



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:38 pm GMT

PDB ID : 4V6M
EMDB ID: : EMD-1858
Title : Structure of the ribosome-SecYE complex in the membrane environment
Authors : Frauenfeld, J.; Gumbart, J.; van der Sluis, E.O.; Funes, S.; Gartmann, M.;
Beatrix, B.; Mielke, T.; Berninghausen, O.; Becker, T.; Schulten, K.; Beck-
mann, R.
Deposited on : 2011-02-08
Resolution : 7.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

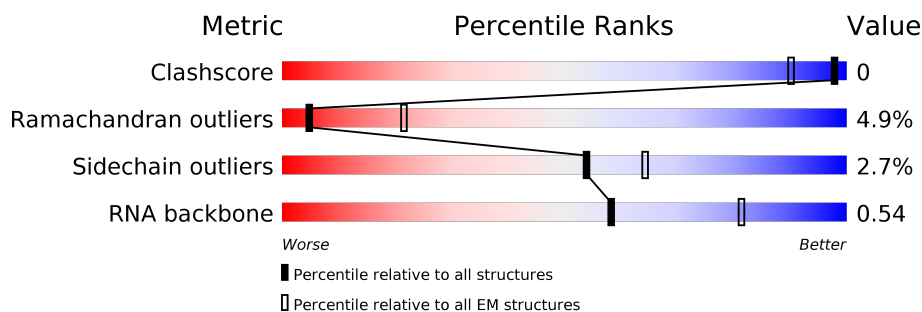
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.10 Å.

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




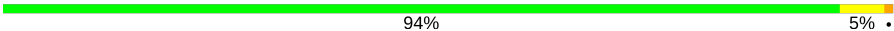

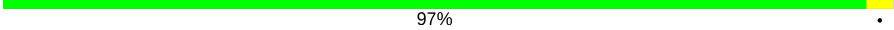
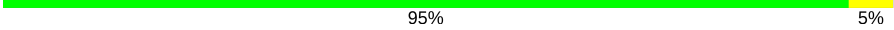


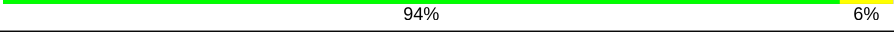
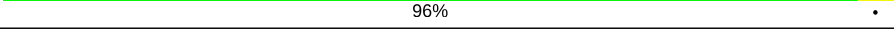


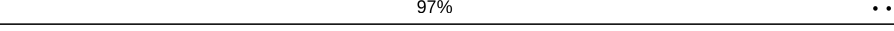
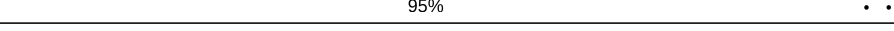


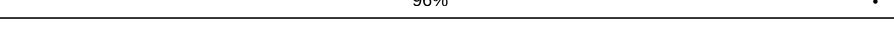
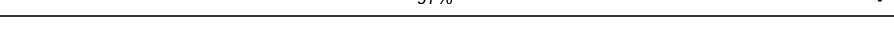
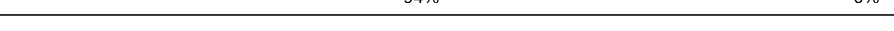
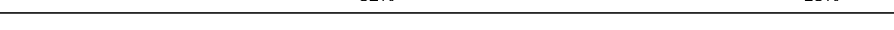
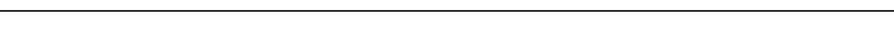
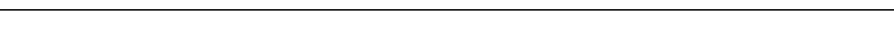
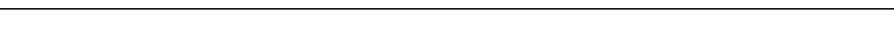
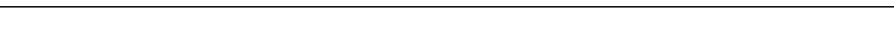
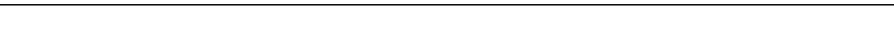

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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

Mol	Chain	Length	Quality of chain
1	AA	1542	78% 19% .
2	AX	11	9% 45% 45%
3	AV	77	77% 23%
4	AZ	98	76% 23% .
5	A0	200	96% 5%
5	A1	200	95% 5% .
6	AB	240	94% 5% .
7	AC	232	90% 9% .





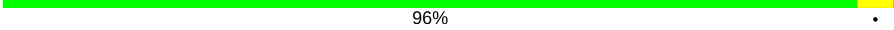
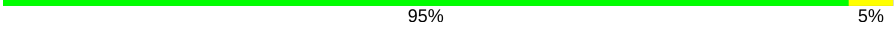

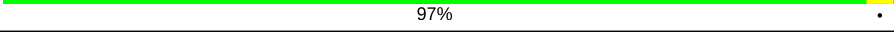


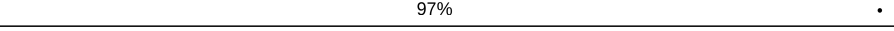

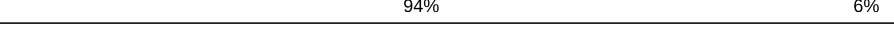
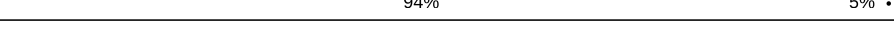


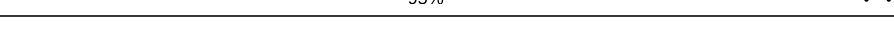
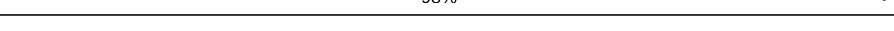
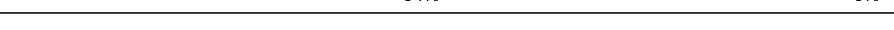
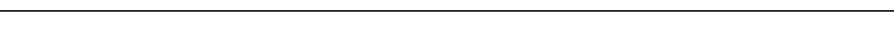
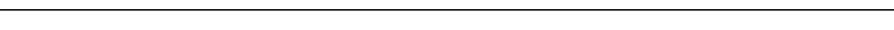
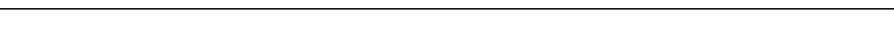
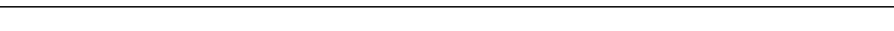
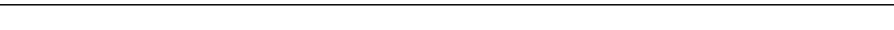

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Mol	Chain	Length	Quality of chain
8	AD	205	 91% 9%
9	AE	166	 94% 5%
10	AF	135	 93% 7%
11	AG	178	 97%
12	AH	129	 95% 5%
13	AI	129	 90% 9%
14	AJ	103	 88% 12%
15	AK	128	 94% 6%
16	AL	123	 96%
17	AM	117	 92% 7%
18	AN	100	 88% 12%
19	AO	88	 97%
20	AP	82	 95%
21	AQ	83	 87% 13%
22	AR	74	 92% 8%
23	AS	91	 96%
24	AT	86	 97%
25	AU	70	 94% 6%
26	B7	120	 82% 18%
27	B8	2904	 80% 18%
28	BA	435	 80% 16%
29	BB	116	 89% 10%
30	B5	234	 95% 5%
31	B6	272	 93% 6%
32	BD	209	 90% 10%

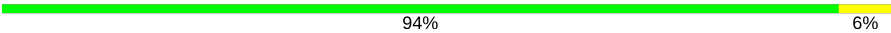

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Mol	Chain	Length	Quality of chain
33	BE	201	 94% 6%
34	BF	178	 90% 9% .
35	BG	176	 93% 7% .
36	BH	149	 88% 11% .
37	BI	141	 96% . .
38	BJ	142	 95% 5%
39	BK	123	 91% 9%
40	BL	144	 97% . .
41	BM	136	 92% 7% .
42	BN	127	 89% 11%
43	BO	117	 97% .
44	BP	114	 91% 9%
45	BQ	117	 94% 6%
46	BR	103	 94% 5% .
47	BS	110	 92% 7% .
48	BT	100	 89% 9% .
49	BU	103	 95% . .
50	BV	94	 98% .
51	BW	84	 94% 6%
52	BX	77	 91% 9%
53	BY	63	 95% 5%
54	BZ	58	 93% 7%
55	B0	56	 96% .
56	B1	54	 94% 6%
57	B2	46	 87% 11% .

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Mol	Chain	Length	Quality of chain
58	B3	64	 94%6%
59	B4	38	 92%8%

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
60	PEV	A0	308	X	-	-	-
60	PEV	A0	314	X	-	-	-
60	PEV	A0	323	X	-	-	-
60	PEV	A1	301	X	-	-	-
60	PEV	A1	305	X	-	-	-
60	PEV	A1	313	X	-	-	-
60	PEV	A1	317	X	-	-	-
60	PEV	AZ	204	X	-	-	-
60	PEV	B8	3001	X	-	-	-
60	PEV	BA	502	X	-	-	-
60	PEV	BA	508	X	-	-	-
60	PEV	BA	526	X	-	-	-
60	PEV	BA	530	X	-	-	-
60	PEV	BA	533	-	-	X	-
60	PEV	BA	535	X	-	-	-
60	PEV	BA	537	X	-	-	-
60	PEV	BA	538	X	-	-	-
60	PEV	BB	202	X	-	-	-
60	PEV	BB	206	X	-	-	-
61	PGV	A0	304	X	-	-	-
61	PGV	A0	305	X	-	-	-
61	PGV	A0	306	X	-	-	-
61	PGV	A0	317	X	-	-	-
61	PGV	A0	318	X	-	-	-
61	PGV	A0	325	X	-	-	-
61	PGV	A0	327	X	-	-	-
61	PGV	A0	328	X	-	-	-
61	PGV	A0	331	X	-	-	-
61	PGV	A0	332	X	-	-	-
61	PGV	A1	303	X	-	-	-
61	PGV	A1	311	X	-	-	-
61	PGV	A1	315	X	-	-	-
61	PGV	A1	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	PGV	AZ	205	X	-	-	-
61	PGV	AZ	207	X	-	-	-
61	PGV	B8	3005	X	-	-	-
61	PGV	BA	501	X	-	-	-
61	PGV	BA	505	X	-	-	-
61	PGV	BA	512	X	-	-	-
61	PGV	BA	515	X	-	-	-
61	PGV	BA	516	X	-	-	-
61	PGV	BA	522	X	-	-	-
61	PGV	BA	536	X	-	-	-
61	PGV	BA	540	X	-	-	-
61	PGV	BB	203	X	-	-	-
61	PGV	BB	204	X	-	-	-
61	PGV	BB	205	X	-	-	-
61	PGV	BB	207	X	-	-	-
61	PGV	BB	208	X	-	-	-
61	PGV	BB	213	X	-	-	-
61	PGV	BB	217	X	-	-	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 163040 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	1542	Total	C	N	O	P	0	0
			33080	14754	6064	10720	1542		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AX	11	Total	C	N	O	P	0	0
			231	103	39	78	11		

- Molecule 3 is a RNA chain called FtsQ nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AV	77	Total	C	N	O	P	0	0
			1649	733	297	542	77		

- Molecule 4 is a protein called Cell division protein FtsQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AZ	98	Total	C	N	O	S	0	0
			779	496	142	138	3		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	104	GLN	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	105	HIS	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	106	ALA	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	107	ARG	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	108	LEU	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	109	ASP	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	110	LYS	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	111	PRO	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	112	GLY	-	EXPRESSION TAG	UNP Q8X9Y5

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Chain	Residue	Modelled	Actual	Comment	Reference
AZ	113	ALA	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	114	ARG	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	115	HIS	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	116	PRO	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	117	CYS	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	118	TRP	-	EXPRESSION TAG	UNP Q8X9Y5
AZ	119	PRO	-	EXPRESSION TAG	UNP Q8X9Y5

- Molecule 5 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A0	200	Total	C	N	O	S	0	0
			1640	1028	290	319	3		
5	A1	200	Total	C	N	O	S	0	0
			1640	1028	290	319	3		

- Molecule 6 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AB	240	Total	C	N	O	S	0	0
			1872	1180	332	352	8		

- Molecule 7 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AC	232	Total	C	N	O	S	0	0
			1822	1149	346	323	4		

- Molecule 8 is a protein called 30S ribosomal protein S4.

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

- Molecule 9 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AE	166	Total	C	N	O	S	0	0
			1225	761	232	226	6		

- Molecule 10 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AF	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AG	178	Total	C	N	O	S	0	0
			1400	874	269	253	4		

- Molecule 12 is a protein called 30S ribosomal protein S8.

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

- Molecule 13 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AI	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 14 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AJ	103	Total	C	N	O	S	0	0
			825	514	158	151	2		

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AK	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 16 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 17 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AM	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 18 is a protein called 30S ribosomal protein S14.

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

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AO	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	79	ARG	GLN	CONFLICT	UNP P0ADZ4

- Molecule 20 is a protein called 30S ribosomal protein S16.

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

- Molecule 21 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AQ	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 22 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	91	Total	C	N	O	S	0	0
			727	464	139	122	2		

- Molecule 24 is a protein called 30S ribosomal protein S20.

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

- Molecule 25 is a protein called 30S ribosomal protein S21.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B7	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 27 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B8	2904	Total	C	N	O	P	0	0
			62341	27810	11469	20158	2904		

- Molecule 28 is a protein called Preprotein translocase secY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	435	Total	C	N	O	S	0	0
			3362	2221	553	571	17		

- Molecule 29 is a protein called Preprotein translocase secE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BB	116	Total	C	N	O	S	0	0
			889	587	154	145	3		

- Molecule 30 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 31 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B6	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 33 is a protein called 50S ribosomal protein L4.

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

- Molecule 34 is a protein called 50S ribosomal protein L5.

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

- Molecule 35 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 36 is a protein called 50S ribosomal protein L9.

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

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 38 is a protein called 50S ribosomal protein L13.

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

- Molecule 39 is a protein called 50S ribosomal protein L14.

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

- Molecule 40 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BL	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BN	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

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

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BT	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 49 is a protein called 50S ribosomal protein L24.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BW	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 52 is a protein called 50S ribosomal protein L28.

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 54 is a protein called 50S ribosomal protein L30.

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

- Molecule 55 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 56 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	B1	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 57 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

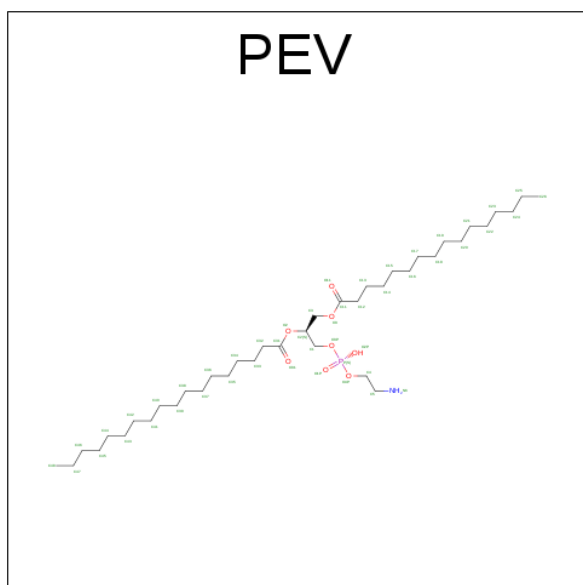
- Molecule 58 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 59 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 60 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C₃₉H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	AZ	1	Total	C	N	O	P	0
			245	195	5	40	5	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	

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Mol	Chain	Residues	Atoms					AltConf
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A0	1	Total	C	N	O	P	0
			1078	858	22	176	22	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	

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Mol	Chain	Residues	Atoms					AltConf
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	A1	1	Total	C	N	O	P	0
			1225	975	25	200	25	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	B8	1	Total	C	N	O	P	0
			294	234	6	48	6	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	

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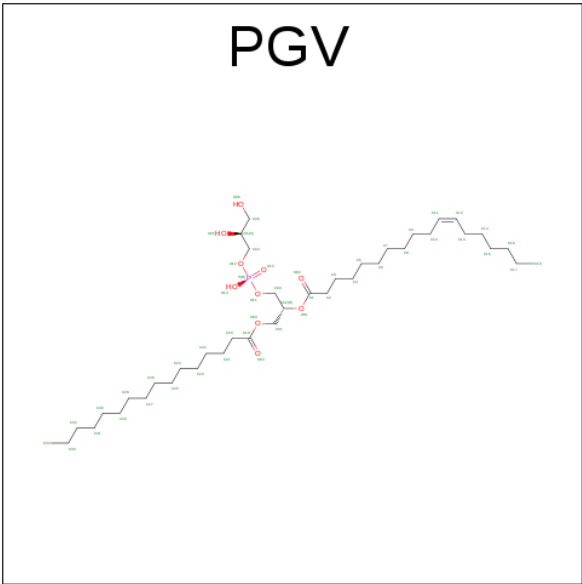
Mol	Chain	Residues	Atoms					AltConf
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BA	1	Total	C	N	O	P	0
			1568	1248	32	256	32	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	

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Mol	Chain	Residues	Atoms					AltConf
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	
60	BB	1	Total	C	N	O	P	0
			539	429	11	88	11	

- Molecule 61 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
61	AZ	1	Total	C	O	P	0
			102	80	20	2	
61	AZ	1	Total	C	O	P	0
			102	80	20	2	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A0	1	Total	C	O	P	0
			510	400	100	10	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	A1	1	Total	C	O	P	0
			204	160	40	4	
61	B8	1	Total	C	O	P	0
			51	40	10	1	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	

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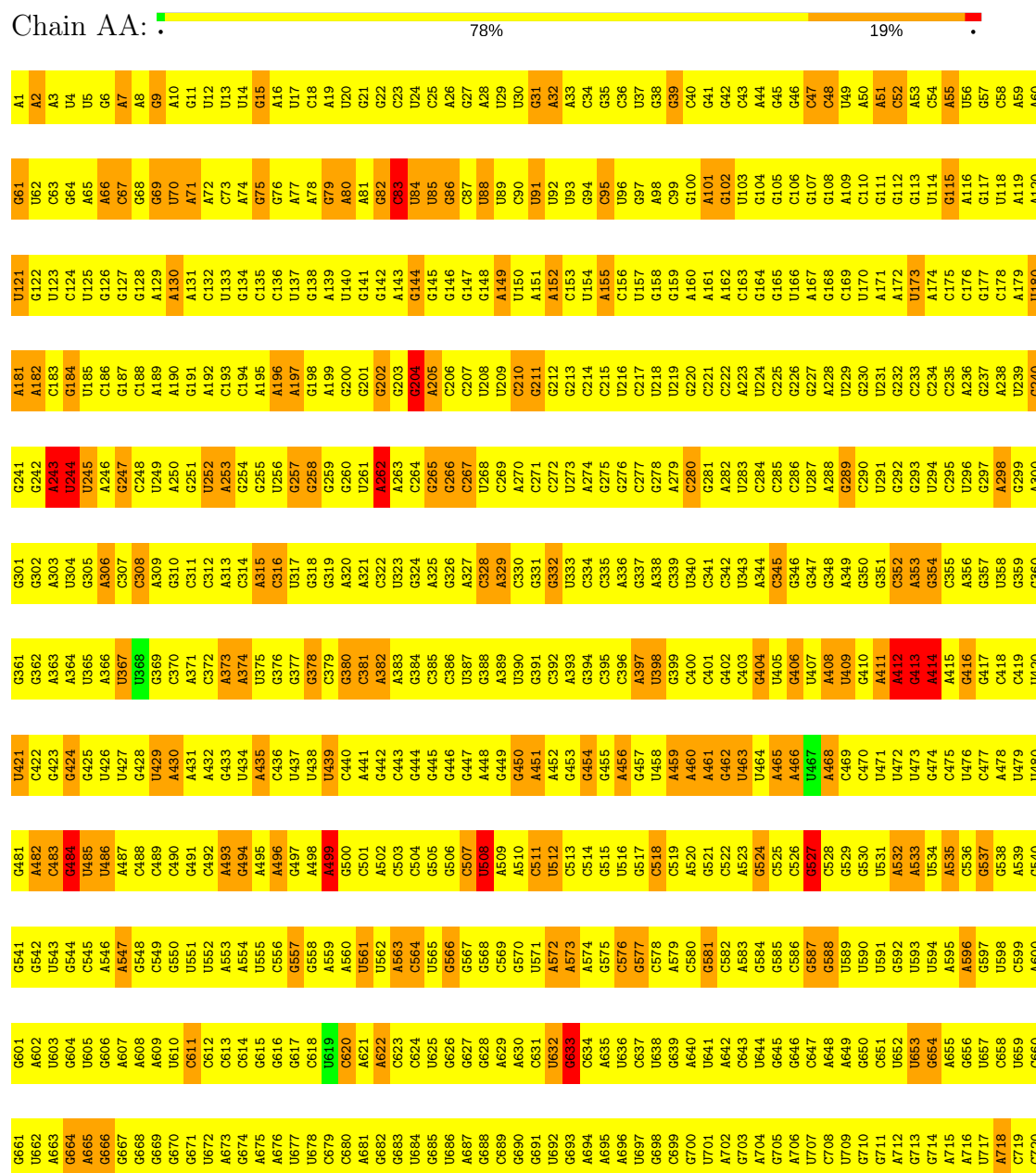
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Mol	Chain	Residues	Atoms				AltConf
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BA	1	Total	C	O	P	0
			408	320	80	8	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	
61	BB	1	Total	C	O	P	0
			357	280	70	7	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S RIBOSOMAL RNA



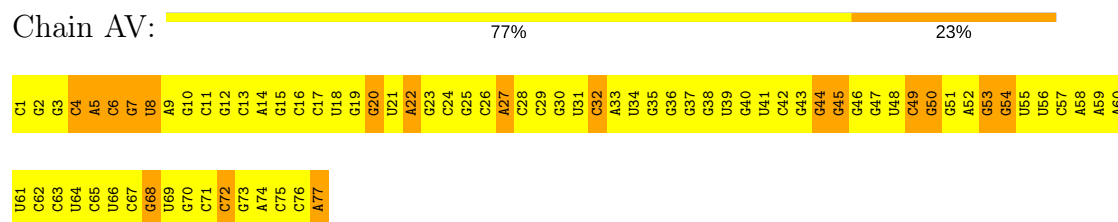
A1502	G1442	C1382	C1322	C1262	U1202	G1142	A1082	A1022	C962	G902	C841	A781	G721
A1503	C1443	C1383	G1323	C1263	C1203	G1143	U1083	U1023	G963	G903	U842	A782	G722
G1504	U1444	C1384	A1324	C1264	A1204	G1144	U1084	G1024	U964	U904	U843	C783	G723
U1505	U1445	G1385	C1325	C1265	U1205	U1145	U1085	U1025	U965	U905	G844	A784	G724
A1506	A1446	G1386	U1326	G1266	G1206	A1146	U1086	G1026	G966	A906	A845	G785	G725
A1507	A1447	G1387	C1327	C1267	G1207	C1147	G1087	G1027	C967	A907	G846	G786	G726
A1508	C1448	C1388	C1328	G1268	C1208	U1148	G1088	U1028	A968	A908	G847	A787	G727
U1509	C1449	C1389	A1329	A1269	C1209	C1149	G1089	C1029	C969	A909	C848	U788	A728
C1510	U1450	U1390	U1330	G1270	C1210	A1150	U1090	U1030	C970	C910	G849	U789	A729
U1511	U1451	G1391	A1331	A1271	U1211	A1151	U1091	C1031	G971	U850	U850	A790	G730
U1512	C1452	G1392	C1332	G1272	U1212	A1152	A1092	G1032	C972	C912	G851	G791	G731
A1513	G1453	U1393	A1333	A1273	A1213	G1153	A1093	G1033	G973	A913	G852	A792	C732
G1514	A1454	A1394	C1334	A1274	C1214	G1154	G1094	G1034	G974	A914	C853	U793	G733
G1515	G1455	C1395	U1335	A1275	G1215	A1155	U1095	A1035	A975	A915	U854	A794	G734
G1516	A1456	A1396	C1336	G1276	A1216	G1156	C1096	A1036	G976	U916	U855	C795	C735
G1517	G1457	C1397	G1337	C1277	C1217	A1157	C1097	C1037	A977	G917	C856	C796	C736
A1518	G1458	A1398	G1338	G1278	C1218	U1158	C1098	A978	C979	A918	C857	C797	C737
A1519	G1459	C1399	A1339	G1279	A1219	U1159	G1099	G1039	C979	A919	G858	U798	C738
C1520	C1460	U1400	A1340	A1280	G1220	G1160	C1100	U1040	C980	U920	G859	G799	C739
C1521	G1461	C1401	U1341	C1281	G1221	C1161	A1101	G1041	U981	U921	A860	G800	U740
U1522	C1462	G1402	C1342	C1282	G1222	C1162	A1102	A1042	U982	G922	G861	U801	G741
G1523	U1463	C1403	G1343	U1283	C1223	A1163	C1103	G1043	A983	A923	C862	A802	G742
C1524	U1464	C1404	C1344	C1284	U1224	G1164	G1104	A1044	C984	C924	U863	G803	A743
G1525	A1465	U1405	A1345	A1285	A1225	U1165	A1105	G1045	C985	G925	A864	U804	C744
G1526	C1466	G1406	G1346	U1286	G1226	G1166	G1106	A1046	U986	G926	A865	C805	G745
U1527	C1467	C1407	G1347	A1287	A1227	A1167	C1107	G1047	C987	G927	C866	C806	A746
U1528	A1468	A1408	U1348	U1288	C1228	U1168	G1108	G1048	G988	G928	G867	A807	A747
G1529	C1469	C1409	A1349	A1289	A1229	U1169	C1109	U1049	U989	G929	C868	C808	G748
G1530	U1470	A1410	A1350	G1290	C1230	A1170	A1110	G1050	C990	C930	G869	G809	A749
A1531	C1471	C1411	U1351	U1291	G1231	A1171	A1111	C1051	U991	C931	C810	C810	C750
U1532	U1472	C1412	C1352	G1292	U1232	C1172	G1112	U1052	U992	C932	C811	C811	C751
C1533	C1473	A1413	G1353	C1293	G1233	U1173	C1113	G1053	G993	C933	A872	G812	G752
A1534	U1474	U1414	U1354	G1294	C1234	C1174	C1114	C1054	A994	C934	A873	U813	A753
C1535	G1475	G1415	G1355	U1295	C1235	G1175	U1115	A1055	C995	A935	U875	A814	C754
C1536	A1476	C1416	G1356	C1296	A1236	U1176	U1116	U1056	C996	C936	C876	A815	G755
G1537	U1477	G1417	A1357	G1297	C1237	G1177	A1117	G1057	U997	A937	G877	A816	C756
C1538	U1478	A1418	U1358	U1298	A1238	G1178	U1118	G1058	C998	A938	A878	C817	U757
U1539	C1479	G1419	C1359	A1299	A1239	A1179	C1119	C1059	C999	C939	C818	G818	C758
U1540	A1480	U1420	A1360	G1300	U1240	A1180	C1120	U1060	A1000	C940	C880	A819	A759
U1541	U1481	G1421	G1361	U1301	G1241	G1181	U1121	G1061	G981	G941	G881	U820	G760
A1542	C1482	G1422	A1362	C1302	G1242	G1182	U1122	U1062	G982	G942	C882	G821	U761
	A1483	G1423	A1363	C1303	C1243	U1183	U1123	G1063	G983	U943	C883	U822	U762
	C1484	U1424	G1364	G1304	G1244	G1184	G1124	G1064	A1004	G944	U884	C823	G763
	U1485	U1425	G1365	G1305	C1245	G1185	U1125	U1065	A1005	G945	G885	G824	C764
	G1486	G1426	C1366	A1306	A1246	G1186	U1126	C1066	G986	A946	G886	A825	G765
	G1487	C1427	C1367	U1307	U1247	G1187	G1127	A1067	G987	G947	G887	C826	A766
	G1488	A1428	A1368	U1308	A1248	A1188	C1128	G1068	G988	C948	G888	U827	A767
	G1489	C1429	C1369	G1309	C1249	U1189	C1129	U1069	A989	A949	A889	U828	A768
	U1490	A1430	G1370	G1310	A1250	G1190	A1130	U1070	G890	U950	G890	G829	G769
	G1491	A1431	G1371	A1311	A1251	A1191	G1131	C1071	U891	G951	U891	G830	C770
	A1492	G1432	U1372	G1312	A1252	C1192	C1132	G1072	A892	U952	A892	A831	G771
	A1493	A1433	G1373	U1313	G1253	G1193	G1133	U1073	C993	G953	C993	G832	G772
	G1494	A1434	A1374	C1314	A1254	U1194	G1134	G1074	G894	G954	G894	G833	G773
	U1495	G1435	A1375	U1315	G1255	C1195	U1135	U1075	G895	U955	G895	U834	G774
	C1496	U1436	G1376	G1316	A1256	A1196	C1136	U1076	C996	U956	C996	U835	G775
	G1497	A1437	U1377	C1317	A1257	A1197	C1137	G1077	C997	U957	C997	G836	G776
	U1498	C1438	C1378	A1318	G1258	G1198	G1138	U1078	G998	A958	G998	U837	A777
	A1499	U1439	G1379	C1319	C1259	U1199	G1139	G1079	C999	A959	C999	G838	G778
	U1500	U1440	U1380	C1320	G1260	C1200	C1140	A1080	U960	U960	A900	C839	C779
	C1501	A1441	U1381	U1321	A1261	A1201	C1141	A1081	A1021	U961	A901	C840	A780

• Molecule 2: mRNA

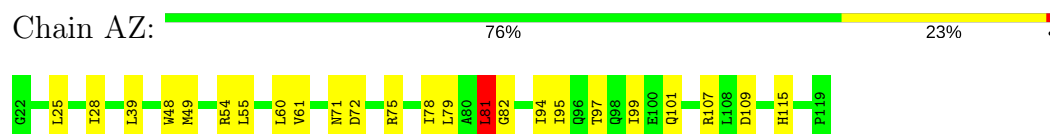
Chain AX: 9% 45% 45%

U12
C13
G14
C15
C16
C17
C18
U19
G20
A21
A22

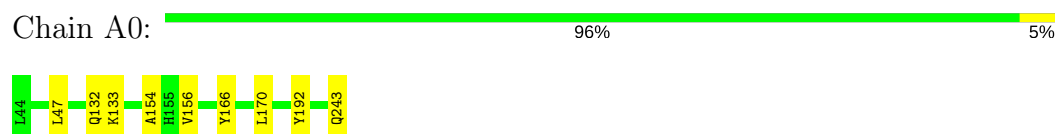
- Molecule 3: FtsQ nascent chain



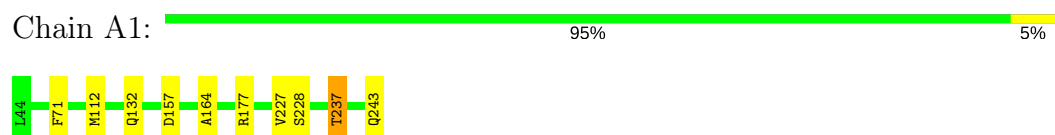
- Molecule 4: Cell division protein FtsQ



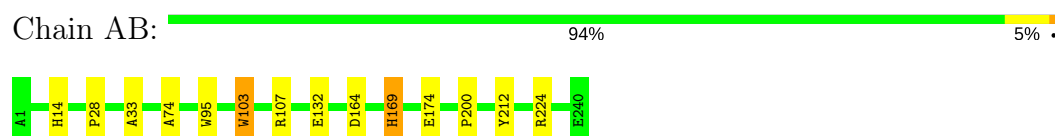
- Molecule 5: Apolipoprotein A-I



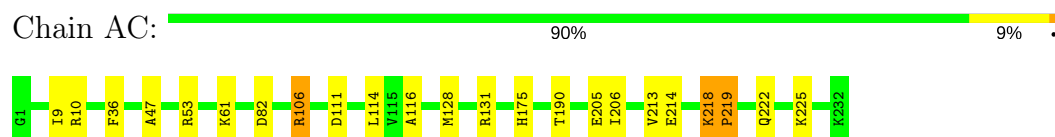
- Molecule 5: Apolipoprotein A-I



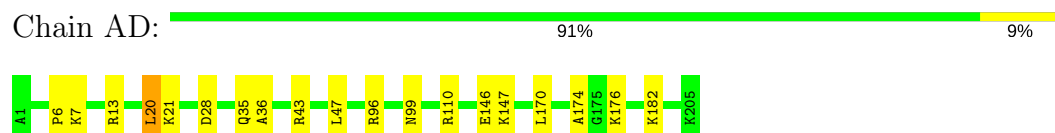
- Molecule 6: 30S ribosomal protein S2



- Molecule 7: 30S ribosomal protein S3



- Molecule 8: 30S ribosomal protein S4



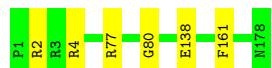
• Molecule 9: 30S ribosomal protein S5

Chain AE:  94% 5%

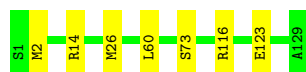
• Molecule 10: 30S ribosomal protein S6

Chain AF:  93% 7%


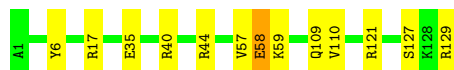
• Molecule 11: 30S ribosomal protein S7

Chain AG:  97%


• Molecule 12: 30S ribosomal protein S8

Chain AH:  95% 5%

• Molecule 13: 30S ribosomal protein S9

Chain AI:  90% 9%

• Molecule 14: 30S ribosomal protein S10

Chain AJ:  88% 12%

• Molecule 15: 30S ribosomal protein S11

Chain AK:  94% 6%

• Molecule 16: 30S ribosomal protein S12

Chain AL:  96% .



- Molecule 17: 30S ribosomal protein S13

Chain AM:  92% 7% .



- Molecule 18: 30S ribosomal protein S14

Chain AN:  88% 12%



- Molecule 19: 30S ribosomal protein S15

Chain AO:  97% ..




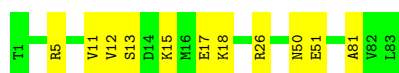
- Molecule 20: 30S ribosomal protein S16

Chain AP:  95% ..



- Molecule 21: 30S ribosomal protein S17

Chain AQ:  87% 13%



- Molecule 22: 30S ribosomal protein S18

Chain AR:  92% 8%



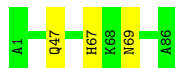
- Molecule 23: 30S ribosomal protein S19

Chain AS:  96% .



- Molecule 24: 30S ribosomal protein S20

Chain AT: 97%



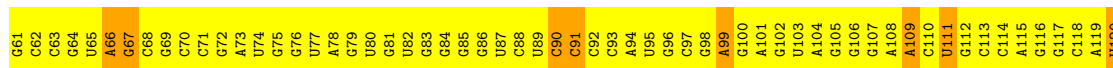
- Molecule 25: 30S ribosomal protein S21

Chain AU: 94%



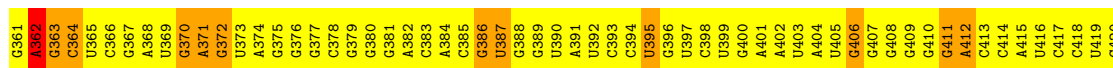
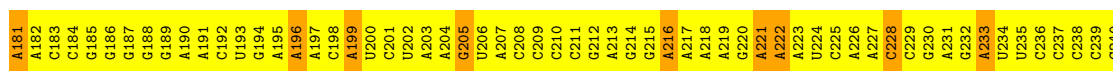
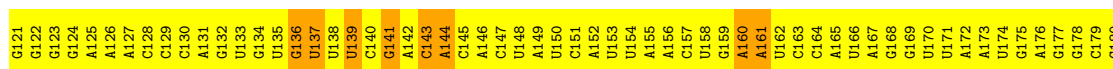
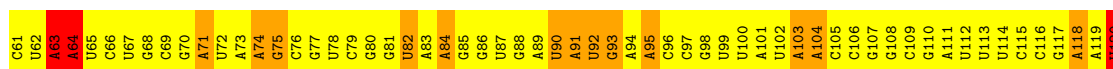
- Molecule 26: 5S RIBOSOMAL RNA

Chain B7: 82%



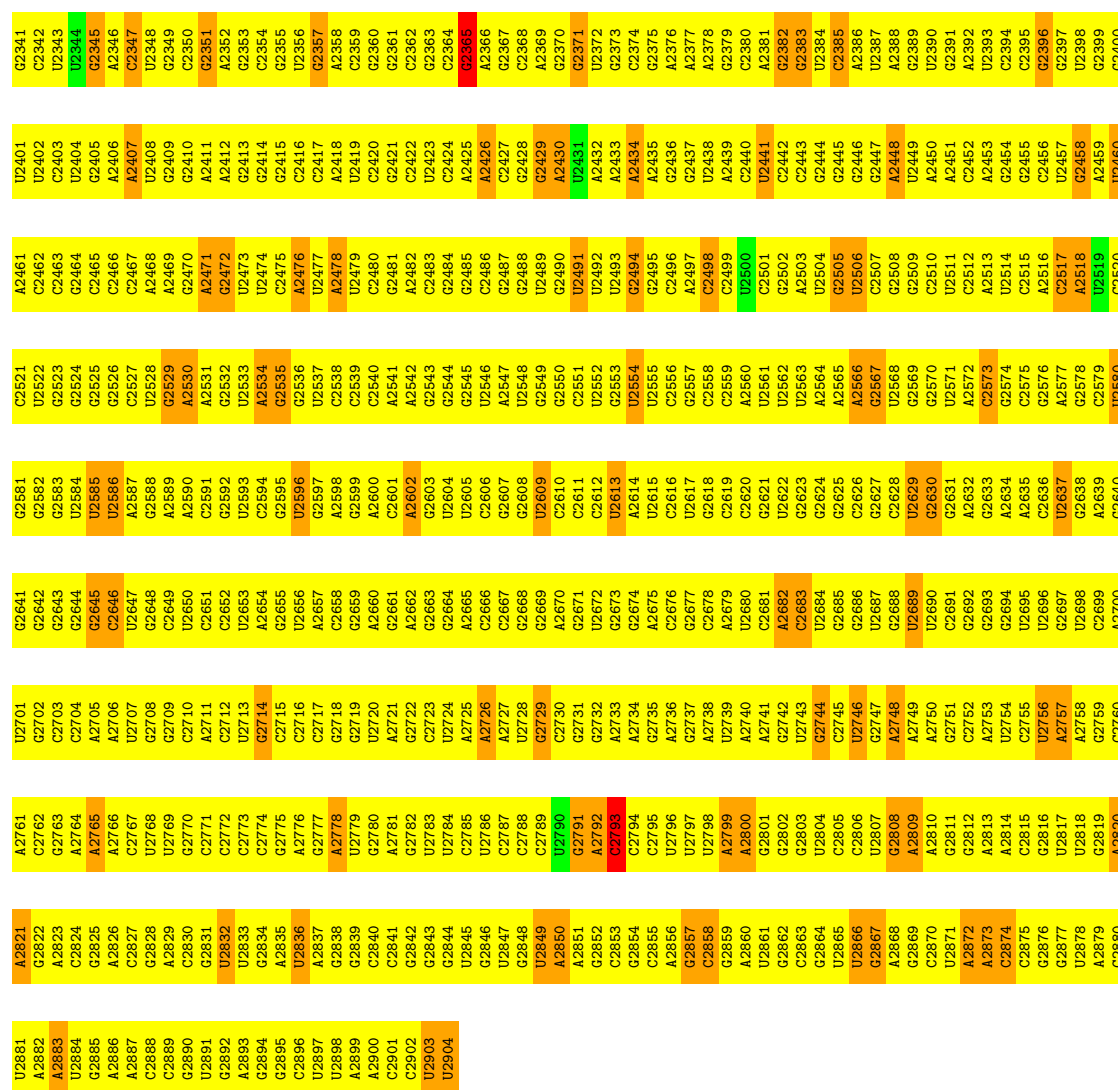
- Molecule 27: 23S RIBOSOMAL RNA

Chain B8: 80%



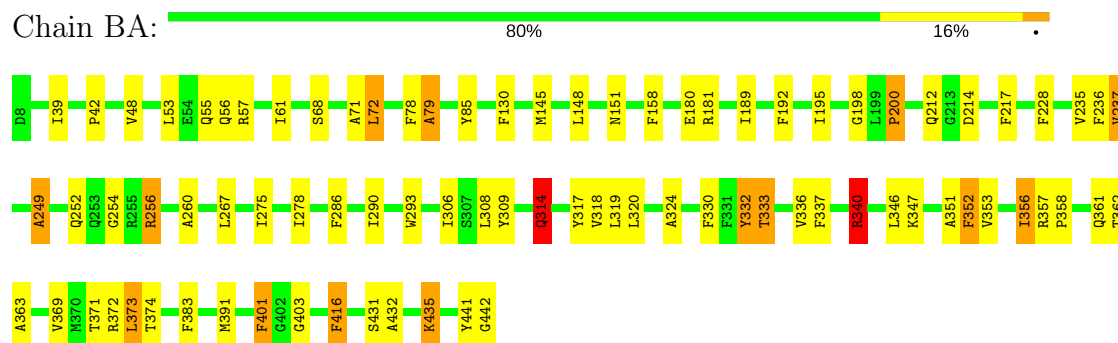
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C1323	A1263	A1203	A1143	U1083	G1023	U963	C903	G843	A783	A723	G663	A603	C943	A483	A423
G1324	A1264	A1204	A1144	U1084	G1024	U964	C904	A844	A784	A724	G664	G604	C944	A484	A424
U1325	A1265	G1205	C1145	A1085	G1025	C965	A905	U845	A785	A725	U665	U606	U546	C486	C426
U1326	G1266	A1206	C1146	U1086	G1026	G966	A906	U846	A786	A726	U666	U607	U547	C487	C427
A1327	U1267	C1207	A1147	G1087	A1027	U967	C907	U847	A787	A727	U667	U608	G548	C488	U428
A1328	A1268	C1208	U1148	A1088	A1028	C968	C908	C848	A788	A728	U668	A609	G549	C489	A429
U1329	A1269	G1209	G1149	U1089	A1029	G969	A909	A849	A789	A729	G669	A610	C550	C490	A430
C1330	C1270	G1210	A1150	G1090	C1030	U970	A910	U850	U790	A730	A670	C611	C551	C491	U431
G1331	C1271	C1211	A1151	G1091	G1031	G971	A911	C851	C791	A731	C671	G612	U552	A492	A432
U1332	A1272	G1212	C1152	C1092	A1032	A972	C912	U852	A792	A732	C672	A613	C553	C493	U433
G1333	U1273	A1213	C1153	G1093	U1033	A973	C913	C853	A793	A733	C673	A614	U554	C494	U434
A1334	A1274	A1214	G1154	U1094	G1034	G974	G914	C854	A794	A734	G674	U615	U555	C495	C435
C1335	A1275	G1215	A1155	A1095	U1035	A975	C915	G855	C795	A735	A675	A616	A556	C496	C436
U1336	A1276	G1216	A1156	U1096	G1036	G976	G916	G856	A796	A736	A676	G617	C557	C497	U437
G1337	C1277	U1217	U1157	U1097	G1037	G977	A917	G857	C797	A737	A677	G618	U558	C498	A438
U1338	C1278	G1218	C1158	A1098	G1038	G978	A918	G858	A798	A738	C678	G619	C559	U499	A439
C1339	G1279	U1219	U1159	G1099	A1039	A979	U919	G859	C799	A739	C679	G620	C560	G500	C440
U1340	G1280	G1220	G1160	C1100	A1040	A980	A920	U860	A800	A740	C680	G621	U561	A501	U441
G1341	C1281	C1221	C1161	U1101	G1041	A981	C921	A861	A801	U741	C681	G622	U562	A502	G442
A1342	U1282	G1222	G1162	C1102	G1042	C982	C922	G862	A802	A742	G682	C623	A563	A503	A443
G1343	G1283	C1223	A1163	A1103	C1043	A983	G923	A863	U803	A743	U683	C624	C564	A504	C444
U1344	A1284	U1224	C1164	C1104	C1044	A984	G924	G864	A804	U744	G684	G625	C565	A505	C445
C1345	A1285	G1225	U1165	U1105	C1045	C985	A925	C865	G805	A745	U685	G626	U566	G506	G446
A1346	A1286	A1226	G1166	G1106	A1046	C986	G926	A866	C906	U746	U686	A627	U567	A507	A447
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G1349	C1289	C1229	A1169	C1109	C1049	G989	U929	G869	G809	A749	U689	G630	C570	C510	U450
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C1351	C1291	U1231	G1171	A1111	G1051	C991	U931	U871	U811	A751	C691	A632	U572	G512	A452
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A1353	C1293	C1233	U1173	U1113	G1053	G993	A933	C873	C813	A753	U693	C634	A574	A514	A454
G1354	U1294	U1234	A1174	C1114	A1054	C994	G934	G874	C814	U754	U694	C635	A575	A515	C455
C1355	C1295	G1235	A1175	G1115	G1055	C995	A935	G875	C815	A755	U695	G636	U576	C516	C456
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A1358	G1298	G1238	C1178	C1118	U1058	C998	G938	A878	G818	A758	C698	U639	G579	U519	U459
U1359	G1299	G1239	G1179	U1119	G1059	U999	G939	G879	A819	A759	A699	G640	U580	G520	A460
G1360	C1300	U1240	U1180	G1120	U1060	A1000	G940	G880	A820	A760	G700	U641	U581	U521	C461
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C1362	A1302	U1242	G1182	G1122	G1062	G1002	G942	G882	G822	U762	U702	A643	A583	C523	C463
G1363	C1303	C1243	U1183	C1123	G1063	G1003	A943	U883	C823	A763	U703	A644	C584	G524	U464
A1364	A1304	A1244	U1184	G1124	C1064	U1004	C944	U884	U824	A764	G704	C645	G585	U525	G465
C1365	C1305	G1245	G1185	G1125	U1065	C1005	A945	C885	A825	A765	A705	U646	A586	A526	A466
U1366	A1306	A1246	G1186	A1126	U1066	C1006	C946	A886	U826	U766	A706	G647	A587	C527	G467
A1367	C1307	G1247	U1187	C1127	A1067	C1007	A947	U887	U827	U767	G707	G648	U588	A528	G468
G1368	A1308	G1248	U1188	G1128	G1068	A1008	C948	C888	U828	A768	G708	G649	U589	A529	C469
C1369	C1309	U1249	A1189	A1129	A1069	A1009	G949	C889	A829	U769	U709	C650	A590	G530	A470
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A2301	A2241	U2181	G2121	G2061	C2001	A1941	C1881	A1821	C1761	A1701	A1641	G1581	U1521	C1461	G1401
U2302	G2242	U2182	U2122	A2062	G2002	C1942	U1882	G1822	A1762	G1702	G1642	C1582	A1522	C1462	U1402
G2303	C2243	A2183	G2123	C2063	A2003	U1943	U1883	G1823	G1763	C1703	G1643	A1583	U1523	C1463	A1403
U2304	U2244	A2184	G2124	C2064	G2004	U1944	G1884	G1824	C1764	C1704	C1644	U1584	G1524	G1464	C1404
G2305	U2245	U2185	G2125	C2065	A2005	G1945	A1885	U1825	U1765	A1705	G1645	C1585	A1525	G1465	U1405
C2306	G2246	G2186	A2126	C2066	C2006	U1946	U1886	G1826	G1766	C1706	C1646	A1586	C1526	U1466	U1406
G2307	A2247	U2187	G2127	G2067	U2007	C1947	G1887	U1827	U1767	U1707	U1647	G1587	C1527	U1467	G1407
C2308	C2248	U2188	G2128	C2068	C2008	G1948	G1888	G1828	C1768	C1708	U1648	A1588	A1528	U1468	G1408
A2309	U2249	U2189	C2129	G2069	A2009	G1949	A1889	A1829	U1769	U1709	G1649	U1589	G1529	A1469	U1409
C2310	G2250	G2190	U2130	A2070	C2010	G1950	A1890	C1830	G1770	G1710	A1650	A1590	G1530	C1470	U1410
A2311	G2251	A2191	U2131	A2071	U2011	U1951	G1891	G1831	C1771	U1711	G1651	A1591	C1531	G1471	U1411
G2312	G2252	U2192	U2132	C2072	A1952	A1952	C1892	G1832	A1772	U1712	A1652	C1592	A1532	C1472	U1412
C2313	G2253	G2193	C2133	C2073	A2013	G1953	C1893	C1833	A1773	U1713	G1653	A1593	C1533	C1473	A1413
A2314	C2254	U2194	A2134	U2074	G1954	A1954	C1894	A1834	C1774	U1714	A1654	U1594	U1534	U1474	A1414
G2315	G2255	U2195	A2135	U2075	A2015	G1955	C1895	C1835	U1775	G1715	A1655	C1595	A1535	G1475	U1415
G2316	G2256	C2196	G2136	U2076	U2016	U1956	G1896	C1836	G1776	U1716	C1656	A1596	C1536	U1476	G1416
A2317	U2257	U2197	U2137	A2077	U2017	G1957	G1897	C1837	U1777	U1717	U1657	A1597	G1537	U1477	C1417
G2318	C2258	A2198	G2138	C2078	G2018	C1958	U1898	C1838	U1778	G1718	C1658	A1598	G1538	G1478	G1418
U2319	U2259	A2199	U2139	C2079	A2019	G1959	A1899	G1839	U1779	G1719	G1659	U1599	U1539	G1479	A1419
C2320	C2260	C2200	G2140	A2080	A2020	A1960	A1900	G1840	A1780	U1720	G1660	C1600	G1540	C1480	A1420
U2321	G2261	G2201	G2141	U2081	C2021	C1961	A1901	U1841	U1781	G1721	G1661	G1601	C1541	U1481	G1421
U2322	U2262	U2202	A2142	A2082	U2022	C1962	C1902	G1842	U1782	A1722	G1662	U1602	U1542	G1482	G1422
G2323	C2263	G2203	C2143	G2083	C2023	U1963	G1903	C1843	A1783	G1723	G1663	A1603	G1543	G1483	G1423
C2324	C2264	G2204	G2144	C2084	G2024	G1964	G1904	C1844	A1784	G1724	A1664	C1604	A1544	U1484	G1424
G2325	U2265	A2205	C2145	U2085	C2025	C1965	C1905	G1845	A1785	U1725	A1665	C1605	A1545	U1485	G1425
A2326	A2266	C2206	C2146	U2086	U2026	A1966	G1906	G1846	A1786	G1726	G1666	C1606	A1546	U1486	G1426
C2327	U2267	C2207	A2147	G2087	G2027	C1967	G1907	A1847	A1787	G1727	G1667	C1607	C1547	U1487	A1427
A2328	A2268	C2208	G2148	A2088	U2028	G1968	C1908	A1848	C1788	G1728	A1668	A1608	A1548	C1488	C1428
U2329	G2269	G2209	U2149	C2089	G2029	A1969	C1909	G1849	A1789	U1729	A1669	A1609	A1549	G1489	G1429
G2330	A2270	U2210	C2150	A2090	A2030	U1970	G1910	G1850	C1790	G1730	C1670	A1610	C1550	A1490	G1430
C2331	G2271	A2211	U2151	C2091	A2031	U1971	U1911	U1851	A1791	G1731	U1671	C1611	A1551	G1491	A1431
C2332	U2272	A2212	G2152	U2092	G2032	A1972	A1912	U1852	A1792	C1732	A1672	C1612	A1552	G1492	G1432
A2333	A2273	U2213	C2153	A2093	A2033	G1973	A1913	A1853	G1793	G1733	G1673	C1613	A1553	C1493	A1433
U2334	A2274	C2214	A2154	A2094	U2034	C1974	A1914	A1854	A1794	G1734	G1674	A1614	U1554	A1494	A1434
G2335	C2275	G2215	A2155	A2095	G2035	U1975	U1915	A1855	A1795	A1735	C1675	C1615	G1555	A1495	G1435
A2336	G2276	G2216	U2156	C2096	G2036	U1976	A1916	U1856	U1796	G1736	A1676	A1616	C1556	A1496	G1436
G2337	G2277	G2217	G2157	A2097	A2037	A1977	U1917	G1857	G1797	G1737	A1677	C1617	C1557	U1497	C1437
C2338	A2278	G2218	A2158	U2098	G2038	A1978	A1918	A1858	U1798	G1738	A1678	A1618	C1558	C1498	U1438
U2339	G2279	U2219	C2159	U2099	U2039	A1979	A1919	U1859	G1799	A1739	A1679	U1559	U1559	A1439	G1439
A2340	G2280	U2220	C2160	G2100	G2040	G1980	G1860		C1800	G1740		G1620	G1560	G1500	



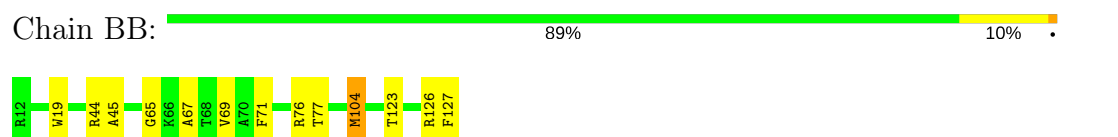
- Molecule 28: Preprotein translocase secY subunit

Chain BA:



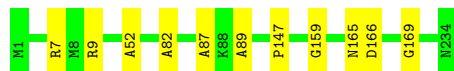
- Molecule 29: Preprotein translocase secE subunit

Chain BB:



- Molecule 30: 50S ribosomal protein L1

Chain B5:  95% 5%



- Molecule 31: 50S ribosomal protein L2

Chain B6:  93% 6%



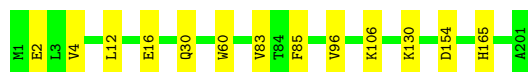
- Molecule 32: 50S ribosomal protein L3

Chain BD:  90% 10%



- Molecule 33: 50S ribosomal protein L4

Chain BE:  94% 6%



- Molecule 34: 50S ribosomal protein L5

Chain BF:  90% 9%



- Molecule 35: 50S ribosomal protein L6

Chain BG:  93% 7%



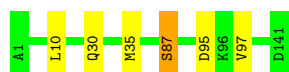
- Molecule 36: 50S ribosomal protein L9

Chain BH:  88% 11%



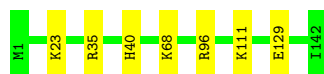
- Molecule 37: 50S ribosomal protein L11

Chain BI:  96% ..



- Molecule 38: 50S ribosomal protein L13

Chain BJ:  95% 5%



- Molecule 39: 50S ribosomal protein L14

Chain BK:  91% 9%



- Molecule 40: 50S ribosomal protein L15

Chain BL:  97% ..



- Molecule 41: 50S ribosomal protein L16

Chain BM:  92% 7% .



- Molecule 42: 50S ribosomal protein L17

Chain BN:  89% 11%



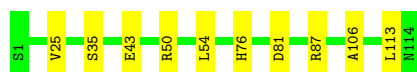
- Molecule 43: 50S ribosomal protein L18

Chain BO:  97% .



- Molecule 44: 50S ribosomal protein L19

Chain BP:  91% 9%



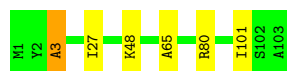
- Molecule 45: 50S ribosomal protein L20

Chain BQ: 94% 6%



- Molecule 46: 50S ribosomal protein L21

Chain BR: 94% 5%



- Molecule 47: 50S ribosomal protein L22

Chain BS: 92% 7%



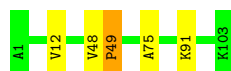
- Molecule 48: 50S ribosomal protein L23

Chain BT: 89% 9%



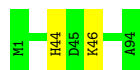
- Molecule 49: 50S ribosomal protein L24

Chain BU: 95%



- Molecule 50: 50S ribosomal protein L25

Chain BV: 98%

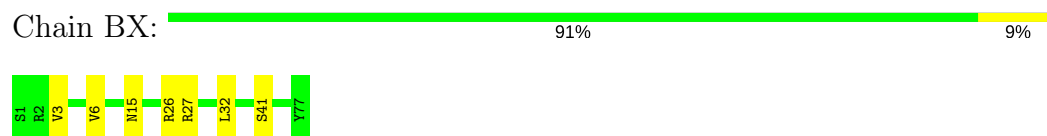


- Molecule 51: 50S ribosomal protein L27

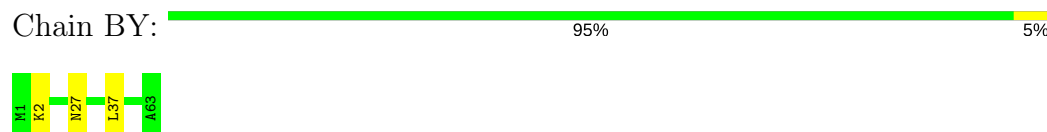
Chain BW: 94% 6%



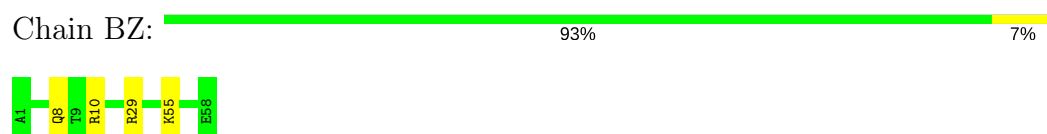
- Molecule 52: 50S ribosomal protein L28



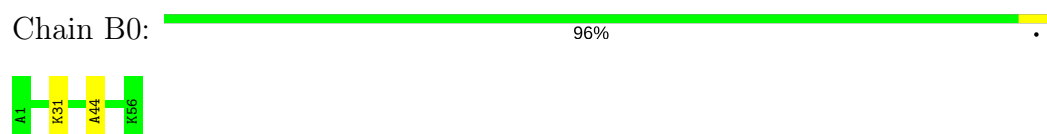
- Molecule 53: 50S ribosomal protein L29



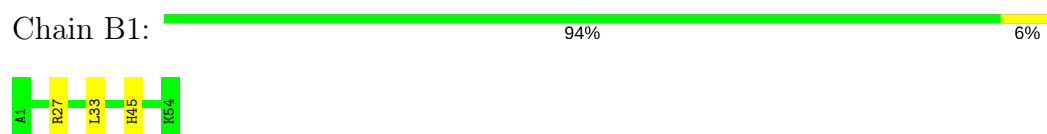
- Molecule 54: 50S ribosomal protein L30



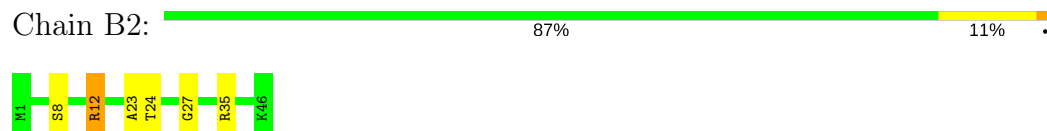
- Molecule 55: 50S ribosomal protein L32



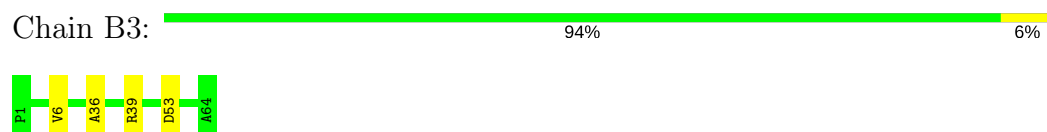
- Molecule 56: 50S ribosomal protein L33



- Molecule 57: 50S ribosomal protein L34



- Molecule 58: 50S ribosomal protein L35



- Molecule 59: 50S ribosomal protein L36





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	85664	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI Polara 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	38000	Depositor
Image detector	Kodak SO163	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, PEV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	AA	1.60	46/37039 (0.1%)	2.50	4339/57778 (7.5%)
10	AF	0.99	0/1121	1.06	0/1509
11	AG	1.03	0/1422	1.01	2/1908 (0.1%)
12	AH	0.96	0/989	1.01	0/1326
13	AI	1.12	0/1048	1.01	0/1394
14	AJ	1.03	0/835	1.03	0/1127
15	AK	1.05	0/982	1.05	0/1323
16	AL	1.07	0/969	1.01	0/1300
17	AM	1.05	0/919	0.99	1/1226 (0.1%)
18	AN	1.07	0/817	1.05	1/1088 (0.1%)
19	AO	1.06	0/724	0.92	0/966
2	AX	1.56	0/256	2.32	28/394 (7.1%)
20	AP	1.07	0/659	1.03	0/884
21	AQ	0.99	0/681	1.05	0/913
22	AR	1.14	0/637	1.05	2/851 (0.2%)
23	AS	0.96	0/744	0.96	0/995
24	AT	0.96	0/676	0.94	0/895
25	AU	1.18	0/598	0.99	0/792
26	B7	1.59	2/2873 (0.1%)	2.49	325/4478 (7.3%)
27	B8	1.60	100/69822 (0.1%)	2.50	8171/108926 (7.5%)
28	BA	1.68	7/3439 (0.2%)	1.14	15/4662 (0.3%)
29	BB	0.98	1/902 (0.1%)	1.05	1/1228 (0.1%)
3	AV	1.61	1/1842 (0.1%)	2.43	211/2870 (7.4%)
30	B5	0.92	0/1748	0.97	0/2355
31	B6	1.04	0/2131	1.03	1/2863 (0.0%)
32	BD	0.97	0/1586	1.08	4/2134 (0.2%)
33	BE	0.95	0/1571	1.01	2/2113 (0.1%)
34	BF	1.01	0/1444	1.06	1/1937 (0.1%)
35	BG	0.96	0/1343	1.06	4/1816 (0.2%)
36	BH	0.93	0/1122	1.05	0/1515
37	BI	0.86	0/1046	1.00	1/1410 (0.1%)
38	BJ	0.97	0/1152	1.01	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BK	1.03	0/956	1.03	0/1279
4	AZ	0.98	0/795	1.16	0/1082
40	BL	1.04	0/1062	0.98	1/1413 (0.1%)
41	BM	1.03	0/1093	1.06	2/1460 (0.1%)
42	BN	1.10	0/1021	1.03	1/1364 (0.1%)
43	BO	1.07	0/910	0.98	0/1219
44	BP	1.06	0/929	1.03	0/1242
45	BQ	1.09	0/960	1.00	2/1278 (0.2%)
46	BR	1.01	0/829	1.07	1/1107 (0.1%)
47	BS	0.99	0/864	1.04	1/1156 (0.1%)
48	BT	0.98	0/794	1.09	1/1060 (0.1%)
49	BU	0.96	0/797	1.04	0/1062
5	A0	0.96	1/1667 (0.1%)	0.95	3/2240 (0.1%)
5	A1	0.97	1/1667 (0.1%)	0.95	0/2240
50	BV	0.96	0/766	1.02	0/1025
51	BW	1.04	0/642	1.05	0/848
52	BX	1.09	0/635	1.04	0/848
53	BY	1.00	0/510	0.90	0/677
54	BZ	0.99	0/453	0.99	0/605
55	B0	1.05	0/450	0.97	0/599
56	B1	0.93	0/448	1.01	0/594
57	B2	1.25	0/380	1.06	0/498
58	B3	0.98	0/513	0.98	0/676
59	B4	1.20	2/303 (0.7%)	1.03	0/397
6	AB	0.92	0/1904	0.98	1/2565 (0.0%)
7	AC	1.00	0/1852	1.06	1/2490 (0.0%)
8	AD	1.04	0/1665	0.99	0/2227
9	AE	0.97	0/1239	1.03	0/1664
All	All	1.44	161/169241 (0.1%)	2.16	13123/251442 (5.2%)

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	72
12	AH	0	1
13	AI	0	1
26	B7	0	2
27	B8	0	100
28	BA	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	AV	0	2
34	BF	0	1
36	BH	0	1
49	BU	0	1
5	A1	0	1
57	B2	0	1
7	AC	0	1
All	All	0	189

The worst 5 of 161 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BA	416	PHE	CG-CD2	41.52	2.01	1.38
28	BA	416	PHE	CG-CD1	39.62	1.98	1.38
28	BA	416	PHE	CE2-CZ	30.78	1.95	1.37
28	BA	416	PHE	CE1-CZ	30.54	1.95	1.37
28	BA	416	PHE	CD2-CE2	27.89	1.95	1.39

The worst 5 of 13123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	85	U	P-O3'-C3'	19.51	143.11	119.70
27	B8	670	A	P-O3'-C3'	17.35	140.52	119.70
27	B8	2076	U	P-O3'-C3'	15.69	138.53	119.70
27	B8	6	A	N1-C6-N6	14.72	127.43	118.60
1	AA	1252	A	N1-C6-N6	14.43	127.26	118.60

There are no chirality outliers.

5 of 189 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	102	G	Sidechain
1	AA	115	G	Sidechain
1	AA	13	U	Sidechain
1	AA	69	G	Sidechain
1	AA	95	C	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	33080	0	16649	21	0
2	AX	231	0	120	0	0
3	AV	1649	0	834	1	0
4	AZ	779	0	798	4	0
5	A0	1640	0	1641	0	0
5	A1	1640	0	1641	0	0
6	AB	1872	0	1885	3	0
7	AC	1822	0	1913	2	0
8	AD	1643	0	1710	1	0
9	AE	1225	0	1273	1	0
10	AF	1101	0	1050	1	0
11	AG	1400	0	1449	0	0
12	AH	979	0	1034	1	0
13	AI	1036	0	1084	0	0
14	AJ	825	0	865	2	0
15	AK	965	0	997	0	0
16	AL	955	0	1019	2	0
17	AM	910	0	981	0	0
18	AN	805	0	847	1	0
19	AO	716	0	742	0	0
20	AP	649	0	666	2	0
21	AQ	672	0	716	1	0
22	AR	626	0	651	0	0
23	AS	727	0	769	0	0
24	AT	670	0	722	2	0
25	AU	590	0	631	1	0
26	B7	2570	0	1301	0	0
27	B8	62341	0	31354	41	0
28	BA	3362	0	3511	38	0
29	BB	889	0	982	1	0
30	B5	1733	0	1824	1	0
31	B6	2092	0	2170	2	0
32	BD	1565	0	1616	1	0
33	BE	1552	0	1619	1	0
34	BF	1420	0	1460	1	0
35	BG	1323	0	1374	0	0
36	BH	1111	0	1148	2	0
37	BI	1032	0	1088	0	0
38	BJ	1129	0	1162	0	0
39	BK	947	0	1023	0	0
40	BL	1053	0	1129	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	BM	1074	0	1157	1	0
42	BN	1008	0	1045	1	0
43	BO	900	0	935	0	0
44	BP	917	0	965	0	0
45	BQ	947	0	1022	0	0
46	BR	816	0	839	1	0
47	BS	857	0	922	0	0
48	BT	787	0	846	0	0
49	BU	789	0	847	0	0
50	BV	753	0	780	0	0
51	BW	634	0	656	0	0
52	BX	625	0	655	0	0
53	BY	509	0	543	0	0
54	BZ	449	0	491	0	0
55	B0	444	0	461	0	0
56	B1	441	0	485	2	0
57	B2	377	0	418	1	0
58	B3	504	0	574	1	0
59	B4	302	0	343	0	0
60	A0	1078	0	1694	1	0
60	A1	1225	0	1925	4	0
60	AZ	245	0	385	0	0
60	B8	294	0	462	2	0
60	BA	1568	0	2464	34	0
60	BB	539	0	847	0	0
61	A0	510	0	760	0	0
61	A1	204	0	304	2	0
61	AZ	102	0	152	0	0
61	B8	51	0	76	0	0
61	BA	408	0	608	1	0
61	BB	357	0	532	0	0
All	All	163040	0	119641	141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 141 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)
28:BA:416:PHE:CE1	28:BA:416:PHE:CD1	1.92	1.58
28:BA:416:PHE:CD2	28:BA:416:PHE:CE2	1.95	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BA:416:PHE:CZ	28:BA:416:PHE:CE2	1.95	1.53
28:BA:416:PHE:CE1	28:BA:416:PHE:CZ	1.95	1.51
28:BA:416:PHE:CD1	28:BA:416:PHE:CG	1.98	1.49

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	
4	AZ	96/98 (98%)	74 (77%)	13 (14%)	9 (9%)	1	14
5	A0	198/200 (99%)	174 (88%)	20 (10%)	4 (2%)	9	46
5	A1	198/200 (99%)	169 (85%)	23 (12%)	6 (3%)	5	37
6	AB	238/240 (99%)	190 (80%)	42 (18%)	6 (2%)	6	41
7	AC	230/232 (99%)	184 (80%)	31 (14%)	15 (6%)	1	22
8	AD	203/205 (99%)	163 (80%)	28 (14%)	12 (6%)	2	23
9	AE	164/166 (99%)	137 (84%)	21 (13%)	6 (4%)	4	33
10	AF	133/135 (98%)	109 (82%)	22 (16%)	2 (2%)	12	53
11	AG	176/178 (99%)	142 (81%)	29 (16%)	5 (3%)	6	39
12	AH	127/129 (98%)	102 (80%)	23 (18%)	2 (2%)	11	51
13	AI	127/129 (98%)	108 (85%)	11 (9%)	8 (6%)	1	22
14	AJ	101/103 (98%)	85 (84%)	9 (9%)	7 (7%)	1	20
15	AK	126/128 (98%)	106 (84%)	15 (12%)	5 (4%)	3	31
16	AL	121/123 (98%)	108 (89%)	12 (10%)	1 (1%)	22	67
17	AM	115/117 (98%)	96 (84%)	13 (11%)	6 (5%)	2	26
18	AN	98/100 (98%)	81 (83%)	9 (9%)	8 (8%)	1	16
19	AO	86/88 (98%)	79 (92%)	5 (6%)	2 (2%)	7	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AP	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	6	41
21	AQ	81/83 (98%)	67 (83%)	8 (10%)	6 (7%)	1	18
22	AR	72/74 (97%)	59 (82%)	9 (12%)	4 (6%)	2	25
23	AS	89/91 (98%)	73 (82%)	12 (14%)	4 (4%)	3	29
24	AT	84/86 (98%)	76 (90%)	7 (8%)	1 (1%)	15	57
25	AU	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
28	BA	433/435 (100%)	313 (72%)	66 (15%)	54 (12%)	0	7
29	BB	114/116 (98%)	96 (84%)	12 (10%)	6 (5%)	2	26
30	B5	232/234 (99%)	211 (91%)	15 (6%)	6 (3%)	6	40
31	B6	270/272 (99%)	227 (84%)	31 (12%)	12 (4%)	3	29
32	BD	207/209 (99%)	172 (83%)	24 (12%)	11 (5%)	2	26
33	BE	199/201 (99%)	169 (85%)	20 (10%)	10 (5%)	2	27
34	BF	176/178 (99%)	137 (78%)	27 (15%)	12 (7%)	1	20
35	BG	174/176 (99%)	137 (79%)	28 (16%)	9 (5%)	2	26
36	BH	147/149 (99%)	108 (74%)	31 (21%)	8 (5%)	2	25
37	BI	139/141 (99%)	125 (90%)	11 (8%)	3 (2%)	8	44
38	BJ	140/142 (99%)	117 (84%)	19 (14%)	4 (3%)	5	38
39	BK	121/123 (98%)	99 (82%)	16 (13%)	6 (5%)	2	27
40	BL	142/144 (99%)	129 (91%)	10 (7%)	3 (2%)	8	45
41	BM	134/136 (98%)	107 (80%)	17 (13%)	10 (8%)	1	18
42	BN	125/127 (98%)	104 (83%)	12 (10%)	9 (7%)	1	19
43	BO	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	6	40
44	BP	112/114 (98%)	94 (84%)	11 (10%)	7 (6%)	1	22
45	BQ	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	2	26
46	BR	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	2	27
47	BS	108/110 (98%)	81 (75%)	18 (17%)	9 (8%)	1	16
48	BT	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	1	19
49	BU	101/103 (98%)	84 (83%)	14 (14%)	3 (3%)	5	37
50	BV	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	17	60
51	BW	82/84 (98%)	59 (72%)	19 (23%)	4 (5%)	2	27
52	BX	75/77 (97%)	57 (76%)	12 (16%)	6 (8%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	BY	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	4	35
54	BZ	56/58 (97%)	49 (88%)	4 (7%)	3 (5%)	2	25
55	B0	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	9	47
56	B1	52/54 (96%)	46 (88%)	5 (10%)	1 (2%)	9	47
57	B2	44/46 (96%)	31 (70%)	10 (23%)	3 (7%)	1	20
58	B3	62/64 (97%)	52 (84%)	9 (14%)	1 (2%)	11	51
59	B4	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	39
All	All	7128/7238 (98%)	5877 (82%)	904 (13%)	347 (5%)	5	27

5 of 347 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AZ	48	TRP
4	AZ	61	VAL
4	AZ	81	LEU
5	A1	177	ARG
7	AC	206	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
4	AZ	85/85 (100%)	72 (85%)	13 (15%)	3	19
5	A0	176/176 (100%)	174 (99%)	2 (1%)	78	89
5	A1	176/176 (100%)	173 (98%)	3 (2%)	66	84
6	AB	198/198 (100%)	194 (98%)	4 (2%)	60	82
7	AC	189/189 (100%)	183 (97%)	6 (3%)	44	70
8	AD	172/172 (100%)	166 (96%)	6 (4%)	41	69
9	AE	125/125 (100%)	122 (98%)	3 (2%)	54	78
10	AF	116/116 (100%)	111 (96%)	5 (4%)	33	64
11	AG	146/146 (100%)	146 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AH	104/104 (100%)	101 (97%)	3 (3%)	48	73
13	AI	106/106 (100%)	101 (95%)	5 (5%)	30	62
14	AJ	90/90 (100%)	88 (98%)	2 (2%)	57	79
15	AK	98/98 (100%)	95 (97%)	3 (3%)	45	71
16	AL	103/103 (100%)	102 (99%)	1 (1%)	80	90
17	AM	95/95 (100%)	92 (97%)	3 (3%)	44	70
18	AN	83/83 (100%)	81 (98%)	2 (2%)	54	78
19	AO	76/76 (100%)	74 (97%)	2 (3%)	51	75
20	AP	65/65 (100%)	65 (100%)	0	100	100
21	AQ	77/77 (100%)	74 (96%)	3 (4%)	37	66
22	AR	64/64 (100%)	63 (98%)	1 (2%)	68	85
23	AS	78/78 (100%)	78 (100%)	0	100	100
24	AT	65/65 (100%)	65 (100%)	0	100	100
25	AU	60/60 (100%)	58 (97%)	2 (3%)	43	70
28	BA	353/353 (100%)	326 (92%)	27 (8%)	15	47
29	BB	92/92 (100%)	88 (96%)	4 (4%)	33	64
30	B5	181/181 (100%)	178 (98%)	3 (2%)	66	84
31	B6	217/217 (100%)	212 (98%)	5 (2%)	56	79
32	BD	164/164 (100%)	158 (96%)	6 (4%)	39	68
33	BE	165/165 (100%)	164 (99%)	1 (1%)	89	94
34	BF	149/149 (100%)	145 (97%)	4 (3%)	50	74
35	BG	137/137 (100%)	134 (98%)	3 (2%)	57	79
36	BH	114/114 (100%)	108 (95%)	6 (5%)	26	59
37	BI	109/109 (100%)	106 (97%)	3 (3%)	49	74
38	BJ	116/116 (100%)	113 (97%)	3 (3%)	51	75
39	BK	104/104 (100%)	99 (95%)	5 (5%)	30	61
40	BL	103/103 (100%)	102 (99%)	1 (1%)	80	90
41	BM	109/109 (100%)	109 (100%)	0	100	100
42	BN	103/103 (100%)	100 (97%)	3 (3%)	48	73
43	BO	87/87 (100%)	87 (100%)	0	100	100
44	BP	99/99 (100%)	96 (97%)	3 (3%)	46	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BQ	89/89 (100%)	89 (100%)	0	100	100
46	BR	84/84 (100%)	84 (100%)	0	100	100
47	BS	93/93 (100%)	93 (100%)	0	100	100
48	BT	84/84 (100%)	79 (94%)	5 (6%)	22	55
49	BU	84/84 (100%)	82 (98%)	2 (2%)	54	78
50	BV	78/78 (100%)	77 (99%)	1 (1%)	73	87
51	BW	62/62 (100%)	61 (98%)	1 (2%)	68	85
52	BX	67/67 (100%)	66 (98%)	1 (2%)	70	85
53	BY	55/55 (100%)	54 (98%)	1 (2%)	64	84
54	BZ	48/48 (100%)	47 (98%)	1 (2%)	59	80
55	B0	47/47 (100%)	46 (98%)	1 (2%)	59	80
56	B1	48/48 (100%)	47 (98%)	1 (2%)	59	80
57	B2	38/38 (100%)	37 (97%)	1 (3%)	51	75
58	B3	51/51 (100%)	50 (98%)	1 (2%)	60	82
59	B4	34/34 (100%)	34 (100%)	0	100	100
All	All	5911/5911 (100%)	5749 (97%)	162 (3%)	54	74

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	BA	180	GLU
28	BA	357	ARG
48	BT	69	ARG
28	BA	192	PHE
28	BA	290	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
28	BA	212	GLN
33	BE	92	HIS
50	BV	88	HIS
31	B6	52	HIS
31	B6	229	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1541/1542 (99%)	273 (17%)	0
2	AX	10/11 (90%)	5 (50%)	0
26	B7	119/120 (99%)	19 (15%)	0
27	B8	2903/2904 (99%)	442 (15%)	0
3	AV	76/77 (98%)	14 (18%)	0
All	All	4649/4654 (99%)	753 (16%)	0

5 of 753 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	5	U
1	AA	7	A
1	AA	9	G
1	AA	15	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

133 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	A0	301	-	48,48,48	0.78	1 (2%)	50,53,53	0.69	2 (4%)
60	PEV	A0	302	-	48,48,48	0.78	2 (4%)	50,53,53	0.70	2 (4%)
60	PEV	A0	303	-	48,48,48	0.80	2 (4%)	50,53,53	0.70	2 (4%)
61	PGV	A0	304	-	50,50,50	1.09	3 (6%)	51,56,56	0.87	2 (3%)
61	PGV	A0	305	-	50,50,50	1.07	2 (4%)	51,56,56	0.79	2 (3%)
61	PGV	A0	306	-	50,50,50	1.08	2 (4%)	51,56,56	0.81	2 (3%)
60	PEV	A0	307	-	48,48,48	0.77	1 (2%)	50,53,53	0.65	2 (4%)
60	PEV	A0	308	-	48,48,48	0.79	2 (4%)	50,53,53	0.75	2 (4%)
60	PEV	A0	309	-	48,48,48	0.80	2 (4%)	50,53,53	0.69	2 (4%)
60	PEV	A0	310	-	48,48,48	0.79	2 (4%)	50,53,53	0.84	2 (4%)
60	PEV	A0	311	-	48,48,48	0.78	1 (2%)	50,53,53	0.67	2 (4%)
60	PEV	A0	312	-	48,48,48	0.79	1 (2%)	50,53,53	0.61	2 (4%)
60	PEV	A0	313	-	48,48,48	0.81	2 (4%)	50,53,53	0.74	2 (4%)
60	PEV	A0	314	-	48,48,48	0.80	2 (4%)	50,53,53	0.70	2 (4%)
60	PEV	A0	315	-	48,48,48	0.76	1 (2%)	50,53,53	0.64	2 (4%)
60	PEV	A0	316	-	48,48,48	0.80	1 (2%)	50,53,53	0.84	2 (4%)
61	PGV	A0	317	-	50,50,50	1.08	2 (4%)	51,56,56	0.90	2 (3%)
61	PGV	A0	318	-	50,50,50	1.09	2 (4%)	51,56,56	0.80	2 (3%)
60	PEV	A0	319	-	48,48,48	0.79	1 (2%)	50,53,53	0.74	2 (4%)
60	PEV	A0	320	-	48,48,48	0.80	1 (2%)	50,53,53	0.65	2 (4%)
60	PEV	A0	321	-	48,48,48	0.79	1 (2%)	50,53,53	0.83	4 (8%)
60	PEV	A0	322	-	48,48,48	0.79	1 (2%)	50,53,53	0.75	2 (4%)
60	PEV	A0	323	-	48,48,48	0.77	1 (2%)	50,53,53	0.71	2 (4%)
60	PEV	A0	324	-	48,48,48	0.79	2 (4%)	50,53,53	0.71	2 (4%)
61	PGV	A0	325	-	50,50,50	1.09	2 (4%)	51,56,56	0.92	2 (3%)
60	PEV	A0	326	-	48,48,48	0.76	1 (2%)	50,53,53	0.71	2 (4%)
61	PGV	A0	327	-	50,50,50	1.10	2 (4%)	51,56,56	0.77	2 (3%)
61	PGV	A0	328	-	50,50,50	1.08	2 (4%)	51,56,56	0.82	2 (3%)
60	PEV	A0	329	-	48,48,48	0.78	1 (2%)	50,53,53	0.72	2 (4%)
60	PEV	A0	330	-	48,48,48	0.78	1 (2%)	50,53,53	0.66	2 (4%)
61	PGV	A0	331	-	50,50,50	1.07	2 (4%)	51,56,56	0.83	2 (3%)
61	PGV	A0	332	-	50,50,50	1.09	2 (4%)	51,56,56	0.82	2 (3%)
60	PEV	A1	301	-	48,48,48	0.78	2 (4%)	50,53,53	0.72	2 (4%)
60	PEV	A1	302	-	48,48,48	0.79	2 (4%)	50,53,53	0.72	2 (4%)
61	PGV	A1	303	-	50,50,50	1.08	2 (4%)	51,56,56	0.81	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	A1	304	-	48,48,48	0.77	1 (2%)	50,53,53	0.63	2 (4%)
60	PEV	A1	305	-	48,48,48	0.78	1 (2%)	50,53,53	0.69	2 (4%)
60	PEV	A1	306	-	48,48,48	0.79	1 (2%)	50,53,53	0.63	2 (4%)
60	PEV	A1	307	-	48,48,48	0.78	1 (2%)	50,53,53	0.69	2 (4%)
60	PEV	A1	308	-	48,48,48	0.80	2 (4%)	50,53,53	0.65	2 (4%)
60	PEV	A1	309	-	48,48,48	0.78	2 (4%)	50,53,53	0.74	2 (4%)
60	PEV	A1	310	-	48,48,48	0.77	2 (4%)	50,53,53	0.73	2 (4%)
61	PGV	A1	311	-	50,50,50	1.09	2 (4%)	51,56,56	0.87	2 (3%)
60	PEV	A1	312	-	48,48,48	0.78	2 (4%)	50,53,53	0.68	2 (4%)
60	PEV	A1	313	-	48,48,48	0.77	1 (2%)	50,53,53	0.73	2 (4%)
60	PEV	A1	314	-	48,48,48	0.78	1 (2%)	50,53,53	0.70	2 (4%)
61	PGV	A1	315	-	50,50,50	1.10	4 (8%)	51,56,56	0.86	2 (3%)
60	PEV	A1	316	-	48,48,48	0.78	2 (4%)	50,53,53	0.75	2 (4%)
60	PEV	A1	317	-	48,48,48	0.79	2 (4%)	50,53,53	0.70	3 (6%)
61	PGV	A1	318	-	50,50,50	1.09	2 (4%)	51,56,56	0.85	2 (3%)
60	PEV	A1	319	-	48,48,48	0.78	1 (2%)	50,53,53	0.66	1 (2%)
60	PEV	A1	320	-	48,48,48	0.79	2 (4%)	50,53,53	0.71	2 (4%)
60	PEV	A1	321	-	48,48,48	0.79	1 (2%)	50,53,53	0.68	2 (4%)
60	PEV	A1	322	-	48,48,48	0.76	1 (2%)	50,53,53	0.70	2 (4%)
60	PEV	A1	323	-	48,48,48	0.76	1 (2%)	50,53,53	0.67	2 (4%)
60	PEV	A1	324	-	48,48,48	0.79	1 (2%)	50,53,53	0.65	2 (4%)
60	PEV	A1	325	-	48,48,48	0.78	1 (2%)	50,53,53	0.66	2 (4%)
60	PEV	A1	326	-	48,48,48	0.77	1 (2%)	50,53,53	0.69	2 (4%)
60	PEV	A1	327	-	48,48,48	0.77	1 (2%)	50,53,53	0.68	2 (4%)
60	PEV	A1	328	-	48,48,48	0.76	1 (2%)	50,53,53	0.68	2 (4%)
60	PEV	A1	329	-	48,48,48	0.79	2 (4%)	50,53,53	0.72	2 (4%)
60	PEV	AZ	201	-	48,48,48	0.75	1 (2%)	50,53,53	0.70	2 (4%)
60	PEV	AZ	202	-	48,48,48	0.77	1 (2%)	50,53,53	0.72	2 (4%)
60	PEV	AZ	203	-	48,48,48	0.78	1 (2%)	50,53,53	0.62	2 (4%)
60	PEV	AZ	204	-	48,48,48	0.78	1 (2%)	50,53,53	0.68	2 (4%)
61	PGV	AZ	205	-	50,50,50	1.08	2 (4%)	51,56,56	0.82	2 (3%)
60	PEV	AZ	206	-	48,48,48	0.78	1 (2%)	50,53,53	0.62	2 (4%)
61	PGV	AZ	207	-	50,50,50	1.08	2 (4%)	51,56,56	0.81	2 (3%)
60	PEV	B8	3001	-	48,48,48	0.79	2 (4%)	50,53,53	0.72	2 (4%)
60	PEV	B8	3002	-	48,48,48	0.77	1 (2%)	50,53,53	0.66	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	B8	3003	-	48,48,48	0.79	1 (2%)	50,53,53	0.72	2 (4%)
60	PEV	B8	3004	-	48,48,48	0.78	1 (2%)	50,53,53	0.70	2 (4%)
61	PGV	B8	3005	-	50,50,50	1.08	2 (4%)	51,56,56	0.78	2 (3%)
60	PEV	B8	3006	-	48,48,48	0.79	1 (2%)	50,53,53	0.67	2 (4%)
60	PEV	B8	3007	-	48,48,48	0.77	1 (2%)	50,53,53	0.64	2 (4%)
61	PGV	BA	501	-	50,50,50	1.08	2 (4%)	51,56,56	0.87	2 (3%)
60	PEV	BA	502	-	48,48,48	0.77	1 (2%)	50,53,53	0.71	2 (4%)
60	PEV	BA	503	-	48,48,48	0.80	3 (6%)	50,53,53	0.74	2 (4%)
60	PEV	BA	504	-	48,48,48	0.79	2 (4%)	50,53,53	0.80	2 (4%)
61	PGV	BA	505	-	50,50,50	1.08	2 (4%)	51,56,56	0.83	2 (3%)
60	PEV	BA	506	-	48,48,48	0.74	1 (2%)	50,53,53	0.70	2 (4%)
60	PEV	BA	507	-	48,48,48	0.78	1 (2%)	50,53,53	0.69	2 (4%)
60	PEV	BA	508	-	48,48,48	0.78	1 (2%)	50,53,53	0.68	2 (4%)
60	PEV	BA	509	-	48,48,48	0.80	2 (4%)	50,53,53	0.75	2 (4%)
60	PEV	BA	510	-	48,48,48	0.77	1 (2%)	50,53,53	0.70	2 (4%)
60	PEV	BA	511	-	48,48,48	0.75	1 (2%)	50,53,53	0.70	2 (4%)
61	PGV	BA	512	-	50,50,50	1.07	2 (4%)	51,56,56	0.81	2 (3%)
60	PEV	BA	513	-	48,48,48	0.78	1 (2%)	50,53,53	0.69	2 (4%)
60	PEV	BA	514	-	48,48,48	0.80	2 (4%)	50,53,53	0.76	2 (4%)
61	PGV	BA	515	-	50,50,50	1.08	2 (4%)	51,56,56	0.80	2 (3%)
61	PGV	BA	516	-	50,50,50	1.09	2 (4%)	51,56,56	0.75	2 (3%)
60	PEV	BA	517	-	48,48,48	0.78	1 (2%)	50,53,53	0.69	2 (4%)
60	PEV	BA	518	-	48,48,48	0.77	1 (2%)	50,53,53	0.67	2 (4%)
60	PEV	BA	519	-	48,48,48	0.79	2 (4%)	50,53,53	0.74	2 (4%)
60	PEV	BA	520	-	48,48,48	0.78	1 (2%)	50,53,53	0.64	2 (4%)
60	PEV	BA	521	-	48,48,48	0.78	2 (4%)	50,53,53	0.67	2 (4%)
61	PGV	BA	522	-	50,50,50	1.09	2 (4%)	51,56,56	0.76	2 (3%)
60	PEV	BA	523	-	48,48,48	0.78	1 (2%)	50,53,53	0.74	2 (4%)
60	PEV	BA	524	-	48,48,48	0.80	2 (4%)	50,53,53	0.71	2 (4%)
60	PEV	BA	525	-	48,48,48	0.79	2 (4%)	50,53,53	0.75	2 (4%)
60	PEV	BA	526	-	48,48,48	0.77	1 (2%)	50,53,53	0.69	2 (4%)
60	PEV	BA	527	-	48,48,48	0.79	1 (2%)	50,53,53	0.76	2 (4%)
60	PEV	BA	528	-	48,48,48	0.78	1 (2%)	50,53,53	0.72	2 (4%)
60	PEV	BA	529	-	48,48,48	0.80	2 (4%)	50,53,53	0.70	2 (4%)
60	PEV	BA	530	-	48,48,48	0.78	1 (2%)	50,53,53	0.67	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PEV	BA	531	-	48,48,48	0.77	1 (2%)	50,53,53	0.66	2 (4%)
60	PEV	BA	532	-	48,48,48	0.76	1 (2%)	50,53,53	0.75	2 (4%)
60	PEV	BA	533	-	48,48,48	2.66	1 (2%)	50,53,53	1.32	2 (4%)
60	PEV	BA	534	-	48,48,48	0.82	3 (6%)	50,53,53	0.77	3 (6%)
60	PEV	BA	535	-	48,48,48	0.78	1 (2%)	50,53,53	0.67	2 (4%)
61	PGV	BA	536	-	50,50,50	1.08	2 (4%)	51,56,56	0.79	2 (3%)
60	PEV	BA	537	-	48,48,48	0.81	2 (4%)	50,53,53	0.75	2 (4%)
60	PEV	BA	538	-	48,48,48	0.75	1 (2%)	50,53,53	0.65	2 (4%)
60	PEV	BA	539	-	48,48,48	0.79	2 (4%)	50,53,53	0.80	2 (4%)
61	PGV	BA	540	-	50,50,50	1.07	2 (4%)	51,56,56	0.83	2 (3%)
60	PEV	BB	201	-	48,48,48	0.79	1 (2%)	50,53,53	0.70	2 (4%)
60	PEV	BB	202	-	48,48,48	0.78	2 (4%)	50,53,53	0.71	2 (4%)
61	PGV	BB	203	-	50,50,50	1.09	2 (4%)	51,56,56	0.83	2 (3%)
61	PGV	BB	204	-	50,50,50	1.09	3 (6%)	51,56,56	0.87	3 (5%)
61	PGV	BB	205	-	50,50,50	1.07	2 (4%)	51,56,56	0.87	2 (3%)
60	PEV	BB	206	-	48,48,48	0.78	1 (2%)	50,53,53	0.69	2 (4%)
61	PGV	BB	207	-	50,50,50	1.09	2 (4%)	51,56,56	0.83	2 (3%)
61	PGV	BB	208	-	50,50,50	1.09	2 (4%)	51,56,56	0.80	2 (3%)
60	PEV	BB	209	-	48,48,48	0.76	1 (2%)	50,53,53	0.69	2 (4%)
60	PEV	BB	210	-	48,48,48	0.77	1 (2%)	50,53,53	0.73	2 (4%)
60	PEV	BB	211	-	48,48,48	0.77	1 (2%)	50,53,53	0.72	2 (4%)
60	PEV	BB	212	-	48,48,48	0.78	1 (2%)	50,53,53	0.66	2 (4%)
61	PGV	BB	213	-	50,50,50	1.09	2 (4%)	51,56,56	0.86	2 (3%)
60	PEV	BB	214	-	48,48,48	0.78	1 (2%)	50,53,53	0.71	2 (4%)
60	PEV	BB	215	-	48,48,48	0.77	1 (2%)	50,53,53	0.70	2 (4%)
60	PEV	BB	216	-	48,48,48	0.78	2 (4%)	50,53,53	0.78	2 (4%)
61	PGV	BB	217	-	50,50,50	1.08	2 (4%)	51,56,56	0.82	2 (3%)
60	PEV	BB	218	-	48,48,48	0.77	1 (2%)	50,53,53	0.71	2 (4%)

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
60	PEV	A0	301	-	-	0/52/52/52	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	A0	302	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	303	-	-	0/52/52/52	0/0/0/0
61	PGV	A0	304	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	A0	305	-	1/1/5/7	0/55/55/55	0/0/0/0
61	PGV	A0	306	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A0	307	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	308	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A0	309	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	310	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	311	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	312	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	313	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	314	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A0	315	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	316	-	-	0/52/52/52	0/0/0/0
61	PGV	A0	317	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	A0	318	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A0	319	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	320	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	321	-	-	2/52/52/52	0/0/0/0
60	PEV	A0	322	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	323	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A0	324	-	-	0/52/52/52	0/0/0/0
61	PGV	A0	325	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A0	326	-	-	0/52/52/52	0/0/0/0
61	PGV	A0	327	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	A0	328	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A0	329	-	-	0/52/52/52	0/0/0/0
60	PEV	A0	330	-	-	0/52/52/52	0/0/0/0
61	PGV	A0	331	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	A0	332	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A1	301	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A1	302	-	-	0/52/52/52	0/0/0/0
61	PGV	A1	303	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A1	304	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	305	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A1	306	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	307	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	308	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	309	-	-	0/52/52/52	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	A1	310	-	-	0/52/52/52	0/0/0/0
61	PGV	A1	311	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A1	312	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	313	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	A1	314	-	-	0/52/52/52	0/0/0/0
61	PGV	A1	315	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A1	316	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	317	-	1/1/4/4	0/52/52/52	0/0/0/0
61	PGV	A1	318	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	A1	319	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	320	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	321	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	322	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	323	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	324	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	325	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	326	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	327	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	328	-	-	0/52/52/52	0/0/0/0
60	PEV	A1	329	-	-	0/52/52/52	0/0/0/0
60	PEV	AZ	201	-	-	0/52/52/52	0/0/0/0
60	PEV	AZ	202	-	-	0/52/52/52	0/0/0/0
60	PEV	AZ	203	-	-	0/52/52/52	0/0/0/0
60	PEV	AZ	204	-	1/1/4/4	0/52/52/52	0/0/0/0
61	PGV	AZ	205	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	AZ	206	-	-	0/52/52/52	0/0/0/0
61	PGV	AZ	207	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	B8	3001	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	B8	3002	-	-	0/52/52/52	0/0/0/0
60	PEV	B8	3003	-	-	0/52/52/52	0/0/0/0
60	PEV	B8	3004	-	-	0/52/52/52	0/0/0/0
61	PGV	B8	3005	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	B8	3006	-	-	0/52/52/52	0/0/0/0
60	PEV	B8	3007	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	501	-	1/1/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	502	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	503	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	504	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	505	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	506	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	507	-	-	0/52/52/52	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PEV	BA	508	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	509	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	510	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	511	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	512	-	1/1/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	513	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	514	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	515	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	BA	516	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	517	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	518	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	519	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	520	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	521	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	522	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	523	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	524	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	525	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	526	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	527	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	528	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	529	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	530	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	531	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	532	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	533	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	534	-	-	0/52/52/52	0/0/0/0
60	PEV	BA	535	-	1/1/4/4	0/52/52/52	0/0/0/0
61	PGV	BA	536	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BA	537	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	538	-	1/1/4/4	0/52/52/52	0/0/0/0
60	PEV	BA	539	-	-	0/52/52/52	0/0/0/0
61	PGV	BA	540	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BB	201	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	202	-	1/1/4/4	0/52/52/52	0/0/0/0
61	PGV	BB	203	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	BB	204	-	2/2/5/7	0/55/55/55	0/0/0/0
61	PGV	BB	205	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BB	206	-	1/1/4/4	0/52/52/52	0/0/0/0
61	PGV	BB	207	-	2/2/5/7	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PGV	BB	208	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BB	209	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	210	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	211	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	212	-	-	0/52/52/52	0/0/0/0
61	PGV	BB	213	-	1/1/5/7	0/55/55/55	0/0/0/0
60	PEV	BB	214	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	215	-	-	0/52/52/52	0/0/0/0
60	PEV	BB	216	-	-	0/52/52/52	0/0/0/0
61	PGV	BB	217	-	2/2/5/7	0/55/55/55	0/0/0/0
60	PEV	BB	218	-	-	0/52/52/52	0/0/0/0

The worst 5 of 204 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BA	516	PGV	C9-C10	-4.69	1.34	1.52
61	BB	213	PGV	C9-C10	-4.67	1.34	1.52
61	BA	522	PGV	C9-C10	-4.63	1.34	1.52
61	A1	315	PGV	C9-C10	-4.62	1.34	1.52
61	BB	204	PGV	C9-C10	-4.62	1.34	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	BB	204	PGV	O01-C1-C2	-2.06	107.28	111.55
60	A1	317	PEV	O3-C3-C2	2.01	113.72	108.66
60	A0	321	PEV	O2-C31-C32	2.02	115.75	111.55
60	A1	304	PEV	C39-C40-C41	2.09	125.24	114.45
60	AZ	203	PEV	C38-C39-C40	2.10	125.25	114.45

5 of 78 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
60	A1	301	PEV	C2
61	BA	540	PGV	C05
61	BA	540	PGV	C02
61	A1	318	PGV	C05
61	A1	318	PGV	C02

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	A0	321	PEV	C2-O2-C31-O31
60	A0	321	PEV	C2-O2-C31-C32

There are no ring outliers.

17 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	A0	315	PEV	1	0
60	A1	301	PEV	1	0
60	A1	302	PEV	1	0
61	A1	303	PGV	1	0
61	A1	315	PGV	1	0
60	A1	319	PEV	1	0
60	A1	323	PEV	1	0
60	B8	3001	PEV	1	0
60	B8	3002	PEV	2	0
60	BA	503	PEV	1	0
61	BA	512	PGV	1	0
60	BA	513	PEV	1	0
60	BA	514	PEV	1	0
60	BA	520	PEV	1	0
60	BA	526	PEV	1	0
60	BA	531	PEV	1	0
60	BA	533	PEV	29	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.