



wwPDB EM Validation Summary Report ⓘ

Mar 11, 2025 – 03:52 pm GMT

PDB ID : 6ZTN
EMDB ID : EMD-11421
Title : E. coli 70S-RNAP expressome complex in NusG-coupled state (42 nt intervening mRNA)
Authors : Webster, M.W.; Takacs, M.; Weixlbaumer, A.
Deposited on : 2020-07-20
Resolution : 3.90 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

A user guide is available at

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

The types of validation reports are described at

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

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

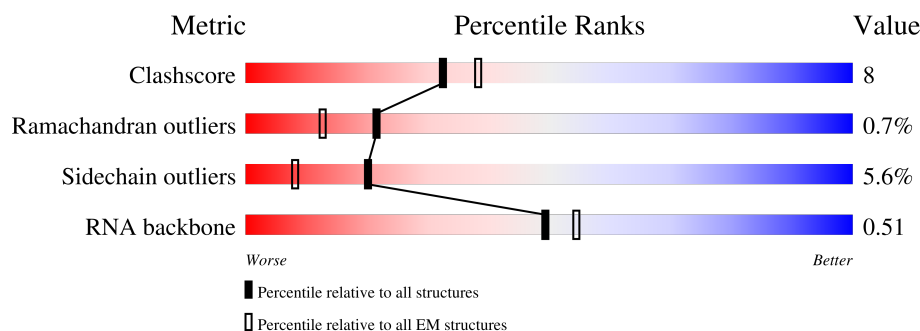
EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 3.90 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.


















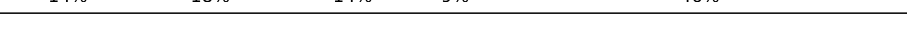









Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 ≥ 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	57% 33% 8% ..
2	AB	241	73% 19% • 6%
3	AC	233	67% 21% • 10%
4	AD	206	74% 24% •
5	AE	167	69% 19% 5% 7%
6	AF	131	44% 31% 5% 21%
7	AG	156	73% 23% ..












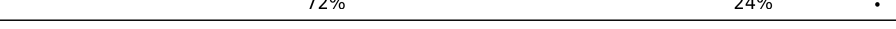













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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	57	
23	AW	77	
24	AX	76	
24	AZ	76	
25	BA	2904	
26	BB	120	
27	BC	273	
28	BD	209	
29	BE	201	
30	BF	179	
31	BG	177	

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Mol	Chain	Length	Quality of chain
32	BH	149	 66% 30% .
33	BK	142	 85% 14% .
34	BL	123	 81% 18% .
35	BM	144	 77% 21% .
36	BN	136	 79% 21% .
37	BO	127	 73% 18% . 6%
38	BP	117	 72% 26% .
39	BQ	115	 77% 20% ..
40	BR	118	 81% 18% ..
41	BS	103	 72% 28%
42	BT	110	 77% 20% .
43	BU	100	 72% 24% .
44	BV	104	 70% 27% ..
45	BW	94	 76% 23% .
46	BX	85	 76% 12% . 11%
47	BY	78	 67% 31% ..
48	BZ	63	 73% 24% ..
49	B1	59	 73% 25% .
50	B2	57	 68% 28% ..
51	B3	55	 85% 9% . .
52	B4	46	 78% 22%
53	B5	65	 75% 20% ..
54	B6	50	 58% 16% . 24%
55	CA	329	 60% 9% 30%
55	CB	329	 57% 8% . 33%

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Mol	Chain	Length	Quality of chain
56	CC	1342	 78%17%••
57	CD	1407	 77%17%•5%
58	CE	91	 47%9%44%
59	CN	39	 26%41%10%23%
60	CT	39	 8%51%18%23%
61	CF	181	 45%9%46%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	7MG	AZ	46	-	-	X	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 174624 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	57	Total	C	N	O	0	0
			474	298	90	86		

- 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	31	Total	C	N	O	P	0	0
			656	294	117	214	31		

- 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 1630	C 730	N 290	O 533	P 76	S 1	0	0
24	AZ	76	Total 1630	C 730	N 290	O 533	P 76	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	2899	Total	C	N	O	P	0	0
			62248	27776	11451	20122	2899		

- 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 DNA-directed RNA polymerase subunit alpha.

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

- Molecule 56 is a protein called DNA-directed RNA polymerase subunit beta.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CE	51	Total	C	N	O	S	0	0
			399	246	77	75	1		

- Molecule 59 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CN	30	Total	C	N	O	P	0	0
			615	294	114	178	29		

- Molecule 60 is a DNA chain called Template DNA strand.

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

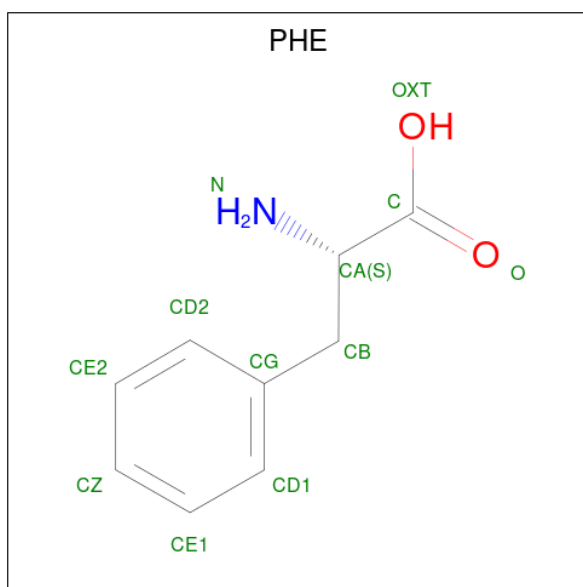
- Molecule 61 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CF	98	Total	C	N	O	S	0	0
			790	505	139	140	6		

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

Mol	Chain	Residues	Atoms		AltConf
62	AA	139	Total	Mg	0
			139	139	
62	AL	3	Total	Mg	0
			3	3	
62	AT	1	Total	Mg	0
			1	1	
62	AV	1	Total	Mg	0
			1	1	
62	AW	4	Total	Mg	0
			4	4	
62	AX	1	Total	Mg	0
			1	1	
62	BA	318	Total	Mg	0
			318	318	
62	BB	9	Total	Mg	0
			9	9	
62	BC	3	Total	Mg	0
			3	3	
62	BD	1	Total	Mg	0
			1	1	
62	BN	1	Total	Mg	0
			1	1	
62	BR	1	Total	Mg	0
			1	1	
62	BX	1	Total	Mg	0
			1	1	
62	B2	1	Total	Mg	0
			1	1	
62	B5	1	Total	Mg	0
			1	1	
62	B6	1	Total	Mg	0
			1	1	
62	CD	1	Total	Mg	0
			1	1	

- Molecule 63 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



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

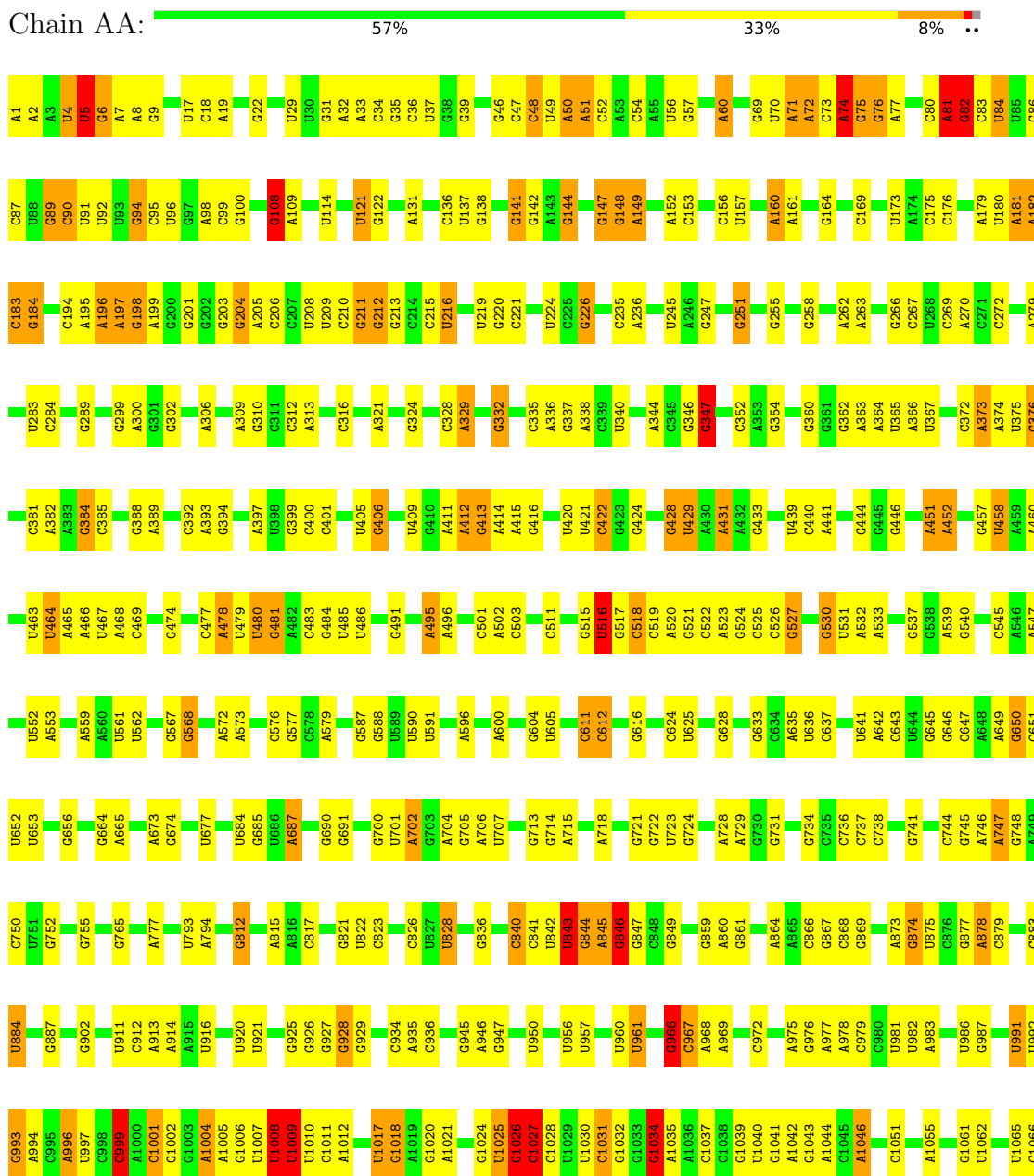
- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

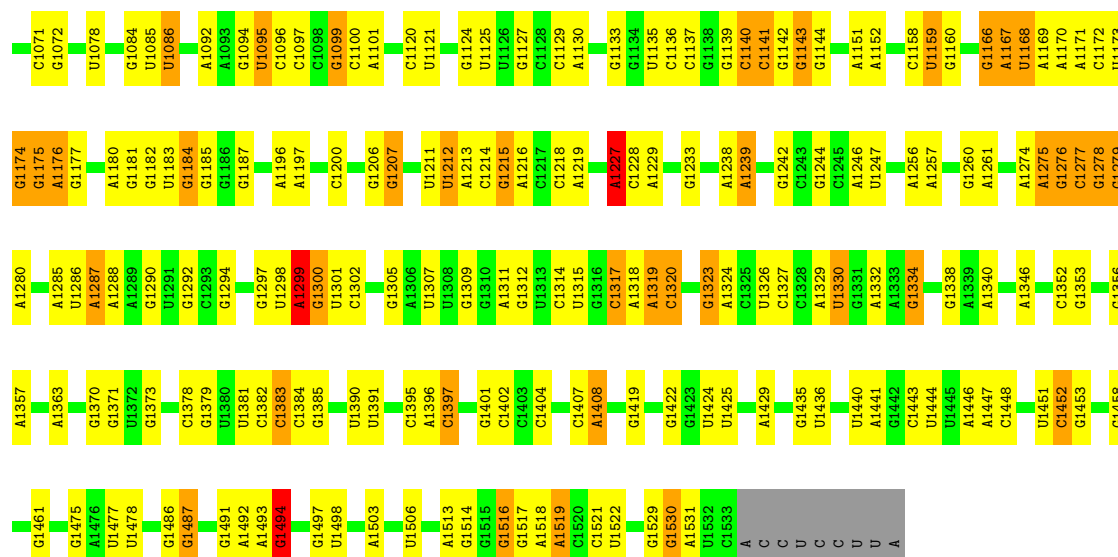
Mol	Chain	Residues	Atoms		AltConf
64	CD	2	Total	Zn	0
			2	2	

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.

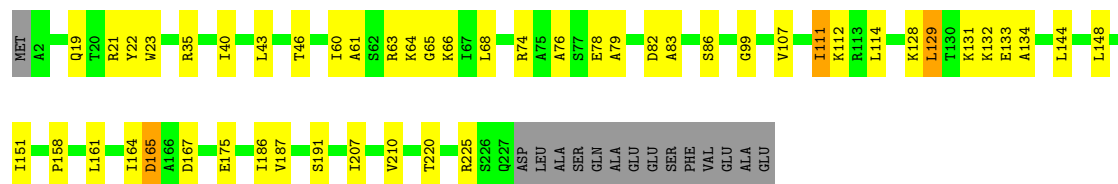
• Molecule 1: 16S ribosomal RNA





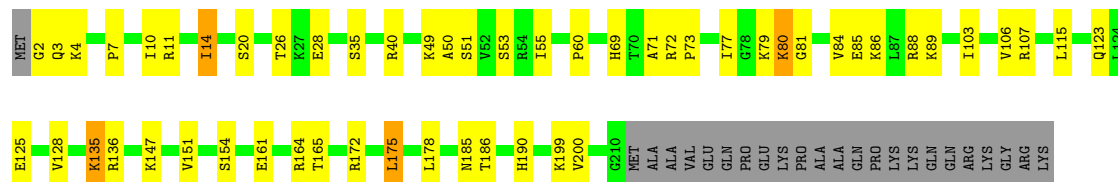
• Molecule 2: 30S ribosomal protein S2

Chain AB: 73% 19% • 6%



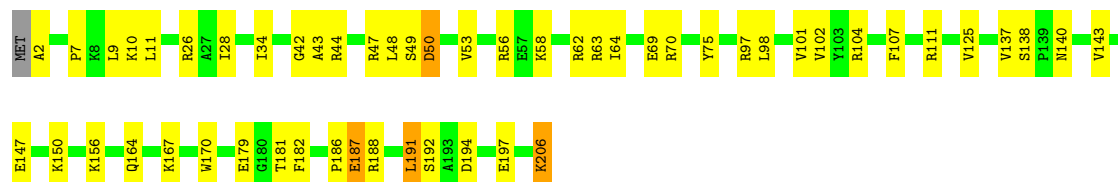
• Molecule 3: 30S ribosomal protein S3

Chain AC: 67% 21% • 10%



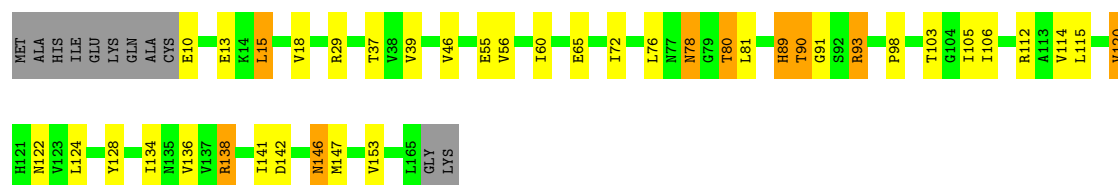
• Molecule 4: 30S ribosomal protein S4

Chain AD: 74% 24% •



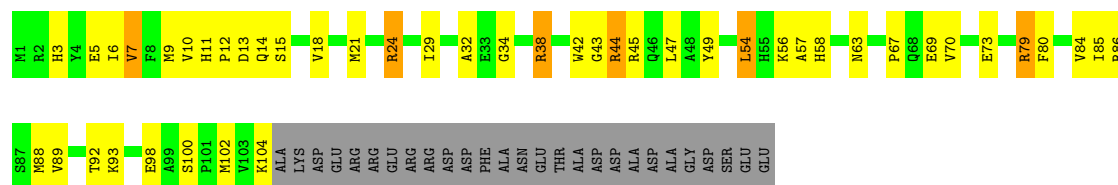
• Molecule 5: 30S ribosomal protein S5

Chain AE: 



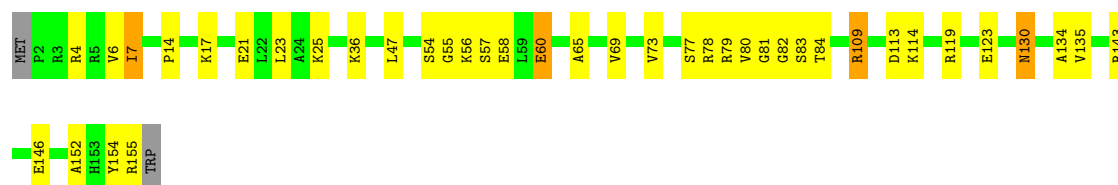
- Molecule 6: 30S ribosomal protein S6

Chain AF: 




- Molecule 7: 30S ribosomal protein S7

Chain AG: 



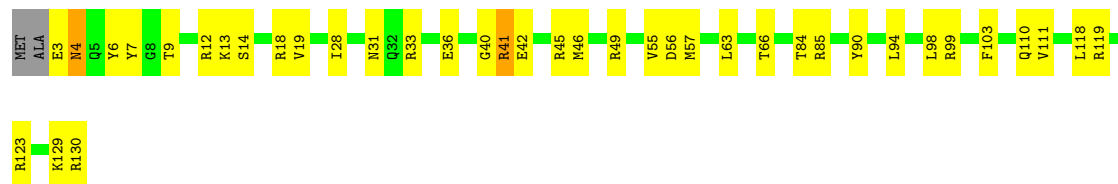
- Molecule 8: 30S ribosomal protein S8

Chain AH: 



- Molecule 9: 30S ribosomal protein S9

Chain AI: 



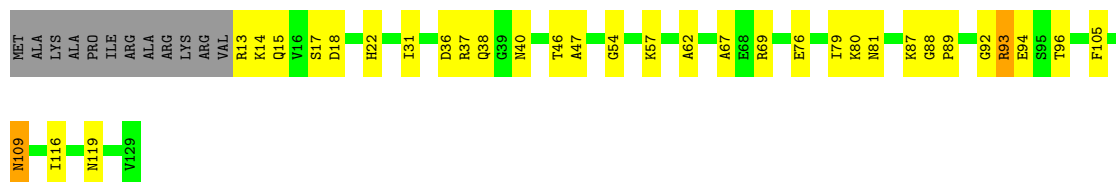
- Molecule 10: 30S ribosomal protein S10

Chain AJ: 



- Molecule 11: 30S ribosomal protein S11

Chain AK: 65% 24% 9%



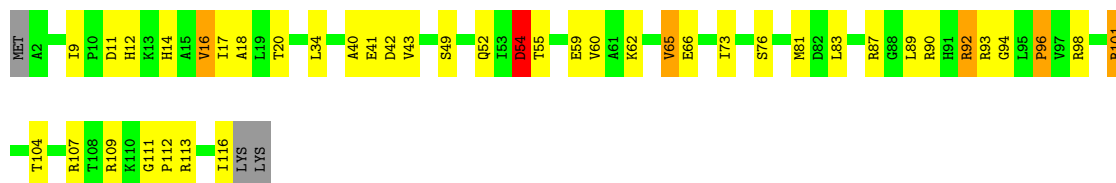
- Molecule 12: 30S ribosomal protein S12

Chain AL: 64% 31% ..



- Molecule 13: 30S ribosomal protein S13

Chain AM: 62% 31% ..



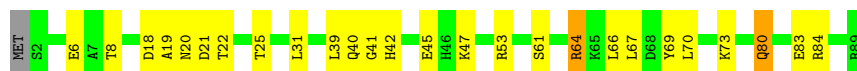
- Molecule 14: 30S ribosomal protein S14

Chain AN: 78% 20% ..




- Molecule 15: 30S ribosomal protein S15

Chain AO: 70% 27% ..




- Molecule 16: 30S ribosomal protein S16

Chain AP:  83% 17%



- Molecule 17: 30S ribosomal protein S17

Chain AQ:  75% 20% 5%



- Molecule 18: 30S ribosomal protein S18

Chain AR:  45% 27% 24%




- Molecule 19: 30S ribosomal protein S19

Chain AS:  65% 23% 10%




- Molecule 20: 30S ribosomal protein S20

Chain AT:  80% 15%

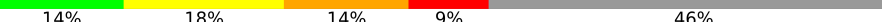


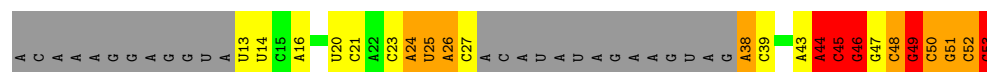
- Molecule 21: 30S ribosomal protein S21

Chain AU:  82% 15%



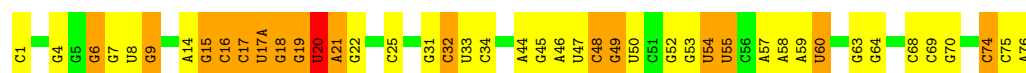
- Molecule 22: mRNA

Chain AV:  14% 18% 14% 9% 46%



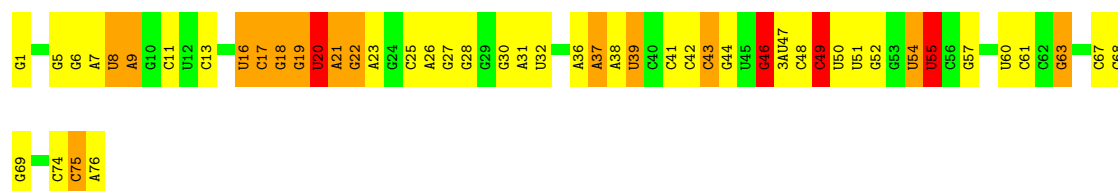
- Molecule 23: tRNA(fmet) P-site

Chain AW: 

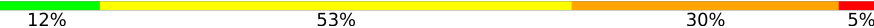


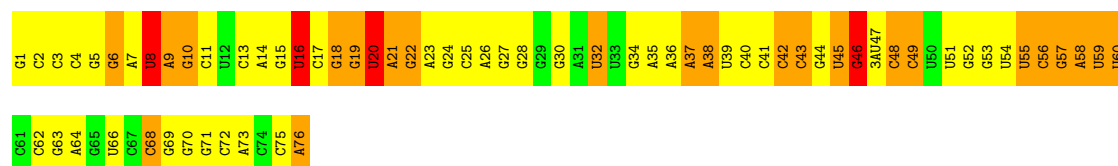
• Molecule 24: Phe-NH-tRNA(Phe) A-site

Chain AX: 



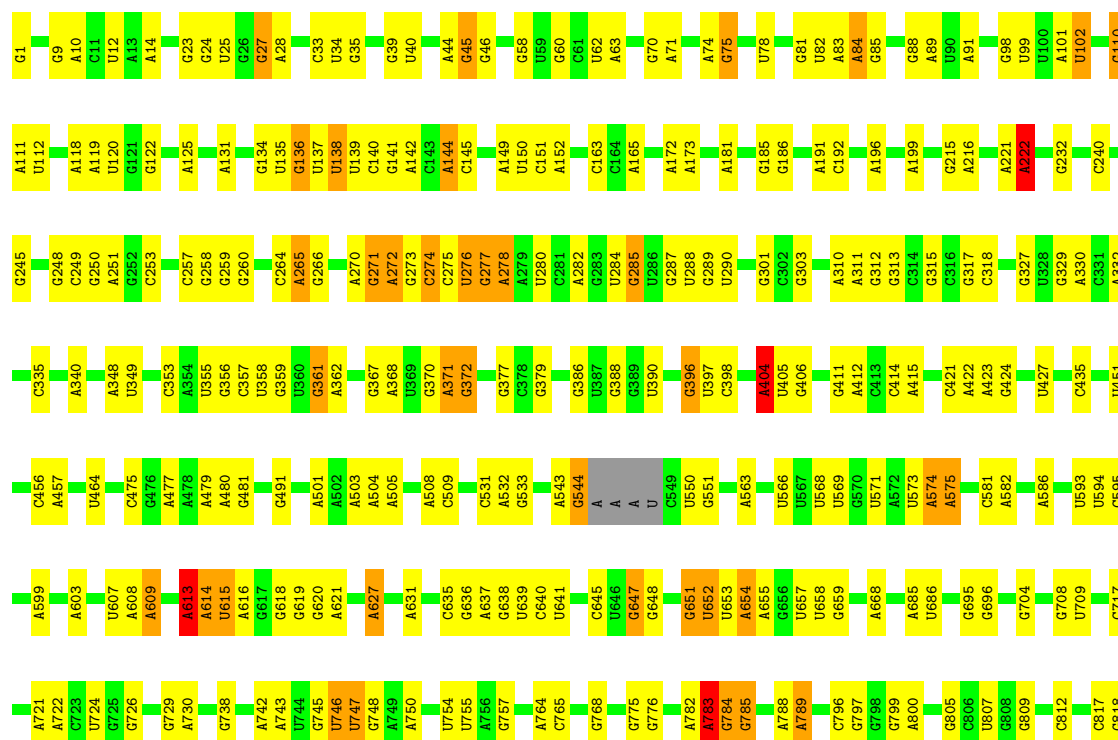
• Molecule 24: Phe-NH-tRNA(Phe) A-site

Chain AZ: 



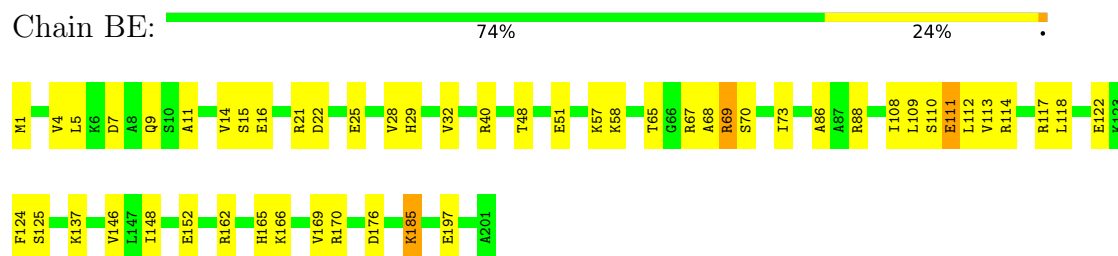
• Molecule 25: 23S ribosomal RNA

Chain BA: 

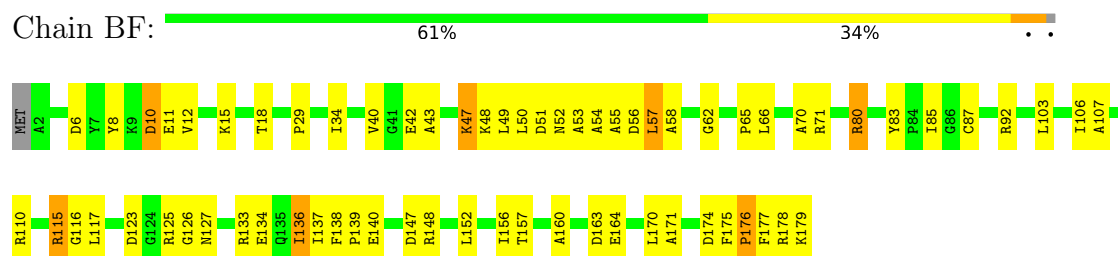


A2212	A2213	U2139	C2065	U1834	U1735	U1599	G1524	G1421	A1322	G1186	A1095	G1026	G924	A819
G2245	U2213	G2140	C2066	G1835	U1736	C1600	A1525	G1422	C1323	G1187	A1096	A1027	A925	U827
A2225	A2226	G2141	C1967	A1848	G1737	C1607	C1526	C1428	U1326	C1196	A1103	A1028	A926	U828
A2227	A2228	C2145	A2070	G1857	G1738	A1608	A1528	G1432	G1333	G1197	C1104	U1033	U931	A833
U2229	U2229	A2147	C2072	A1858	G1740	A1609	A1529	A1433	G1334	U1198	U1105	G1034	U932	G834
		G2148	C2073	U1859	G1741	A1610	G1530	A1434	G1334	U1199	G1106	U1035	U933	U839
G2234	G2234	U2149	U2074	G1860	G1742	G1613	C1531	G1452	U1344	A1204	U1108	G1037	G940	C840
G2238	G2238	C2150	U2075	G1861	G1743	A1614	U1534	A1453	C1345	A1205	C1109	G1038	A941	A845
G2239	G2239	U2151	U2085	G1862	A1744	A1618	U1535	G1454	G1349	G1206	A1110	A1039	U941	U846
		C2152	U2086	U1863	A1745	G1619	C1536	G1455	C1350		A1111	A1040	A945	A847
		C2153	G2087	U1864	G1750	G1622	G1537	G1456	C1351	U1211	G1112	C1043	A946	U847
U2243	U2243	U2155		C1868	G1752	G1623	G1540	U1457	U1352	G1216	U1113	C1044	C946	C848
U2244	U2244	C2156	G2093	C1869		G1623	G1540	U1458	A1353	G1217	G1115	C1045	A947	A849
U2245	U2245	G2157		C1870	A1755	A1630	G1543	G1459	A1354	G1218	G1116	A1046	C948	
G2246	G2246	A2158	C2096	A1871	G1756	U1647	G1544	U1460	G1360	G1223	C1118	A1043	G953	G855
A2247	A2247	G2159	U2097	A1872	U1757	U1648	A1544	A1474	G1361	G1232	U1119	A1050	G954	G856
		C2160	U2098	G1873	U1758	G1649	A1545	U1477	G1362	G1233	C1118	A1051	G955	G857
G2250	G2250	C2161	U2099	C1874	U1758	G1651	A1548	A1478	G1363	G1234	U1120	A1052	G956	G858
G2251	G2251	G2162	A1998	C1875	U1759	G1657	A1549	U1481	G1364	G1235	U1121	A1053	G957	G859
G2252	G2252	A2163	A1999	A1876	C1761	A1650	A1549	G1482	G1365	G1236	U1122	C1052	U958	
G2253	G2253	A2163	C1999	A1876	U1761	G1651	A1549	G1483	G1366	G1237	U1123	C1053	U959	U870
		C2164	G2000	A1877	C1764	G1651	U1554	U1486	A1367	A1237	A1126	A1054	A960	U871
		C2165	C2001	G1878	U1773	C1656	U1554	U1487	G1368	G1238	A1127	A1055	A961	U872
G2258	G2258	G2168	G2002	A1885	C1774	U1657	C1558	U1497	G1371	G1248	U1128	G1056	C962	
A2266	A2266	A2170	A2009	C1905	U1775	G1660	U1559	U1498	G1371	G1249	U1129	G1057	U963	C876
A2267	A2267	G2171	G2010	C1906	A1779	G1661	U1563	U1481	G1378	C1251	G1131	A1058	G969	A877
A2268	A2268	A2172	U2022	G1907	C1790	G1674	C1564	G1483	G1379	G1252	U1130	A1059	U970	A878
		C2173	C2023	U1911	A1791	G1674	C1565	U1490	G1380	A1253	A1133	U1060		
G2279	G2279	A2174	U2026	U1912	A1794	A1677	A1566	U1486	G1383	A1254	A1134	U1061	C974	G881
G2280	G2280	C2175	U2030	A1913	C1795	A1678	G1567	U1487	A1383	G1255	U1135	G1062	C974	G882
A2281	A2281	A2176	A2033	C1914	U1796	A1679	G1568	U1488	G1384	G1256	U1136	C1064	A979	G883
G2282	G2282	C2177	A2031	3TD1915	G1797	A1679	A1569	U1498	A1385			U1065		U884
G2283	G2283	C2178	C2032	A1916	U1798	G1703	A1570	C1493	A1392	U1263	U1141	U1066	C982	C885
A2284	A2284	C2179	C2032	A1917	U1799	G1703	A1571	A1494	A1392	A1264	A1142	A1067	C982	A886
C2285	C2285	U2180	A2033	U1917	G1799	G1707	U1578	A1495	A1395	A1265	A1143	G1068	A983	U887
G2286	G2286	U2181	U2034	A1918	C1800	G1707	A1579	A1496	A1395	A1266	A1144	A1069	A984	C888
A2287	A2287	U2182	U2034	A1919	A1801	G1713	A1580	U1497	U1400	G1271	U1174	A1070	C985	C889
		A2183	A2037	G1929	A1802	U1714	G1581	U1498	G1401	A1272	U1175	A1083	C994	G891
G2288	G2288	C2184	G2038	G1930	A1803	G1715	C1582	C1499	U1402	U1273	U1176	A1084	C995	A892
G2289	G2289	U2185	G2038	U1931	A1808	G1718	A1583	G1500	A1403	G1292	U1177	A1085	C996	C893
G2290	G2290	G2186	C2043	A1932	A1809	G1719	U1584	U1506	A1404	G1293	U1178	A1086	A999	U894
U2291	U2291	U2187	C2044	G1933	A1810	U1720	C1585	C1507	U1405	C1293	C1170	A1087	U999	A896
G2292	G2292	U2188	C2045	G1933	A1811	U1721	A1586	A1508	U1406	G1300	G1171	U1078	C1005	C897
G2294	G2294	U2189	A2051	A1936	G1812	G1721	G1587	A1509	G1407	A1301	U1172	C1079	U1010	C898
G2295	G2295	G2190	A2052	A1937	G1813	G1724	G1588	U1510	U1408	A1302	U1173	A1080	A1010	A899
U2296	U2296	G2197	A2052	A1938	G1814	G1725	U1589	G1511	U1409	G1310	U1174	U1083	G1011	
A2297	A2297	U2197	C2055	U1939	C1816	U1725	A1590	C1512	G1410	G1310	U1175	A1083	G1012	C908
A2298	A2298	A2198	G2056	U1943	G1826	C1728	C1591	A1515	A1413	C1167	U1176	A1084	A909	A910
U2299	U2299	U2199	G2056	U1943	G1827	U1729	C1592	A1516	A1414	G1168	U1177	A1085	C1013	
C2300	C2300	C2200	A2059	U1955	U1827	C1730	U1593	U1415	U1415	U1169	G1178	A1086	U1019	G914
C2301	C2301	A2134	A2060	U1955	G1828	G1731	U1594	U1416	U1416	C1314	G1179	A1087	U1022	C915
G2303	G2303	A2135	G2061	U1960	A1829	G1732	C1595	G1517	G1417	C1315	U1180	A1088	G1023	
U2304	U2304	G2136	A2062	A1960	A1830	G1733	A1596	G1518	C1417	C1320	U1181	A1089	U1022	G923
G2305	G2305	U2210	C2063	C1961	G1733	G1734	A1597	G1519	A1420	A1321	G1182	A1090		

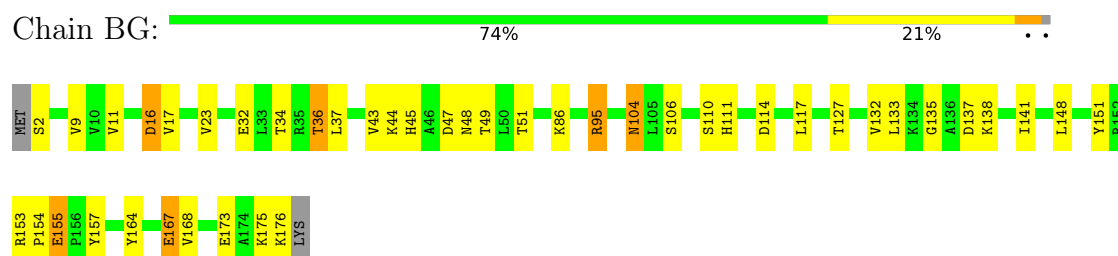
- Molecule 29: 50S ribosomal protein L4



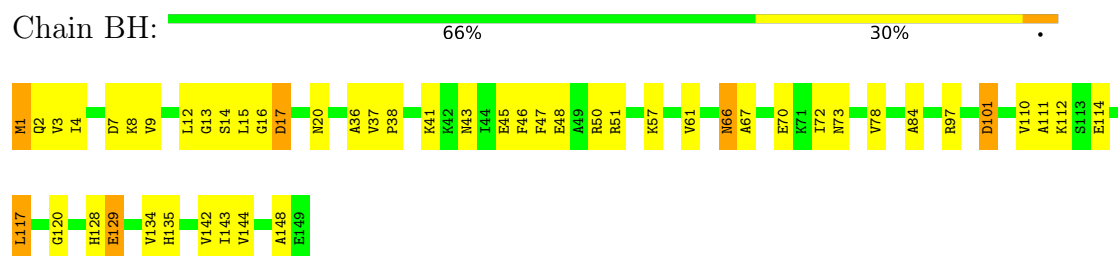
- Molecule 30: 50S ribosomal protein L5



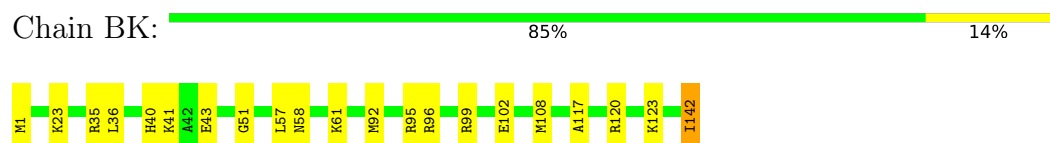
- Molecule 31: 50S ribosomal protein L6




- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L13




- Molecule 34: 50S ribosomal protein L14

Chain BL:  81% 18% .




- Molecule 35: 50S ribosomal protein L15

Chain BM:  77% 21% .



- Molecule 36: 50S ribosomal protein L16

Chain BN:  79% 21% .



- Molecule 37: 50S ribosomal protein L17

Chain BO:  73% 18% 6% .




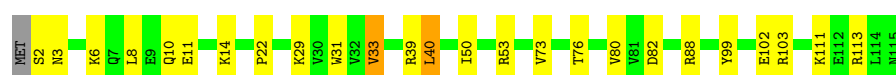
- Molecule 38: 50S ribosomal protein L18

Chain BP:  72% 26% .




- Molecule 39: 50S ribosomal protein L19

Chain BQ:  77% 20% ..



- Molecule 40: 50S ribosomal protein L20

Chain BR:  81% 18% ..




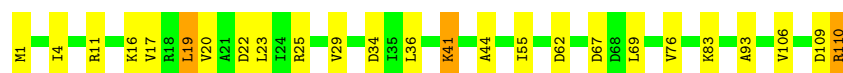
- Molecule 41: 50S ribosomal protein L21

Chain BS:  72% 28%




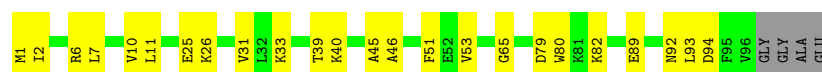
- Molecule 42: 50S ribosomal protein L22

Chain BT:  77% 20%



- Molecule 43: 50S ribosomal protein L23

Chain BU:  72% 24%




- Molecule 44: 50S ribosomal protein L24

Chain BV:  70% 27%




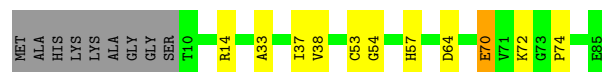
- Molecule 45: 50S ribosomal protein L25

Chain BW:  76% 23%



- Molecule 46: 50S ribosomal protein L27

Chain BX:  76% 12% 11%



- Molecule 47: 50S ribosomal protein L28

Chain BY:  67% 31%



- Molecule 48: 50S ribosomal protein L29

Chain BZ:  73% 24% ..



- Molecule 49: 50S ribosomal protein L30

Chain B1:  73% 25% .




- Molecule 50: 50S ribosomal protein L32

Chain B2:  68% 28% ..




- Molecule 51: 50S ribosomal protein L33

Chain B3:  85% 9% . .



- Molecule 52: 50S ribosomal protein L34

Chain B4:  78% 22%



- Molecule 53: 50S ribosomal protein L35

Chain B5:  75% 20% ..



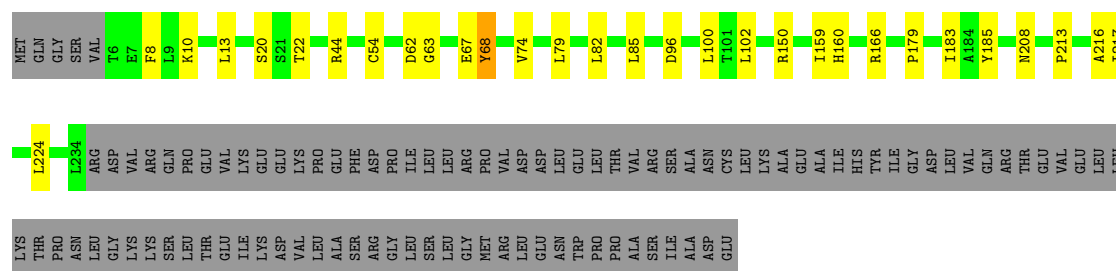
- Molecule 54: 50S ribosomal protein L36

Chain B6:  58% 16% . 24%



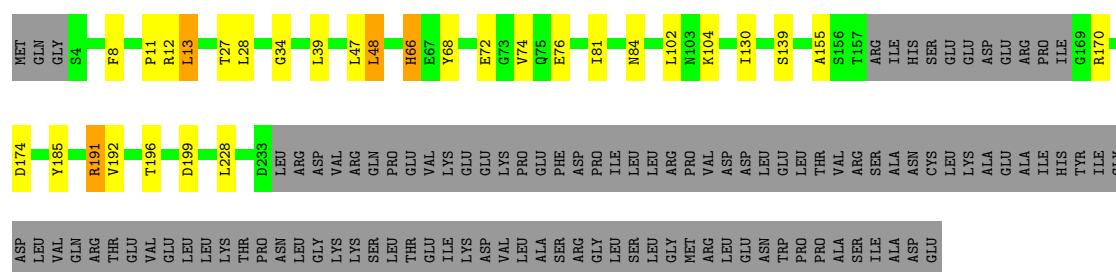
- Molecule 55: DNA-directed RNA polymerase subunit alpha

Chain CA: 




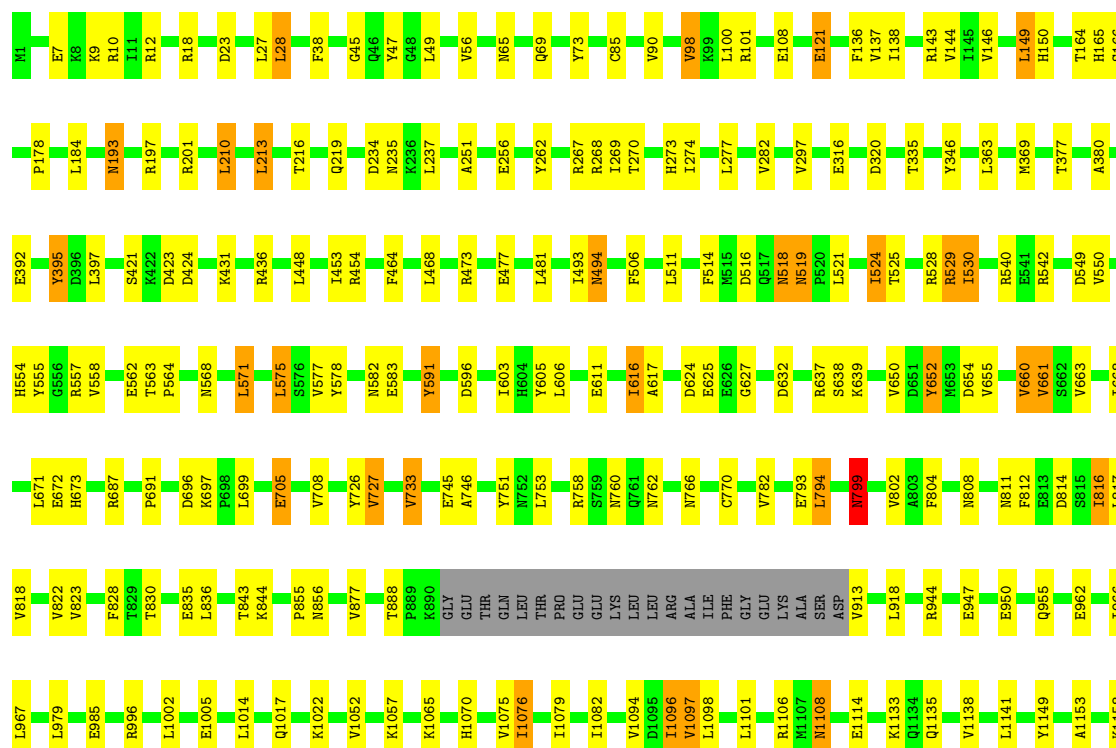
- Molecule 55: DNA-directed RNA polymerase subunit alpha

Chain CB: 




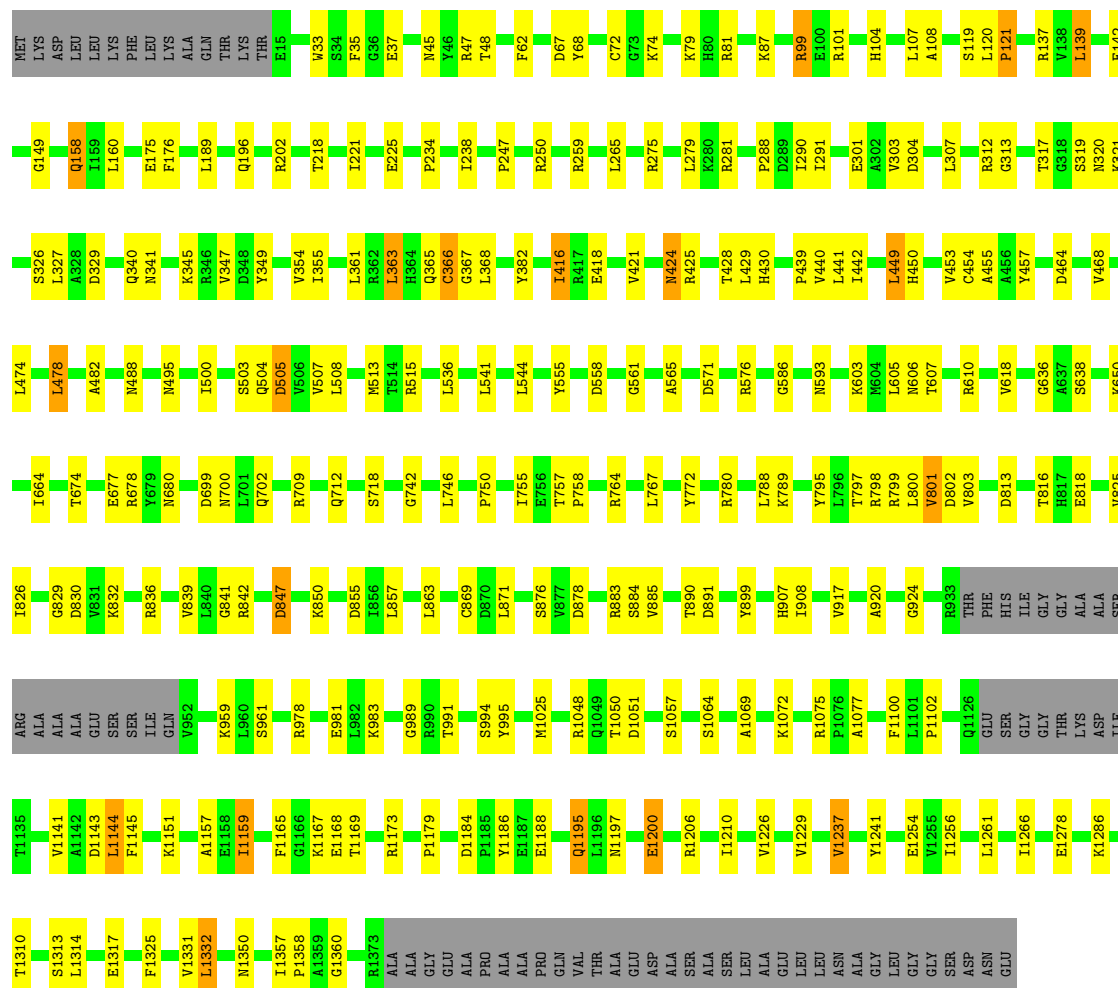
- Molecule 56: DNA-directed RNA polymerase subunit beta

Chain CC: 



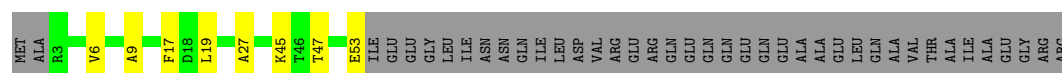
- Molecule 57: DNA-directed RNA polymerase subunit beta'

Chain CD:  77% 17% 5%



- Molecule 58: DNA-directed RNA polymerase subunit omega

Chain CE: 



- Molecule 59: Non-template DNA strand

Chain CN:



● Molecule 60: Template DNA strand



● Molecule 61: Transcription termination/antitermination protein NusG



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34590	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: OMG, UR3, 2MA, 6MZ, MA6, 5MC, 1MG, 7MG, 5MU, D2T, PSU, 2MG, 4SU, MG, 4OC, MIA, ZN, 3TD, OMU, MEQ, H2U, 4D4, 3AU, G7M, OMC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.73	1/36569 (0.0%)	1.04	74/57044 (0.1%)
2	AB	0.32	0/1796	0.56	0/2420
3	AC	0.36	0/1667	0.57	0/2246
4	AD	0.34	0/1665	0.53	0/2227
5	AE	0.37	0/1161	0.59	0/1563
6	AF	0.38	0/867	0.55	0/1171
7	AG	0.32	0/1230	0.62	2/1649 (0.1%)
8	AH	0.37	0/989	0.53	0/1326
9	AI	0.36	0/1043	0.62	0/1387
10	AJ	0.35	0/810	0.70	0/1094
11	AK	0.35	0/893	0.57	0/1205
12	AL	0.41	0/954	0.71	0/1279
13	AM	0.33	0/900	0.62	1/1204 (0.1%)
14	AN	0.34	0/817	0.52	0/1088
15	AO	0.36	0/722	0.58	0/964
16	AP	0.32	0/659	0.54	0/884
17	AQ	0.35	0/657	0.58	0/881
18	AR	0.37	0/481	0.65	1/645 (0.2%)
19	AS	0.35	0/680	0.59	0/915
20	AT	0.32	0/676	0.45	0/895
21	AU	0.34	0/598	0.51	0/792
22	AV	1.68	20/731 (2.7%)	1.62	23/1133 (2.0%)
23	AW	0.75	1/1725 (0.1%)	0.98	0/2687
24	AX	0.61	1/1584 (0.1%)	0.87	1/2463 (0.0%)
24	AZ	0.54	1/1584 (0.1%)	0.96	1/2463 (0.0%)
25	BA	0.82	0/69140	1.03	115/107854 (0.1%)
26	BB	0.61	0/2872	0.94	1/4478 (0.0%)
27	BC	0.43	0/2131	0.66	1/2863 (0.0%)
28	BD	0.39	0/1576	0.57	0/2119
29	BE	0.39	0/1571	0.62	2/2113 (0.1%)
30	BF	0.35	0/1444	0.62	0/1937

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	BG	0.33	0/1333	0.57	0/1805
32	BH	0.31	0/1122	0.66	1/1515 (0.1%)
33	BK	0.38	0/1152	0.54	0/1551
34	BL	0.39	0/956	0.60	0/1279
35	BM	0.36	0/1061	0.61	0/1412
36	BN	0.38	0/1081	0.57	0/1443
37	BO	0.38	0/973	0.60	0/1301
38	BP	0.32	0/910	0.58	0/1219
39	BQ	0.38	0/929	0.58	0/1242
40	BR	0.47	0/960	0.54	0/1278
41	BS	0.41	0/829	0.65	0/1107
42	BT	0.38	0/864	0.57	0/1156
43	BU	0.36	0/771	0.58	0/1031
44	BV	0.34	0/797	0.53	0/1062
45	BW	0.36	0/766	0.60	1/1025 (0.1%)
46	BX	0.39	0/589	0.57	0/779
47	BY	0.40	0/635	0.50	0/848
48	BZ	0.31	0/502	0.48	0/667
49	B1	0.34	0/453	0.55	0/605
50	B2	0.40	0/450	0.74	0/599
51	B3	0.33	0/443	0.66	0/587
52	B4	0.37	0/379	0.49	0/496
53	B5	0.39	0/513	0.63	0/676
54	B6	0.35	0/302	0.55	0/397
55	CA	1.02	3/1797 (0.2%)	0.87	0/2436
55	CB	0.74	1/1703 (0.1%)	0.81	4/2308 (0.2%)
56	CC	1.28	79/10581 (0.7%)	0.92	22/14275 (0.2%)
57	CD	1.02	36/10532 (0.3%)	0.87	12/14219 (0.1%)
58	CE	0.48	0/401	0.75	0/540
59	CN	1.55	6/690 (0.9%)	1.17	4/1064 (0.4%)
60	CT	2.23	21/676 (3.1%)	1.25	9/1039 (0.9%)
61	CF	0.41	0/808	0.58	0/1088
All	All	0.78	170/186150 (0.1%)	0.93	275/275038 (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	6
5	AE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	AM	0	1
25	BA	0	2
27	BC	0	1
37	BO	0	1
46	BX	0	1
53	B5	0	1
57	CD	0	1
All	All	0	15

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	1	G	OP3-P	-10.82	1.48	1.61
23	AW	1	C	OP3-P	-10.78	1.48	1.61
24	AZ	1	G	OP3-P	-10.67	1.48	1.61
60	CT	14	DC	C3'-O3'	-9.25	1.31	1.44
60	CT	18	DC	C3'-O3'	-8.52	1.32	1.44

The worst 5 of 275 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1027	C	C6-N1-C2	-27.34	109.36	120.30
1	AA	1027	C	C2-N1-C1'	18.55	139.21	118.80
1	AA	1027	C	C5-C6-N1	16.26	129.13	121.00
1	AA	1027	C	C6-N1-C1'	-15.50	102.20	120.80
1	AA	206	C	C6-N1-C2	-14.18	114.63	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1027	C	Sidechain
1	AA	60	A	Sidechain
1	AA	81	A	Sidechain
1	AA	82	G	Sidechain
1	AA	884	U	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32909	0	16575	402	0
2	AB	1765	0	1792	32	0
3	AC	1640	0	1713	48	0
4	AD	1643	0	1707	31	0
5	AE	1148	0	1195	20	0
6	AF	848	0	846	35	0
7	AG	1214	0	1267	20	0
8	AH	979	0	1031	18	0
9	AI	1031	0	1076	23	0
10	AJ	800	0	839	25	0
11	AK	877	0	887	20	0
12	AL	951	0	1012	26	0
13	AM	891	0	952	27	0
14	AN	805	0	844	15	0
15	AO	714	0	734	17	0
16	AP	649	0	666	8	0
17	AQ	648	0	691	10	0
18	AR	474	0	494	16	0
19	AS	663	0	688	20	0
20	AT	670	0	719	11	0
21	AU	590	0	629	6	0
22	AV	656	0	336	24	0
23	AW	1645	0	842	24	0
24	AX	1630	0	838	35	0
24	AZ	1630	0	839	64	0
25	BA	62248	0	31319	678	0
26	BB	2569	0	1300	32	0
27	BC	2092	0	2167	27	0
28	BD	1566	0	1618	28	0
29	BE	1552	0	1618	30	0
30	BF	1420	0	1457	53	0
31	BG	1313	0	1358	24	0
32	BH	1111	0	1148	29	0
33	BK	1129	0	1162	13	0
34	BL	947	0	1023	10	0
35	BM	1052	0	1127	20	0
36	BN	1075	0	1155	17	0
37	BO	960	0	1000	18	0
38	BP	900	0	935	23	0
39	BQ	917	0	962	14	0
40	BR	947	0	1018	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	BS	816	0	839	18	0
42	BT	857	0	922	14	0
43	BU	764	0	829	15	0
44	BV	789	0	844	17	0
45	BW	753	0	780	12	0
46	BX	582	0	598	6	0
47	BY	625	0	652	17	0
48	BZ	501	0	531	12	0
49	B1	449	0	488	6	0
50	B2	444	0	458	13	0
51	B3	436	0	477	5	0
52	B4	376	0	414	5	0
53	B5	504	0	572	9	0
54	B6	301	0	343	5	0
55	CA	1775	0	1800	17	0
55	CB	1684	0	1713	15	0
56	CC	10415	0	10432	154	0
57	CD	10375	0	10597	197	0
58	CE	399	0	417	4	0
59	CN	615	0	335	40	0
60	CT	606	0	338	43	0
61	CF	790	0	782	51	0
62	AA	139	0	0	1	0
62	AL	3	0	0	0	0
62	AT	1	0	0	0	0
62	AV	1	0	0	0	0
62	AW	4	0	0	0	0
62	AX	1	0	0	0	0
62	B2	1	0	0	0	0
62	B5	1	0	0	0	0
62	B6	1	0	0	0	0
62	BA	318	0	0	0	0
62	BB	9	0	0	0	0
62	BC	3	0	0	0	0
62	BD	1	0	0	0	0
62	BN	1	0	0	0	0
62	BR	1	0	0	0	0
62	BX	1	0	0	0	0
62	CD	1	0	0	0	0
63	AX	11	0	8	0	0
64	CD	2	0	0	0	0
All	All	174624	0	124748	2410	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 8.

The worst 5 of 2410 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)
59:CN:18:DG:H3'	61:CF:90:MET:CB	1.24	1.46
59:CN:18:DG:C3'	61:CF:90:MET:HB3	0.99	1.41
3:AC:77:ILE:CD1	57:CD:79:LYS:HG3	1.55	1.36
25:BA:1869:G:N2	25:BA:1872:A:C5	2.05	1.25
57:CD:1100:PHE:CD2	57:CD:1200:GLU:HB3	1.71	1.24

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%)	209 (93%)	14 (6%)	1 (0%)	30	65
3	AC	207/233 (89%)	193 (93%)	10 (5%)	4 (2%)	6	34
4	AD	203/206 (98%)	192 (95%)	10 (5%)	1 (0%)	25	60
5	AE	154/167 (92%)	143 (93%)	10 (6%)	1 (1%)	22	57
6	AF	102/131 (78%)	96 (94%)	6 (6%)	0	100	100
7	AG	152/156 (97%)	139 (91%)	11 (7%)	2 (1%)	10	41
8	AH	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	16	51
9	AI	126/130 (97%)	110 (87%)	13 (10%)	3 (2%)	5	30
10	AJ	98/103 (95%)	89 (91%)	7 (7%)	2 (2%)	6	33
11	AK	115/129 (89%)	100 (87%)	14 (12%)	1 (1%)	14	48
12	AL	119/124 (96%)	110 (92%)	7 (6%)	2 (2%)	7	36
13	AM	113/118 (96%)	108 (96%)	4 (4%)	1 (1%)	14	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	AN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	11	43
16	AP	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	AQ	78/84 (93%)	72 (92%)	6 (8%)	0	100	100
18	AR	55/75 (73%)	52 (94%)	2 (4%)	1 (2%)	7	35
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%)	67 (98%)	1 (2%)	0	100	100
27	BC	270/273 (99%)	249 (92%)	18 (7%)	3 (1%)	12	45
28	BD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	25	60
29	BE	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
30	BF	176/179 (98%)	165 (94%)	8 (4%)	3 (2%)	7	36
31	BG	173/177 (98%)	159 (92%)	13 (8%)	1 (1%)	22	57
32	BH	147/149 (99%)	128 (87%)	18 (12%)	1 (1%)	19	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%)	130 (92%)	10 (7%)	2 (1%)	9	39
36	BN	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
37	BO	118/127 (93%)	107 (91%)	11 (9%)	0	100	100
38	BP	115/117 (98%)	107 (93%)	7 (6%)	1 (1%)	14	48
39	BQ	112/115 (97%)	104 (93%)	7 (6%)	1 (1%)	14	48
40	BR	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
41	BS	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	13	46
42	BT	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
43	BU	94/100 (94%)	88 (94%)	6 (6%)	0	100	100
44	BV	101/104 (97%)	97 (96%)	3 (3%)	1 (1%)	13	46
45	BW	92/94 (98%)	91 (99%)	1 (1%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	B2	54/57 (95%)	50 (93%)	3 (6%)	1 (2%)	6	34
51	B3	51/55 (93%)	48 (94%)	3 (6%)	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%)	8	37
54	B6	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
55	CA	227/329 (69%)	217 (96%)	10 (4%)	0	100	100
55	CB	215/329 (65%)	201 (94%)	13 (6%)	1 (0%)	25	60
56	CC	1316/1342 (98%)	1201 (91%)	100 (8%)	15 (1%)	12	45
57	CD	1327/1407 (94%)	1222 (92%)	96 (7%)	9 (1%)	19	54
58	CE	49/91 (54%)	40 (82%)	8 (16%)	1 (2%)	6	33
61	CF	94/181 (52%)	88 (94%)	6 (6%)	0	100	100
All	All	8773/9507 (92%)	8169 (93%)	540 (6%)	64 (1%)	21	54

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	80	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%)	179 (96%)	8 (4%)	25	49
3	AC	171/190 (90%)	156 (91%)	15 (9%)	8	29
4	AD	172/173 (99%)	157 (91%)	15 (9%)	8	30
5	AE	118/126 (94%)	100 (85%)	18 (15%)	2	13
6	AF	91/112 (81%)	83 (91%)	8 (9%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	127/129 (98%)	113 (89%)	14 (11%)	5	21
8	AH	104/105 (99%)	97 (93%)	7 (7%)	13	38
9	AI	106/107 (99%)	99 (93%)	7 (7%)	14	38
10	AJ	87/90 (97%)	81 (93%)	6 (7%)	13	37
11	AK	90/99 (91%)	83 (92%)	7 (8%)	10	33
12	AL	102/103 (99%)	90 (88%)	12 (12%)	4	20
13	AM	93/96 (97%)	85 (91%)	8 (9%)	8	31
14	AN	83/84 (99%)	78 (94%)	5 (6%)	16	41
15	AO	76/77 (99%)	70 (92%)	6 (8%)	10	33
16	AP	65/65 (100%)	61 (94%)	4 (6%)	15	40
17	AQ	74/78 (95%)	70 (95%)	4 (5%)	18	44
18	AR	50/65 (77%)	47 (94%)	3 (6%)	16	41
19	AS	72/79 (91%)	70 (97%)	2 (3%)	38	59
20	AT	65/66 (98%)	58 (89%)	7 (11%)	5	22
21	AU	60/61 (98%)	57 (95%)	3 (5%)	20	45
27	BC	217/218 (100%)	209 (96%)	8 (4%)	29	53
28	BD	163/163 (100%)	155 (95%)	8 (5%)	21	46
29	BE	165/165 (100%)	153 (93%)	12 (7%)	11	35
30	BF	149/150 (99%)	137 (92%)	12 (8%)	9	33
31	BG	136/138 (99%)	122 (90%)	14 (10%)	6	23
32	BH	114/114 (100%)	103 (90%)	11 (10%)	7	25
33	BK	116/116 (100%)	110 (95%)	6 (5%)	19	45
34	BL	104/104 (100%)	95 (91%)	9 (9%)	8	30
35	BM	103/103 (100%)	94 (91%)	9 (9%)	8	30
36	BN	108/108 (100%)	103 (95%)	5 (5%)	23	47
37	BO	100/103 (97%)	93 (93%)	7 (7%)	12	36
38	BP	87/87 (100%)	80 (92%)	7 (8%)	10	33
39	BQ	99/100 (99%)	94 (95%)	5 (5%)	20	45
40	BR	89/90 (99%)	84 (94%)	5 (6%)	17	43
41	BS	84/84 (100%)	79 (94%)	5 (6%)	16	41
42	BT	93/93 (100%)	86 (92%)	7 (8%)	11	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BU	83/84 (99%)	80 (96%)	3 (4%)	30	54
44	BV	84/85 (99%)	77 (92%)	7 (8%)	9	32
45	BW	78/78 (100%)	74 (95%)	4 (5%)	20	45
46	BX	58/63 (92%)	57 (98%)	1 (2%)	56	72
47	BY	67/68 (98%)	65 (97%)	2 (3%)	36	58
48	BZ	54/55 (98%)	51 (94%)	3 (6%)	17	43
49	B1	48/49 (98%)	44 (92%)	4 (8%)	9	32
50	B2	47/48 (98%)	42 (89%)	5 (11%)	5	22
51	B3	48/49 (98%)	45 (94%)	3 (6%)	15	40
52	B4	37/38 (97%)	35 (95%)	2 (5%)	18	44
53	B5	51/52 (98%)	48 (94%)	3 (6%)	16	41
54	B6	34/44 (77%)	32 (94%)	2 (6%)	16	41
55	CA	197/286 (69%)	191 (97%)	6 (3%)	36	58
55	CB	187/286 (65%)	180 (96%)	7 (4%)	29	53
56	CC	1139/1157 (98%)	1099 (96%)	40 (4%)	31	54
57	CD	1118/1168 (96%)	1090 (98%)	28 (2%)	42	62
58	CE	43/75 (57%)	42 (98%)	1 (2%)	45	64
61	CF	86/158 (54%)	85 (99%)	1 (1%)	67	78
All	All	7379/7883 (94%)	6968 (94%)	411 (6%)	20	43

5 of 411 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	BL	18	ARG
42	BT	83	LYS
57	CD	802	ASP
34	BL	123	LEU
38	BP	2	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
36	BN	13	HIS
56	CC	235	ASN
57	CD	1367	GLN

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Mol	Chain	Res	Type
57	CD	1197	ASN
29	BE	165	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	294 (19%)	32 (2%)
22	AV	29/57 (50%)	10 (34%)	1 (3%)
23	AW	76/77 (98%)	22 (28%)	8 (10%)
24	AX	73/76 (96%)	24 (32%)	2 (2%)
24	AZ	73/76 (96%)	30 (41%)	0
25	BA	2893/2904 (99%)	544 (18%)	66 (2%)
26	BB	119/120 (99%)	12 (10%)	0
All	All	4792/4852 (98%)	936 (19%)	109 (2%)

5 of 936 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	19	A

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	764	A
25	BA	1109	C
25	BA	2296	U
25	BA	784	G
25	BA	984	A

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

63 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	G7M	AA	527	1	20,26,27	2.29	7 (35%)	17,39,42	1.20	2 (11%)
28	MEQ	BD	150	28	8,9,10	0.91	0	5,10,12	1.07	1 (20%)
24	5MU	AX	54	24	19,22,23	1.36	3 (15%)	28,32,35	2.16	8 (28%)
24	3AU	AX	47	24	18,21,29	3.38	8 (44%)	26,30,43	1.67	5 (19%)
25	2MA	BA	2503	62,25	19,25,26	3.41	8 (42%)	21,37,40	2.37	3 (14%)
25	PSU	BA	2604	62,25	18,21,22	1.04	3 (16%)	22,30,33	1.84	4 (18%)
1	MA6	AA	1519	1	18,26,27	1.40	3 (16%)	19,38,41	3.85	2 (10%)
1	2MG	AA	966	1	18,26,27	2.31	7 (38%)	16,38,41	1.60	4 (25%)
24	PSU	AX	39	24	18,21,22	1.01	1 (5%)	22,30,33	1.90	5 (22%)
24	PSU	AX	55	24	18,21,22	1.04	1 (5%)	22,30,33	1.82	5 (22%)
25	OMG	BA	2251	23,25	18,26,27	2.59	8 (44%)	19,38,41	1.61	4 (21%)
25	PSU	BA	2605	62,25	18,21,22	1.00	2 (11%)	22,30,33	2.03	5 (22%)
1	2MG	AA	1516	1	18,26,27	2.19	7 (38%)	16,38,41	1.62	4 (25%)
24	PSU	AX	32	24	18,21,22	1.04	1 (5%)	22,30,33	1.58	3 (13%)
12	D2T	AL	89	12	7,9,10	1.08	0	6,11,13	2.06	2 (33%)
24	7MG	AZ	46	24	22,26,27	3.74	10 (45%)	29,39,42	1.96	8 (27%)
24	H2U	AZ	16	24	18,21,22	3.01	5 (27%)	21,30,33	2.01	5 (23%)
25	PSU	BA	2457	25	18,21,22	1.09	2 (11%)	22,30,33	2.16	6 (27%)
24	H2U	AX	20	24	18,21,22	3.19	5 (27%)	21,30,33	2.00	5 (23%)
25	6MZ	BA	1618	25	18,25,26	1.91	3 (16%)	16,36,39	2.35	4 (25%)
25	H2U	BA	2449	25	18,21,22	2.89	5 (27%)	21,30,33	2.31	5 (23%)
25	3TD	BA	1915	25	18,22,23	4.46	10 (55%)	22,32,35	1.98	4 (18%)
24	4SU	AZ	8	24	18,21,22	4.17	8 (44%)	26,30,33	2.14	5 (19%)
1	PSU	AA	516	1	18,21,22	1.02	1 (5%)	22,30,33	2.10	6 (27%)
23	H2U	AW	20	23	18,21,22	3.07	5 (27%)	21,30,33	2.28	5 (23%)
25	PSU	BA	2580	25	18,21,22	1.04	3 (16%)	22,30,33	2.25	7 (31%)
25	5MU	BA	747	25	19,22,23	1.39	4 (21%)	28,32,35	2.23	6 (21%)
24	7MG	AX	46	24	22,26,27	3.79	10 (45%)	29,39,42	2.08	9 (31%)
24	H2U	AX	16	24	18,21,22	3.04	5 (27%)	21,30,33	2.05	5 (23%)
24	4SU	AX	8	24	18,21,22	4.05	8 (44%)	26,30,33	2.32	5 (19%)
24	MIA	AX	37	24	22,29,32	2.82	4 (18%)	22,41,47	3.01	7 (31%)
23	5MU	AW	54	23	19,22,23	1.41	5 (26%)	28,32,35	2.27	10 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	1MG	BA	745	25	18,26,27	2.61	6 (33%)	19,39,42	1.45	4 (21%)
25	OMC	BA	2498	25	19,22,23	2.84	7 (36%)	26,31,34	0.75	1 (3%)
1	2MG	AA	1207	1,62	18,26,27	2.29	7 (38%)	16,38,41	1.65	4 (25%)
24	PSU	AZ	55	24	18,21,22	1.10	1 (5%)	22,30,33	1.83	4 (18%)
25	PSU	BA	746	62,25	18,21,22	1.02	2 (11%)	22,30,33	2.03	6 (27%)
36	4D4	BN	81	36	9,11,12	2.49	3 (33%)	8,13,15	0.74	0
1	5MC	AA	967	1	18,22,23	3.96	7 (38%)	26,32,35	1.13	2 (7%)
25	2MG	BA	2445	25	18,26,27	2.24	7 (38%)	16,38,41	1.61	4 (25%)
24	H2U	AZ	20	24	18,21,22	3.05	5 (27%)	21,30,33	2.04	5 (23%)
23	4SU	AW	8	23	18,21,22	4.04	8 (44%)	26,30,33	2.50	4 (15%)
24	PSU	AZ	32	24	18,21,22	1.00	1 (5%)	22,30,33	1.72	4 (18%)
25	PSU	BA	1911	25	18,21,22	1.07	2 (11%)	22,30,33	1.94	5 (22%)
1	MA6	AA	1518	1	18,26,27	1.39	3 (16%)	19,38,41	4.32	3 (15%)
25	5MC	BA	1962	25	18,22,23	3.83	7 (38%)	26,32,35	1.17	1 (3%)
25	6MZ	BA	2030	25	18,25,26	1.86	3 (16%)	16,36,39	2.65	3 (18%)
24	MIA	AZ	37	24	22,29,32	2.81	4 (18%)	22,41,47	2.97	6 (27%)
23	OMC	AW	32	23	19,22,23	2.90	8 (42%)	26,31,34	0.79	0
24	5MU	AZ	54	24	19,22,23	1.41	6 (31%)	28,32,35	2.04	6 (21%)
1	5MC	AA	1407	1	18,22,23	3.81	7 (38%)	26,32,35	1.02	1 (3%)
25	PSU	BA	2504	25	18,21,22	1.10	3 (16%)	22,30,33	2.16	5 (22%)
24	3AU	AZ	47	24	18,21,29	3.42	8 (44%)	26,30,43	1.64	5 (19%)
1	4OC	AA	1402	1,62	20,23,24	3.35	9 (45%)	26,32,35	1.00	2 (7%)
1	UR3	AA	1498	1	19,22,23	2.50	6 (31%)	26,32,35	1.40	1 (3%)
23	PSU	AW	55	23	18,21,22	1.01	1 (5%)	22,30,33	1.91	6 (27%)
25	PSU	BA	955	62,25	18,21,22	1.14	2 (11%)	22,30,33	1.82	4 (18%)
24	PSU	AZ	39	24	18,21,22	1.02	1 (5%)	22,30,33	1.83	4 (18%)
25	2MG	BA	1835	25	18,26,27	2.28	7 (38%)	16,38,41	1.65	4 (25%)
25	PSU	BA	1917	25	18,21,22	0.99	2 (11%)	22,30,33	1.91	5 (22%)
25	5MU	BA	1939	62,25	19,22,23	1.44	4 (21%)	28,32,35	2.39	6 (21%)
25	G7M	BA	2069	25	20,26,27	2.25	8 (40%)	17,39,42	1.18	1 (5%)
25	OMU	BA	2552	25	19,22,23	2.90	7 (36%)	26,31,34	1.79	5 (19%)

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	G7M	AA	527	1	-	1/3/25/26	0/3/3/3
28	MEQ	BD	150	28	-	3/8/9/11	-
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
24	3AU	AX	47	24	-	3/7/25/35	0/2/2/2
25	2MA	BA	2503	62,25	-	2/3/25/26	0/3/3/3
25	PSU	BA	2604	62,25	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	6/7/29/30	0/3/3/3
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	2/7/25/26	0/2/2/2
25	OMG	BA	2251	23,25	-	1/5/27/28	0/3/3/3
25	PSU	BA	2605	62,25	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
24	PSU	AX	32	24	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	3/7/12/14	-
24	7MG	AZ	46	24	-	3/7/37/38	0/3/3/3
24	H2U	AZ	16	24	-	3/7/38/39	0/2/2/2
25	PSU	BA	2457	25	-	0/7/25/26	0/2/2/2
24	H2U	AX	20	24	-	5/7/38/39	0/2/2/2
25	6MZ	BA	1618	25	-	2/5/27/28	0/3/3/3
25	H2U	BA	2449	25	-	0/7/38/39	0/2/2/2
25	3TD	BA	1915	25	-	3/7/25/26	0/2/2/2
24	4SU	AZ	8	24	-	7/7/25/26	0/2/2/2
1	PSU	AA	516	1	-	1/7/25/26	0/2/2/2
23	H2U	AW	20	23	-	4/7/38/39	0/2/2/2
25	PSU	BA	2580	25	-	0/7/25/26	0/2/2/2
25	5MU	BA	747	25	-	0/7/25/26	0/2/2/2
24	7MG	AX	46	24	-	1/7/37/38	0/3/3/3
24	H2U	AX	16	24	-	2/7/38/39	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
24	MIA	AX	37	24	-	6/9/31/34	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
25	1MG	BA	745	25	-	0/3/25/26	0/3/3/3
25	OMC	BA	2498	25	-	3/9/27/28	0/2/2/2
1	2MG	AA	1207	1,62	-	1/5/27/28	0/3/3/3
24	PSU	AZ	55	24	-	1/7/25/26	0/2/2/2
25	PSU	BA	746	62,25	-	2/7/25/26	0/2/2/2
36	4D4	BN	81	36	-	4/11/12/14	-
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	2MG	BA	2445	25	-	2/5/27/28	0/3/3/3
24	H2U	AZ	20	24	-	5/7/38/39	0/2/2/2
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
24	PSU	AZ	32	24	-	0/7/25/26	0/2/2/2
25	PSU	BA	1911	25	-	1/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	3/7/29/30	0/3/3/3
25	5MC	BA	1962	25	-	0/7/25/26	0/2/2/2
25	6MZ	BA	2030	25	-	2/5/27/28	0/3/3/3
24	MIA	AZ	37	24	-	8/9/31/34	0/3/3/3
23	OMC	AW	32	23	-	1/9/27/28	0/2/2/2
24	5MU	AZ	54	24	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
25	PSU	BA	2504	25	-	0/7/25/26	0/2/2/2
24	3AU	AZ	47	24	-	1/7/25/35	0/2/2/2
1	4OC	AA	1402	1,62	-	1/9/29/30	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	3/7/25/26	0/2/2/2
25	PSU	BA	955	62,25	-	0/7/25/26	0/2/2/2
24	PSU	AZ	39	24	-	0/7/25/26	0/2/2/2
25	2MG	BA	1835	25	-	0/5/27/28	0/3/3/3
25	PSU	BA	1917	25	-	2/7/25/26	0/2/2/2
25	5MU	BA	1939	62,25	-	2/7/25/26	0/2/2/2
25	G7M	BA	2069	25	-	2/3/25/26	0/3/3/3
25	OMU	BA	2552	25	-	2/9/27/28	0/2/2/2

The worst 5 of 304 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1915	3TD	C6-C5	11.84	1.49	1.35
24	AX	20	H2U	C2-N1	10.31	1.50	1.35
1	AA	967	5MC	C6-C5	9.94	1.50	1.34
25	BA	1915	3TD	C2-N1	9.79	1.49	1.37
1	AA	1407	5MC	C6-C5	9.77	1.50	1.34

The worst 5 of 270 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	MA6	N1-C6-N6	-17.72	98.41	117.06
1	AA	1519	MA6	N1-C6-N6	-15.75	100.48	117.06
24	AZ	37	MIA	C12-C13-C14	-9.98	107.73	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	37	MIA	C12-C13-C14	-9.48	108.69	127.14
23	AW	8	4SU	C4-N3-C2	-8.72	118.87	127.34

There are no chirality outliers.

5 of 109 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	1402	4OC	C1'-C2'-O2'-CM2
1	AA	1518	MA6	C5-C6-N6-C10
1	AA	1518	MA6	N1-C6-N6-C10

There are no ring outliers.

39 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	527	G7M	1	0
28	BD	150	MEQ	1	0
24	AX	54	5MU	1	0
25	BA	2503	2MA	1	0
25	BA	2604	PSU	1	0
1	AA	1519	MA6	1	0
1	AA	966	2MG	2	0
24	AX	39	PSU	1	0
24	AX	55	PSU	1	0
25	BA	2251	OMG	1	0
25	BA	2605	PSU	2	0
1	AA	1516	2MG	1	0
12	AL	89	D2T	2	0
24	AZ	46	7MG	9	0
24	AZ	16	H2U	2	0
24	AX	20	H2U	4	0
25	BA	1618	6MZ	3	0
25	BA	2449	H2U	1	0
25	BA	1915	3TD	3	0
24	AZ	8	4SU	1	0
1	AA	516	PSU	1	0
23	AW	20	H2U	3	0
24	AX	46	7MG	3	0
24	AX	37	MIA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	54	5MU	2	0
25	BA	2498	OMC	1	0
1	AA	1207	2MG	2	0
24	AZ	55	PSU	1	0
36	BN	81	4D4	1	0
1	AA	967	5MC	2	0
24	AZ	20	H2U	3	0
24	AZ	32	PSU	1	0
25	BA	2030	6MZ	1	0
24	AZ	37	MIA	3	0
23	AW	32	OMC	1	0
23	AW	55	PSU	1	0
25	BA	1917	PSU	2	0
25	BA	2069	G7M	1	0
25	BA	2552	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 490 ligands modelled in this entry, 489 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	102	24	10,11,12	0.59	0	10,13,15	0.27	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	102	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
63	AX	102	PHE	CA-CB-CG-CD1
63	AX	102	PHE	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
57	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	1.19