wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 06:54 PM EST

PDB ID	:	1VQ7
Title	:	The structure of the transition state analogue "DCA" bound to the large ribosomal subunit of haloarcula marismortui
Authors	:	Schmeing, T.M.; Steitz, T.A.
Deposited on	:	2004-12-16
Resolution	:	2.50 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

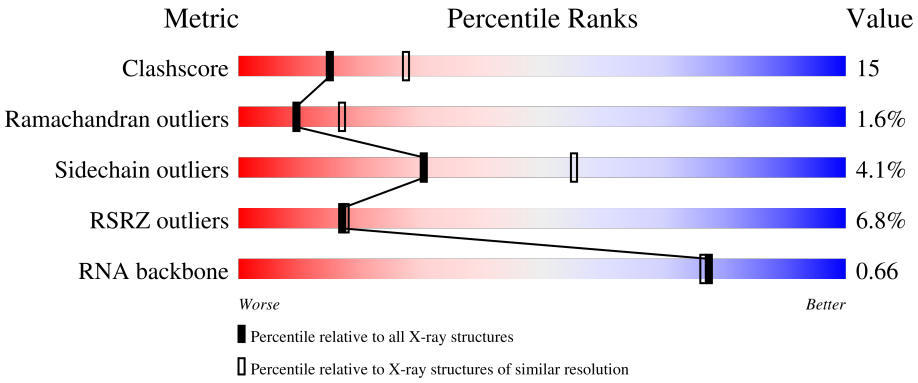
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 of 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 <=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	0	2922	2% 60% 29% 5% • 6%
2	9	122	4% 58% 32% 8% •
3	4	8	38% 62%
4	A	240	7% 64% 30% • •
5	B	338	3% 50% 44% 5%

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Mol	Chain	Length	Quality of chain
6	C	246	2% 62% 33% 5%
7	D	177	42% 34% 40% 6% 21%
8	E	178	15% 53% 43%
9	F	120	22% 62% 32%
10	G	348	5% 5% 92%
11	H	171	5% 58% 33% 6%
12	J	145	61% 30% 6%
13	K	132	2% 61% 36%
14	L	165	17% 51% 34% 12%
15	M	194	% 71% 27%
16	N	187	19% 49% 45% 6%
17	O	116	3% 71% 26%
18	P	149	3% 58% 36%
19	Q	96	2% 72% 25%
20	R	155	67% 28%
21	S	85	2% 64% 31% 5%
22	T	120	2% 54% 40% 5%
23	U	66	3% 41% 39% 20%
24	V	71	31% 42% 45% 8%
25	W	154	49% 47%
26	X	92	13% 50% 35% 11%
27	Y	241	3% 39% 18% 41%
28	Z	83	6% 53% 33% 12%
29	1	57	72% 26%
30	2	50	28% 54% 36% 8%

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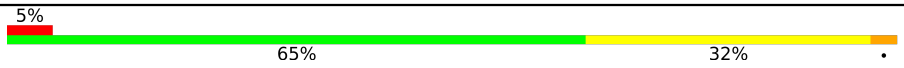
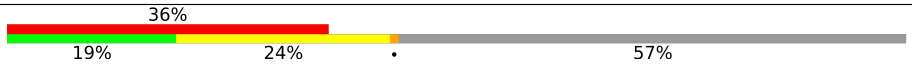
Mol	Chain	Length	Quality of chain
31	3	92	
32	I	162	

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
33	MG	0	8092	-	-	-	X
35	NA	S	9112	-	-	-	X

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99063 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 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2754	59021	26350	10878	19048	2745	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	9	122	2600	1160	472	847	121	0	0	0

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(5AA)P*(2OP)P*(PAE)P*AP*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	8	130	63	23	39	5	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	237	1753	1072	352	324	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 8 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501
M	194	ALA	GLY	conflict	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	115	Total 865	C 529	N 161	O 175	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	143	Total 1136	C 683	N 229	O 224	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	95	Total 735	C 450	N 141	O 144	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	150	Total 1149	C 713	N 209	O 223	S 4	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	81	Total 641	C 389	N 111	O 138	S 3	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	119	Total 950	C 568	N 180	O 202	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	53	Total 410	C 244	N 75	O 86	S 5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 26 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 27 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	Y	142	Total	C	N	O	0	0	0
			1130	686	228	216			

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
33	9	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	3	Total	K	0	0
			3	3		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	72	Total Na 72 72	0	0
35	9	2	Total Na 2 2	0	0
35	A	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	H	2	Total Na 2 2	0	0
35	J	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	T	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	11	Total Cl 11 11	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5809	Total O 5809 5809	0	0
38	9	137	Total O 137 137	0	0
38	4	8	Total O 8 8	0	0
38	A	119	Total O 119 119	0	0
38	B	153	Total O 153 153	0	0
38	C	168	Total O 168 168	0	0
38	D	47	Total O 47 47	0	0
38	E	43	Total O 43 43	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	F	23	Total O 23 23	0	0
38	G	18	Total O 18 18	0	0
38	H	65	Total O 65 65	0	0
38	J	51	Total O 51 51	0	0
38	K	58	Total O 58 58	0	0
38	L	82	Total O 82 82	0	0
38	M	116	Total O 116 116	0	0
38	N	63	Total O 63 63	0	0
38	O	42	Total O 42 42	0	0
38	P	64	Total O 64 64	0	0
38	Q	51	Total O 51 51	0	0
38	R	84	Total O 84 84	0	0
38	S	30	Total O 30 30	0	0
38	T	42	Total O 42 42	0	0
38	U	29	Total O 29 29	0	0
38	V	14	Total O 14 14	0	0
38	W	68	Total O 68 68	0	0
38	X	27	Total O 27 27	0	0
38	Y	96	Total O 96 96	0	0
38	Z	32	Total O 32 32	0	0
38	1	53	Total O 53 53	0	0

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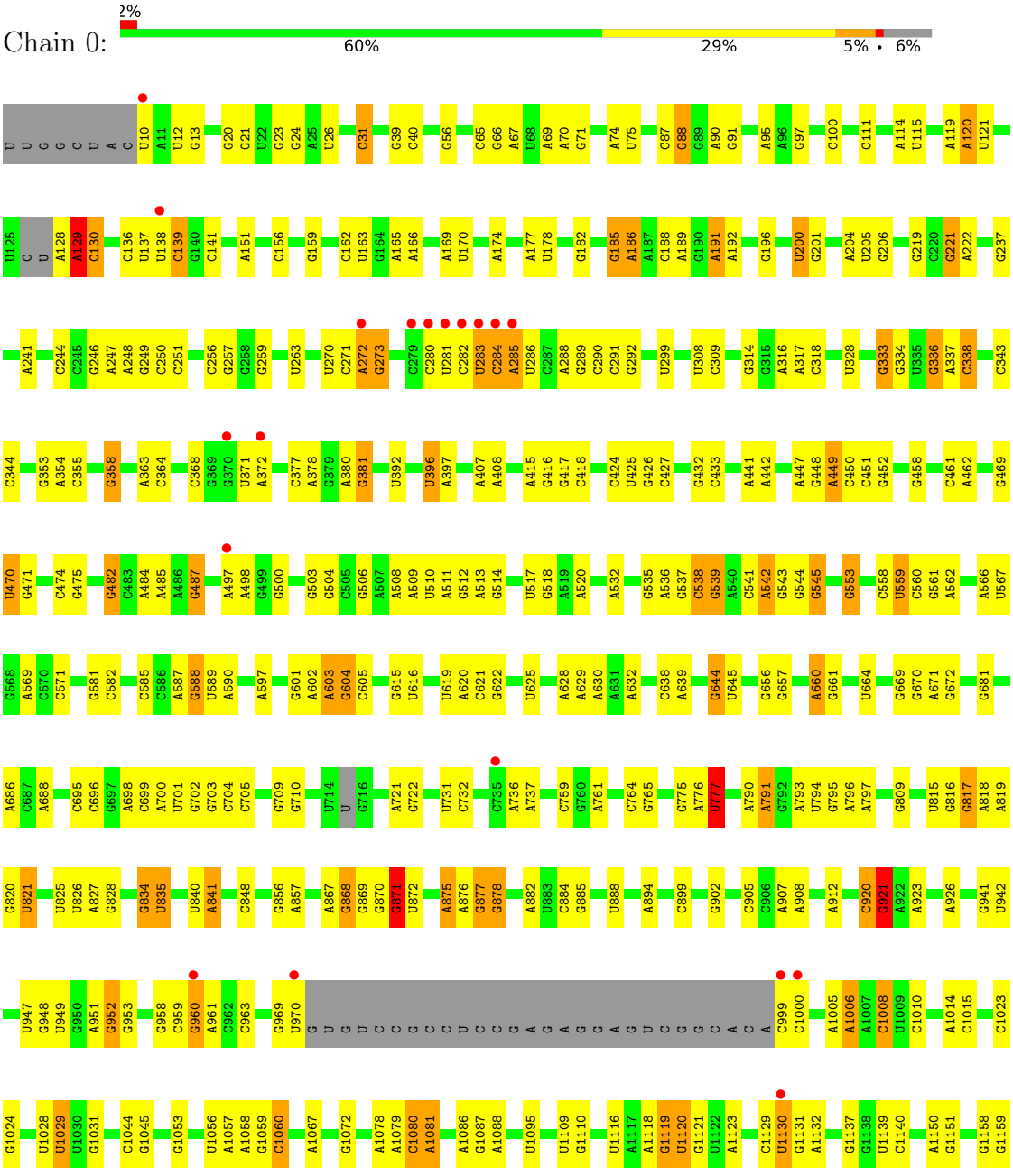
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	2	40	Total O 40 40	0	0
38	3	74	Total O 74 74	0	0
38	I	9	Total O 9 9	0	0

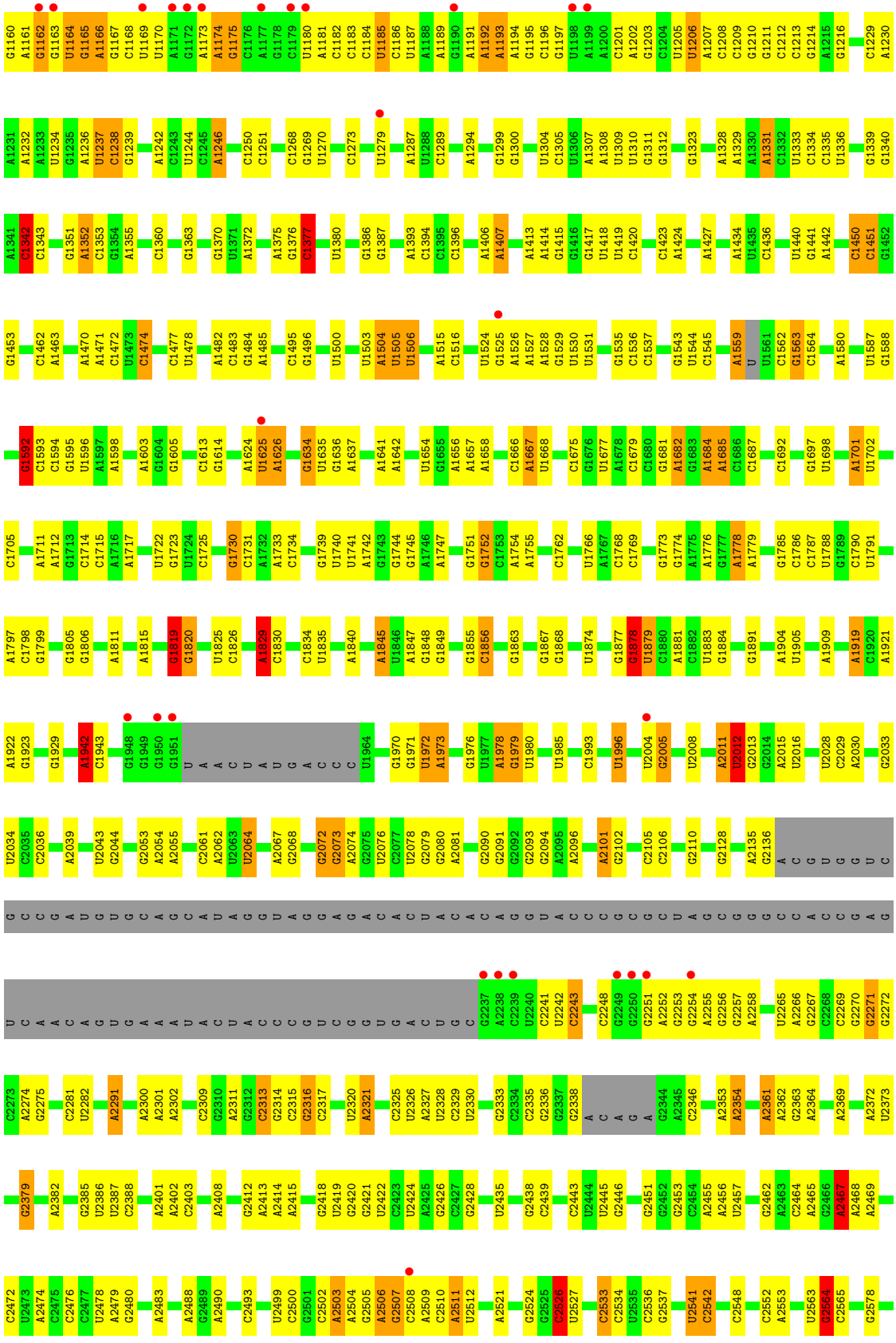
3 Residue-property plots (i)

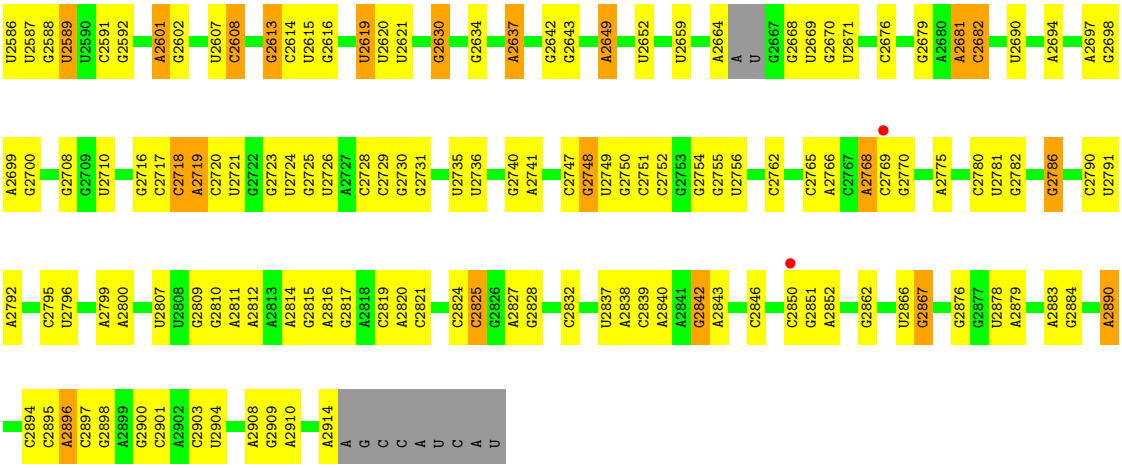
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 23S ribosomal rna

Chain 0:

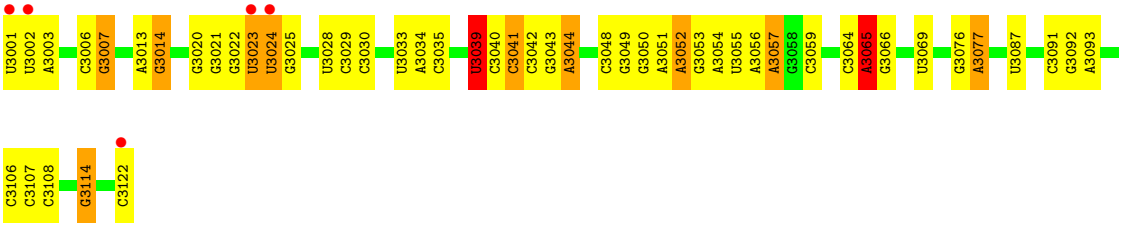






• Molecule 2: 5S ribosomal RNA

Chain 9:

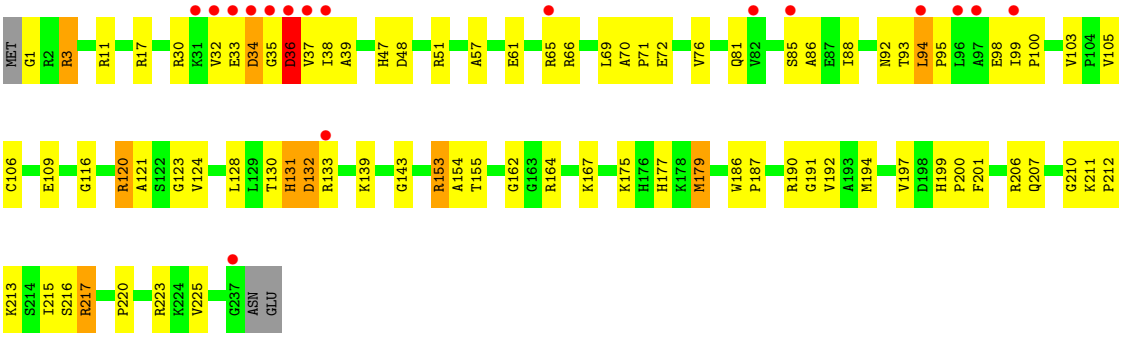


• Molecule 3: 5'-R(*CP*CP*(5AA)P*(2OP)P*(PAE)P*AP*C*C)-3')

Chain 4:

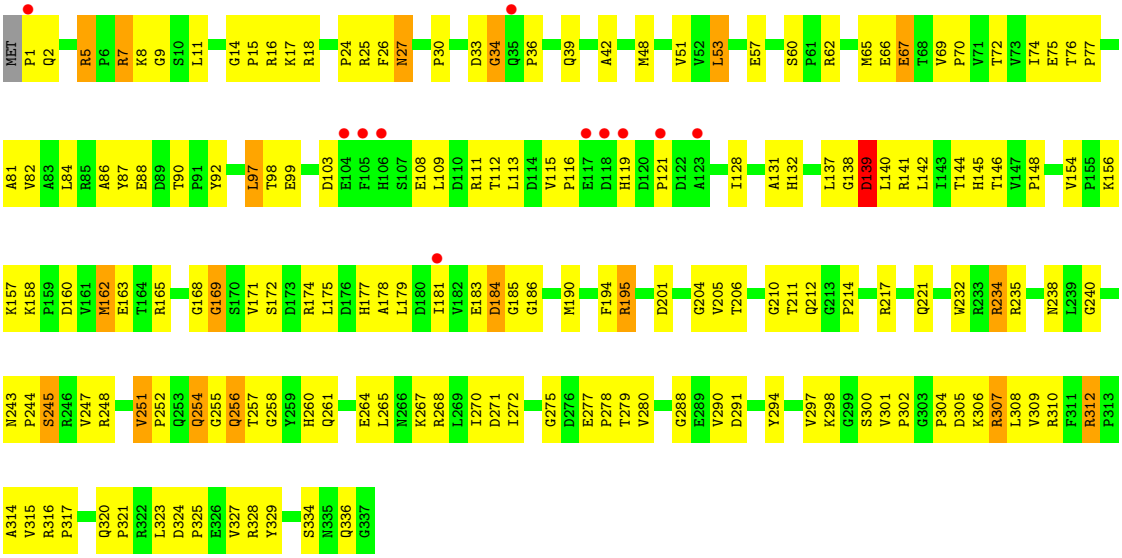
• Molecule 4: 50S ribosomal protein L2P

Chain A:



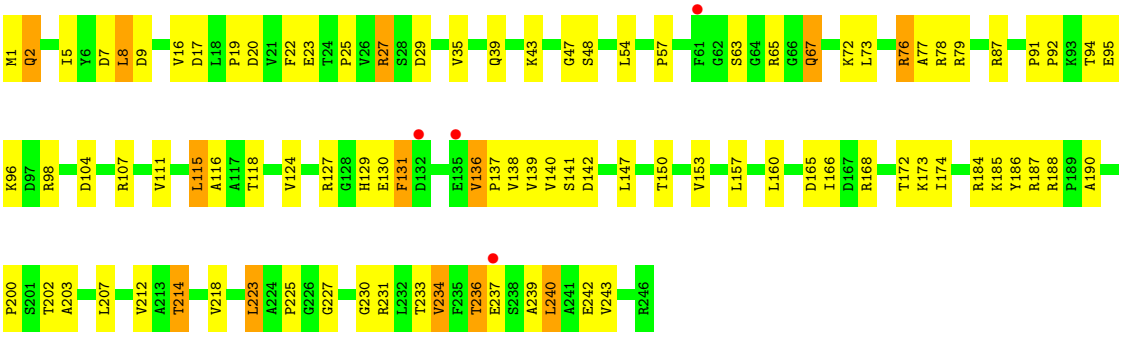
• Molecule 5: 50S ribosomal protein L3P

Chain B:



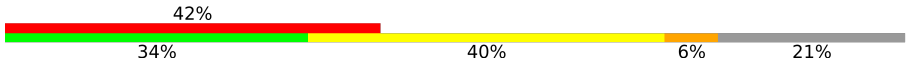
• Molecule 6: 50S ribosomal protein L4E

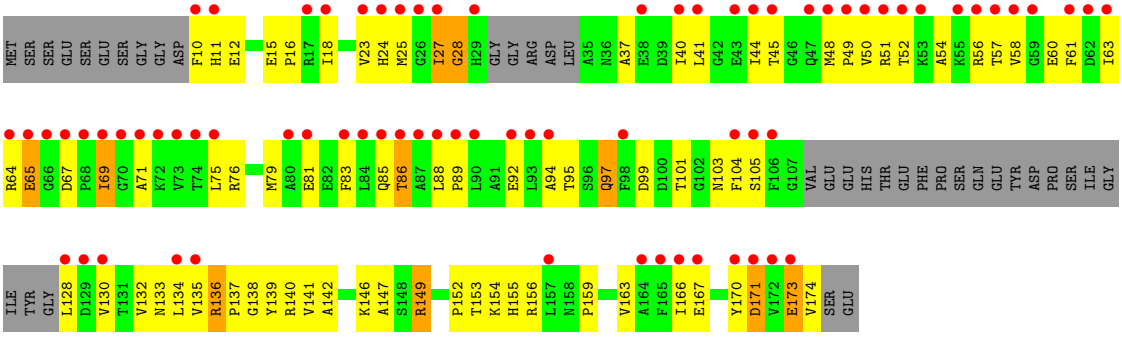
Chain C:



• Molecule 7: 50S ribosomal protein L5P

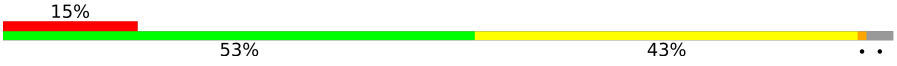
Chain D:

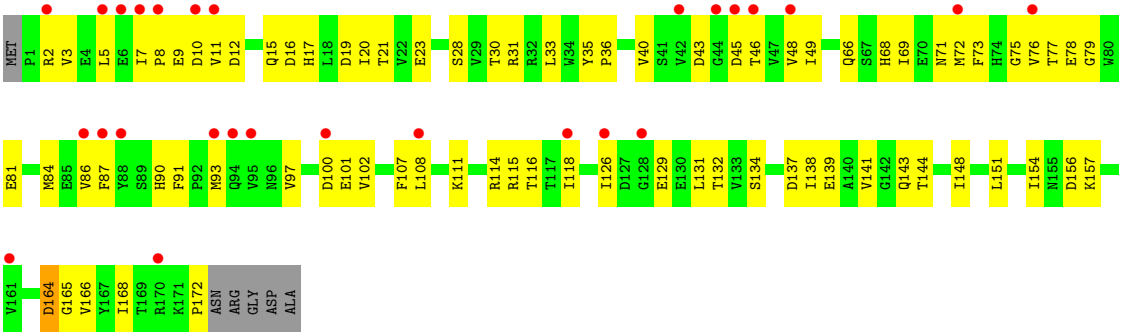




• Molecule 8: 50S ribosomal protein L6P

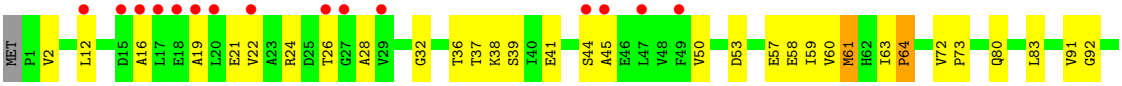
Chain E:

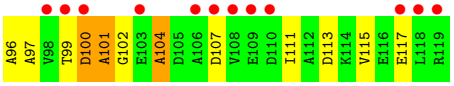




• Molecule 9: 50S ribosomal protein L7AE

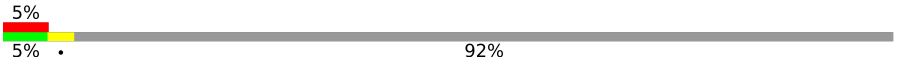
Chain F:

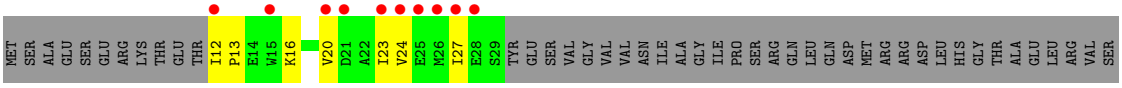


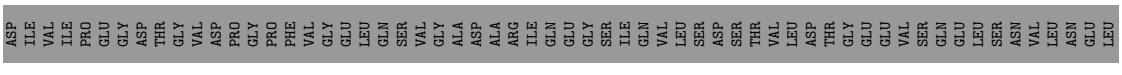


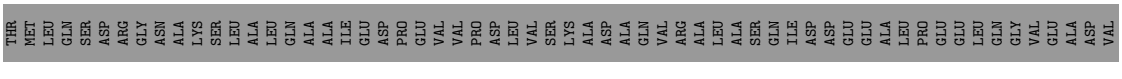
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:



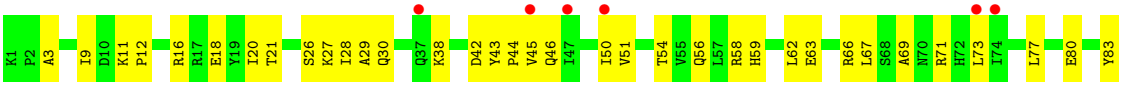


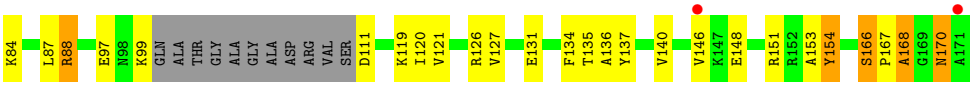




• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

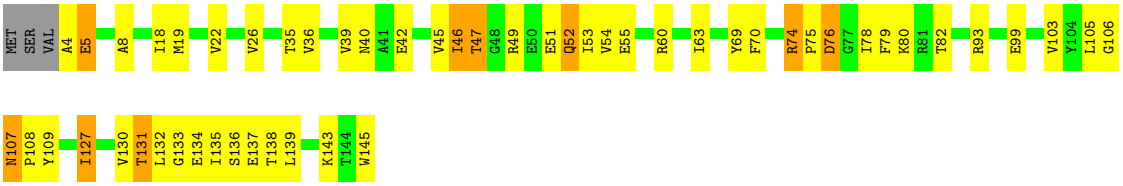
Chain H:





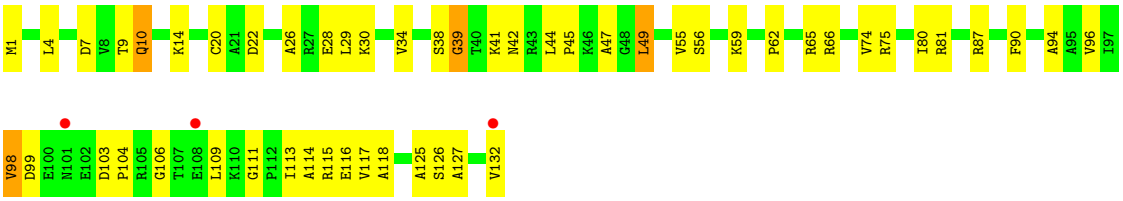
• Molecule 12: 50S ribosomal protein L13P

Chain J:



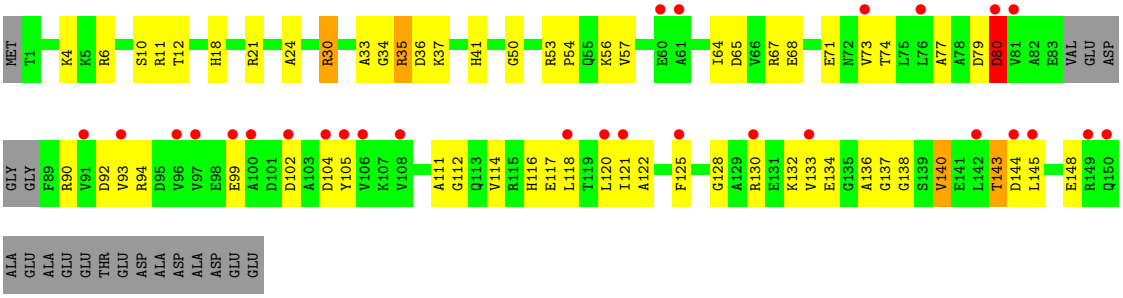
• Molecule 13: 50S ribosomal protein L14P

Chain K:



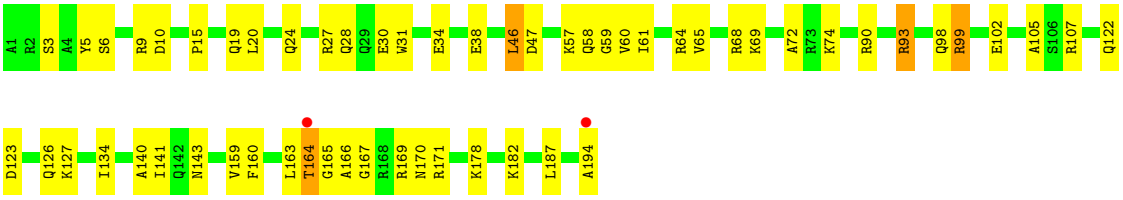
• Molecule 14: 50S ribosomal protein L15P

Chain L:

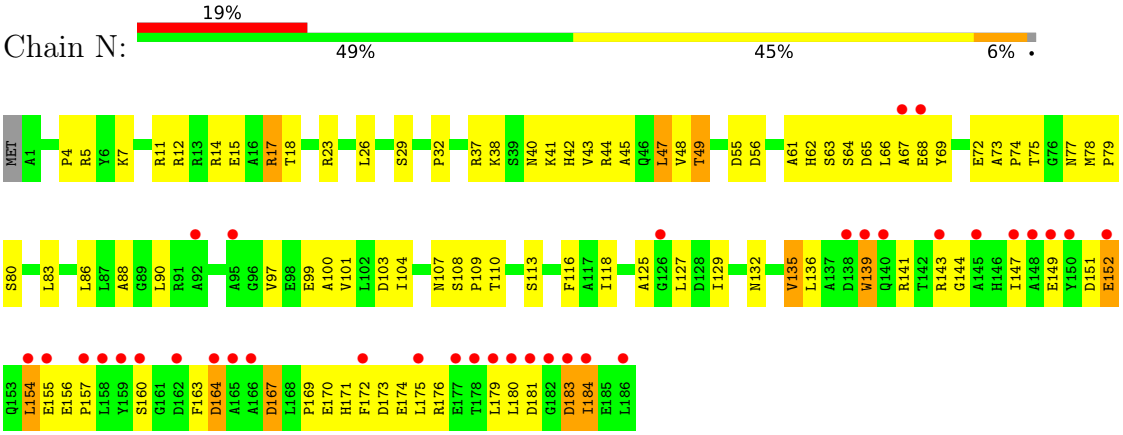


• Molecule 15: 50S Ribosomal Protein L15E

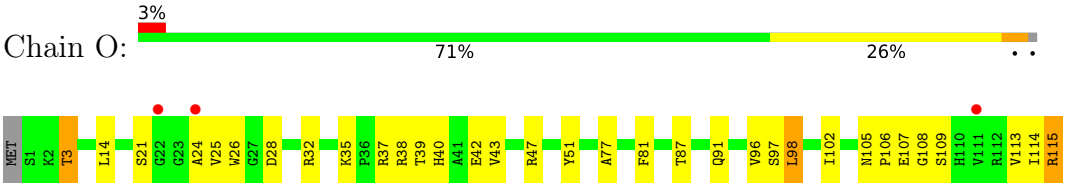
Chain M:



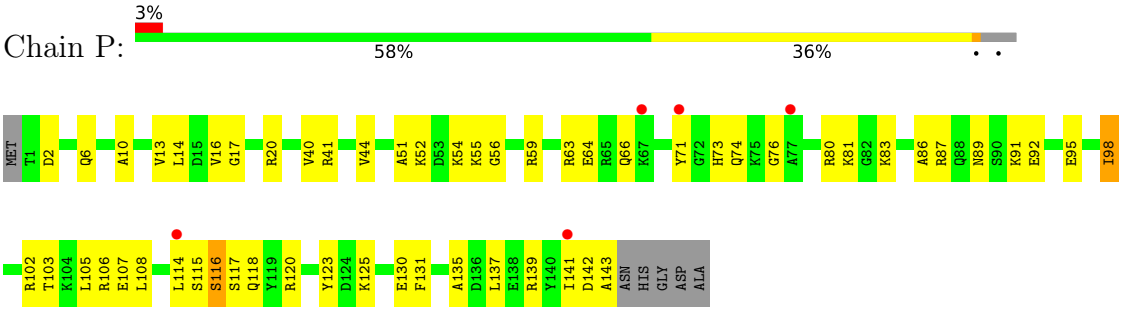
• Molecule 16: 50S ribosomal protein L18P



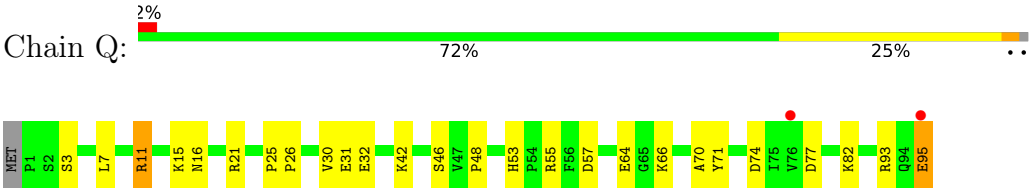
• Molecule 17: 50S ribosomal protein L18e



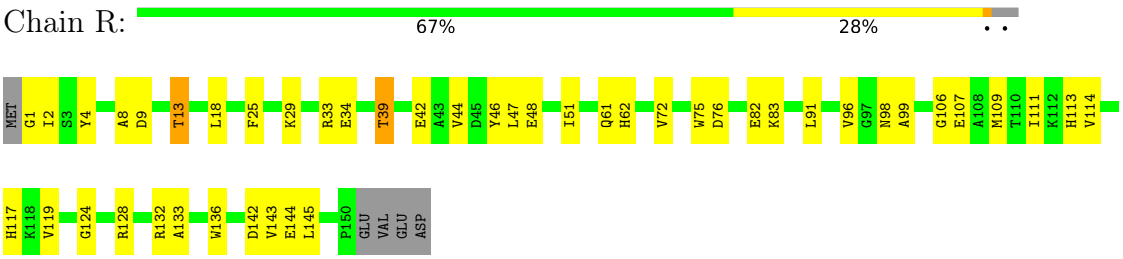
• Molecule 18: 50S ribosomal protein L19E



• Molecule 19: 50S ribosomal protein L21e

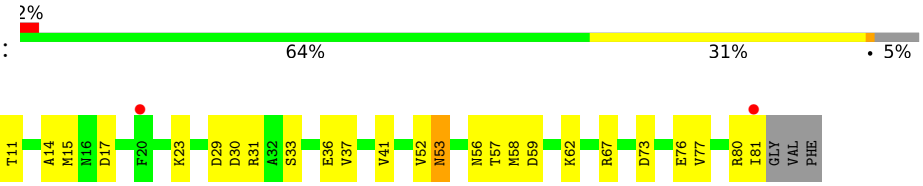


• Molecule 20: 50S ribosomal protein L22P



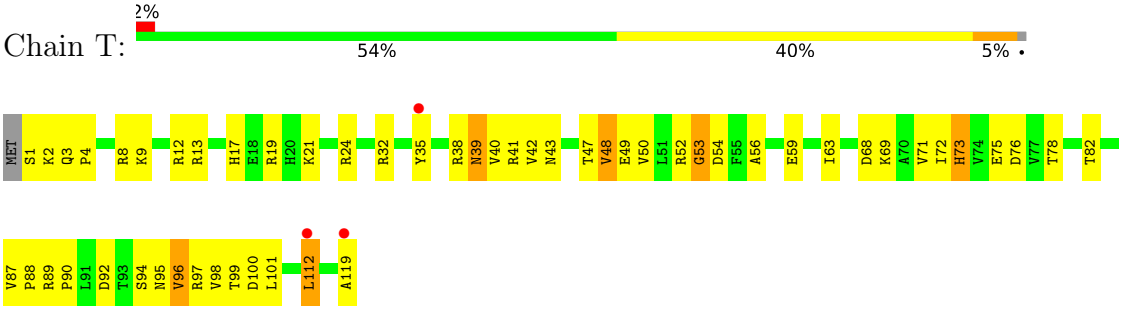
• Molecule 21: 50S ribosomal protein L23P

Chain S:



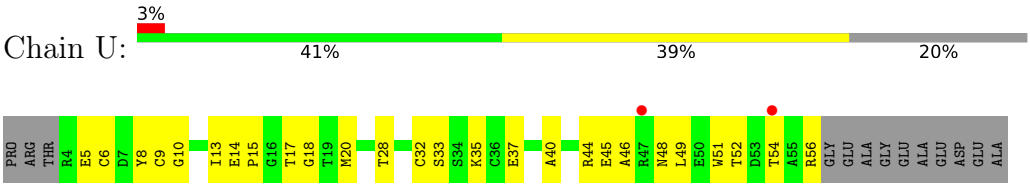
• Molecule 22: 50S ribosomal protein L24P

Chain T:



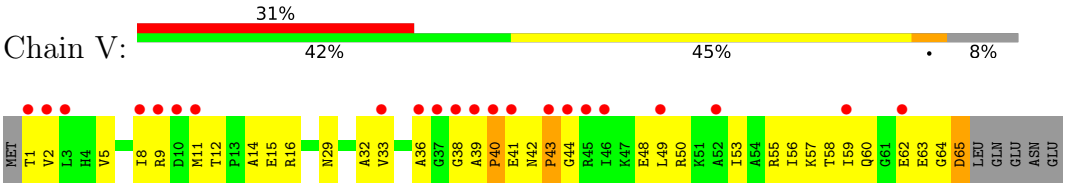
• Molecule 23: 50S ribosomal protein L24E

Chain U:



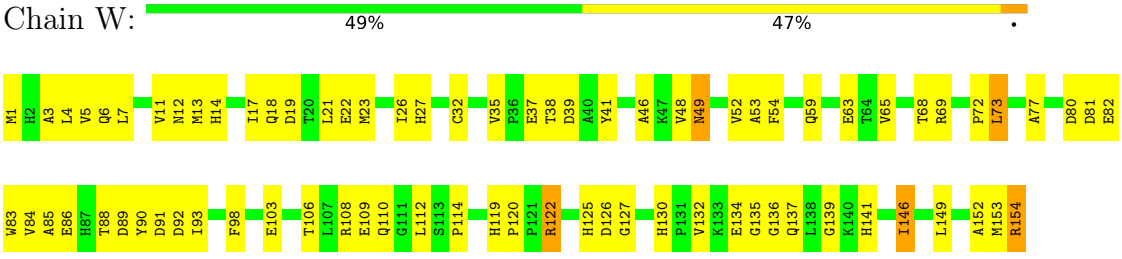
• Molecule 24: 50S ribosomal protein L29P

Chain V:



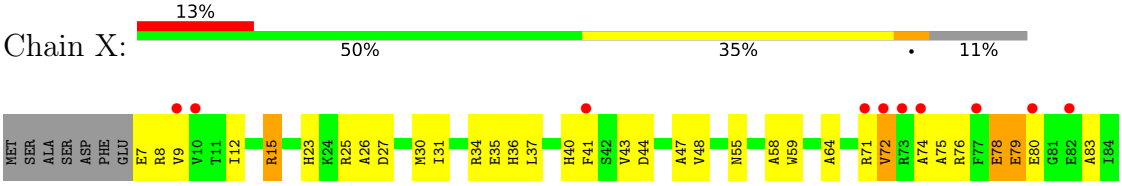
• Molecule 25: 50S ribosomal protein L30P

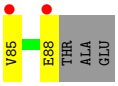
Chain W:



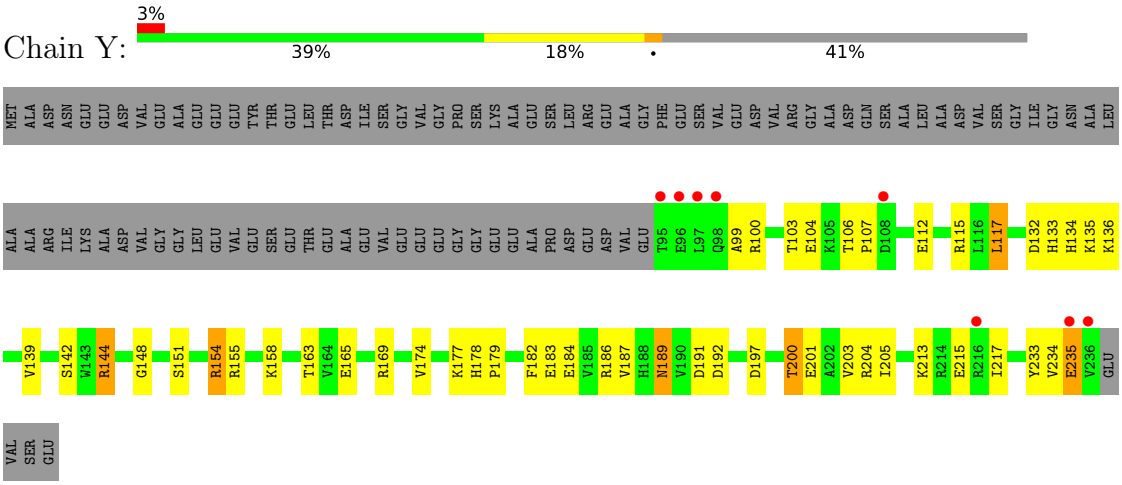
• Molecule 26: 50S ribosomal protein L31e

Chain X:

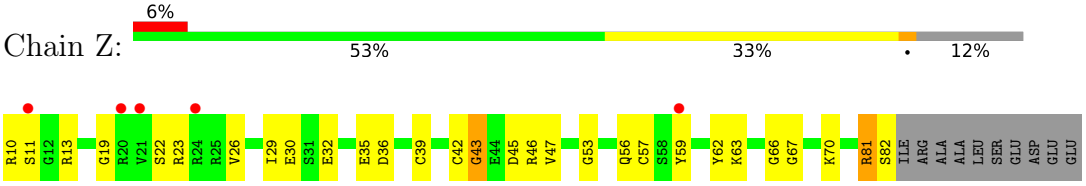




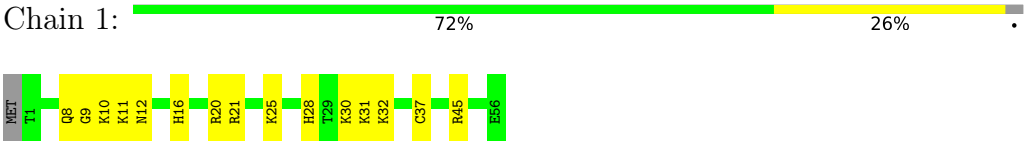
• Molecule 27: 50S ribosomal protein L32E



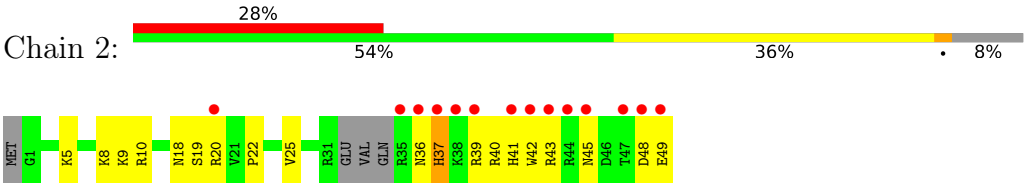
• Molecule 28: 50S ribosomal protein L37Ae



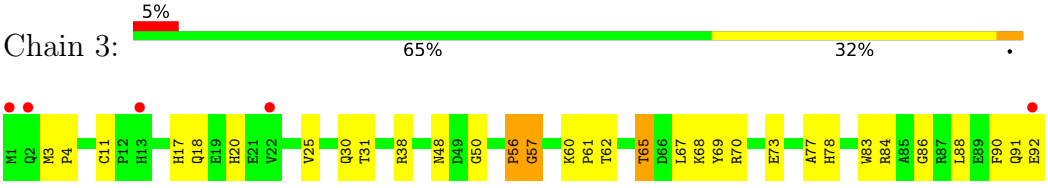
• Molecule 29: 50S ribosomal protein L37e



• Molecule 30: 50S ribosomal protein L39e

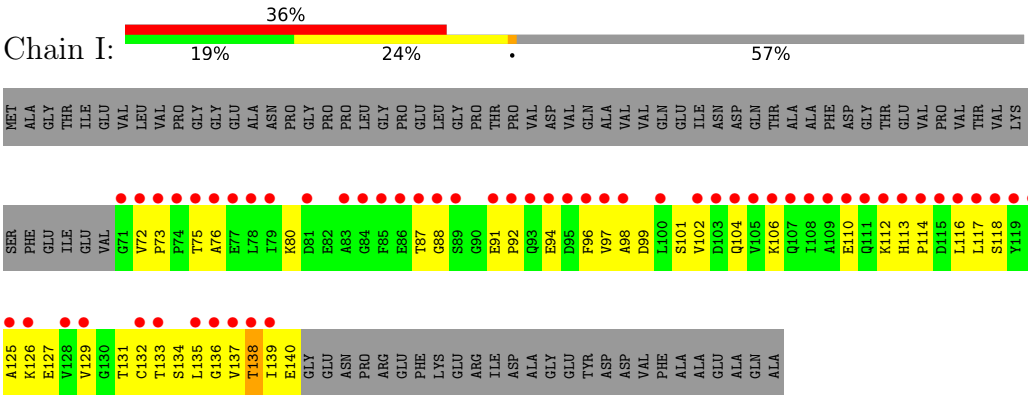


• Molecule 31: 50S ribosomal protein L44E



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P

Chain I:


36%
19%
24%
57%
MET ALA GLY THR ILE GLU VAL LEU VAL PRO GLY GLY GLU ALA ASN PRO GLY PRO PRO LEU GLY PRO GLU LEU GLY PRO THR PRO VAL ASP VAL GLN ALA VAL VAL GLN GLU ILE ASN ASP GLN THR ALA ALA PHE ASP GLY THR GLU VAL PRO VAL THR VAL LYS TYR ASP ASP GLY
SER PHE GLU ILE GLU VAL G71 V72 P73 P74 T75 A76 E77 L78 I79 K80 D81 E82 A83 G84 F85 E86 T87 G88 S89 G90 E91 P92 Q93 E94 D95 F96 V97 A98 D99 L100 S101 V102 D103 Q104 V105 K106 Q107 I108 A109 E110 Q111 K112 H113 P114 D115 L116 L117 S118 Y119 D120 L121 T122 N123 A124
A125 K126 E127 V128 V129 G130 T131 C132 T133 S134 L135 G136 V137 T138 I139 E140 GLY GLU ASN PRO ARG GLU PHE LYS GLU ARG ILE ASP ALA GLY GLU TYR ASP ASP VAL PHE ALA ALA GLU ALA GLN ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.15Å 300.13Å 573.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-2.50) 89.0 (49.61-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.244 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 58.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	99063	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, 5AA, OMG, OMU, UR3, PSU, NA, CD, 1MA, 2OP, CL, PAE, 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	0	0.37	0/65959	0.69	23/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.43	0/102	0.65	0/149
4	A	0.33	0/1786	0.65	0/2408
5	B	0.32	0/2690	0.63	0/3652
6	C	0.38	0/1884	0.66	0/2551
7	D	0.30	0/1111	0.54	0/1498
8	E	0.31	0/1382	0.57	0/1880
9	F	0.31	0/901	0.55	0/1224
10	G	0.27	0/241	0.45	0/324
11	H	0.33	0/1287	0.65	0/1725
12	J	0.35	0/1136	0.60	0/1530
13	K	0.34	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.65	0/1509
15	M	0.35	0/1584	0.62	0/2119
16	N	0.29	0/1474	0.63	0/1999
17	O	0.34	0/874	0.60	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.35	0/749	0.67	0/1005
20	R	0.36	0/1172	0.63	0/1578
21	S	0.33	0/648	0.60	0/875
22	T	0.31	0/958	0.63	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.29	0/502	0.53	0/675
25	W	0.33	0/1219	0.63	0/1655
26	X	0.33	0/664	0.58	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.36	0/589	0.65	0/787
29	1	0.41	0/438	0.66	0/578
30	2	0.32	0/401	0.52	0/529
31	3	0.39	0/771	0.61	0/1024
32	I	0.31	0/526	0.54	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.36	0/98794	0.67	24/147726 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	54
2	9	0	3
All	All	1	57

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1563	G	C2'-C3'-O3'	9.68	130.79	109.50
1	0	1942	A	C5'-C4'-C3'	8.39	129.43	116.00
1	0	1979	G	C2'-C3'-O3'	7.72	126.49	109.50
1	0	871	G	C5'-C4'-O4'	-7.18	100.48	109.10
2	9	3039	U	N1-C1'-C2'	7.03	123.14	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	174	A	Sidechain
1	0	191	A	Sidechain
1	0	221	G	Sidechain
1	0	246	G	Sidechain
1	0	26	U	Sidechain

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	813	0
2	9	2600	0	1326	57	0
3	4	130	0	77	5	0
4	A	1753	0	1766	106	0
5	B	2625	0	2533	167	0
6	C	1859	0	1816	100	0
7	D	1094	0	1085	85	0
8	E	1357	0	1266	84	0
9	F	890	0	843	43	0
10	G	240	0	231	14	0
11	H	1266	0	1268	64	0
12	J	1120	0	1098	73	0
13	K	992	0	1031	57	0
14	L	1118	0	1076	53	0
15	M	1560	0	1568	58	0
16	N	1445	0	1401	104	0
17	O	865	0	873	32	0
18	P	1136	0	1123	51	0
19	Q	735	0	729	21	0
20	R	1149	0	1122	60	0
21	S	641	0	605	21	0
22	T	950	0	923	56	0
23	U	410	0	364	29	0
24	V	499	0	511	35	0
25	W	1196	0	1137	95	0
26	X	654	0	653	34	0
27	Y	1130	0	1133	56	0
28	Z	578	0	539	25	0
29	1	431	0	426	21	0
30	2	396	0	413	28	0
31	3	755	0	728	27	0
32	I	519	0	500	47	0
33	0	108	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	1	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	0	72	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	11	0	0	1	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5809	0	0	103	0
38	1	53	0	0	2	0
38	2	40	0	0	3	0
38	3	74	0	0	4	0
38	4	8	0	0	1	0
38	9	137	0	0	5	0
38	A	119	0	0	13	0
38	B	153	0	0	15	0
38	C	168	0	0	12	0
38	D	47	0	0	10	0
38	E	43	0	0	7	0
38	F	23	0	0	3	0
38	G	18	0	0	2	0
38	H	65	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	I	9	0	0	2	0
38	J	51	0	0	4	0
38	K	58	0	0	6	0
38	L	82	0	0	12	0
38	M	116	0	0	5	0
38	N	63	0	0	10	0
38	O	42	0	0	3	0
38	P	64	0	0	3	0
38	Q	51	0	0	3	0
38	R	84	0	0	3	0
38	S	30	0	0	1	0
38	T	42	0	0	2	0
38	U	29	0	0	2	0
38	V	14	0	0	1	0
38	W	68	0	0	2	0
38	X	27	0	0	2	0
38	Y	96	0	0	5	0
38	Z	32	0	0	2	0
All	All	99063	0	59977	2271	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 2271 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)
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.28	1.16
1:0:156:C:H5"	15:M:171:ARG:HD3	1.29	1.14
5:B:62:ARG:HA	5:B:65:MET:HE3	1.29	1.14
1:0:1160:G:H5'	1:0:1161:A:H5'	1.20	1.11
1:0:1242:A:H5'	12:J:82:THR:HG23	1.34	1.09

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
4	A	235/240 (98%)	210 (89%)	21 (9%)	4 (2%)	9 16
5	B	335/338 (99%)	298 (89%)	31 (9%)	6 (2%)	8 14
6	C	244/246 (99%)	218 (89%)	25 (10%)	1 (0%)	34 54
7	D	134/177 (76%)	101 (75%)	23 (17%)	10 (8%)	1 1
8	E	170/178 (96%)	158 (93%)	12 (7%)	0	100 100
9	F	117/120 (98%)	108 (92%)	3 (3%)	6 (5%)	2 2
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100 100
11	H	156/171 (91%)	145 (93%)	8 (5%)	3 (2%)	8 13
12	J	140/145 (97%)	131 (94%)	7 (5%)	2 (1%)	11 20
13	K	130/132 (98%)	116 (89%)	11 (8%)	3 (2%)	6 10
14	L	141/165 (86%)	121 (86%)	16 (11%)	4 (3%)	5 7
15	M	192/194 (99%)	183 (95%)	9 (5%)	0	100 100
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	3 4
17	O	113/116 (97%)	107 (95%)	5 (4%)	1 (1%)	17 31
18	P	141/149 (95%)	138 (98%)	2 (1%)	1 (1%)	22 39
19	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100 100
20	R	148/155 (96%)	137 (93%)	11 (7%)	0	100 100
21	S	79/85 (93%)	76 (96%)	3 (4%)	0	100 100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	17 31
23	U	51/66 (77%)	46 (90%)	5 (10%)	0	100 100
24	V	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	4 5
25	W	152/154 (99%)	142 (93%)	9 (6%)	1 (1%)	22 39
26	X	80/92 (87%)	70 (88%)	9 (11%)	1 (1%)	12 21
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100 100
28	Z	71/83 (86%)	60 (84%)	9 (13%)	2 (3%)	5 7
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100 100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	6 9
31	3	90/92 (98%)	87 (97%)	1 (1%)	2 (2%)	6 10
32	I	68/162 (42%)	50 (74%)	17 (25%)	1 (2%)	10 18
All	All	3705/4430 (84%)	3373 (91%)	273 (7%)	59 (2%)	9 17

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	36	ASP
4	A	37	VAL
5	B	34	GLY
5	B	139	ASP
5	B	184	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
4	A	179/182 (98%)	170 (95%)	9 (5%)	24	46
5	B	282/283 (100%)	266 (94%)	16 (6%)	20	39
6	C	193/193 (100%)	178 (92%)	15 (8%)	12	24
7	D	117/148 (79%)	111 (95%)	6 (5%)	24	45
8	E	152/156 (97%)	151 (99%)	1 (1%)	84	94
9	F	93/94 (99%)	93 (100%)	0	100	100
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	124 (94%)	8 (6%)	18	36
12	J	118/121 (98%)	109 (92%)	9 (8%)	13	25
13	K	106/106 (100%)	102 (96%)	4 (4%)	33	58
14	L	113/127 (89%)	107 (95%)	6 (5%)	22	43
15	M	158/158 (100%)	153 (97%)	5 (3%)	39	65
16	N	149/150 (99%)	142 (95%)	7 (5%)	26	49
17	O	93/94 (99%)	89 (96%)	4 (4%)	29	53
18	P	113/117 (97%)	110 (97%)	3 (3%)	44	71
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	58
20	R	117/122 (96%)	115 (98%)	2 (2%)	60	82
21	S	71/74 (96%)	70 (99%)	1 (1%)	67	86
22	T	105/106 (99%)	99 (94%)	6 (6%)	20	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	U	44/52 (85%)	44 (100%)	0	100 100
24	V	51/57 (90%)	49 (96%)	2 (4%)	32 57
25	W	130/130 (100%)	126 (97%)	4 (3%)	40 67
26	X	66/74 (89%)	62 (94%)	4 (6%)	18 36
27	Y	120/196 (61%)	112 (93%)	8 (7%)	16 31
28	Z	60/68 (88%)	60 (100%)	0	100 100
29	1	46/47 (98%)	46 (100%)	0	100 100
30	2	42/46 (91%)	41 (98%)	1 (2%)	49 74
31	3	79/79 (100%)	77 (98%)	2 (2%)	47 73
32	I	58/130 (45%)	58 (100%)	0	100 100
All	All	3093/3611 (86%)	2967 (96%)	126 (4%)	30 55

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	52	GLN
25	W	154	ARG
14	L	99	GLU
25	W	146	ILE
27	Y	163	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
22	T	39	ASN
27	Y	133	HIS
23	U	48	ASN
25	W	110	GLN
29	1	8	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	32 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
3	4	1/8 (12%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2867/3052 (93%)	251 (8%)	33 (1%)

5 of 251 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2649	A
1	0	2718	C
2	9	3065	A
1	0	1237	U
1	0	1232	A

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMG	0	2588	3,1	18,26,27	1.04	2 (11%)	19,38,41	0.71	1 (5%)
1	OMU	0	2587	1	19,22,23	0.24	0	26,31,34	0.35	0
1	1MA	0	628	1	16,25,26	1.37	3 (18%)	18,37,40	1.15	2 (11%)
3	5AA	4	76	3,1	18,26,27	1.09	1 (5%)	15,38,41	0.80	1 (6%)
1	PSU	0	2621	1	18,21,22	1.49	2 (11%)	22,30,33	1.31	3 (13%)
1	UR3	0	2619	1	19,22,23	0.36	0	26,32,35	0.66	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	3,1	-	0/5/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
3	5AA	4	76	3,1	-	0/7/29/30	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.97	1.43	1.36
1	0	628	1MA	C2-N3	3.67	1.33	1.29
3	4	76	5AA	C3'-N3'	-3.38	1.42	1.47
1	0	628	1MA	C6-N6	2.67	1.34	1.27
1	0	2621	PSU	C6-C5	2.59	1.38	1.35

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	C6-C5-C4	3.66	120.75	118.20
1	0	2621	PSU	C6-N1-C2	-3.02	119.60	122.68
1	0	628	1MA	N1-C2-N3	2.83	129.32	126.02
1	0	2621	PSU	O2-C2-N1	2.61	125.66	122.79
1	0	628	1MA	C5-C6-N1	2.46	117.56	113.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	2619	UR3	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 234 ligands modelled in this entry, 234 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)

There are no chain breaks in this entry.

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, 95^{th} 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	0	2749/2922 (94%)	-0.49	48 (1%) 70 72	24, 49, 93, 155	0
2	9	122/122 (100%)	-0.29	5 (4%) 37 40	45, 66, 91, 152	0
3	4	5/8 (62%)	-0.71	0 100 100	41, 45, 47, 49	0
4	A	237/240 (98%)	0.39	17 (7%) 15 16	30, 51, 89, 114	0
5	B	337/338 (99%)	0.30	11 (3%) 46 50	31, 61, 90, 100	0
6	C	246/246 (100%)	-0.05	4 (1%) 72 74	28, 48, 71, 82	0
7	D	140/177 (79%)	2.54	74 (52%) 0 0	59, 106, 130, 136	0
8	E	172/178 (96%)	1.10	27 (15%) 2 1	52, 76, 101, 111	0
9	F	119/120 (99%)	0.99	27 (22%) 0 0	52, 74, 100, 116	0
10	G	29/348 (8%)	2.64	19 (65%) 0 0	74, 92, 104, 108	0
11	H	160/171 (93%)	0.39	8 (5%) 28 30	42, 60, 91, 100	0
12	J	142/145 (97%)	0.13	0 100 100	40, 56, 76, 99	0
13	K	132/132 (100%)	0.20	3 (2%) 60 63	35, 58, 80, 85	0
14	L	145/165 (87%)	0.85	28 (19%) 1 1	28, 69, 114, 127	0
15	M	194/194 (100%)	0.04	2 (1%) 82 84	32, 43, 59, 66	0
16	N	186/187 (99%)	0.84	36 (19%) 1 1	40, 64, 113, 119	0
17	O	115/116 (99%)	0.15	3 (2%) 56 59	39, 58, 75, 90	0
18	P	143/149 (95%)	0.30	5 (3%) 44 47	43, 58, 70, 78	0
19	Q	95/96 (98%)	0.14	2 (2%) 63 66	38, 47, 60, 72	0
20	R	150/155 (96%)	-0.07	0 100 100	33, 48, 65, 76	0
21	S	81/85 (95%)	0.19	2 (2%) 57 61	45, 59, 78, 88	0
22	T	119/120 (99%)	0.42	3 (2%) 57 61	40, 58, 85, 96	0
23	U	53/66 (80%)	0.28	2 (3%) 40 43	46, 62, 76, 86	0
24	V	65/71 (91%)	1.62	22 (33%) 0 0	56, 76, 112, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	0.07	0 100 100	39, 55, 74, 86	0
26	X	82/92 (89%)	0.65	12 (14%) 2 2	46, 63, 85, 101	0
27	Y	142/241 (58%)	0.27	8 (5%) 24 25	30, 49, 70, 92	0
28	Z	73/83 (87%)	0.18	5 (6%) 17 17	46, 60, 76, 94	0
29	1	56/57 (98%)	-0.35	0 100 100	27, 34, 39, 52	0
30	2	46/50 (92%)	1.61	14 (30%) 0 0	36, 65, 120, 122	0
31	3	92/92 (100%)	0.32	5 (5%) 25 27	35, 55, 71, 87	0
32	I	70/162 (43%)	4.52	59 (84%) 0 0	108, 126, 148, 149	0
All	All	6651/7482 (88%)	0.11	451 (6%) 17 17	24, 55, 103, 155	0

The worst 5 of 451 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	96	PHE	15.2
32	I	133	THR	13.6
24	V	1	THR	13.1
32	I	102	VAL	12.5
32	I	93	GLN	11.6

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	OMU	0	2587	21/22	0.98	0.13	31,34,37,38	0
1	OMG	0	2588	24/25	0.98	0.13	30,34,37,38	0
1	PSU	0	2621	20/21	0.98	0.13	28,31,39,40	0
1	UR3	0	2619	21/22	0.99	0.15	33,38,40,43	0
1	1MA	0	628	23/24	0.99	0.16	31,35,37,38	0
3	5AA	4	76	24/25	0.99	0.14	39,44,45,46	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
35	NA	9	9151	1/1	0.51	0.14	76,76,76,76	0
34	K	0	9003	1/1	0.62	0.31	82,82,82,82	0
33	MG	9	8095	1/1	0.63	0.11	72,72,72,72	0
35	NA	0	9182	1/1	0.65	0.28	74,74,74,74	0
33	MG	0	8092	1/1	0.76	0.48	95,95,95,95	0
35	NA	S	9112	1/1	0.78	0.49	76,76,76,76	0
33	MG	0	8085	1/1	0.79	0.25	93,93,93,93	0
33	MG	0	8114	1/1	0.80	0.13	64,64,64,64	0
33	MG	0	8045	1/1	0.80	0.23	65,65,65,65	0
35	NA	H	9122	1/1	0.81	0.25	77,77,77,77	0
35	NA	0	9172	1/1	0.82	0.31	59,59,59,59	0
35	NA	0	9171	1/1	0.82	0.26	60,60,60,60	0
35	NA	0	9184	1/1	0.82	0.10	75,75,75,75	0
35	NA	0	9163	1/1	0.83	0.35	71,71,71,71	0
33	MG	0	8090	1/1	0.83	0.39	80,80,80,80	0
35	NA	0	9186	1/1	0.84	0.32	75,75,75,75	0
35	NA	0	9174	1/1	0.84	0.25	59,59,59,59	0
35	NA	0	9116	1/1	0.84	0.13	36,36,36,36	0
33	MG	0	8082	1/1	0.84	0.14	66,66,66,66	0
35	NA	0	9124	1/1	0.85	0.09	59,59,59,59	0
35	NA	0	9141	1/1	0.85	0.12	46,46,46,46	0
33	MG	0	8049	1/1	0.85	0.39	90,90,90,90	0
35	NA	0	9117	1/1	0.86	0.21	72,72,72,72	0
35	NA	0	9185	1/1	0.86	0.36	60,60,60,60	0
33	MG	0	8047	1/1	0.86	0.18	102,102,102,102	0
33	MG	0	8071	1/1	0.87	0.08	53,53,53,53	0
35	NA	R	9137	1/1	0.87	0.08	42,42,42,42	0
33	MG	0	8104	1/1	0.87	0.17	53,53,53,53	0
33	MG	0	8107	1/1	0.88	0.06	45,45,45,45	0
35	NA	0	9150	1/1	0.88	0.21	44,44,44,44	0
33	MG	0	8030	1/1	0.88	0.11	35,35,35,35	0
35	NA	0	9165	1/1	0.88	0.18	39,39,39,39	0
35	NA	0	9113	1/1	0.88	0.14	59,59,59,59	0
33	MG	0	8076	1/1	0.89	0.11	57,57,57,57	0
35	NA	0	9126	1/1	0.89	0.14	40,40,40,40	0
33	MG	0	8053	1/1	0.89	0.09	51,51,51,51	0
35	NA	0	9142	1/1	0.89	0.22	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	8050	1/1	0.89	0.07	63,63,63,63	0
33	MG	3	8078	1/1	0.89	0.07	46,46,46,46	0
35	NA	0	9166	1/1	0.90	0.12	77,77,77,77	0
35	NA	0	9129	1/1	0.90	0.14	53,53,53,53	0
33	MG	0	8043	1/1	0.90	0.09	42,42,42,42	0
36	CL	J	9302	1/1	0.90	0.13	70,70,70,70	0
37	CD	O	9205	1/1	0.90	0.07	137,137,137,137	0
33	MG	0	8101	1/1	0.91	0.17	69,69,69,69	0
33	MG	0	8051	1/1	0.91	0.12	56,56,56,56	0
35	NA	B	9158	1/1	0.91	1.05	69,69,69,69	0
35	NA	0	9119	1/1	0.91	0.13	42,42,42,42	0
35	NA	0	9176	1/1	0.91	0.23	43,43,43,43	0
33	MG	0	8048	1/1	0.91	0.13	60,60,60,60	0
36	CL	0	9315	1/1	0.91	0.21	69,69,69,69	0
36	CL	0	9322	1/1	0.91	0.31	76,76,76,76	0
35	NA	0	9107	1/1	0.91	0.13	43,43,43,43	0
33	MG	0	8057	1/1	0.91	0.13	39,39,39,39	0
37	CD	3	9204	1/1	0.91	0.10	62,62,62,62	0
33	MG	0	8059	1/1	0.92	0.09	51,51,51,51	0
34	K	0	9001	1/1	0.92	0.09	66,66,66,66	0
35	NA	J	9146	1/1	0.92	0.14	37,37,37,37	0
35	NA	0	9167	1/1	0.92	0.09	40,40,40,40	0
33	MG	0	8014	1/1	0.92	0.10	42,42,42,42	0
35	NA	0	9138	1/1	0.93	0.12	51,51,51,51	0
33	MG	0	8072	1/1	0.93	0.20	51,51,51,51	0
33	MG	0	8113	1/1	0.93	0.10	45,45,45,45	0
35	NA	L	9180	1/1	0.93	0.38	50,50,50,50	0
33	MG	0	8042	1/1	0.93	0.07	45,45,45,45	0
35	NA	0	9181	1/1	0.93	0.14	51,51,51,51	0
36	CL	0	9314	1/1	0.93	0.09	50,50,50,50	0
35	NA	0	9155	1/1	0.93	0.25	60,60,60,60	0
33	MG	0	8116	1/1	0.93	0.07	50,50,50,50	0
36	CL	J	9301	1/1	0.93	0.12	72,72,72,72	0
35	NA	0	9105	1/1	0.93	0.13	35,35,35,35	0
36	CL	L	9310	1/1	0.93	0.09	58,58,58,58	0
36	CL	O	9308	1/1	0.93	0.11	68,68,68,68	0
33	MG	0	8118	1/1	0.93	0.10	63,63,63,63	0
35	NA	0	9111	1/1	0.93	0.24	65,65,65,65	0
35	NA	0	9108	1/1	0.94	0.12	48,48,48,48	0
35	NA	0	9175	1/1	0.94	0.23	42,42,42,42	0
35	NA	0	9156	1/1	0.94	0.21	50,50,50,50	0
35	NA	0	9177	1/1	0.94	0.22	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	9159	1/1	0.94	0.19	50,50,50,50	0
33	MG	0	8080	1/1	0.94	0.06	37,37,37,37	0
33	MG	0	8001	1/1	0.94	0.07	36,36,36,36	0
35	NA	0	9114	1/1	0.94	0.16	66,66,66,66	0
33	MG	0	8075	1/1	0.94	0.05	39,39,39,39	0
33	MG	0	8106	1/1	0.94	0.10	51,51,51,51	0
35	NA	9	9183	1/1	0.94	0.11	55,55,55,55	0
36	CL	3	9304	1/1	0.94	0.06	47,47,47,47	0
33	MG	0	8040	1/1	0.94	0.09	45,45,45,45	0
35	NA	0	9173	1/1	0.94	0.14	42,42,42,42	0
35	NA	0	9164	1/1	0.95	0.16	52,52,52,52	0
35	NA	0	9125	1/1	0.95	0.18	64,64,64,64	0
33	MG	0	8062	1/1	0.95	0.10	53,53,53,53	0
33	MG	0	8063	1/1	0.95	0.09	53,53,53,53	0
35	NA	0	9169	1/1	0.95	0.15	46,46,46,46	0
35	NA	0	9170	1/1	0.95	0.41	61,61,61,61	0
35	NA	0	9135	1/1	0.95	0.20	43,43,43,43	0
33	MG	0	8013	1/1	0.95	0.23	33,33,33,33	0
35	NA	0	9140	1/1	0.95	0.33	49,49,49,49	0
33	MG	0	8008	1/1	0.95	0.08	35,35,35,35	0
35	NA	0	9115	1/1	0.95	0.14	37,37,37,37	0
33	MG	0	8041	1/1	0.95	0.23	59,59,59,59	0
35	NA	0	9102	1/1	0.95	0.13	42,42,42,42	0
33	MG	0	8115	1/1	0.95	0.14	52,52,52,52	0
35	NA	0	9157	1/1	0.95	0.07	60,60,60,60	0
35	NA	0	9121	1/1	0.95	0.26	50,50,50,50	0
35	NA	0	9161	1/1	0.95	0.25	49,49,49,49	0
33	MG	0	8046	1/1	0.95	0.04	52,52,52,52	0
35	NA	0	9106	1/1	0.96	0.17	34,34,34,34	0
35	NA	A	9145	1/1	0.96	0.18	39,39,39,39	0
33	MG	0	8023	1/1	0.96	0.20	53,53,53,53	0
35	NA	C	9104	1/1	0.96	0.09	32,32,32,32	0
35	NA	0	9136	1/1	0.96	0.08	53,53,53,53	0
33	MG	0	8093	1/1	0.96	0.13	56,56,56,56	0
33	MG	0	8094	1/1	0.96	0.16	62,62,62,62	0
33	MG	0	8100	1/1	0.96	0.10	68,68,68,68	0
33	MG	0	8027	1/1	0.96	0.12	44,44,44,44	0
36	CL	0	9303	1/1	0.96	0.15	54,54,54,54	0
36	CL	0	9313	1/1	0.96	0.14	62,62,62,62	0
33	MG	9	8052	1/1	0.96	0.07	50,50,50,50	0
33	MG	0	8103	1/1	0.96	0.20	66,66,66,66	0
36	CL	0	9316	1/1	0.96	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	8006	1/1	0.96	0.09	32,32,32,32	0
36	CL	B	9319	1/1	0.96	0.14	47,47,47,47	0
33	MG	0	8088	1/1	0.96	0.06	39,39,39,39	0
34	K	0	9002	1/1	0.96	0.06	43,43,43,43	0
35	NA	0	9160	1/1	0.96	0.24	41,41,41,41	0
33	MG	0	8037	1/1	0.96	0.10	46,46,46,46	0
33	MG	0	8111	1/1	0.96	0.08	57,57,57,57	0
33	MG	0	8112	1/1	0.96	0.05	37,37,37,37	0
35	NA	0	9127	1/1	0.96	0.18	39,39,39,39	0
33	MG	0	8039	1/1	0.97	0.08	49,49,49,49	0
33	MG	0	8098	1/1	0.97	0.11	45,45,45,45	0
35	NA	0	9168	1/1	0.97	0.13	52,52,52,52	0
35	NA	0	9110	1/1	0.97	0.14	37,37,37,37	0
33	MG	0	8019	1/1	0.97	0.10	33,33,33,33	0
33	MG	0	8060	1/1	0.97	0.20	39,39,39,39	0
33	MG	0	8102	1/1	0.97	0.08	51,51,51,51	0
33	MG	0	8020	1/1	0.97	0.14	32,32,32,32	0
33	MG	0	8021	1/1	0.97	0.14	25,25,25,25	0
33	MG	0	8066	1/1	0.97	0.17	114,114,114,114	0
35	NA	0	9118	1/1	0.97	0.12	54,54,54,54	0
33	MG	0	8067	1/1	0.97	0.12	52,52,52,52	0
35	NA	0	9178	1/1	0.97	0.31	53,53,53,53	0
35	NA	0	9179	1/1	0.97	0.20	57,57,57,57	0
33	MG	0	8108	1/1	0.97	0.09	56,56,56,56	0
33	MG	0	8070	1/1	0.97	0.12	53,53,53,53	0
33	MG	0	8022	1/1	0.97	0.06	35,35,35,35	0
33	MG	0	8044	1/1	0.97	0.06	47,47,47,47	0
33	MG	0	8003	1/1	0.97	0.13	26,26,26,26	0
33	MG	0	8024	1/1	0.97	0.15	49,49,49,49	0
35	NA	0	9130	1/1	0.97	0.09	36,36,36,36	0
35	NA	0	9131	1/1	0.97	0.13	35,35,35,35	0
35	NA	0	9133	1/1	0.97	0.16	27,27,27,27	0
35	NA	0	9134	1/1	0.97	0.14	34,34,34,34	0
33	MG	0	8002	1/1	0.97	0.03	28,28,28,28	0
33	MG	0	8007	1/1	0.97	0.08	23,23,23,23	0
33	MG	0	8084	1/1	0.97	0.11	40,40,40,40	0
33	MG	0	8032	1/1	0.97	0.16	39,39,39,39	0
33	MG	4	8119	1/1	0.97	0.08	41,41,41,41	0
33	MG	A	8065	1/1	0.97	0.14	42,42,42,42	0
35	NA	0	9149	1/1	0.97	0.09	36,36,36,36	0
33	MG	B	8055	1/1	0.97	0.20	60,60,60,60	0
35	NA	0	9152	1/1	0.97	0.30	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	Y	8109	1/1	0.97	0.08	40,40,40,40	0
33	MG	0	8086	1/1	0.97	0.07	50,50,50,50	0
33	MG	0	8087	1/1	0.97	0.21	57,57,57,57	0
33	MG	0	8035	1/1	0.97	0.08	50,50,50,50	0
33	MG	0	8036	1/1	0.97	0.14	39,39,39,39	0
36	CL	J	9321	1/1	0.97	0.15	54,54,54,54	0
35	NA	0	9101	1/1	0.97	0.22	46,46,46,46	0
36	CL	N	9307	1/1	0.97	0.16	61,61,61,61	0
35	NA	0	9162	1/1	0.97	0.26	58,58,58,58	0
33	MG	0	8091	1/1	0.97	0.07	74,74,74,74	0
33	MG	0	8018	1/1	0.97	0.13	40,40,40,40	0
33	MG	0	8054	1/1	0.97	0.11	24,24,24,24	0
33	MG	0	8079	1/1	0.98	0.12	28,28,28,28	0
35	NA	0	9153	1/1	0.98	0.05	17,17,17,17	0
35	NA	0	9154	1/1	0.98	0.09	26,26,26,26	0
33	MG	0	8038	1/1	0.98	0.17	28,28,28,28	0
33	MG	0	8028	1/1	0.98	0.15	43,43,43,43	0
33	MG	B	8056	1/1	0.98	0.15	49,49,49,49	0
35	NA	0	9120	1/1	0.98	0.14	56,56,56,56	0
33	MG	K	8069	1/1	0.98	0.11	41,41,41,41	0
35	NA	H	9109	1/1	0.98	0.13	31,31,31,31	0
33	MG	0	8012	1/1	0.98	0.15	35,35,35,35	0
33	MG	0	8015	1/1	0.98	0.10	30,30,30,30	0
33	MG	0	8033	1/1	0.98	0.08	39,39,39,39	0
35	NA	M	9147	1/1	0.98	0.13	18,18,18,18	0
35	NA	Q	9148	1/1	0.98	0.20	36,36,36,36	0
33	MG	0	8068	1/1	0.98	0.06	58,58,58,58	0
35	NA	0	9128	1/1	0.98	0.08	40,40,40,40	0
33	MG	0	8034	1/1	0.98	0.12	39,39,39,39	0
36	CL	0	9305	1/1	0.98	0.10	52,52,52,52	0
36	CL	0	9311	1/1	0.98	0.14	51,51,51,51	0
33	MG	0	8110	1/1	0.98	0.06	34,34,34,34	0
33	MG	0	8089	1/1	0.98	0.06	60,60,60,60	0
35	NA	0	9132	1/1	0.98	0.09	29,29,29,29	0
35	NA	0	9103	1/1	0.98	0.15	44,44,44,44	0
36	CL	0	9320	1/1	0.98	0.11	48,48,48,48	0
33	MG	0	8016	1/1	0.98	0.19	35,35,35,35	0
36	CL	A	9309	1/1	0.98	0.21	58,58,58,58	0
33	MG	0	8026	1/1	0.98	0.12	24,24,24,24	0
33	MG	0	8074	1/1	0.98	0.07	34,34,34,34	0
33	MG	0	8058	1/1	0.98	0.16	45,45,45,45	0
35	NA	0	9139	1/1	0.98	0.09	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	8017	1/1	0.98	0.10	31,31,31,31	0
33	MG	0	8117	1/1	0.98	0.07	32,32,32,32	0
33	MG	0	8096	1/1	0.98	0.09	38,38,38,38	0
36	CL	R	9306	1/1	0.98	0.12	53,53,53,53	0
35	NA	0	9144	1/1	0.98	0.06	35,35,35,35	0
33	MG	0	8077	1/1	0.98	0.10	29,29,29,29	0
33	MG	0	8099	1/1	0.98	0.14	59,59,59,59	0
33	MG	0	8011	1/1	0.99	0.11	23,23,23,23	0
33	MG	0	8064	1/1	0.99	0.12	25,25,25,25	0
33	MG	0	8005	1/1	0.99	0.09	24,24,24,24	0
36	CL	0	9317	1/1	0.99	0.05	61,61,61,61	0
33	MG	0	8029	1/1	0.99	0.19	32,32,32,32	0
35	NA	0	9123	1/1	0.99	0.13	52,52,52,52	0
33	MG	0	8081	1/1	0.99	0.14	43,43,43,43	0
33	MG	0	8004	1/1	0.99	0.08	33,33,33,33	0
33	MG	0	8083	1/1	0.99	0.08	35,35,35,35	0
33	MG	0	8097	1/1	0.99	0.10	45,45,45,45	0
33	MG	T	8073	1/1	0.99	0.05	49,49,49,49	0
33	MG	0	8031	1/1	0.99	0.08	30,30,30,30	0
36	CL	M	9318	1/1	0.99	0.13	36,36,36,36	0
35	NA	T	9143	1/1	0.99	0.06	31,31,31,31	0
33	MG	0	8009	1/1	0.99	0.10	31,31,31,31	0
33	MG	0	8025	1/1	0.99	0.13	48,48,48,48	0
33	MG	0	8061	1/1	0.99	0.09	34,34,34,34	0
36	CL	0	9312	1/1	0.99	0.07	52,52,52,52	0
37	CD	U	9201	1/1	0.99	0.06	73,73,73,73	0
37	CD	Z	9203	1/1	0.99	0.08	61,61,61,61	0
37	CD	1	9202	1/1	0.99	0.02	54,54,54,54	0
33	MG	0	8010	1/1	0.99	0.07	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.