



## wwPDB EM Validation Summary Report ⓘ

Mar 11, 2025 – 12:44 pm GMT

PDB ID : 6ZTO  
EMDB ID : EMD-11422  
Title : E. coli 70S-RNAP expressome complex in uncoupled state 1  
Authors : Webster, M.W.; Takacs, M.; Weixlbaumer, A.  
Deposited on : 2020-07-20  
Resolution : 3.00 Å (reported)  
Based on initial models : 4YBB, 6ALH

This is a wwPDB EM 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

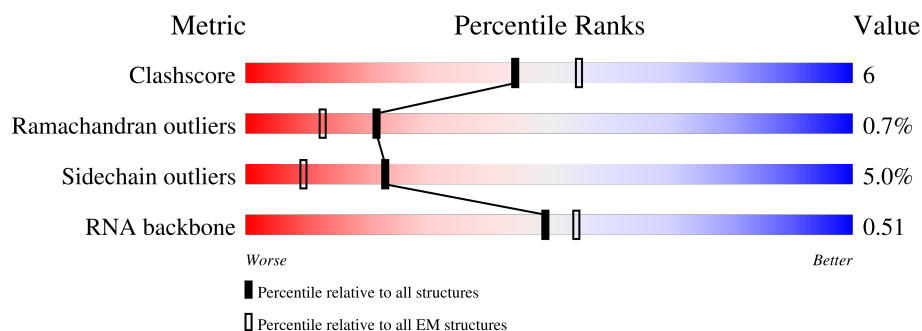
EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

# 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 3.00 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.











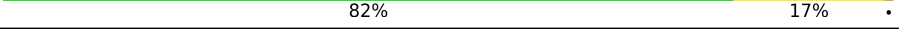

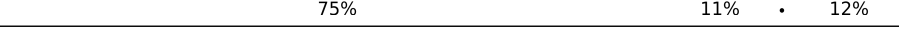
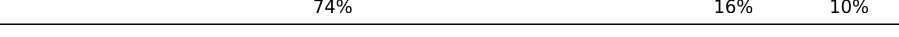

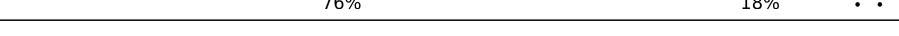
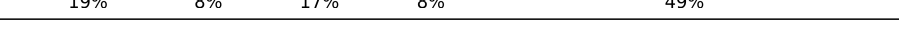

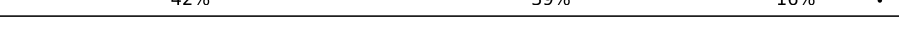

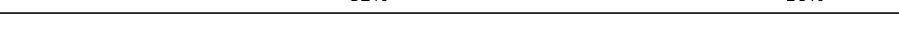






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	AA	1542	65% 27% 7% ..
2	AB	241	71% 20% . 6%
3	AC	233	67% 22% . 10%
4	AD	206	72% 26% .
5	AE	167	74% 19% . 7%
6	AF	131	49% 27% . 21%
7	AG	156	78% 19% ..


























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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	53	
23	AW	77	
24	AX	76	
25	BA	2904	
26	BB	120	
27	BC	273	
28	BD	209	
29	BE	201	
30	BF	179	
31	BG	177	
32	BH	149	



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Mol	Chain	Length	Quality of chain
33	BK	142	 84% 16%
34	BL	123	 84% 15% .
35	BM	144	 83% 16% .
36	BN	136	 82% 18%
37	BO	127	 80% 12% . 6%
38	BP	117	 68% 29% .
39	BQ	115	 81% 17% ..
40	BR	118	 81% 18% ..
41	BS	103	 80% 20%
42	BT	110	 70% 28% .
43	BU	100	 79% 16% . .
44	BV	104	 75% 22% ..
45	BW	94	 81% 17% .
46	BX	85	 81% 6% . 11%
47	BY	78	 82% 17% .
48	BZ	63	 76% 21% . .
49	B1	59	 76% 20% . .
50	B2	57	 79% 19% .
51	B3	55	 67% 25% . .
52	B4	46	 83% 13% .
53	B5	65	 80% 14% 5% .
54	B6	50	 58% 16% . 24%
55	B7	70	 74% 23% .
56	CN	39	 23% 44% 10% 23%
57	CT	39	 13% 41% 23% 23%

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Mol	Chain	Length	Quality of chain
58	CA	329	
58	CB	329	
59	CC	1342	
60	CD	1407	
61	CE	91	

## 2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 172846 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1533	Total	C	N	O	P	0	0
			32909	14684	6037	10655	1533		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	226	Total	C	N	O	S	0	0
			1765	1116	317	324	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	209	Total	C	N	O	S	0	0
			1640	1038	308	291	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	156	Total	C	N	O	S	0	0
			1148	715	217	210	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	9	CYS	GLY	conflict	UNP A0A090BZW5

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	100	Total	C	N	O	S	0	0
			800	500	153	146	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	66	Total	C	N	O	S	0	0
			545	344	102	98	1		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.



Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	27	Total	C	N	O	P	0	0
			572	256	102	187	27		

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 24 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0
			1630	730	290	533	76	1		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	2900	Total	C	N	O	P	0	0
			62270	27786	11456	20128	2900		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BC	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BG	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

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

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BM	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	77	VAL	ILE	conflict	UNP P02413

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BN	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BO	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BP	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BU	96	Total	C	N	O	S	0	0
			764	484	142	136	2		

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	BV	103	Total	C	N	O	0	0
			789	498	148	143		

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BZ	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	B3	53	Total	C	N	O	0	0
			436	281	80	75		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	46	Total	C	N	O	S	0	0
			376	228	89	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B5	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B6	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B7	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 56 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	CN	30	Total	C	N	O	P	0	0
			618	294	114	180	30		

- Molecule 57 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	CT	30	Total	C	N	O	P	0	0
			606	288	105	183	30		

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CA	229	Total	C	N	O	S	0	0
			1775	1106	313	350	6		
58	CB	219	Total	C	N	O	S	0	0
			1684	1051	295	332	6		

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CC	1320	Total	C	N	O	S	0	0
			10415	6535	1815	2021	44		

- Molecule 60 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CD	1333	Total	C	N	O	S	0	0
			10375	6518	1851	1956	50		

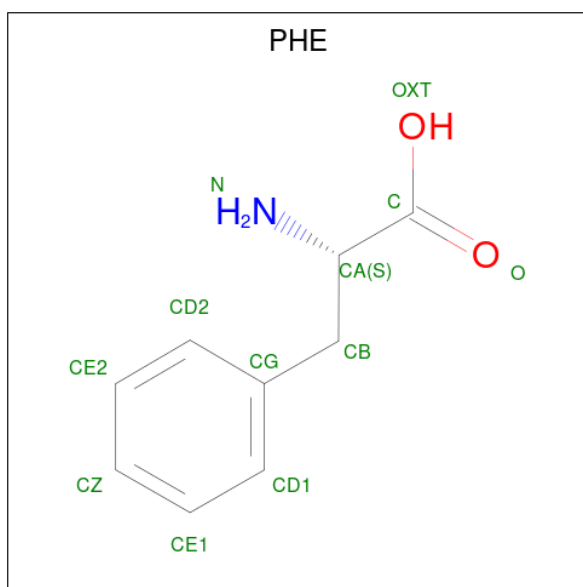
- Molecule 61 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CE	61	Total	C	N	O	S	0	0
			478	295	90	92	1		

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	AA	143	Total	Mg	0
			143	143	
62	AI	1	Total	Mg	0
			1	1	
62	AL	1	Total	Mg	0
			1	1	
62	AM	1	Total	Mg	0
			1	1	
62	AW	5	Total	Mg	0
			5	5	
62	AX	1	Total	Mg	0
			1	1	
62	BA	317	Total	Mg	0
			317	317	
62	BB	9	Total	Mg	0
			9	9	
62	BC	3	Total	Mg	0
			3	3	
62	BN	1	Total	Mg	0
			1	1	
62	BO	1	Total	Mg	0
			1	1	
62	BQ	1	Total	Mg	0
			1	1	
62	BV	1	Total	Mg	0
			1	1	
62	BX	1	Total	Mg	0
			1	1	
62	CD	1	Total	Mg	0
			1	1	

- Molecule 63 is PHENYLALANINE (three-letter code: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
63	AX	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

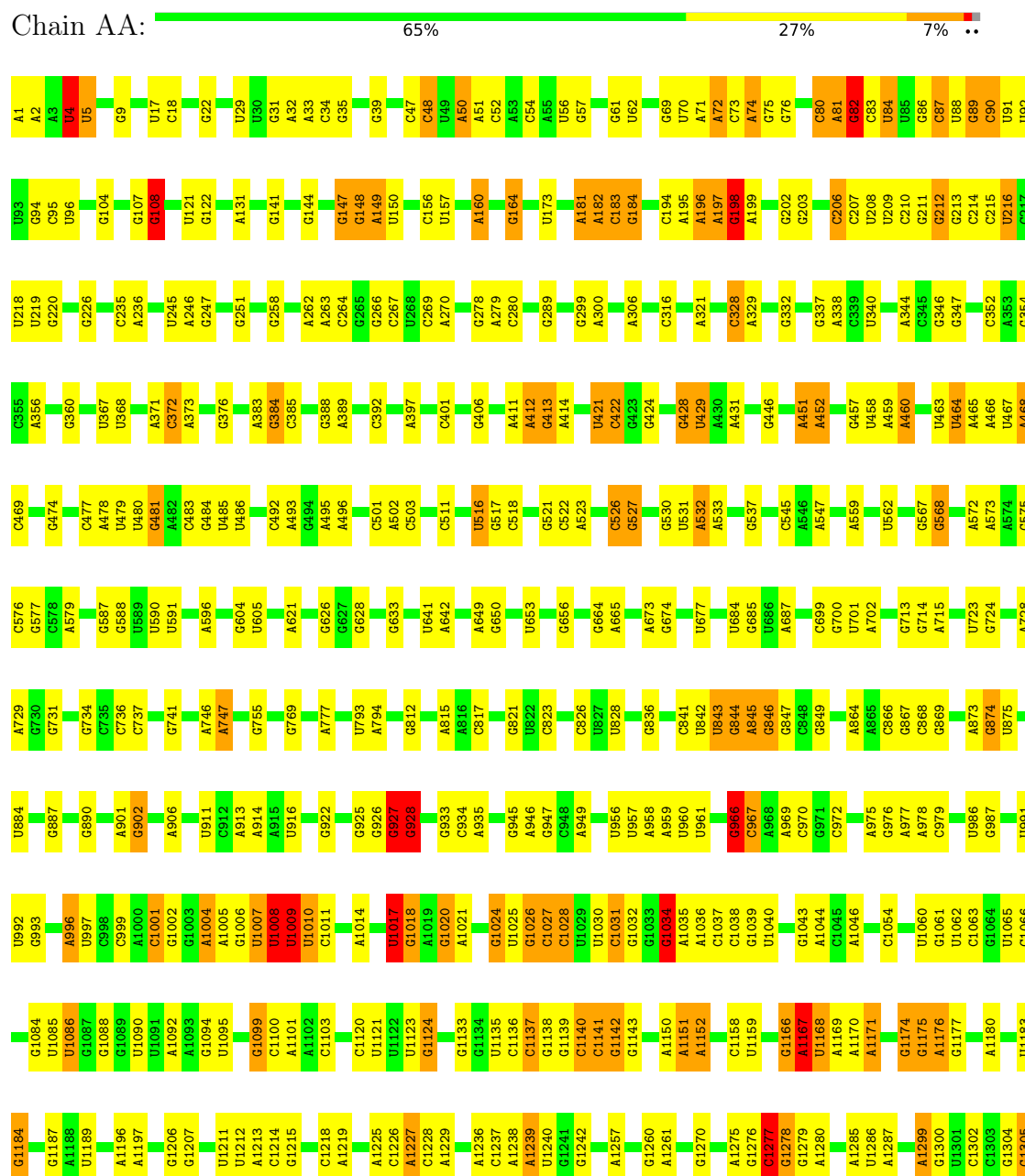
Mol	Chain	Residues	Atoms		AltConf
64	B6	1	Total	Zn	0
			1	1	
64	B7	1	Total	Zn	0
			1	1	
64	CD	2	Total	Zn	0
			2	2	

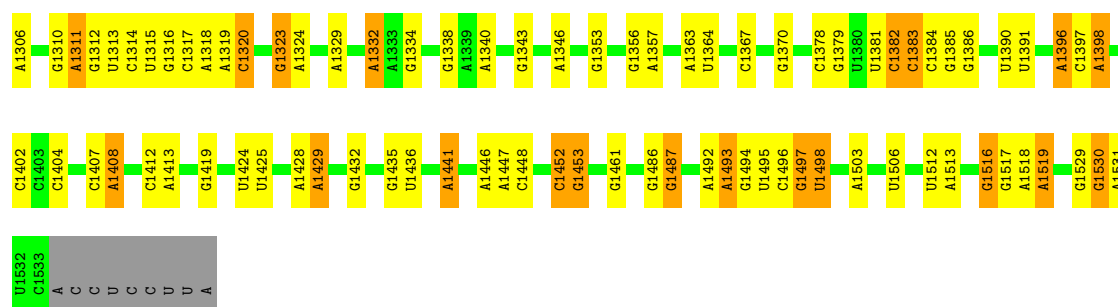


### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

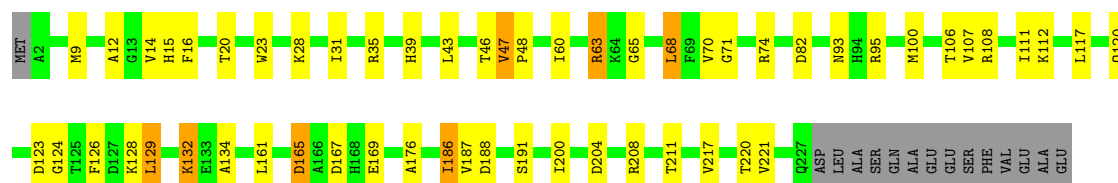
#### • Molecule 1: 16S ribosomal RNA





• Molecule 2: 30S ribosomal protein S2

Chain AB: 71% 20% 6%



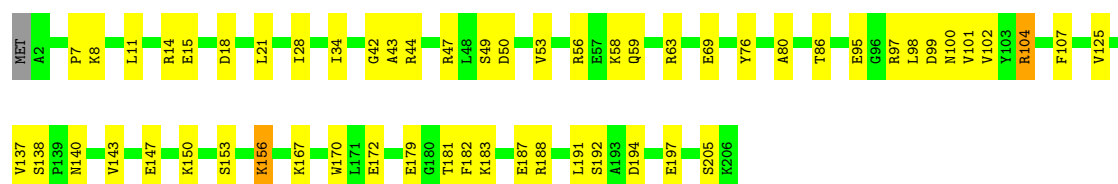
• Molecule 3: 30S ribosomal protein S3

Chain AC: 67% 22% 10%



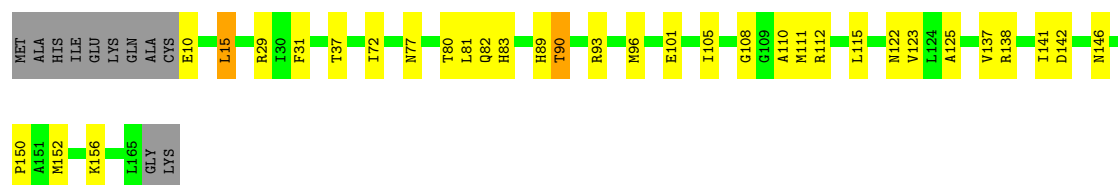
• Molecule 4: 30S ribosomal protein S4

Chain AD: 72% 26%

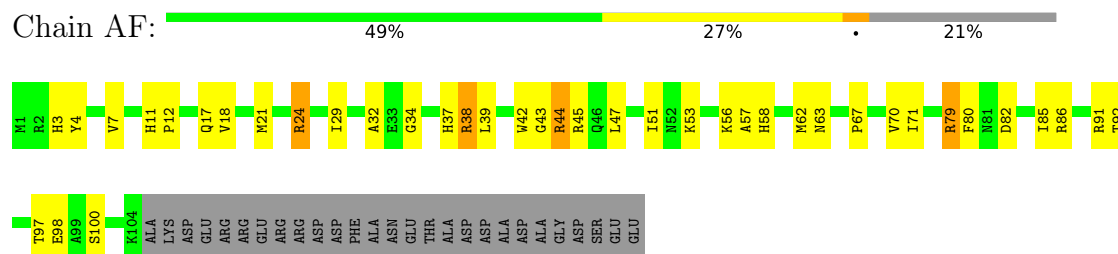


• Molecule 5: 30S ribosomal protein S5

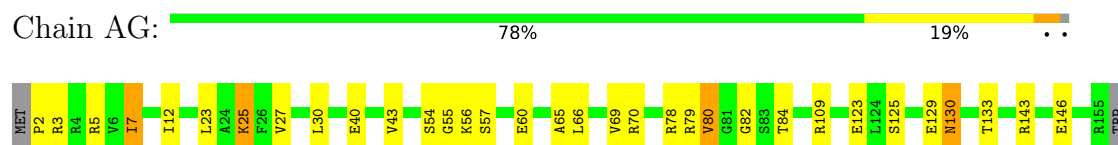
Chain AE: 74% 19% 7%



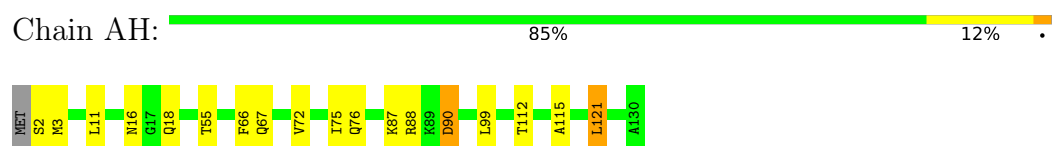
- Molecule 6: 30S ribosomal protein S6



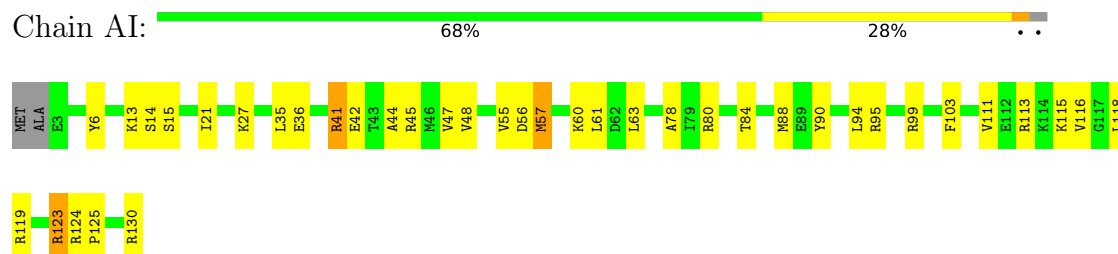
- Molecule 7: 30S ribosomal protein S7



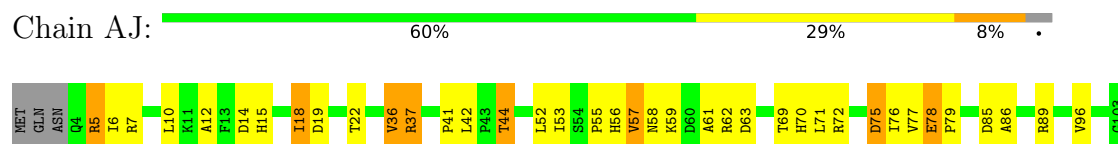
- Molecule 8: 30S ribosomal protein S8



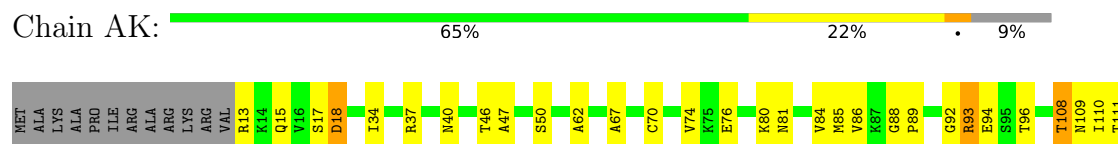
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11





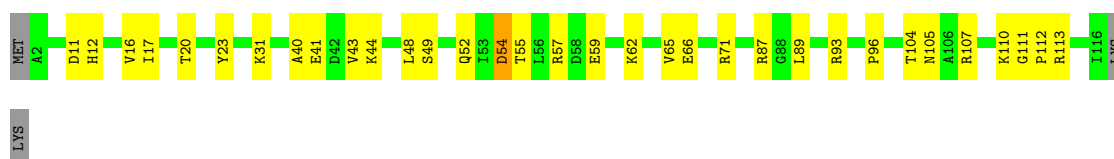
- Molecule 12: 30S ribosomal protein S12

Chain AL: 73% 22% . . .



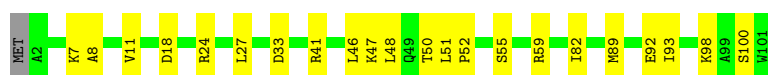
- Molecule 13: 30S ribosomal protein S13

Chain AM: 69% 27% . .



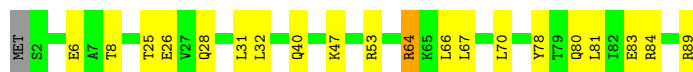
- Molecule 14: 30S ribosomal protein S14

Chain AN: 77% 22% .



- Molecule 15: 30S ribosomal protein S15

Chain AO: 76% 21% . .



- Molecule 16: 30S ribosomal protein S16

Chain AP: 82% 17% .




- Molecule 17: 30S ribosomal protein S17

Chain AQ: 82% 11% 5%




- Molecule 18: 30S ribosomal protein S18

Chain AR:  75% 11% 12%




- Molecule 19: 30S ribosomal protein S19

Chain AS:  74% 16% 10%




- Molecule 20: 30S ribosomal protein S20

Chain AT:  86% 8% 5%



- Molecule 21: 30S ribosomal protein S21

Chain AU:  76% 18% 6%



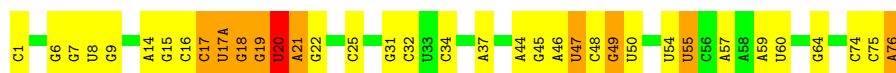
- Molecule 22: mRNA

Chain AV:  19% 8% 17% 8% 49%



- Molecule 23: tRNA(fmet) P-site

Chain AW:  53% 34% 12%




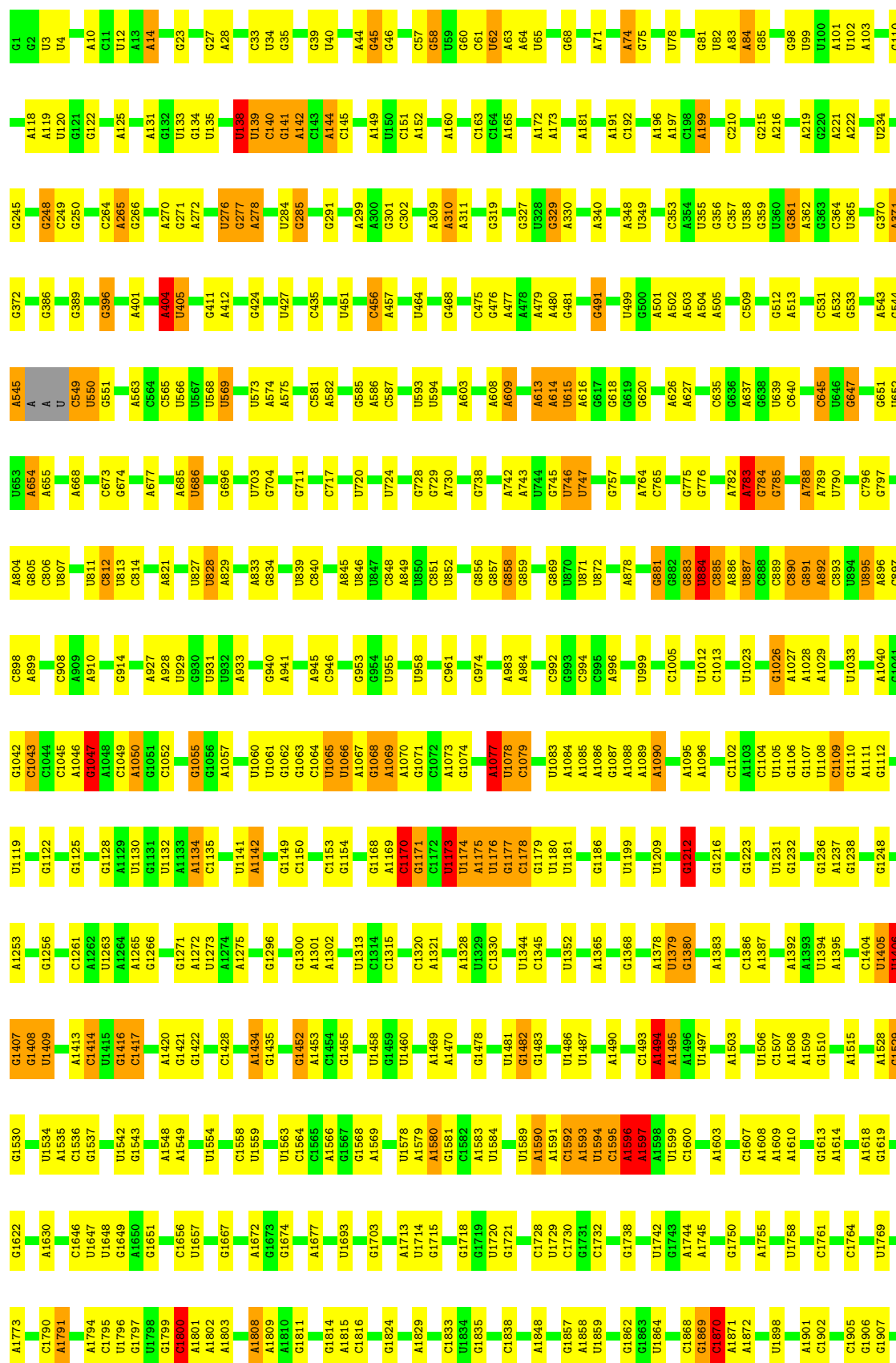
- Molecule 24: Phe-NH-tRNA(Phe) A-site

Chain AX:  42% 39% 16%



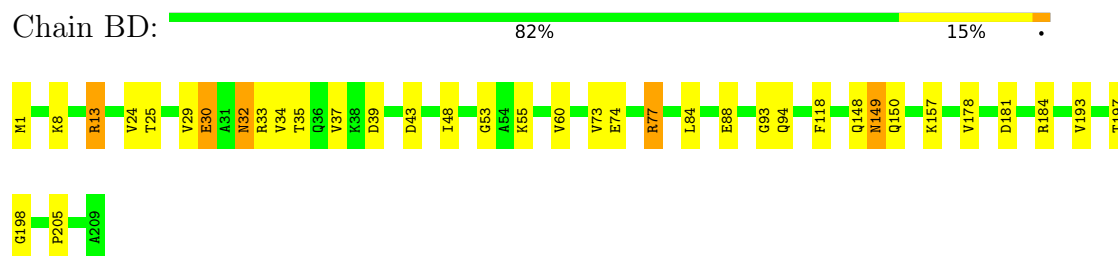
- Molecule 25: 23S ribosomal RNA

Chain BA:  66% 27% 6%

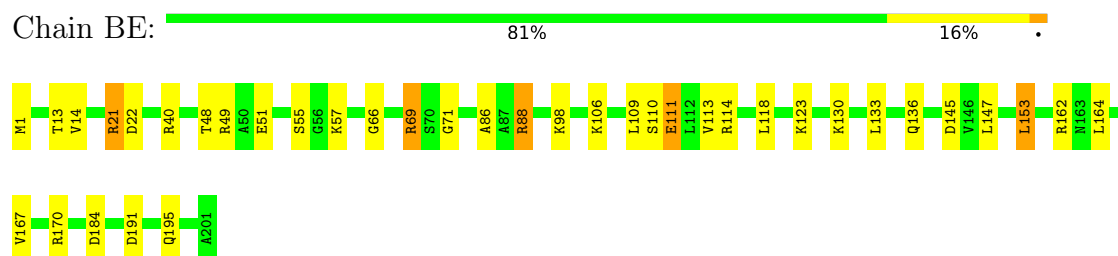




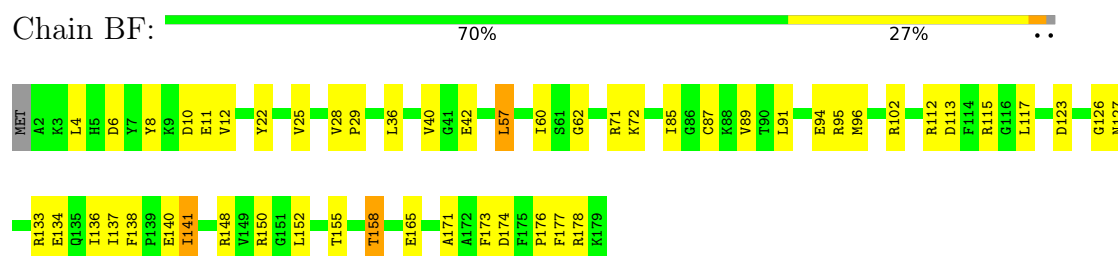
- Molecule 28: 50S ribosomal protein L3



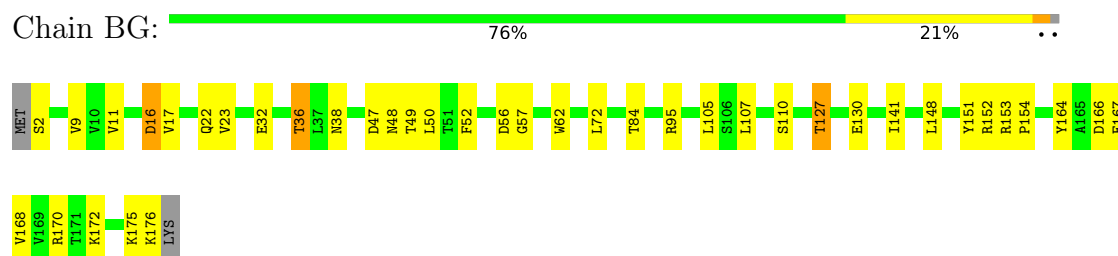
- Molecule 29: 50S ribosomal protein L4



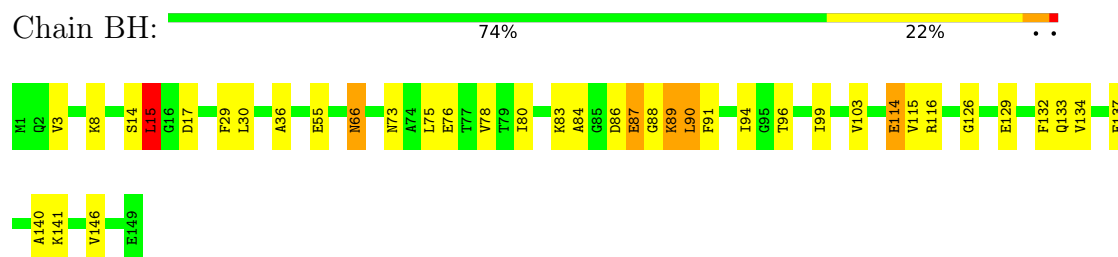
- Molecule 30: 50S ribosomal protein L5



- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9






- Molecule 33: 50S ribosomal protein L13

Chain BK:  84% 16%



- Molecule 34: 50S ribosomal protein L14

Chain BL:  84% 15%




- Molecule 35: 50S ribosomal protein L15

Chain BM:  83% 16%




- Molecule 36: 50S ribosomal protein L16

Chain BN:  82% 18%



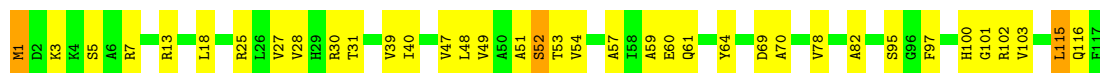
- Molecule 37: 50S ribosomal protein L17

Chain BO:  80% 12% 6%




- Molecule 38: 50S ribosomal protein L18

Chain BP:  68% 29%




- Molecule 39: 50S ribosomal protein L19

Chain BQ:  81% 17%




- Molecule 40: 50S ribosomal protein L20

Chain BR:  81% 18% ..



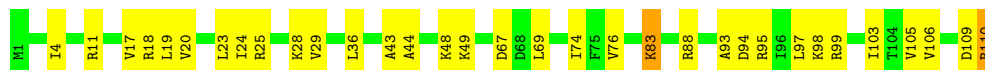
- Molecule 41: 50S ribosomal protein L21

Chain BS:  80% 20%




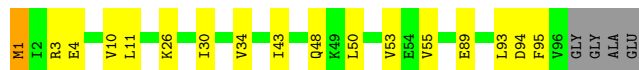
- Molecule 42: 50S ribosomal protein L22

Chain BT:  70% 28% .




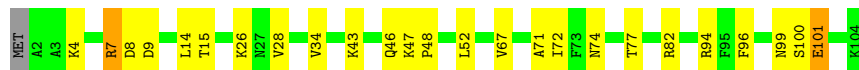
- Molecule 43: 50S ribosomal protein L23

Chain BU:  79% 16% . .




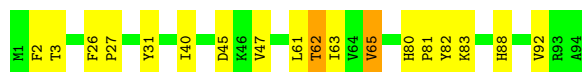
- Molecule 44: 50S ribosomal protein L24

Chain BV:  75% 22% ..




- Molecule 45: 50S ribosomal protein L25

Chain BW:  81% 17% .




- Molecule 46: 50S ribosomal protein L27

Chain BX:  81% 6% . 11%




- Molecule 47: 50S ribosomal protein L28

Chain BY:  82% 17%




- Molecule 48: 50S ribosomal protein L29

Chain BZ:  76% 21%




- Molecule 49: 50S ribosomal protein L30

Chain B1:  76% 20%



- Molecule 50: 50S ribosomal protein L32

Chain B2:  79% 19%




- Molecule 51: 50S ribosomal protein L33

Chain B3:  67% 25%




- Molecule 52: 50S ribosomal protein L34

Chain B4:  83% 13%




- Molecule 53: 50S ribosomal protein L35

Chain B5:  80% 14% 5%



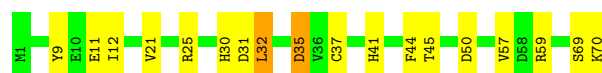
- Molecule 54: 50S ribosomal protein L36

Chain B6:  58% 16% 24%



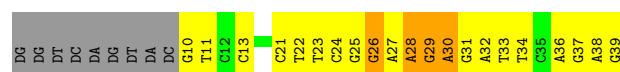
- Molecule 55: 50S ribosomal protein L31

Chain B7:  74% 23%



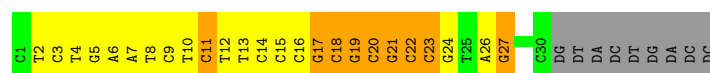
- Molecule 56: Non-template DNA strand

Chain CN:  23% 44% 10% 23%



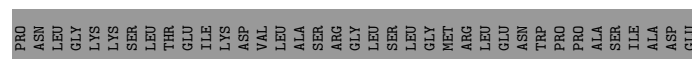
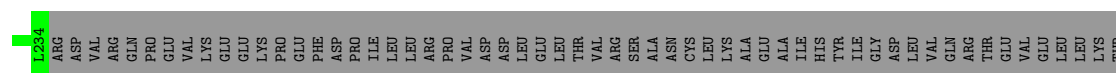
- Molecule 57: Template DNA strand

Chain CT:  13% 41% 23% 23%



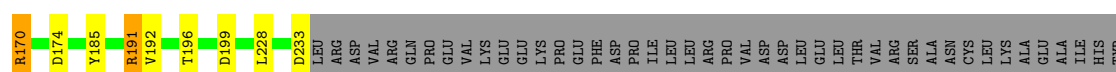
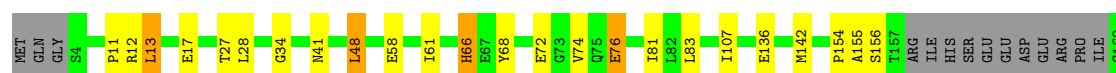
- Molecule 58: DNA-directed RNA polymerase subunit alpha

Chain CA:  60% 9% 30%




- Molecule 58: DNA-directed RNA polymerase subunit alpha

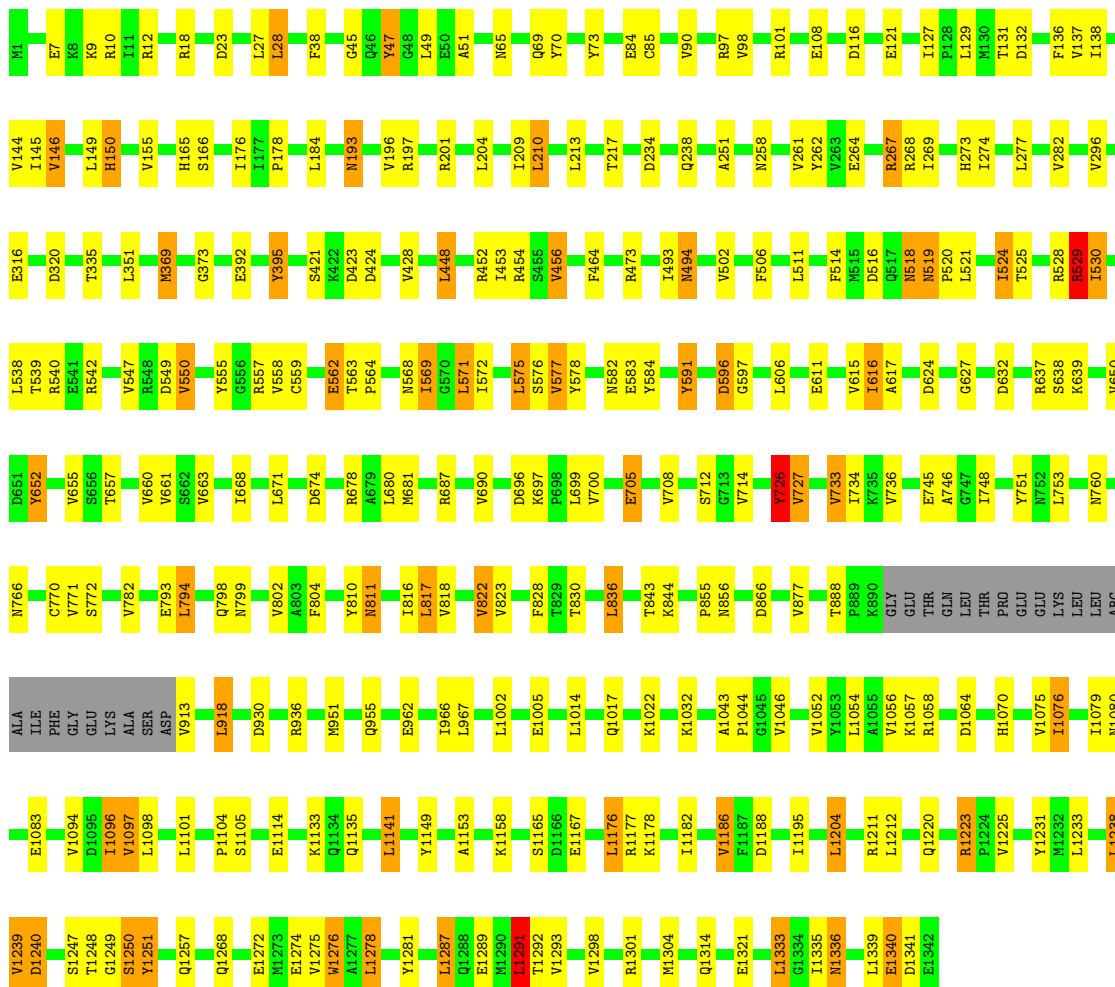
Chain CB:  57% 8% 33%




ILE GLY ASP LEU VAL GLN ARG THR LEU VAL GLY LEU LYS THR PRO ASN LEU GLY LYS LYS SER LEU THR LEU GLY ILE LYS ASP VAL LEU LEU SER ALA SER ARG GLY LEU SER LEU GLY MET ARG LEU LEU ASP ASN TRP PRO PRO ALA ILE SER ILE ASP GLU

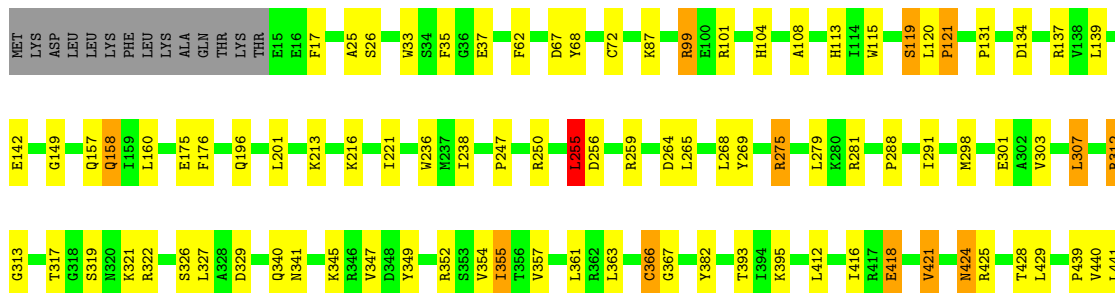
• Molecule 59: DNA-directed RNA polymerase subunit beta

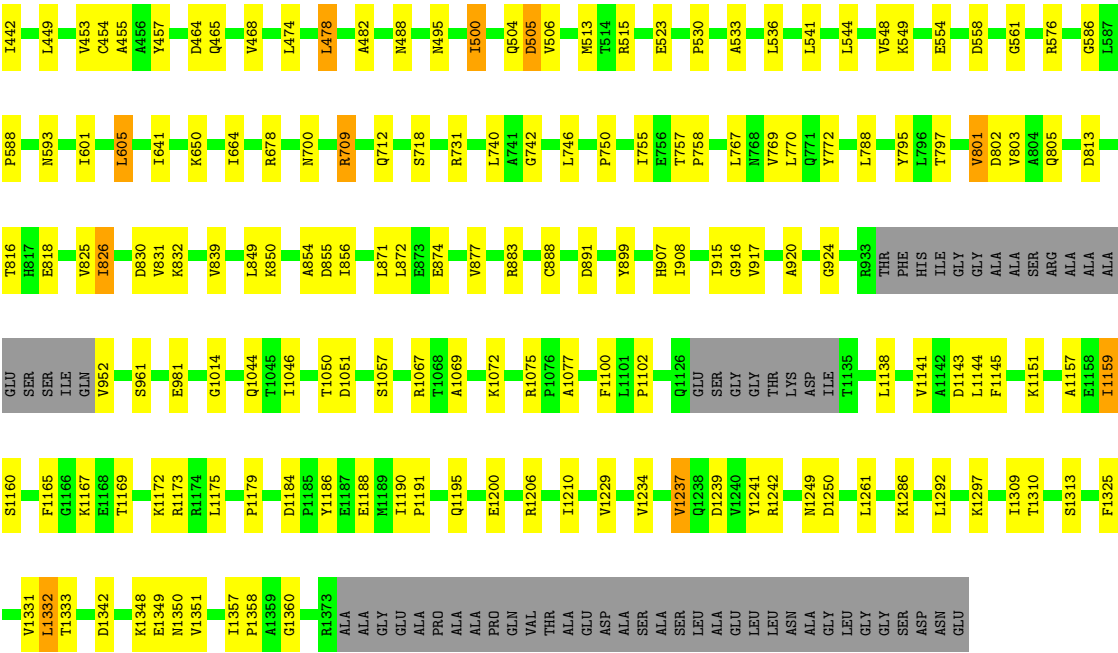
Chain CC:  76% 18%



• Molecule 60: DNA-directed RNA polymerase subunit beta'

Chain CD:  77% 16% 5%





● Molecule 61: DNA-directed RNA polymerase subunit omega



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, OMC, 4D4, 3TD, 4OC, PSU, UR3, G7M, MA6, 4SU, 2MG, OMG, MG, D2T, H2U, 5MC, 6MZ, 1MG, 7MG, 2MA, 3AU, MEQ, ZN, 5MU, MIA

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	1.04	0/36569	0.95	44/57044 (0.1%)
2	AB	0.34	0/1796	0.53	0/2420
3	AC	0.52	0/1667	0.60	0/2246
4	AD	0.40	0/1665	0.54	0/2227
5	AE	0.45	0/1161	0.60	0/1563
6	AF	0.41	0/867	0.59	0/1171
7	AG	0.38	0/1230	0.59	2/1649 (0.1%)
8	AH	0.43	0/989	0.55	1/1326 (0.1%)
9	AI	0.56	0/1043	0.67	0/1387
10	AJ	0.50	0/810	0.69	0/1094
11	AK	0.39	0/893	0.56	0/1205
12	AL	0.48	0/954	0.68	0/1279
13	AM	0.43	0/900	0.62	1/1204 (0.1%)
14	AN	0.52	0/817	0.55	0/1088
15	AO	0.39	0/722	0.53	0/964
16	AP	0.48	0/659	0.54	0/884
17	AQ	0.45	0/657	0.59	0/881
18	AR	0.41	0/554	0.65	1/743 (0.1%)
19	AS	0.51	0/680	0.62	0/915
20	AT	0.41	0/676	0.53	0/895
21	AU	0.35	0/598	0.54	0/792
22	AV	1.98	28/637 (4.4%)	1.78	32/987 (3.2%)
23	AW	0.75	1/1725 (0.1%)	0.94	1/2687 (0.0%)
24	AX	0.58	1/1584 (0.1%)	0.84	1/2463 (0.0%)
25	BA	0.87	2/69165 (0.0%)	0.94	80/107893 (0.1%)
26	BB	0.74	0/2872	0.86	3/4478 (0.1%)
27	BC	0.46	0/2131	0.59	0/2863
28	BD	0.45	0/1576	0.57	0/2119
29	BE	0.40	0/1571	0.60	2/2113 (0.1%)
30	BF	0.35	0/1444	0.53	0/1937
31	BG	0.37	0/1333	0.57	0/1805



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	BH	0.29	0/1122	0.62	1/1515 (0.1%)
33	BK	0.43	0/1152	0.53	0/1551
34	BL	0.44	0/956	0.62	0/1279
35	BM	0.41	0/1061	0.62	0/1412
36	BN	0.41	0/1081	0.55	0/1443
37	BO	0.45	0/973	0.61	0/1301
38	BP	0.38	0/910	0.59	0/1219
39	BQ	0.43	0/929	0.56	0/1242
40	BR	0.51	0/960	0.56	0/1278
41	BS	0.44	0/829	0.62	0/1107
42	BT	0.41	0/864	0.60	0/1156
43	BU	0.38	0/771	0.53	0/1031
44	BV	0.38	0/797	0.53	0/1062
45	BW	0.40	0/766	0.56	0/1025
46	BX	0.43	0/589	0.52	0/779
47	BY	0.43	0/635	0.53	0/848
48	BZ	0.32	0/502	0.53	0/667
49	B1	0.37	0/453	0.56	0/605
50	B2	0.43	0/450	0.60	0/599
51	B3	0.34	0/443	0.61	0/587
52	B4	0.42	0/379	0.55	0/496
53	B5	0.40	0/513	0.62	0/676
54	B6	0.46	0/302	0.58	0/397
55	B7	0.31	0/559	0.67	0/745
56	CN	1.77	12/693 (1.7%)	1.24	3/1068 (0.3%)
57	CT	2.53	38/676 (5.6%)	1.33	9/1039 (0.9%)
58	CA	1.13	7/1797 (0.4%)	0.91	2/2436 (0.1%)
58	CB	0.80	1/1703 (0.1%)	0.86	3/2308 (0.1%)
59	CC	1.41	120/10581 (1.1%)	0.97	31/14275 (0.2%)
60	CD	1.12	58/10532 (0.6%)	0.91	15/14219 (0.1%)
61	CE	0.55	0/480	0.73	0/647
All	All	0.90	268/184403 (0.1%)	0.88	232/272334 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
5	AE	0	1
13	AM	0	1

*Continued on next page...*

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	AV	0	1
25	BA	0	1
37	BO	0	1
46	BX	0	1
53	B5	0	1
All	All	0	8

The worst 5 of 268 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	1	C	OP3-P	-10.67	1.48	1.61
24	AX	1	G	OP3-P	-10.59	1.48	1.61
57	CT	18	DC	C3'-O3'	-10.26	1.30	1.44
60	CD	1357	ILE	C-N	-9.72	1.15	1.34
57	CT	14	DC	C3'-O3'	-9.51	1.31	1.44

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1027	C	C2-N1-C1'	12.29	132.32	118.80
57	CT	19	DG	O4'-C1'-N9	10.11	115.07	108.00
1	AA	1027	C	C6-N1-C1'	-9.76	109.09	120.80
22	AV	52	C	C6-N1-C2	-9.48	116.51	120.30
1	AA	812	G	O4'-C1'-N9	9.05	115.44	108.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1034	G	Sidechain
5	AE	89	HIS	Peptide
13	AM	65	VAL	Peptide
22	AV	45	C	Sidechain
25	BA	138	U	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32909	0	16580	275	0
2	AB	1765	0	1792	36	0
3	AC	1640	0	1713	27	0
4	AD	1643	0	1707	31	0
5	AE	1148	0	1195	19	0
6	AF	848	0	846	29	0
7	AG	1214	0	1267	18	0
8	AH	979	0	1031	10	0
9	AI	1031	0	1076	30	0
10	AJ	800	0	839	28	0
11	AK	877	0	887	25	0
12	AL	951	0	1012	25	0
13	AM	891	0	952	21	0
14	AN	805	0	844	13	0
15	AO	714	0	734	11	0
16	AP	649	0	666	8	0
17	AQ	648	0	691	6	0
18	AR	545	0	560	5	0
19	AS	663	0	688	11	0
20	AT	670	0	719	11	0
21	AU	590	0	629	12	0
22	AV	572	0	294	20	0
23	AW	1645	0	842	13	0
24	AX	1630	0	838	30	0
25	BA	62270	0	31335	443	0
26	BB	2569	0	1301	9	0
27	BC	2092	0	2167	32	0
28	BD	1566	0	1618	24	0
29	BE	1552	0	1618	23	0
30	BF	1420	0	1457	32	0
31	BG	1313	0	1358	20	0
32	BH	1111	0	1148	31	0
33	BK	1129	0	1162	10	0
34	BL	947	0	1023	11	0
35	BM	1052	0	1127	11	0
36	BN	1075	0	1155	13	0
37	BO	960	0	1000	12	0
38	BP	900	0	935	22	0
39	BQ	917	0	962	13	0
40	BR	947	0	1019	16	0
41	BS	816	0	839	10	0
42	BT	857	0	922	26	0
43	BU	764	0	829	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	789	0	843	14	0
45	BW	753	0	780	11	0
46	BX	582	0	598	4	0
47	BY	625	0	652	6	0
48	BZ	501	0	531	8	0
49	B1	449	0	488	6	0
50	B2	444	0	458	7	0
51	B3	436	0	477	13	0
52	B4	376	0	414	7	0
53	B5	504	0	572	9	0
54	B6	301	0	340	4	0
55	B7	549	0	551	14	0
56	CN	618	0	339	29	0
57	CT	606	0	338	37	0
58	CA	1775	0	1800	17	0
58	CB	1684	0	1713	19	0
59	CC	10415	0	10432	164	0
60	CD	10375	0	10597	147	0
61	CE	478	0	496	7	0
62	AA	143	0	0	0	0
62	AI	1	0	0	0	0
62	AL	1	0	0	0	0
62	AM	1	0	0	0	0
62	AW	5	0	0	0	0
62	AX	1	0	0	0	0
62	BA	317	0	0	0	0
62	BB	9	0	0	0	0
62	BC	3	0	0	0	0
62	BN	1	0	0	0	0
62	BO	1	0	0	0	0
62	BQ	1	0	0	0	0
62	BV	1	0	0	0	0
62	BX	1	0	0	0	0
62	CD	1	0	0	0	0
63	AX	11	0	8	1	0
64	B6	1	0	0	0	0
64	B7	1	0	0	0	0
64	CD	2	0	0	0	0
All	All	172846	0	123804	1795	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 6.

The worst 5 of 1795 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)
25:BA:2285:C:OP2	51:B3:6:ARG:NH1	1.99	0.94
1:AA:481:G:O2'	1:AA:483:C:N4	2.01	0.93
25:BA:1936:A:H2	25:BA:1943:U:H3	1.16	0.92
1:AA:411:A:H4'	1:AA:412:A:H5'	1.53	0.90
18:AR:36:SER:HA	18:AR:72:ASP:HB2	1.52	0.90

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	
2	AB	224/241 (93%)	210 (94%)	13 (6%)	1 (0%)	30	66
3	AC	207/233 (89%)	197 (95%)	6 (3%)	4 (2%)	6	31
4	AD	203/206 (98%)	192 (95%)	10 (5%)	1 (0%)	25	61
5	AE	154/167 (92%)	145 (94%)	7 (4%)	2 (1%)	10	39
6	AF	102/131 (78%)	97 (95%)	5 (5%)	0	100	100
7	AG	152/156 (97%)	144 (95%)	6 (4%)	2 (1%)	10	39
8	AH	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
9	AI	126/130 (97%)	111 (88%)	12 (10%)	3 (2%)	5	25
10	AJ	98/103 (95%)	90 (92%)	5 (5%)	3 (3%)	3	19
11	AK	115/129 (89%)	100 (87%)	14 (12%)	1 (1%)	14	49
12	AL	119/124 (96%)	109 (92%)	8 (7%)	2 (2%)	7	33
13	AM	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	AN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	AO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	AP	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	AQ	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
18	AR	64/75 (85%)	61 (95%)	2 (3%)	1 (2%)	8	34
19	AS	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
20	AT	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	AU	68/71 (96%)	68 (100%)	0	0	100	100
27	BC	270/273 (99%)	249 (92%)	18 (7%)	3 (1%)	12	44
28	BD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	25	61
29	BE	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
30	BF	176/179 (98%)	163 (93%)	10 (6%)	3 (2%)	7	33
31	BG	173/177 (98%)	159 (92%)	13 (8%)	1 (1%)	22	57
32	BH	147/149 (99%)	134 (91%)	10 (7%)	3 (2%)	6	29
33	BK	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
34	BL	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
35	BM	142/144 (99%)	132 (93%)	8 (6%)	2 (1%)	9	37
36	BN	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
37	BO	118/127 (93%)	108 (92%)	10 (8%)	0	100	100
38	BP	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	14	49
39	BQ	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
40	BR	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
41	BS	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	13	46
42	BT	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	BU	94/100 (94%)	88 (94%)	5 (5%)	1 (1%)	12	44
44	BV	101/104 (97%)	97 (96%)	3 (3%)	1 (1%)	13	46
45	BW	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	BX	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
47	BY	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
48	BZ	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
49	B1	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
50	B2	54/57 (95%)	54 (100%)	0	0	100	100
51	B3	51/55 (93%)	47 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	B4	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
53	B5	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	8	34
54	B6	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
55	B7	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
58	CA	227/329 (69%)	217 (96%)	10 (4%)	0	100	100
58	CB	215/329 (65%)	204 (95%)	10 (5%)	1 (0%)	25	61
59	CC	1316/1342 (98%)	1196 (91%)	111 (8%)	9 (1%)	19	54
60	CD	1327/1407 (94%)	1222 (92%)	95 (7%)	10 (1%)	16	51
61	CE	59/91 (65%)	53 (90%)	4 (7%)	2 (3%)	3	17
All	All	8766/9396 (93%)	8198 (94%)	508 (6%)	60 (1%)	21	54

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	AG	56	LYS
9	AI	56	ASP
10	AJ	57	VAL
11	AK	93	ARG
12	AL	88	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	
2	AB	187/199 (94%)	174 (93%)	13 (7%)	12	41
3	AC	171/190 (90%)	161 (94%)	10 (6%)	17	48
4	AD	172/173 (99%)	162 (94%)	10 (6%)	17	48
5	AE	118/126 (94%)	110 (93%)	8 (7%)	13	42
6	AF	91/112 (81%)	85 (93%)	6 (7%)	14	43
7	AG	127/129 (98%)	119 (94%)	8 (6%)	15	45
8	AH	104/105 (99%)	97 (93%)	7 (7%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AI	106/107 (99%)	101 (95%)	5 (5%)	22	56
10	AJ	87/90 (97%)	78 (90%)	9 (10%)	6	24
11	AK	90/99 (91%)	82 (91%)	8 (9%)	8	31
12	AL	102/103 (99%)	95 (93%)	7 (7%)	13	42
13	AM	93/96 (97%)	88 (95%)	5 (5%)	18	50
14	AN	83/84 (99%)	78 (94%)	5 (6%)	16	47
15	AO	76/77 (99%)	73 (96%)	3 (4%)	27	61
16	AP	65/65 (100%)	61 (94%)	4 (6%)	15	45
17	AQ	74/78 (95%)	70 (95%)	4 (5%)	18	50
18	AR	57/65 (88%)	54 (95%)	3 (5%)	19	51
19	AS	72/79 (91%)	71 (99%)	1 (1%)	62	83
20	AT	65/66 (98%)	59 (91%)	6 (9%)	7	29
21	AU	60/61 (98%)	54 (90%)	6 (10%)	6	25
27	BC	217/218 (100%)	212 (98%)	5 (2%)	45	75
28	BD	163/163 (100%)	155 (95%)	8 (5%)	21	54
29	BE	165/165 (100%)	155 (94%)	10 (6%)	15	46
30	BF	149/150 (99%)	139 (93%)	10 (7%)	13	43
31	BG	136/138 (99%)	124 (91%)	12 (9%)	8	31
32	BH	114/114 (100%)	106 (93%)	8 (7%)	12	41
33	BK	116/116 (100%)	111 (96%)	5 (4%)	25	58
34	BL	104/104 (100%)	98 (94%)	6 (6%)	17	48
35	BM	103/103 (100%)	95 (92%)	8 (8%)	10	36
36	BN	108/108 (100%)	102 (94%)	6 (6%)	17	49
37	BO	100/103 (97%)	95 (95%)	5 (5%)	20	53
38	BP	87/87 (100%)	81 (93%)	6 (7%)	13	42
39	BQ	99/100 (99%)	92 (93%)	7 (7%)	12	40
40	BR	89/90 (99%)	84 (94%)	5 (6%)	17	49
41	BS	84/84 (100%)	79 (94%)	5 (6%)	16	47
42	BT	93/93 (100%)	87 (94%)	6 (6%)	14	43
43	BU	83/84 (99%)	79 (95%)	4 (5%)	21	55
44	BV	84/85 (99%)	78 (93%)	6 (7%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BW	78/78 (100%)	74 (95%)	4 (5%)	20	53
46	BX	58/63 (92%)	57 (98%)	1 (2%)	56	81
47	BY	67/68 (98%)	64 (96%)	3 (4%)	23	57
48	BZ	54/55 (98%)	51 (94%)	3 (6%)	17	49
49	B1	48/49 (98%)	45 (94%)	3 (6%)	15	45
50	B2	47/48 (98%)	46 (98%)	1 (2%)	48	77
51	B3	48/49 (98%)	43 (90%)	5 (10%)	5	23
52	B4	37/38 (97%)	34 (92%)	3 (8%)	9	34
53	B5	51/52 (98%)	47 (92%)	4 (8%)	10	36
54	B6	34/44 (77%)	30 (88%)	4 (12%)	4	19
55	B7	62/62 (100%)	59 (95%)	3 (5%)	21	55
58	CA	197/286 (69%)	193 (98%)	4 (2%)	50	78
58	CB	187/286 (65%)	177 (95%)	10 (5%)	19	51
59	CC	1139/1157 (98%)	1097 (96%)	42 (4%)	29	63
60	CD	1118/1168 (96%)	1097 (98%)	21 (2%)	52	79
61	CE	52/75 (69%)	48 (92%)	4 (8%)	10	37
All	All	7371/7787 (95%)	7006 (95%)	365 (5%)	23	53

5 of 365 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	BS	39	LEU
58	CA	101	THR
42	BT	109	ASP
48	BZ	59	GLU
59	CC	108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
44	BV	54	GLN
44	BV	74	ASN
32	BH	73	ASN
41	BS	43	ASN
43	BU	48	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	292 (19%)	28 (1%)
22	AV	25/53 (47%)	9 (36%)	1 (4%)
23	AW	76/77 (98%)	22 (28%)	8 (10%)
24	AX	73/76 (96%)	16 (21%)	1 (1%)
25	BA	2895/2904 (99%)	557 (19%)	65 (2%)
26	BB	120/120 (100%)	12 (10%)	1 (0%)
All	All	4718/4772 (98%)	908 (19%)	104 (2%)

5 of 908 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	22	G
1	AA	29	U

5 of 104 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	984	A
25	BA	1379	U
25	BA	2756	U
25	BA	1060	U
25	BA	1111	A

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

53 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
23	H2U	AW	20	23	18,21,22	3.00	5 (27%)	21,30,33	2.25	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	MIA	AX	37	24	22,29,32	2.86	4 (18%)	22,41,47	2.73	7 (31%)
25	OMG	BA	2251	23,25	18,26,27	2.56	8 (44%)	19,38,41	1.54	4 (21%)
25	G7M	BA	2069	25	20,26,27	2.28	8 (40%)	17,39,42	1.31	3 (17%)
23	4SU	AW	8	23	18,21,22	4.08	8 (44%)	26,30,33	2.30	5 (19%)
25	2MG	BA	2445	25	18,26,27	2.24	7 (38%)	16,38,41	1.75	4 (25%)
25	5MU	BA	747	25	19,22,23	1.40	4 (21%)	28,32,35	2.28	6 (21%)
25	6MZ	BA	2030	25	18,25,26	1.92	2 (11%)	16,36,39	2.50	3 (18%)
23	5MU	AW	54	23	19,22,23	1.39	5 (26%)	28,32,35	2.11	6 (21%)
25	PSU	BA	2580	25	18,21,22	1.09	3 (16%)	22,30,33	2.07	6 (27%)
1	MA6	AA	1518	1	18,26,27	1.33	3 (16%)	19,38,41	4.05	2 (10%)
36	4D4	BN	81	36	9,11,12	2.51	3 (33%)	8,13,15	0.83	0
1	2MG	AA	1516	1	18,26,27	2.27	7 (38%)	16,38,41	1.64	4 (25%)
25	2MA	BA	2503	62,25	19,25,26	3.47	9 (47%)	21,37,40	2.23	4 (19%)
24	4SU	AX	8	24	18,21,22	4.08	8 (44%)	26,30,33	2.34	5 (19%)
25	OMC	BA	2498	62,25	19,22,23	2.81	7 (36%)	26,31,34	0.96	1 (3%)
1	5MC	AA	967	1	18,22,23	3.75	7 (38%)	26,32,35	1.04	2 (7%)
25	5MU	BA	1939	62,25	19,22,23	1.46	4 (21%)	28,32,35	2.32	6 (21%)
25	PSU	BA	2504	25	18,21,22	1.04	1 (5%)	22,30,33	1.91	4 (18%)
25	OMU	BA	2552	25	19,22,23	2.83	7 (36%)	26,31,34	1.76	4 (15%)
24	H2U	AX	16	24	18,21,22	3.02	5 (27%)	21,30,33	2.05	5 (23%)
1	MA6	AA	1519	1	18,26,27	1.33	3 (16%)	19,38,41	4.10	2 (10%)
1	UR3	AA	1498	1	19,22,23	2.50	6 (31%)	26,32,35	1.25	2 (7%)
24	PSU	AX	39	24	18,21,22	1.05	1 (5%)	22,30,33	1.85	5 (22%)
24	3AU	AX	47	24	18,21,29	3.43	8 (44%)	26,30,43	1.72	5 (19%)
23	OMC	AW	32	23	19,22,23	2.81	8 (42%)	26,31,34	0.78	0
25	PSU	BA	2457	25	18,21,22	1.12	2 (11%)	22,30,33	2.00	5 (22%)
25	PSU	BA	1917	25	18,21,22	1.07	2 (11%)	22,30,33	1.87	5 (22%)
25	PSU	BA	1911	25	18,21,22	1.09	1 (5%)	22,30,33	1.85	4 (18%)
25	5MC	BA	1962	25	18,22,23	3.75	7 (38%)	26,32,35	1.08	4 (15%)
1	2MG	AA	1207	1,62	18,26,27	2.32	7 (38%)	16,38,41	1.72	4 (25%)
24	PSU	AX	55	24	18,21,22	1.05	1 (5%)	22,30,33	1.87	5 (22%)
25	PSU	BA	746	62,25	18,21,22	1.07	3 (16%)	22,30,33	1.97	7 (31%)
1	G7M	AA	527	1	20,26,27	2.17	8 (40%)	17,39,42	1.32	2 (11%)
24	H2U	AX	20	24	18,21,22	3.12	5 (27%)	21,30,33	1.95	5 (23%)
25	PSU	BA	955	25	18,21,22	1.11	2 (11%)	22,30,33	1.94	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	AA	516	1	18,21,22	1.14	2 (11%)	22,30,33	2.15	6 (27%)
1	2MG	AA	966	1	18,26,27	2.30	7 (38%)	16,38,41	1.75	5 (31%)
1	4OC	AA	1402	1,62	20,23,24	3.24	9 (45%)	26,32,35	0.97	1 (3%)
23	PSU	AW	55	23	18,21,22	1.07	1 (5%)	22,30,33	1.86	6 (27%)
12	D2T	AL	89	12	7,9,10	1.01	0	6,11,13	2.45	4 (66%)
1	5MC	AA	1407	1	18,22,23	3.77	7 (38%)	26,32,35	1.07	2 (7%)
25	3TD	BA	1915	25	18,22,23	4.42	10 (55%)	22,32,35	2.19	4 (18%)
25	PSU	BA	2604	25	18,21,22	1.05	1 (5%)	22,30,33	1.91	5 (22%)
24	PSU	AX	32	24	18,21,22	1.01	1 (5%)	22,30,33	1.72	4 (18%)
25	6MZ	BA	1618	25	18,25,26	1.86	3 (16%)	16,36,39	2.37	4 (25%)
28	MEQ	BD	150	28	8,9,10	0.89	0	5,10,12	0.55	0
25	H2U	BA	2449	25	18,21,22	2.85	5 (27%)	21,30,33	2.13	5 (23%)
25	1MG	BA	745	25	18,26,27	2.60	5 (27%)	19,39,42	1.45	3 (15%)
25	PSU	BA	2605	25	18,21,22	1.08	2 (11%)	22,30,33	1.90	4 (18%)
25	2MG	BA	1835	25	18,26,27	2.26	7 (38%)	16,38,41	1.79	4 (25%)
24	5MU	AX	54	24	19,22,23	1.36	5 (26%)	28,32,35	2.06	7 (25%)
24	7MG	AX	46	24	22,26,27	3.86	10 (45%)	29,39,42	2.00	9 (31%)

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
23	H2U	AW	20	23	-	2/7/38/39	0/2/2/2
24	MIA	AX	37	24	-	4/9/31/34	0/3/3/3
25	OMG	BA	2251	23,25	-	1/5/27/28	0/3/3/3
25	G7M	BA	2069	25	-	2/3/25/26	0/3/3/3
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
25	2MG	BA	2445	25	-	2/5/27/28	0/3/3/3
25	5MU	BA	747	25	-	0/7/25/26	0/2/2/2
25	6MZ	BA	2030	25	-	2/5/27/28	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
25	PSU	BA	2580	25	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
36	4D4	BN	81	36	-	7/11/12/14	-
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	2MA	BA	2503	62,25	-	2/3/25/26	0/3/3/3
24	4SU	AX	8	24	-	2/7/25/26	0/2/2/2
25	OMC	BA	2498	62,25	-	2/9/27/28	0/2/2/2
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2
25	5MU	BA	1939	62,25	-	2/7/25/26	0/2/2/2
25	PSU	BA	2504	25	-	0/7/25/26	0/2/2/2
25	OMU	BA	2552	25	-	2/9/27/28	0/2/2/2
24	H2U	AX	16	24	-	3/7/38/39	0/2/2/2
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
24	3AU	AX	47	24	-	2/7/25/35	0/2/2/2
23	OMC	AW	32	23	-	0/9/27/28	0/2/2/2
25	PSU	BA	2457	25	-	0/7/25/26	0/2/2/2
25	PSU	BA	1917	25	-	2/7/25/26	0/2/2/2
25	PSU	BA	1911	25	-	1/7/25/26	0/2/2/2
25	5MC	BA	1962	25	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1,62	-	1/5/27/28	0/3/3/3
24	PSU	AX	55	24	-	1/7/25/26	0/2/2/2
25	PSU	BA	746	62,25	-	2/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	1/3/25/26	0/3/3/3
24	H2U	AX	20	24	-	3/7/38/39	0/2/2/2
25	PSU	BA	955	25	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	1	-	2/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
1	4OC	AA	1402	1,62	-	0/9/29/30	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/7/12/14	-
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
25	3TD	BA	1915	25	-	2/7/25/26	0/2/2/2
25	PSU	BA	2604	25	-	0/7/25/26	0/2/2/2
24	PSU	AX	32	24	-	0/7/25/26	0/2/2/2
25	6MZ	BA	1618	25	-	2/5/27/28	0/3/3/3
28	MEQ	BD	150	28	-	2/8/9/11	-
25	H2U	BA	2449	25	-	0/7/38/39	0/2/2/2
25	1MG	BA	745	25	-	0/3/25/26	0/3/3/3
25	PSU	BA	2605	25	-	0/7/25/26	0/2/2/2
25	2MG	BA	1835	25	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
24	7MG	AX	46	24	-	3/7/37/38	0/3/3/3

The worst 5 of 254 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1915	3TD	C6-C5	11.77	1.49	1.35
24	AX	37	MIA	C13-C14	9.69	1.60	1.32
25	BA	1915	3TD	C2-N1	9.63	1.49	1.37
1	AA	1407	5MC	C6-C5	9.59	1.50	1.34
24	AX	20	H2U	C2-N1	9.57	1.49	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	MA6	N1-C6-N6	-16.64	99.54	117.06
1	AA	1518	MA6	N1-C6-N6	-16.52	99.67	117.06
24	AX	8	4SU	C4-N3-C2	-8.27	119.31	127.34
24	AX	37	MIA	C12-C13-C14	-8.16	111.27	127.14
23	AW	8	4SU	C4-N3-C2	-8.08	119.49	127.34

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
24	AX	37	MIA	C12-C13-C14-C15
24	AX	37	MIA	C12-C13-C14-C16

There are no ring outliers.

21 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	20	H2U	2	0
24	AX	37	MIA	3	0
25	BA	2251	OMG	1	0
25	BA	2069	G7M	2	0
25	BA	2030	6MZ	1	0
1	AA	1516	2MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	BA	2503	2MA	1	0
24	AX	8	4SU	1	0
1	AA	967	5MC	1	0
24	AX	16	H2U	3	0
1	AA	1519	MA6	1	0
1	AA	1498	UR3	1	0
25	BA	1917	PSU	3	0
1	AA	527	G7M	2	0
1	AA	966	2MG	2	0
23	AW	55	PSU	1	0
12	AL	89	D2T	2	0
25	BA	1915	3TD	1	0
28	BD	150	MEQ	2	0
25	BA	2605	PSU	1	0
24	AX	54	5MU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 492 ligands modelled in this entry, 491 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
63	PHE	AX	101	24	10,11,12	0.62	0	10,13,15	0.22	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
63	PHE	AX	101	24	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	AX	101	PHE	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
60	CD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	1357:ILE	C	1358:PRO	N	1.15