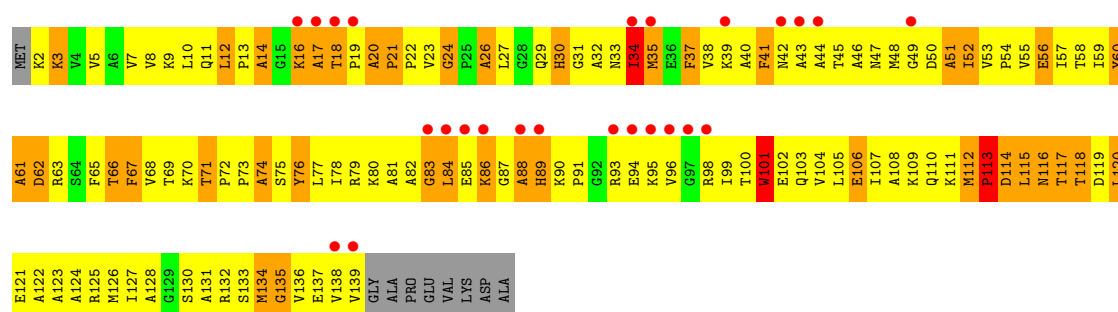
Chain BF:





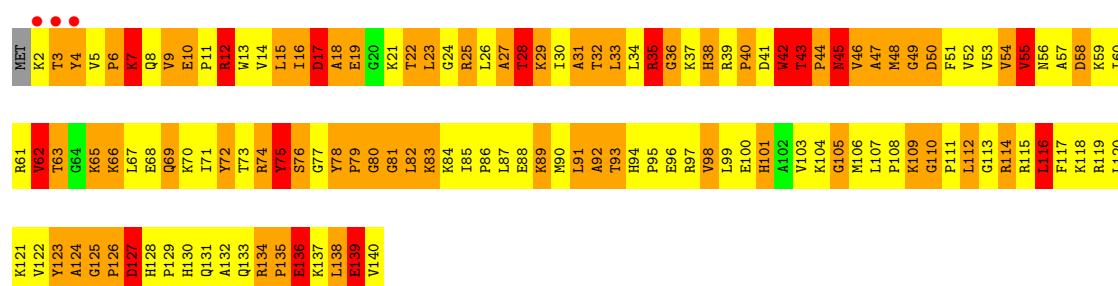
- Molecule 33: 50S ribosomal protein L11

Chain BL:



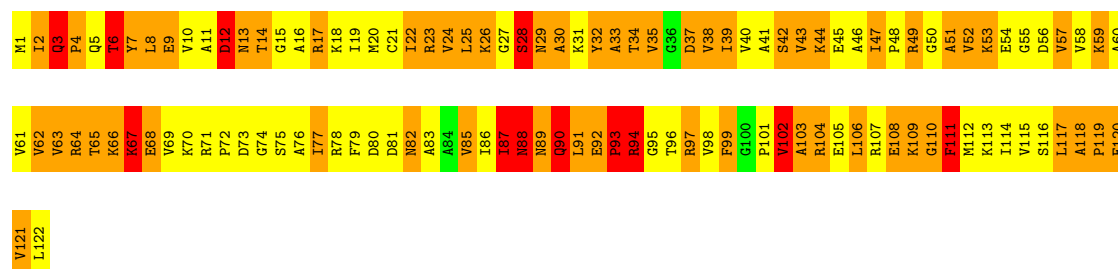
- Molecule 34: 50S ribosomal protein L13

Chain BM:



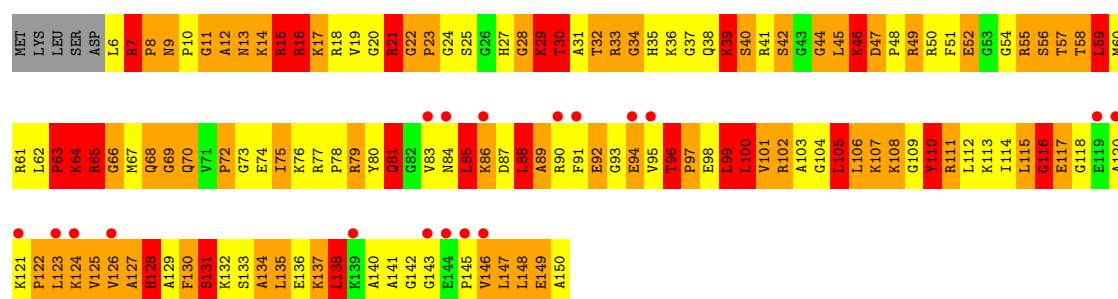
- Molecule 35: 50S ribosomal protein L14

Chain BN:



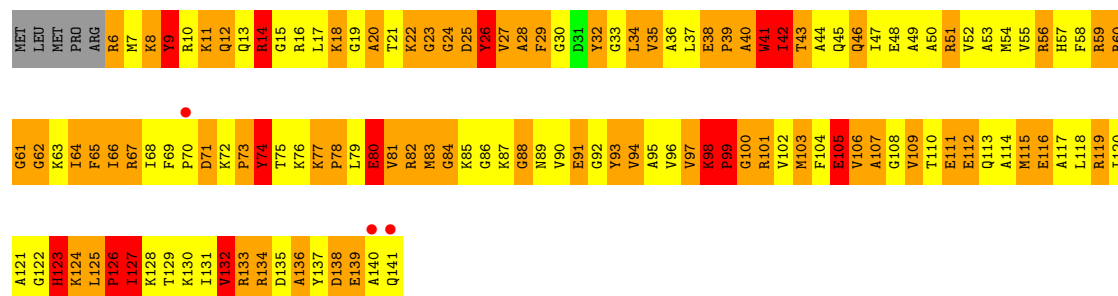
- Molecule 36: 50S ribosomal protein L15

Chain BO:



- Molecule 37: 50S ribosomal protein L16

Chain BP:



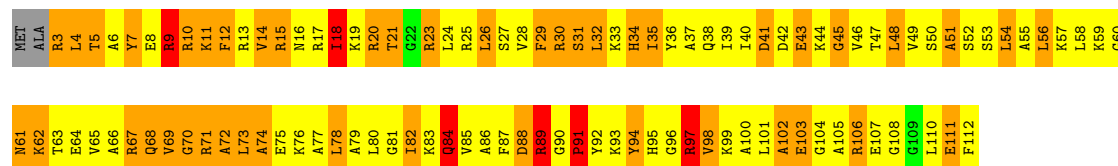
- Molecule 38: 50S ribosomal protein L17

Chain BQ:



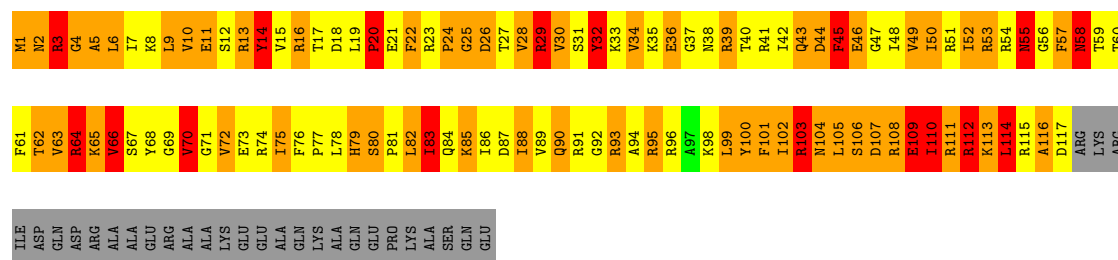
- Molecule 39: 50S ribosomal protein L18

Chain BR:



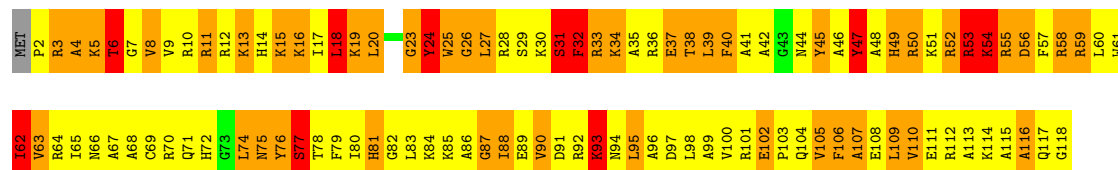
- Molecule 40: 50S ribosomal protein L19

Chain BS:



- Molecule 41: 50S ribosomal protein L20

Chain BT:



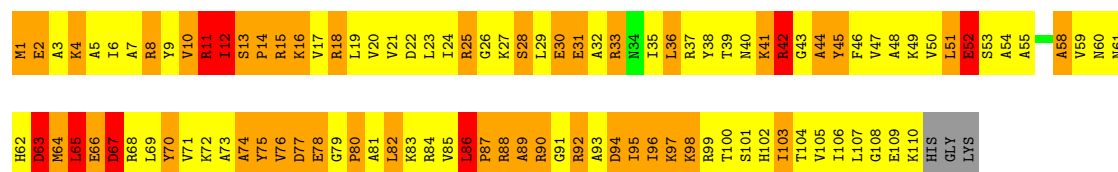
- Molecule 42: 50S ribosomal protein L21

Chain BU:



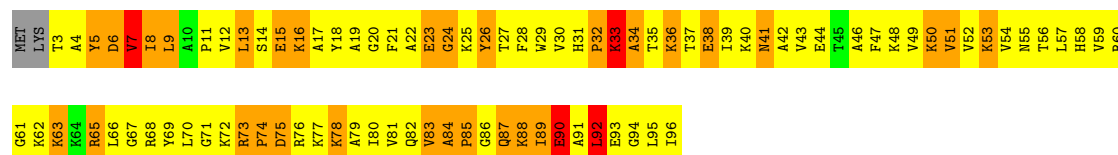
- Molecule 43: 50S ribosomal protein L22

Chain BV:



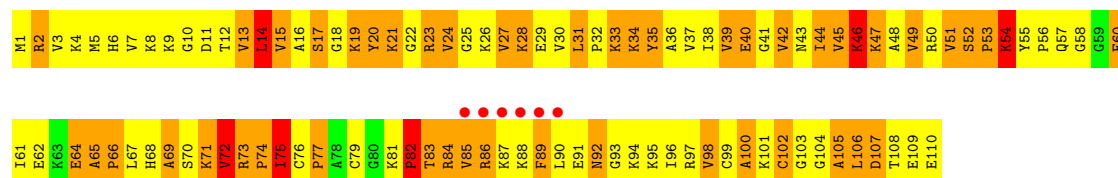
- Molecule 44: 50S ribosomal protein L23

Chain BW:



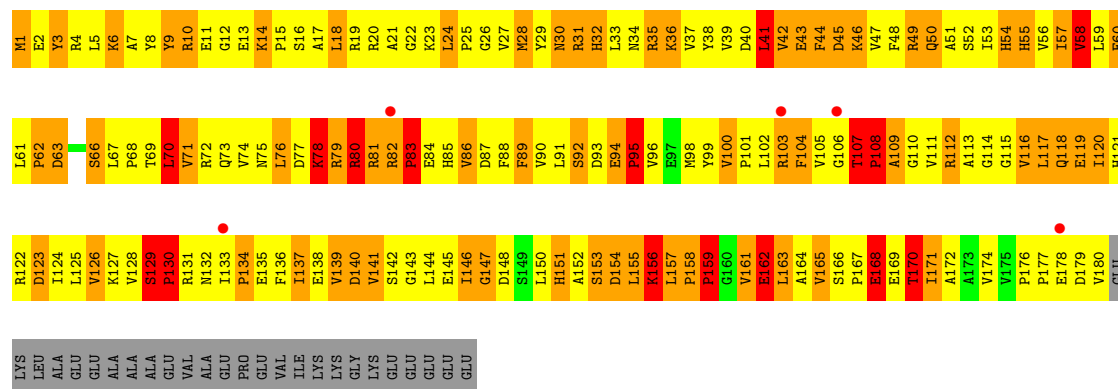
- Molecule 45: 50S ribosomal protein L24

Chain BX:



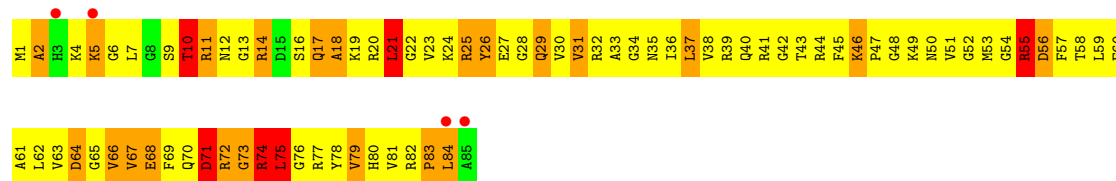
- Molecule 46: 50S ribosomal protein L25

Chain BY:



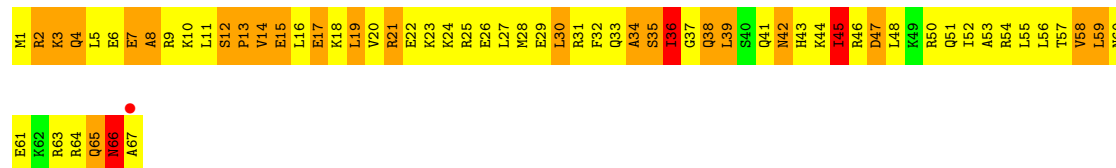
- Molecule 47: 50S ribosomal protein L27

Chain BZ:



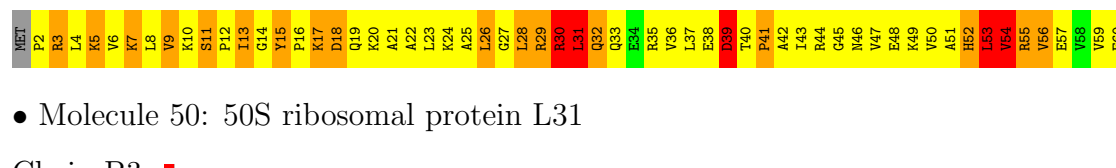
- Molecule 48: 50S ribosomal protein L29

Chain B1:



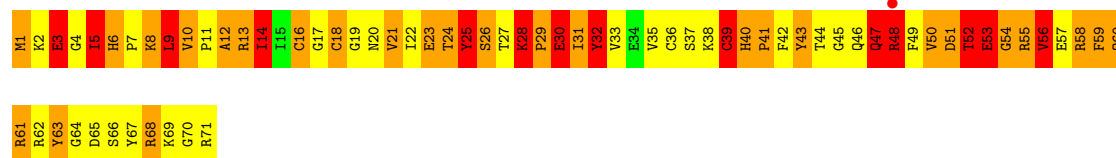
- Molecule 49: 50S ribosomal protein L30

Chain B2:



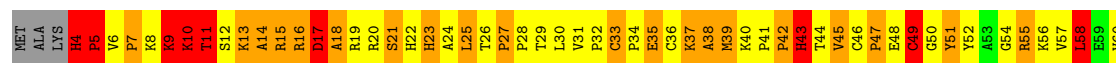
- Molecule 50: 50S ribosomal protein L31

Chain B3:



- Molecule 51: 50S ribosomal protein L32

Chain B4:



- Molecule 52: 50S ribosomal protein L33

Chain B5:



- Molecule 53: 50S ribosomal protein L34

Chain B6:

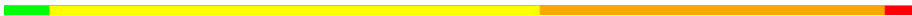


● Molecule 54: 50S ribosomal protein L35

Chain B7: 



● Molecule 55: 50S ribosomal protein L36

Chain B8: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	509.52Å 509.52Å 804.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.00 430.52 – 4.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (300.00-5.00) 96.7 (430.52-4.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 4.88Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.263 , 0.323 0.356 , 0.374	Depositor DCC
$R_{free}$ test set	10549 reflections (4.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.08 , 20.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	1 of 252174 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	149044	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	AA	0.94	48/36438 (0.1%)	1.12	150/56869 (0.3%)
2	AC	1.00	1/1814 (0.1%)	0.92	3/2825 (0.1%)
3	AD	0.80	1/1813 (0.1%)	0.94	3/2823 (0.1%)
4	AE	0.65	0/1935	1.02	3/2609 (0.1%)
5	AF	0.55	0/1636	0.98	4/2205 (0.2%)
6	AG	0.68	1/1733 (0.1%)	1.07	5/2318 (0.2%)
7	AH	0.68	0/1162	1.06	2/1564 (0.1%)
8	AI	0.68	0/856	1.01	3/1154 (0.3%)
9	AJ	0.60	0/1276	0.90	0/1709
10	AK	0.68	0/1136	1.10	5/1527 (0.3%)
11	AL	0.54	0/1029	0.87	0/1379
12	AM	0.49	0/807	0.88	0/1085
13	AN	0.73	0/900	1.06	3/1213 (0.2%)
14	AO	0.67	0/986	1.12	6/1320 (0.5%)
15	AP	0.53	0/1008	0.90	2/1347 (0.1%)
16	AQ	0.57	0/501	1.01	1/664 (0.2%)
17	AR	0.71	0/745	1.00	1/992 (0.1%)
18	AS	0.72	0/716	1.05	3/963 (0.3%)
19	AT	0.73	0/870	1.07	2/1159 (0.2%)
20	AU	0.64	0/603	1.02	3/799 (0.4%)
21	AV	0.55	0/661	0.94	0/890
22	AW	0.77	0/765	1.03	1/1007 (0.1%)
23	AX	0.48	0/212	0.85	1/277 (0.4%)
24	BA	1.06	154/69685 (0.2%)	1.16	463/108786 (0.4%)
25	BB	0.86	4/2954 (0.1%)	1.01	8/4606 (0.2%)
26	BC	0.50	0/1775	0.89	2/2393 (0.1%)
27	BD	0.83	3/2174 (0.1%)	1.25	12/2927 (0.4%)
28	BE	0.86	2/1611 (0.1%)	1.29	13/2171 (0.6%)
29	BF	0.69	0/1660	1.11	8/2247 (0.4%)
30	BG	0.63	0/1507	1.05	4/2027 (0.2%)
31	BH	0.62	0/1354	1.06	5/1831 (0.3%)
32	BK	0.69	0/1170	1.08	2/1581 (0.1%)
33	BL	0.49	0/1044	0.90	1/1415 (0.1%)
34	BM	0.83	1/1140 (0.1%)	1.19	8/1537 (0.5%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	BN	1.00	0/942	1.39	8/1268 (0.6%)
36	BO	0.79	0/1123	1.27	15/1493 (1.0%)
37	BP	0.85	1/1100 (0.1%)	1.27	6/1470 (0.4%)
38	BQ	0.69	0/974	1.08	2/1302 (0.2%)
39	BR	0.78	0/887	1.11	2/1180 (0.2%)
40	BS	0.95	0/990	1.44	13/1325 (1.0%)
41	BT	0.79	0/982	1.18	6/1306 (0.5%)
42	BU	0.90	1/790 (0.1%)	1.44	11/1057 (1.0%)
43	BV	0.78	0/886	1.11	2/1189 (0.2%)
44	BW	0.57	0/756	0.91	0/1015
45	BX	0.53	0/857	1.09	4/1142 (0.4%)
46	BY	0.66	0/1467	1.13	6/1992 (0.3%)
47	BZ	0.72	0/679	1.11	2/902 (0.2%)
48	B1	0.64	0/569	0.91	0/751
49	B2	0.63	0/474	1.08	1/635 (0.2%)
50	B3	1.00	2/594 (0.3%)	1.37	8/795 (1.0%)
51	B4	0.74	1/459 (0.2%)	1.12	2/621 (0.3%)
52	B5	0.91	0/433	1.61	7/576 (1.2%)
53	B6	0.81	0/438	1.03	1/575 (0.2%)
54	B7	0.70	0/523	1.23	3/690 (0.4%)
55	B8	0.69	0/310	1.19	2/407 (0.5%)
All	All	0.93	220/161909 (0.1%)	1.13	828/241910 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	217
2	AC	0	13
3	AD	0	7
5	AF	0	1
10	AK	0	1
13	AN	0	1
24	BA	0	546
25	BB	0	16
27	BD	0	2
28	BE	0	1
29	BF	0	1
31	BH	0	1
37	BP	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	BS	0	2
42	BU	0	2
43	BV	0	1
44	BW	0	1
50	B3	0	2
All	All	0	818

The worst 5 of 220 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1203	G	O3'-P	-34.70	1.19	1.61
24	BA	607	U	N3-C4	-31.59	1.10	1.38
24	BA	2501	C	O3'-P	24.61	1.90	1.61
24	BA	607	U	C2-N3	-22.10	1.22	1.37
1	AA	173	U	O3'-P	19.93	1.85	1.61

The worst 5 of 828 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1064	G	N1-C2-N2	-70.70	52.57	116.20
1	AA	1064	G	N3-C2-N2	58.69	160.98	119.90
24	BA	607	U	N3-C4-O4	-29.32	98.87	119.40
24	BA	1203	G	P-O3'-C3'	27.75	153.00	119.70
1	AA	1064	G	N1-C2-N3	-25.80	108.42	123.90

There are no chirality outliers.

5 of 818 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	21	G	Sidechain
1	AA	24	U	Sidechain
1	AA	6	G	Sidechain
1	AA	7	G	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32554	0	16429	6468	0
2	AC	1624	0	826	363	0
3	AD	1623	0	821	385	0
4	AE	1900	0	1951	934	0
5	AF	1612	0	1677	695	0
6	AG	1703	0	1763	800	0
7	AH	1146	0	1207	493	0
8	AI	843	0	857	370	0
9	AJ	1257	0	1296	561	0
10	AK	1116	0	1177	644	0
11	AL	1010	0	1037	460	0
12	AM	794	0	840	363	0
13	AN	885	0	904	407	0
14	AO	970	0	1057	440	0
15	AP	997	0	1072	511	0
16	AQ	492	0	529	255	0
17	AR	734	0	771	300	0
18	AS	700	0	720	308	0
19	AT	857	0	930	415	0
20	AU	597	0	668	331	0
21	AV	647	0	673	300	0
22	AW	763	0	861	356	0
23	AX	208	0	221	83	0
24	BA	62218	0	31353	15020	0
25	BB	2641	0	1337	589	1
26	BC	1742	0	1796	854	0
27	BD	2124	0	2207	1514	0
28	BE	1578	0	1647	1071	0
29	BF	1625	0	1666	891	0
30	BG	1482	0	1546	966	0
31	BH	1328	0	1408	737	0
32	BK	1155	0	1244	550	0
33	BL	1025	0	1074	489	0
34	BM	1113	0	1183	765	0
35	BN	932	0	994	688	0
36	BO	1106	0	1183	834	0
37	BP	1080	0	1127	704	0
38	BQ	960	0	1021	511	0
39	BR	877	0	938	586	0
40	BS	976	0	1033	667	0
41	BT	964	0	1022	665	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BU	779	0	852	580	0
43	BV	876	0	941	448	0
44	BW	742	0	800	376	0
45	BX	844	0	930	504	0
46	BY	1435	0	1463	735	0
47	BZ	670	0	700	371	0
48	B1	567	0	621	314	0
49	B2	469	0	518	304	0
50	B3	581	0	577	360	0
51	B4	445	0	459	296	0
52	B5	426	0	452	291	0
53	B6	430	0	480	261	0
54	B7	515	0	587	388	0
55	B8	307	0	335	148	0
All	All	149044	0	101781	45453	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 182.

The worst 5 of 45453 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
46:BY:27:VAL:HG23	46:BY:85:HIS:CE1	1.45	1.50
46:BY:27:VAL:CG2	46:BY:85:HIS:CE1	1.95	1.45
35:BN:64:ARG:HH11	35:BN:68:GLU:N	1.15	1.44
24:BA:775:G:H2'	24:BA:794:G:C8	1.54	1.42
24:BA:1201:C:N4	24:BA:1241:A:H61	1.15	1.39

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:BB:-1:A:O2'	25:BB:-1:A:O2'[15_545]	2.14	0.06

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
4	AE	232/256 (91%)	119 (51%)	48 (21%)	65 (28%)	0	1
5	AF	204/239 (85%)	117 (57%)	41 (20%)	46 (22%)	0	3
6	AG	206/209 (99%)	99 (48%)	52 (25%)	55 (27%)	0	2
7	AH	148/162 (91%)	89 (60%)	26 (18%)	33 (22%)	0	3
8	AI	99/101 (98%)	62 (63%)	14 (14%)	23 (23%)	0	3
9	AJ	153/156 (98%)	65 (42%)	45 (29%)	43 (28%)	0	1
10	AK	136/138 (99%)	71 (52%)	28 (21%)	37 (27%)	0	1
11	AL	125/128 (98%)	57 (46%)	38 (30%)	30 (24%)	0	2
12	AM	96/105 (91%)	53 (55%)	21 (22%)	22 (23%)	0	3
13	AN	117/129 (91%)	63 (54%)	28 (24%)	26 (22%)	0	3
14	AO	122/132 (92%)	60 (49%)	29 (24%)	33 (27%)	0	2
15	AP	123/126 (98%)	64 (52%)	33 (27%)	26 (21%)	0	4
16	AQ	58/61 (95%)	24 (41%)	16 (28%)	18 (31%)	0	1
17	AR	86/89 (97%)	43 (50%)	26 (30%)	17 (20%)	0	4
18	AS	81/88 (92%)	46 (57%)	22 (27%)	13 (16%)	0	8
19	AT	102/105 (97%)	63 (62%)	20 (20%)	19 (19%)	0	5
20	AU	71/88 (81%)	29 (41%)	23 (32%)	19 (27%)	0	2
21	AV	78/93 (84%)	32 (41%)	24 (31%)	22 (28%)	0	1
22	AW	97/106 (92%)	31 (32%)	43 (44%)	23 (24%)	0	3
23	AX	22/27 (82%)	11 (50%)	5 (23%)	6 (27%)	0	1
26	BC	226/229 (99%)	110 (49%)	62 (27%)	54 (24%)	0	3
27	BD	270/276 (98%)	110 (41%)	66 (24%)	94 (35%)	0	0
28	BE	204/206 (99%)	108 (53%)	40 (20%)	56 (28%)	0	1
29	BF	206/210 (98%)	106 (52%)	45 (22%)	55 (27%)	0	2
30	BG	180/182 (99%)	71 (39%)	52 (29%)	57 (32%)	0	0
31	BH	172/180 (96%)	75 (44%)	50 (29%)	47 (27%)	0	1
32	BK	146/148 (99%)	85 (58%)	36 (25%)	25 (17%)	0	7
33	BL	136/147 (92%)	68 (50%)	38 (28%)	30 (22%)	0	3
34	BM	137/140 (98%)	63 (46%)	28 (20%)	46 (34%)	0	0
35	BN	120/122 (98%)	60 (50%)	24 (20%)	36 (30%)	0	1
36	BO	143/150 (95%)	52 (36%)	40 (28%)	51 (36%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BP	134/141 (95%)	53 (40%)	36 (27%)	45 (34%)	0	0
38	BQ	115/118 (98%)	60 (52%)	37 (32%)	18 (16%)	0	8
39	BR	108/112 (96%)	43 (40%)	35 (32%)	30 (28%)	0	1
40	BS	115/146 (79%)	55 (48%)	27 (24%)	33 (29%)	0	1
41	BT	115/118 (98%)	46 (40%)	40 (35%)	29 (25%)	0	2
42	BU	99/101 (98%)	53 (54%)	19 (19%)	27 (27%)	0	1
43	BV	108/113 (96%)	64 (59%)	20 (18%)	24 (22%)	0	3
44	BW	92/96 (96%)	53 (58%)	18 (20%)	21 (23%)	0	3
45	BX	108/110 (98%)	39 (36%)	34 (32%)	35 (32%)	0	0
46	BY	178/206 (86%)	85 (48%)	50 (28%)	43 (24%)	0	2
47	BZ	83/85 (98%)	48 (58%)	20 (24%)	15 (18%)	0	6
48	B1	65/67 (97%)	30 (46%)	20 (31%)	15 (23%)	0	3
49	B2	57/60 (95%)	33 (58%)	12 (21%)	12 (21%)	0	4
50	B3	69/71 (97%)	20 (29%)	23 (33%)	26 (38%)	0	0
51	B4	55/60 (92%)	14 (26%)	22 (40%)	19 (34%)	0	0
52	B5	47/54 (87%)	15 (32%)	8 (17%)	24 (51%)	0	0
53	B6	47/49 (96%)	18 (38%)	14 (30%)	15 (32%)	0	0
54	B7	62/65 (95%)	23 (37%)	18 (29%)	21 (34%)	0	0
55	B8	35/37 (95%)	21 (60%)	6 (17%)	8 (23%)	0	3
All	All	5988/6337 (94%)	2879 (48%)	1522 (25%)	1587 (26%)	0	2

5 of 1587 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	13	ALA
4	AE	15	VAL
4	AE	17	PHE
4	AE	20	GLU
4	AE	42	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	
4	AE	202/220 (92%)	142 (70%)	60 (30%)	0	5
5	AF	160/188 (85%)	122 (76%)	38 (24%)	1	9
6	AG	180/181 (99%)	130 (72%)	50 (28%)	0	6
7	AH	115/123 (94%)	70 (61%)	45 (39%)	0	1
8	AI	90/90 (100%)	59 (66%)	31 (34%)	0	3
9	AJ	126/127 (99%)	97 (77%)	29 (23%)	1	10
10	AK	119/119 (100%)	76 (64%)	43 (36%)	0	2
11	AL	98/99 (99%)	74 (76%)	24 (24%)	1	9
12	AM	88/92 (96%)	61 (69%)	27 (31%)	0	5
13	AN	90/99 (91%)	70 (78%)	20 (22%)	1	11
14	AO	104/109 (95%)	79 (76%)	25 (24%)	1	9
15	AP	100/101 (99%)	73 (73%)	27 (27%)	1	6
16	AQ	49/50 (98%)	36 (74%)	13 (26%)	1	7
17	AR	79/80 (99%)	56 (71%)	23 (29%)	0	5
18	AS	72/74 (97%)	45 (62%)	27 (38%)	0	1
19	AT	96/97 (99%)	69 (72%)	27 (28%)	0	5
20	AU	64/77 (83%)	50 (78%)	14 (22%)	1	11
21	AV	71/80 (89%)	57 (80%)	14 (20%)	2	15
22	AW	76/82 (93%)	57 (75%)	19 (25%)	1	8
23	AX	19/22 (86%)	16 (84%)	3 (16%)	4	27
26	BC	180/181 (99%)	145 (81%)	35 (19%)	2	16
27	BD	215/218 (99%)	146 (68%)	69 (32%)	0	4
28	BE	166/166 (100%)	95 (57%)	71 (43%)	0	1
29	BF	164/166 (99%)	106 (65%)	58 (35%)	0	2
30	BG	156/156 (100%)	113 (72%)	43 (28%)	0	6
31	BH	143/148 (97%)	91 (64%)	52 (36%)	0	2
32	BK	124/124 (100%)	88 (71%)	36 (29%)	0	5
33	BL	105/111 (95%)	86 (82%)	19 (18%)	2	19
34	BM	118/119 (99%)	82 (70%)	36 (30%)	0	5
35	BN	100/100 (100%)	60 (60%)	40 (40%)	0	1
36	BO	111/116 (96%)	66 (60%)	45 (40%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BP	106/111 (96%)	68 (64%)	38 (36%)	0	2
38	BQ	100/101 (99%)	73 (73%)	27 (27%)	1	6
39	BR	87/88 (99%)	61 (70%)	26 (30%)	0	5
40	BS	105/127 (83%)	65 (62%)	40 (38%)	0	1
41	BT	93/94 (99%)	61 (66%)	32 (34%)	0	3
42	BU	82/82 (100%)	55 (67%)	27 (33%)	0	3
43	BV	90/92 (98%)	56 (62%)	34 (38%)	0	1
44	BW	76/78 (97%)	59 (78%)	17 (22%)	1	11
45	BX	91/91 (100%)	71 (78%)	20 (22%)	1	11
46	BY	159/179 (89%)	107 (67%)	52 (33%)	0	4
47	BZ	67/67 (100%)	49 (73%)	18 (27%)	1	7
48	B1	62/62 (100%)	49 (79%)	13 (21%)	1	12
49	B2	51/52 (98%)	37 (72%)	14 (28%)	0	6
50	B3	63/63 (100%)	42 (67%)	21 (33%)	0	3
51	B4	50/52 (96%)	33 (66%)	17 (34%)	0	3
52	B5	48/52 (92%)	32 (67%)	16 (33%)	0	3
53	B6	42/42 (100%)	29 (69%)	13 (31%)	0	4
54	B7	54/55 (98%)	39 (72%)	15 (28%)	0	6
55	B8	34/34 (100%)	25 (74%)	9 (26%)	1	7
All	All	5040/5237 (96%)	3528 (70%)	1512 (30%)	0	5

5 of 1512 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	BE	57	LYS
31	BH	52	VAL
48	B1	7	GLU
28	BE	119	ARG
29	BF	119	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 190 such sidechains are listed below:

Mol	Chain	Res	Type
26	BC	56	GLN

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Mol	Chain	Res	Type
29	BF	169	ASN
50	B3	20	ASN
26	BC	225	ASN
28	BE	54	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1515/1522 (99%)	430 (28%)	157 (10%)
2	AC	75/77 (97%)	29 (38%)	6 (8%)
24	BA	2888/2916 (99%)	1218 (42%)	265 (9%)
25	BB	122/123 (99%)	49 (40%)	4 (3%)
3	AD	75/76 (98%)	27 (36%)	4 (5%)
All	All	4675/4714 (99%)	1753 (37%)	436 (9%)

5 of 1753 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	14	U

5 of 436 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	350	U
24	BA	776	G
24	BA	2491	U
24	BA	442	G
24	BA	620	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	BA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	2501:C	O3'	2502:G	P	1.90
1	BA	1203:G	O3'	1204:A	P	1.19

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1515/1522 (99%)	-0.72	3 (0%) 93 89	88, 158, 260, 350	0
2	AC	76/77 (98%)	-0.70	1 (1%) 74 61	133, 166, 216, 249	0
3	AD	76/76 (100%)	-0.53	0 100 100	219, 265, 316, 334	0
4	AE	234/256 (91%)	-0.11	3 (1%) 74 61	122, 163, 221, 265	0
5	AF	206/239 (86%)	-0.06	1 (0%) 88 79	143, 182, 210, 228	0
6	AG	208/209 (99%)	-0.26	0 100 100	106, 148, 170, 187	0
7	AH	150/162 (92%)	-0.04	0 100 100	114, 139, 171, 200	0
8	AI	101/101 (100%)	0.54	4 (3%) 36 33	121, 150, 168, 203	0
9	AJ	155/156 (99%)	0.11	0 100 100	155, 180, 208, 214	0
10	AK	138/138 (100%)	-0.31	0 100 100	113, 133, 153, 160	0
11	AL	127/128 (99%)	0.18	2 (1%) 68 57	161, 225, 247, 255	0
12	AM	98/105 (93%)	0.38	8 (8%) 12 17	146, 208, 237, 240	0
13	AN	119/129 (92%)	0.24	2 (1%) 67 55	114, 142, 176, 206	0
14	AO	124/132 (93%)	0.27	2 (1%) 68 57	96, 129, 162, 184	0
15	AP	125/126 (99%)	-0.13	2 (1%) 68 57	167, 194, 223, 230	0
16	AQ	60/61 (98%)	-0.11	0 100 100	163, 188, 203, 206	0
17	AR	88/89 (98%)	-0.33	0 100 100	113, 131, 168, 183	0
18	AS	83/88 (94%)	-0.45	0 100 100	104, 128, 155, 185	0
19	AT	104/105 (99%)	-0.43	0 100 100	98, 126, 169, 215	0
20	AU	73/88 (82%)	-0.14	6 (8%) 12 17	109, 136, 190, 224	0
21	AV	80/93 (86%)	0.38	3 (3%) 38 35	175, 198, 217, 222	0
22	AW	99/106 (93%)	-0.33	0 100 100	105, 134, 163, 166	0
23	AX	24/27 (88%)	-0.17	0 100 100	168, 210, 224, 229	0
24	BA	2889/2916 (99%)	-0.69	2 (0%) 93 91	63, 155, 266, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	BB	123/123 (100%)	-0.58	0 100 100	146, 209, 257, 291	0
26	BC	228/229 (99%)	0.36	16 (7%) 16 20	220, 256, 308, 312	0
27	BD	272/276 (98%)	0.62	19 (6%) 16 20	80, 125, 153, 198	0
28	BE	206/206 (100%)	-0.05	2 (0%) 79 67	69, 117, 172, 224	0
29	BF	208/210 (99%)	-0.11	0 100 100	111, 179, 215, 231	0
30	BG	182/182 (100%)	-0.06	5 (2%) 52 43	160, 198, 226, 240	0
31	BH	174/180 (96%)	-0.01	3 (1%) 67 55	146, 186, 216, 238	0
32	BK	148/148 (100%)	-0.30	0 100 100	135, 161, 188, 190	0
33	BL	138/147 (93%)	0.86	25 (18%) 2 5	277, 307, 330, 334	0
34	BM	139/140 (99%)	0.04	3 (2%) 59 48	107, 133, 167, 183	0
35	BN	122/122 (100%)	0.03	0 100 100	78, 106, 140, 154	0
36	BO	145/150 (96%)	0.56	18 (12%) 5 10	106, 190, 227, 239	0
37	BP	136/141 (96%)	0.11	3 (2%) 59 48	109, 141, 173, 186	0
38	BQ	117/118 (99%)	-0.14	0 100 100	91, 124, 157, 173	0
39	BR	110/112 (98%)	-0.38	0 100 100	152, 183, 210, 248	0
40	BS	117/146 (80%)	0.20	0 100 100	83, 127, 165, 184	0
41	BT	117/118 (99%)	0.13	0 100 100	100, 138, 152, 158	0
42	BU	101/101 (100%)	0.76	8 (7%) 13 18	104, 160, 186, 197	0
43	BV	110/113 (97%)	0.10	0 100 100	110, 143, 179, 195	0
44	BW	94/96 (97%)	-0.08	0 100 100	153, 170, 232, 237	0
45	BX	110/110 (100%)	0.04	6 (5%) 24 25	157, 199, 247, 273	0
46	BY	180/206 (87%)	0.42	5 (2%) 50 42	142, 190, 211, 226	0
47	BZ	85/85 (100%)	-0.24	4 (4%) 30 29	139, 166, 181, 197	0
48	B1	67/67 (100%)	0.24	1 (1%) 70 58	172, 186, 199, 209	0
49	B2	59/60 (98%)	-0.18	0 100 100	127, 163, 188, 202	0
50	B3	71/71 (100%)	-0.13	1 (1%) 72 59	127, 160, 176, 185	0
51	B4	57/60 (95%)	-0.06	0 100 100	96, 147, 217, 241	0
52	B5	49/54 (90%)	0.43	3 (6%) 21 23	141, 163, 183, 198	0
53	B6	49/49 (100%)	0.25	0 100 100	87, 145, 164, 188	0
54	B7	64/65 (98%)	-0.04	0 100 100	113, 131, 153, 165	0
55	B8	37/37 (100%)	-0.38	0 100 100	146, 157, 169, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	10767/11051 (97%)	-0.26	161 (1%) 70 58	63, 160, 260, 350	0

The worst 5 of 161 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	BL	85	GLU	6.1
33	BL	84	LEU	6.0
36	BO	119	GLU	4.9
26	BC	89	ALA	4.7
33	BL	94	GLU	4.4

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.