wwPDB EM Validation Summary Report (i)

Apr 16, 2024 – 09:45 am BST

PDB ID	:	6ZTM
EMDB ID	:	EMD-11420
Title	:	E. coli 70S-RNAP expressome complex in collided state without NusG
Authors	:	Webster, M.W.; Takacs, M.; Weixlbaumer, A.
Deposited on	:	2020-07-20
Resolution	:	3.30 Å(reported)
Based on initial models	:	6ALH, 4YBB

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

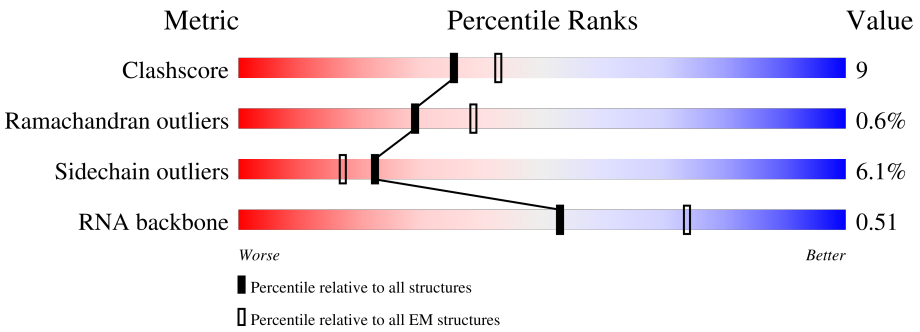
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	AA	1542	58% 33% 7% ••
2	AB	241	71% 20% • 6%
3	AC	233	58% 27% 5% 10%
4	AD	206	66% 30% •
5	AE	167	65% 25% •• 7%
6	AF	131	49% 24% 6% 21%
7	AG	156	65% 29% • •

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Mol	Chain	Length	Quality of chain
8	AH	130	70% 25% 5%
9	AI	130	55% 38% 5%
10	AJ	103	48% 41% 9%
11	AK	129	66% 23% 10%
12	AL	124	69% 26%
13	AM	118	61% 33%
14	AN	101	71% 26%
15	AO	89	70% 26%
16	AP	82	89% 11%
17	AQ	84	68% 20% 6% 6%
18	AR	75	47% 21% 28%
19	AS	92	61% 27% 10%
20	AT	87	76% 20%
21	AU	71	69% 25%
22	AV	57	16% 14% 16% 7% 47%
23	AW	77	48% 30% 21%
24	AX	76	33% 51% 12%
25	BA	2904	63% 28% 7%
26	BB	120	67% 30%
27	BC	273	77% 21%
28	BD	209	78% 19%
29	BE	201	75% 23%
30	BF	179	54% 41% 5%
31	BG	177	70% 26%
32	BH	149	64% 31% 5%

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Mol	Chain	Length	Quality of chain
33	BK	142	80% 18% •
34	BL	123	71% 28% •
35	BM	144	72% 25% •
36	BN	136	71% 29%
37	BO	127	77% 14% • 6%
38	BP	117	64% 33% •
39	BQ	115	72% 24% • •
40	BR	118	80% 19% • •
41	BS	103	71% 28% •
42	BT	110	76% 22% •
43	BU	100	68% 21% 6% 5%
44	BV	104	74% 24% • •
45	BW	94	71% 27% • •
46	BX	85	74% 13% • 11%
47	BY	78	72% 27% •
48	BZ	63	81% 14% • •
49	B1	59	69% 24% 5% •
50	B2	57	60% 33% 5% •
51	B3	55	64% 31% • •
52	B4	46	76% 24%
53	B5	65	68% 29% • •
54	B6	50	58% 18% 24%
55	CN	39	26% 41% 10% 23%
56	CT	39	15% 36% 26% 23%
57	CA	329	60% 8% • 30%

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Mol	Chain	Length	Quality of chain
57	CB	329	56% 9% • 33%
58	CC	1342	76% 18% • •
59	CD	1407	77% 17% • 5%

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 171689 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
			Total	C	N	O	P		
1	AA	1533	32907	14682	6037	10655	1533	0	0

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
6	AF	104	848	536	153	152	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AG	153	1203	750	231	218	4	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AK	116	866	534	170	159	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AL	122	949	587	195	163	4	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AQ	79	641	406	120	112	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	AR	54	443	281	81	81	0	0

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

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

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

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

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	AV	30	636	285	115	206	30	0	0

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
24	AX	76	1624	724	290	533	76	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	BA	2901	62290	27795	11458	20136	2901	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
36	BN	136	1075	686	205	178	6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BU	95	757	479	141	135	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	B4	46	377	228	90	57	2	0	0

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

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

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

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

- Molecule 55 is a DNA chain called Non-template DNA strand.

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

- Molecule 56 is a DNA chain called Template DNA strand.

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

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit alpha.

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

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

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

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

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

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	AA	119	119	119	0
			Total	Mg	
60	AW	2	2	2	0

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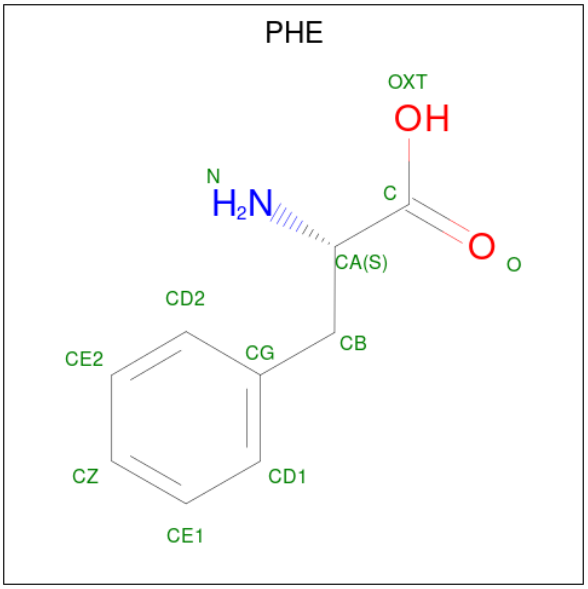
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	BA	294	294	294	0
			Total	Mg	
60	BB	2	2	2	0
			Total	Mg	
60	BC	1	1	1	0
			Total	Mg	
60	BO	1	1	1	0
			Total	Mg	
60	B2	1	1	1	0
			Total	Mg	
60	CD	1	1	1	0

- Molecule 61 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



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

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

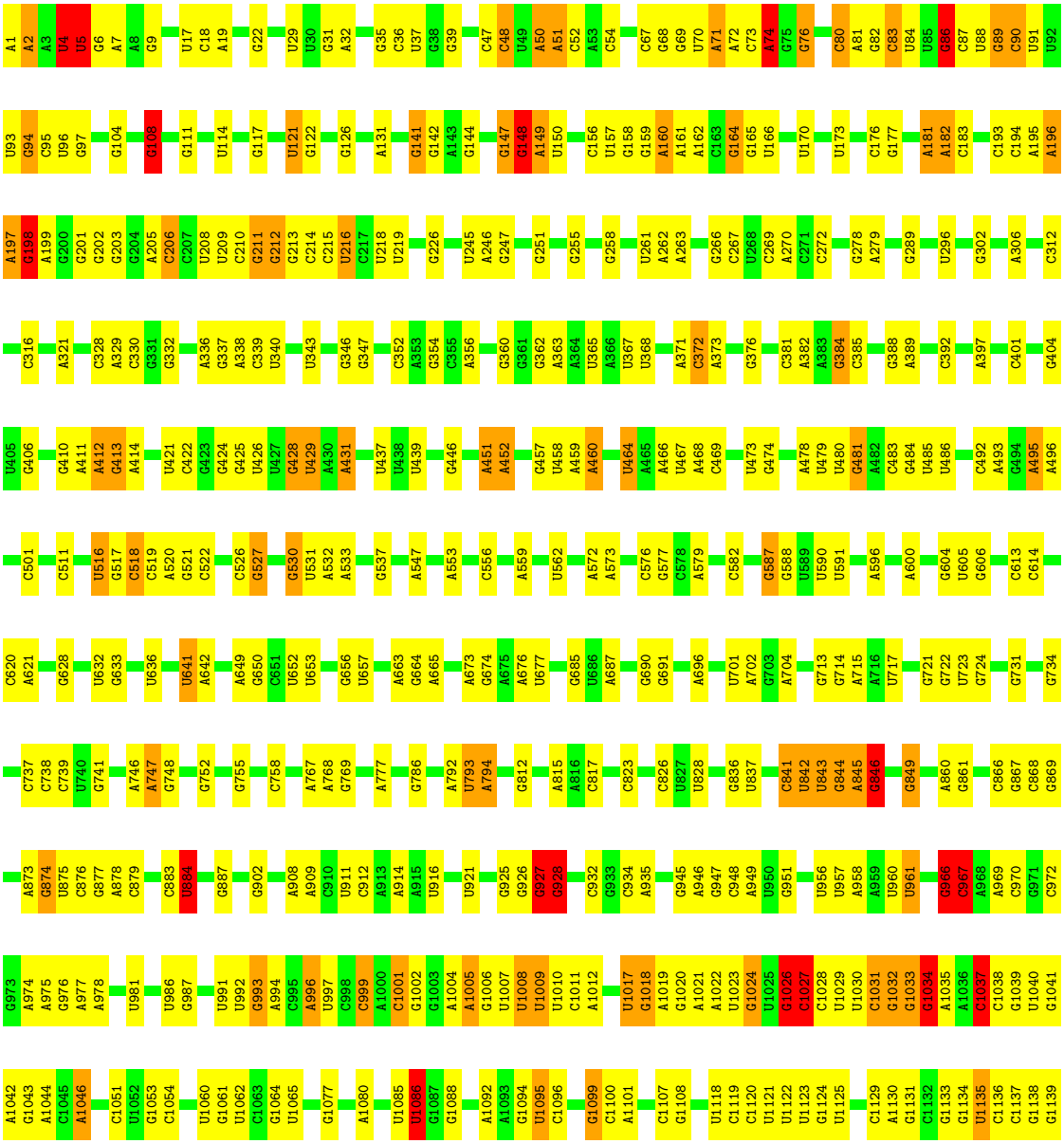
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
62	B6	1	1	1	0
			Total	Zn	
62	CD	2	2	2	0

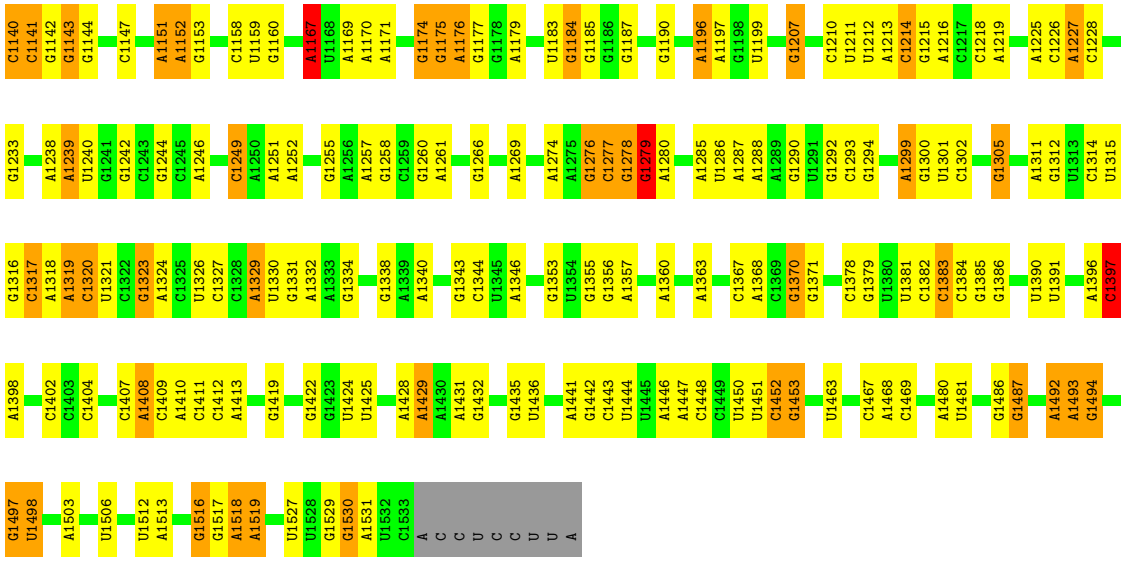
3 Residue-property plots (i)

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

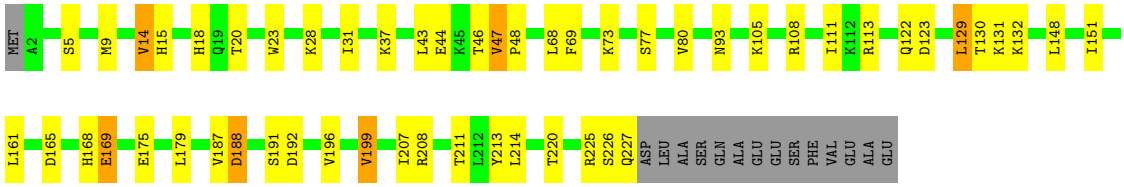
Chain AA: 58% 33% 7% ••





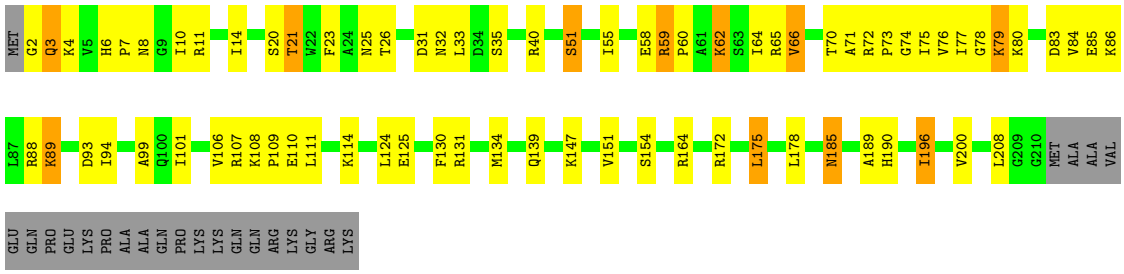
- Molecule 2: 30S ribosomal protein S2

Chain AB:



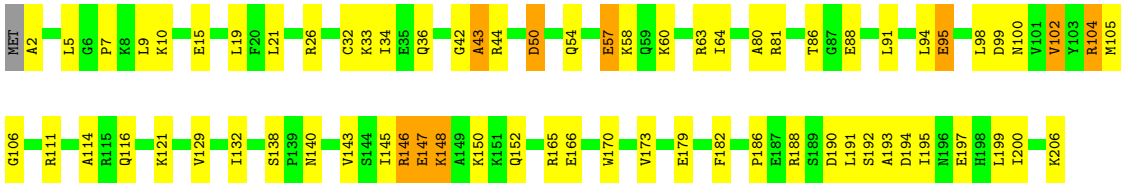
- Molecule 3: 30S ribosomal protein S3

Chain AC:



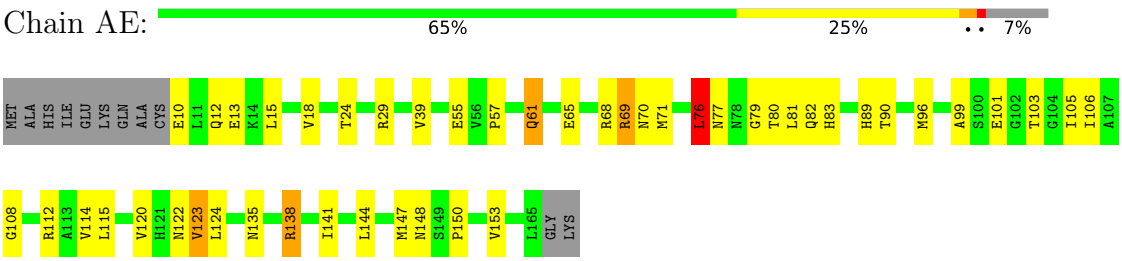
- Molecule 4: 30S ribosomal protein S4

Chain AD:



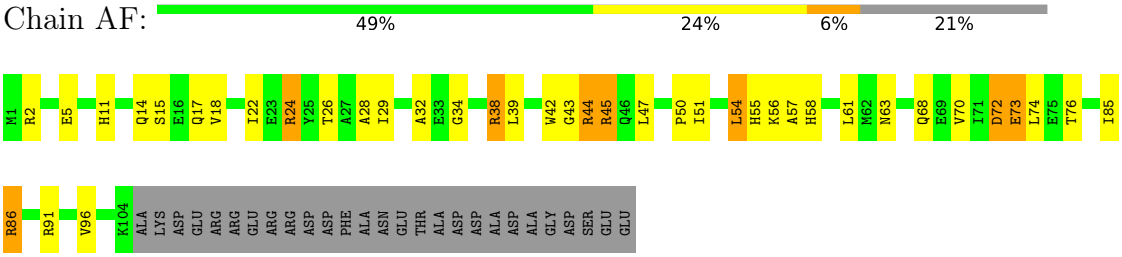
- Molecule 5: 30S ribosomal protein S5

Chain AE:



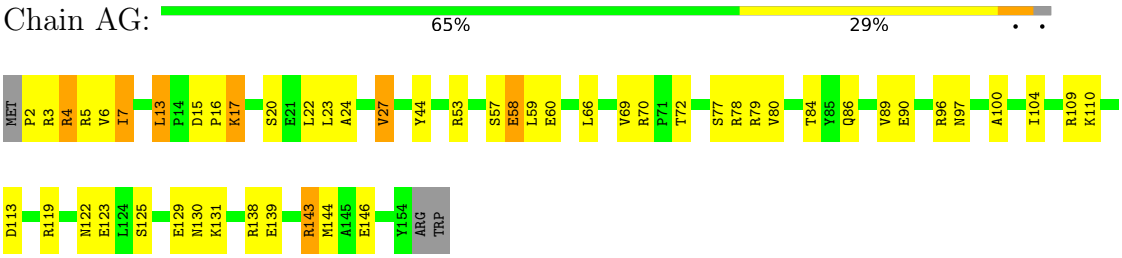
- Molecule 6: 30S ribosomal protein S6

Chain AF:



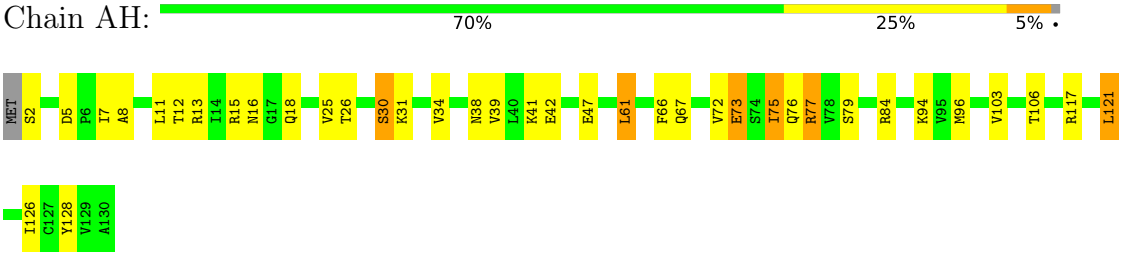
- Molecule 7: 30S ribosomal protein S7

Chain AG:



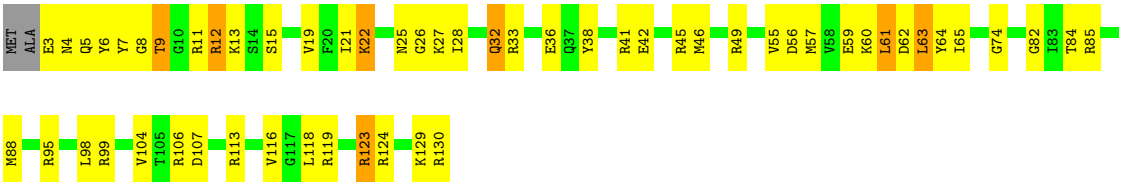
- Molecule 8: 30S ribosomal protein S8

Chain AH:



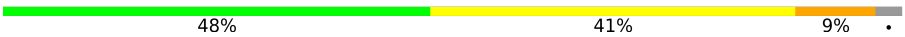
- Molecule 9: 30S ribosomal protein S9

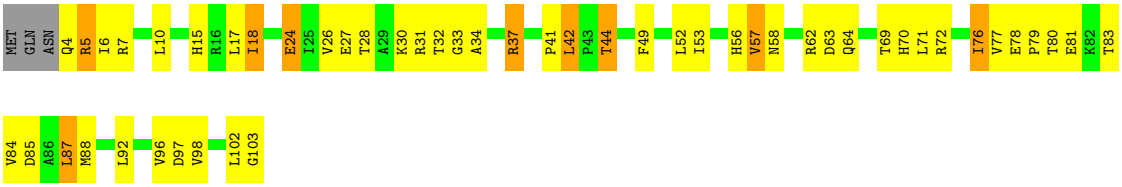
Chain AI:



- Molecule 10: 30S ribosomal protein S10

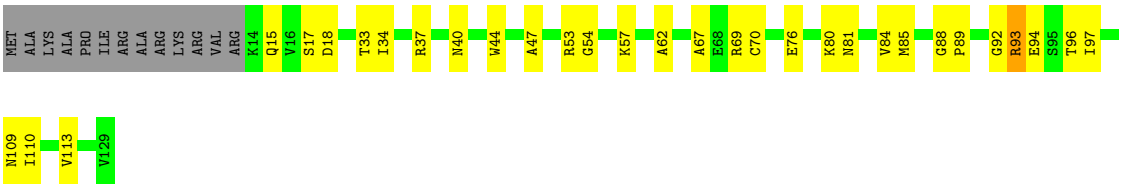
Chain AJ:





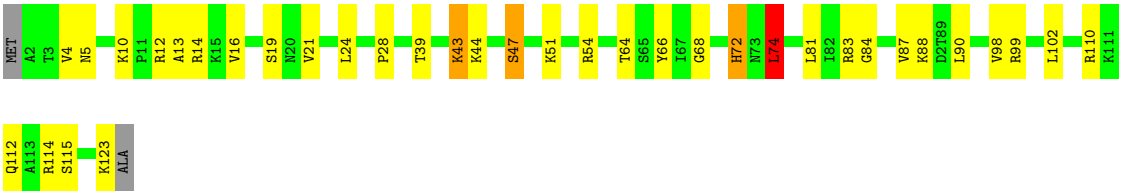
- Molecule 11: 30S ribosomal protein S11

Chain AK:



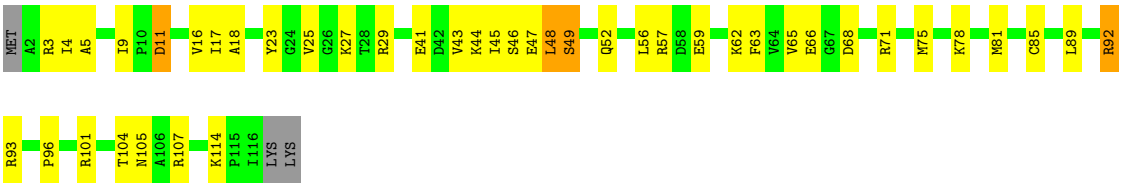
- Molecule 12: 30S ribosomal protein S12

Chain AL:



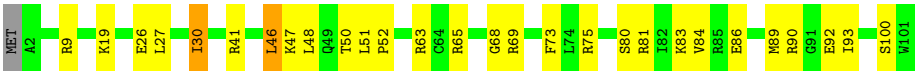
- Molecule 13: 30S ribosomal protein S13

Chain AM:



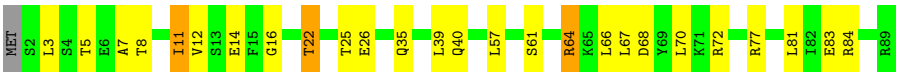
- Molecule 14: 30S ribosomal protein S14

Chain AN:



- Molecule 15: 30S ribosomal protein S15

Chain AO: 70% 26%



• Molecule 16: 30S ribosomal protein S16

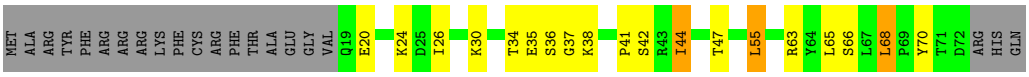
Chain AP: 89% 11%

• Molecule 17: 30S ribosomal protein S17

Chain AQ: 68% 20% 6% 6%

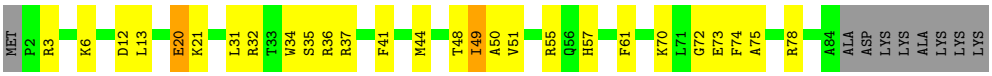
• Molecule 18: 30S ribosomal protein S18

Chain AR: 47% 21% 28%



• Molecule 19: 30S ribosomal protein S19

Chain AS: 61% 27% 10%

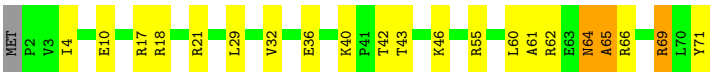


• Molecule 20: 30S ribosomal protein S20

Chain AT: 76% 20%

• Molecule 21: 30S ribosomal protein S21

Chain AU: 69% 25%



• Molecule 22: mRNA

Chain AV: 16% 14% 16% 7% 47%

A C A A A G G A G G U A U U14 C15 A16 U19 C23 A24 U25 A26 C27 A C A U A U A U A G A C A C A34 C37 A38 A39 A40 C41 G42 G43 C44 G45 C46 G47 C48 G49

• Molecule 23: tRNA(fmet) P-site

Chain AW: 48% 30% 21%

C1 G2 G6 G7 U8 A14 G15 C16 C17 U17A G18 G19 U20 A21 G22 C25 G31 C32 U33 A44 G45 A46 U47 C48 G49 U50 G53 U54 U55 C56 A57 A58 A59 U60 C61 G64 C69 G70 C74 C75 A76

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

Chain AX: 33% 51% 12%

G1 G5 G6 A7 U8 A9 G10 C11 U12 C13 A14 G15 U16 C17 G18 G19 U20 A21 G22 A23 G24 C25 A26 G27 G28 U32 U33 G34 A35 A36 A37 A38 U39 C40 C41 C42 C43 G44 U45 G46 3AU47 C48 C49 U50 U51 G52 G53 U54 U55 C56 G57 A58 U59 G63 A64 G65 U66

G71 C74 C75 A76

• Molecule 25: 23S ribosomal RNA

Chain BA: 63% 28% 7%

G1 A10 C11 U12 A13 A14 U18 G23 G27 A28 C33 U34 G35 G39 U40 A44 G45 G46 A52 A53 G58 U59 G60 C61 U62 A63 A64 U65 C66 U67 G68 A71 U72 A73 A74 G75 U78 G81 U82 A83 A84 G85 U92 G93 G98 U99

U100 A101 U102 G110 A111 U112 A118 A119 U120 G121 G122 A125 A131 C132 U133 G134 U135 G136 U137 U138 U139 C140 G141 A142 C143 A144 C145 A149 C163 C164 A165 U166 A167 G168 A172 A173 A181 A191 C192 A196 A197 C198 A199 U200 C201 A207 C208 C209 C210

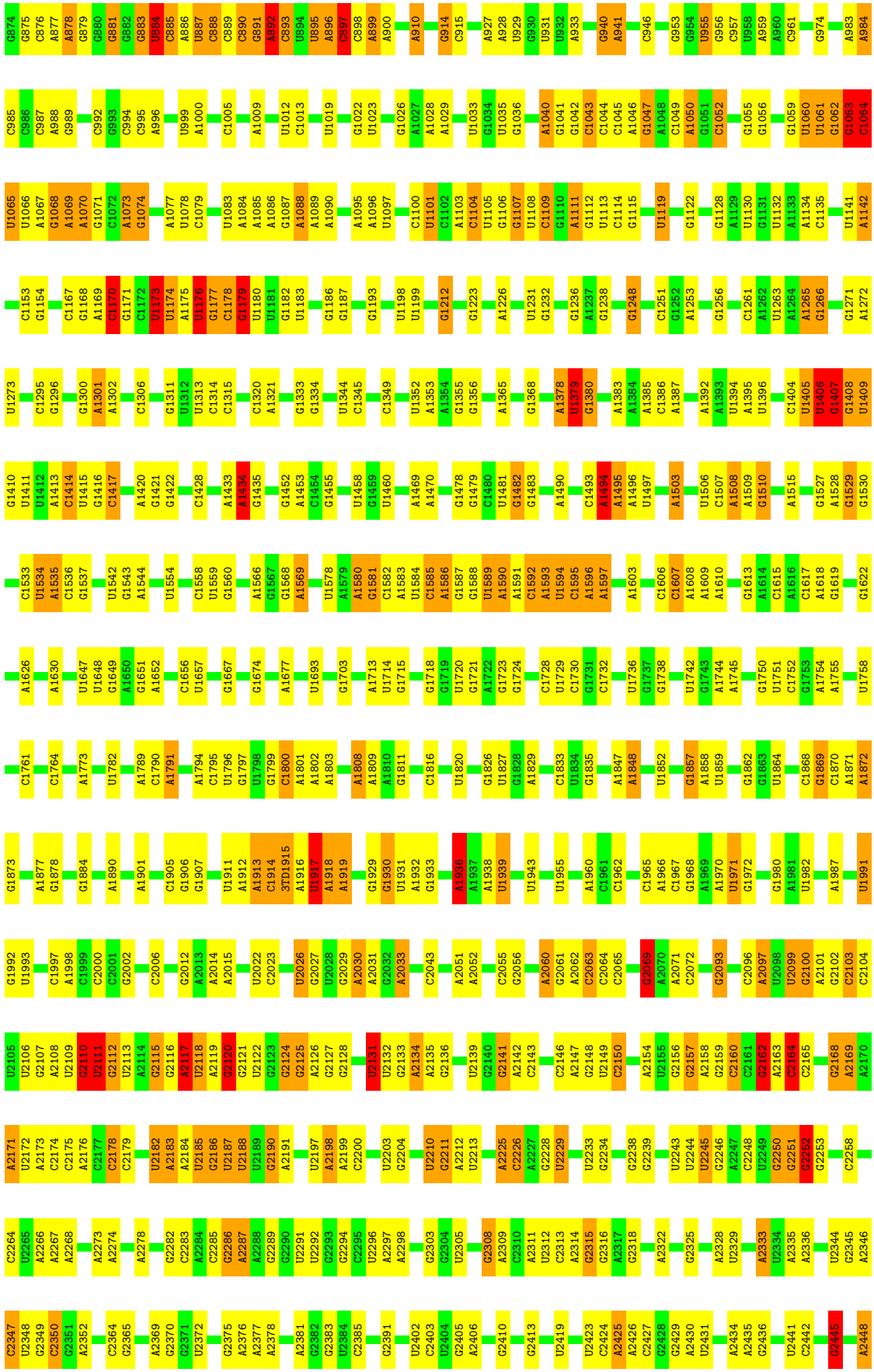
G215 A216 A219 G220 A221 A222 U234 C239 C240 A241 A244 G245 G248 C249 G250 G263 C264 A265 G266 A270 G271 A272 G273 C274 C275 U276 G277 A278 A279 U280 U284 G285 G289 U290 G301 C302 A310 A311 G327 U328 G329 A330 C335 C353 A354

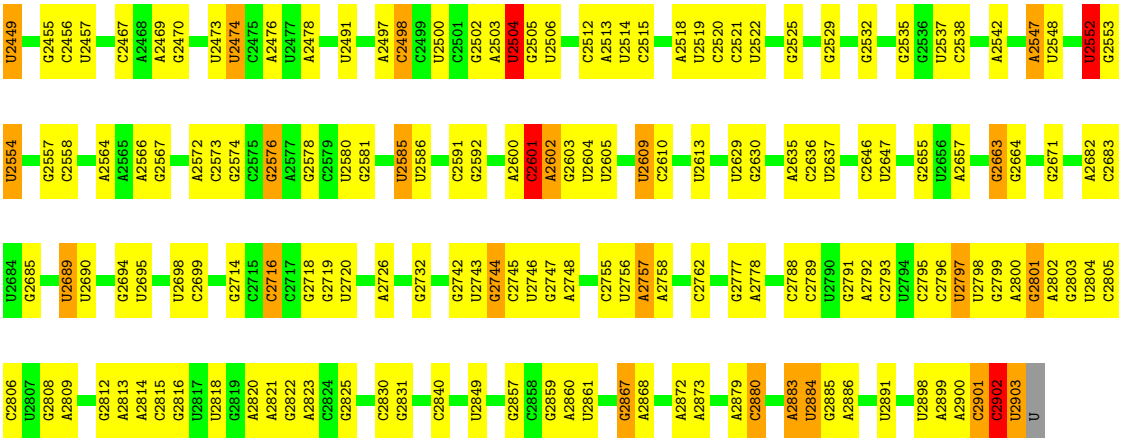
U355 G356 C357 U358 G359 U360 G361 A362 U365 C366 G370 A371 G386 G389 G396 G400 U403 A404 U405 G411 A412 C413 C414 A415 G424 U427 C435 A443 C444 U451 C456 G463 U464 G465 A466 G467 G468 C475 G476 A477 A478 A479 A480 G481

A482 A483 G491 G495 U499 G500 A501 A502 A503 A504 A505 A508 C509 A529 G530 C531 A532 G533 U534 G535 A543 G544 A545 A A U548 C549 U550 G551 A563 U567 U568 U569 U573 A574 A575 U580 G585 A586 U593 U594 C595 A603 A609 A613

A614 U615 A616 G617 G618 G622 A626 A627 A637 G638 U639 C640 C645 U646 G647 G651 U652 U653 A654 A655 A668 A677 A685 U686 A693 G696 G711 C717 A721 A722 C723 U724 G728 G729 A730 G738 A742 A743 U744 G745 U746 U747 A752

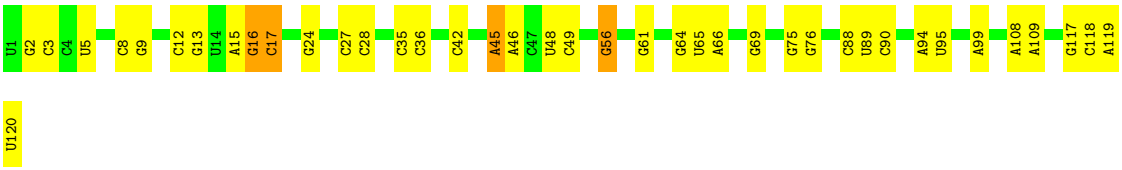
G757 A764 C765 G768 G775 G776 A782 A783 G784 G785 A788 A789 U790 C791 A792 A804 G805 C806 U811 C812 U827 U828 A829 A833 G834 U839 C840 U846 U847 C848 A849 U850 C851 U852 G856 G857 G858 G859 A866 C867 U868 G869 U870 U871 U872 C873





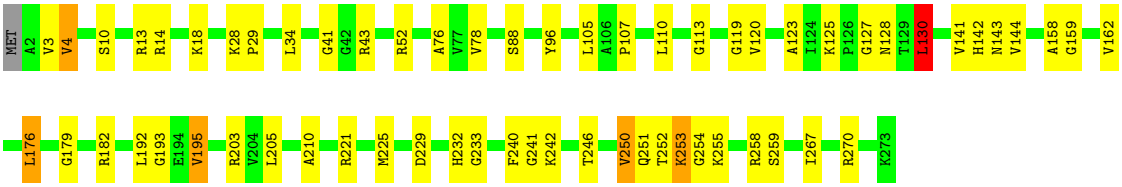
- Molecule 26: 5S ribosomal RNA

Chain BB:



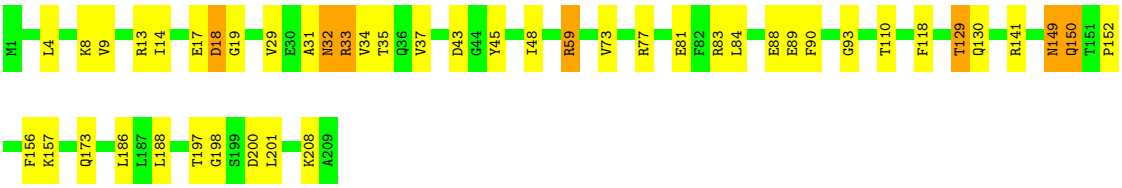
- Molecule 27: 50S ribosomal protein L2

Chain BC:



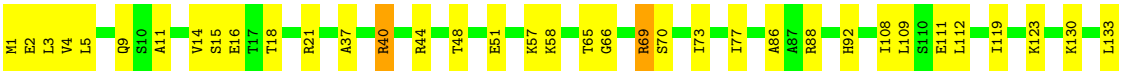
- Molecule 28: 50S ribosomal protein L3

Chain BD:



- Molecule 29: 50S ribosomal protein L4

Chain BE:



E144 D145 I148 E152 F158 K166 V169 R170 D176 S179 D184 Q195 V196 E197 E198 A201

- Molecule 30: 50S ribosomal protein L5

Chain BF: 54% 41% 5%

MET A2 H5 Y8 E11 V12 V13 K14 K15 V25 V28 V31 I34 T35 L36 V40 G41 E42 A43 I44 A45 D46 K47 K48 L49 L50 A53 A54 A55 D56 L57 A58 A59 I60 S61 G62 Q63 K64 P65 L66 I67 S73 F77 K78 I79 R80 Y83 P84

I85 G86 C87 L91 E94 R95 M96 W97 E98 F99 F100 E101 R102 L103 I104 A107 R110 D113 F114 R115 S118 A119 K120 D123 G126 E134 Q135 I136 E140 I141 D142 Y143 V146 R150 G151 L152 T155 I156 T157 T158 D163 E164 L169 L170 A171

D174 F175 P176 F177 R178 K179

- Molecule 31: 50S ribosomal protein L6

Chain BG: 70% 26%

MET S2 R3 V4 V10 D16 V23 I24 E32 R35 T36 L37 N38 D39 A40 V41 D47 N48 T49 F52 G53 P54 W62 A63 Q64 T67 A68 R69 L72 M75 V76 V79 F83 T84 K85 K86 R95 A96 A97 L105 S106 L107 S110 H111

D114 L117 A123 E124 C125 P126 T127 E130 G135 I141 A145 L148 Y151 R152 E155 K160 Y164 E167 R170 E173 K176 LYS

- Molecule 32: 50S ribosomal protein L9

Chain BH: 64% 31% 5%

M1 I4 L5 L6 D7 K8 N11 L12 G13 S14 L15 Q18 V19 N20 V21 V37 F46 F47 E48 A49 R50 R51 E55 L58 A59 E60 A64 A65 N66 A67 R68 A69 E70 K71 I72 N73 A74 L75 E76 T77 V78 K83 A84 E87 G88 K89 L90 F91 R97

D101 A102 V103 T104 G107 V108 K112 V115 R116 L117 G120 S131 F132 Q133 F139 A140 K141 V144 E149

- Molecule 33: 50S ribosomal protein L13

Chain BK: 80% 18%

M1 K2 T3 E9 T30 E31 L36 K39 H40 K41 T50 G51 V56 L57 D60 K61 K68 T78 K85 R96 R99 M108 R116 A117 R120 K123 V124 E129 D141 I142

- Molecule 34: 50S ribosomal protein L14

Chain BL: 71% 28%

M1 Q5 A11 D12 N13 S14 G15 A16 R17 R18 C21 G34 V35 G36 D37 K40 I41 I47 P48 R49 V57 L58 K59 V62 V63 R64 K67 R70 G74 S75 V76 I77 R78 N89 R98 I99 F100 G101 P102 L107 R108 K111 I116

L123

- Molecule 35: 50S ribosomal protein L15

Chain BM: 72% 25% •

M1 R2 T5 A9 S12 K13 K14 K17 R21 L27 G28 K29 T30 R33 K36 G37 S40 L57 L61 P62 K63 T67 K70 E76 V77 R78 L79 S80 D81 K84 V85 V89 A98 N99 F107 I111 L112 A113 G114 E115 V116

V120 R123 R126 K129 R132 I142 E143 E144

- Molecule 36: 50S ribosomal protein L16

Chain BN: 71% 29%

M1 L2 Q3 K8 H13 K14 G15 R16 N17 R18 G19 L20 D25 F31 G32 L33 K34 A35 V36 G37 R38 R55 R59 W64 I65 R66 V67 K71 P77 L78 A79 V80 4D481 W92 I96 Q97 P98 L102 Y103 E104 M105 D106 G107 E110 E115 A116

F117 K123 K127 F130 V131 T132 K133 T134 V135 M136

- Molecule 37: 50S ribosomal protein L17

Chain BO: 77% 14% • 6%

M1 R2 K5 R8 N13 M20 F21 M24 L38 P39 L44 E49 T53 L54 L65 R69 E82 R86 R90 C100 G101 P109 M110 E120 LYS ALA GLU ALA ALA ALA GLU

- Molecule 38: 50S ribosomal protein L18

Chain BP: 64% 33% •

M1 D2 S5 A6 R7 R13 A14 R15 R25 L26 V27 R30 T31 H34 I35 Y36 A37 Q38 Y39 I40 V47 L48 V49 A50 A51 S52 E55 K56 A57 E60 Q61 N67 K68 D69 V74 V78 R81 D89 F92 S95 G96 F97 Q98 Y99 H100

G101 R102 V103 L106 A107 R111 Q116 F117

- Molecule 39: 50S ribosomal protein L19

Chain BQ: 72% 24% • •

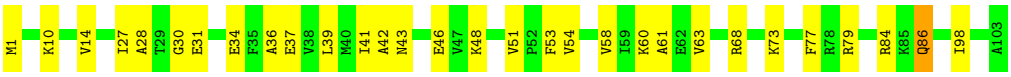
MET S2 N3 I4 L8 E11 Q12 M13 K14 S19 V26 V32 V33 E34 R39 L40 R51 N52 R53 V73 S78 P79 V80 R88 R89 G90 A91 Y98 Y99 L100 R101 E102 R103 T104 R109 I110 K111 E112 R113 L114 N115

- Molecule 40: 50S ribosomal protein L20

Chain BR: 80% 19% ••

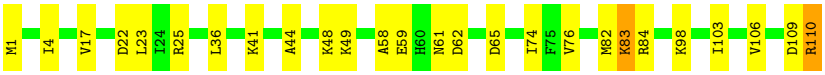
• Molecule 41: 50S ribosomal protein L21

Chain BS: 71% 28% •



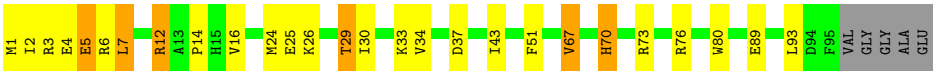
• Molecule 42: 50S ribosomal protein L22

Chain BT: 76% 22% •



• Molecule 43: 50S ribosomal protein L23

Chain BU: 68% 21% 6% 5%



• Molecule 44: 50S ribosomal protein L24

Chain BV: 74% 24% ••

• Molecule 45: 50S ribosomal protein L25

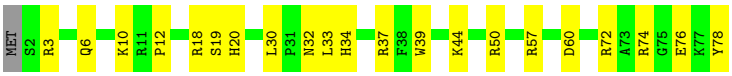
Chain BW: 71% 27% ••

• Molecule 46: 50S ribosomal protein L27

Chain BX: 74% 13% • 11%

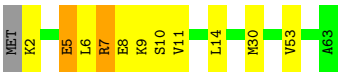
• Molecule 47: 50S ribosomal protein L28

Chain BY: 72% 27%



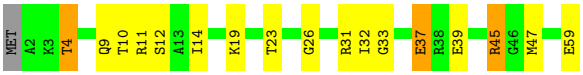
• Molecule 48: 50S ribosomal protein L29

Chain BZ: 81% 14%



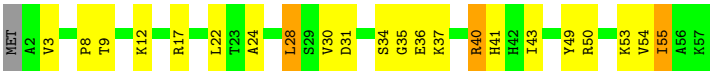
• Molecule 49: 50S ribosomal protein L30

Chain B1: 69% 24% 5%



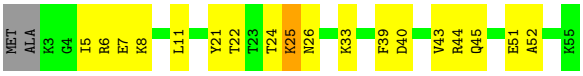
• Molecule 50: 50S ribosomal protein L32

Chain B2: 60% 33% 5%



• Molecule 51: 50S ribosomal protein L33

Chain B3: 64% 31%

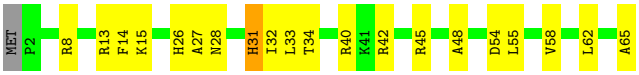


• Molecule 52: 50S ribosomal protein L34

Chain B4: 76% 24%

• Molecule 53: 50S ribosomal protein L35

Chain B5: 68% 29%



• Molecule 54: 50S ribosomal protein L36

Chain B6: 58% 18% 24%

M1 K2 C14 K15 I23 R24 A29 K32 H33 K34 Q37 G38 LEU ILE PHE SER HIS ILE PHE LEU ALA LYS LEU GLY

• Molecule 55: Non-template DNA strand

Chain CN: 26% 41% 10% 23%

DG DG DT DC DA DG DT DA DC G10 T11 C12 C13 C21 T22 T23 C24 G25 G26 A27 A28 G29 A30 G31 A32 T33 T34 C35 A36 G37 A38 G39

• Molecule 56: Template DNA strand

Chain CT: 15% 36% 26% 23%

C1 T2 C3 T4 G5 A6 A7 T8 C9 T10 C11 T12 T13 C14 C15 C16 G17 C18 G19 C20 G21 C22 C23 A26 G27 C30 DG DT DA DC DT DG DA DC DC

• Molecule 57: DNA-directed RNA polymerase subunit alpha

Chain CA: 60% 8% • 30%

MET GLN GLY SER VAL T6 E7 F8 L9 K10 P11 R12 L13 L31 C54 E58 D62 G63 E67 Y68 V74 L79 L85 E97 T101 L102 N103 C131 R166 R170 P179 V180 M205 E206 T207 N208 P213 A216 I217 R218 L234 ARG

ASP VAL ARG GLN PRO GLU VAL LYS GLU GLU LYS PRO GLU PHE ASP PRO ILE LEU LEU ARG PRO VAL ASP ASP LEU GLU LEU THR VAL ARG SER ALA ASN CYS LEU LYS ALA GLU ALA ILE HIS TYR ILE GLY ASP LEU VAL GLN ARG THR GLU VAL GLU LEU LEU LYS THR PRO ASN LEU

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

• Molecule 57: DNA-directed RNA polymerase subunit alpha

Chain CB: 56% 9% • 33%

MET GLN GLY S4 P11 R12 L13 E17 T27 L28 G34 N41 A42 L43 L48 E58 I61 H66 E67 Y68 E72 G73 V74 Q75 E76 I81 L82 L83 I107 E136 M142 P154 A155 S156 T157 ARG ILE HIS SER GLU GLU ASP GLU ARG PRO

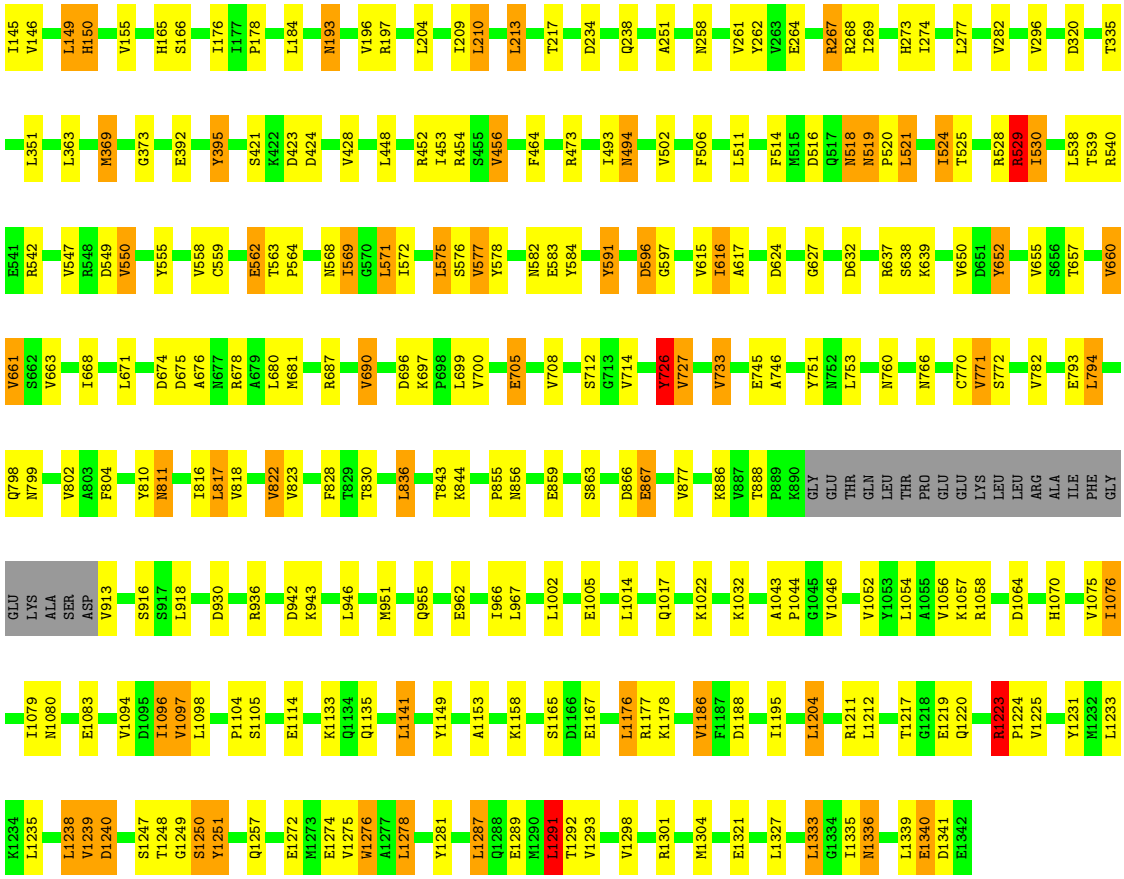
ILE G169 R170 D174 Y185 R191 V192 T196 D199 L228 D233 LEU ARG ASP VAL ARG GLN PRO GLU VAL LYS GLU GLU LYS PRO GLU PHE ASP PRO ILE LEU LEU ARG PRO VAL ASP ASP LEU GLU LEU THR VAL ARG SER ALA ASN CYS LEU LYS ALA GLU ALA ILE

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

• Molecule 58: DNA-directed RNA polymerase subunit beta

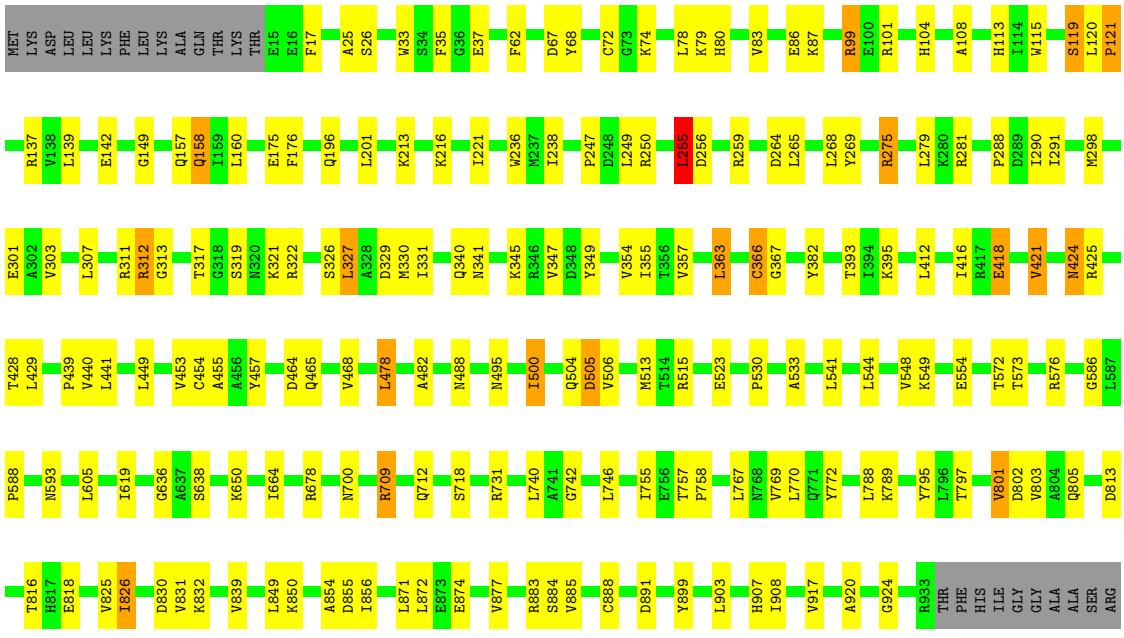
Chain CC: 76% 18% • •

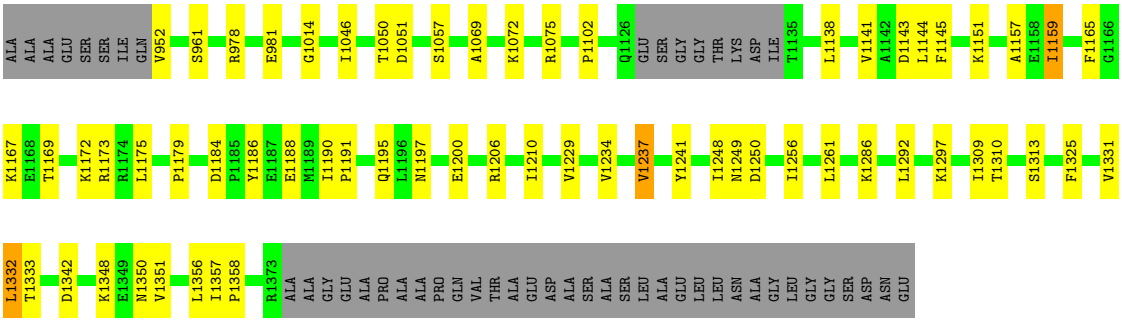
M1 E7 K8 K9 R10 I11 R12 R18 D23 L27 L28 F38 G45 Q46 Y47 G48 L49 E50 A51 N65 Q69 Y70 Y73 E84 C85 V90 V98 R101 E108 D116 I127 P128 L129 M130 T131 D132 N133 G134 T135 F136 V137 I138 V144



- Molecule 59: DNA-directed RNA polymerase subunit beta'

Chain CD: 77% 17% • 5%




ALA
ALA
ALA
GLU
SER
SER
ILE
GLN
V952
S961
R978
E981
G1014
I1046
T1050
D1051
S1057
A1069
K1072
R1075
P1102
Q1126
GLU
SER
GLY
GLY
THR
LYS
ASP
ILE
T1135
L1138
V1141
A1142
D1143
L1144
F1145
K1151
A1157
E1158
I1159
F1165
G1166
K1167
E1168
T1169
K1172
R1173
R1174
L1175
P1179
D1184
P1185
Y1186
E1187
E1188
M1189
I1190
P1191
Q1195
L1196
N1197
E1200
R1206
I1210
V1229
V1234
V1237
Y1241
I1248
N1249
D1250
I1256
L1261
K1286
L1292
K1297
I1309
T1310
S1313
F1325
V1331
L1332
T1333
D1342
K1348
E1349
N1350
V1351
L1356
I1357
P1358
R1373
ALA
ALA
GLY
GLU
ALA
PRO
ALA
ALA
PRO
GLN
VAL
THR
ALA
GLU
ASP
ALA
SER
ALA
SER
LEU
ALA
GLU
LEU
LEU
ASN
ALA
GLY
LEU
GLY
GLY
SER
ASP
ASN
GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18552	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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

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

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	1.13	1/36569 (0.0%)	1.04	68/57044 (0.1%)
2	AB	0.35	0/1796	0.56	0/2420
3	AC	0.42	0/1667	0.58	0/2246
4	AD	0.51	0/1665	0.62	0/2227
5	AE	0.50	0/1161	0.68	1/1563 (0.1%)
6	AF	0.44	0/867	0.58	0/1171
7	AG	0.34	0/1219	0.61	1/1635 (0.1%)
8	AH	0.54	0/989	0.60	1/1326 (0.1%)
9	AI	0.43	0/1043	0.62	0/1387
10	AJ	0.41	0/810	0.70	1/1094 (0.1%)
11	AK	0.40	0/882	0.57	0/1191
12	AL	0.59	0/954	0.72	1/1279 (0.1%)
13	AM	0.36	0/900	0.55	0/1204
14	AN	0.40	0/817	0.52	0/1088
15	AO	0.45	0/722	0.56	0/964
16	AP	0.63	0/659	0.62	0/884
17	AQ	0.53	0/650	0.71	1/871 (0.1%)
18	AR	0.43	0/449	0.47	0/604
19	AS	0.42	0/680	0.58	0/915
20	AT	0.47	0/676	0.53	0/895
21	AU	0.37	0/598	0.57	1/792 (0.1%)
22	AV	1.89	28/709 (3.9%)	1.72	32/1099 (2.9%)
23	AW	0.73	1/1725 (0.1%)	1.04	2/2687 (0.1%)
24	AX	0.60	1/1584 (0.1%)	0.85	0/2463
25	BA	1.01	2/69187 (0.0%)	1.01	148/107927 (0.1%)
26	BB	0.72	0/2872	0.90	1/4478 (0.0%)
27	BC	0.50	0/2131	0.64	1/2863 (0.0%)
28	BD	0.47	0/1576	0.60	0/2119
29	BE	0.44	0/1571	0.65	2/2113 (0.1%)
30	BF	0.33	0/1444	0.59	0/1937
31	BG	0.38	0/1333	0.59	0/1805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	BH	0.30	0/1122	0.65	2/1515 (0.1%)
33	BK	0.47	0/1152	0.54	0/1551
34	BL	0.46	0/956	0.62	0/1279
35	BM	0.44	0/1061	0.64	0/1412
36	BN	0.43	0/1081	0.57	0/1443
37	BO	0.46	0/973	0.62	0/1301
38	BP	0.36	0/910	0.59	0/1219
39	BQ	0.43	0/929	0.58	0/1242
40	BR	0.59	0/960	0.56	0/1278
41	BS	0.48	0/829	0.67	0/1107
42	BT	0.43	0/864	0.58	0/1156
43	BU	0.41	0/764	0.57	0/1021
44	BV	0.41	0/797	0.58	0/1062
45	BW	0.42	0/766	0.61	1/1025 (0.1%)
46	BX	0.45	0/589	0.56	0/779
47	BY	0.46	0/635	0.52	0/848
48	BZ	0.34	0/502	0.51	0/667
49	B1	0.40	0/453	0.61	0/605
50	B2	0.47	0/450	0.73	0/599
51	B3	0.36	0/443	0.65	0/587
52	B4	0.48	0/380	0.61	0/498
53	B5	0.40	0/513	0.65	0/676
54	B6	0.47	0/302	0.65	0/397
55	CN	1.77	13/693 (1.9%)	1.24	3/1068 (0.3%)
56	CT	2.53	39/676 (5.8%)	1.33	9/1039 (0.9%)
57	CA	1.13	7/1797 (0.4%)	0.91	2/2436 (0.1%)
57	CB	0.80	1/1703 (0.1%)	0.86	3/2308 (0.1%)
58	CC	1.41	120/10581 (1.1%)	0.97	31/14275 (0.2%)
59	CD	1.12	58/10532 (0.6%)	0.91	15/14219 (0.1%)
All	All	0.98	271/183318 (0.1%)	0.94	327/270903 (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	3
10	AJ	0	1
12	AL	0	1
13	AM	0	2
22	AV	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	BA	0	2
27	BC	0	1
37	BO	0	1
46	BX	0	1
53	B5	0	1
All	All	0	14

The worst 5 of 271 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	1	C	OP3-P	-10.65	1.48	1.61
24	AX	1	G	OP3-P	-10.51	1.48	1.61
56	CT	18	DC	C3'-O3'	-10.28	1.30	1.44
59	CD	1357	ILE	C-N	-9.69	1.15	1.34
56	CT	14	DC	C3'-O3'	-9.60	1.31	1.44

The worst 5 of 327 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1027	C	C6-N1-C2	-25.80	109.98	120.30
1	AA	1027	C	C2-N1-C1'	18.88	139.57	118.80
1	AA	1027	C	C5-C6-N1	18.21	130.11	121.00
1	AA	1027	C	C6-N1-C1'	-15.29	102.45	120.80
25	BA	2131	U	O4'-C1'-N1	-14.14	96.89	108.20

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1027	C	Sidechain
1	AA	1034	G	Sidechain
1	AA	884	U	Sidechain
10	AJ	42	LEU	Mainchain
12	AL	43	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32907	0	16571	400	0
2	AB	1765	0	1792	35	0
3	AC	1640	0	1713	99	0
4	AD	1643	0	1706	58	0
5	AE	1148	0	1195	40	0
6	AF	848	0	846	31	0
7	AG	1203	0	1254	34	0
8	AH	979	0	1031	26	0
9	AI	1031	0	1076	50	0
10	AJ	800	0	839	39	0
11	AK	866	0	874	17	0
12	AL	949	0	1008	24	0
13	AM	891	0	952	37	0
14	AN	805	0	844	21	0
15	AO	714	0	734	13	0
16	AP	649	0	666	4	0
17	AQ	641	0	682	13	0
18	AR	443	0	466	14	0
19	AS	663	0	688	21	0
20	AT	670	0	719	14	0
21	AU	590	0	629	19	0
22	AV	636	0	327	19	0
23	AW	1645	0	842	26	0
24	AX	1624	0	823	35	0
25	BA	62290	0	31344	614	0
26	BB	2569	0	1301	24	0
27	BC	2092	0	2167	40	0
28	BD	1566	0	1618	31	0
29	BE	1552	0	1618	28	0
30	BF	1420	0	1457	63	0
31	BG	1313	0	1358	34	0
32	BH	1111	0	1148	35	0
33	BK	1129	0	1162	17	0
34	BL	947	0	1023	25	0
35	BM	1052	0	1127	26	0
36	BN	1075	0	1153	23	0
37	BO	960	0	999	15	0
38	BP	900	0	935	26	0
39	BQ	917	0	962	23	0
40	BR	947	0	1019	20	0
41	BS	816	0	839	15	0
42	BT	857	0	922	17	0
43	BU	757	0	820	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	789	0	844	18	0
45	BW	753	0	780	17	0
46	BX	582	0	599	8	0
47	BY	625	0	652	13	0
48	BZ	501	0	531	7	0
49	B1	449	0	488	9	0
50	B2	444	0	458	17	0
51	B3	436	0	477	13	0
52	B4	377	0	418	10	0
53	B5	504	0	572	14	0
54	B6	301	0	341	7	0
55	CN	618	0	339	27	0
56	CT	606	0	338	36	0
57	CA	1775	0	1800	15	0
57	CB	1684	0	1713	19	0
58	CC	10415	0	10432	214	0
59	CD	10375	0	10597	176	0
60	AA	119	0	0	0	0
60	AW	2	0	0	0	0
60	B2	1	0	0	0	0
60	BA	294	0	0	0	0
60	BB	2	0	0	0	0
60	BC	1	0	0	0	0
60	BO	1	0	0	0	0
60	CD	1	0	0	0	0
61	AX	11	0	8	1	0
62	B6	1	0	0	0	0
62	CD	2	0	0	0	0
All	All	171689	0	122636	2452	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 9.

The worst 5 of 2452 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)
3:AC:109:PRO:HD2	58:CC:859:GLU:CG	1.58	1.34
4:AD:193:ALA:CA	59:CD:86:GLU:OE2	1.73	1.32
5:AE:10:GLU:HG3	59:CD:78:LEU:CD1	1.77	1.15
3:AC:109:PRO:HD2	58:CC:859:GLU:HG3	1.21	1.15
4:AD:191:LEU:O	59:CD:86:GLU:OE1	1.60	1.15

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%)	208 (93%)	15 (7%)	1 (0%)	34	66
3	AC	207/233 (89%)	194 (94%)	10 (5%)	3 (1%)	11	38
4	AD	203/206 (98%)	193 (95%)	9 (4%)	1 (0%)	29	61
5	AE	154/167 (92%)	143 (93%)	10 (6%)	1 (1%)	25	57
6	AF	102/131 (78%)	95 (93%)	7 (7%)	0	100	100
7	AG	151/156 (97%)	142 (94%)	8 (5%)	1 (1%)	22	54
8	AH	127/130 (98%)	117 (92%)	9 (7%)	1 (1%)	19	51
9	AI	126/130 (97%)	115 (91%)	9 (7%)	2 (2%)	9	36
10	AJ	98/103 (95%)	88 (90%)	7 (7%)	3 (3%)	4	23
11	AK	114/129 (88%)	99 (87%)	14 (12%)	1 (1%)	17	48
12	AL	119/124 (96%)	109 (92%)	8 (7%)	2 (2%)	9	35
13	AM	113/118 (96%)	106 (94%)	6 (5%)	1 (1%)	17	48
14	AN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	AO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	AP	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
17	AQ	77/84 (92%)	70 (91%)	7 (9%)	0	100	100
18	AR	52/75 (69%)	50 (96%)	2 (4%)	0	100	100
19	AS	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
20	AT	84/87 (97%)	84 (100%)	0	0	100	100
21	AU	68/71 (96%)	66 (97%)	1 (2%)	1 (2%)	10	38
27	BC	270/273 (99%)	249 (92%)	18 (7%)	3 (1%)	14	45
28	BD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BE	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
30	BF	176/179 (98%)	162 (92%)	14 (8%)	0	100	100
31	BG	173/177 (98%)	158 (91%)	15 (9%)	0	100	100
32	BH	147/149 (99%)	132 (90%)	14 (10%)	1 (1%)	22	54
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%)	11	38
36	BN	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
37	BO	118/127 (93%)	105 (89%)	13 (11%)	0	100	100
38	BP	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	17	48
39	BQ	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
40	BR	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
41	BS	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	15	46
42	BT	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	BU	93/100 (93%)	88 (95%)	5 (5%)	0	100	100
44	BV	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	15	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%)	57 (95%)	3 (5%)	0	100	100
49	B1	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
50	B2	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
51	B3	51/55 (93%)	49 (96%)	2 (4%)	0	100	100
52	B4	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
53	B5	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	9	36
54	B6	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
57	CA	227/329 (69%)	217 (96%)	10 (4%)	0	100	100
57	CB	215/329 (65%)	204 (95%)	10 (5%)	1 (0%)	29	61
58	CC	1316/1342 (98%)	1197 (91%)	110 (8%)	9 (1%)	22	54
59	CD	1327/1407 (94%)	1222 (92%)	95 (7%)	10 (1%)	19	51
All	All	8623/9235 (93%)	8034 (93%)	540 (6%)	49 (1%)	29	57

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	AI	13	LYS
9	AI	56	ASP
11	AK	93	ARG
12	AL	88	LYS
27	BC	241	GLY

5.3.2 Protein sidechains (i)

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%)	175 (94%)	12 (6%)	17	46
3	AC	171/190 (90%)	153 (90%)	18 (10%)	7	25
4	AD	172/173 (99%)	154 (90%)	18 (10%)	7	25
5	AE	118/126 (94%)	107 (91%)	11 (9%)	9	30
6	AF	91/112 (81%)	83 (91%)	8 (9%)	10	33
7	AG	126/129 (98%)	111 (88%)	15 (12%)	5	21
8	AH	104/105 (99%)	97 (93%)	7 (7%)	16	45
9	AI	106/107 (99%)	97 (92%)	9 (8%)	10	35
10	AJ	87/90 (97%)	75 (86%)	12 (14%)	3	16
11	AK	89/99 (90%)	85 (96%)	4 (4%)	27	58
12	AL	102/103 (99%)	90 (88%)	12 (12%)	5	21
13	AM	93/96 (97%)	86 (92%)	7 (8%)	13	39
14	AN	83/84 (99%)	77 (93%)	6 (7%)	14	41
15	AO	76/77 (99%)	67 (88%)	9 (12%)	5	21
16	AP	65/65 (100%)	63 (97%)	2 (3%)	40	67
17	AQ	73/78 (94%)	63 (86%)	10 (14%)	3	16
18	AR	47/65 (72%)	43 (92%)	4 (8%)	10	35
19	AS	72/79 (91%)	69 (96%)	3 (4%)	30	60
20	AT	65/66 (98%)	58 (89%)	7 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AU	60/61 (98%)	58 (97%)	2 (3%)	38	66
27	BC	217/218 (100%)	207 (95%)	10 (5%)	27	58
28	BD	163/163 (100%)	151 (93%)	12 (7%)	13	40
29	BE	165/165 (100%)	150 (91%)	15 (9%)	9	31
30	BF	149/150 (99%)	135 (91%)	14 (9%)	8	30
31	BG	136/138 (99%)	122 (90%)	14 (10%)	7	26
32	BH	114/114 (100%)	100 (88%)	14 (12%)	4	20
33	BK	116/116 (100%)	108 (93%)	8 (7%)	15	44
34	BL	104/104 (100%)	96 (92%)	8 (8%)	13	38
35	BM	103/103 (100%)	92 (89%)	11 (11%)	6	25
36	BN	108/108 (100%)	103 (95%)	5 (5%)	27	58
37	BO	100/103 (97%)	95 (95%)	5 (5%)	24	55
38	BP	87/87 (100%)	80 (92%)	7 (8%)	12	37
39	BQ	99/100 (99%)	91 (92%)	8 (8%)	11	36
40	BR	89/90 (99%)	84 (94%)	5 (6%)	21	52
41	BS	84/84 (100%)	78 (93%)	6 (7%)	14	42
42	BT	93/93 (100%)	88 (95%)	5 (5%)	22	53
43	BU	82/84 (98%)	73 (89%)	9 (11%)	6	24
44	BV	84/85 (99%)	81 (96%)	3 (4%)	35	63
45	BW	78/78 (100%)	72 (92%)	6 (8%)	13	38
46	BX	58/63 (92%)	55 (95%)	3 (5%)	23	54
47	BY	67/68 (98%)	66 (98%)	1 (2%)	65	81
48	BZ	54/55 (98%)	52 (96%)	2 (4%)	34	63
49	B1	48/49 (98%)	41 (85%)	7 (15%)	3	14
50	B2	47/48 (98%)	42 (89%)	5 (11%)	6	25
51	B3	48/49 (98%)	46 (96%)	2 (4%)	30	60
52	B4	38/38 (100%)	36 (95%)	2 (5%)	22	53
53	B5	51/52 (98%)	50 (98%)	1 (2%)	55	76
54	B6	34/44 (77%)	34 (100%)	0	100	100
57	CA	197/286 (69%)	193 (98%)	4 (2%)	55	76
57	CB	187/286 (65%)	177 (95%)	10 (5%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	CC	1139/1157 (98%)	1096 (96%)	43 (4%)	33	62
59	CD	1118/1168 (96%)	1097 (98%)	21 (2%)	57	77
All	All	7244/7650 (95%)	6802 (94%)	442 (6%)	22	48

5 of 442 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	BG	69	ARG
36	BN	127	LYS
59	CD	1167	LYS
58	CC	830	THR
31	BG	155	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
5	AE	70	ASN
6	AF	11	HIS
9	AI	31	ASN
39	BQ	115	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	288 (18%)	32 (2%)
22	AV	28/57 (49%)	12 (42%)	1 (3%)
23	AW	76/77 (98%)	21 (27%)	6 (7%)
24	AX	73/76 (96%)	18 (24%)	0
25	BA	2895/2904 (99%)	552 (19%)	66 (2%)
26	BB	119/120 (99%)	15 (12%)	0
All	All	4720/4776 (98%)	906 (19%)	105 (2%)

5 of 906 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	19	A

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Mol	Chain	Res	Type
1	AA	22	G

5 of 105 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	884	U
25	BA	1344	U
25	BA	2601	C
25	BA	984	A
25	BA	1109	C

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

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	$\#\|Z\| > 2$
1	4OC	AA	1402	1,60	20,23,24	3.29	9 (45%)	26,32,35	1.05	3 (11%)
25	PSU	BA	746	25,60	18,21,22	1.12	3 (16%)	22,30,33	2.04	6 (27%)
1	G7M	AA	527	1	20,26,27	2.24	8 (40%)	17,39,42	1.31	2 (11%)
24	H2U	AX	20	24	18,21,22	3.21	5 (27%)	21,30,33	1.90	5 (23%)
25	5MU	BA	747	25	19,22,23	1.41	4 (21%)	28,32,35	2.25	6 (21%)
25	G7M	BA	2069	25	20,26,27	2.21	8 (40%)	17,39,42	1.24	1 (5%)
24	PSU	AX	39	24	18,21,22	1.11	2 (11%)	22,30,33	1.86	4 (18%)
25	PSU	BA	2457	25	18,21,22	1.06	2 (11%)	22,30,33	2.09	6 (27%)
24	3AU	AX	47	24	18,21,29	3.41	8 (44%)	26,30,43	1.66	4 (15%)
24	H2U	AX	16	24	18,21,22	2.99	5 (27%)	21,30,33	1.94	5 (23%)
23	H2U	AW	20	23	18,21,22	3.05	5 (27%)	21,30,33	2.03	4 (19%)
1	5MC	AA	1407	1	18,22,23	3.75	7 (38%)	26,32,35	1.03	1 (3%)
25	5MC	BA	1962	25	18,22,23	3.70	7 (38%)	26,32,35	1.11	1 (3%)
25	PSU	BA	2580	25	18,21,22	1.09	2 (11%)	22,30,33	2.27	8 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MA6	AA	1518	1	18,26,27	1.40	3 (16%)	19,38,41	3.96	2 (10%)
24	PSU	AX	32	24	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
24	7MG	AX	46	24	20,25,27	3.16	10 (50%)	27,37,42	2.05	7 (25%)
23	4SU	AW	8	23	18,21,22	4.08	8 (44%)	26,30,33	2.21	5 (19%)
25	2MG	BA	2445	29,25	18,26,27	2.18	7 (38%)	16,38,41	1.63	4 (25%)
1	MA6	AA	1519	1	18,26,27	1.35	3 (16%)	19,38,41	4.51	2 (10%)
1	2MG	AA	1516	1	18,26,27	2.20	7 (38%)	16,38,41	1.65	4 (25%)
25	OMU	BA	2552	25	19,22,23	2.80	6 (31%)	26,31,34	1.85	5 (19%)
1	PSU	AA	516	1,60	18,21,22	1.03	2 (11%)	22,30,33	2.04	7 (31%)
1	2MG	AA	966	1	18,25,27	2.54	8 (44%)	19,37,41	1.69	5 (26%)
1	5MC	AA	967	1	18,22,23	3.85	7 (38%)	26,32,35	1.11	2 (7%)
28	MEQ	BD	150	28	8,9,10	0.94	0	5,10,12	0.97	1 (20%)
25	6MZ	BA	1618	25	18,25,26	1.96	3 (16%)	16,36,39	2.19	3 (18%)
25	PSU	BA	2604	25	18,21,22	1.04	2 (11%)	22,30,33	1.90	5 (22%)
23	OMC	AW	32	23	19,22,23	2.90	8 (42%)	26,31,34	0.82	0
12	D2T	AL	89	12	6,7,10	1.02	0	5,8,13	1.07	0
25	PSU	BA	2605	25	18,21,22	1.08	2 (11%)	22,30,33	1.88	3 (13%)
25	3TD	BA	1915	25	18,22,23	4.39	10 (55%)	22,32,35	2.04	4 (18%)
24	PSU	AX	55	24	18,21,22	1.01	1 (5%)	22,30,33	1.94	5 (22%)
24	4SU	AX	8	24	18,21,22	4.03	8 (44%)	26,30,33	2.20	4 (15%)
23	PSU	AW	55	23	18,21,22	1.03	1 (5%)	22,30,33	1.96	5 (22%)
25	5MU	BA	1939	25,60	19,22,23	1.45	3 (15%)	28,32,35	2.36	6 (21%)
25	PSU	BA	2504	25,60	18,21,22	1.12	3 (16%)	22,30,33	2.11	6 (27%)
25	2MG	BA	1835	25	18,26,27	2.23	7 (38%)	16,38,41	1.57	4 (25%)
36	4D4	BN	81	36	9,11,12	2.47	3 (33%)	8,13,15	0.84	0
25	OMC	BA	2498	25,60	19,22,23	2.69	7 (36%)	26,31,34	0.84	1 (3%)
25	OMG	BA	2251	25,23	18,26,27	2.54	8 (44%)	19,38,41	1.48	4 (21%)
1	2MG	AA	1207	1	18,25,27	2.49	8 (44%)	19,37,41	1.66	5 (26%)
25	1MG	BA	745	25	18,26,27	2.55	4 (22%)	19,39,42	1.52	4 (21%)
25	6MZ	BA	2030	25	18,25,26	1.95	3 (16%)	16,36,39	2.61	4 (25%)
25	PSU	BA	1917	25	18,21,22	1.00	3 (16%)	22,30,33	1.90	5 (22%)
1	UR3	AA	1498	1	19,22,23	2.40	6 (31%)	26,32,35	1.29	1 (3%)
25	PSU	BA	955	25,36	18,21,22	1.17	3 (16%)	22,30,33	1.94	5 (22%)
25	PSU	BA	1911	25	18,21,22	1.11	2 (11%)	22,30,33	1.87	4 (18%)
24	MIA	AX	37	24	18,24,32	1.48	3 (16%)	18,35,47	1.53	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	H2U	BA	2449	25	18,21,22	2.74	5 (27%)	21,30,33	2.10	5 (23%)
24	5MU	AX	54	24	19,22,23	1.37	4 (21%)	28,32,35	2.11	6 (21%)
25	2MA	BA	2503	25,60	17,25,26	2.58	6 (35%)	17,37,40	1.45	4 (23%)
23	5MU	AW	54	23	19,22,23	1.38	5 (26%)	28,32,35	2.20	8 (28%)

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
1	4OC	AA	1402	1,60	-	0/9/29/30	0/2/2/2
25	PSU	BA	746	25,60	-	1/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	1/3/25/26	0/3/3/3
24	H2U	AX	20	24	-	5/7/38/39	0/2/2/2
25	5MU	BA	747	25	-	0/7/25/26	0/2/2/2
25	G7M	BA	2069	25	-	2/3/25/26	0/3/3/3
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
25	PSU	BA	2457	25	-	0/7/25/26	0/2/2/2
24	3AU	AX	47	24	-	0/7/25/35	0/2/2/2
24	H2U	AX	16	24	-	1/7/38/39	0/2/2/2
23	H2U	AW	20	23	-	7/7/38/39	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
25	5MC	BA	1962	25	-	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	-	3/7/29/30	0/3/3/3
24	PSU	AX	32	24	-	0/7/25/26	0/2/2/2
24	7MG	AX	46	24	-	4/7/34/38	0/3/3/3
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
25	2MG	BA	2445	29,25	-	2/5/27/28	0/3/3/3
1	MA6	AA	1519	1	-	6/7/29/30	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
25	OMU	BA	2552	25	-	2/9/27/28	0/2/2/2
1	PSU	AA	516	1,60	-	2/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/3/25/28	0/3/3/3
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2
28	MEQ	BD	150	28	-	3/8/9/11	-
25	6MZ	BA	1618	25	-	2/5/27/28	0/3/3/3
25	PSU	BA	2604	25	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMC	AW	32	23	-	0/9/27/28	0/2/2/2
12	D2T	AL	89	12	-	1/5/6/14	-
25	PSU	BA	2605	25	-	0/7/25/26	0/2/2/2
25	3TD	BA	1915	25	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	2/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	1/7/25/26	0/2/2/2
25	5MU	BA	1939	25,60	-	2/7/25/26	0/2/2/2
25	PSU	BA	2504	25,60	-	0/7/25/26	0/2/2/2
25	2MG	BA	1835	25	-	0/5/27/28	0/3/3/3
36	4D4	BN	81	36	-	7/11/12/14	-
25	OMC	BA	2498	25,60	-	2/9/27/28	0/2/2/2
25	OMG	BA	2251	25,23	-	0/5/27/28	0/3/3/3
1	2MG	AA	1207	1	-	2/3/25/28	0/3/3/3
25	1MG	BA	745	25	-	0/3/25/26	0/3/3/3
25	6MZ	BA	2030	25	-	2/5/27/28	0/3/3/3
25	PSU	BA	1917	25	-	2/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
25	PSU	BA	955	25,36	-	0/7/25/26	0/2/2/2
25	PSU	BA	1911	25	-	1/7/25/26	0/2/2/2
24	MIA	AX	37	24	-	0/3/25/34	0/3/3/3
25	H2U	BA	2449	25	-	0/7/38/39	0/2/2/2
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
25	2MA	BA	2503	25,60	-	2/3/25/26	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2

The worst 5 of 255 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1915	3TD	C6-C5	11.44	1.48	1.35
24	AX	20	H2U	C2-N1	10.34	1.50	1.35
25	BA	1915	3TD	C2-N1	9.65	1.49	1.37
23	AW	20	H2U	C2-N1	9.55	1.49	1.35
1	AA	967	5MC	C6-C5	9.49	1.50	1.34

The worst 5 of 207 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1519	MA6	N1-C6-N6	-18.57	97.51	117.06
1	AA	1518	MA6	N1-C6-N6	-16.24	99.97	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AW	8	4SU	C4-N3-C2	-7.77	119.79	127.34
24	AX	8	4SU	C4-N3-C2	-7.50	120.05	127.34
25	BA	2030	6MZ	C9-N6-C6	-7.37	116.52	122.87

There are no chirality outliers.

5 of 70 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	1518	MA6	C5-C6-N6-C9
1	AA	1518	MA6	C5-C6-N6-C10
1	AA	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	527	G7M	2	0
24	AX	20	H2U	2	0
25	BA	747	5MU	1	0
25	BA	2069	G7M	1	0
24	AX	16	H2U	1	0
1	AA	1518	MA6	2	0
24	AX	46	7MG	1	0
25	BA	2445	2MG	1	0
1	AA	1519	MA6	1	0
1	AA	1516	2MG	1	0
25	BA	2552	OMU	3	0
1	AA	966	2MG	2	0
1	AA	967	5MC	1	0
28	BD	150	MEQ	3	0
25	BA	1915	3TD	3	0
24	AX	8	4SU	2	0
23	AW	55	PSU	1	0
25	BA	2504	PSU	1	0
1	AA	1207	2MG	2	0
25	BA	2030	6MZ	1	0
25	BA	1917	PSU	3	0
1	AA	1498	UR3	1	0
25	BA	955	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AX	37	MIA	2	0
25	BA	2449	H2U	2	0
23	AW	54	5MU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 425 ligands modelled in this entry, 424 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	$\#\|Z\| > 2$
61	PHE	AX	101	24	10,11,12	0.49	0	10,13,15	0.24	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
61	PHE	AX	101	24	-	2/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	AX	101	PHE	CA-CB-CG-CD1
61	AX	101	PHE	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	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
59	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

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11420. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

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

7 Map analysis (i)

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

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit (i)

This section was not generated.