wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:58 PM GMT

PDB ID	:	1QVF
Title	:	Structure of a deacylated tRNA minihelix bound to the E site of the large ribosomal subunit of Haloarcula marismortui
Authors	:	Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2003-08-27
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

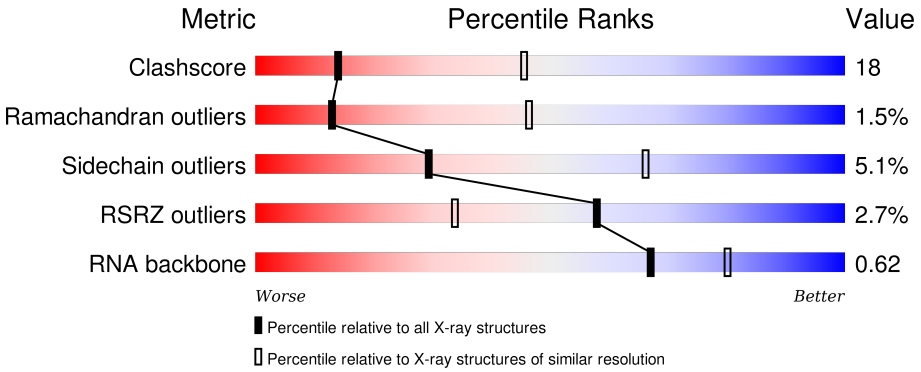
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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. 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	% 57% 29% 7% • 6%
2	9	122	4% 45% 39% 13% •
3	3	28	29% 18% 18% 7% 57%
4	A	239	3% 60% 33% 6% •
5	B	337	% 53% 41% 6%

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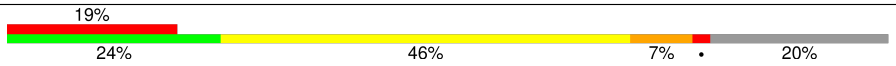
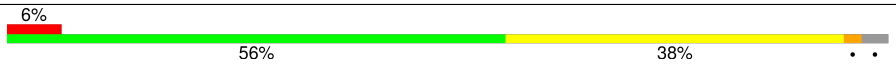
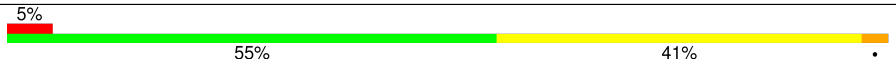
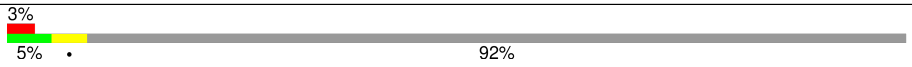
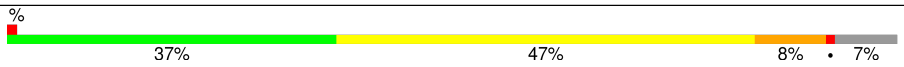
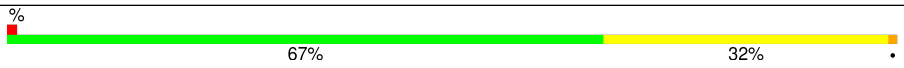
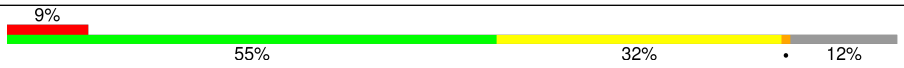
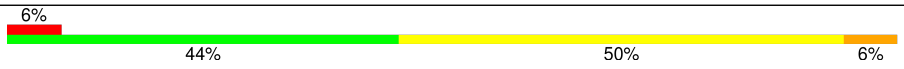
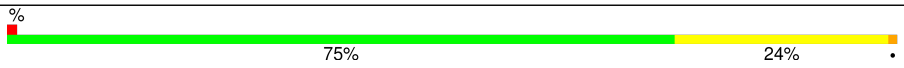
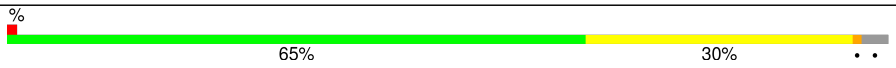
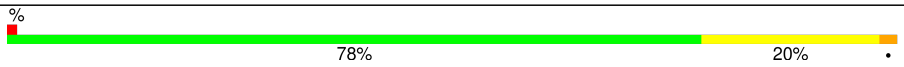
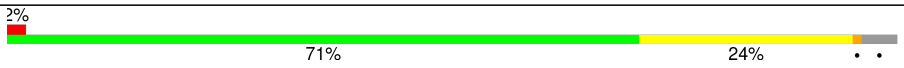
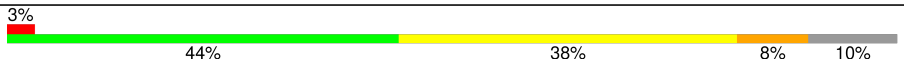
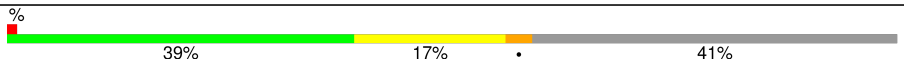
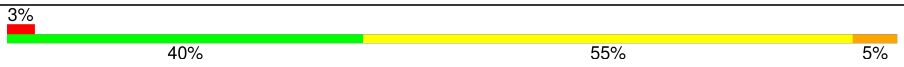
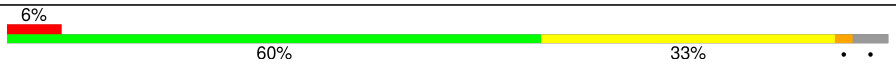
Mol	Chain	Length	Quality of chain
6	C	246	
7	D	176	
8	E	177	
9	F	119	
10	G	348	
11	H	167	
12	I	145	
13	J	132	
14	K	164	
15	L	194	
16	M	186	
17	N	115	
18	O	148	
19	P	95	
20	Q	154	
21	R	84	
22	S	119	
23	T	66	
24	U	70	
25	V	154	
26	W	91	
27	X	240	
28	Y	73	
29	Z	56	
30	1	48	

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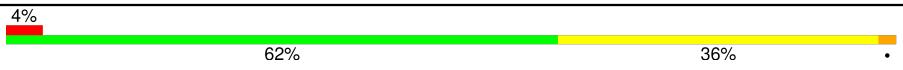
Mol	Chain	Length	Quality of chain
31	2	92	

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
32	MG	0	8044	-	-	-	X
32	MG	0	8064	-	-	-	X
32	MG	0	8112	-	-	-	X
32	MG	0	8114	-	-	-	X
32	MG	2	8118	-	-	-	X
32	MG	A	8065	-	-	-	X
33	K	0	8202	-	-	-	X
34	NA	0	8303	-	-	-	X
34	NA	0	8321	-	-	-	X
34	NA	0	8323	-	-	-	X
34	NA	0	8325	-	-	-	X
34	NA	0	8326	-	-	-	X
34	NA	0	8331	-	-	-	X
34	NA	0	8332	-	-	-	X
34	NA	0	8340	-	-	-	X
34	NA	0	8343	-	-	-	X
34	NA	0	8350	-	-	-	X
34	NA	0	8356	-	-	-	X
34	NA	0	8361	-	-	-	X
34	NA	0	8362	-	-	-	X
34	NA	0	8364	-	-	-	X
34	NA	0	8365	-	-	-	X
34	NA	0	8366	-	-	-	X
34	NA	0	8368	-	-	-	X
34	NA	0	8371	-	-	-	X
34	NA	0	8372	-	-	-	X
34	NA	0	8373	-	-	-	X
34	NA	0	8374	-	-	-	X
34	NA	0	8378	-	-	-	X
34	NA	0	8379	-	-	-	X
34	NA	0	8381	-	-	-	X
34	NA	0	8382	-	-	-	X
34	NA	9	8383	-	-	-	X
34	NA	K	8380	-	-	-	X
34	NA	Q	8386	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	0	8505	-	-	-	X
35	CL	0	8515	-	-	-	X
35	CL	B	8519	-	-	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98648 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	59017	26346	10878	19048	2745	0	0	0

- 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 Deacylated tRNA minihelix.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	3	12	257	114	47	84	12	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	1754	1072	352	325	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	337	2624	1616	493	510	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	DELETION	UNP P20279
B	310	ARG	PHE	CONFLICT	UNP P20279

- 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
			1858	1131	344	382	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
			885	552	141	191	1			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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 L10 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	I	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	K	145	Total	C	N	O	0	0	0
			1114	668	222	224			

- Molecule 15 is a protein called L15 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	M	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	N	115	Total	C	N	O	0	0	0
			864	529	161	174			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	O	143	Total	C	N	O	0	0	0
			1133	680	230	223			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	CONFLICT	UNP P14119

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	P	95	Total	C	N	O	0	0	0
			734	450	141	143			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	S	119	Total	C	N	O	0	0	0
			949	568	180	201			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	U	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	V	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	W	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	X	142	Total	C	N	O	0	0	0
			1130	686	228	216			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	Z	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	ARG	DELETION	UNP P22452

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	109	Total Mg 109 109	0	0
32	J	1	Total Mg 1 1	0	0
32	Y	1	Total Mg 1 1	0	0
32	B	1	Total Mg 1 1	0	0
32	A	2	Total Mg 2 2	0	0
32	X	1	Total Mg 1 1	0	0
32	2	2	Total Mg 2 2	0	0
32	9	1	Total Mg 1 1	0	0
32	S	1	Total Mg 1 1	0	0

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	72	Total Na 72 72	0	0
34	P	1	Total Na 1 1	0	0
34	Q	3	Total Na 3 3	0	0
34	K	1	Total Na 1 1	0	0
34	H	2	Total Na 2 2	0	0
34	I	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	A	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	R	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0
34	L	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	Q	1	Total Cl 1 1	0	0
35	K	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	I	3	Total Cl 3 3	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	X	1	Total Cl 1 1	0	0
35	2	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	Z	1	Total Cd 1 1	0	0
36	Y	1	Total Cd 1 1	0	0
36	T	1	Total Cd 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	2	1	Total Cd 1 1	0	0
36	N	1	Total Cd 1 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	5836	Total O 5836 5836	0	0
37	9	138	Total O 138 138	0	0
37	3	3	Total O 3 3	0	0
37	A	124	Total O 124 124	0	0
37	B	150	Total O 150 150	0	0
37	C	166	Total O 166 166	0	0
37	D	49	Total O 49 49	0	0
37	E	42	Total O 42 42	0	0
37	F	26	Total O 26 26	0	0
37	G	21	Total O 21 21	0	0
37	H	75	Total O 75 75	0	0
37	I	52	Total O 52 52	0	0
37	J	56	Total O 56 56	0	0
37	K	79	Total O 79 79	0	0
37	L	127	Total O 127 127	0	0
37	M	67	Total O 67 67	0	0
37	N	42	Total O 42 42	0	0

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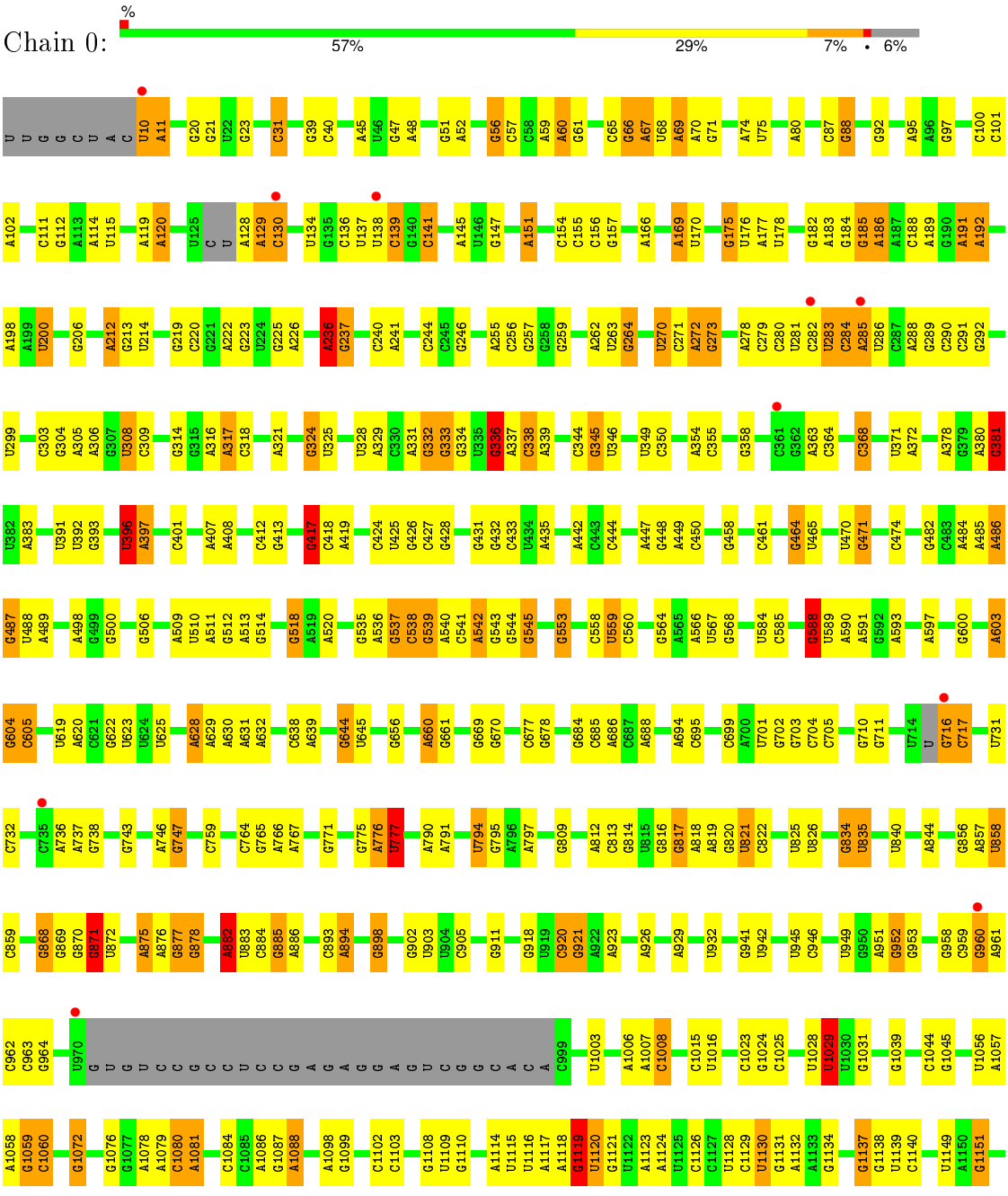
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	62	Total O 62 62	0	0
37	P	52	Total O 52 52	0	0
37	Q	82	Total O 82 82	0	0
37	R	35	Total O 35 35	0	0
37	S	41	Total O 41 41	0	0
37	T	23	Total O 23 23	0	0
37	U	14	Total O 14 14	0	0
37	V	69	Total O 69 69	0	0
37	W	29	Total O 29 29	0	0
37	X	85	Total O 85 85	0	0
37	Y	38	Total O 38 38	0	0
37	Z	56	Total O 56 56	0	0
37	1	42	Total O 42 42	0	0
37	2	58	Total O 58 58	0	0

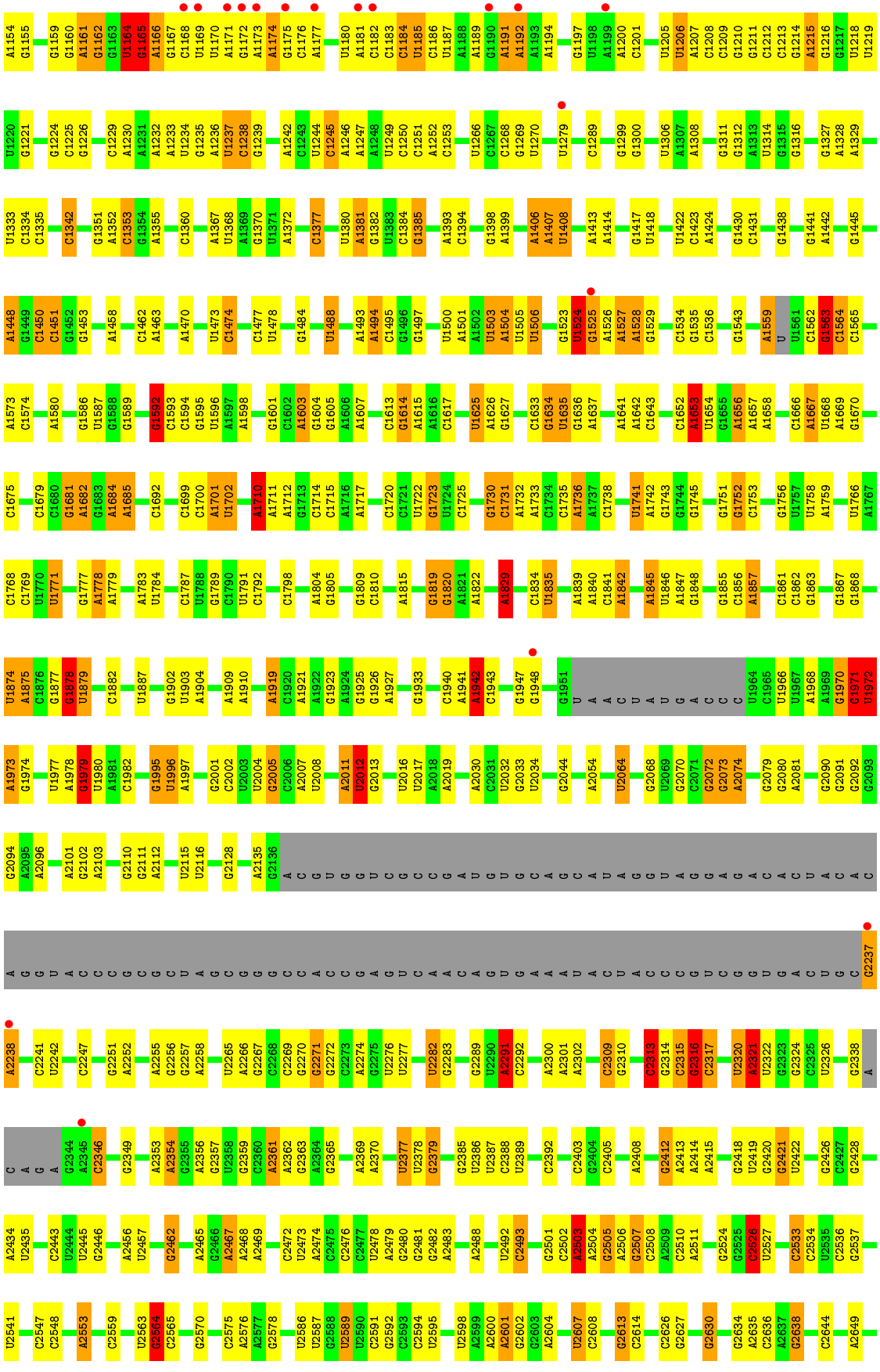
3 Residue-property plots (i)

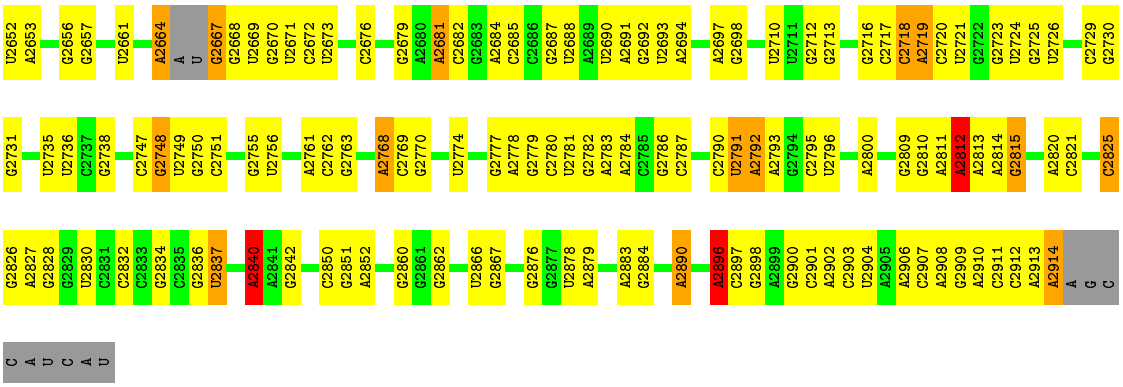
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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:

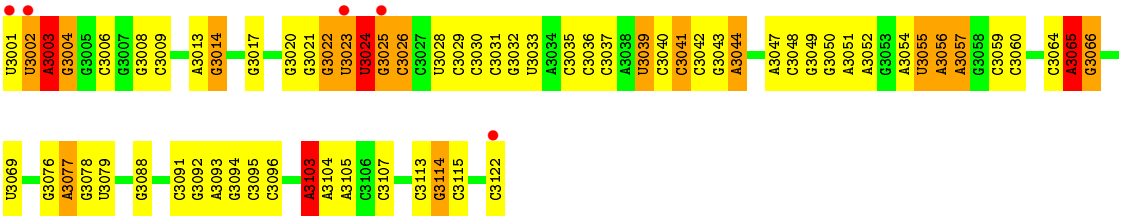






• Molecule 2: 5S ribosomal RNA

Chain 9:

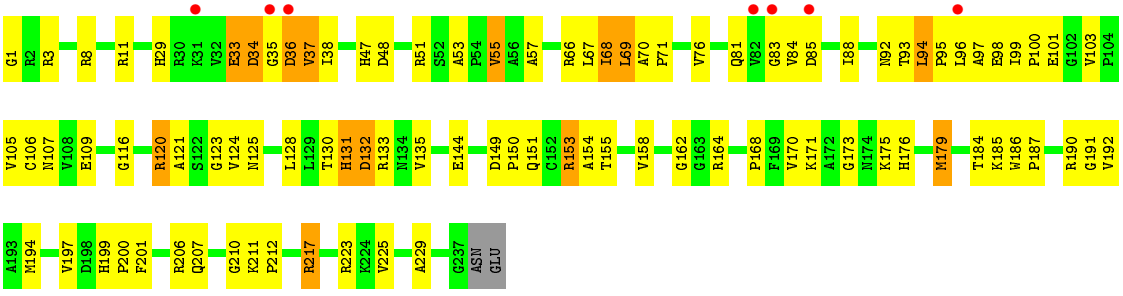


• Molecule 3: Deacylated tRNA minihelix

Chain 3:

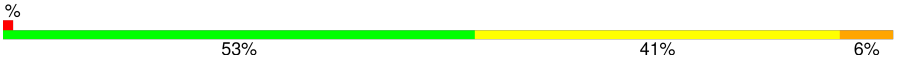
• Molecule 4: 50S ribosomal protein L2P

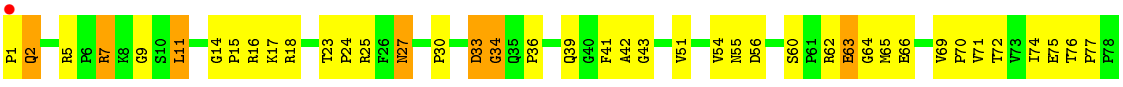
Chain A:

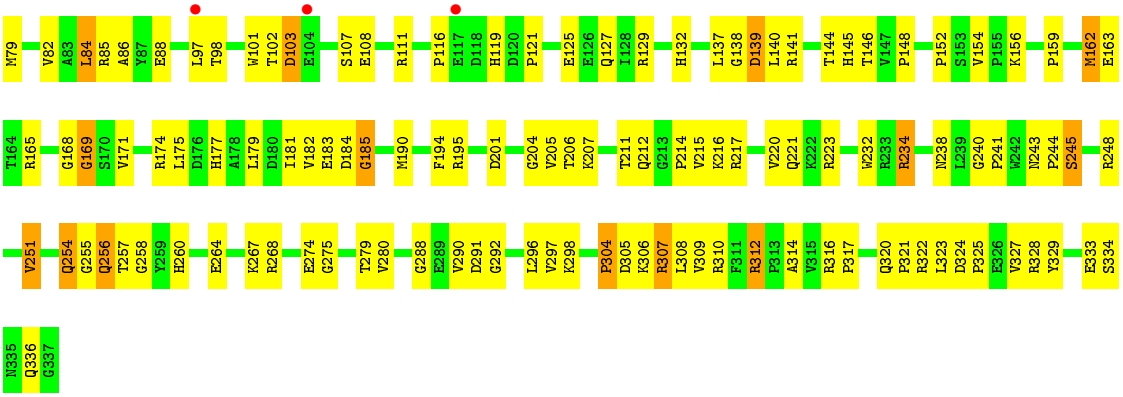


• Molecule 5: 50S ribosomal protein L3P

Chain B:

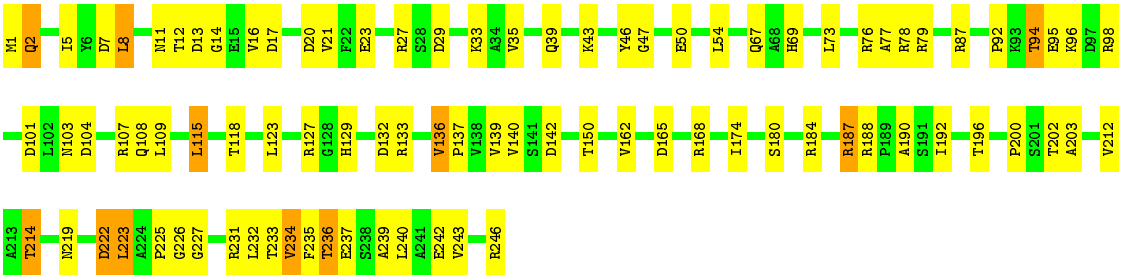






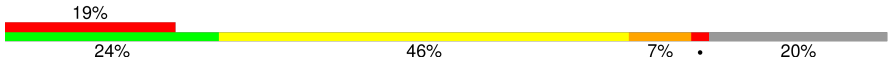
• Molecule 6: 50S ribosomal protein L4E

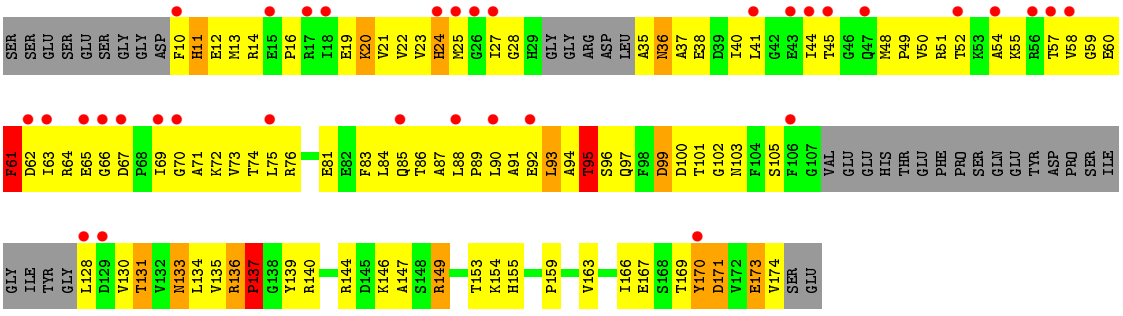
Chain C:



• Molecule 7: 50S ribosomal protein L5P

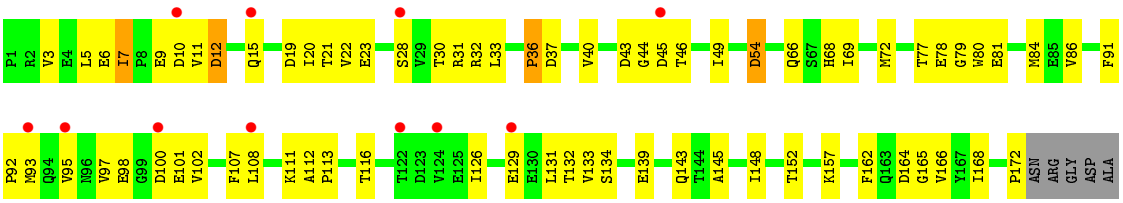
Chain D:





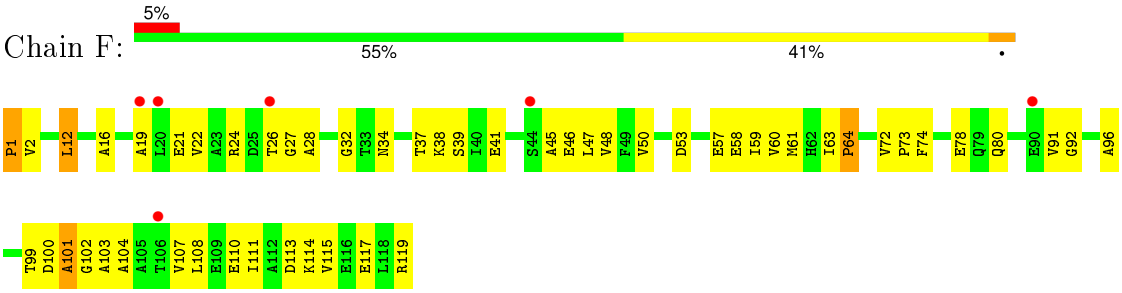
• Molecule 8: 50S ribosomal protein L6P

Chain E:



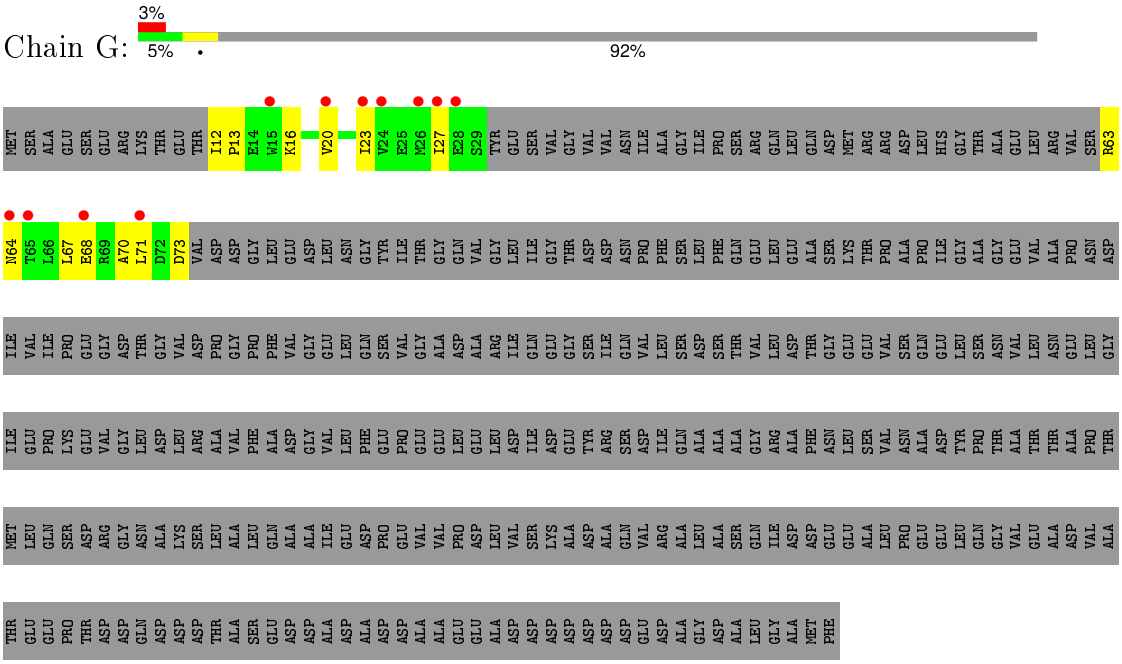
• Molecule 9: 50S ribosomal protein L7Ae

Chain F:



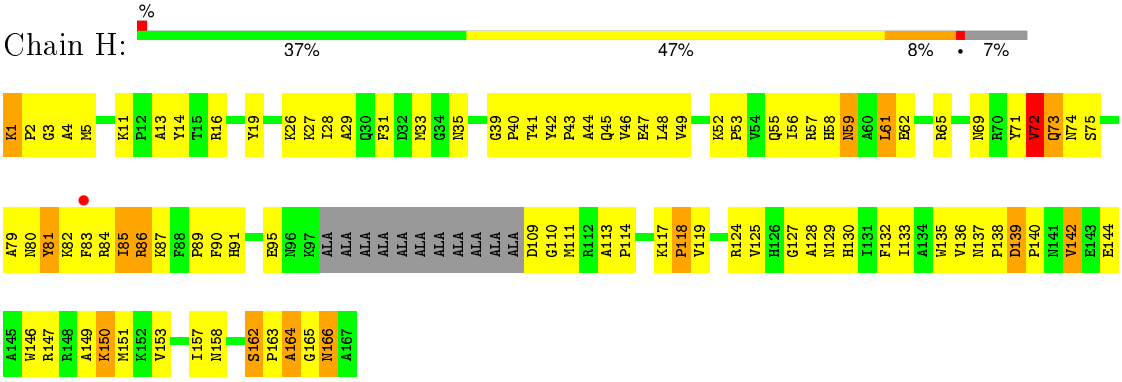
• Molecule 10: 50S RIBOSOMAL PROTEIN L10E

Chain G:



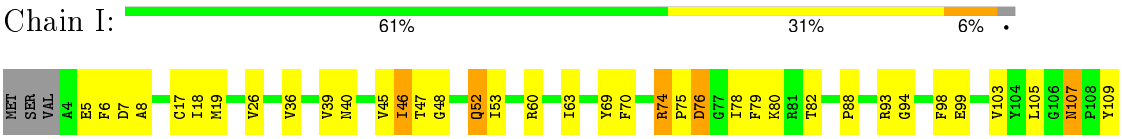
• Molecule 11: L10 Ribosomal Protein

Chain H:



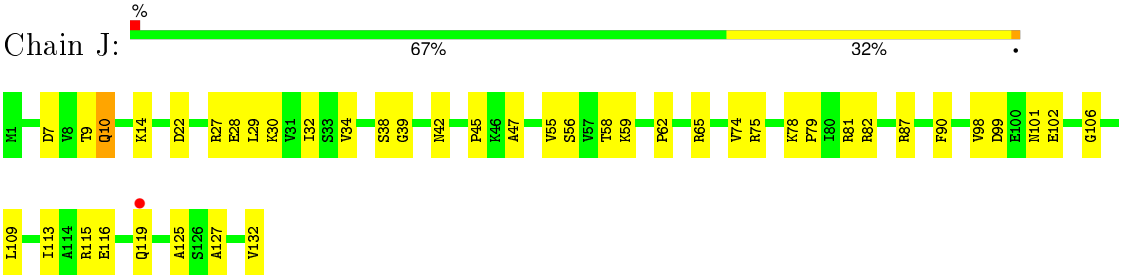
• Molecule 12: 50S ribosomal protein L13P

Chain I:



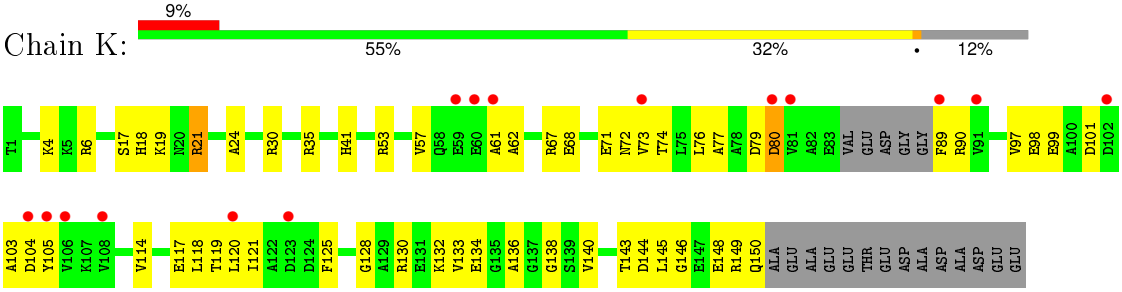
• Molecule 13: 50S ribosomal protein L14P

Chain J:



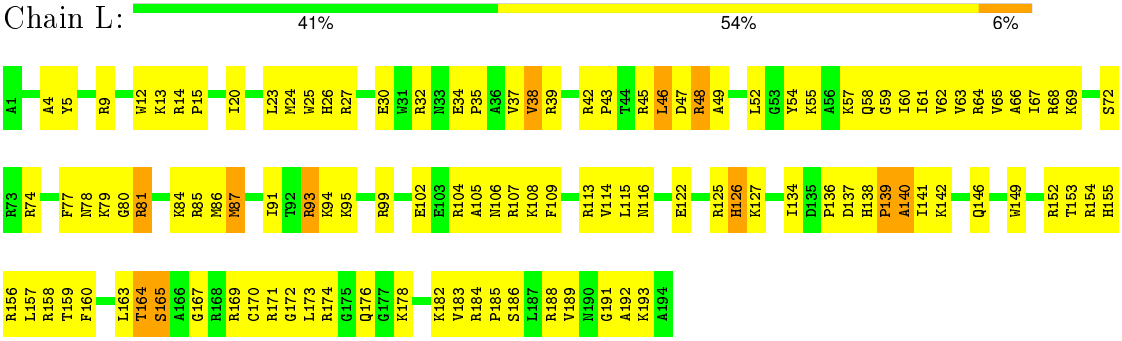
• Molecule 14: 50S ribosomal protein L15P

Chain K:



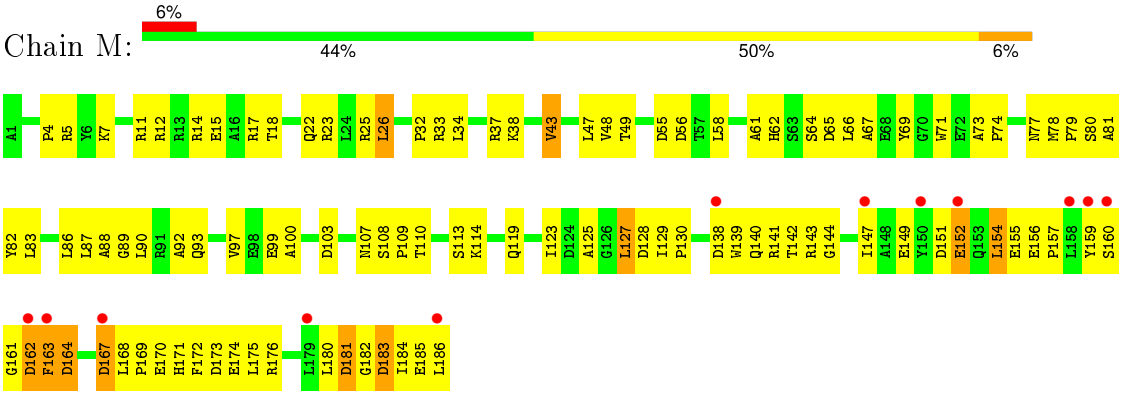
• Molecule 15: L15 Ribosomal Protein

Chain L:



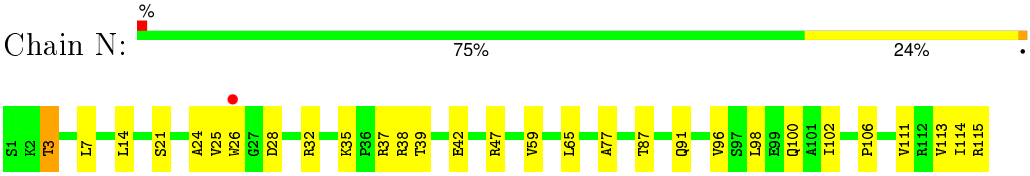
• Molecule 16: 50S ribosomal protein L18P

Chain M:



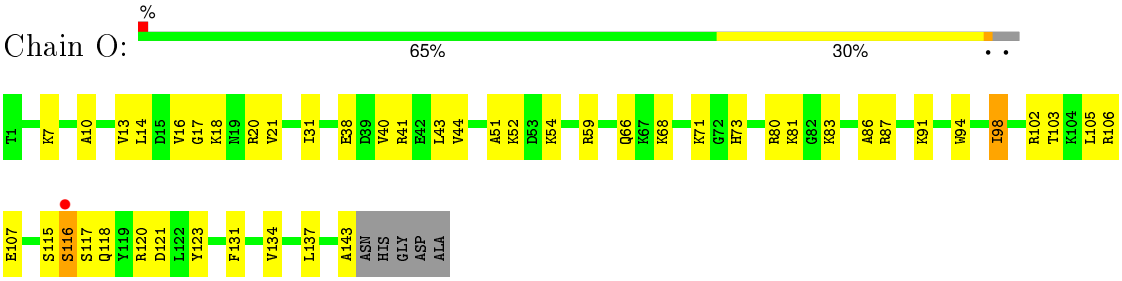
• Molecule 17: 50S ribosomal protein L18e

Chain N:



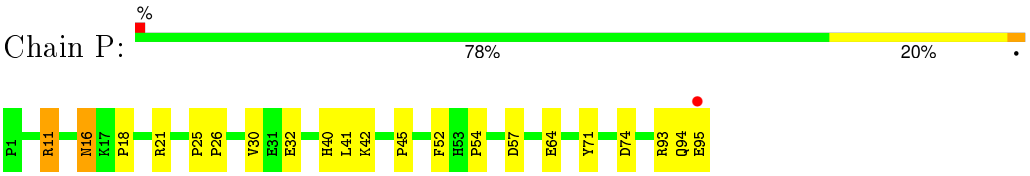
• Molecule 18: 50S ribosomal protein L19E

Chain O:



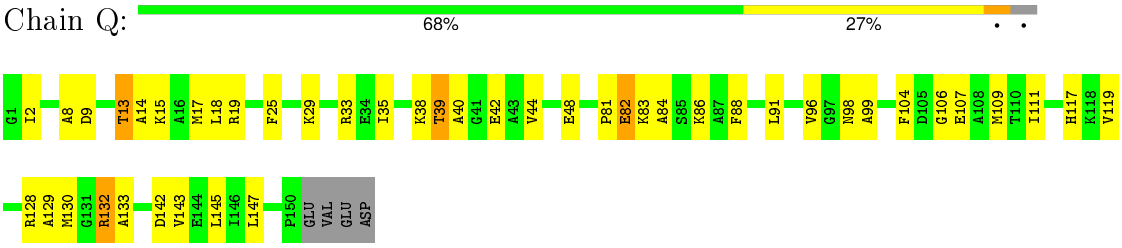
• Molecule 19: 50S ribosomal protein L21e

Chain P:



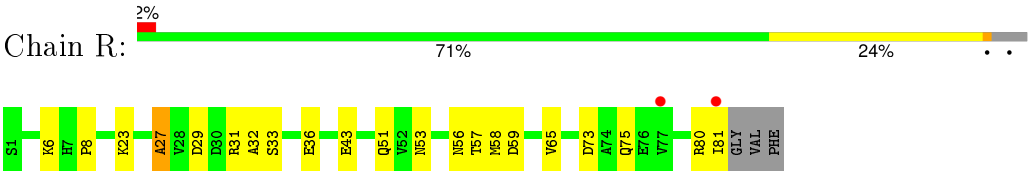
• Molecule 20: 50S ribosomal protein L22P

Chain Q:



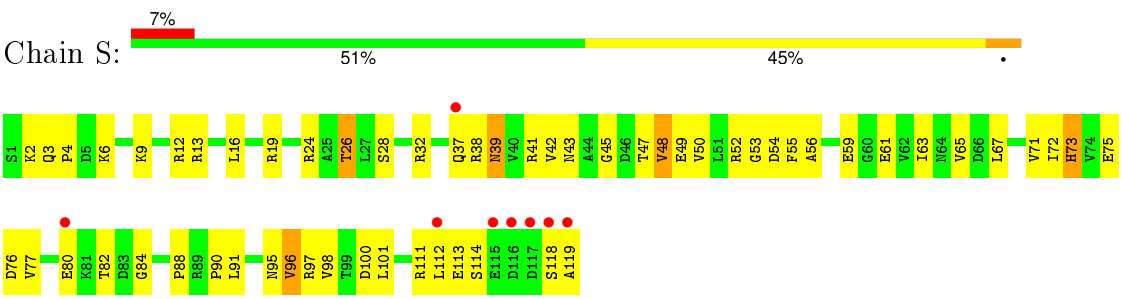
• Molecule 21: 50S ribosomal protein L23P

Chain R:



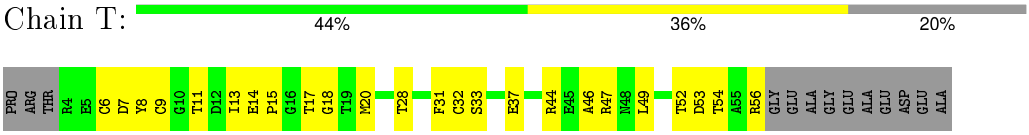
• Molecule 22: 50S ribosomal protein L24P

Chain S:



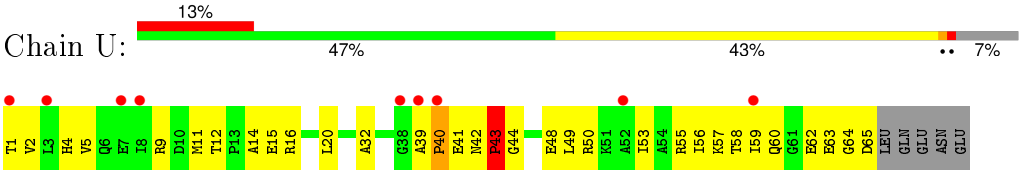
- Molecule 23: 50S ribosomal protein L24E

Chain T:



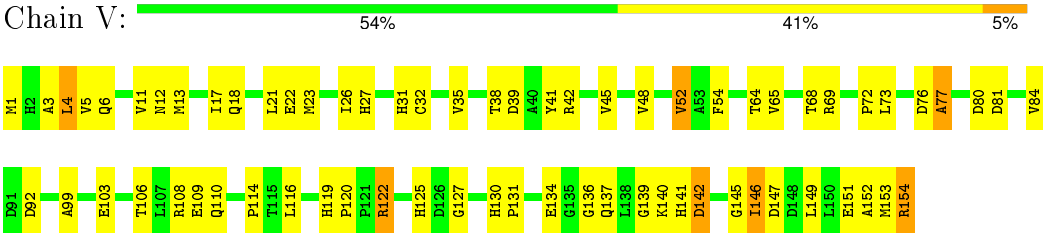
- Molecule 24: 50S ribosomal protein L29P

Chain U:



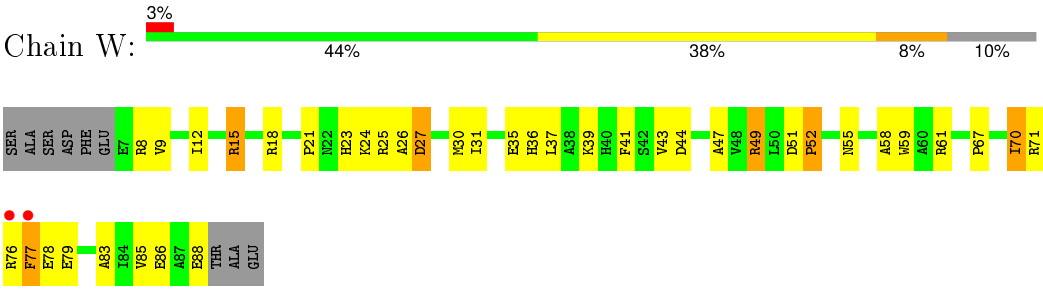
- Molecule 25: 50S ribosomal protein L30P

Chain V:



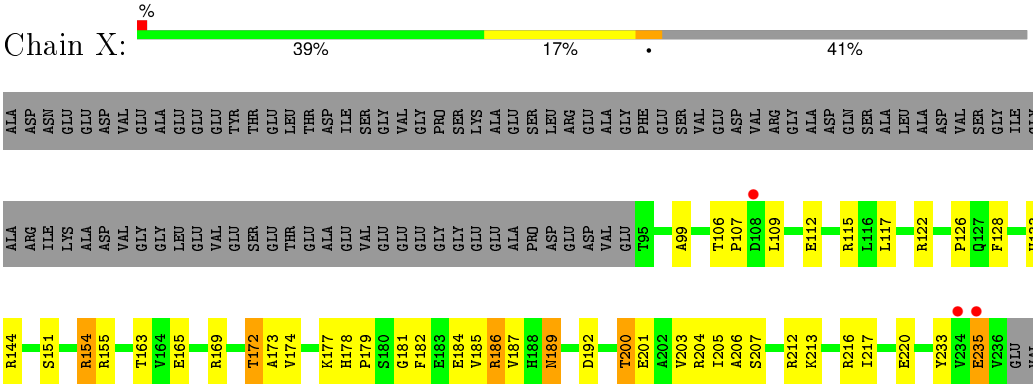
- Molecule 26: 50S ribosomal protein L31e

Chain W:



- Molecule 27: 50S ribosomal protein L32E

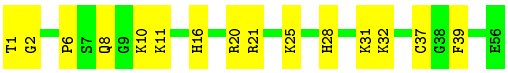
Chain X:



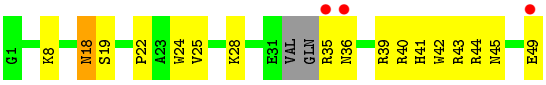
- Molecule 28: L37Ae 50S ribosomal protein

Chain Y:

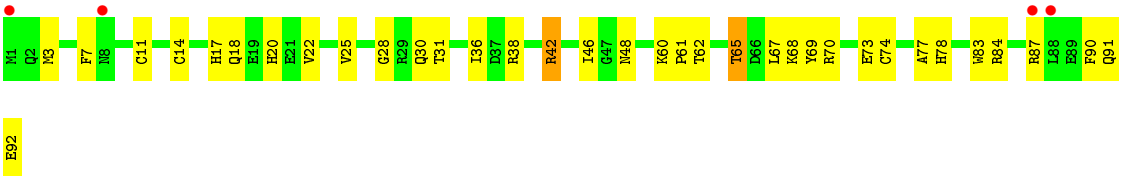
• Molecule 29: 50S ribosomal protein L37e



• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.52Å 300.82Å 574.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.04 – 3.11	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 91.3 (50.04-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 3.13Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.239 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	61.4	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 73.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 327197 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	98648	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, MG, CD, K, CL

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	0.78	1/66076 (0.0%)	0.88	85/103052 (0.1%)
2	9	0.69	0/2905	0.87	5/4528 (0.1%)
3	3	1.07	1/285 (0.4%)	0.93	0/438
4	A	0.52	0/1787	0.74	0/2409
5	B	0.56	0/2689	0.74	0/3652
6	C	0.61	0/1883	0.76	0/2551
7	D	0.47	0/1111	0.66	0/1498
8	E	0.55	0/1382	0.67	0/1880
9	F	0.50	0/896	0.65	0/1219
10	G	0.50	0/241	0.57	0/324
11	H	0.60	0/1246	0.84	2/1686 (0.1%)
12	I	0.64	1/1135 (0.1%)	0.72	0/1530
13	J	0.55	0/1003	0.76	0/1351
14	K	0.51	0/1126	0.77	0/1504
15	L	0.62	0/1633	0.78	2/2180 (0.1%)
16	M	0.48	0/1473	0.72	0/1999
17	N	0.58	0/873	0.71	0/1181
18	O	0.55	0/1143	0.66	0/1521
19	P	0.59	0/748	0.76	0/1005
20	Q	0.63	0/1172	0.75	0/1578
21	R	0.52	0/648	0.68	1/875 (0.1%)
22	S	0.51	0/957	0.73	0/1289
23	T	0.55	0/417	0.69	0/562
24	U	0.47	0/502	0.62	0/675
25	V	0.58	0/1218	0.72	0/1655
26	W	0.59	0/664	0.70	0/895
27	X	0.58	0/1146	0.75	0/1536
28	Y	0.58	0/575	0.77	0/763
29	Z	0.61	0/437	0.75	0/578
30	1	0.51	0/398	0.64	0/527
31	2	0.57	0/771	0.66	0/1024
All	All	0.72	3/98540 (0.0%)	0.84	95/147465 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	83
2	9	0	2
3	3	0	1
11	H	0	1
25	V	0	1
All	All	0	88

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	1	G	OP3-P	-5.80	1.54	1.61
1	0	2812	A	C5-C6	-5.75	1.35	1.41
12	I	17	CYS	CB-SG	-5.43	1.73	1.81

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1165	G	O5'-P-OP1	-23.72	82.23	110.70
1	0	1165	G	O5'-P-OP2	-17.27	89.97	110.70
1	0	1164	U	OP1-P-O3'	-17.09	67.61	105.20
1	0	1164	U	OP2-P-O3'	-16.44	69.02	105.20
1	0	1942	A	C5'-C4'-C3'	9.02	130.43	116.00

There are no chirality outliers.

5 of 88 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	246	G	Sidechain
1	0	308	U	Sidechain
1	0	324	G	Sidechain
1	0	332	G	Sidechain
1	0	48	A	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	59017	0	29799	943	0
2	9	2600	0	1326	92	0
3	3	257	0	133	3	0
4	A	1754	0	1763	123	0
5	B	2624	0	2533	178	0
6	C	1858	0	1816	118	0
7	D	1094	0	1085	139	0
8	E	1357	0	1266	79	0
9	F	885	0	854	62	0
10	G	240	0	231	21	0
11	H	1215	0	1215	148	0
12	I	1119	0	1098	61	0
13	J	993	0	1027	52	0
14	K	1114	0	1072	57	0
15	L	1605	0	1676	151	0
16	M	1444	0	1401	126	0
17	N	864	0	873	28	0
18	O	1133	0	1127	49	0
19	P	734	0	728	18	0
20	Q	1149	0	1122	52	0
21	R	641	0	605	22	0
22	S	949	0	923	59	0
23	T	410	0	364	36	0
24	U	499	0	511	29	0
25	V	1195	0	1137	97	0
26	W	654	0	653	48	0
27	X	1130	0	1133	64	0
28	Y	563	0	597	58	0
29	Z	430	0	426	24	0
30	1	393	0	406	25	0
31	2	755	0	728	34	0
32	0	109	0	0	0	0
32	2	2	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	J	1	0	0	0	0
32	S	1	0	0	0	0
32	X	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	0	72	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	2	0	0	0	0
34	I	1	0	0	0	0
34	K	1	0	0	0	0
34	L	1	0	0	0	0
34	P	1	0	0	0	0
34	Q	3	0	0	0	0
34	R	1	0	0	0	0
35	0	10	0	0	0	0
35	2	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	I	3	0	0	1	0
35	K	1	0	0	0	0
35	L	1	0	0	1	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	Q	1	0	0	0	0
35	X	1	0	0	0	0
36	2	1	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	Y	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5836	0	0	198	0
37	1	42	0	0	5	0
37	2	58	0	0	6	0
37	3	3	0	0	0	0
37	9	138	0	0	16	0
37	A	124	0	0	18	0
37	B	150	0	0	27	0
37	C	166	0	0	31	0
37	D	49	0	0	20	0
37	E	42	0	0	15	0
37	F	26	0	0	12	0
37	G	21	0	0	6	0
37	H	75	0	0	20	0
37	I	52	0	0	6	0
37	J	56	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	K	79	0	0	18	0
37	L	127	0	0	22	0
37	M	67	0	0	15	0
37	N	42	0	0	5	0
37	O	62	0	0	4	0
37	P	52	0	0	3	0
37	Q	82	0	0	7	0
37	R	35	0	0	6	0
37	S	41	0	0	10	0
37	T	23	0	0	6	0
37	U	14	0	0	2	0
37	V	69	0	0	10	0
37	W	29	0	0	5	0
37	X	85	0	0	18	0
37	Y	38	0	0	13	0
37	Z	56	0	0	4	0
All	All	98648	0	59628	2743	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 18.

The worst 5 of 2743 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:86:ARG:NH1	11:H:133:ILE:HG13	1.59	1.17
1:0:1160:G:H5'	1:0:1161:A:H5'	1.29	1.15
2:9:3024:U:O2'	2:9:3025:G:H4'	1.50	1.11
6:C:236:THR:HG22	6:C:239:ALA:H	1.02	1.11
1:0:960:G:H4'	37:0:6875:HOH:O	1.47	1.11

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	235/239 (98%)	210 (89%)	22 (9%)	3 (1%)	15 50
5	B	335/337 (99%)	306 (91%)	22 (7%)	7 (2%)	9 37
6	C	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	39 75
7	D	134/176 (76%)	96 (72%)	25 (19%)	13 (10%)	1 4
8	E	170/177 (96%)	162 (95%)	7 (4%)	1 (1%)	30 68
9	F	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	11 43
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100 100
11	H	152/167 (91%)	134 (88%)	12 (8%)	6 (4%)	4 22
12	I	140/145 (97%)	128 (91%)	9 (6%)	3 (2%)	9 37
13	J	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	24 63
14	K	141/164 (86%)	119 (84%)	20 (14%)	2 (1%)	14 48
15	L	192/194 (99%)	173 (90%)	17 (9%)	2 (1%)	19 58
16	M	184/186 (99%)	165 (90%)	13 (7%)	6 (3%)	5 26
17	N	113/115 (98%)	110 (97%)	3 (3%)	0	100 100
18	O	141/148 (95%)	136 (96%)	4 (3%)	1 (1%)	26 65
19	P	93/95 (98%)	87 (94%)	6 (6%)	0	100 100
20	Q	148/154 (96%)	141 (95%)	6 (4%)	1 (1%)	26 65
21	R	79/84 (94%)	74 (94%)	5 (6%)	0	100 100
22	S	117/119 (98%)	111 (95%)	6 (5%)	0	100 100
23	T	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	9 38
24	U	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	5 26
25	V	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	26 65
26	W	80/91 (88%)	72 (90%)	6 (8%)	2 (2%)	7 32
27	X	140/240 (58%)	138 (99%)	2 (1%)	0	100 100
28	Y	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	14 48
29	Z	54/56 (96%)	52 (96%)	2 (4%)	0	100 100
30	1	42/48 (88%)	42 (100%)	0	0	100 100
31	2	90/92 (98%)	87 (97%)	3 (3%)	0	100 100
All	All	3633/4235 (86%)	3327 (92%)	250 (7%)	56 (2%)	13 46

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	139	ASP
7	D	93	LEU
7	D	95	THR
7	D	137	PRO
7	D	173	GLU

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	179/181 (99%)	167 (93%)	12 (7%)	20	56
5	B	282/282 (100%)	264 (94%)	18 (6%)	22	57
6	C	193/193 (100%)	180 (93%)	13 (7%)	20	56
7	D	117/147 (80%)	107 (92%)	10 (8%)	13	45
8	E	152/155 (98%)	146 (96%)	6 (4%)	39	75
9	F	92/92 (100%)	90 (98%)	2 (2%)	60	85
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	122/122 (100%)	110 (90%)	12 (10%)	10	36
12	I	118/121 (98%)	107 (91%)	11 (9%)	11	39
13	J	106/106 (100%)	103 (97%)	3 (3%)	51	82
14	K	112/126 (89%)	109 (97%)	3 (3%)	52	82
15	L	166/166 (100%)	157 (95%)	9 (5%)	27	64
16	M	149/149 (100%)	143 (96%)	6 (4%)	38	75
17	N	93/93 (100%)	91 (98%)	2 (2%)	60	85
18	O	113/116 (97%)	110 (97%)	3 (3%)	52	82
19	P	79/79 (100%)	74 (94%)	5 (6%)	22	58
20	Q	117/121 (97%)	113 (97%)	4 (3%)	44	79
21	R	71/73 (97%)	71 (100%)	0	100	100
22	S	105/105 (100%)	100 (95%)	5 (5%)	31	69
23	T	44/52 (85%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	U	51/56 (91%)	50 (98%)	1 (2%)	63 86
25	V	130/130 (100%)	122 (94%)	8 (6%)	23 59
26	W	66/73 (90%)	61 (92%)	5 (8%)	16 51
27	X	120/195 (62%)	111 (92%)	9 (8%)	17 51
28	Y	56/56 (100%)	52 (93%)	4 (7%)	18 54
29	Z	46/46 (100%)	46 (100%)	0	100 100
30	1	42/44 (96%)	41 (98%)	1 (2%)	57 84
31	2	79/79 (100%)	76 (96%)	3 (4%)	40 76
All	All	3027/3441 (88%)	2872 (95%)	155 (5%)	29 66

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	H	142	VAL
13	J	98	VAL
27	X	189	ASN
11	H	166	ASN
12	I	107	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
14	K	42	ASN
18	O	66	GLN
29	Z	28	HIS
15	L	26	HIS
15	L	176	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2748/2922 (94%)	278 (10%)	96 (3%)
2	9	121/122 (99%)	20 (16%)	7 (5%)
3	3	10/28 (35%)	3 (30%)	0
All	All	2879/3072 (93%)	301 (10%)	103 (3%)

5 of 301 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A

5 of 103 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1450	C
1	0	1856	C
1	0	2902	A
1	0	1488	U
1	0	1653	A

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 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

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	2754/2922 (94%)	-0.14	28 (1%) 84 69	28, 55, 104, 159	0
2	9	122/122 (100%)	0.11	5 (4%) 41 19	37, 71, 106, 162	0
3	3	12/28 (42%)	2.70	8 (66%) 0 0	80, 132, 141, 145	0
4	A	237/239 (99%)	0.10	7 (2%) 54 29	36, 64, 100, 123	0
5	B	337/337 (100%)	-0.10	4 (1%) 81 64	32, 65, 90, 100	0
6	C	246/246 (100%)	-0.15	0 100 100	27, 58, 84, 91	0
7	D	140/176 (79%)	1.21	34 (24%) 1 0	66, 110, 129, 134	0
8	E	172/177 (97%)	0.64	11 (6%) 23 9	49, 75, 99, 106	0
9	F	119/119 (100%)	0.50	6 (5%) 32 13	62, 87, 111, 120	0
10	G	29/348 (8%)	1.72	11 (37%) 0 0	79, 97, 104, 106	0
11	H	156/167 (93%)	0.12	1 (0%) 90 80	36, 62, 87, 94	0
12	I	142/145 (97%)	-0.12	0 100 100	42, 55, 80, 99	0
13	J	132/132 (100%)	0.03	1 (0%) 87 75	42, 64, 89, 97	0
14	K	145/164 (88%)	0.41	15 (10%) 9 3	33, 82, 117, 125	0
15	L	194/194 (100%)	-0.19	0 100 100	40, 58, 78, 90	0
16	M	186/186 (100%)	0.51	12 (6%) 22 8	48, 80, 122, 133	0
17	N	115/115 (100%)	0.12	1 (0%) 85 72	54, 69, 86, 89	0
18	O	143/148 (96%)	0.20	1 (0%) 89 78	45, 68, 85, 94	0
19	P	95/95 (100%)	-0.07	1 (1%) 82 66	38, 55, 72, 90	0
20	Q	150/154 (97%)	-0.10	0 100 100	36, 51, 74, 84	0
21	R	81/84 (96%)	0.17	2 (2%) 61 37	56, 77, 96, 100	0
22	S	119/119 (100%)	0.42	8 (6%) 21 7	50, 70, 97, 117	0
23	T	53/66 (80%)	0.19	0 100 100	53, 67, 83, 91	0
24	U	65/70 (92%)	0.94	9 (13%) 4 2	64, 90, 123, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	V	154/154 (100%)	-0.27	0 100 100	38, 53, 74, 84	0
26	W	82/91 (90%)	0.31	3 (3%) 45 22	51, 66, 87, 107	0
27	X	142/240 (59%)	0.04	3 (2%) 67 44	31, 54, 75, 96	0
28	Y	73/73 (100%)	0.02	2 (2%) 58 34	57, 73, 87, 95	0
29	Z	56/56 (100%)	-0.37	0 100 100	34, 44, 51, 53	0
30	1	46/48 (95%)	0.41	3 (6%) 22 8	48, 80, 110, 119	0
31	2	92/92 (100%)	0.35	4 (4%) 39 18	47, 68, 82, 97	0
All	All	6589/7307 (90%)	0.05	180 (2%) 58 34	27, 62, 106, 162	0

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	U	1	THR	9.6
2	9	3001	U	7.8
16	M	186	LEU	7.5
22	S	119	ALA	5.8
10	G	23	ILE	5.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
34	NA	0	8356	1/1	0.90	0.64	44.54	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	NA	0	8362	1/1	0.83	0.46	41.51	59,59,59,59	0
32	MG	0	8114	1/1	0.73	1.12	40.68	93,93,93,93	0
34	NA	9	8383	1/1	0.87	1.06	34.61	71,71,71,71	0
34	NA	0	8374	1/1	0.97	0.90	34.05	62,62,62,62	0
34	NA	0	8303	1/1	0.78	0.57	33.38	58,58,58,58	0
34	NA	0	8332	1/1	0.76	0.48	26.57	47,47,47,47	0
35	CL	0	8505	1/1	0.93	0.52	23.81	69,69,69,69	0
34	NA	0	8378	1/1	0.94	0.73	21.13	38,38,38,38	0
32	MG	0	8064	1/1	0.97	0.42	18.63	37,37,37,37	0
34	NA	0	8373	1/1	0.84	0.62	17.25	58,58,58,58	0
35	CL	0	8515	1/1	0.74	0.42	16.96	107,107,107,107	0
34	NA	0	8326	1/1	0.85	0.72	15.15	98,98,98,98	0
34	NA	K	8380	1/1	0.88	0.50	15.04	63,63,63,63	0
34	NA	0	8361	1/1	0.90	0.41	14.95	44,44,44,44	0
34	NA	0	8371	1/1	0.67	0.39	14.57	51,51,51,51	0
34	NA	0	8321	1/1	0.93	0.49	13.14	42,42,42,42	0
34	NA	0	8372	1/1	0.91	0.46	11.86	66,66,66,66	0
34	NA	0	8379	1/1	0.93	0.25	10.83	53,53,53,53	0
33	K	0	8202	1/1	0.93	0.28	8.41	76,76,76,76	0
34	NA	0	8331	1/1	0.98	0.25	8.37	66,66,66,66	0
35	CL	B	8519	1/1	0.96	0.34	8.21	65,65,65,65	0
34	NA	0	8340	1/1	0.90	0.39	7.63	47,47,47,47	0
34	NA	0	8323	1/1	0.93	0.25	7.56	50,50,50,50	0
32	MG	0	8044	1/1	0.95	0.22	7.25	74,74,74,74	0
34	NA	0	8325	1/1	0.93	0.21	7.20	56,56,56,56	0
32	MG	2	8118	1/1	0.57	0.43	6.95	70,70,70,70	0
34	NA	Q	8386	1/1	0.80	0.44	6.54	82,82,82,82	0
32	MG	A	8065	1/1	0.90	0.40	5.99	38,38,38,38	0
34	NA	0	8368	1/1	0.84	0.21	5.53	58,58,58,58	0
34	NA	0	8365	1/1	0.84	0.41	5.48	62,62,62,62	0
34	NA	0	8382	1/1	0.88	0.24	4.84	99,99,99,99	0
34	NA	0	8364	1/1	0.90	0.20	3.30	51,51,51,51	0
34	NA	0	8366	1/1	0.87	0.36	3.19	66,66,66,66	0
34	NA	0	8381	1/1	0.71	0.22	2.94	76,76,76,76	0
34	NA	0	8350	1/1	0.97	0.16	2.65	36,36,36,36	0
32	MG	0	8112	1/1	0.93	0.22	2.50	59,59,59,59	0
34	NA	0	8343	1/1	0.95	0.30	2.39	40,40,40,40	0
35	CL	N	8508	1/1	0.86	0.36	1.79	92,92,92,92	0
32	MG	0	8013	1/1	0.98	0.17	1.11	57,57,57,57	0
35	CL	I	8521	1/1	0.83	0.22	0.91	66,66,66,66	0
34	NA	0	8335	1/1	0.98	0.17	0.46	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	NA	0	8324	1/1	0.77	0.24	0.40	55,55,55,55	0
35	CL	0	8512	1/1	0.98	0.20	0.19	50,50,50,50	0
32	MG	0	8110	1/1	0.98	0.16	-0.01	30,30,30,30	0
32	MG	0	8018	1/1	0.98	0.15	-0.25	48,48,48,48	0
33	K	0	8201	1/1	0.98	0.16	-0.26	89,89,89,89	0
34	NA	0	8339	1/1	0.95	0.15	-0.31	25,25,25,25	0
34	NA	0	8333	1/1	0.83	0.15	-0.37	52,52,52,52	0
32	MG	0	8053	1/1	0.84	0.14	-0.39	59,59,59,59	0
35	CL	2	8504	1/1	0.86	0.26	-0.56	67,67,67,67	0
34	NA	0	8353	1/1	0.98	0.16	-0.70	49,49,49,49	0
34	NA	C	8304	1/1	0.89	0.16	-0.87	41,41,41,41	0
35	CL	L	8518	1/1	0.92	0.19	-1.05	55,55,55,55	0
32	MG	0	8086	1/1	0.98	0.11	-1.17	67,67,67,67	0
34	NA	0	8317	1/1	0.97	0.11	-1.24	51,51,51,51	0
36	CD	Y	8403	1/1	0.98	0.09	-1.35	79,79,79,79	0
34	NA	I	8346	1/1	0.95	0.16	-1.38	43,43,43,43	0
32	MG	0	8088	1/1	0.96	0.14	-1.47	36,36,36,36	0
36	CD	2	8404	1/1	0.98	0.08	-1.51	74,74,74,74	0
34	NA	Q	8337	1/1	0.86	0.12	-1.54	57,57,57,57	0
34	NA	Q	8338	1/1	0.95	0.12	-1.63	68,68,68,68	0
32	MG	S	8073	1/1	0.95	0.22	-1.78	59,59,59,59	0
32	MG	2	8078	1/1	0.98	0.07	-1.80	46,46,46,46	0
36	CD	Z	8402	1/1	1.00	0.07	-1.81	68,68,68,68	0
34	NA	H	8309	1/1	0.95	0.08	-1.94	24,24,24,24	0
32	MG	0	8056	1/1	0.98	0.13	-2.04	67,67,67,67	0
32	MG	0	8067	1/1	0.98	0.15	-2.08	57,57,57,57	0
32	MG	0	8108	1/1	0.98	0.14	-2.11	83,83,83,83	0
32	MG	0	8057	1/1	0.96	0.14	-2.13	38,38,38,38	0
32	MG	0	8107	1/1	0.95	0.10	-2.14	61,61,61,61	0
32	MG	0	8015	1/1	0.95	0.11	-2.16	23,23,23,23	0
34	NA	0	8308	1/1	0.95	0.13	-2.45	46,46,46,46	0
34	NA	0	8314	1/1	0.95	0.10	-2.54	32,32,32,32	0
34	NA	P	8348	1/1	0.96	0.11	-2.59	34,34,34,34	0
36	CD	T	8401	1/1	0.99	0.07	-2.67	82,82,82,82	0
32	MG	0	8074	1/1	0.99	0.07	-2.72	27,27,27,27	0
32	MG	0	8077	1/1	0.99	0.09	-2.73	34,34,34,34	0
32	MG	0	8058	1/1	1.00	0.11	-2.76	41,41,41,41	0
32	MG	0	8010	1/1	0.99	0.11	-2.88	34,34,34,34	0
34	NA	A	8345	1/1	0.97	0.12	-2.88	53,53,53,53	0
34	NA	0	8376	1/1	0.98	0.12	-3.26	53,53,53,53	0
32	MG	0	8059	1/1	0.95	0.11	-3.34	76,76,76,76	0
34	NA	L	8347	1/1	0.93	0.11	-3.49	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	0	8033	1/1	0.97	0.09	-3.62	29,29,29,29	0
32	MG	0	8039	1/1	0.98	0.06	-3.68	53,53,53,53	0
34	NA	0	8327	1/1	0.91	0.12	-3.74	44,44,44,44	0
32	MG	0	8096	1/1	0.96	0.11	-3.86	49,49,49,49	0
32	MG	0	8004	1/1	0.97	0.05	-3.86	60,60,60,60	0
32	MG	0	8017	1/1	0.99	0.03	-4.08	34,34,34,34	0
32	MG	0	8035	1/1	0.99	0.10	-4.18	55,55,55,55	0
32	MG	0	8062	1/1	0.98	0.08	-4.29	63,63,63,63	0
32	MG	0	8071	1/1	0.94	0.09	-4.42	100,100,100,100	0
32	MG	B	8055	1/1	0.98	0.04	-4.45	37,37,37,37	0
32	MG	X	8109	1/1	0.98	0.07	-4.66	34,34,34,34	0
32	MG	0	8008	1/1	0.95	0.09	-4.75	45,45,45,45	0
34	NA	0	8344	1/1	0.95	0.05	-4.83	31,31,31,31	0
32	MG	0	8060	1/1	0.99	0.11	-5.03	38,38,38,38	0
34	NA	0	8305	1/1	0.96	0.11	-5.07	44,44,44,44	0
32	MG	0	8084	1/1	0.89	0.10	-5.14	30,30,30,30	0
32	MG	0	8027	1/1	0.99	0.03	-5.19	43,43,43,43	0
32	MG	0	8003	1/1	0.98	0.07	-5.82	26,26,26,26	0
32	MG	0	8002	1/1	0.99	0.06	-5.91	43,43,43,43	0
32	MG	0	8001	1/1	0.92	0.09	-6.13	43,43,43,43	0
32	MG	0	8021	1/1	0.99	0.07	-6.19	28,28,28,28	0
32	MG	0	8012	1/1	0.97	0.07	-6.25	33,33,33,33	0
32	MG	0	8038	1/1	0.99	0.09	-6.28	47,47,47,47	0
32	MG	0	8020	1/1	0.98	0.08	-6.53	29,29,29,29	0
32	MG	0	8080	1/1	0.98	0.09	-6.94	44,44,44,44	0
34	NA	0	8320	1/1	0.97	0.10	-7.72	25,25,25,25	0
32	MG	0	8032	1/1	0.99	0.07	-7.85	42,42,42,42	0
32	MG	0	8019	1/1	0.99	0.08	-8.33	41,41,41,41	0
32	MG	0	8007	1/1	0.97	0.07	-8.86	25,25,25,25	0
32	MG	0	8054	1/1	0.94	0.10	-9.27	25,25,25,25	0
32	MG	0	8052	1/1	0.97	0.10	-10.79	36,36,36,36	0
32	MG	0	8014	1/1	0.98	0.03	-10.92	24,24,24,24	0
32	MG	0	8006	1/1	0.98	0.05	-11.76	57,57,57,57	0
32	MG	0	8042	1/1	0.99	0.14	-	52,52,52,52	0
34	NA	0	8310	1/1	0.78	0.56	-	35,35,35,35	0
34	NA	0	8301	1/1	0.89	0.16	-	44,44,44,44	0
32	MG	0	8119	1/1	0.17	0.95	-	112,112,112,112	0
32	MG	0	8085	1/1	0.94	0.20	-	91,91,91,91	0
32	MG	0	8040	1/1	0.94	0.09	-	67,67,67,67	0
34	NA	0	8375	1/1	0.93	0.31	-	85,85,85,85	0
32	MG	0	8036	1/1	0.99	0.06	-	45,45,45,45	0
34	NA	R	8312	1/1	0.23	0.77	-	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	CL	0	8517	1/1	0.93	0.20	-	56,56,56,56	0
34	NA	0	8352	1/1	0.74	0.54	-	54,54,54,54	0
32	MG	0	8117	1/1	0.98	0.07	-	37,37,37,37	0
32	MG	0	8102	1/1	0.92	0.25	-	48,48,48,48	0
32	MG	0	8076	1/1	0.90	0.14	-	96,96,96,96	0
36	CD	N	8405	1/1	0.95	0.07	-	118,118,118,118	0
35	CL	X	8520	1/1	0.92	0.20	-	47,47,47,47	0
34	NA	0	8306	1/1	0.93	0.72	-	57,57,57,57	0
32	MG	0	8050	1/1	0.94	0.19	-	71,71,71,71	0
32	MG	0	8011	1/1	0.95	0.40	-	1,1,1,1	0
32	MG	0	8101	1/1	0.94	0.13	-	48,48,48,48	0
32	MG	0	8047	1/1	0.98	0.07	-	74,74,74,74	0
32	MG	A	8066	1/1	0.95	0.07	-	60,60,60,60	0
32	MG	0	8028	1/1	0.90	0.07	-	52,52,52,52	0
35	CL	M	8507	1/1	0.95	0.15	-	66,66,66,66	0
34	NA	0	8313	1/1	0.98	0.11	-	57,57,57,57	0
32	MG	0	8104	1/1	0.92	0.11	-	52,52,52,52	0
34	NA	0	8377	1/1	0.86	0.25	-	77,77,77,77	0
32	MG	0	8103	1/1	0.80	0.34	-	67,67,67,67	0
32	MG	0	8009	1/1	0.97	0.08	-	18,18,18,18	0
34	NA	0	8367	1/1	0.77	0.26	-	60,60,60,60	0
32	MG	0	8037	1/1	0.98	0.10	-	72,72,72,72	0
32	MG	0	8048	1/1	0.98	0.11	-	33,33,33,33	0
32	MG	0	8099	1/1	0.93	0.12	-	57,57,57,57	0
35	CL	0	8516	1/1	0.97	0.20	-	51,51,51,51	0
34	NA	0	8349	1/1	0.96	0.16	-	59,59,59,59	0
34	NA	0	8370	1/1	0.95	0.31	-	53,53,53,53	0
32	MG	0	8097	1/1	0.99	0.17	-	36,36,36,36	0
32	MG	0	8030	1/1	0.99	0.12	-	44,44,44,44	0
32	MG	0	8023	1/1	0.90	0.14	-	35,35,35,35	0
32	MG	0	8093	1/1	0.96	0.11	-	38,38,38,38	0
32	MG	0	8106	1/1	0.96	0.12	-	45,45,45,45	0
32	MG	0	8022	1/1	0.99	0.04	-	41,41,41,41	0
32	MG	9	8095	1/1	0.98	0.08	-	80,80,80,80	0
35	CL	I	8501	1/1	0.97	0.24	-	80,80,80,80	0
34	NA	0	8318	1/1	0.97	0.23	-	38,38,38,38	0
34	NA	0	8328	1/1	0.87	0.56	-	51,51,51,51	0
35	CL	0	8503	1/1	0.86	0.31	-	61,61,61,61	0
34	NA	0	8342	1/1	0.90	0.23	-	46,46,46,46	0
35	CL	K	8510	1/1	0.89	0.20	-	75,75,75,75	0
34	NA	0	8307	1/1	0.82	0.26	-	55,55,55,55	0
35	CL	A	8509	1/1	0.94	0.26	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	NA	0	8354	1/1	0.82	0.35	-	51,51,51,51	0
32	MG	J	8069	1/1	0.90	0.14	-	72,72,72,72	0
32	MG	0	8072	1/1	0.98	0.15	-	114,114,114,114	0
32	MG	0	8016	1/1	0.99	0.11	-	55,55,55,55	0
32	MG	0	8094	1/1	0.97	0.08	-	63,63,63,63	0
32	MG	0	8049	1/1	0.89	0.21	-	59,59,59,59	0
32	MG	Y	8105	1/1	0.82	0.26	-	28,28,28,28	0
32	MG	0	8026	1/1	0.98	0.08	-	35,35,35,35	0
35	CL	0	8513	1/1	0.88	0.18	-	68,68,68,68	0
34	NA	0	8357	1/1	0.96	0.10	-	66,66,66,66	0
35	CL	0	8511	1/1	0.94	0.58	-	87,87,87,87	0
32	MG	0	8029	1/1	0.99	0.10	-	73,73,73,73	0
32	MG	0	8075	1/1	0.87	0.10	-	56,56,56,56	0
34	NA	0	8330	1/1	0.93	0.32	-	38,38,38,38	0
35	CL	Q	8506	1/1	0.94	0.19	-	68,68,68,68	0
34	NA	0	8334	1/1	0.85	0.07	-	39,39,39,39	0
34	NA	0	8319	1/1	0.97	0.08	-	40,40,40,40	0
32	MG	0	8089	1/1	0.96	0.28	-	84,84,84,84	0
34	NA	0	8336	1/1	0.97	0.09	-	48,48,48,48	0
32	MG	0	8111	1/1	0.95	0.12	-	45,45,45,45	0
34	NA	0	8311	1/1	0.93	0.13	-	48,48,48,48	0
32	MG	0	8045	1/1	0.98	0.09	-	70,70,70,70	0
32	MG	0	8113	1/1	0.98	0.10	-	53,53,53,53	0
32	MG	0	8046	1/1	0.94	0.09	-	80,80,80,80	0
34	NA	0	8369	1/1	0.73	0.48	-	84,84,84,84	0
32	MG	0	8041	1/1	0.97	0.15	-	62,62,62,62	0
32	MG	0	8005	1/1	0.98	0.09	-	66,66,66,66	0
34	NA	0	8341	1/1	0.30	0.30	-	52,52,52,52	0
32	MG	0	8087	1/1	0.92	0.16	-	60,60,60,60	0
32	MG	0	8091	1/1	0.98	0.05	-	47,47,47,47	0
32	MG	0	8090	1/1	0.97	0.12	-	46,46,46,46	0
32	MG	0	8116	1/1	0.93	0.12	-	58,58,58,58	0
32	MG	0	8043	1/1	0.94	0.07	-	48,48,48,48	0
34	NA	0	8360	1/1	0.88	0.89	-	47,47,47,47	0
32	MG	0	8051	1/1	0.92	0.23	-	89,89,89,89	0
32	MG	0	8115	1/1	0.93	0.11	-	58,58,58,58	0
34	NA	0	8329	1/1	0.67	0.55	-	108,108,108,108	0
34	NA	0	8355	1/1	0.93	0.67	-	50,50,50,50	0
35	CL	0	8514	1/1	0.95	0.20	-	54,54,54,54	0
35	CL	0	8522	1/1	0.90	0.41	-	89,89,89,89	0
32	MG	0	8079	1/1	0.98	0.10	-	38,38,38,38	0
32	MG	0	8061	1/1	0.95	0.05	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	0	8031	1/1	0.99	0.04	-	43,43,43,43	0
32	MG	0	8092	1/1	0.89	0.24	-	89,89,89,89	0
34	NA	0	8384	1/1	0.57	1.07	-	122,122,122,122	0
32	MG	0	8081	1/1	0.88	0.11	-	79,79,79,79	0
32	MG	0	8025	1/1	0.90	0.12	-	32,32,32,32	0
34	NA	0	8385	1/1	0.77	0.47	-	72,72,72,72	0
32	MG	0	8063	1/1	0.96	0.06	-	107,107,107,107	0
32	MG	0	8070	1/1	0.97	0.24	-	63,63,63,63	0
34	NA	0	8302	1/1	0.89	0.20	-	52,52,52,52	0
34	NA	0	8359	1/1	0.93	0.59	-	72,72,72,72	0
32	MG	0	8024	1/1	0.87	0.64	-	187,187,187,187	0
34	NA	9	8351	1/1	0.25	0.39	-	91,91,91,91	0
34	NA	0	8316	1/1	0.99	0.22	-	47,47,47,47	0
34	NA	0	8315	1/1	0.97	0.17	-	65,65,65,65	0
32	MG	0	8034	1/1	0.99	0.07	-	42,42,42,42	0
32	MG	0	8100	1/1	0.89	0.20	-	99,99,99,99	0
32	MG	0	8098	1/1	0.98	0.29	-	50,50,50,50	0
32	MG	0	8082	1/1	0.91	0.23	-	58,58,58,58	0
35	CL	I	8502	1/1	0.97	0.10	-	74,74,74,74	0
34	NA	H	8322	1/1	0.87	0.40	-	59,59,59,59	0
34	NA	0	8358	1/1	0.93	0.66	-	91,91,91,91	0
32	MG	0	8083	1/1	0.95	0.13	-	58,58,58,58	0
34	NA	0	8363	1/1	0.49	0.84	-	68,68,68,68	0
32	MG	0	8068	1/1	0.98	0.09	-	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.