



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 02:29 pm BST

PDB ID : 6BY1
Title : E. coli pH03H9 complex
Authors : Amiri, H.; Noller, H.F.
Deposited on : 2017-12-19
Resolution : 3.94 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

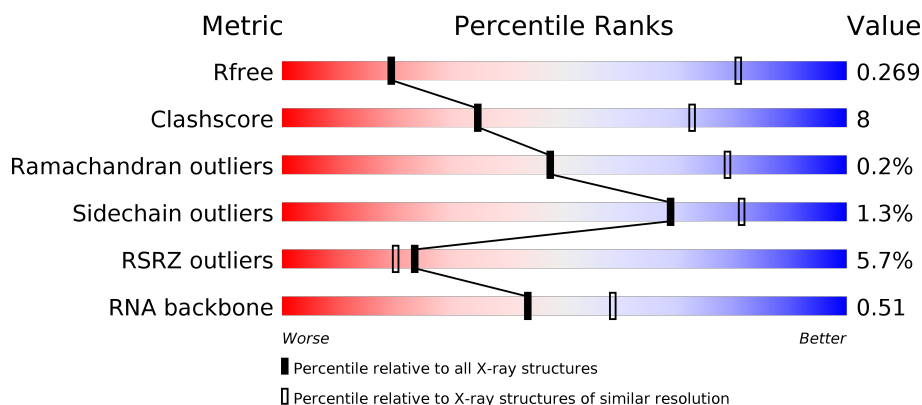
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 Å.

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



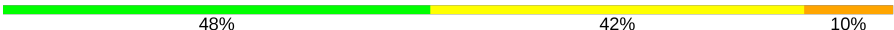

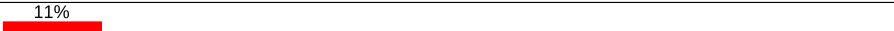
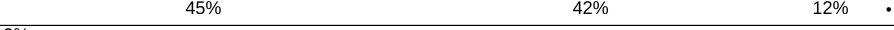



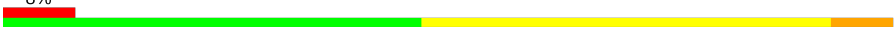
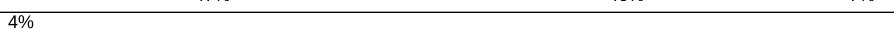


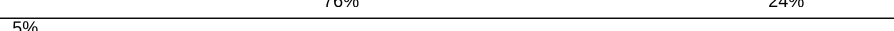




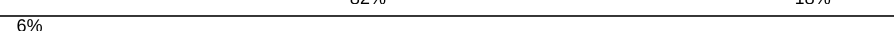








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)
RNA backbone	3102	1041 (4.84-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1541	<div> <div>45%</div> <div>44%</div> <div>10%</div> </div>
1	BA	1541	<div> <div>44%</div> <div>45%</div> <div>9%</div> </div>
2	CA	2904	<div> <div>52%</div> <div>39%</div> <div>8%</div> </div>
2	DA	2904	<div> <div>48%</div> <div>42%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
3	CB	118	
3	DB	118	
4	AV	76	
4	AW	76	
4	AY	76	
4	BV	76	
4	BW	76	
5	CC	271	
5	DC	271	
6	CD	209	
6	DD	209	
7	CE	181	
7	DE	181	
8	CF	177	
8	DF	177	
9	CG	176	
9	DG	176	
10	CH	149	
10	DH	149	
11	C5	109	
12	CI	72	
12	DI	72	
13	CJ	142	
13	DJ	142	
14	CK	122	

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Mol	Chain	Length	Quality of chain
14	DK	122	
15	CL	143	
15	DL	143	
16	CM	136	
16	DM	136	
17	CN	121	
17	DN	121	
18	CO	116	
18	DO	116	
19	CP	114	
19	DP	114	
20	CQ	117	
20	DQ	117	
21	CR	103	
21	DR	103	
22	CS	110	
22	DS	110	
23	CT	93	
23	DT	93	
24	CU	102	
24	DU	102	
25	CV	94	
25	DV	94	
26	CW	75	
26	DW	75	

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Mol	Chain	Length	Quality of chain
27	CX	77	<div> <div>4%</div> <div>86%</div> <div>13%</div> </div>
27	DX	77	<div> <div>5%</div> <div>81%</div> <div>19%</div> </div>
28	CY	63	<div> <div>87%</div> <div>10%</div> </div>
28	DY	63	<div> <div>5%</div> <div>76%</div> <div>24%</div> </div>
29	CZ	58	<div> <div>3%</div> <div>76%</div> <div>22%</div> </div>
29	DZ	58	<div> <div>9%</div> <div>81%</div> <div>19%</div> </div>
30	C0	39	<div> <div>15%</div> <div>69%</div> <div>31%</div> </div>
30	D0	39	<div> <div>26%</div> <div>59%</div> <div>36%</div> <div>5%</div> </div>
31	C1	56	<div> <div>82%</div> <div>18%</div> </div>
31	D1	56	<div> <div>79%</div> <div>21%</div> </div>
32	C2	50	<div> <div>62%</div> <div>78%</div> <div>22%</div> </div>
32	D2	50	<div> <div>78%</div> <div>80%</div> <div>20%</div> </div>
33	C3	46	<div> <div>80%</div> <div>20%</div> </div>
33	D3	46	<div> <div>76%</div> <div>22%</div> </div>
34	C4	62	<div> <div>19%</div> <div>79%</div> <div>19%</div> </div>
34	D4	62	<div> <div>39%</div> <div>77%</div> <div>23%</div> </div>
35	C6	38	<div> <div>68%</div> <div>32%</div> </div>
35	D6	38	<div> <div>34%</div> <div>55%</div> <div>45%</div> </div>
36	AX	46	<div> <div>33%</div> <div>26%</div> <div>33%</div> <div>7%</div> <div>35%</div> </div>
36	BX	46	<div> <div>37%</div> <div>33%</div> <div>30%</div> <div>35%</div> </div>
37	AB	225	<div> <div>12%</div> <div>83%</div> <div>17%</div> </div>
37	BB	225	<div> <div>7%</div> <div>80%</div> <div>19%</div> </div>
38	AC	206	<div> <div>%</div> <div>83%</div> <div>15%</div> </div>
38	BC	206	<div> <div>10%</div> <div>74%</div> <div>25%</div> </div>
39	AD	205	<div> <div>12%</div> <div>73%</div> <div>26%</div> </div>

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Mol	Chain	Length	Quality of chain
39	BD	205	
40	AE	150	
40	BE	150	
41	AF	100	
41	BF	100	
42	AG	179	
42	BG	179	
43	AH	129	
43	BH	129	
44	AI	130	
44	BI	130	
45	AJ	98	
45	BJ	98	
46	AK	117	
46	BK	117	
47	AL	123	
47	BL	123	
48	AM	114	
48	BM	114	
49	AN	101	
49	BN	101	
50	AO	89	
50	BO	89	
51	AP	82	
51	BP	82	

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Mol	Chain	Length	Quality of chain
52	AQ	80	
52	BQ	80	
53	AR	55	
53	BR	55	
54	AS	79	
54	BS	79	
55	AT	85	
55	BT	85	

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
56	MG	AA	1640	-	-	-	X
56	MG	AA	1644	-	-	-	X
56	MG	BA	1608	-	-	-	X
56	MG	BA	1620	-	-	-	X
56	MG	BA	1628	-	-	-	X
56	MG	CA	3068	-	-	-	X
56	MG	DA	3094	-	-	-	X

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 296390 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1540	Total	C	N	O	P	0	1	0
			33037	14735	6057	10705	1540			
1	BA	1541	Total	C	N	O	P	0	0	0
			33057	14744	6059	10713	1541			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CA	2867	Total	C	N	O	P	0	0	0
			61550	27457	11328	19898	2867			
2	DA	2869	Total	C	N	O	P	0	0	0
			61593	27477	11339	19908	2869			

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
3	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 4 is a RNA chain called Valine-specific transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AV	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			
4	AY	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			
4	AW	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			
4	BV	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	BW	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	CC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
5	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
6	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	CE	181	Total	C	N	O	S	0	0	0
			1404	881	261	258	4			
7	DE	180	Total	C	N	O	S	0	0	0
			1393	875	257	257	4			

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	CF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
8	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
9	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
10	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	C5	109	Total	C	N	O	S	0	0	0
			825	521	149	151	4			

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	CI	71	Total	C	N	O	S	0	0	0
			511	313	93	102	3			
12	DI	72	Total	C	N	O	S	0	0	0
			518	317	94	104	3			

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	CJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
13	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	CK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
14	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	CL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	CM	135	Total	C	N	O	S	0	0	0
			1065	681	204	175	5			
16	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	CN	121	Total	C	N	O	S	0	0	0
			969	599	198	167	5			
17	DN	121	Total	C	N	O	S	0	0	0
			969	599	198	167	5			

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	CO	116	Total	C	N	O		0	0	0
			892	552	178	162				
18	DO	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	CP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
19	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	CQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
20	DQ	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
21	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	CS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
22	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	CT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
23	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	CU	102	Total	C	N	O	0	0	0
			780	492	146	142			
24	DU	102	Total	C	N	O	0	0	0
			780	492	146	142			

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	CV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
25	DV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CW	75	Total	C	N	O	S	0	0	0
			574	356	116	101	1			
26	DW	75	Total	C	N	O	S	0	0	0
			574	356	116	101	1			

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	CX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
27	DX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CY	61	Total	C	N	O	S	0	0	0
			499	308	97	92	2			
28	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
29	DZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	C0	39	Total	C	N	O	S	0	0	0
			293	179	52	57	5			
30	D0	39	Total	C	N	O	S	0	0	0
			293	179	52	57	5			

- Molecule 31 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	C1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	C2	50	Total	C	N	O		0	0	0
			410	263	75	72				
32	D2	50	Total	C	N	O		0	0	0
			410	263	75	72				

- Molecule 33 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	C3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
33	D3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 34 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	C4	61	Total	C	N	O	S	0	0	0
			479	306	102	69	2			
34	D4	62	Total	C	N	O	S	0	0	0
			486	311	103	70	2			

- Molecule 35 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	C6	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
35	D6	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 36 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AX	30	Total	C	N	O	P	0	0	0
			653	293	130	200	30			
36	BX	30	Total	C	N	O	P	0	0	0
			653	293	130	200	30			

- Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AB	225	Total	C	N	O	S	0	0	0
			1757	1111	315	323	8			
37	BB	225	Total	C	N	O	S	0	0	0
			1757	1111	315	323	8			

- Molecule 38 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
38	BC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			
40	BE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 41 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
41	BF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AG	135	Total	C	N	O	S	0	0	0
			1058	659	203	192	4			
42	BG	132	Total	C	N	O	S	0	0	0
			1035	644	200	187	4			

- Molecule 43 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AH	128	Total	C	N	O	S	0	0	0
			973	613	172	182	6			
43	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 44 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AI	124	Total	C	N	O	S	0	0	0
			995	619	199	174	3			
44	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			
45	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 46 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	AK	116	Total	C	N	O	S	0	0	0
			869	535	173	158	3			
46	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 47 is a protein called 30S ribosomal protein S12.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 48 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
48	BM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 49 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
49	BN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 50 is a protein called 30S ribosomal protein S15.

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

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
52	BQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
53	BR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
54	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
55	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DQ	1	Total	Mg	0	0
			1	1		
56	CN	2	Total	Mg	0	0
			2	2		
56	CA	167	Total	Mg	0	0
			167	167		
56	C4	1	Total	Mg	0	0
			1	1		
56	CB	3	Total	Mg	0	0
			3	3		
56	CC	1	Total	Mg	0	0
			1	1		
56	AA	50	Total	Mg	0	0
			50	50		
56	CQ	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DA	166	Total 166	Mg 166	0	0
56	BA	49	Total 49	Mg 49	0	0
56	DN	1	Total 1	Mg 1	0	0
56	DB	3	Total 3	Mg 3	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	D0	1	Total 1	Zn 1	0	0
57	C0	1	Total 1	Zn 1	0	0
57	D6	1	Total 1	Zn 1	0	0
57	C6	1	Total 1	Zn 1	0	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	481	Total 481	O 481	0	0
58	CA	1106	Total 1106	O 1106	0	0
58	CB	49	Total 49	O 49	0	0
58	AV	28	Total 28	O 28	0	0
58	AY	5	Total 5	O 5	0	0
58	CC	13	Total 13	O 13	0	0
58	CD	10	Total 10	O 10	0	0
58	CE	16	Total 16	O 16	0	0
58	CF	14	Total 14	O 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CG	18	Total 18	O 18	0	0
58	CH	8	Total 8	O 8	0	0
58	C5	7	Total 7	O 7	0	0
58	CI	4	Total 4	O 4	0	0
58	CJ	9	Total 9	O 9	0	0
58	CK	7	Total 7	O 7	0	0
58	CL	8	Total 8	O 8	0	0
58	CM	4	Total 4	O 4	0	0
58	CN	6	Total 6	O 6	0	0
58	CO	8	Total 8	O 8	0	0
58	CP	8	Total 8	O 8	0	0
58	CQ	2	Total 2	O 2	0	0
58	CR	7	Total 7	O 7	0	0
58	CS	3	Total 3	O 3	0	0
58	CT	7	Total 7	O 7	0	0
58	CU	13	Total 13	O 13	0	0
58	CV	10	Total 10	O 10	0	0
58	CW	4	Total 4	O 4	0	0
58	CX	3	Total 3	O 3	0	0
58	CY	3	Total 3	O 3	0	0
58	CZ	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	C1	5	Total 5	O 5	0	0
58	C2	1	Total 1	O 1	0	0
58	C3	2	Total 2	O 2	0	0
58	C4	2	Total 2	O 2	0	0
58	C6	3	Total 3	O 3	0	0
58	AX	4	Total 4	O 4	0	0
58	AW	32	Total 32	O 32	0	0
58	AB	7	Total 7	O 7	0	0
58	AC	15	Total 15	O 15	0	0
58	AD	10	Total 10	O 10	0	0
58	AE	12	Total 12	O 12	0	0
58	AF	6	Total 6	O 6	0	0
58	AG	5	Total 5	O 5	0	0
58	AH	7	Total 7	O 7	0	0
58	AI	6	Total 6	O 6	0	0
58	AJ	4	Total 4	O 4	0	0
58	AK	10	Total 10	O 10	0	0
58	AL	9	Total 9	O 9	0	0
58	AM	6	Total 6	O 6	0	0
58	AN	3	Total 3	O 3	0	0
58	AO	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AP	4	Total 4	O 4	0	0
58	AQ	8	Total 8	O 8	0	0
58	AR	1	Total 1	O 1	0	0
58	AS	4	Total 4	O 4	0	0
58	AT	4	Total 4	O 4	0	0
58	BA	461	Total 461	O 461	0	0
58	DA	1005	Total 1005	O 1005	0	0
58	DB	32	Total 32	O 32	0	0
58	BV	13	Total 13	O 13	0	0
58	DC	28	Total 28	O 28	0	0
58	DD	15	Total 15	O 15	0	0
58	DE	12	Total 12	O 12	0	0
58	DF	4	Total 4	O 4	0	0
58	DG	6	Total 6	O 6	0	0
58	DH	4	Total 4	O 4	0	0
58	DJ	3	Total 3	O 3	0	0
58	DK	5	Total 5	O 5	0	0
58	DL	10	Total 10	O 10	0	0
58	DM	6	Total 6	O 6	0	0
58	DN	6	Total 6	O 6	0	0
58	DO	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DP	6	Total 6	O 6	0	0
58	DQ	5	Total 5	O 5	0	0
58	DR	13	Total 13	O 13	0	0
58	DS	9	Total 9	O 9	0	0
58	DT	10	Total 10	O 10	0	0
58	DU	14	Total 14	O 14	0	0
58	DV	7	Total 7	O 7	0	0
58	DW	3	Total 3	O 3	0	0
58	DX	3	Total 3	O 3	0	0
58	DY	7	Total 7	O 7	0	0
58	DZ	2	Total 2	O 2	0	0
58	D0	2	Total 2	O 2	0	0
58	D1	11	Total 11	O 11	0	0
58	D2	2	Total 2	O 2	0	0
58	D3	2	Total 2	O 2	0	0
58	D6	1	Total 1	O 1	0	0
58	BX	5	Total 5	O 5	0	0
58	BW	23	Total 23	O 23	0	0
58	BB	2	Total 2	O 2	0	0
58	BC	8	Total 8	O 8	0	0
58	BD	24	Total 24	O 24	0	0

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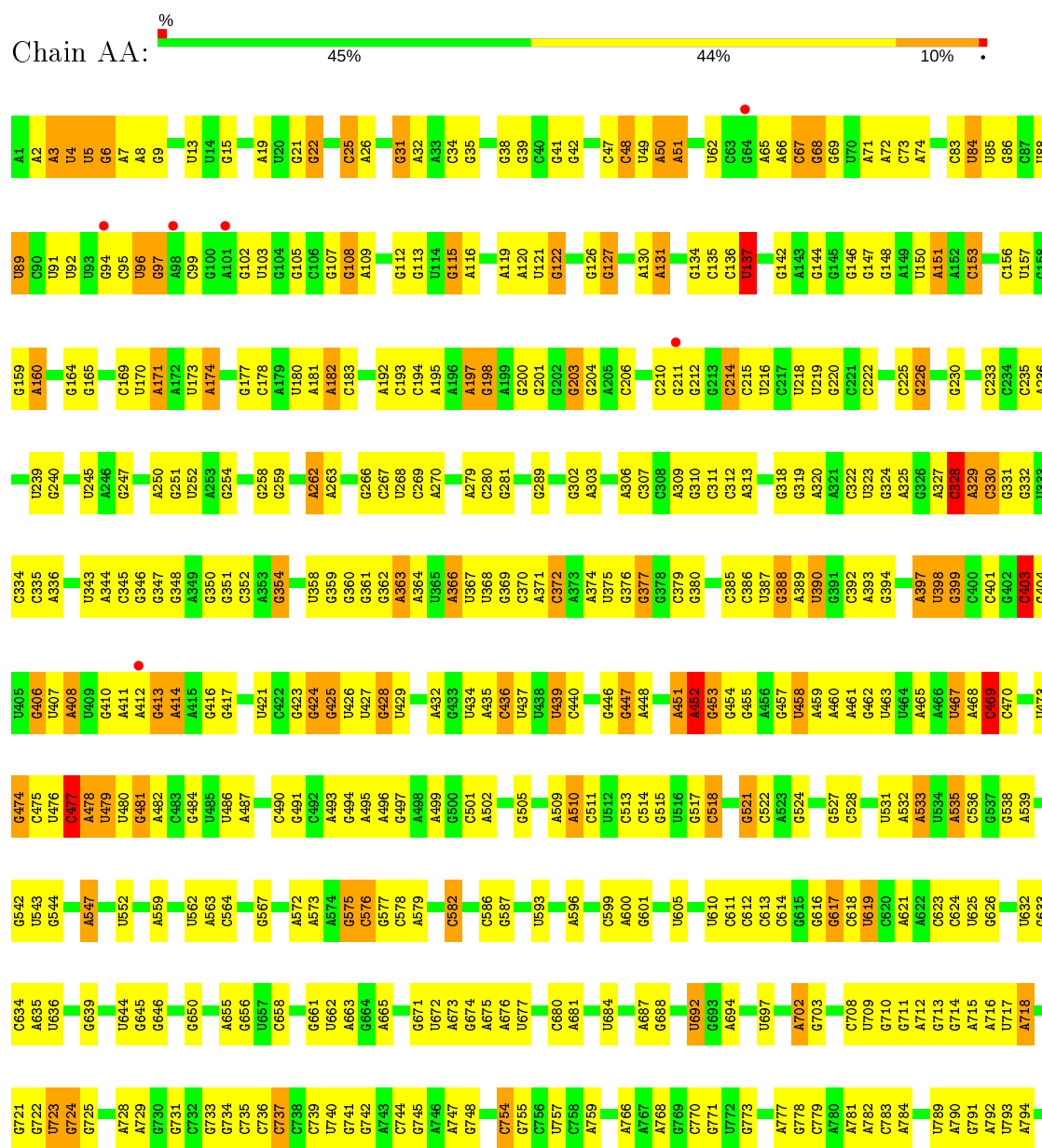
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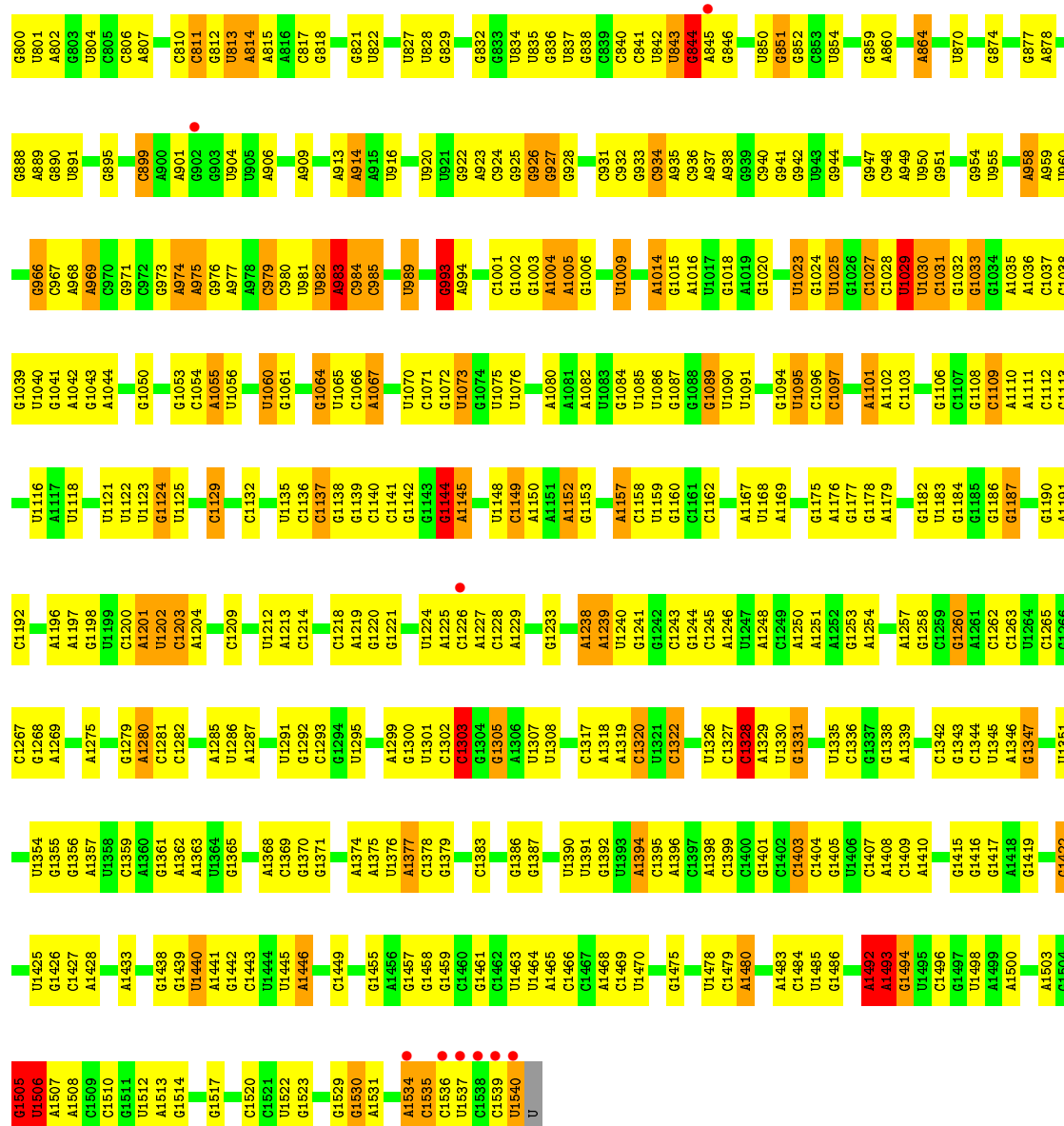
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BE	18	Total 18	O 18	0	0
58	BF	6	Total 6	O 6	0	0
58	BG	4	Total 4	O 4	0	0
58	BH	12	Total 12	O 12	0	0
58	BI	9	Total 9	O 9	0	0
58	BJ	8	Total 8	O 8	0	0
58	BK	5	Total 5	O 5	0	0
58	BL	8	Total 8	O 8	0	0
58	BM	6	Total 6	O 6	0	0
58	BN	5	Total 5	O 5	0	0
58	BO	2	Total 2	O 2	0	0
58	BP	5	Total 5	O 5	0	0
58	BQ	10	Total 10	O 10	0	0
58	BR	1	Total 1	O 1	0	0
58	BS	3	Total 3	O 3	0	0
58	BT	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

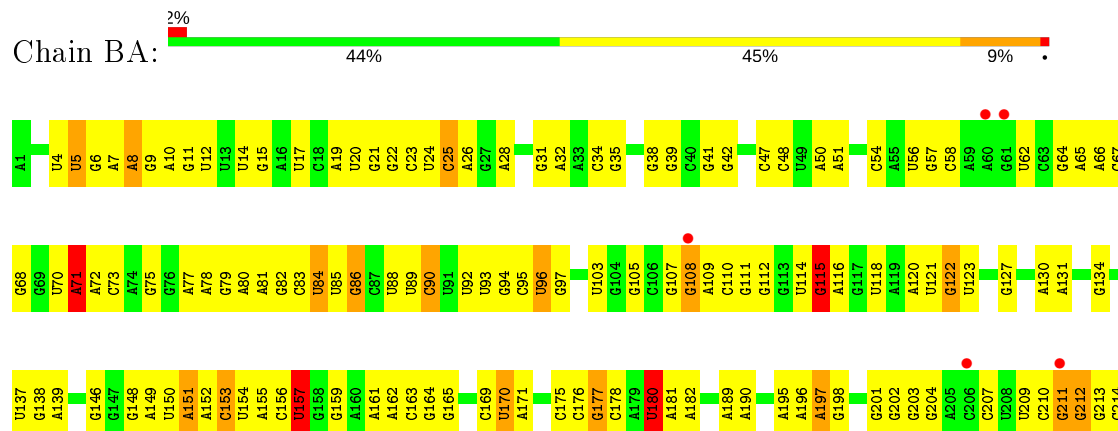
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S ribosomal RNA

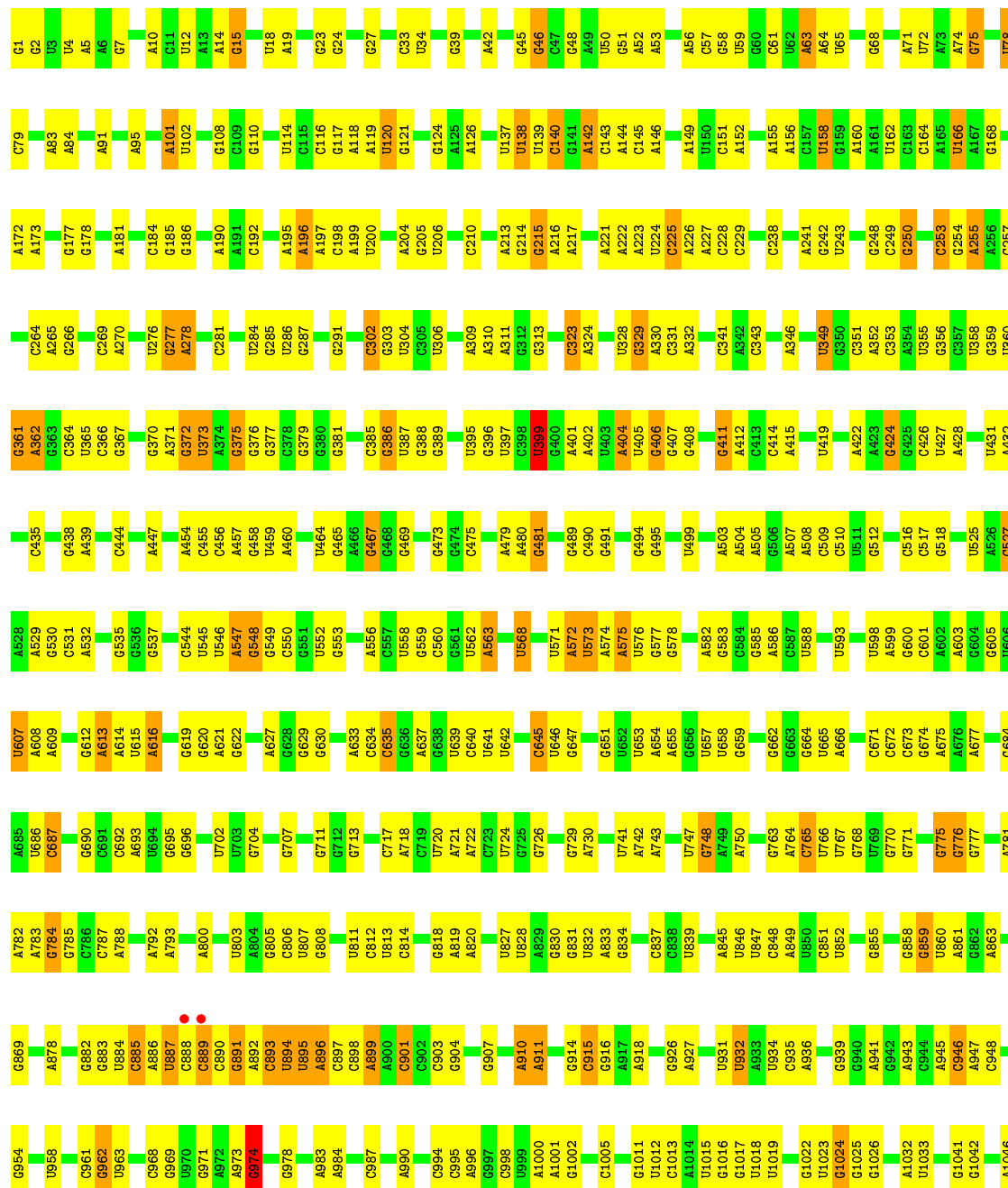




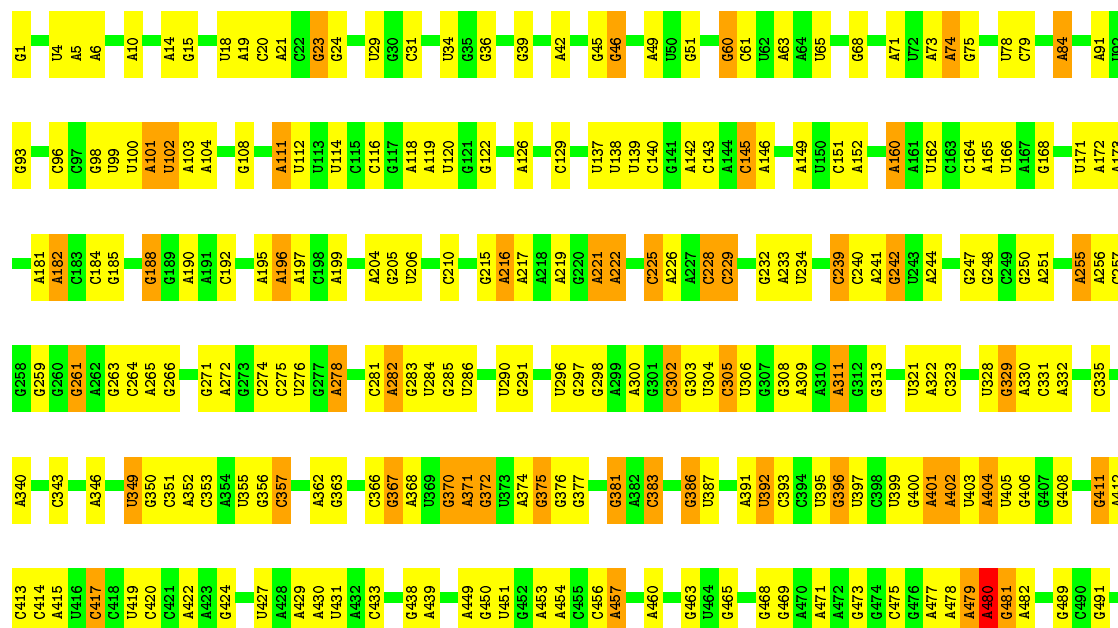
• Molecule 1: 16S ribosomal RNA



U1348	A1275	G1039	A988	G887	C806	G719	C632	C545	U464	A383	G299	C215
A1349	G1279	U1040	A969	G888	A907	G720	U632	A946	A465	G384	A300	U216
A1350	G1280	A1042	C970	A889	A907	G721	U633	A547	A466	U387	A306	C217
G1352	G1281	G1043	C972	U891	G809	G722	A635	U548	U467	U387	A306	U218
G1353	G1282	A1044	G973	A892	G809	G723	A635	C549	A468	A389	C311	U219
U1354	G1283	G1045	A974	G895	U813	G724	U639	G550	C469	U390	C321	C221
G1355	U1286	G1053	A975	G895	A814	A728	U639	U551	G474	G391	A315	C222
A1287	A1287	C1054	G976	G895	A815	A729	A642	U552	C475	C392	C316	A223
A1288	A1288	U1056	C979	G898	A816	G730	A643	A553	U476	A393	A321	G226
U1358	A1289	G1057	C980	A900	C817	G731	U644	C556	C477	G394	C322	G230
C1359	G1290	G1058	U981	A900	A818	G734	U647	A559	U478	C395	A325	U231
A1360	U1291	C1059	U982	U904	U820	C737	A648	A560	U480	C396	A325	G230
G1361	G1292	U1060	A983	U904	G821	C738	U652	U561	G481	A397	A325	U231
A1362	U1293	G1061	C984	A909	U822	C739	U652	A563	A482	U398	C328	C235
U1364	U1298	U1065	C985	A913	G823	C740	U652	C564	C483	C401	A329	A236
A1365	A1299	C1066	U989	A914	G824	U740	U664	A565	C484	G402	A329	G237
C1366	G1300	U1069	A915	A915	U827	G741	U665	U565	U485	C403	G332	A238
C1367	U1301	C1069	U916	A916	U828	G742	U666	A566	U486	G404	G335	A243
A1368	C1302	U1070	G983	A917	G829	A743	U667	A567	A487	U405	C335	U244
C1369	G1303	C1071	A994	A918	G829	G744	U668	A572	C488	G406	A336	U245
G1370	G1304	G1072	C995	A919	U837	G745	U672	A573	C489	U407	A344	A246
G1371	A1305	U1077	A996	U920	G836	A746	U673	A574	C490	G410	C345	G247
U1372	U1306	G1078	C999	U921	G837	A747	U674	A575	C491	A411	C346	C248
A1377	U1308	U1079	A922	G922	G838	G748	U676	C576	C492	G412	G347	U249
C1378	A1311	A1080	A923	A923	C941	U751	A676	A577	A495	G413	G348	U250
G1379	G1312	U1089	U918	G925	U843	C754	U682	C578	A496	U421	A349	G251
C1380	U1313	U1090	A1004	G926	G844	G755	U683	C580	C497	G423	G350	U252
C1383	G1314	U1086	A1005	G927	A845	C756	U686	C581	U498	G424	C351	A253
G1386	C1317	G1087	U1008	G928	G846	U757	U687	C582	A500	G425	C352	C254
G1387	A1318	U1089	U1009	G928	G847	C758	U688	C583	C501	U426	A353	G255
U1390	G1320	U1090	C1011	C931	G848	U762	C689	C585	A502	U427	C355	G258
C1391	U1321	U1095	A1012	C934	U850	G763	U692	C588	U428	U429	A356	G259
A1392	C1322	C1096	A1013	A938	G851	C764	U693	C589	A509	U432	U358	G260
C1393	G1323	C1097	A1016	G939	G852	G769	U694	C596	C511	A432	G359	U261
C1395	A1324	U1098	U1017	U942	U854	C770	A695	A596	C517	C436	C361	A262
A1396	G1327	A1101	G1020	G945	U855	G771	U697	A597	C518	U437	A362	C264
C1397	C1328	C1102	A1021	A946	G859	G776	U701	U598	C519	U438	A363	G265
A1398	A1256	C1103	A1022	G947	A860	A777	A702	C599	A520	U439	A364	C267
C1399	G1257	G1106	U1023	C948	G861	A781	G703	A600	G521	U447	U367	U268
U1400	G1258	C1107	G1024	A949	U861	A782	G703	G601	U524	U451	C370	C269
G1401	C1259	G1108	U1025	U950	A864	A782	U707	U605	A452	A452	A371	G275
G1402	G1260	C1109	G1027	G951	A865	G786	C708	G606	A453	C372	C372	A279
C1403	A1261	C1112	U1029	U952	G869	U793	U709	A607	G454	G454	C373	C280
C1404	U1335	U1115	U1030	G953	U870	A794	G710	C611	A532	G455	C373	G281
G1405	C1336	U1116	C1031	U957	U871	C795	A712	C618	A533	U458	G376	C284
C1407	G1337	A1197	G1032	U957	C876	C796	G713	U619	C536	A459	G377	C284
A1408	U1266	A1197	G1033	A958	G877	G799	A715	C620	A460	C378	G378	G289
C1409	C1342	U1117	G1034	U959	G881	G800	U716	A621	A461	G380	C379	C289
C1410	G1343	U1118	A1035	U960	C882	U801	A717	C624	G462	C381	G380	U296
G1411	U1344	G1124	A1036	U965	C882	A802	A718				A382	
C1412	U1345	U1125	G1037	U965	C882							
A1413	A1346	U1126	C1038	U965	C882							
U1414	G1347											



G2162	A2101	U2022	U1926	C1833	A1744	A1854	A1570	G1483	U1390	G1300	G1221	G1125	G1047
A2163	G2102	C2023	A1927	C1837	G1753	G1860	A1571	A1490	U1391	A1301	U1222	A1126	A1057
C	C2103	G2024	A1928	C	A1754	G1860	A1572	G1491	A1392	A1302	G1223	A1129	U1060
U	C2104	C2025	G1929	C1843	A1759	A1665	U1576	C1492	A1393	C1306	U1224	U1130	U1061
U	U2105	U2028	U1931	G1845	C1760	G1666	C1577	C1493	A1394	U1309	A1225	G1131	G1062
U	U2106	G2029	G	G1846	C1761	G1667	G1581	A1496	A1395	G1310	A1226	U1132	G1063
G	U2107	A2030	A1936	G1847	A1762	G1667	C1582	C1499	U1396	U1231	G1227	A1133	U1064
A	A2108	A2031	A1937	G1848	C1764	G1672	C1583	C1499	U1397	G1312	U1232	A1134	U1065
A	U2109	A2032	A1938	G1849	C1765	G1673	U1584	C1500	C1398	U1313	G	U1066	U1066
U	G2110	A2033	U1939	A1847	C1766	G1674	C1585	G1501	A1403	C1314	G1235	G1139	A1067
G	U	U2034	U1940	U1854	A1773	G1675	C1586	A1504	U1406	C1315	G	U1068	A1068
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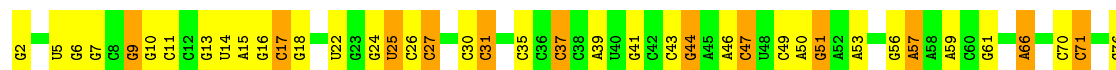




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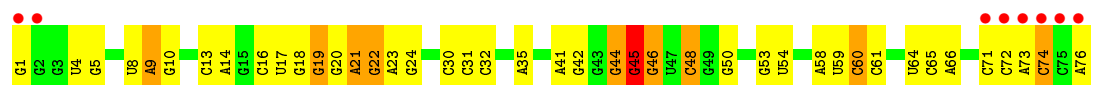
- Molecule 3: 5S ribosomal RNA



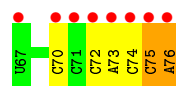
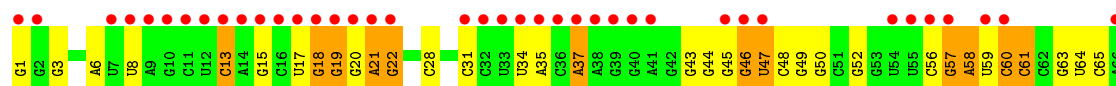
- Molecule 3: 5S ribosomal RNA



- Molecule 4: Valine-specific transfer RNA



- Molecule 4: Valine-specific transfer RNA



- Molecule 4: Valine-specific transfer RNA



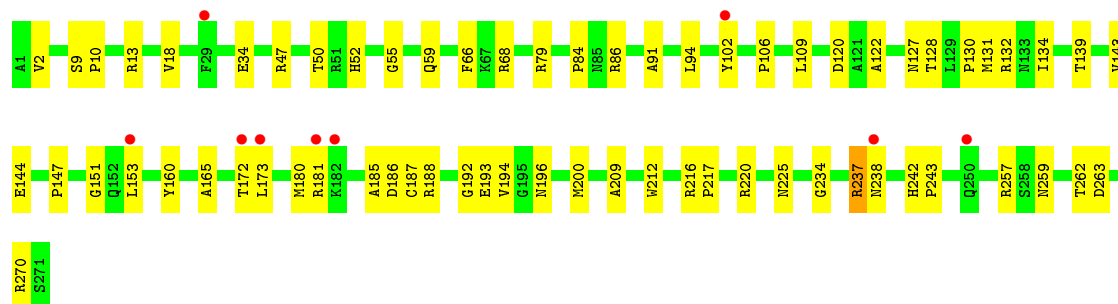
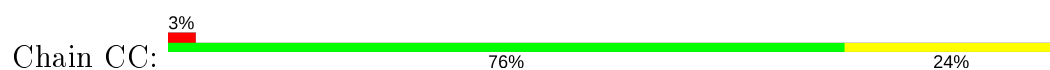
- Molecule 4: Valine-specific transfer RNA



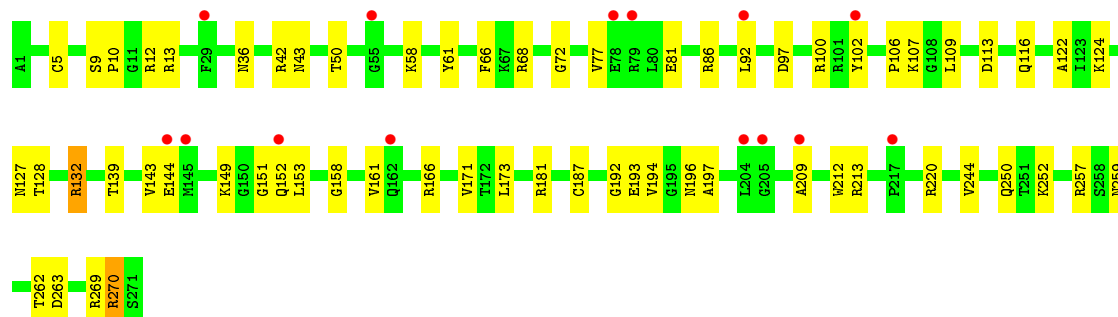
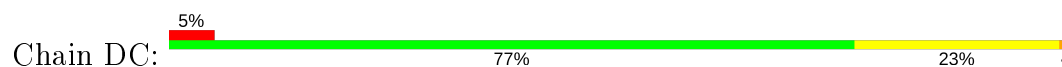
• Molecule 4: Valine-specific transfer RNA



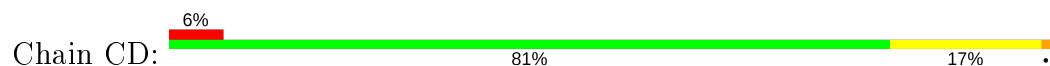
• Molecule 5: 50S ribosomal protein L2

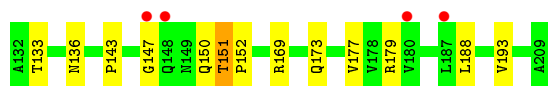


• Molecule 5: 50S ribosomal protein L2

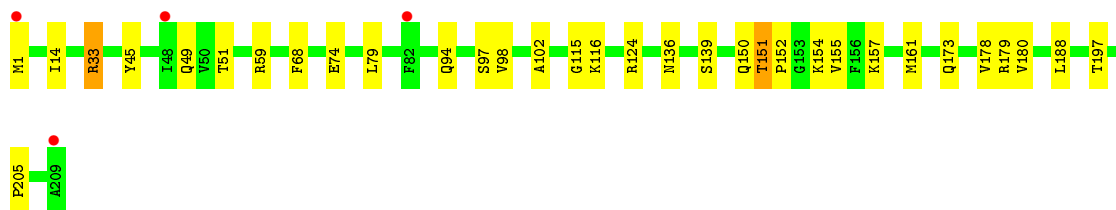
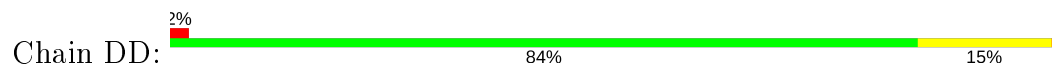


• Molecule 6: 50S ribosomal protein L3

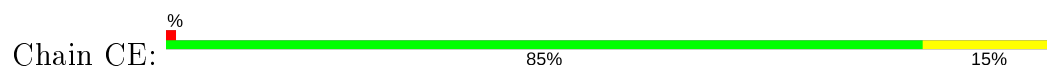




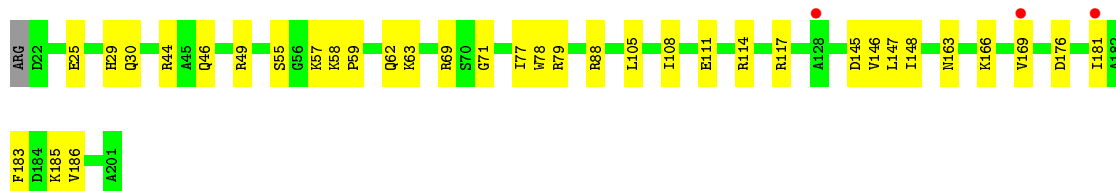
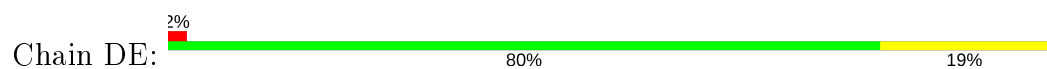
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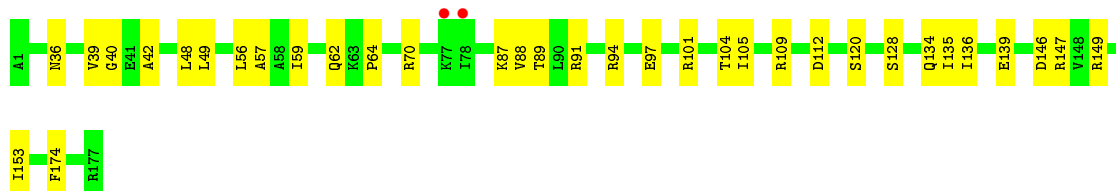
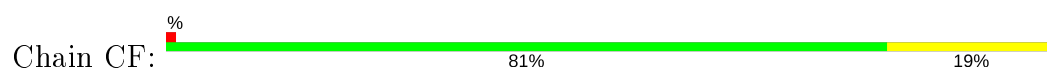
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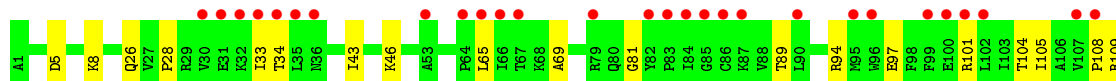
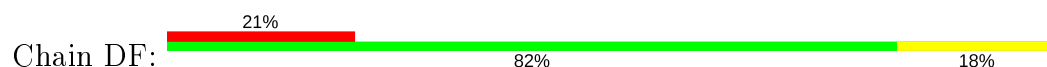
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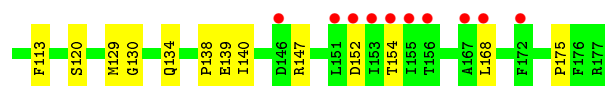


- Molecule 8: 50S ribosomal protein L5

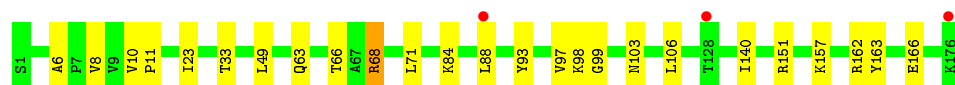
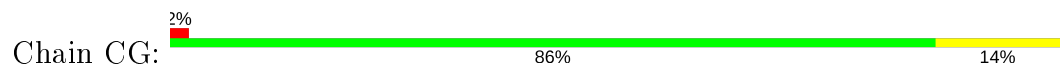


- Molecule 8: 50S ribosomal protein L5

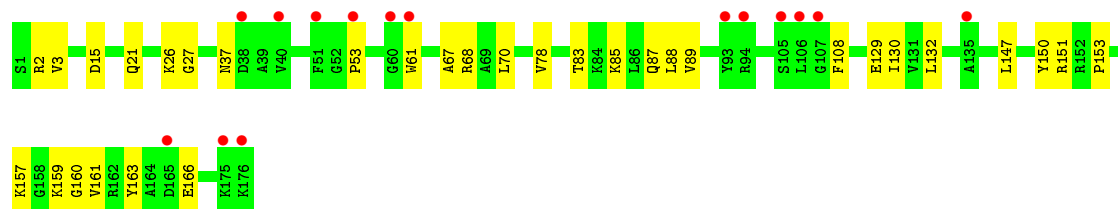
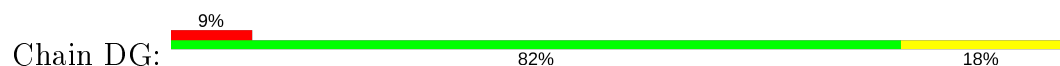




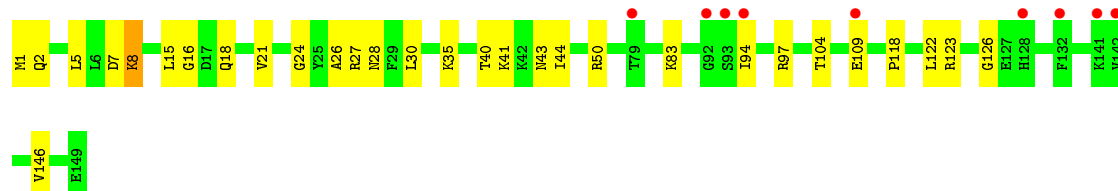
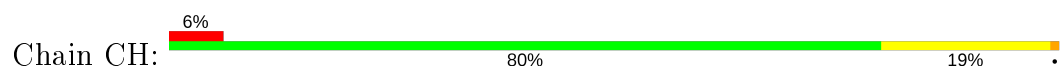
- Molecule 9: 50S ribosomal protein L6



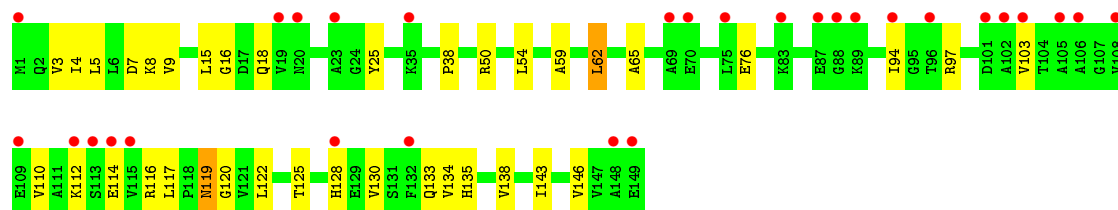
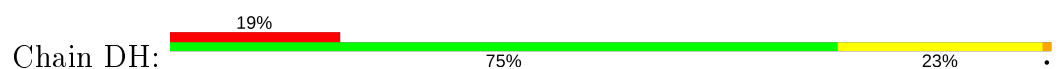
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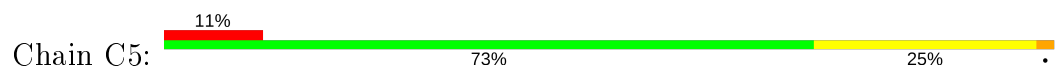
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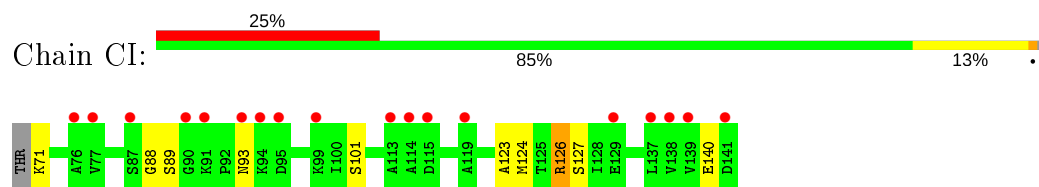
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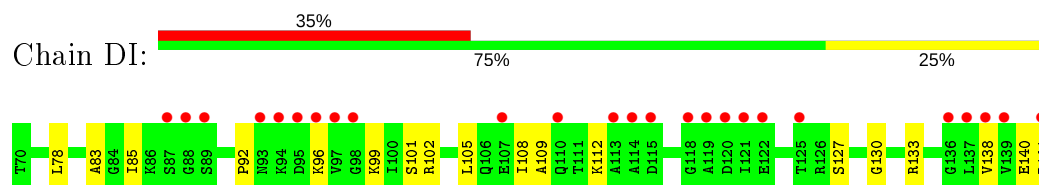
- Molecule 11: 50S ribosomal protein L10



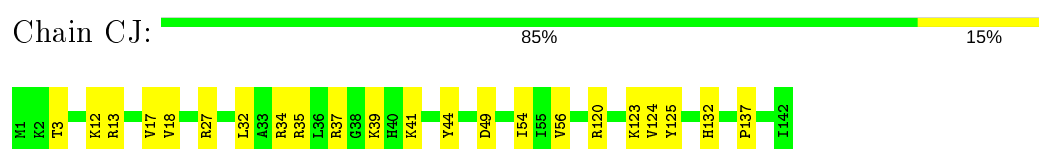
- Molecule 12: 50S ribosomal protein L11



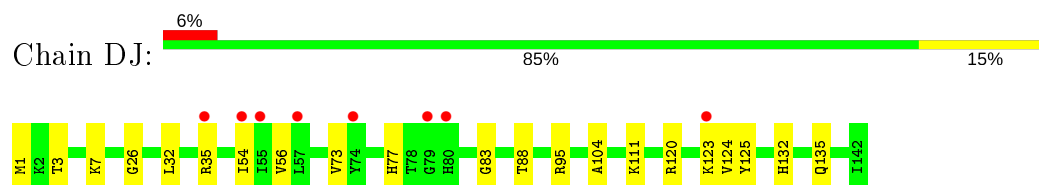
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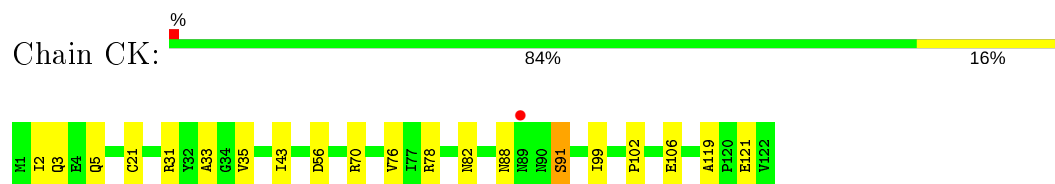
- Molecule 13: 50S ribosomal protein L13



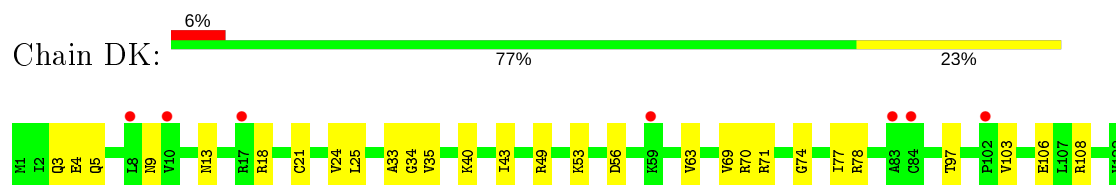
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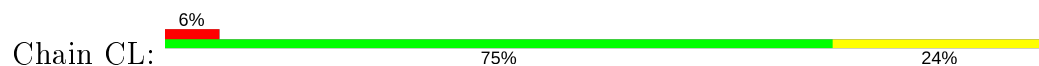
- Molecule 14: 50S ribosomal protein L14

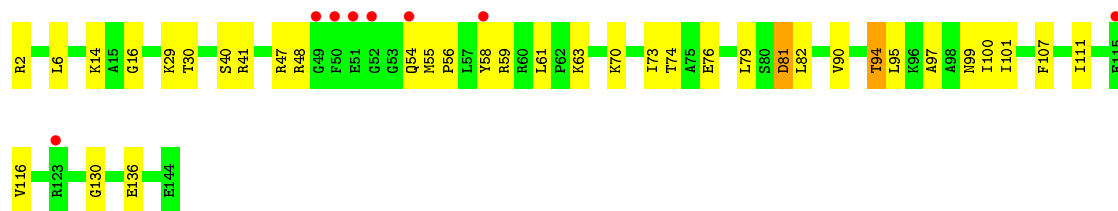


- Molecule 14: 50S ribosomal protein L14

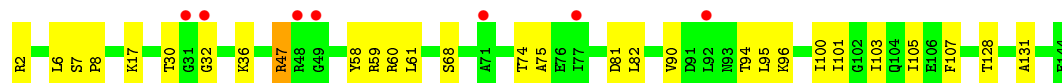
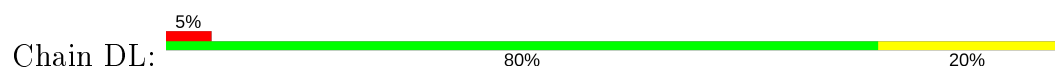


- Molecule 15: 50S ribosomal protein L15





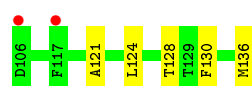
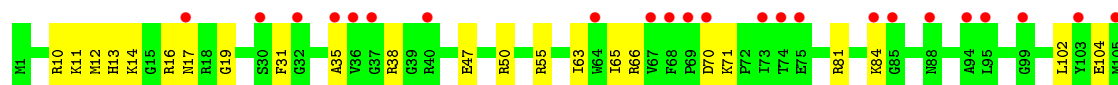
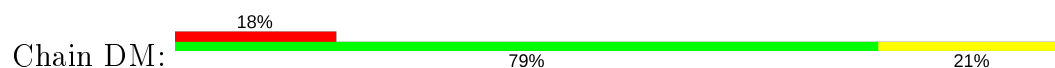
- Molecule 15: 50S ribosomal protein L15



- Molecule 16: 50S ribosomal protein L16



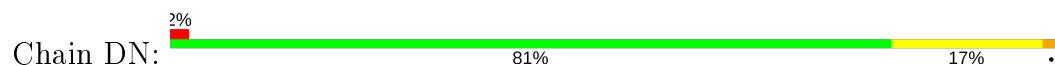
- Molecule 16: 50S ribosomal protein L16



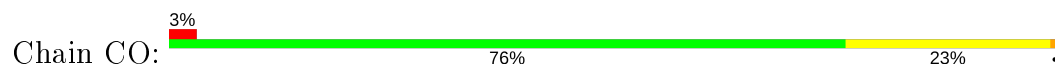
- Molecule 17: 50S ribosomal protein L17

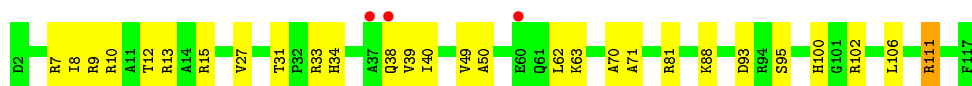


- Molecule 17: 50S ribosomal protein L17

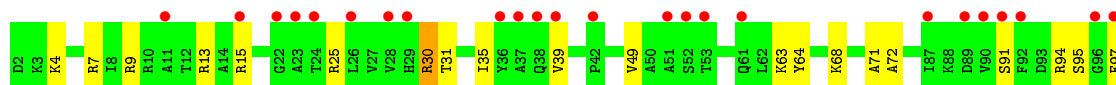
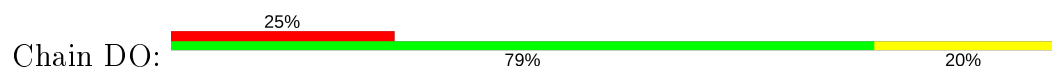


- Molecule 18: 50S ribosomal protein L18

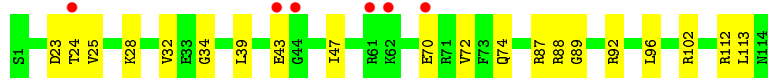
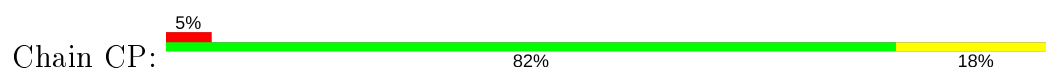




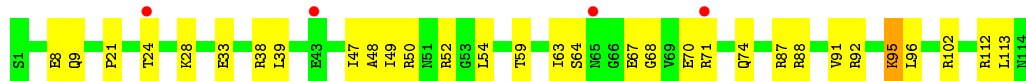
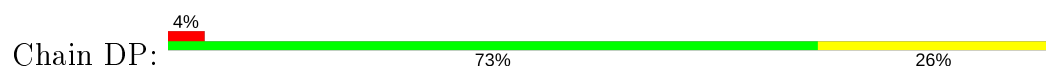
- Molecule 18: 50S ribosomal protein L18



- Molecule 19: 50S ribosomal protein L19



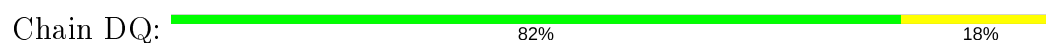
- Molecule 19: 50S ribosomal protein L19



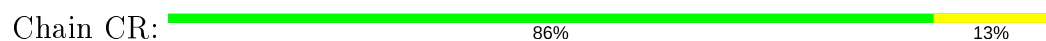
- Molecule 20: 50S ribosomal protein L20



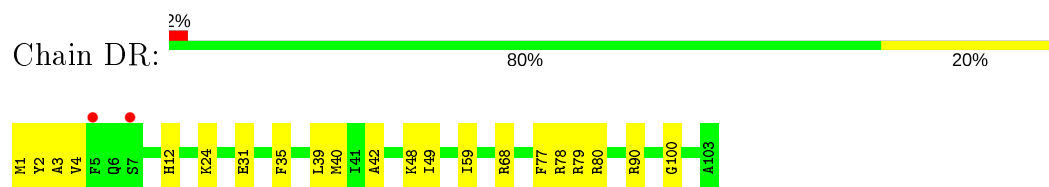
- Molecule 20: 50S ribosomal protein L20



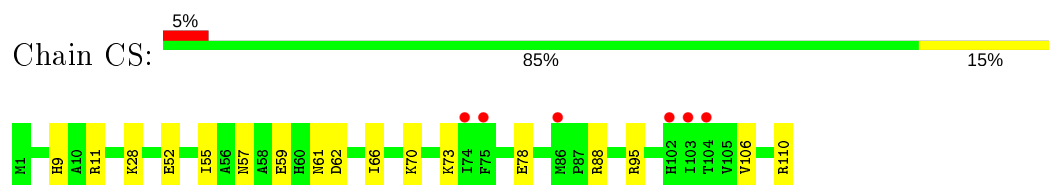
- Molecule 21: 50S ribosomal protein L21



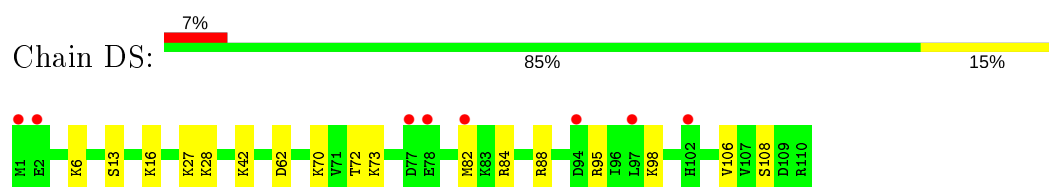
- Molecule 21: 50S ribosomal protein L21



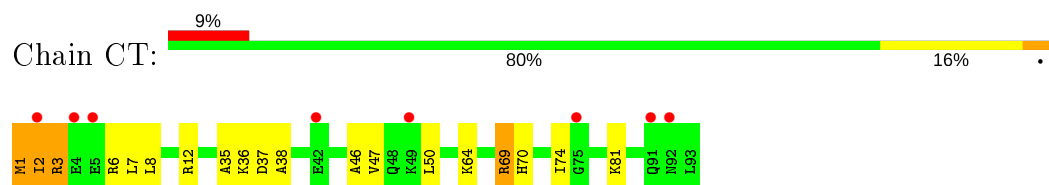
- Molecule 22: 50S ribosomal protein L22



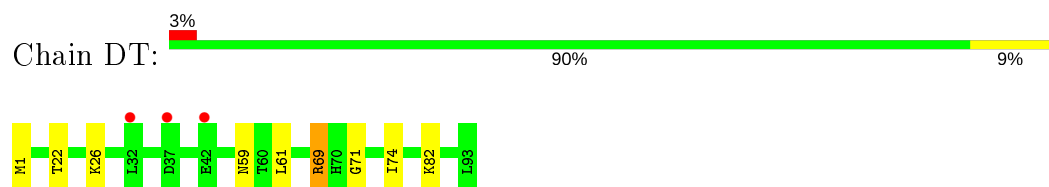
- Molecule 22: 50S ribosomal protein L22



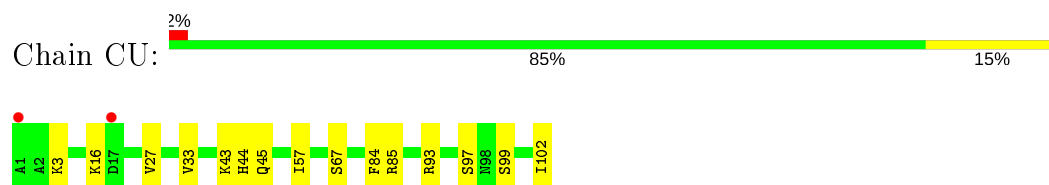
- Molecule 23: 50S ribosomal protein L23



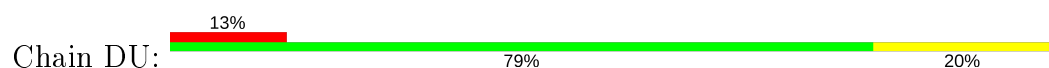
- Molecule 23: 50S ribosomal protein L23

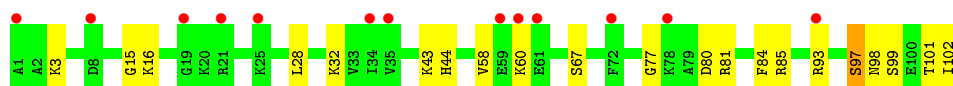


- Molecule 24: 50S ribosomal protein L24

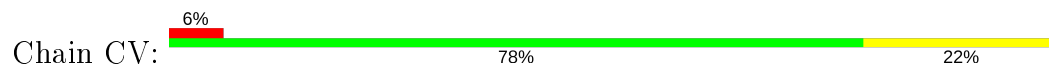


- Molecule 24: 50S ribosomal protein L24

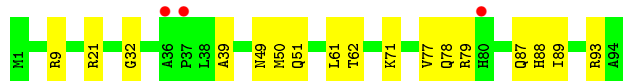
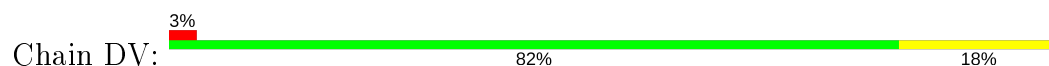




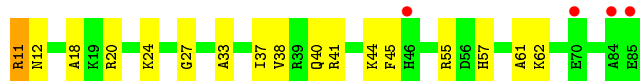
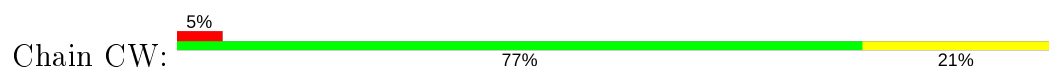
- Molecule 25: 50S ribosomal protein L25



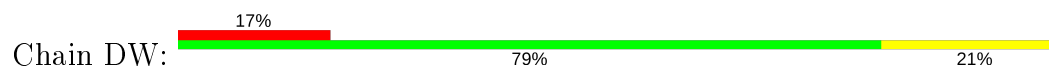
- Molecule 25: 50S ribosomal protein L25



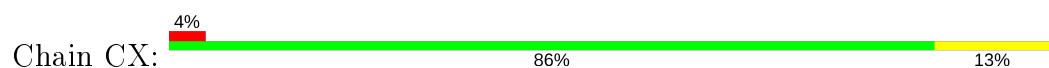
- Molecule 26: 50S ribosomal protein L27



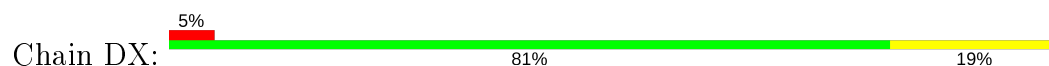
- Molecule 26: 50S ribosomal protein L27




- Molecule 27: 50S ribosomal protein L28



- Molecule 27: 50S ribosomal protein L28




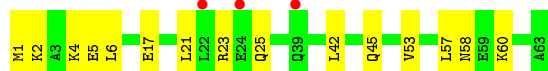
- Molecule 28: 50S ribosomal protein L29

Chain CY:  87% 10%




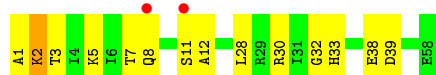
- Molecule 28: 50S ribosomal protein L29

Chain DY:  5% 76% 24%




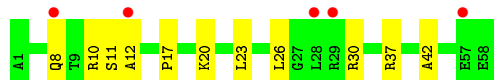
- Molecule 29: 50S ribosomal protein L30

Chain CZ:  3% 76% 22%



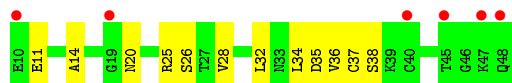
- Molecule 29: 50S ribosomal protein L30

Chain DZ:  9% 81% 19%



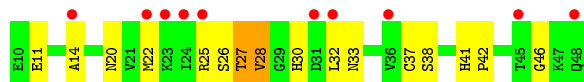
- Molecule 30: 50S ribosomal protein L31

Chain C0:  15% 69% 31%




- Molecule 30: 50S ribosomal protein L31

Chain D0:  26% 59% 36% 5%




- Molecule 31: 50S ribosomal protein L32

Chain C1:  82% 18%




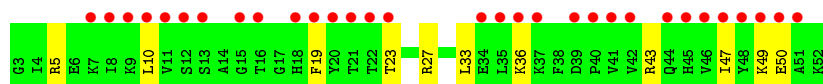
- Molecule 31: 50S ribosomal protein L32

Chain D1:  79% 21%




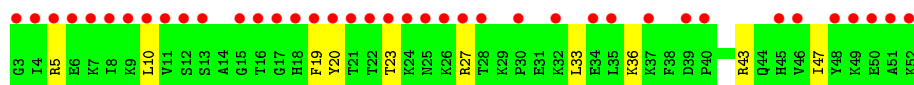
- Molecule 32: 50S ribosomal protein L33

Chain C2:  62% 78% 22%




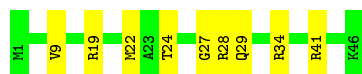
- Molecule 32: 50S ribosomal protein L33

Chain D2:  78% 80% 20%




- Molecule 33: 50S ribosomal protein L34

Chain C3:  80% 20%




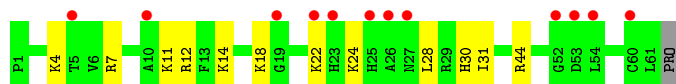
- Molecule 33: 50S ribosomal protein L34

Chain D3:  76% 22%




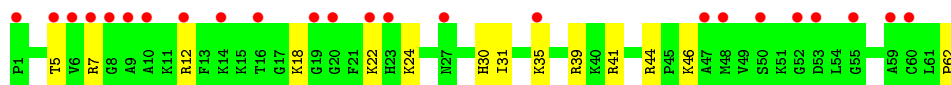
- Molecule 34: 50S ribosomal protein L35

Chain C4:  19% 79% 19%




- Molecule 34: 50S ribosomal protein L35

Chain D4:  39% 77% 23%



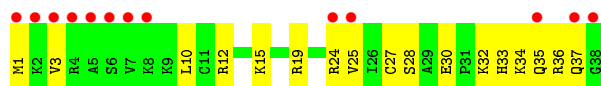
- Molecule 35: 50S ribosomal protein L36

Chain C6:  68% 32%




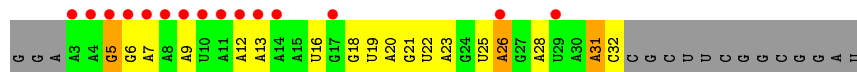
- Molecule 35: 50S ribosomal protein L36

Chain D6:  34% 55% 45%



- Molecule 36: Messenger RNA

Chain AX:  33% 26% 33% 7% 35%




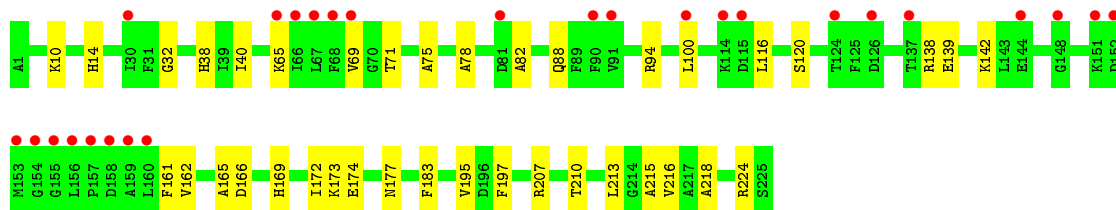
- Molecule 36: Messenger RNA

Chain BX:  37% 33% 30% 35%




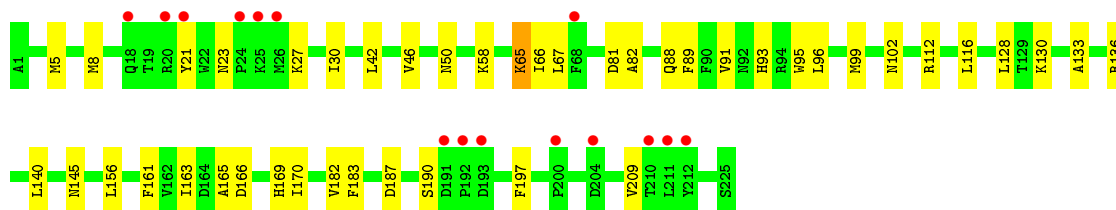
- Molecule 37: 30S ribosomal protein S2

Chain AB:  12% 83% 17%

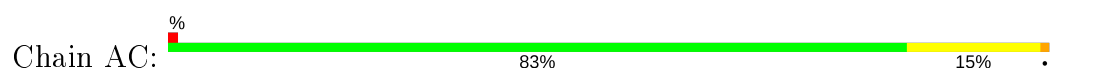


- Molecule 37: 30S ribosomal protein S2

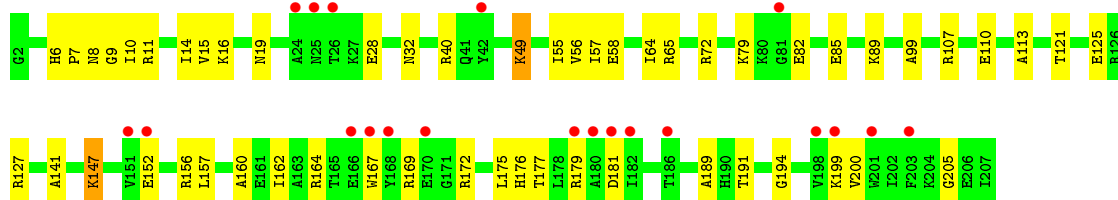
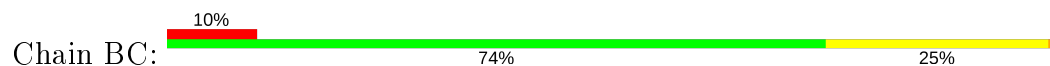
Chain BB:  7% 80% 19%



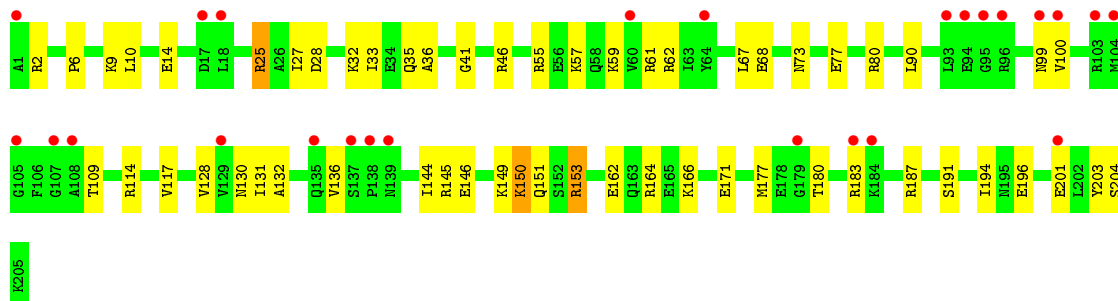
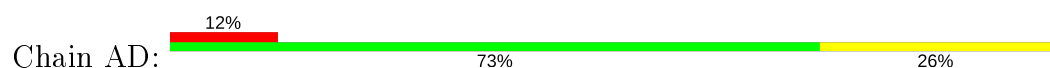
- Molecule 38: 30S ribosomal protein S3



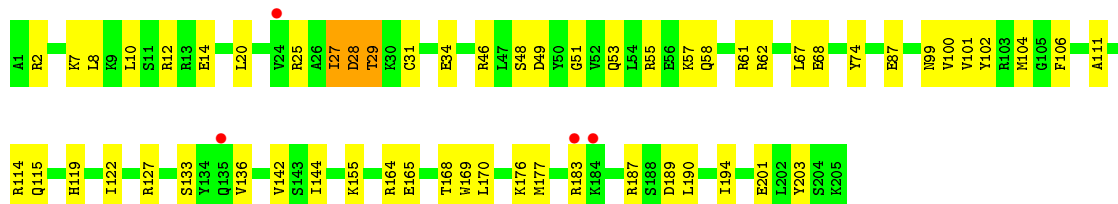
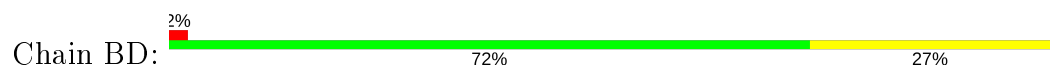
- Molecule 38: 30S ribosomal protein S3



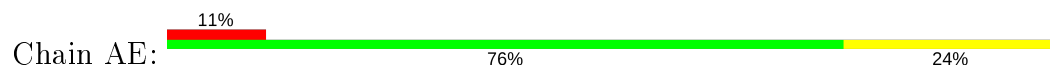
- Molecule 39: 30S ribosomal protein S4

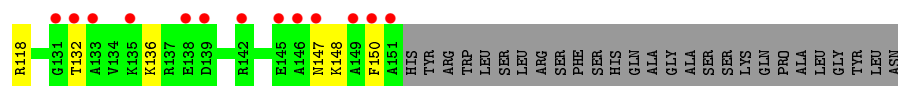


- Molecule 39: 30S ribosomal protein S4

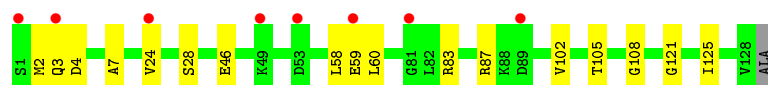
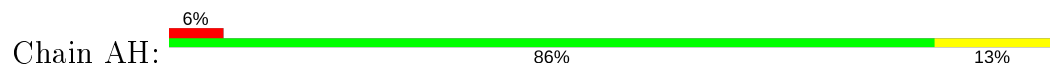


- Molecule 40: 30S ribosomal protein S5

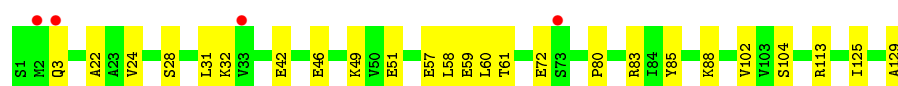
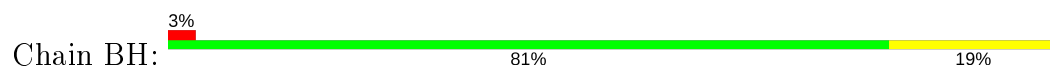




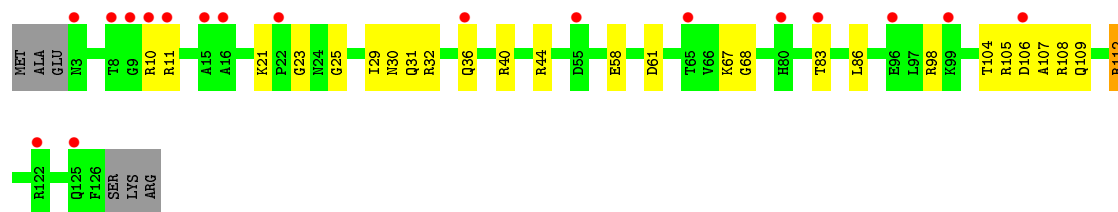
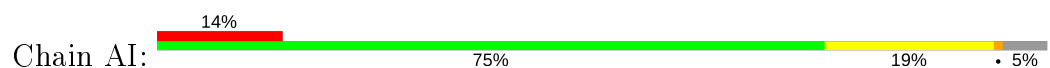
- Molecule 43: 30S ribosomal protein S8



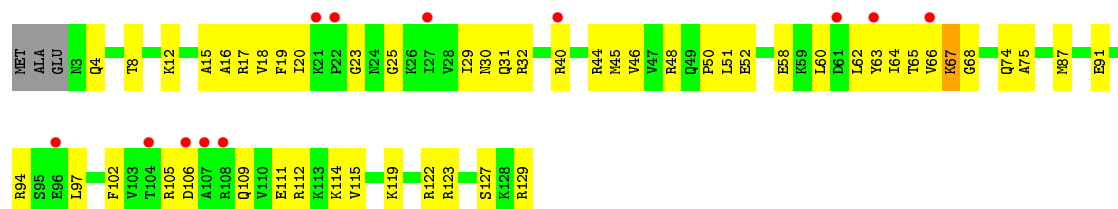
- Molecule 43: 30S ribosomal protein S8



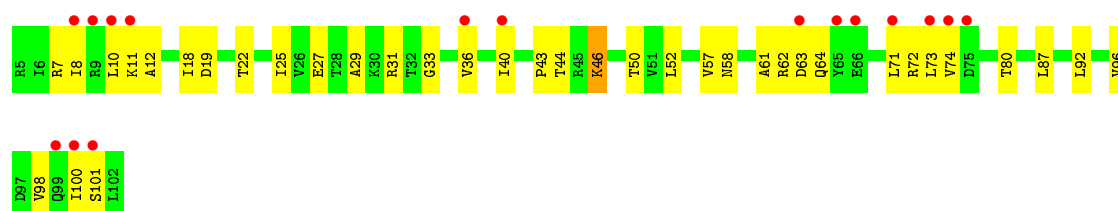
- Molecule 44: 30S ribosomal protein S9



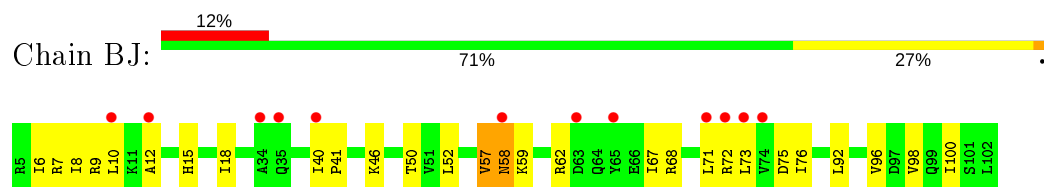
- Molecule 44: 30S ribosomal protein S9



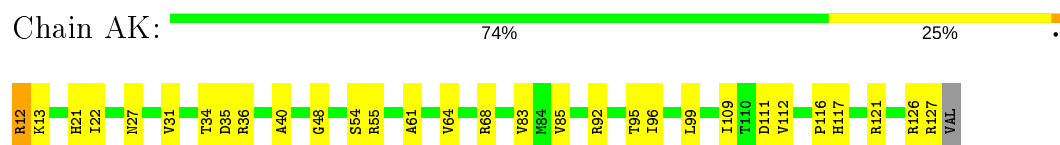
- Molecule 45: 30S ribosomal protein S10



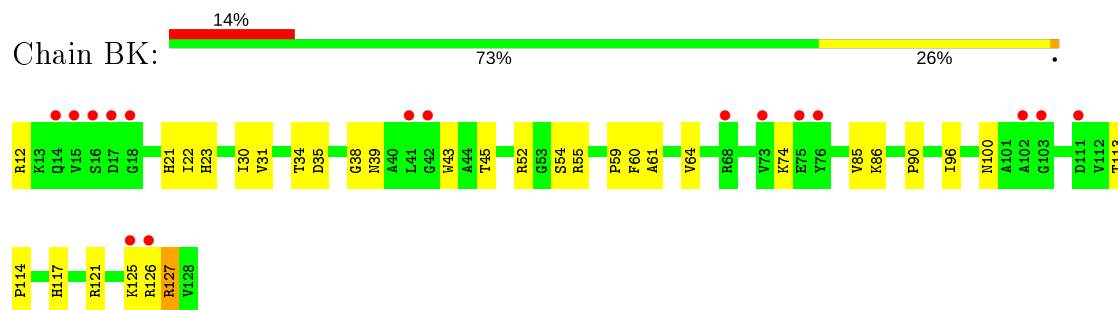
- Molecule 45: 30S ribosomal protein S10



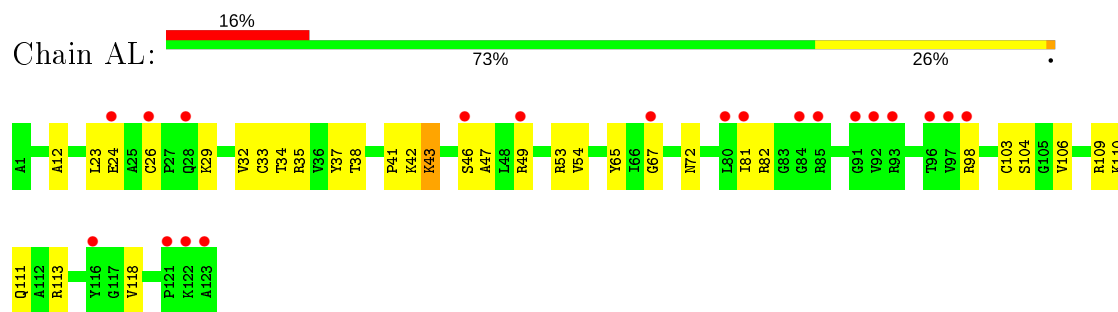
- Molecule 46: 30S ribosomal protein S11



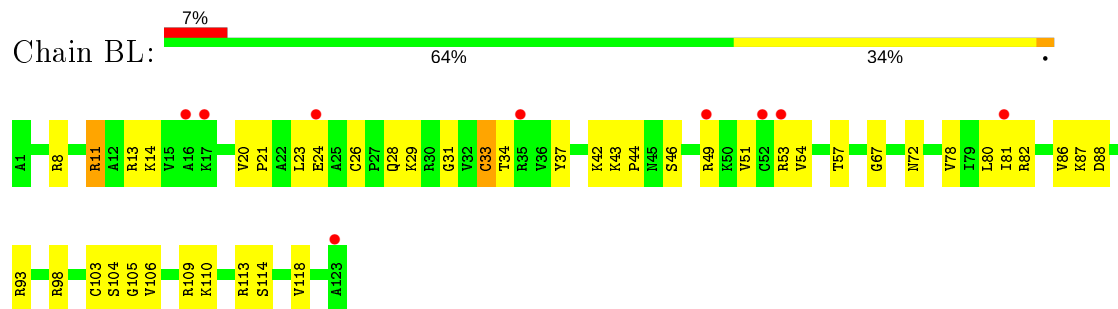
- Molecule 46: 30S ribosomal protein S11



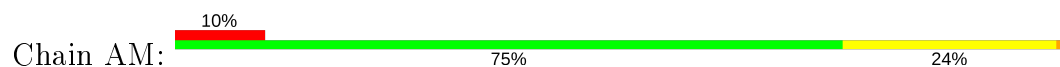
- Molecule 47: 30S ribosomal protein S12

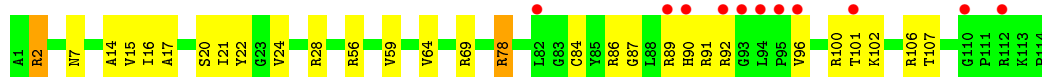


- Molecule 47: 30S ribosomal protein S12

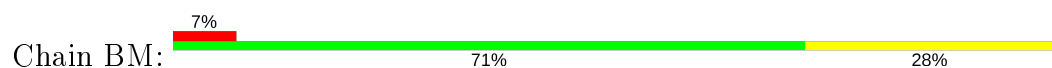


- Molecule 48: 30S ribosomal protein S13

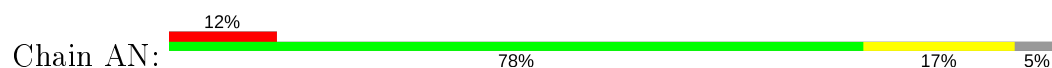




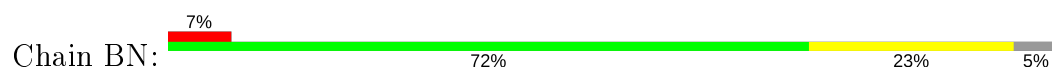
- Molecule 48: 30S ribosomal protein S13



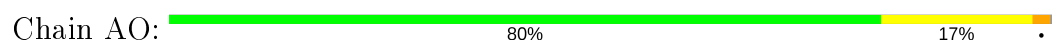
- Molecule 49: 30S ribosomal protein S14



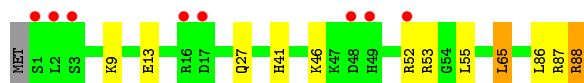
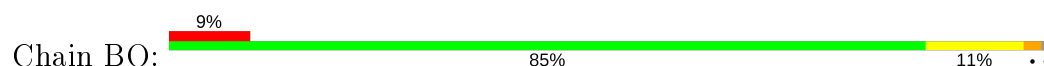
- Molecule 49: 30S ribosomal protein S14



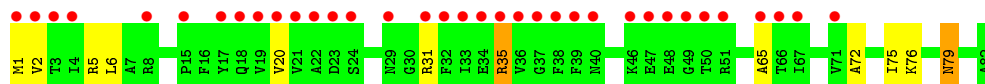
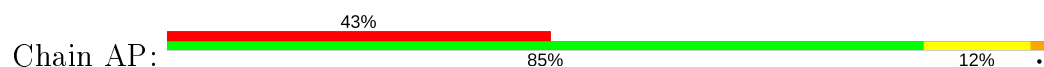
- Molecule 50: 30S ribosomal protein S15



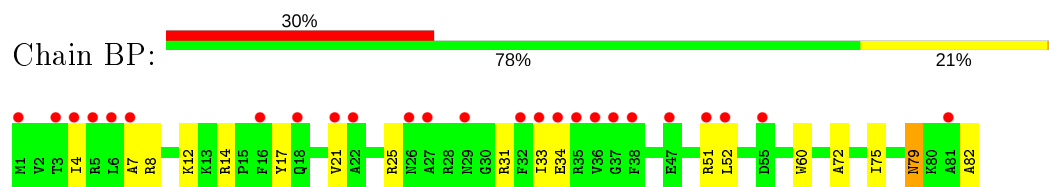
- Molecule 50: 30S ribosomal protein S15



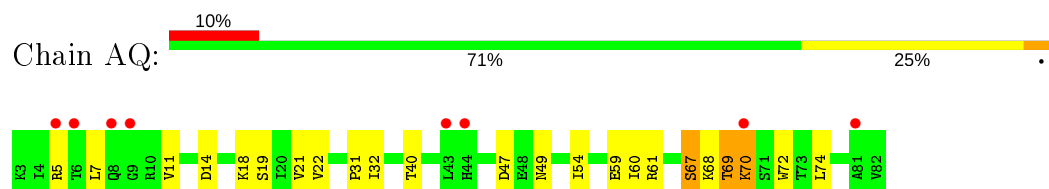
- Molecule 51: 30S ribosomal protein S16



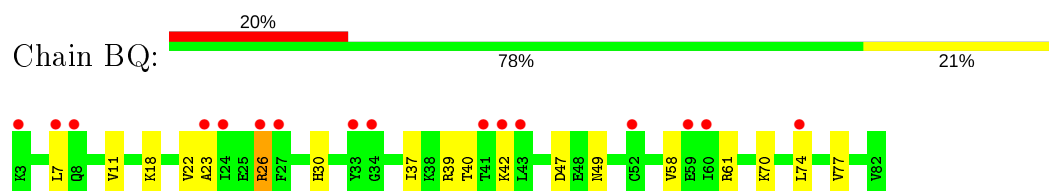
- Molecule 51: 30S ribosomal protein S16



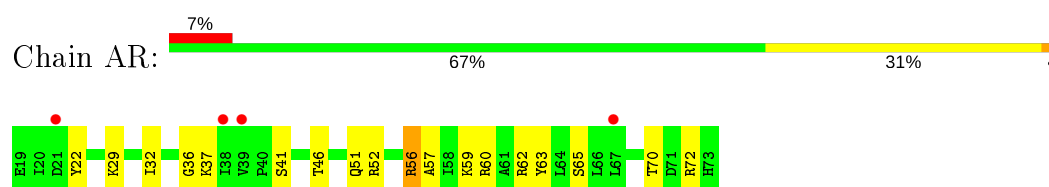
- Molecule 52: 30S ribosomal protein S17



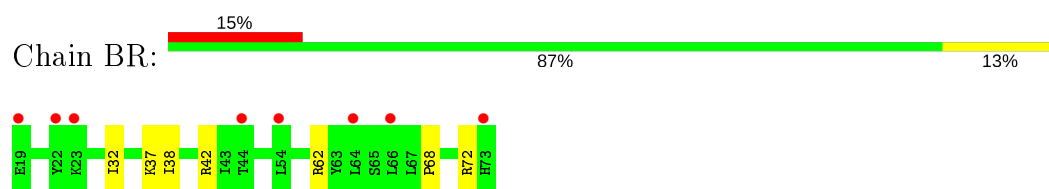
- Molecule 52: 30S ribosomal protein S17



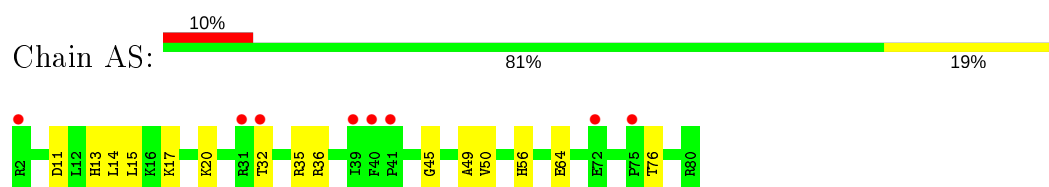
- Molecule 53: 30S ribosomal protein S18



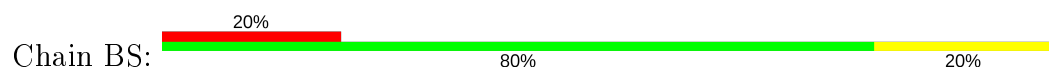
- Molecule 53: 30S ribosomal protein S18

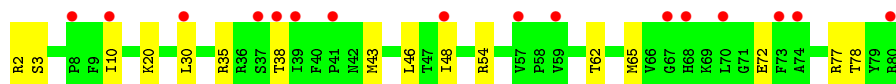


- Molecule 54: 30S ribosomal protein S19

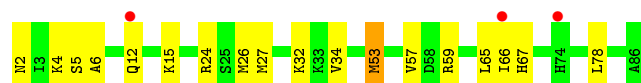
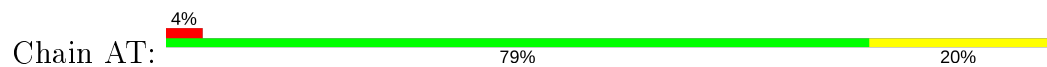


- Molecule 54: 30S ribosomal protein S19

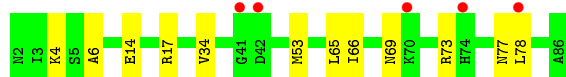
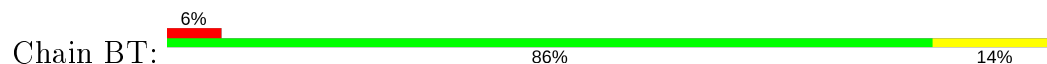




- Molecule 55: 30S ribosomal protein S20



- Molecule 55: 30S ribosomal protein S20



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.66Å 433.91Å 623.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.99 – 3.94 59.99 – 3.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.99-3.94) 99.9 (59.99-3.94)	Depositor EDS
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.249 , 0.269 0.249 , 0.269	Depositor DCC
R_{free} test set	10092 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	137.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	296390	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.44	0/36967	1.12	179/57663 (0.3%)
1	BA	0.47	0/37009	1.18	224/57723 (0.4%)
2	CA	0.49	2/68933 (0.0%)	1.10	263/107532 (0.2%)
2	DA	0.45	1/68974 (0.0%)	1.11	303/107576 (0.3%)
3	CB	0.47	0/2828	1.14	19/4410 (0.4%)
3	DB	0.39	0/2828	1.14	21/4410 (0.5%)
4	AV	0.47	1/1813 (0.1%)	1.16	18/2823 (0.6%)
4	AW	0.51	1/1813 (0.1%)	1.22	21/2823 (0.7%)
4	AY	0.42	1/1813 (0.1%)	1.06	5/2823 (0.2%)
4	BV	0.47	1/1813 (0.1%)	1.10	10/2823 (0.4%)
4	BW	0.48	1/1813 (0.1%)	1.18	13/2823 (0.5%)
5	CC	0.32	0/2122	0.60	0/2852
5	DC	0.31	0/2122	0.61	0/2852
6	CD	0.36	0/1586	0.60	0/2134
6	DD	0.33	0/1586	0.59	0/2134
7	CE	0.31	0/1422	0.57	0/1911
7	DE	0.30	0/1411	0.53	0/1897
8	CF	0.35	0/1435	0.64	0/1926
8	DF	0.36	0/1435	0.63	0/1926
9	CG	0.33	0/1343	0.55	0/1816
9	DG	0.30	0/1343	0.55	0/1816
10	CH	0.30	0/1121	0.62	0/1515
10	DH	0.32	0/1121	0.65	1/1515 (0.1%)
11	C5	0.31	0/835	0.63	0/1123
12	CI	0.29	0/513	0.54	0/684
12	DI	0.30	0/520	0.62	0/694
13	CJ	0.33	0/1152	0.55	0/1551
13	DJ	0.32	0/1152	0.53	0/1551
14	CK	0.33	0/948	0.61	0/1268
14	DK	0.33	0/948	0.63	0/1268
15	CL	0.32	0/1054	0.68	1/1403 (0.1%)
15	DL	0.30	0/1054	0.65	1/1403 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	CM	0.34	0/1084	0.66	1/1450 (0.1%)
16	DM	0.33	0/1093	0.65	1/1460 (0.1%)
17	CN	0.31	0/982	0.61	0/1312
17	DN	0.31	0/982	0.62	0/1312
18	CO	0.30	0/902	0.57	0/1209
18	DO	0.31	0/902	0.65	0/1209
19	CP	0.32	0/929	0.57	1/1242 (0.1%)
19	DP	0.31	0/929	0.59	1/1242 (0.1%)
20	CQ	0.34	0/960	0.50	0/1278
20	DQ	0.30	0/960	0.47	0/1278
21	CR	0.33	0/829	0.62	0/1107
21	DR	0.30	0/829	0.60	0/1107
22	CS	0.32	0/864	0.56	0/1156
22	DS	0.29	0/864	0.54	0/1156
23	CT	0.32	0/745	0.59	0/994
23	DT	0.29	0/745	0.57	0/994
24	CU	0.35	0/788	0.65	1/1051 (0.1%)
24	DU	0.33	0/788	0.63	1/1051 (0.1%)
25	CV	0.33	0/766	0.58	0/1025
25	DV	0.29	0/766	0.56	0/1025
26	CW	0.32	0/581	0.53	0/769
26	DW	0.31	0/581	0.55	0/769
27	CX	0.34	0/635	0.57	0/848
27	DX	0.29	0/635	0.53	0/848
28	CY	0.30	0/500	0.64	0/665
28	DY	0.29	0/510	0.61	0/677
29	CZ	0.30	0/453	0.56	0/605
29	DZ	0.30	0/453	0.58	0/605
30	C0	0.54	0/297	1.05	2/398 (0.5%)
30	D0	0.65	1/297 (0.3%)	0.89	1/398 (0.3%)
31	C1	0.32	0/450	0.61	0/599
31	D1	0.28	0/450	0.59	0/599
32	C2	0.30	0/417	0.61	0/554
32	D2	0.28	0/417	0.60	0/554
33	C3	0.30	0/380	0.53	0/498
33	D3	0.30	0/380	0.54	0/498
34	C4	0.30	0/486	0.57	0/639
34	D4	0.29	0/494	0.59	0/651
35	C6	0.36	0/303	0.65	0/397
35	D6	0.33	0/303	0.61	0/397
36	AX	0.43	0/735	1.26	7/1145 (0.6%)
36	BX	0.55	1/735 (0.1%)	1.34	9/1145 (0.8%)
37	AB	0.31	0/1788	0.60	0/2408

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	BB	0.31	0/1788	0.64	1/2408 (0.0%)
38	AC	0.31	0/1652	0.60	1/2225 (0.0%)
38	BC	0.30	0/1652	0.56	0/2225
39	AD	0.31	0/1665	0.65	1/2227 (0.0%)
39	BD	0.34	0/1665	0.65	0/2227
40	AE	0.33	0/1119	0.68	0/1504
40	BE	0.34	0/1119	0.69	0/1504
41	AF	0.32	0/836	0.64	0/1128
41	BF	0.32	0/836	0.69	1/1128 (0.1%)
42	AG	0.29	0/1069	0.54	0/1430
42	BG	0.28	0/1046	0.56	0/1398
43	AH	0.30	0/983	0.55	0/1319
43	BH	0.30	0/989	0.54	0/1326
44	AI	0.29	0/1007	0.60	0/1342
44	BI	0.29	0/1034	0.62	0/1375
45	AJ	0.29	0/797	0.70	1/1077 (0.1%)
45	BJ	0.29	0/797	0.67	1/1077 (0.1%)
46	AK	0.31	0/885	0.58	0/1195
46	BK	0.29	0/893	0.60	0/1205
47	AL	0.30	0/969	0.67	1/1300 (0.1%)
47	BL	0.32	0/969	0.65	1/1300 (0.1%)
48	AM	0.36	0/893	0.73	2/1193 (0.2%)
48	BM	0.44	1/893 (0.1%)	0.68	1/1193 (0.1%)
49	AN	0.29	0/785	0.60	0/1043
49	BN	0.28	0/785	0.60	0/1043
50	AO	0.30	0/722	0.63	0/964
50	BO	0.27	0/722	0.62	1/964 (0.1%)
51	AP	0.29	0/659	0.64	0/884
51	BP	0.30	0/659	0.62	0/884
52	AQ	0.35	0/658	0.75	1/881 (0.1%)
52	BQ	0.32	0/658	0.69	0/881
53	AR	0.28	0/463	0.56	0/621
53	BR	0.27	0/463	0.55	0/621
54	AS	0.30	0/653	0.59	0/877
54	BS	0.28	0/653	0.58	0/877
55	AT	0.29	0/671	0.57	0/888
55	BT	0.30	0/671	0.55	0/888
All	All	0.43	11/317592 (0.0%)	1.02	1117/475614 (0.2%)

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
5	CC	0	2
6	CD	0	1
6	DD	0	1
8	CF	0	1
10	DH	0	2
11	C5	0	1
14	CK	0	1
14	DK	0	1
15	CL	0	1
19	DP	0	1
23	CT	0	1
23	DT	0	1
25	DV	0	1
33	D3	0	1
34	C4	0	1
34	D4	0	1
37	AB	0	1
38	AC	0	1
39	AD	0	2
39	BD	0	2
40	BE	0	2
41	AF	0	1
41	BF	0	1
42	AG	0	1
45	BJ	0	1
48	AM	0	1
49	AN	0	1
52	AQ	0	1
52	BQ	0	1
All	All	0	34

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BW	1	G	OP3-P	-10.75	1.48	1.61
4	BV	1	G	OP3-P	-10.71	1.48	1.61
4	AV	1	G	OP3-P	-10.67	1.48	1.61
4	AY	1	G	OP3-P	-10.64	1.48	1.61
4	AW	1	G	OP3-P	-10.49	1.48	1.61

The worst 5 of 1117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	71	A	OP2-P-O3'	-33.97	30.46	105.20
2	DA	2219	U	O5'-P-OP1	-27.34	77.89	110.70
2	DA	2219	U	OP1-P-OP2	-24.36	83.07	119.60
2	DA	2219	U	O5'-P-OP2	19.93	134.61	110.70
2	CA	1521	G	OP2-P-O3'	-15.81	70.41	105.20

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	C5	89	PRO	Peptide
5	CC	120	ASP	Peptide
5	CC	237	ARG	Peptide
6	CD	151	THR	Peptide
8	CF	174	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	33037	0	16628	487	3
1	BA	33057	0	16640	516	0
2	CA	61550	0	30959	698	0
2	DA	61593	0	30990	812	3
3	CB	2529	0	1281	36	0
3	DB	2529	0	1281	34	0
4	AV	1623	0	823	18	0
4	AW	1623	0	823	28	0
4	AY	1623	0	823	12	0
4	BV	1623	0	823	19	0
4	BW	1623	0	823	20	0
5	CC	2083	0	2157	48	0
5	DC	2083	0	2157	46	0
6	CD	1565	0	1616	30	2
6	DD	1565	0	1616	25	0
7	CE	1404	0	1466	22	0
7	DE	1393	0	1453	24	0
8	CF	1411	0	1447	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	DF	1411	0	1447	23	0
9	CG	1323	0	1374	15	0
9	DG	1323	0	1374	17	0
10	CH	1110	0	1148	17	0
10	DH	1110	0	1148	24	3
11	C5	825	0	856	17	0
12	CI	511	0	544	7	0
12	DI	518	0	551	12	0
13	CJ	1129	0	1162	15	0
13	DJ	1129	0	1162	15	0
14	CK	939	0	1012	14	0
14	DK	939	0	1012	16	0
15	CL	1045	0	1117	24	1
15	DL	1045	0	1117	23	0
16	CM	1065	0	1148	7	0
16	DM	1074	0	1157	20	0
17	CN	969	0	1012	32	0
17	DN	969	0	1013	20	0
18	CO	892	0	923	21	2
18	DO	892	0	923	15	0
19	CP	917	0	965	14	0
19	DP	917	0	965	22	0
20	CQ	947	0	1022	13	0
20	DQ	947	0	1022	20	0
21	CR	816	0	839	10	0
21	DR	816	0	839	17	2
22	CS	857	0	922	12	0
22	DS	857	0	922	12	0
23	CT	739	0	807	14	0
23	DT	739	0	807	5	0
24	CU	780	0	834	10	0
24	DU	780	0	834	16	0
25	CV	753	0	780	16	0
25	DV	753	0	780	12	0
26	CW	574	0	592	16	0
26	DW	574	0	592	14	0
27	CX	625	0	655	10	0
27	DX	625	0	655	11	0
28	CY	499	0	535	6	0
28	DY	509	0	543	9	0
29	CZ	449	0	491	16	1
29	DZ	449	0	491	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	C0	293	0	283	9	0
30	D0	293	0	284	18	0
31	C1	444	0	461	9	1
31	D1	444	0	461	9	0
32	C2	410	0	440	7	0
32	D2	410	0	440	7	0
33	C3	377	0	418	6	0
33	D3	377	0	418	8	0
34	C4	479	0	553	10	0
34	D4	486	0	560	10	0
35	C6	302	0	340	8	0
35	D6	302	0	340	11	0
36	AX	653	0	325	29	0
36	BX	653	0	325	24	0
37	AB	1757	0	1787	23	0
37	BB	1757	0	1787	25	0
38	AC	1625	0	1696	28	0
38	BC	1625	0	1696	40	0
39	AD	1643	0	1710	46	3
39	BD	1643	0	1710	41	0
40	AE	1106	0	1148	24	0
40	BE	1106	0	1148	21	0
41	AF	818	0	808	18	0
41	BF	818	0	808	13	3
42	AG	1058	0	1111	19	0
42	BG	1035	0	1087	16	0
43	AH	973	0	1029	11	0
43	BH	979	0	1034	20	0
44	AI	995	0	1039	42	0
44	BI	1022	0	1070	51	0
45	AJ	787	0	828	27	0
45	BJ	787	0	828	19	0
46	AK	869	0	878	23	0
46	BK	877	0	887	23	0
47	AL	955	0	1019	21	0
47	BL	955	0	1019	33	0
48	AM	884	0	944	23	0
48	BM	884	0	944	34	0
49	AN	774	0	827	12	0
49	BN	774	0	827	19	0
50	AO	714	0	737	23	0
50	BO	714	0	737	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	AP	649	0	666	9	0
51	BP	649	0	666	12	0
52	AQ	649	0	691	13	0
52	BQ	649	0	691	11	0
53	AR	456	0	478	15	0
53	BR	456	0	478	5	0
54	AS	638	0	665	16	0
54	BS	638	0	665	16	0
55	AT	665	0	714	14	0
55	BT	665	0	714	7	0
56	AA	50	0	0	0	0
56	BA	49	0	0	0	0
56	C4	1	0	0	0	0
56	CA	167	0	0	0	0
56	CB	3	0	0	0	0
56	CC	1	0	0	0	0
56	CN	2	0	0	0	0
56	CQ	1	0	0	0	0
56	DA	166	0	0	0	0
56	DB	3	0	0	0	0
56	DN	1	0	0	0	0
56	DQ	1	0	0	0	0
57	C0	1	0	0	0	0
57	C6	1	0	0	0	0
57	D0	1	0	0	0	0
57	D6	1	0	0	0	0
58	AA	481	0	0	8	0
58	AB	7	0	0	0	0
58	AC	15	0	0	0	0
58	AD	10	0	0	1	0
58	AE	12	0	0	1	0
58	AF	6	0	0	0	0
58	AG	5	0	0	0	0
58	AH	7	0	0	1	0
58	AI	6	0	0	0	0
58	AJ	4	0	0	0	0
58	AK	10	0	0	2	0
58	AL	9	0	0	0	0
58	AM	6	0	0	0	0
58	AN	3	0	0	0	0
58	AO	7	0	0	1	0
58	AP	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	AQ	8	0	0	1	0
58	AR	1	0	0	0	0
58	AS	4	0	0	1	0
58	AT	4	0	0	1	0
58	AV	28	0	0	0	0
58	AW	32	0	0	0	0
58	AX	4	0	0	0	0
58	AY	5	0	0	0	0
58	BA	461	0	0	14	0
58	BB	2	0	0	0	0
58	BC	8	0	0	1	0
58	BD	24	0	0	2	0
58	BE	18	0	0	0	0
58	BF	6	0	0	0	0
58	BG	4	0	0	0	0
58	BH	12	0	0	2	0
58	BI	9	0	0	0	0
58	BJ	8	0	0	1	0
58	BK	5	0	0	0	0
58	BL	8	0	0	0	0
58	BM	6	0	0	1	0
58	BN	5	0	0	0	0
58	BO	2	0	0	1	0
58	BP	5	0	0	1	0
58	BQ	10	0	0	0	0
58	BR	1	0	0	1	0
58	BS	3	0	0	0	0
58	BT	2	0	0	0	0
58	BV	13	0	0	0	0
58	BW	23	0	0	0	0
58	BX	5	0	0	0	0
58	C1	5	0	0	0	0
58	C2	1	0	0	0	0
58	C3	2	0	0	0	0
58	C4	2	0	0	0	0
58	C5	7	0	0	0	0
58	C6	3	0	0	0	0
58	CA	1106	0	0	22	0
58	CB	49	0	0	1	0
58	CC	13	0	0	0	0
58	CD	10	0	0	0	0
58	CE	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	CF	14	0	0	2	0
58	CG	18	0	0	0	0
58	CH	8	0	0	1	0
58	CI	4	0	0	0	0
58	CJ	9	0	0	0	0
58	CK	7	0	0	0	0
58	CL	8	0	0	1	0
58	CM	4	0	0	0	0
58	CN	6	0	0	2	0
58	CO	8	0	0	2	0
58	CP	8	0	0	0	0
58	CQ	2	0	0	0	0
58	CR	7	0	0	0	0
58	CS	3	0	0	0	0
58	CT	7	0	0	1	0
58	CU	13	0	0	0	0
58	CV	10	0	0	5	0
58	CW	4	0	0	0	0
58	CX	3	0	0	0	0
58	CY	3	0	0	0	0
58	CZ	1	0	0	0	0
58	D0	2	0	0	2	0
58	D1	11	0	0	0	0
58	D2	2	0	0	0	0
58	D3	2	0	0	0	0
58	D6	1	0	0	0	0
58	DA	1005	0	0	22	0
58	DB	32	0	0	1	0
58	DC	28	0	0	1	0
58	DD	15	0	0	0	0
58	DE	12	0	0	0	0
58	DF	4	0	0	0	0
58	DG	6	0	0	0	0
58	DH	4	0	0	0	0
58	DJ	3	0	0	0	0
58	DK	5	0	0	0	0
58	DL	10	0	0	0	0
58	DM	6	0	0	1	0
58	DN	6	0	0	0	0
58	DO	4	0	0	0	0
58	DP	6	0	0	0	0
58	DQ	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	DR	13	0	0	0	0
58	DS	9	0	0	0	0
58	DT	10	0	0	0	0
58	DU	14	0	0	1	0
58	DV	7	0	0	0	0
58	DW	3	0	0	0	0
58	DX	3	0	0	1	0
58	DY	7	0	0	0	0
58	DZ	2	0	0	0	0
All	All	296390	0	195117	3829	12

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 3829 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)
1:BA:1029:U:O2'	1:BA:1033:G:N2	1.59	1.29
30:D0:46:GLY:HA2	58:D0:201:HOH:O	1.29	1.28
2:CA:2278:A:OP2	26:CW:12:ASN:ND2	1.73	1.19
50:AO:2:LEU:HD13	50:AO:34:GLN:NE2	1.58	1.18
17:CN:94:TYR:C	17:CN:116:VAL:HG23	1.72	1.08

The worst 5 of 12 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CO:111:ARG:NH1	21:DR:31:GLU:OE1[3_445]	1.60	0.60
29:CZ:5:LYS:NZ	31:C1:34:GLY:O[4_445]	1.69	0.51
39:AD:164:ARG:CD	41:BF:14:GLN:OE1[4_455]	1.79	0.41
1:AA:368:U:N3	10:DH:97:ARG:NH1[4_455]	1.88	0.32
39:AD:25:ARG:O	41:BF:13:ASP:OD2[4_455]	1.93	0.27

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 X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CC	269/271 (99%)	240 (89%)	29 (11%)	0	100	100
5	DC	269/271 (99%)	249 (93%)	20 (7%)	0	100	100
6	CD	207/209 (99%)	192 (93%)	13 (6%)	2 (1%)	15	52
6	DD	207/209 (99%)	195 (94%)	11 (5%)	1 (0%)	29	66
7	CE	179/181 (99%)	172 (96%)	7 (4%)	0	100	100
7	DE	178/181 (98%)	169 (95%)	9 (5%)	0	100	100
8	CF	175/177 (99%)	150 (86%)	25 (14%)	0	100	100
8	DF	175/177 (99%)	152 (87%)	23 (13%)	0	100	100
9	CG	174/176 (99%)	163 (94%)	11 (6%)	0	100	100
9	DG	174/176 (99%)	162 (93%)	12 (7%)	0	100	100
10	CH	147/149 (99%)	120 (82%)	26 (18%)	1 (1%)	22	60
10	DH	147/149 (99%)	118 (80%)	29 (20%)	0	100	100
11	C5	107/109 (98%)	91 (85%)	16 (15%)	0	100	100
12	CI	69/72 (96%)	65 (94%)	4 (6%)	0	100	100
12	DI	70/72 (97%)	59 (84%)	11 (16%)	0	100	100
13	CJ	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
13	DJ	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
14	CK	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
14	DK	120/122 (98%)	104 (87%)	16 (13%)	0	100	100
15	CL	141/143 (99%)	122 (86%)	19 (14%)	0	100	100
15	DL	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
16	CM	133/136 (98%)	127 (96%)	4 (3%)	2 (2%)	10	45
16	DM	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
17	CN	119/121 (98%)	108 (91%)	11 (9%)	0	100	100
17	DN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	9	42
18	CO	114/116 (98%)	105 (92%)	9 (8%)	0	100	100
18	DO	114/116 (98%)	100 (88%)	13 (11%)	1 (1%)	17	54
19	CP	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
19	DP	112/114 (98%)	104 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	CQ	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
20	DQ	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
21	CR	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
21	DR	101/103 (98%)	90 (89%)	11 (11%)	0	100	100
22	CS	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
22	DS	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
23	CT	91/93 (98%)	84 (92%)	6 (7%)	1 (1%)	14	50
23	DT	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
24	CU	100/102 (98%)	86 (86%)	14 (14%)	0	100	100
24	DU	100/102 (98%)	85 (85%)	14 (14%)	1 (1%)	15	52
25	CV	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
25	DV	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
26	CW	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
26	DW	73/75 (97%)	64 (88%)	9 (12%)	0	100	100
27	CX	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
27	DX	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
28	CY	59/63 (94%)	52 (88%)	7 (12%)	0	100	100
28	DY	61/63 (97%)	54 (88%)	6 (10%)	1 (2%)	9	44
29	CZ	56/58 (97%)	53 (95%)	2 (4%)	1 (2%)	8	41
29	DZ	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
30	C0	37/39 (95%)	33 (89%)	4 (11%)	0	100	100
30	D0	37/39 (95%)	33 (89%)	4 (11%)	0	100	100
31	C1	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
31	D1	54/56 (96%)	48 (89%)	6 (11%)	0	100	100
32	C2	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
32	D2	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
33	C3	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
33	D3	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
34	C4	59/62 (95%)	52 (88%)	6 (10%)	1 (2%)	9	42
34	D4	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	9	42
35	C6	36/38 (95%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	D6	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
37	AB	223/225 (99%)	198 (89%)	25 (11%)	0	100	100
37	BB	223/225 (99%)	186 (83%)	37 (17%)	0	100	100
38	AC	204/206 (99%)	174 (85%)	30 (15%)	0	100	100
38	BC	204/206 (99%)	186 (91%)	18 (9%)	0	100	100
39	AD	203/205 (99%)	179 (88%)	24 (12%)	0	100	100
39	BD	203/205 (99%)	174 (86%)	27 (13%)	2 (1%)	15	52
40	AE	148/150 (99%)	117 (79%)	31 (21%)	0	100	100
40	BE	148/150 (99%)	122 (82%)	26 (18%)	0	100	100
41	AF	98/100 (98%)	80 (82%)	17 (17%)	1 (1%)	15	52
41	BF	98/100 (98%)	79 (81%)	18 (18%)	1 (1%)	15	52
42	AG	131/179 (73%)	117 (89%)	14 (11%)	0	100	100
42	BG	128/179 (72%)	117 (91%)	11 (9%)	0	100	100
43	AH	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
43	BH	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
44	AI	122/130 (94%)	107 (88%)	15 (12%)	0	100	100
44	BI	125/130 (96%)	104 (83%)	21 (17%)	0	100	100
45	AJ	96/98 (98%)	85 (88%)	11 (12%)	0	100	100
45	BJ	96/98 (98%)	80 (83%)	15 (16%)	1 (1%)	15	52
46	AK	114/117 (97%)	101 (89%)	13 (11%)	0	100	100
46	BK	115/117 (98%)	99 (86%)	16 (14%)	0	100	100
47	AL	121/123 (98%)	104 (86%)	16 (13%)	1 (1%)	19	57
47	BL	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
48	AM	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
48	BM	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
49	AN	92/101 (91%)	80 (87%)	12 (13%)	0	100	100
49	BN	92/101 (91%)	77 (84%)	15 (16%)	0	100	100
50	AO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13	49
50	BO	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
51	AP	80/82 (98%)	71 (89%)	8 (10%)	1 (1%)	12	47
51	BP	80/82 (98%)	68 (85%)	11 (14%)	1 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	AQ	78/80 (98%)	64 (82%)	12 (15%)	2 (3%)	5	34
52	BQ	78/80 (98%)	63 (81%)	15 (19%)	0	100	100
53	AR	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
53	BR	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
54	AS	77/79 (98%)	65 (84%)	12 (16%)	0	100	100
54	BS	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
55	AT	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
55	BT	83/85 (98%)	75 (90%)	8 (10%)	0	100	100
All	All	11101/11427 (97%)	9933 (90%)	1142 (10%)	26 (0%)	47	79

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	CT	3	ARG
41	AF	55	HIS
52	AQ	70	LYS
17	DN	118	ARG
39	BD	28	ASP

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CC	216/216 (100%)	214 (99%)	2 (1%)	78	87
5	DC	216/216 (100%)	213 (99%)	3 (1%)	67	80
6	CD	164/164 (100%)	163 (99%)	1 (1%)	86	91
6	DD	164/164 (100%)	163 (99%)	1 (1%)	86	91
7	CE	148/148 (100%)	147 (99%)	1 (1%)	84	90
7	DE	147/148 (99%)	145 (99%)	2 (1%)	67	80
8	CF	148/148 (100%)	148 (100%)	0	100	100
8	DF	148/148 (100%)	147 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CG	137/137 (100%)	136 (99%)	1 (1%)	84	90
9	DG	137/137 (100%)	136 (99%)	1 (1%)	84	90
10	CH	114/114 (100%)	110 (96%)	4 (4%)	36	61
10	DH	114/114 (100%)	113 (99%)	1 (1%)	78	87
11	C5	83/83 (100%)	81 (98%)	2 (2%)	49	69
12	CI	53/54 (98%)	50 (94%)	3 (6%)	20	49
12	DI	54/54 (100%)	54 (100%)	0	100	100
13	CJ	116/116 (100%)	115 (99%)	1 (1%)	78	87
13	DJ	116/116 (100%)	114 (98%)	2 (2%)	60	78
14	CK	103/103 (100%)	103 (100%)	0	100	100
14	DK	103/103 (100%)	101 (98%)	2 (2%)	57	75
15	CL	102/102 (100%)	99 (97%)	3 (3%)	42	64
15	DL	102/102 (100%)	100 (98%)	2 (2%)	55	73
16	CM	108/109 (99%)	108 (100%)	0	100	100
16	DM	109/109 (100%)	108 (99%)	1 (1%)	78	87
17	CN	101/101 (100%)	100 (99%)	1 (1%)	76	85
17	DN	101/101 (100%)	101 (100%)	0	100	100
18	CO	86/86 (100%)	84 (98%)	2 (2%)	50	70
18	DO	86/86 (100%)	84 (98%)	2 (2%)	50	70
19	CP	99/99 (100%)	99 (100%)	0	100	100
19	DP	99/99 (100%)	98 (99%)	1 (1%)	76	85
20	CQ	89/89 (100%)	89 (100%)	0	100	100
20	DQ	89/89 (100%)	89 (100%)	0	100	100
21	CR	84/84 (100%)	83 (99%)	1 (1%)	71	83
21	DR	84/84 (100%)	84 (100%)	0	100	100
22	CS	93/93 (100%)	92 (99%)	1 (1%)	73	84
22	DS	93/93 (100%)	92 (99%)	1 (1%)	73	84
23	CT	80/80 (100%)	78 (98%)	2 (2%)	47	68
23	DT	80/80 (100%)	79 (99%)	1 (1%)	69	81
24	CU	83/83 (100%)	83 (100%)	0	100	100
24	DU	83/83 (100%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	CV	78/78 (100%)	78 (100%)	0	100	100
25	DV	78/78 (100%)	77 (99%)	1 (1%)	69	81
26	CW	57/57 (100%)	56 (98%)	1 (2%)	59	77
26	DW	57/57 (100%)	57 (100%)	0	100	100
27	CX	67/67 (100%)	66 (98%)	1 (2%)	65	79
27	DX	67/67 (100%)	66 (98%)	1 (2%)	65	79
28	CY	55/55 (100%)	55 (100%)	0	100	100
28	DY	55/55 (100%)	55 (100%)	0	100	100
29	CZ	48/48 (100%)	47 (98%)	1 (2%)	53	72
29	DZ	48/48 (100%)	48 (100%)	0	100	100
30	C0	35/35 (100%)	35 (100%)	0	100	100
30	D0	35/35 (100%)	34 (97%)	1 (3%)	42	64
31	C1	47/47 (100%)	47 (100%)	0	100	100
31	D1	47/47 (100%)	47 (100%)	0	100	100
32	C2	45/45 (100%)	44 (98%)	1 (2%)	52	71
32	D2	45/45 (100%)	44 (98%)	1 (2%)	52	71
33	C3	38/38 (100%)	37 (97%)	1 (3%)	46	67
33	D3	38/38 (100%)	37 (97%)	1 (3%)	46	67
34	C4	49/50 (98%)	49 (100%)	0	100	100
34	D4	50/50 (100%)	49 (98%)	1 (2%)	55	73
35	C6	34/34 (100%)	34 (100%)	0	100	100
35	D6	34/34 (100%)	34 (100%)	0	100	100
37	AB	186/186 (100%)	185 (100%)	1 (0%)	88	93
37	BB	186/186 (100%)	182 (98%)	4 (2%)	52	71
38	AC	170/170 (100%)	169 (99%)	1 (1%)	86	91
38	BC	170/170 (100%)	165 (97%)	5 (3%)	42	64
39	AD	172/172 (100%)	168 (98%)	4 (2%)	50	70
39	BD	172/172 (100%)	167 (97%)	5 (3%)	42	64
40	AE	113/113 (100%)	111 (98%)	2 (2%)	59	77
40	BE	113/113 (100%)	109 (96%)	4 (4%)	36	61
41	AF	87/87 (100%)	86 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	BF	87/87 (100%)	86 (99%)	1 (1%)	73	84
42	AG	110/147 (75%)	110 (100%)	0	100	100
42	BG	107/147 (73%)	107 (100%)	0	100	100
43	AH	104/104 (100%)	103 (99%)	1 (1%)	76	85
43	BH	104/104 (100%)	104 (100%)	0	100	100
44	AI	102/107 (95%)	100 (98%)	2 (2%)	55	73
44	BI	105/107 (98%)	102 (97%)	3 (3%)	42	64
45	AJ	86/86 (100%)	85 (99%)	1 (1%)	71	83
45	BJ	86/86 (100%)	85 (99%)	1 (1%)	71	83
46	AK	89/90 (99%)	87 (98%)	2 (2%)	52	71
46	BK	90/90 (100%)	85 (94%)	5 (6%)	21	49
47	AL	103/103 (100%)	102 (99%)	1 (1%)	76	85
47	BL	103/103 (100%)	102 (99%)	1 (1%)	76	85
48	AM	92/92 (100%)	91 (99%)	1 (1%)	73	84
48	BM	92/92 (100%)	92 (100%)	0	100	100
49	AN	79/84 (94%)	79 (100%)	0	100	100
49	BN	79/84 (94%)	79 (100%)	0	100	100
50	AO	76/77 (99%)	74 (97%)	2 (3%)	46	67
50	BO	76/77 (99%)	73 (96%)	3 (4%)	32	58
51	AP	65/65 (100%)	64 (98%)	1 (2%)	65	79
51	BP	65/65 (100%)	65 (100%)	0	100	100
52	AQ	74/74 (100%)	73 (99%)	1 (1%)	67	80
52	BQ	74/74 (100%)	72 (97%)	2 (3%)	44	66
53	AR	48/48 (100%)	47 (98%)	1 (2%)	53	72
53	BR	48/48 (100%)	48 (100%)	0	100	100
54	AS	70/70 (100%)	70 (100%)	0	100	100
54	BS	70/70 (100%)	69 (99%)	1 (1%)	67	80
55	AT	65/65 (100%)	64 (98%)	1 (2%)	65	79
55	BT	65/65 (100%)	64 (98%)	1 (2%)	65	79
All	All	9222/9323 (99%)	9106 (99%)	116 (1%)	69	81

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	AT	53	MET
14	DK	49	ARG
46	BK	127	ARG
5	DC	196	ASN
7	DE	163	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
5	DC	196	ASN
13	DJ	135	GLN
45	BJ	56	HIS
5	DC	225	ASN
9	DG	19	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1536/1541 (99%)	390 (25%)	7 (0%)
1	BA	1536/1541 (99%)	356 (23%)	11 (0%)
2	CA	2862/2904 (98%)	585 (20%)	18 (0%)
2	DA	2856/2904 (98%)	636 (22%)	16 (0%)
3	CB	117/118 (99%)	23 (19%)	0
3	DB	117/118 (99%)	18 (15%)	0
36	AX	29/46 (63%)	2 (6%)	2 (6%)
36	BX	29/46 (63%)	1 (3%)	0
4	AV	75/76 (98%)	21 (28%)	0
4	AW	76/76 (100%)	17 (22%)	2 (2%)
4	AY	75/76 (98%)	32 (42%)	0
4	BV	75/76 (98%)	17 (22%)	0
4	BW	75/76 (98%)	15 (20%)	0
All	All	9458/9598 (98%)	2113 (22%)	56 (0%)

5 of 2113 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	3	A
1	AA	4	U
1	AA	5	U
1	AA	6	G

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	AX	5	G
1	BA	96	U
2	DA	2188	U
36	AX	26	A
4	AW	17	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 449 ligands modelled in this entry, 449 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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
2	DA	9
1	BA	4

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Mol	Chain	Number of breaks
1	AA	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DA	2105:U	O3'	2118:U	P	30.28
1	DA	2185:U	O3'	2186:G	P	7.24
1	DA	2103:C	O3'	2104:C	P	6.01
1	DA	1887:C	O3'	1888:G	P	5.11
1	DA	2140:G	O3'	2141:G	P	3.75

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1540/1541 (99%)	-0.27	15 (0%) 82 74	95, 154, 227, 359	2 (0%)
1	BA	1541/1541 (100%)	-0.25	24 (1%) 72 62	110, 157, 208, 259	3 (0%)
2	CA	2867/2904 (98%)	-0.48	28 (0%) 82 74	69, 94, 175, 298	33 (1%)
2	DA	2869/2904 (98%)	-0.33	45 (1%) 72 62	86, 126, 219, 320	26 (0%)
3	CB	118/118 (100%)	-0.68	0 100 100	81, 108, 131, 159	0
3	DB	118/118 (100%)	-0.52	0 100 100	133, 191, 210, 222	0
4	AV	76/76 (100%)	0.18	8 (10%) 6 6	125, 166, 186, 201	0
4	AW	76/76 (100%)	-0.11	2 (2%) 56 46	119, 157, 180, 196	0
4	AY	76/76 (100%)	3.17	47 (61%) 0 0	120, 227, 240, 243	76 (100%)
4	BV	76/76 (100%)	0.10	6 (7%) 12 11	138, 193, 215, 225	0
4	BW	76/76 (100%)	-0.06	3 (3%) 39 31	142, 195, 208, 221	0
5	CC	271/271 (100%)	0.09	9 (3%) 46 37	71, 99, 117, 127	0
5	DC	271/271 (100%)	0.18	14 (5%) 27 24	98, 122, 143, 158	0
6	CD	209/209 (100%)	0.31	12 (5%) 23 20	70, 90, 110, 165	0
6	DD	209/209 (100%)	0.15	4 (1%) 66 58	89, 113, 130, 143	0
7	CE	181/181 (100%)	-0.05	2 (1%) 80 72	68, 95, 111, 133	0
7	DE	180/181 (99%)	0.13	3 (1%) 70 60	92, 128, 142, 151	0
8	CF	177/177 (100%)	-0.01	2 (1%) 80 72	113, 134, 158, 170	0
8	DF	177/177 (100%)	0.90	38 (21%) 0 1	136, 191, 224, 239	0
9	CG	176/176 (100%)	-0.03	3 (1%) 70 60	88, 105, 120, 148	0
9	DG	176/176 (100%)	0.46	15 (8%) 10 9	132, 150, 165, 176	0
10	CH	149/149 (100%)	0.32	9 (6%) 21 17	101, 151, 164, 168	0
10	DH	149/149 (100%)	1.00	29 (19%) 1 1	139, 210, 238, 243	0
11	C5	109/109 (100%)	0.38	12 (11%) 5 5	131, 173, 190, 197	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
12	CI	71/72 (98%)	1.30	18 (25%) 0 0	191, 212, 223, 225	71 (100%)
12	DI	72/72 (100%)	1.62	25 (34%) 0 0	262, 278, 291, 295	0
13	CJ	142/142 (100%)	0.13	0 100 100	68, 86, 104, 121	0
13	DJ	142/142 (100%)	0.23	8 (5%) 24 21	97, 114, 129, 147	0
14	CK	122/122 (100%)	-0.14	1 (0%) 86 79	77, 92, 114, 125	0
14	DK	122/122 (100%)	0.33	7 (5%) 23 20	97, 114, 129, 139	0
15	CL	143/143 (100%)	0.26	8 (5%) 24 21	74, 99, 116, 130	0
15	DL	143/143 (100%)	0.33	7 (4%) 29 25	98, 150, 167, 182	0
16	CM	135/136 (99%)	0.07	0 100 100	78, 95, 113, 127	0
16	DM	136/136 (100%)	0.96	25 (18%) 1 1	117, 138, 151, 164	0
17	CN	121/121 (100%)	-0.07	0 100 100	72, 87, 99, 100	0
17	DN	121/121 (100%)	0.04	3 (2%) 57 47	89, 106, 122, 146	0
18	CO	116/116 (100%)	0.13	3 (2%) 56 46	93, 111, 126, 131	0
18	DO	116/116 (100%)	1.16	29 (25%) 0 0	169, 188, 201, 208	0
19	CP	114/114 (100%)	0.20	6 (5%) 26 23	76, 96, 125, 135	0
19	DP	114/114 (100%)	0.31	4 (3%) 44 35	108, 121, 142, 154	0
20	CQ	117/117 (100%)	-0.27	0 100 100	68, 80, 97, 112	0
20	DQ	117/117 (100%)	-0.38	0 100 100	84, 108, 120, 127	0
21	CR	103/103 (100%)	0.09	0 100 100	70, 94, 109, 119	0
21	DR	103/103 (100%)	-0.03	2 (1%) 66 58	99, 116, 130, 141	0
22	CS	110/110 (100%)	0.44	6 (5%) 25 22	69, 87, 102, 121	0
22	DS	110/110 (100%)	0.51	8 (7%) 15 12	84, 104, 119, 131	0
23	CT	93/93 (100%)	0.47	8 (8%) 10 9	78, 97, 123, 138	0
23	DT	93/93 (100%)	0.32	3 (3%) 47 37	107, 127, 150, 166	0
24	CU	102/102 (100%)	0.14	2 (1%) 65 56	77, 96, 119, 137	0
24	DU	102/102 (100%)	0.71	13 (12%) 3 4	97, 123, 149, 165	0
25	CV	94/94 (100%)	0.16	6 (6%) 19 15	78, 101, 116, 119	0
25	DV	94/94 (100%)	0.14	3 (3%) 47 37	132, 146, 157, 161	0
26	CW	75/75 (100%)	0.33	4 (5%) 26 23	82, 95, 110, 155	0
26	DW	75/75 (100%)	0.83	13 (17%) 1 2	129, 148, 161, 172	0
27	CX	77/77 (100%)	0.25	3 (3%) 39 31	83, 98, 117, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DX	77/77 (100%)	0.70	4 (5%) 27 24	118, 135, 151, 156	0
28	CY	61/63 (96%)	-0.36	0 100 100	94, 109, 122, 145	0
28	DY	63/63 (100%)	0.11	3 (4%) 30 26	118, 133, 150, 154	0
29	CZ	58/58 (100%)	0.53	2 (3%) 45 36	74, 88, 108, 128	0
29	DZ	58/58 (100%)	0.82	5 (8%) 10 9	121, 137, 146, 152	0
30	C0	39/39 (100%)	0.91	6 (15%) 2 2	150, 167, 178, 182	39 (100%)
30	D0	39/39 (100%)	1.43	10 (25%) 0 0	179, 195, 204, 205	39 (100%)
31	C1	56/56 (100%)	-0.23	0 100 100	67, 91, 115, 127	0
31	D1	56/56 (100%)	-0.19	0 100 100	89, 110, 123, 135	0
32	C2	50/50 (100%)	2.64	31 (62%) 0 0	128, 140, 154, 158	0
32	D2	50/50 (100%)	4.10	39 (78%) 0 0	158, 174, 180, 184	50 (100%)
33	C3	46/46 (100%)	0.04	0 100 100	68, 87, 102, 108	0
33	D3	46/46 (100%)	0.16	0 100 100	101, 110, 120, 140	0
34	C4	61/62 (98%)	1.26	12 (19%) 1 1	79, 108, 121, 123	0
34	D4	62/62 (100%)	1.91	24 (38%) 0 0	135, 160, 171, 175	0
35	C6	38/38 (100%)	0.06	0 100 100	88, 103, 122, 149	0
35	D6	38/38 (100%)	1.27	13 (34%) 0 0	126, 137, 150, 178	0
36	AX	30/46 (65%)	2.49	15 (50%) 0 0	123, 203, 227, 257	1 (3%)
36	BX	30/46 (65%)	2.59	17 (56%) 0 0	140, 188, 233, 239	2 (6%)
37	AB	225/225 (100%)	0.54	27 (12%) 4 5	161, 181, 193, 207	0
37	BB	225/225 (100%)	0.31	15 (6%) 17 14	168, 197, 211, 218	0
38	AC	206/206 (100%)	-0.12	3 (1%) 73 64	147, 163, 176, 198	0
38	BC	206/206 (100%)	0.32	20 (9%) 7 7	140, 159, 171, 180	0
39	AD	205/205 (100%)	0.62	25 (12%) 4 5	138, 166, 180, 185	0
39	BD	205/205 (100%)	0.04	4 (1%) 65 56	126, 144, 156, 172	0
40	AE	150/150 (100%)	0.55	17 (11%) 5 5	121, 145, 160, 165	0
40	BE	150/150 (100%)	0.38	10 (6%) 17 14	126, 149, 161, 171	0
41	AF	100/100 (100%)	-0.28	1 (1%) 82 74	113, 136, 153, 159	0
41	BF	100/100 (100%)	0.63	15 (15%) 2 2	145, 158, 171, 178	0
42	AG	135/179 (75%)	0.66	15 (11%) 5 5	149, 173, 188, 200	0
42	BG	132/179 (73%)	0.79	24 (18%) 1 2	169, 196, 215, 225	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	AH	128/129 (99%)	0.31	8 (6%) 20 16	135, 147, 164, 171	0
43	BH	129/129 (100%)	0.14	4 (3%) 49 38	141, 154, 164, 172	0
44	AI	124/130 (95%)	1.00	18 (14%) 2 3	146, 178, 189, 200	0
44	BI	127/130 (97%)	0.73	12 (9%) 8 8	161, 193, 206, 210	0
45	AJ	98/98 (100%)	0.85	16 (16%) 1 2	149, 182, 197, 200	0
45	BJ	98/98 (100%)	0.65	12 (12%) 4 5	151, 176, 189, 193	0
46	AK	116/117 (99%)	-0.27	0 100 100	96, 131, 147, 161	0
46	BK	117/117 (100%)	0.61	16 (13%) 3 3	142, 170, 187, 192	0
47	AL	123/123 (100%)	0.91	20 (16%) 1 2	116, 134, 148, 176	0
47	BL	123/123 (100%)	0.48	9 (7%) 15 12	111, 128, 142, 153	0
48	AM	114/114 (100%)	0.36	11 (9%) 8 7	135, 168, 206, 227	0
48	BM	114/114 (100%)	0.32	8 (7%) 16 13	164, 190, 212, 243	0
49	AN	96/101 (95%)	0.69	12 (12%) 3 5	147, 168, 180, 189	0
49	BN	96/101 (95%)	0.38	7 (7%) 15 12	153, 166, 177, 185	0
50	AO	88/89 (98%)	-0.03	0 100 100	112, 131, 150, 159	0
50	BO	88/89 (98%)	0.32	8 (9%) 9 8	135, 153, 167, 172	0
51	AP	82/82 (100%)	1.95	35 (42%) 0 0	147, 169, 179, 195	0
51	BP	82/82 (100%)	1.16	25 (30%) 0 0	122, 148, 174, 189	0
52	AQ	80/80 (100%)	0.61	8 (10%) 7 7	126, 151, 163, 170	0
52	BQ	80/80 (100%)	0.94	16 (20%) 1 1	131, 150, 161, 173	0
53	AR	55/55 (100%)	0.66	4 (7%) 15 12	126, 139, 157, 161	0
53	BR	55/55 (100%)	0.94	8 (14%) 2 3	152, 162, 183, 200	0
54	AS	79/79 (100%)	0.64	8 (10%) 7 7	156, 170, 179, 184	0
54	BS	79/79 (100%)	0.91	16 (20%) 1 1	165, 179, 188, 193	0
55	AT	85/85 (100%)	0.15	3 (3%) 44 35	134, 154, 166, 176	0
55	BT	85/85 (100%)	0.74	5 (5%) 22 18	131, 151, 163, 170	0
All	All	20800/21025 (98%)	0.09	1191 (5%) 23 20	67, 135, 203, 359	342 (1%)

The worst 5 of 1191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	DA	2153	C	15.4
2	DA	2145	C	11.7

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Mol	Chain	Res	Type	RSRZ
4	AV	76	A	11.0
30	D0	22	MET	10.7
4	AY	17	U	10.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	AA	1640	1/1	0.06	0.66	127,127,127,127	0
56	MG	AA	1642	1/1	0.44	0.34	122,122,122,122	0
56	MG	AA	1610	1/1	0.50	0.30	114,114,114,114	0
56	MG	AA	1644	1/1	0.56	0.57	164,164,164,164	0
56	MG	BA	1628	1/1	0.56	1.70	120,120,120,120	0
56	MG	BA	1618	1/1	0.57	0.19	144,144,144,144	0
56	MG	DA	3097	1/1	0.64	0.33	78,78,78,78	0
57	ZN	D0	101	1/1	0.66	0.10	210,210,210,210	1
57	ZN	C0	101	1/1	0.67	0.10	177,177,177,177	1
56	MG	DA	3090	1/1	0.70	0.26	60,60,60,60	0
56	MG	BA	1641	1/1	0.70	0.29	134,134,134,134	0
56	MG	DA	3160	1/1	0.71	0.37	78,78,78,78	0
56	MG	DA	3094	1/1	0.72	0.48	77,77,77,77	0
56	MG	AA	1605	1/1	0.72	0.21	155,155,155,155	1
56	MG	CA	3090	1/1	0.72	0.39	83,83,83,83	0
56	MG	CA	3070	1/1	0.72	0.29	76,76,76,76	0
56	MG	CA	3068	1/1	0.73	0.45	101,101,101,101	0
56	MG	BA	1620	1/1	0.73	1.03	104,104,104,104	0
56	MG	BA	1632	1/1	0.74	0.06	191,191,191,191	0
56	MG	BA	1645	1/1	0.76	0.32	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	1636	1/1	0.77	0.35	99,99,99,99	0
56	MG	BA	1608	1/1	0.78	0.46	127,127,127,127	0
56	MG	BA	1639	1/1	0.80	0.18	155,155,155,155	1
56	MG	AA	1606	1/1	0.81	0.12	110,110,110,110	0
56	MG	BA	1649	1/1	0.81	0.15	72,72,72,72	0
56	MG	BA	1604	1/1	0.82	0.10	147,147,147,147	0
56	MG	C4	101	1/1	0.82	0.75	73,73,73,73	0
56	MG	DA	3087	1/1	0.83	0.41	104,104,104,104	0
56	MG	CA	3091	1/1	0.83	0.34	98,98,98,98	0
56	MG	AA	1638	1/1	0.84	0.34	55,55,55,55	0
56	MG	AA	1641	1/1	0.85	0.27	171,171,171,171	0
56	MG	BA	1626	1/1	0.85	0.54	114,114,114,114	0
56	MG	BA	1607	1/1	0.85	1.12	87,87,87,87	0
56	MG	AA	1604	1/1	0.85	0.10	182,182,182,182	1
56	MG	AA	1647	1/1	0.85	0.28	105,105,105,105	0
56	MG	BA	1648	1/1	0.86	0.45	109,109,109,109	0
56	MG	CA	3019	1/1	0.86	0.19	78,78,78,78	1
56	MG	AA	1632	1/1	0.86	0.36	151,151,151,151	0
56	MG	AA	1648	1/1	0.86	0.13	149,149,149,149	0
56	MG	DA	3076	1/1	0.87	0.17	76,76,76,76	1
56	MG	BA	1646	1/1	0.87	0.32	81,81,81,81	0
56	MG	DA	3141	1/1	0.87	0.20	151,151,151,151	1
56	MG	DA	3164	1/1	0.87	0.27	60,60,60,60	0
56	MG	DA	3154	1/1	0.87	0.94	68,68,68,68	0
56	MG	DA	3149	1/1	0.88	0.25	68,68,68,68	0
56	MG	DA	3112	1/1	0.88	0.19	101,101,101,101	0
56	MG	DA	3162	1/1	0.88	0.53	77,77,77,77	0
56	MG	DA	3110	1/1	0.88	0.18	108,108,108,108	0
56	MG	CA	3155	1/1	0.88	0.30	81,81,81,81	1
56	MG	DA	3029	1/1	0.88	0.14	72,72,72,72	1
56	MG	BA	1638	1/1	0.88	0.16	154,154,154,154	0
56	MG	DA	3101	1/1	0.89	0.15	125,125,125,125	1
56	MG	CA	3150	1/1	0.89	0.39	91,91,91,91	0
56	MG	CQ	801	1/1	0.89	0.36	56,56,56,56	0
56	MG	BA	1642	1/1	0.89	0.55	107,107,107,107	0
56	MG	DA	3165	1/1	0.89	1.17	60,60,60,60	0
56	MG	CA	3157	1/1	0.89	0.25	52,52,52,52	0
56	MG	BA	1610	1/1	0.89	0.10	147,147,147,147	0
56	MG	AA	1619	1/1	0.89	0.42	124,124,124,124	0
56	MG	DA	3060	1/1	0.89	0.66	73,73,73,73	1
56	MG	AA	1603	1/1	0.89	0.05	148,148,148,148	1
56	MG	CA	3112	1/1	0.89	0.11	73,73,73,73	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3100	1/1	0.89	0.74	76,76,76,76	0
56	MG	BA	1631	1/1	0.89	0.42	155,155,155,155	0
56	MG	AA	1630	1/1	0.89	0.27	158,158,158,158	0
56	MG	DA	3061	1/1	0.89	0.39	73,73,73,73	0
56	MG	DN	201	1/1	0.90	0.43	84,84,84,84	1
56	MG	BA	1615	1/1	0.90	0.14	115,115,115,115	0
56	MG	DA	3081	1/1	0.90	0.43	55,55,55,55	0
56	MG	BA	1605	1/1	0.90	0.31	104,104,104,104	0
56	MG	DQ	801	1/1	0.90	0.59	60,60,60,60	0
56	MG	DA	3158	1/1	0.90	0.62	64,64,64,64	0
56	MG	BA	1617	1/1	0.90	0.18	124,124,124,124	0
56	MG	CA	3164	1/1	0.90	0.28	60,60,60,60	0
56	MG	CA	3007	1/1	0.90	0.25	88,88,88,88	0
56	MG	DA	3135	1/1	0.91	0.61	92,92,92,92	0
56	MG	CA	3149	1/1	0.91	0.30	95,95,95,95	1
56	MG	AA	1602	1/1	0.91	0.25	177,177,177,177	0
56	MG	CA	3098	1/1	0.91	0.13	98,98,98,98	0
56	MG	CA	3127	1/1	0.91	0.25	42,42,42,42	0
56	MG	CA	3079	1/1	0.91	0.40	64,64,64,64	0
56	MG	BA	1635	1/1	0.91	0.12	141,141,141,141	0
56	MG	CA	3005	1/1	0.91	0.30	90,90,90,90	1
56	MG	CA	3166	1/1	0.91	0.69	60,60,60,60	0
56	MG	AA	1650	1/1	0.91	0.28	86,86,86,86	0
56	MG	BA	1637	1/1	0.91	0.08	150,150,150,150	0
56	MG	CA	3026	1/1	0.91	0.28	70,70,70,70	1
56	MG	DA	3083	1/1	0.91	1.01	73,73,73,73	0
56	MG	DA	3044	1/1	0.91	0.06	125,125,125,125	0
56	MG	DA	3106	1/1	0.91	0.10	90,90,90,90	1
56	MG	DA	3093	1/1	0.92	0.21	76,76,76,76	0
56	MG	DA	3163	1/1	0.92	0.38	60,60,60,60	0
56	MG	CA	3084	1/1	0.92	0.39	85,85,85,85	0
56	MG	DA	3159	1/1	0.92	0.21	95,95,95,95	0
56	MG	DA	3056	1/1	0.92	0.28	84,84,84,84	0
56	MG	DA	3103	1/1	0.92	0.09	95,95,95,95	1
56	MG	BA	1613	1/1	0.92	0.16	88,88,88,88	0
56	MG	CB	202	1/1	0.92	0.19	80,80,80,80	0
56	MG	CA	3087	1/1	0.92	0.27	74,74,74,74	0
56	MG	DA	3161	1/1	0.92	0.27	92,92,92,92	0
56	MG	DA	3128	1/1	0.92	0.14	121,121,121,121	1
56	MG	DA	3091	1/1	0.92	0.47	132,132,132,132	1
56	MG	DA	3026	1/1	0.92	0.17	102,102,102,102	0
56	MG	BA	1644	1/1	0.92	0.58	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DB	203	1/1	0.92	0.23	131,131,131,131	0
56	MG	BA	1647	1/1	0.92	0.36	104,104,104,104	0
56	MG	DA	3132	1/1	0.92	0.22	105,105,105,105	0
56	MG	DA	3152	1/1	0.92	0.38	103,103,103,103	0
56	MG	BA	1625	1/1	0.92	0.18	171,171,171,171	0
56	MG	CA	3165	1/1	0.93	0.78	60,60,60,60	0
56	MG	DA	3139	1/1	0.93	0.09	99,99,99,99	0
56	MG	CA	3001	1/1	0.93	0.26	62,62,62,62	1
56	MG	DA	3072	1/1	0.93	0.26	79,79,79,79	0
57	ZN	C6	101	1/1	0.93	0.09	98,98,98,98	0
56	MG	AA	1627	1/1	0.93	0.25	128,128,128,128	0
56	MG	CA	3160	1/1	0.93	0.15	68,68,68,68	0
56	MG	DA	3030	1/1	0.93	0.14	132,132,132,132	1
56	MG	DA	3043	1/1	0.93	0.17	104,104,104,104	0
56	MG	CA	3042	1/1	0.93	0.12	77,77,77,77	1
56	MG	BA	1621	1/1	0.94	0.24	91,91,91,91	0
56	MG	CA	3011	1/1	0.94	0.18	52,52,52,52	0
56	MG	CA	3151	1/1	0.94	0.51	75,75,75,75	0
56	MG	DA	3155	1/1	0.94	0.23	79,79,79,79	0
56	MG	DA	3002	1/1	0.94	0.15	89,89,89,89	0
56	MG	CA	3113	1/1	0.94	0.32	81,81,81,81	0
56	MG	BA	1606	1/1	0.94	0.34	100,100,100,100	0
56	MG	DA	3049	1/1	0.94	0.27	96,96,96,96	0
56	MG	DA	3150	1/1	0.94	0.18	28,28,28,28	1
56	MG	AA	1634	1/1	0.94	0.13	122,122,122,122	1
56	MG	DA	3013	1/1	0.94	0.42	51,51,51,51	0
56	MG	CA	3008	1/1	0.94	0.24	69,69,69,69	0
56	MG	DA	3037	1/1	0.94	0.73	83,83,83,83	0
56	MG	DA	3017	1/1	0.94	0.34	73,73,73,73	0
56	MG	DA	3140	1/1	0.94	0.21	98,98,98,98	1
56	MG	DA	3007	1/1	0.94	0.10	72,72,72,72	0
56	MG	CA	3142	1/1	0.94	0.26	57,57,57,57	0
56	MG	DA	3020	1/1	0.94	0.14	77,77,77,77	0
56	MG	BA	1629	1/1	0.94	0.17	161,161,161,161	0
56	MG	CA	3030	1/1	0.94	0.09	84,84,84,84	1
56	MG	AA	1613	1/1	0.94	0.42	104,104,104,104	0
56	MG	AA	1629	1/1	0.94	0.98	127,127,127,127	0
56	MG	CA	3040	1/1	0.94	0.25	88,88,88,88	1
56	MG	BA	1643	1/1	0.94	0.15	114,114,114,114	1
56	MG	DA	3092	1/1	0.94	0.24	102,102,102,102	0
56	MG	BA	1623	1/1	0.94	0.15	139,139,139,139	0
56	MG	DA	3005	1/1	0.94	0.07	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3069	1/1	0.94	0.16	166,166,166,166	0
56	MG	DA	3134	1/1	0.94	0.54	67,67,67,67	0
56	MG	DA	3023	1/1	0.94	0.17	100,100,100,100	1
56	MG	DA	3098	1/1	0.94	0.23	84,84,84,84	0
56	MG	CA	3138	1/1	0.94	0.07	102,102,102,102	0
56	MG	DA	3117	1/1	0.94	0.29	95,95,95,95	0
56	MG	DA	3166	1/1	0.94	0.12	137,137,137,137	0
56	MG	CA	3060	1/1	0.94	0.39	48,48,48,48	0
56	MG	CA	3046	1/1	0.94	0.13	77,77,77,77	1
56	MG	DA	3018	1/1	0.94	0.50	95,95,95,95	0
56	MG	CA	3082	1/1	0.94	0.37	84,84,84,84	0
56	MG	AA	1609	1/1	0.94	0.52	127,127,127,127	1
56	MG	CA	3162	1/1	0.94	0.60	56,56,56,56	1
56	MG	CA	3015	1/1	0.94	0.34	87,87,87,87	0
56	MG	CA	3159	1/1	0.95	0.15	93,93,93,93	0
56	MG	DA	3078	1/1	0.95	0.10	151,151,151,151	0
56	MG	AA	1611	1/1	0.95	0.25	165,165,165,165	1
56	MG	DA	3046	1/1	0.95	0.14	111,111,111,111	1
56	MG	DA	3107	1/1	0.95	0.28	112,112,112,112	0
56	MG	CA	3031	1/1	0.95	0.16	66,66,66,66	1
56	MG	AA	1643	1/1	0.95	0.19	85,85,85,85	0
56	MG	CA	3093	1/1	0.95	0.08	100,100,100,100	0
56	MG	CA	3039	1/1	0.95	0.15	62,62,62,62	0
56	MG	DA	3151	1/1	0.95	0.50	88,88,88,88	0
56	MG	AA	1631	1/1	0.95	0.20	148,148,148,148	1
56	MG	DA	3145	1/1	0.95	0.18	30,30,30,30	1
56	MG	CA	3044	1/1	0.95	0.21	86,86,86,86	1
56	MG	AA	1614	1/1	0.95	0.25	103,103,103,103	0
56	MG	CA	3021	1/1	0.95	0.17	78,78,78,78	0
56	MG	CA	3153	1/1	0.95	0.66	73,73,73,73	1
56	MG	BA	1640	1/1	0.95	0.12	145,145,145,145	0
56	MG	DA	3047	1/1	0.95	0.11	122,122,122,122	0
56	MG	BA	1612	1/1	0.95	0.47	116,116,116,116	0
56	MG	DA	3133	1/1	0.95	0.34	77,77,77,77	0
56	MG	DA	3071	1/1	0.95	0.17	101,101,101,101	1
56	MG	AA	1620	1/1	0.95	0.11	160,160,160,160	1
56	MG	DA	3131	1/1	0.95	0.45	78,78,78,78	0
56	MG	DA	3052	1/1	0.95	0.40	54,54,54,54	0
56	MG	AA	1635	1/1	0.95	0.09	133,133,133,133	1
56	MG	CA	3062	1/1	0.95	0.17	90,90,90,90	1
56	MG	CA	3023	1/1	0.95	0.10	80,80,80,80	1
56	MG	AA	1639	1/1	0.95	0.15	137,137,137,137	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3025	1/1	0.95	0.51	88,88,88,88	0
56	MG	DA	3127	1/1	0.95	0.37	43,43,43,43	0
56	MG	CA	3119	1/1	0.96	0.15	81,81,81,81	1
56	MG	CN	201	1/1	0.96	0.12	86,86,86,86	1
56	MG	CA	3156	1/1	0.96	0.26	84,84,84,84	0
56	MG	CA	3017	1/1	0.96	0.21	64,64,64,64	0
56	MG	AA	1622	1/1	0.96	0.20	92,92,92,92	0
56	MG	DA	3136	1/1	0.96	0.46	78,78,78,78	0
56	MG	BA	1601	1/1	0.96	0.21	115,115,115,115	0
56	MG	DA	3051	1/1	0.96	0.33	99,99,99,99	1
56	MG	CA	3148	1/1	0.96	0.18	98,98,98,98	0
56	MG	DA	3075	1/1	0.96	0.19	90,90,90,90	0
56	MG	DA	3119	1/1	0.96	0.11	92,92,92,92	0
56	MG	DA	3137	1/1	0.96	0.44	68,68,68,68	0
56	MG	CA	3051	1/1	0.96	0.11	82,82,82,82	1
56	MG	CA	3104	1/1	0.96	0.18	85,85,85,85	1
56	MG	BA	1624	1/1	0.96	0.08	119,119,119,119	0
56	MG	DA	3108	1/1	0.96	0.16	97,97,97,97	0
56	MG	DA	3004	1/1	0.96	0.09	122,122,122,122	0
56	MG	DA	3105	1/1	0.96	0.10	92,92,92,92	0
56	MG	AA	1633	1/1	0.96	0.07	108,108,108,108	1
56	MG	DA	3070	1/1	0.96	0.14	69,69,69,69	0
56	MG	DA	3016	1/1	0.96	0.17	90,90,90,90	0
56	MG	DA	3122	1/1	0.96	0.17	103,103,103,103	0
56	MG	CA	3088	1/1	0.96	0.39	83,83,83,83	1
56	MG	DA	3063	1/1	0.96	0.16	105,105,105,105	0
56	MG	CA	3013	1/1	0.96	0.57	55,55,55,55	0
56	MG	CA	3120	1/1	0.96	0.09	71,71,71,71	1
56	MG	CA	3134	1/1	0.96	0.27	75,75,75,75	0
56	MG	DA	3123	1/1	0.96	0.11	120,120,120,120	1
56	MG	AA	1616	1/1	0.96	0.34	92,92,92,92	0
56	MG	CA	3037	1/1	0.96	0.31	40,40,40,40	0
56	MG	CA	3129	1/1	0.96	0.18	80,80,80,80	0
56	MG	CA	3154	1/1	0.96	0.28	78,78,78,78	1
56	MG	AA	1636	1/1	0.96	0.10	104,104,104,104	1
56	MG	AA	1607	1/1	0.96	0.35	98,98,98,98	0
56	MG	BA	1627	1/1	0.96	0.45	132,132,132,132	0
56	MG	CA	3128	1/1	0.96	0.16	56,56,56,56	0
56	MG	DA	3019	1/1	0.96	0.11	102,102,102,102	1
56	MG	CA	3100	1/1	0.96	0.36	66,66,66,66	0
56	MG	CN	202	1/1	0.96	0.28	64,64,64,64	0
56	MG	DB	201	1/1	0.96	0.04	204,204,204,204	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3072	1/1	0.96	0.14	73,73,73,73	1
56	MG	CA	3094	1/1	0.96	0.26	74,74,74,74	0
56	MG	CA	3167	1/1	0.96	0.08	102,102,102,102	0
56	MG	CA	3140	1/1	0.96	0.14	61,61,61,61	0
56	MG	AA	1608	1/1	0.96	0.52	106,106,106,106	0
56	MG	AA	1646	1/1	0.96	0.29	132,132,132,132	0
57	ZN	D6	101	1/1	0.96	0.07	128,128,128,128	0
56	MG	CA	3055	1/1	0.97	0.12	71,71,71,71	0
56	MG	CA	3106	1/1	0.97	0.14	82,82,82,82	0
56	MG	AA	1615	1/1	0.97	0.32	103,103,103,103	0
56	MG	CA	3074	1/1	0.97	0.06	70,70,70,70	0
56	MG	DA	3109	1/1	0.97	0.09	123,123,123,123	0
56	MG	DA	3089	1/1	0.97	0.12	115,115,115,115	0
56	MG	CA	3107	1/1	0.97	0.16	83,83,83,83	1
56	MG	CA	3145	1/1	0.97	0.21	69,69,69,69	0
56	MG	CA	3036	1/1	0.97	0.10	80,80,80,80	1
56	MG	BA	1630	1/1	0.97	0.13	160,160,160,160	0
56	MG	CA	3136	1/1	0.97	0.17	66,66,66,66	0
56	MG	BA	1614	1/1	0.97	0.10	128,128,128,128	1
56	MG	CA	3147	1/1	0.97	0.18	93,93,93,93	0
56	MG	DA	3036	1/1	0.97	0.31	102,102,102,102	0
56	MG	DA	3146	1/1	0.97	0.16	96,96,96,96	0
56	MG	DA	3077	1/1	0.97	0.12	90,90,90,90	0
56	MG	AA	1612	1/1	0.97	0.12	128,128,128,128	0
56	MG	CA	3064	1/1	0.97	0.11	70,70,70,70	0
56	MG	DA	3009	1/1	0.97	0.13	106,106,106,106	0
56	MG	DA	3021	1/1	0.97	0.12	92,92,92,92	1
56	MG	CA	3132	1/1	0.97	0.13	67,67,67,67	0
56	MG	CA	3137	1/1	0.97	0.27	67,67,67,67	1
56	MG	CA	3006	1/1	0.97	0.09	90,90,90,90	1
56	MG	BA	1619	1/1	0.97	0.04	133,133,133,133	0
56	MG	DA	3079	1/1	0.97	0.17	144,144,144,144	0
56	MG	DA	3147	1/1	0.97	0.14	100,100,100,100	1
56	MG	CA	3058	1/1	0.97	0.15	74,74,74,74	1
56	MG	DB	202	1/1	0.97	0.27	95,95,95,95	0
56	MG	CC	301	1/1	0.97	0.11	74,74,74,74	0
56	MG	DA	3068	1/1	0.97	0.46	84,84,84,84	0
56	MG	BA	1609	1/1	0.97	0.18	110,110,110,110	0
56	MG	AA	1645	1/1	0.97	0.15	148,148,148,148	0
56	MG	CA	3075	1/1	0.97	0.26	78,78,78,78	1
56	MG	DA	3039	1/1	0.97	0.11	74,74,74,74	0
56	MG	CA	3130	1/1	0.97	0.13	62,62,62,62	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3144	1/1	0.97	0.25	57,57,57,57	0
56	MG	CA	3110	1/1	0.97	0.14	86,86,86,86	1
56	MG	CA	3025	1/1	0.97	0.11	66,66,66,66	1
56	MG	BA	1602	1/1	0.97	0.10	132,132,132,132	0
56	MG	BA	1622	1/1	0.97	0.30	105,105,105,105	0
56	MG	CA	3105	1/1	0.97	0.18	85,85,85,85	1
56	MG	AA	1621	1/1	0.97	0.14	90,90,90,90	0
56	MG	CA	3141	1/1	0.97	0.24	67,67,67,67	1
56	MG	DA	3050	1/1	0.97	0.24	79,79,79,79	0
56	MG	CA	3069	1/1	0.97	0.13	69,69,69,69	0
56	MG	CA	3045	1/1	0.97	0.06	83,83,83,83	1
56	MG	DA	3116	1/1	0.97	0.17	93,93,93,93	1
56	MG	DA	3156	1/1	0.97	0.12	109,109,109,109	0
56	MG	AA	1601	1/1	0.97	0.18	102,102,102,102	0
56	MG	DA	3096	1/1	0.97	0.09	78,78,78,78	1
56	MG	CA	3047	1/1	0.97	0.12	94,94,94,94	0
56	MG	CA	3111	1/1	0.97	0.11	74,74,74,74	0
56	MG	AA	1628	1/1	0.97	0.26	143,143,143,143	0
56	MG	DA	3022	1/1	0.97	0.14	86,86,86,86	0
56	MG	AA	1625	1/1	0.97	0.11	100,100,100,100	1
56	MG	DA	3042	1/1	0.97	0.14	97,97,97,97	0
56	MG	CB	203	1/1	0.97	0.17	77,77,77,77	0
56	MG	CA	3050	1/1	0.97	0.27	56,56,56,56	0
56	MG	CA	3018	1/1	0.97	0.08	90,90,90,90	1
56	MG	CA	3143	1/1	0.97	0.29	63,63,63,63	0
56	MG	DA	3065	1/1	0.97	0.12	85,85,85,85	0
56	MG	DA	3067	1/1	0.97	0.33	129,129,129,129	0
56	MG	DA	3125	1/1	0.97	0.11	92,92,92,92	1
56	MG	DA	3066	1/1	0.97	0.37	81,81,81,81	0
56	MG	DA	3035	1/1	0.97	0.18	96,96,96,96	0
56	MG	CA	3135	1/1	0.97	0.41	55,55,55,55	0
56	MG	BA	1603	1/1	0.97	0.14	121,121,121,121	0
56	MG	BA	1634	1/1	0.97	0.14	129,129,129,129	0
56	MG	DA	3011	1/1	0.97	0.12	80,80,80,80	0
56	MG	DA	3038	1/1	0.98	0.17	75,75,75,75	1
56	MG	CA	3152	1/1	0.98	0.28	57,57,57,57	0
56	MG	DA	3115	1/1	0.98	0.11	139,139,139,139	0
56	MG	CA	3024	1/1	0.98	0.33	59,59,59,59	0
56	MG	DA	3001	1/1	0.98	0.15	71,71,71,71	1
56	MG	DA	3111	1/1	0.98	0.05	108,108,108,108	1
56	MG	DA	3143	1/1	0.98	0.09	53,53,53,53	0
56	MG	DA	3085	1/1	0.98	0.14	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3053	1/1	0.98	0.16	72,72,72,72	1
56	MG	DA	3084	1/1	0.98	0.37	85,85,85,85	0
56	MG	DA	3113	1/1	0.98	0.28	85,85,85,85	0
56	MG	AA	1624	1/1	0.98	0.20	130,130,130,130	0
56	MG	CA	3061	1/1	0.98	0.17	95,95,95,95	1
56	MG	CA	3077	1/1	0.98	0.13	101,101,101,101	0
56	MG	BA	1633	1/1	0.98	0.23	102,102,102,102	0
56	MG	AA	1637	1/1	0.98	0.09	186,186,186,186	0
56	MG	DA	3034	1/1	0.98	0.11	99,99,99,99	0
56	MG	DA	3014	1/1	0.98	0.08	95,95,95,95	1
56	MG	CA	3133	1/1	0.98	0.48	47,47,47,47	0
56	MG	CA	3059	1/1	0.98	0.10	60,60,60,60	0
56	MG	CA	3096	1/1	0.98	0.19	68,68,68,68	1
56	MG	CA	3004	1/1	0.98	0.18	78,78,78,78	0
56	MG	CA	3121	1/1	0.98	0.18	86,86,86,86	1
56	MG	DA	3073	1/1	0.98	0.22	93,93,93,93	1
56	MG	CA	3163	1/1	0.98	0.18	81,81,81,81	1
56	MG	CA	3123	1/1	0.98	0.24	83,83,83,83	1
56	MG	DA	3028	1/1	0.98	0.25	76,76,76,76	0
56	MG	DA	3054	1/1	0.98	0.12	70,70,70,70	0
56	MG	CA	3035	1/1	0.98	0.36	37,37,37,37	0
56	MG	DA	3118	1/1	0.98	0.30	103,103,103,103	0
56	MG	CA	3020	1/1	0.98	0.16	45,45,45,45	1
56	MG	CA	3083	1/1	0.98	0.29	81,81,81,81	1
56	MG	DA	3057	1/1	0.98	0.21	101,101,101,101	0
56	MG	DA	3012	1/1	0.98	0.07	81,81,81,81	0
56	MG	CA	3049	1/1	0.98	0.25	73,73,73,73	0
56	MG	DA	3024	1/1	0.98	0.27	98,98,98,98	0
56	MG	BA	1611	1/1	0.98	0.49	130,130,130,130	0
56	MG	DA	3080	1/1	0.98	0.18	98,98,98,98	1
56	MG	CA	3022	1/1	0.98	0.09	75,75,75,75	1
56	MG	DA	3082	1/1	0.98	0.34	106,106,106,106	0
56	MG	CA	3043	1/1	0.98	0.30	59,59,59,59	0
56	MG	DA	3144	1/1	0.98	0.23	112,112,112,112	0
56	MG	CA	3041	1/1	0.98	0.08	67,67,67,67	1
56	MG	DA	3130	1/1	0.98	0.55	100,100,100,100	0
56	MG	DA	3031	1/1	0.98	0.15	116,116,116,116	0
56	MG	CA	3124	1/1	0.98	0.18	75,75,75,75	1
56	MG	CA	3085	1/1	0.98	0.18	71,71,71,71	0
56	MG	CA	3065	1/1	0.98	0.10	76,76,76,76	1
56	MG	DA	3129	1/1	0.98	0.11	92,92,92,92	1
56	MG	CA	3028	1/1	0.98	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3153	1/1	0.98	0.12	93,93,93,93	0
56	MG	CA	3076	1/1	0.98	0.06	68,68,68,68	0
56	MG	CA	3114	1/1	0.98	0.15	73,73,73,73	1
56	MG	CA	3158	1/1	0.98	0.11	73,73,73,73	0
56	MG	DA	3102	1/1	0.98	0.07	98,98,98,98	1
56	MG	CA	3056	1/1	0.98	0.11	73,73,73,73	0
56	MG	DA	3086	1/1	0.98	0.11	125,125,125,125	1
56	MG	DA	3040	1/1	0.98	0.26	90,90,90,90	1
56	MG	CA	3101	1/1	0.98	0.09	84,84,84,84	0
56	MG	DA	3015	1/1	0.98	0.46	73,73,73,73	0
56	MG	DA	3114	1/1	0.98	0.21	98,98,98,98	1
56	MG	DA	3032	1/1	0.98	0.25	93,93,93,93	0
56	MG	CA	3014	1/1	0.98	0.24	72,72,72,72	1
56	MG	CA	3131	1/1	0.98	0.32	53,53,53,53	0
56	MG	CA	3146	1/1	0.98	0.34	78,78,78,78	0
56	MG	CA	3010	1/1	0.98	0.21	89,89,89,89	1
56	MG	AA	1649	1/1	0.98	0.21	140,140,140,140	0
56	MG	CA	3002	1/1	0.98	0.17	67,67,67,67	1
56	MG	DA	3126	1/1	0.98	0.08	93,93,93,93	0
56	MG	CA	3054	1/1	0.98	0.38	65,65,65,65	0
56	MG	CA	3016	1/1	0.98	0.80	20,20,20,20	0
56	MG	DA	3003	1/1	0.98	0.04	121,121,121,121	0
56	MG	DA	3157	1/1	0.99	0.48	83,83,83,83	0
56	MG	DA	3059	1/1	0.99	0.18	94,94,94,94	1
56	MG	CA	3095	1/1	0.99	0.08	86,86,86,86	1
56	MG	CA	3125	1/1	0.99	0.05	82,82,82,82	1
56	MG	CA	3003	1/1	0.99	0.19	82,82,82,82	0
56	MG	CA	3071	1/1	0.99	0.10	77,77,77,77	0
56	MG	CA	3126	1/1	0.99	0.26	67,67,67,67	0
56	MG	CA	3116	1/1	0.99	0.06	83,83,83,83	1
56	MG	DA	3148	1/1	0.99	0.12	88,88,88,88	0
56	MG	DA	3062	1/1	0.99	0.19	95,95,95,95	1
56	MG	DA	3006	1/1	0.99	0.09	114,114,114,114	1
56	MG	CB	201	1/1	0.99	0.16	113,113,113,113	1
56	MG	CA	3122	1/1	0.99	0.18	77,77,77,77	1
56	MG	CA	3097	1/1	0.99	0.21	67,67,67,67	1
56	MG	DA	3041	1/1	0.99	0.14	100,100,100,100	0
56	MG	BA	1616	1/1	0.99	0.16	136,136,136,136	0
56	MG	DA	3058	1/1	0.99	0.23	83,83,83,83	0
56	MG	CA	3080	1/1	0.99	0.10	62,62,62,62	1
56	MG	CA	3029	1/1	0.99	0.23	57,57,57,57	1
56	MG	CA	3027	1/1	0.99	0.07	74,74,74,74	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3055	1/1	0.99	0.15	85,85,85,85	0
56	MG	DA	3095	1/1	0.99	0.08	76,76,76,76	0
56	MG	CA	3057	1/1	0.99	0.05	78,78,78,78	1
56	MG	CA	3048	1/1	0.99	0.14	80,80,80,80	1
56	MG	CA	3118	1/1	0.99	0.23	82,82,82,82	1
56	MG	DA	3053	1/1	0.99	0.06	98,98,98,98	1
56	MG	DA	3138	1/1	0.99	0.59	58,58,58,58	0
56	MG	AA	1626	1/1	0.99	0.25	107,107,107,107	0
56	MG	DA	3074	1/1	0.99	0.22	92,92,92,92	0
56	MG	CA	3109	1/1	0.99	0.09	90,90,90,90	1
56	MG	CA	3052	1/1	0.99	0.17	76,76,76,76	1
56	MG	CA	3099	1/1	0.99	0.09	84,84,84,84	1
56	MG	CA	3092	1/1	0.99	0.10	85,85,85,85	0
56	MG	AA	1617	1/1	0.99	0.21	107,107,107,107	0
56	MG	CA	3012	1/1	0.99	0.16	67,67,67,67	1
56	MG	AA	1623	1/1	0.99	0.06	104,104,104,104	1
56	MG	DA	3142	1/1	0.99	0.14	100,100,100,100	0
56	MG	CA	3073	1/1	0.99	0.22	73,73,73,73	1
56	MG	CA	3034	1/1	0.99	0.13	68,68,68,68	0
56	MG	CA	3086	1/1	0.99	0.14	93,93,93,93	1
56	MG	DA	3099	1/1	0.99	0.19	114,114,114,114	1
56	MG	CA	3033	1/1	0.99	0.18	65,65,65,65	0
56	MG	CA	3089	1/1	0.99	0.14	92,92,92,92	1
56	MG	CA	3009	1/1	0.99	0.12	69,69,69,69	0
56	MG	CA	3161	1/1	0.99	0.07	97,97,97,97	0
56	MG	CA	3102	1/1	0.99	0.23	55,55,55,55	0
56	MG	CA	3081	1/1	0.99	0.12	73,73,73,73	1
56	MG	DA	3064	1/1	0.99	0.10	95,95,95,95	0
56	MG	CA	3066	1/1	0.99	0.15	80,80,80,80	1
56	MG	CA	3117	1/1	0.99	0.33	49,49,49,49	0
56	MG	DA	3124	1/1	0.99	0.13	104,104,104,104	0
56	MG	DA	3008	1/1	0.99	0.08	103,103,103,103	1
56	MG	DA	3048	1/1	0.99	0.12	93,93,93,93	1
56	MG	DA	3010	1/1	0.99	0.12	97,97,97,97	0
56	MG	CA	3139	1/1	0.99	0.14	88,88,88,88	0
56	MG	DA	3033	1/1	0.99	0.12	104,104,104,104	0
56	MG	DA	3121	1/1	0.99	0.11	100,100,100,100	1
56	MG	DA	3088	1/1	0.99	0.38	88,88,88,88	1
56	MG	CA	3078	1/1	0.99	0.11	102,102,102,102	1
56	MG	DA	3045	1/1	0.99	0.18	102,102,102,102	0
56	MG	DA	3104	1/1	0.99	0.21	101,101,101,101	0
56	MG	DA	3027	1/1	0.99	0.19	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1618	1/1	0.99	0.11	106,106,106,106	1
56	MG	CA	3067	1/1	0.99	0.12	68,68,68,68	1
56	MG	CA	3108	1/1	0.99	0.15	71,71,71,71	0
56	MG	CA	3038	1/1	0.99	0.18	67,67,67,67	0
56	MG	CA	3032	1/1	0.99	0.17	79,79,79,79	0
56	MG	DA	3120	1/1	1.00	0.12	98,98,98,98	0
56	MG	CA	3103	1/1	1.00	0.20	80,80,80,80	1
56	MG	CA	3115	1/1	1.00	0.13	70,70,70,70	1
56	MG	CA	3063	1/1	1.00	0.09	94,94,94,94	1

6.5 Other polymers [i](#)

There are no such residues in this entry.