wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 – 05:27 AM EDT

PDB ID	:	1Q81
Title	:	Crystal Structure of minihelix with 3' puromycin bound to A-site of the 50S ribosomal subunit.
Authors	:	Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2003-08-20
Resolution	:	2.95 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 (i)) were used in the production of this report:

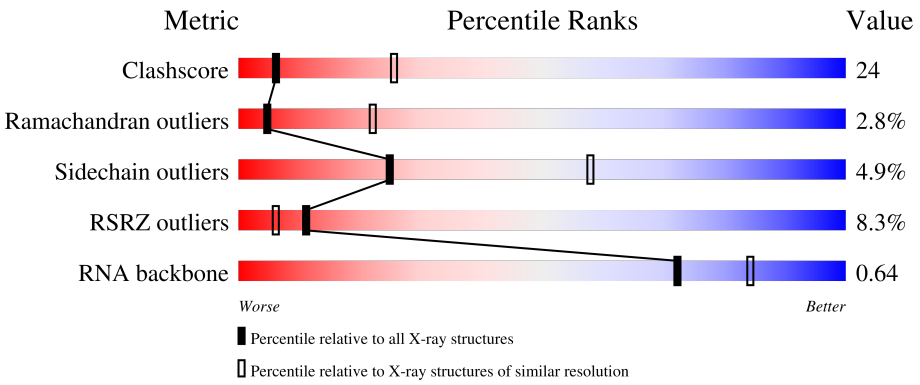
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.95 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	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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	A	2922	2%, 48%, 39%, 7%, 6%
2	B	122	5%, 39%, 48%, 11%, •
3	5	2	100%, 100%
4	C	239	10%, 52%, 41%, 6%, •
5	D	337	%, 45%, 50%, 6%

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Mol	Chain	Length	Quality of chain
6	E	246	%, 50%, 46%
7	F	176	40%, 23%, 48%, 8%, 20%
8	G	177	14%, 46%, 50%
9	H	119	18%, 49%, 47%
10	I	348	5%, 92%
11	J	167	8%, 30%, 54%, 8%, 7%
12	K	145	2%, 47%, 44%, 7%
13	L	132	2%, 48%, 50%
14	M	164	18%, 43%, 42%, 12%
15	N	194	3%, 37%, 56%, 7%
16	O	186	18%, 34%, 57%, 9%
17	P	115	2%, 50%, 47%
18	Q	148	8%, 59%, 36%
19	R	95	%, 62%, 35%
20	S	154	%, 58%, 36%
21	T	84	2%, 64%, 31%
22	U	119	8%, 46%, 50%
23	V	66	23%, 35%, 44%, 20%
24	W	70	26%, 43%, 44%, 6%, 7%
25	X	154	44%, 49%, 6%
26	Y	91	10%, 40%, 44%, 7%, 10%
27	Z	240	3%, 33%, 23%, 41%
28	1	73	55%, 15%, 77%, 8%
29	2	56	62%, 38%
30	3	48	6%, 60%, 33%

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Mol	Chain	Length	Quality of chain
31	4	92	100% 27% 70%

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	4	8078	-	-	-	X
32	MG	4	8114	-	-	-	X
32	MG	A	8024	-	-	-	X
32	MG	A	8070	-	-	-	X
32	MG	A	8097	-	-	-	X
34	NA	A	8355	-	-	-	X
34	NA	A	8359	-	-	-	X
34	NA	A	8377	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	B	8351	-	-	-	X
34	NA	S	8386	-	-	-	X
34	NA	T	8312	-	-	-	X
35	CL	4	8504	-	-	-	X
35	CL	A	8515	-	-	-	X
37	CD	4	8404	-	-	-	X
37	CD	P	8405	-	-	-	X

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 98596 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	A	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	B	122	2600	1160	472	847	121	0	0	0

- Molecule 3 is a RNA chain called minihelix-puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	5	2	40	18	6	14	2	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	C	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	D	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
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	246	1858	1131	344	382	1	0	0	0

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

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

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

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

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	119	885	552	141	191	1	0	0	0

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

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

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

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

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

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

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

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

- Molecule 15 is a protein called L15 Ribosomal Protein.

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	conflict	UNP P14119

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	X	154	1195	737	209	243	6	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	1	73	563	359	111	86	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	2	56	430	258	86	82	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	3	46	393	238	86	68	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	deletion	UNP P22452

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	4	92	755	458	153	137	7	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	108	Total Mg 108 108	0	0
32	B	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	D	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	1	1	Total Mg 1 1	0	0
32	4	2	Total Mg 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	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	A	73	Total Na 73 73	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	J	1	Total Na 1 1	0	0
34	K	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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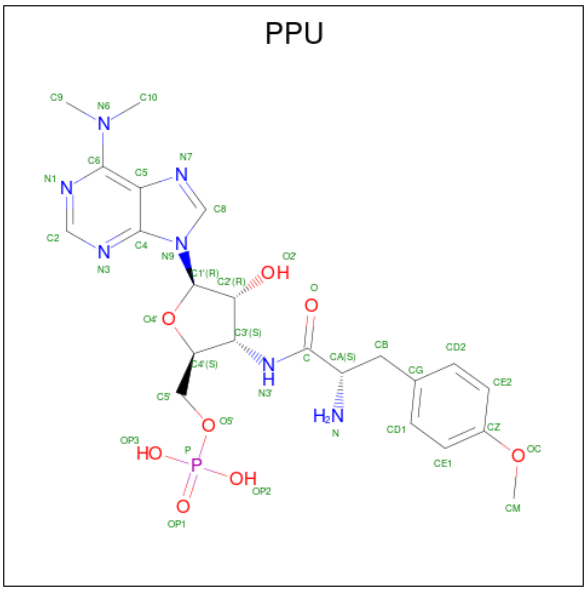
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	0	0
34	T	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	11	Total Cl 11 11	0	0
35	C	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	3	Total Cl 3 3	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	P	1	Total Cl 1 1	0	0
35	S	1	Total Cl 1 1	0	0
35	Z	1	Total Cl 1 1	0	0
35	4	1	Total Cl 1 1	0	0

- Molecule 36 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: $C_{22}H_{30}N_7O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
36	5	1	37	22	7	7	1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
37	P	1	1	1	0	0
37	V	1	1	1	0	0
37	1	1	1	1	0	0
37	2	1	1	1	0	0
37	4	1	1	1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
38	A	5871	5871	5871	0	0
38	B	147	147	147	0	0
38	C	135	135	135	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	155	Total O 155 155	0	0
38	E	171	Total O 171 171	0	0
38	F	51	Total O 51 51	0	0
38	G	44	Total O 44 44	0	0
38	H	26	Total O 26 26	0	0
38	I	20	Total O 20 20	0	0
38	J	77	Total O 77 77	0	0
38	K	55	Total O 55 55	0	0
38	L	63	Total O 63 63	0	0
38	M	90	Total O 90 90	0	0
38	N	125	Total O 125 125	0	0
38	O	64	Total O 64 64	0	0
38	P	44	Total O 44 44	0	0
38	Q	68	Total O 68 68	0	0
38	R	54	Total O 54 54	0	0
38	S	83	Total O 83 83	0	0
38	T	31	Total O 31 31	0	0
38	U	39	Total O 39 39	0	0
38	V	26	Total O 26 26	0	0
38	W	15	Total O 15 15	0	0
38	X	70	Total O 70 70	0	0

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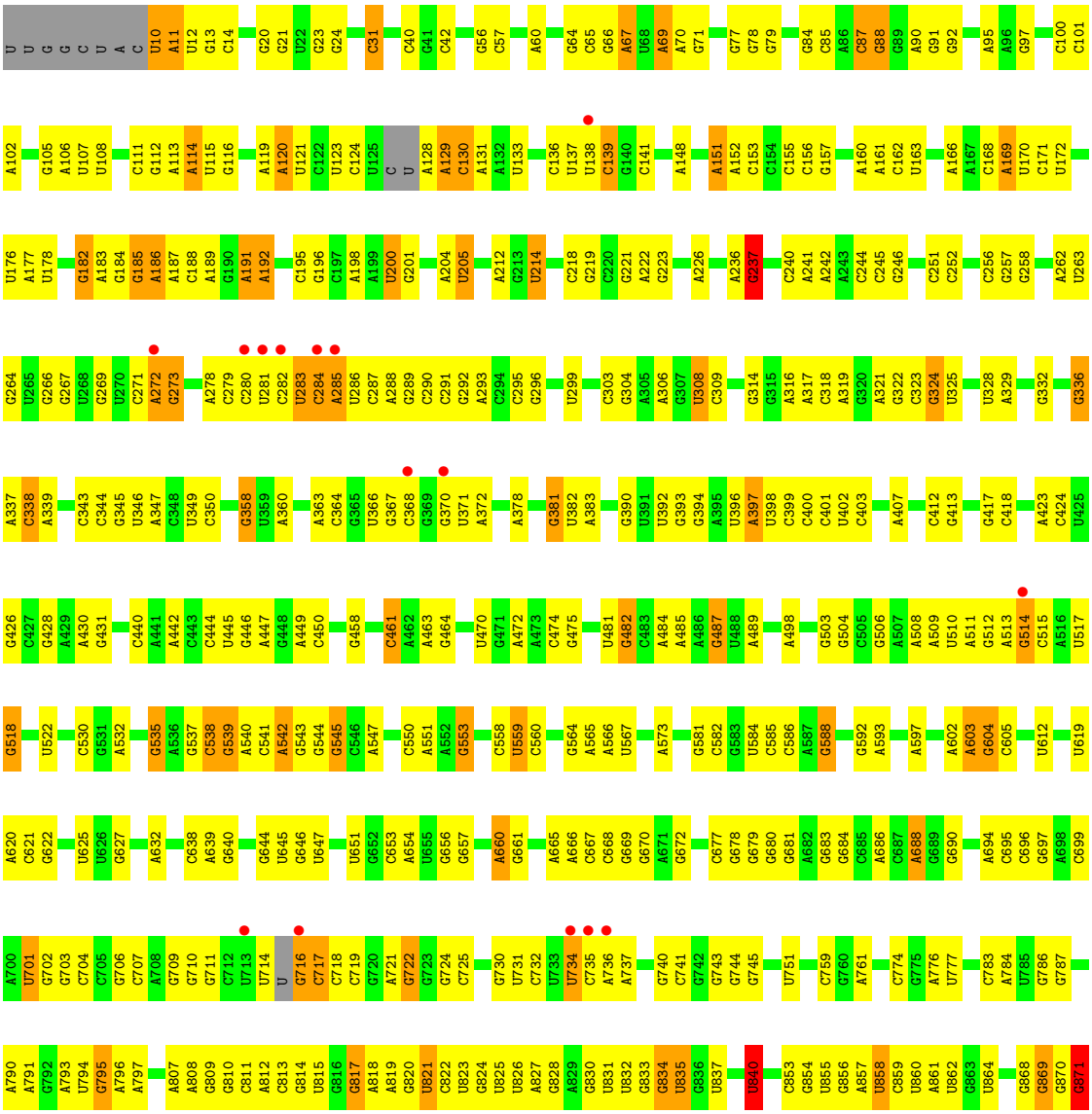
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
38	Y	30	30	30	0	0
			Total	O		
38	Z	102	102	102	0	0
			Total	O		
38	1	38	38	38	0	0
			Total	O		
38	2	56	56	56	0	0
			Total	O		
38	3	47	47	47	0	0
			Total	O		
38	4	72	72	72	0	0

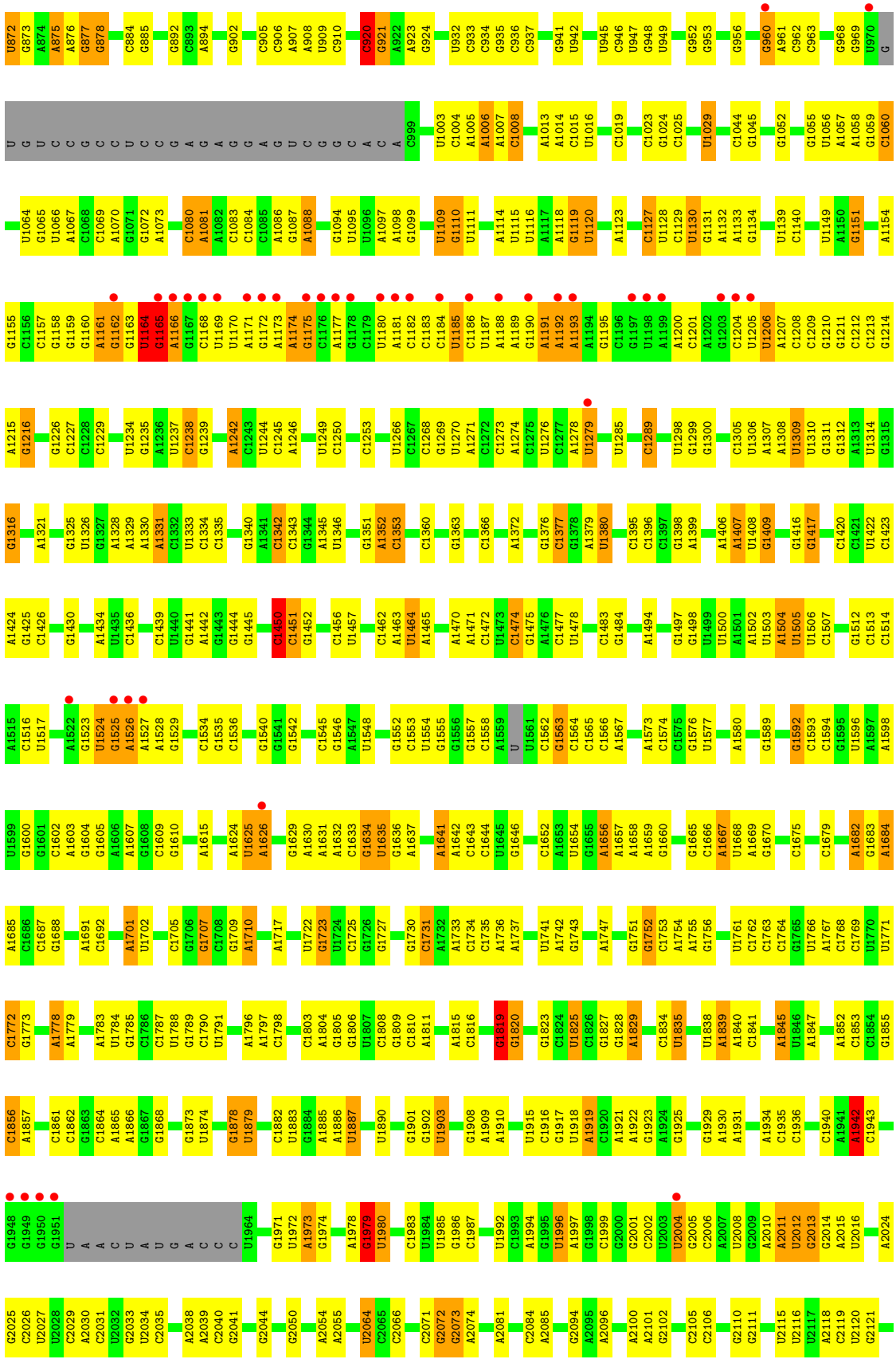
3 Residue-property plots (i)

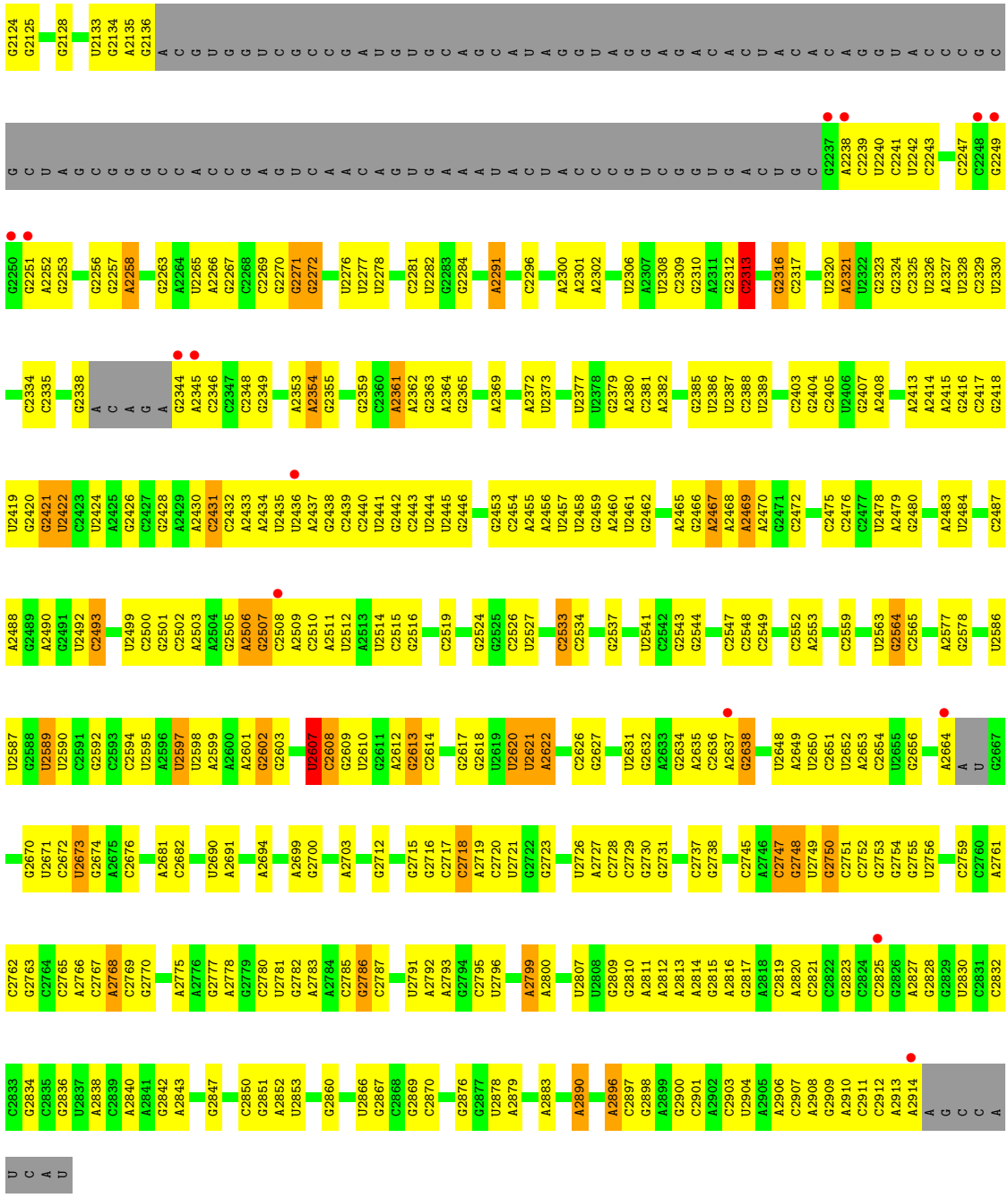
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 A: 2% 48% 39% 7% 6%

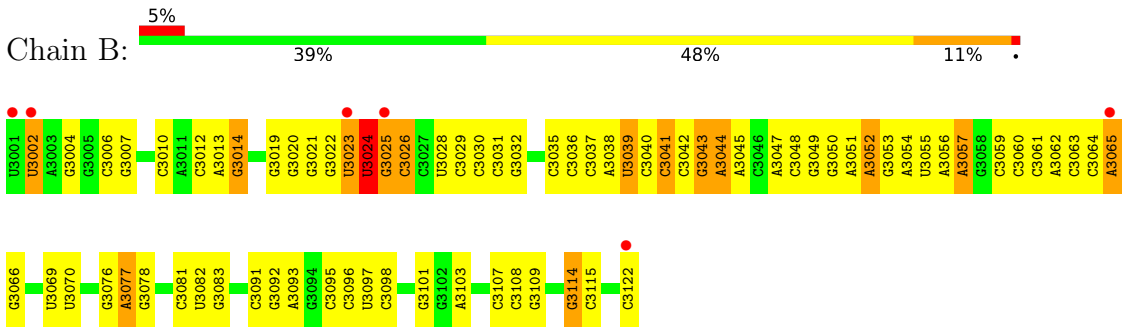






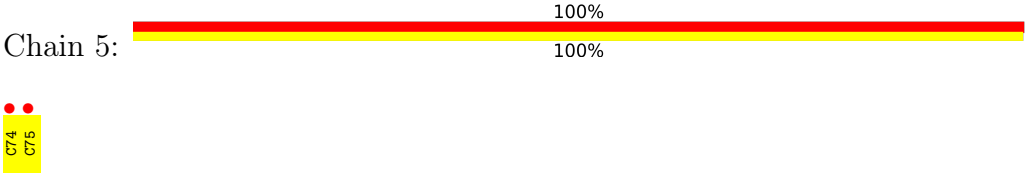
• Molecule 2: 5S ribosomal RNA

Chain B:



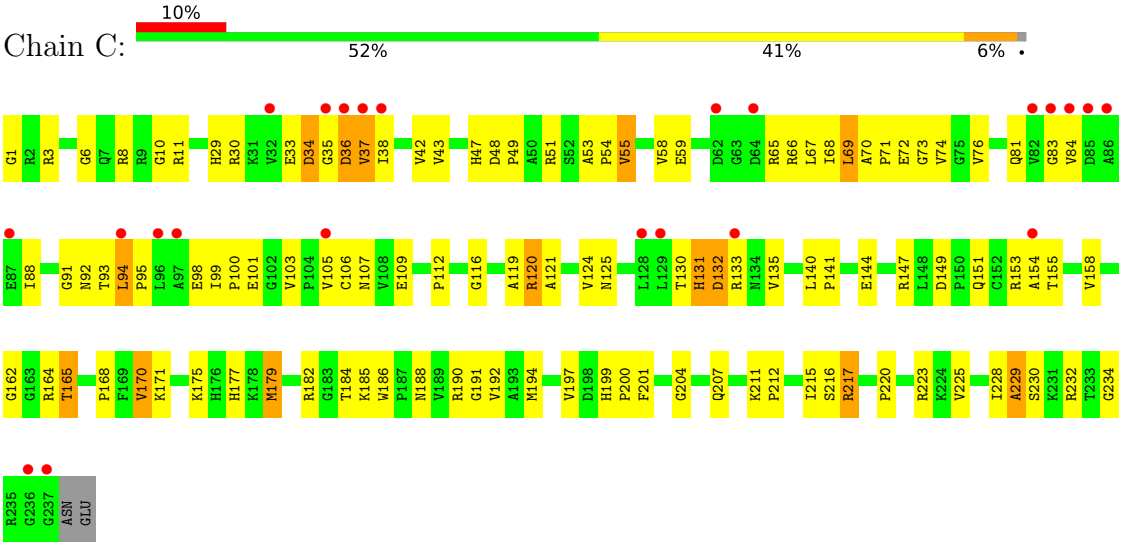
• Molecule 3: minihelix-puromycin

Chain 5:



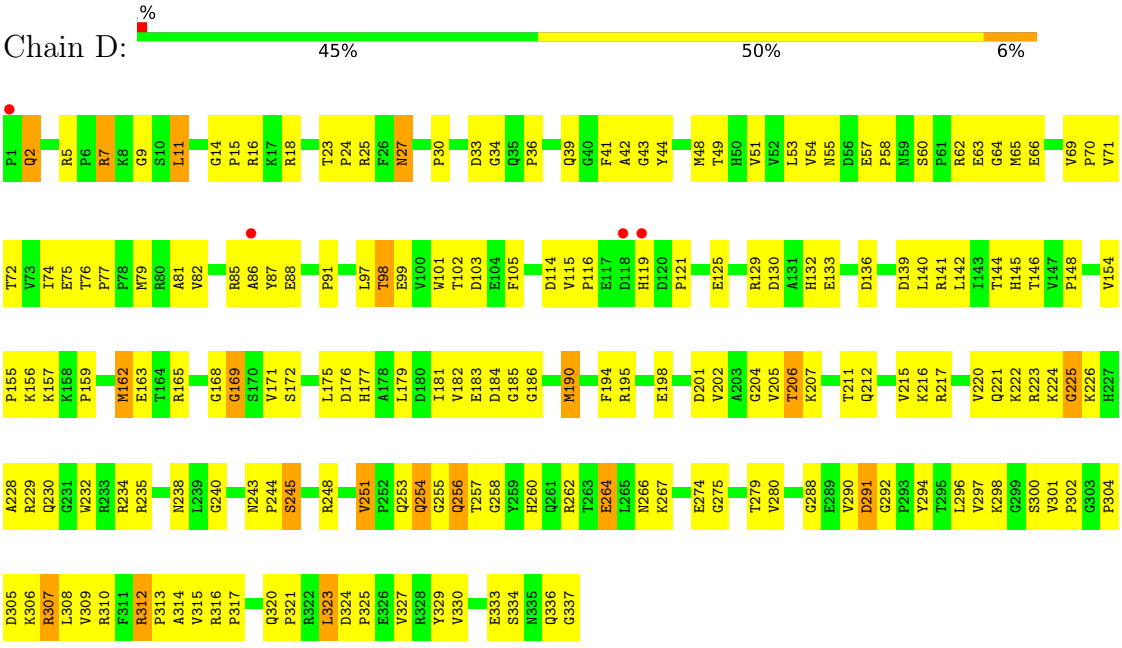
• Molecule 4: 50S ribosomal protein L2P

Chain C:



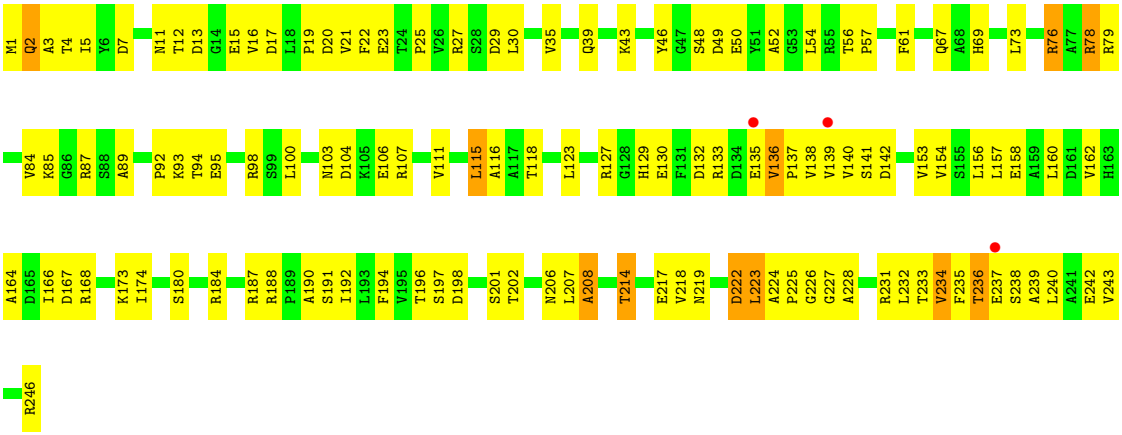
• Molecule 5: 50S ribosomal protein L3P

Chain D:



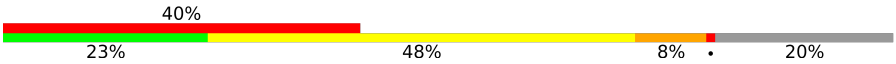
• Molecule 6: 50S ribosomal protein L4E

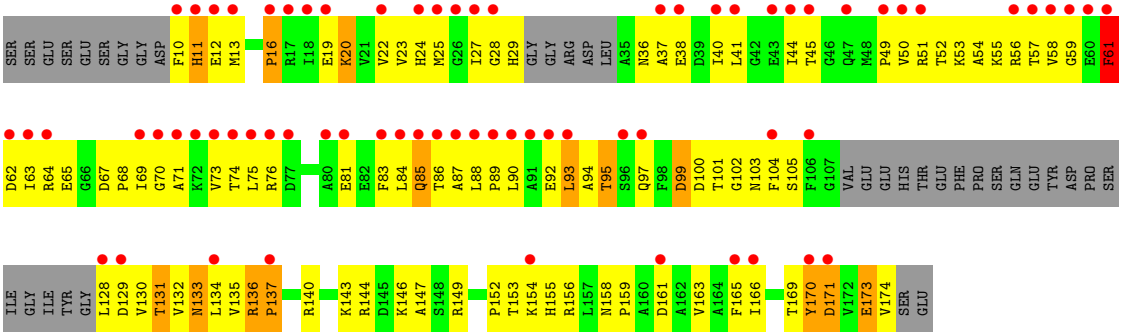
Chain E:



• Molecule 7: 50S ribosomal protein L5P

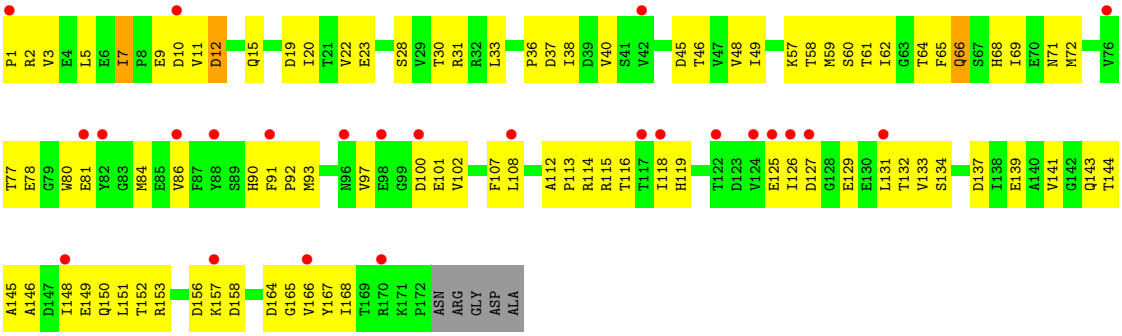
Chain F:





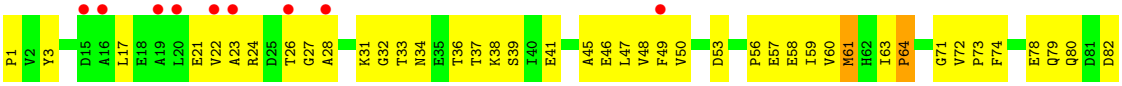
• Molecule 8: 50S ribosomal protein L6P

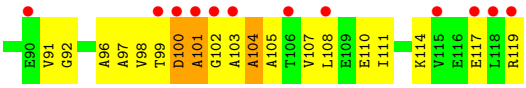
Chain G:



• Molecule 9: 50S ribosomal protein L7Ae

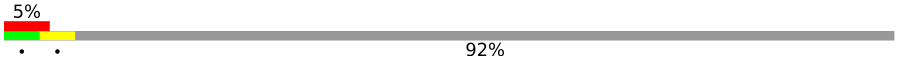
Chain H:

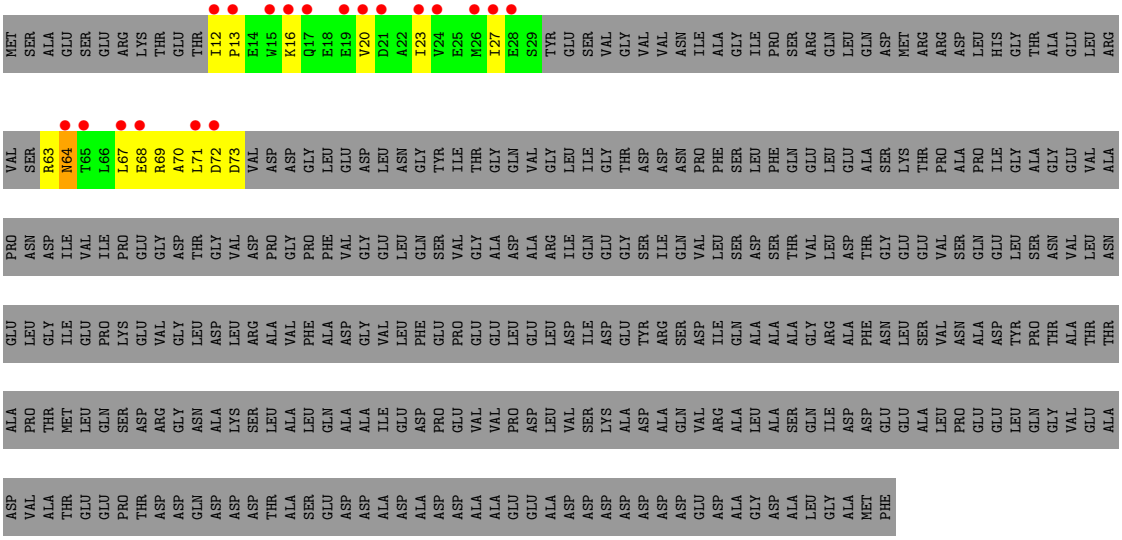




• Molecule 10: Acidic ribosomal protein P0 homolog

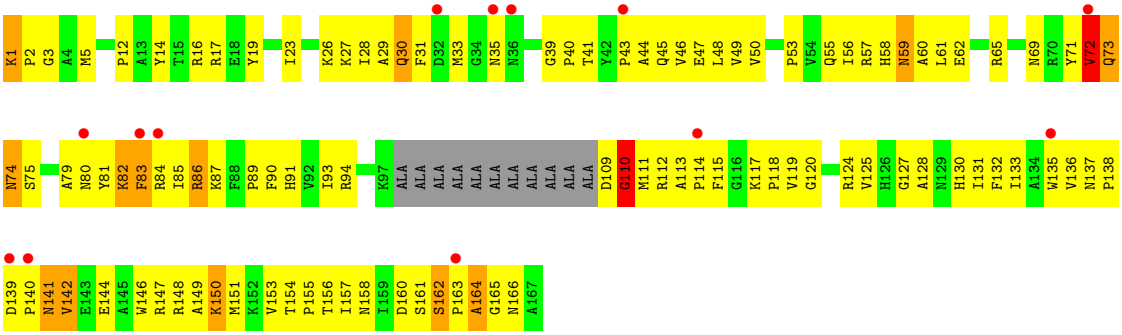
Chain I:





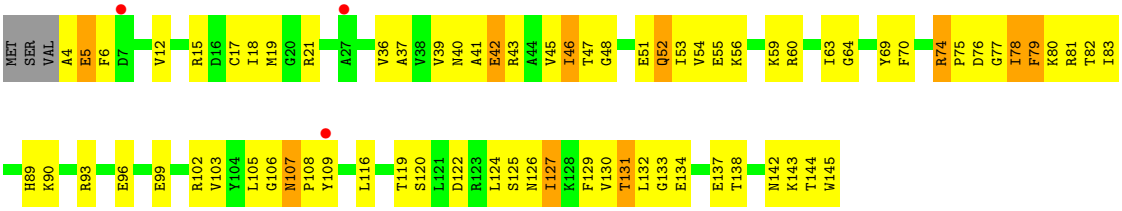
• Molecule 11: L10 Ribosomal Protein

Chain J:



• Molecule 12: 50S ribosomal protein L13P

Chain K:



• Molecule 13: 50S ribosomal protein L14P

Chain L: 2% 48% 50%

M1 E2 A3 L4 D7 V8 T9 Q10 K14 I18 T19 C20 A21 D22 N23 T24 G25 A26 R27 E28 L29 K30 V31 I32 S33 V34 Y37 S38 G39 T40 K41 N42 P45 K46 A47 G48 L49 I53 T54 V55 S56 V57 T58 P62 E63 M64 R65 R66 Q67 V72 V73 V74

R75 I80 R81 R82 F83 D84 G85 T86 R87 V88 K89 F90 N93 V98 D99 E100 N101 E102 G106 P112 I113 A114 R115 E116 V117 A118 Q119 R120 F121 G122 S123 V124 A125 S126 A127 V132

- Molecule 14: 50S ribosomal protein L15P

Chain M: 18% 43% 42% 12%

T1 K4 K5 R6 Q7 S10 R11 T12 H13 G16 S17 H18 R21 R22 H26 R30 G34 R35 H38 E39 F40 H43 E44 P45 L46 G50 R53 P54 V57 Q58 E59 E60 A61 A62 D65 V66 R67 E68 E71 N72 V73 T74 L75 L76 A77 A78

D79 D80 V81 A82 E83 VAL GLU ASP GLY GLY F89 R90 V91 D92 V93 R94 V97 E98 E99 A103 D104 Y105 V106 A111 V114 R115 H116 E117 L118 T119 L120 I121 A122 D123 D124 F125 G128 A129 R130 E131 K132 V133 E134 G135 A136 G137 G138 S139 V140 E141 L142 T143 D144 L145 G146

E147 E148 R149 Q150 ALA GLU ALA GLU GLU THR GLU ASP ALA ASP ALA ASP GLU GLU

- Molecule 15: L15 Ribosomal Protein

Chain N: 3% 37% 56% 7%

A1 R2 S3 A4 Y5 S6 R9 W12 K13 R14 E17 G18 Q19 I20 A21 E22 L23 H26 R27 M28 Q29 E30 W31 R32 N33 E34 P35 A36 V37 V38 R39 P43 T44 R45 L46 D47 R48 A49 R50 S51 L52 K57 Q58 G59 I60 I61 V62 V63 R64 V65 A66 I67 R68 K69

R74 T75 R76 F77 N78 K79 G80 R81 R82 S83 K84 R85 M86 M87 V88 N89 R90 I91 T92 R93 K94 K95 R99 E102 E103 R104 A105 N106 R107 K108 F109 R113 V114 L115 N116 V120 G121 E122 K127 E130 I134 D137 H138 P139 A140 I141 K142 Q146 L147 S148

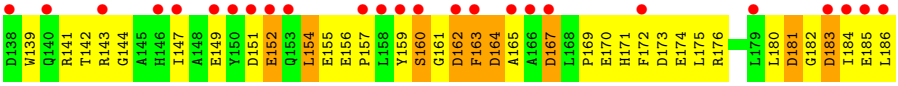
W149 I150 S151 R152 T153 R154 H155 R156 L157 R158 T159 F160 R161 G162 L163 T164 S165 A166 G167 R168 R169 C170 R171 G172 L173 R174 G175 K178 G179 K182 V183 R184 P185 S186 L187 R188 V189 K193 A194

- Molecule 16: 50S ribosomal protein L18P

Chain O: 18% 34% 57% 9%

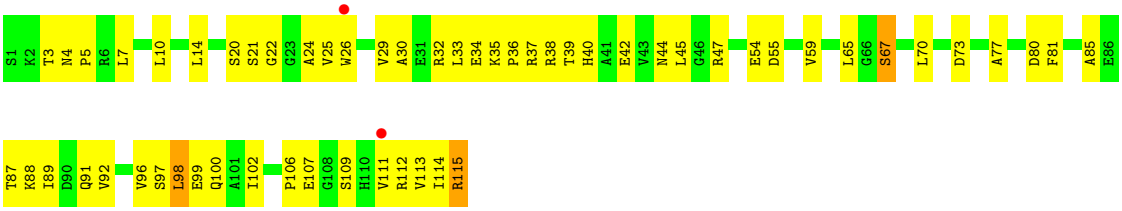
A1 T2 G3 P4 R5 Y6 K7 V8 P9 M10 R11 R12 R13 R14 E15 A16 R17 T18 D19 Y20 H21 Q22 R23 L24 R25 L26 L27 K28 S29 P32 R33 L34 V35 A36 R37 H42 V43 R44 A45 Q46 L47 V48 T49 L50 D55 D56 T57 L58 A61 H62 S63 S64 D65 L66 A67 E68

Y69 G70 W71 E72 A73 P74 T75 G76 N77 M78 P79 S80 A81 Y82 L83 L86 L87 A88 G89 L90 R91 A92 Q93 E94 A95 G96 V97 E98 E99 A100 I104 N107 S108 P109 S113 K114 V115 F116 A117 I118 Q119 E120 I123 D124 A125 G126 L127 D128 I129 N132 V135 L136 A137



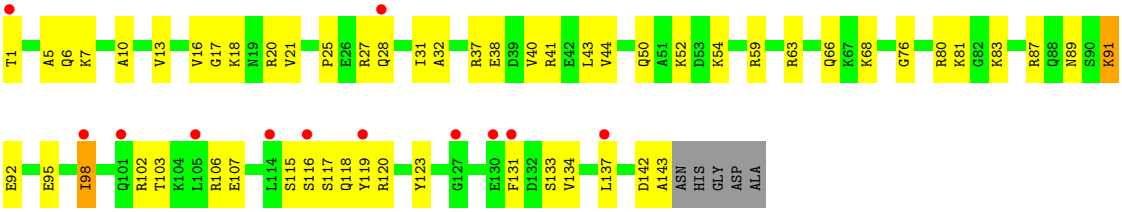
• Molecule 17: 50S ribosomal protein L18e

Chain P:



• Molecule 18: 50S ribosomal protein L19E

Chain Q:

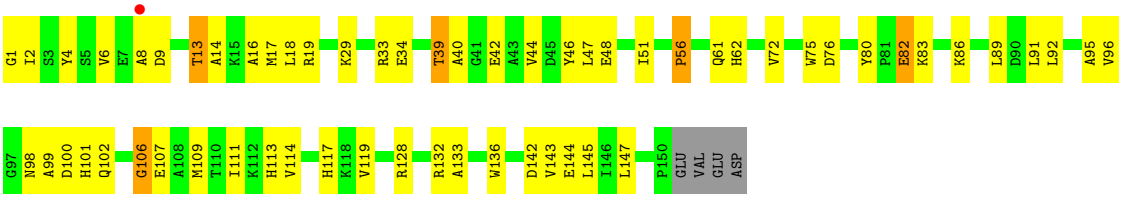


• Molecule 19: 50S ribosomal protein L21e

Chain R:

• Molecule 20: 50S ribosomal protein L22P

Chain S:

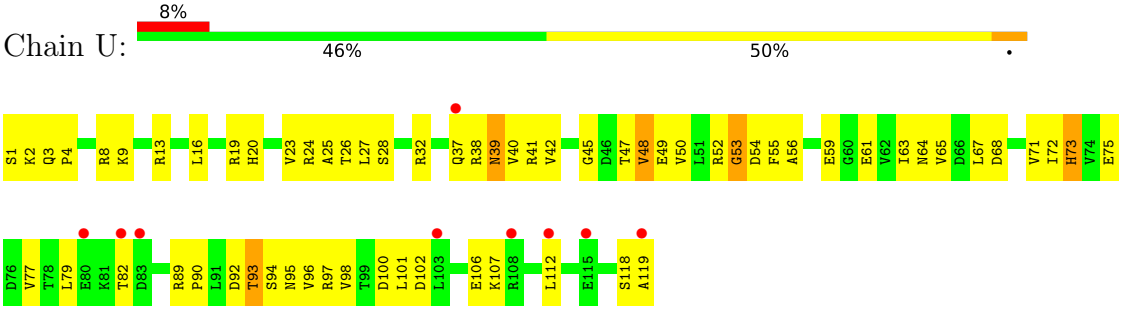


• Molecule 21: 50S ribosomal protein L23P

Chain T:

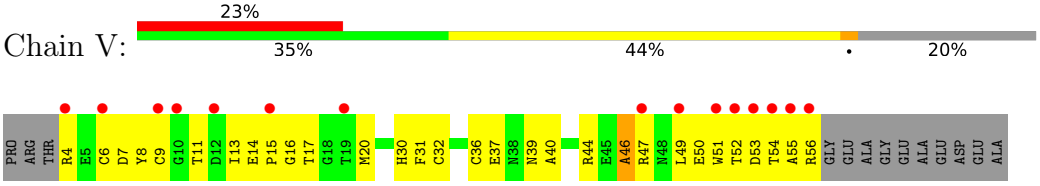
• Molecule 22: 50S ribosomal protein L24P

Chain U:



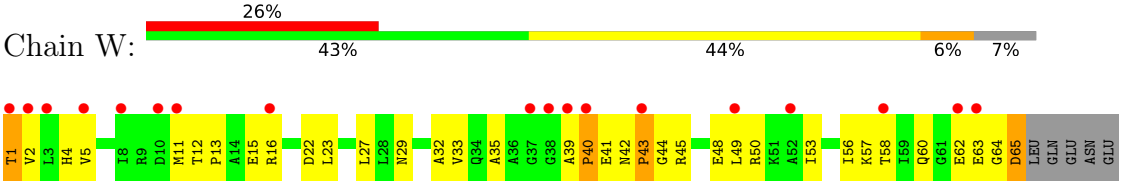
• Molecule 23: 50S ribosomal protein L24E

Chain V:



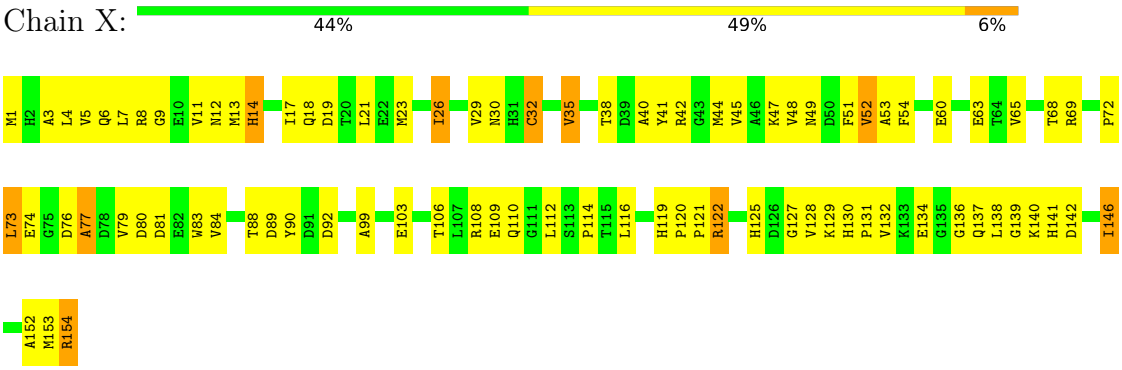
• Molecule 24: 50S ribosomal protein L29P

Chain W:



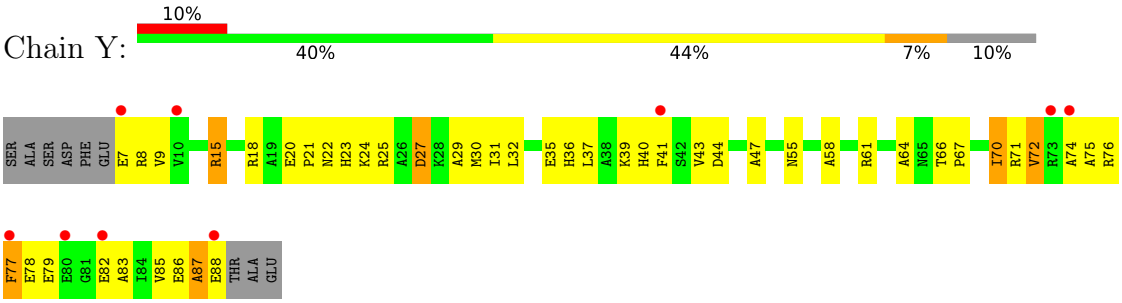
• Molecule 25: 50S ribosomal protein L30P

Chain X:



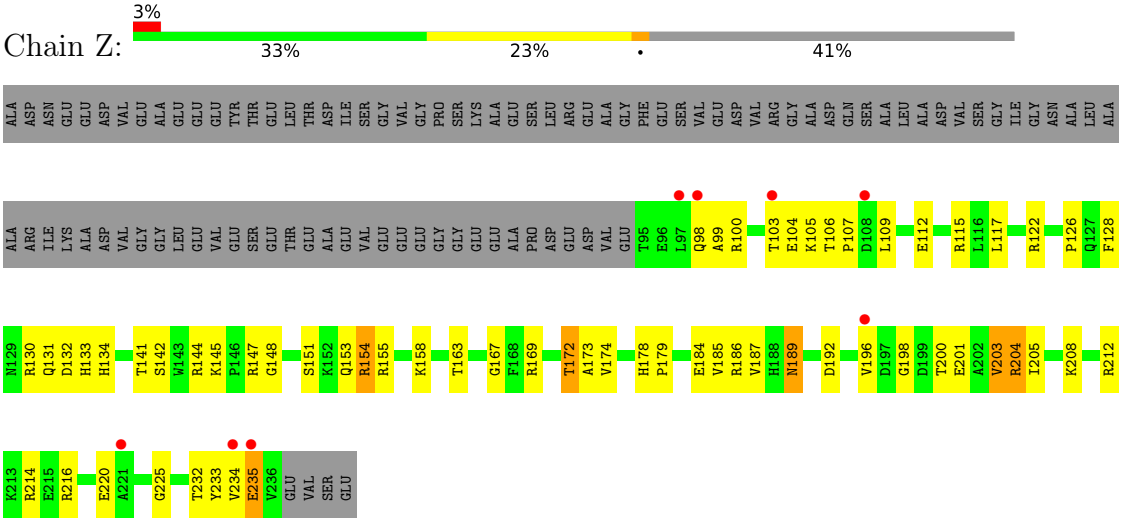
• Molecule 26: 50S ribosomal protein L31e

Chain Y:



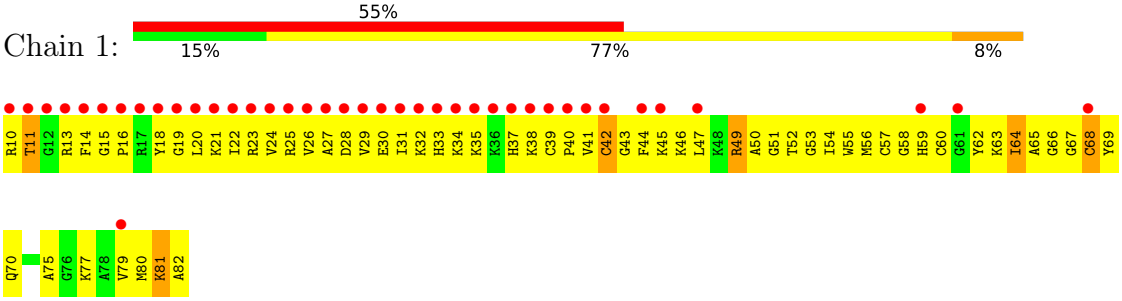
• Molecule 27: 50S ribosomal protein L32E

Chain Z:



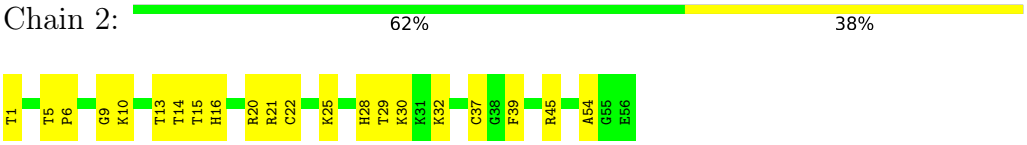
• Molecule 28: L37Ae 50S ribosomal protein

Chain 1:



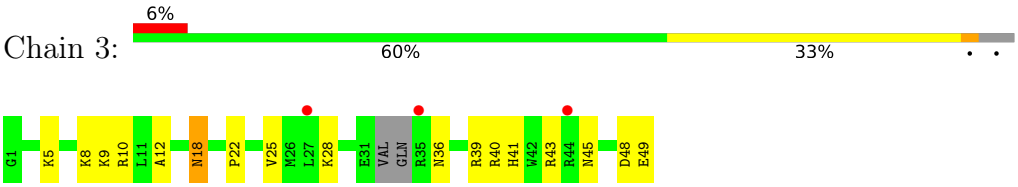
• Molecule 29: 50S ribosomal protein L37e

Chain 2:



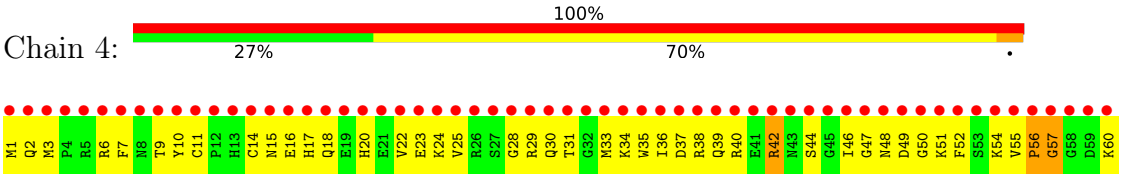
• Molecule 30: 50S ribosomal protein L39e

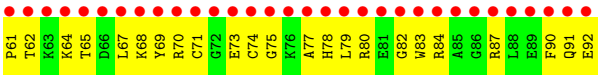
Chain 3:



• Molecule 31: 50S ribosomal protein L44E

Chain 4:




P61
T62
K63
K64
T65
D66
L67
K68
Y69
R70
C71
G72
E73
C74
G75
K76
A77
H78
L79
R80
E81
G82
W83
R84
A85
G86
R87
L88
E89
F90
Q91
E92

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.16Å 301.29Å 575.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.95 53.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.95) 90.6 (53.80-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.80 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.259 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	98596	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: MG, CL, K, NA, CD, PPU

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	A	0.53	6/66076 (0.0%)	0.72	18/103052 (0.0%)
2	B	0.49	0/2905	0.78	3/4528 (0.1%)
3	5	1.19	0/43	0.77	0/64
4	C	0.40	0/1787	0.71	0/2409
5	D	0.39	0/2689	0.69	0/3652
6	E	0.44	0/1883	0.68	0/2551
7	F	0.37	0/1111	0.62	0/1498
8	G	0.38	0/1382	0.62	0/1880
9	H	0.46	1/896 (0.1%)	0.73	3/1219 (0.2%)
10	I	0.42	0/241	0.62	0/324
11	J	0.44	0/1246	0.76	3/1686 (0.2%)
12	K	0.41	0/1135	0.67	0/1530
13	L	0.40	0/1003	0.73	0/1351
14	M	0.41	0/1126	0.72	0/1504
15	N	0.45	0/1633	0.74	2/2180 (0.1%)
16	O	0.36	0/1473	0.69	0/1999
17	P	0.41	0/873	0.71	0/1181
18	Q	0.41	0/1143	0.62	0/1521
19	R	0.42	0/748	0.74	1/1005 (0.1%)
20	S	0.42	0/1172	0.65	0/1578
21	T	0.39	0/648	0.63	0/875
22	U	0.36	0/957	0.66	0/1289
23	V	0.46	0/417	0.65	0/562
24	W	0.33	0/502	0.63	0/675
25	X	0.37	0/1218	0.67	0/1655
26	Y	0.40	0/664	0.66	0/895
27	Z	0.41	0/1146	0.67	0/1536
28	1	0.57	0/575	0.72	0/763
29	2	0.48	0/437	0.69	0/578
30	3	0.35	0/398	0.60	0/527
31	4	0.84	0/771	0.70	0/1024
All	All	0.50	7/98298 (0.0%)	0.71	30/147091 (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	A	0	58
2	B	1	0
All	All	1	58

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2617	G	C3'-O3'	12.86	1.60	1.42
1	A	2617	G	C4'-O4'	-6.15	1.37	1.45
9	H	3	TYR	CG-CD1	6.05	1.47	1.39
1	A	2618	G	P-OP2	-5.70	1.39	1.49
1	A	2617	G	N9-C8	5.65	1.41	1.37

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1165	G	O5'-P-OP2	10.73	123.58	110.70
1	A	1563	G	C2'-C3'-O3'	9.26	129.87	109.50
2	B	3024	U	C2'-C3'-O3'	9.18	129.70	109.50
9	H	3	TYR	CB-CG-CD2	9.11	126.47	121.00
1	A	1164	U	OP1-P-O3'	-8.57	86.34	105.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	3024	U	C3'

5 of 58 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	A	Sidechain
1	A	176	U	Sidechain
1	A	182	G	Sidechain
1	A	205	U	Sidechain
1	A	214	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	A	59017	0	29805	1413	0
2	B	2600	0	1326	101	0
3	5	40	0	22	7	0
4	C	1754	0	1763	136	0
5	D	2624	0	2533	221	0
6	E	1858	0	1816	138	0
7	F	1094	0	1085	149	0
8	G	1357	0	1266	101	0
9	H	885	0	854	76	0
10	I	240	0	231	24	0
11	J	1215	0	1215	172	0
12	K	1119	0	1098	86	0
13	L	993	0	1027	73	0
14	M	1114	0	1072	76	0
15	N	1605	0	1676	178	0
16	O	1444	0	1401	159	0
17	P	864	0	873	74	0
18	Q	1133	0	1127	64	0
19	R	734	0	728	36	0
20	S	1149	0	1122	76	0
21	T	641	0	605	23	0
22	U	949	0	923	76	0
23	V	410	0	367	46	0
24	W	499	0	511	37	0
25	X	1195	0	1137	111	0
26	Y	654	0	653	53	0
27	Z	1130	0	1133	77	0
28	1	563	0	600	89	0
29	2	430	0	426	24	0
30	3	393	0	406	17	0
31	4	755	0	732	108	0
32	1	1	0	0	0	0
32	4	2	0	0	0	0
32	A	108	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	73	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	1	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
35	4	1	0	0	1	0
35	A	11	0	0	3	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	2	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	P	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	5	37	0	28	4	0
37	1	1	0	0	0	0
37	2	1	0	0	0	0
37	4	1	0	0	0	0
37	P	1	0	0	0	0
37	V	1	0	0	0	0
38	1	38	0	0	14	0
38	2	56	0	0	9	0
38	3	47	0	0	2	0
38	4	72	0	0	13	0
38	A	5871	0	0	307	0
38	B	147	0	0	14	0
38	C	135	0	0	24	0
38	D	155	0	0	28	0
38	E	171	0	0	31	0
38	F	51	0	0	25	0
38	G	44	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	26	0	0	12	0
38	I	20	0	0	6	0
38	J	77	0	0	27	0
38	K	55	0	0	5	0
38	L	63	0	0	14	0
38	M	90	0	0	19	0
38	N	125	0	0	27	0
38	O	64	0	0	26	0
38	P	44	0	0	13	0
38	Q	68	0	0	10	0
38	R	54	0	0	5	0
38	S	83	0	0	9	0
38	T	31	0	0	4	0
38	U	39	0	0	8	0
38	V	26	0	0	7	0
38	W	15	0	0	5	0
38	X	70	0	0	14	0
38	Y	30	0	0	5	0
38	Z	102	0	0	19	0
All	All	98596	0	59561	3672	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 24.

The worst 5 of 3672 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)
2:B:3006:C:H5"	16:O:37:ARG:NH1	1.56	1.19
24:W:12:THR:HG22	24:W:15:GLU:HG3	1.28	1.14
6:E:236:THR:HG22	6:E:239:ALA:H	1.10	1.10
11:J:86:ARG:HH11	11:J:133:ILE:HG13	0.99	1.10
6:E:115:LEU:HD13	6:E:223:LEU:HD21	1.30	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	C	235/239 (98%)	199 (85%)	27 (12%)	9 (4%)	3	15
5	D	335/337 (99%)	297 (89%)	28 (8%)	10 (3%)	4	20
6	E	244/246 (99%)	208 (85%)	31 (13%)	5 (2%)	7	30
7	F	134/176 (76%)	98 (73%)	25 (19%)	11 (8%)	1	3
8	G	170/177 (96%)	156 (92%)	13 (8%)	1 (1%)	25	60
9	H	117/119 (98%)	103 (88%)	9 (8%)	5 (4%)	2	12
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	3	14
11	J	152/167 (91%)	128 (84%)	18 (12%)	6 (4%)	3	14
12	K	140/145 (97%)	124 (89%)	11 (8%)	5 (4%)	3	16
13	L	130/132 (98%)	113 (87%)	15 (12%)	2 (2%)	10	38
14	M	141/164 (86%)	114 (81%)	23 (16%)	4 (3%)	5	22
15	N	192/194 (99%)	177 (92%)	10 (5%)	5 (3%)	5	24
16	O	184/186 (99%)	153 (83%)	19 (10%)	12 (6%)	1	5
17	P	113/115 (98%)	105 (93%)	7 (6%)	1 (1%)	17	51
18	Q	141/148 (95%)	129 (92%)	11 (8%)	1 (1%)	22	56
19	R	93/95 (98%)	84 (90%)	9 (10%)	0	100	100
20	S	148/154 (96%)	130 (88%)	14 (10%)	4 (3%)	5	23
21	T	79/84 (94%)	75 (95%)	3 (4%)	1 (1%)	12	41
22	U	117/119 (98%)	106 (91%)	8 (7%)	3 (3%)	5	24
23	V	51/66 (77%)	48 (94%)	1 (2%)	2 (4%)	3	14
24	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4	19
25	X	152/154 (99%)	142 (93%)	6 (4%)	4 (3%)	5	24
26	Y	80/91 (88%)	69 (86%)	8 (10%)	3 (4%)	3	15
27	Z	140/240 (58%)	134 (96%)	5 (4%)	1 (1%)	22	56
28	1	71/73 (97%)	61 (86%)	9 (13%)	1 (1%)	11	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	2	54/56 (96%)	48 (89%)	6 (11%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	82 (91%)	6 (7%)	2 (2%)	6	28
All	All	3633/4235 (86%)	3205 (88%)	327 (9%)	101 (3%)	5	22

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
5	D	206	THR
7	F	93	LEU
7	F	95	THR
7	F	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	C	179/181 (99%)	169 (94%)	10 (6%)	21	53
5	D	282/282 (100%)	265 (94%)	17 (6%)	19	50
6	E	193/193 (100%)	178 (92%)	15 (8%)	12	38
7	F	117/147 (80%)	108 (92%)	9 (8%)	13	39
8	G	152/155 (98%)	149 (98%)	3 (2%)	55	80
9	H	92/92 (100%)	90 (98%)	2 (2%)	52	79
10	I	27/283 (10%)	26 (96%)	1 (4%)	34	66
11	J	122/122 (100%)	111 (91%)	11 (9%)	9	32
12	K	118/121 (98%)	110 (93%)	8 (7%)	16	45
13	L	106/106 (100%)	103 (97%)	3 (3%)	43	74
14	M	112/126 (89%)	108 (96%)	4 (4%)	35	67
15	N	166/166 (100%)	156 (94%)	10 (6%)	19	50
16	O	149/149 (100%)	142 (95%)	7 (5%)	26	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	93/93 (100%)	89 (96%)	4 (4%)	29	62
18	Q	113/116 (97%)	110 (97%)	3 (3%)	44	74
19	R	79/79 (100%)	75 (95%)	4 (5%)	24	56
20	S	117/121 (97%)	114 (97%)	3 (3%)	46	75
21	T	71/73 (97%)	71 (100%)	0	100	100
22	U	105/105 (100%)	102 (97%)	3 (3%)	42	73
23	V	44/52 (85%)	44 (100%)	0	100	100
24	W	51/56 (91%)	48 (94%)	3 (6%)	19	50
25	X	130/130 (100%)	122 (94%)	8 (6%)	18	48
26	Y	66/73 (90%)	63 (96%)	3 (4%)	27	61
27	Z	120/195 (62%)	113 (94%)	7 (6%)	20	51
28	1	56/56 (100%)	49 (88%)	7 (12%)	4	17
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	49	77
31	4	79/79 (100%)	76 (96%)	3 (4%)	33	66
All	All	3027/3441 (88%)	2878 (95%)	149 (5%)	25	58

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	U	48	VAL
28	1	64	ILE
24	W	65	ASP
26	Y	72	VAL
7	F	136	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
20	S	61	GLN
25	X	14	HIS
20	S	98	ASN
22	U	39	ASN
25	X	141	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	246 (8%)	27 (0%)
2	B	121/122 (99%)	17 (14%)	4 (3%)
3	5	1/2 (50%)	0	0
All	All	2869/3046 (94%)	263 (9%)	31 (1%)

5 of 263 RNA backbone outliers are listed below:

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

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1352	A
2	B	3023	U
1	A	1474	C
2	B	3043	G
1	A	2467	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	PPU	5	76	3	32,40,41	2.43	6 (18%)	33,57,60	1.15	3 (9%)

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
36	PPU	5	76	3	-	4/21/43/44	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	76	PPU	C-N3'	9.69	1.55	1.34
36	5	76	PPU	C10-N6	-4.31	1.35	1.45
36	5	76	PPU	C9-N6	-4.22	1.35	1.45
36	5	76	PPU	CE1-CZ	3.95	1.46	1.38
36	5	76	PPU	CE2-CD2	3.53	1.45	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	76	PPU	C3'-N3'-C	-3.76	117.55	123.21
36	5	76	PPU	CM-OC-CZ	2.11	122.08	117.51
36	5	76	PPU	CA-C-N3'	-2.07	113.28	116.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	5	76	PPU	O-C-CA-CB
36	5	76	PPU	N3'-C-CA-CB
36	5	76	PPU	C4'-C3'-N3'-C
36	5	76	PPU	C2'-C3'-N3'-C

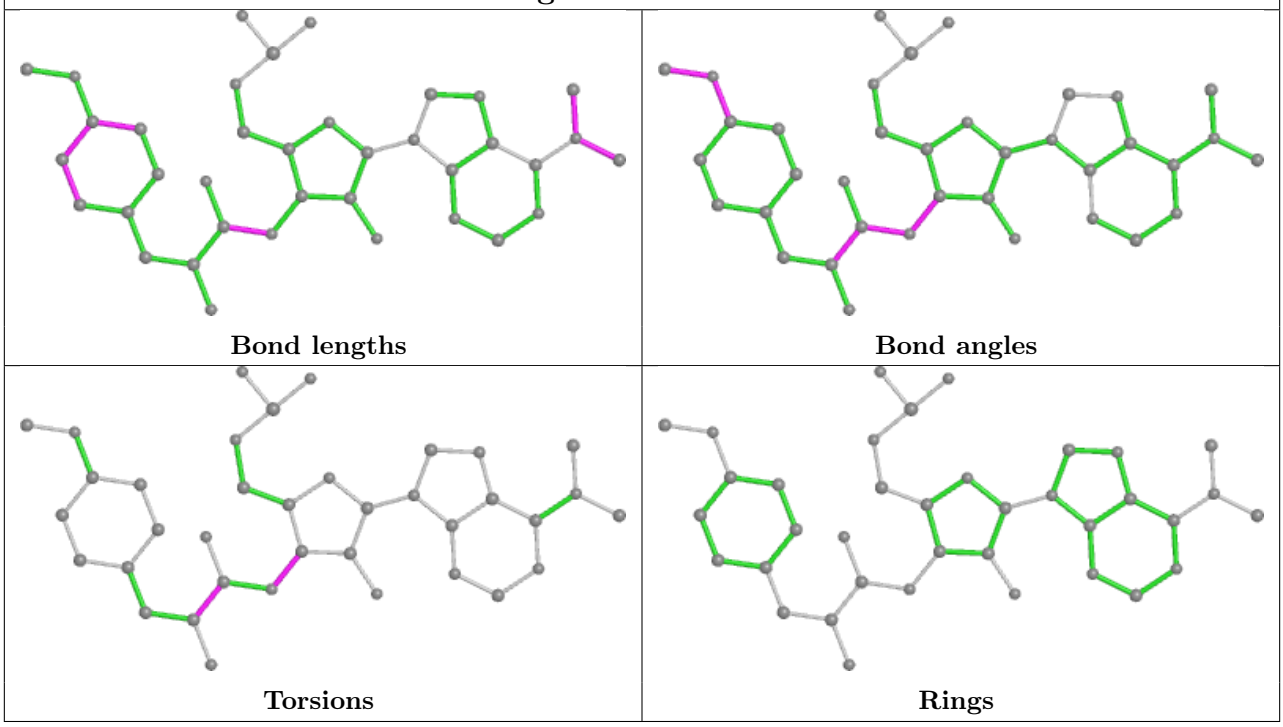
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	76	PPU	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PPU 5 76



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	2754/2922 (94%)	0.08	70 (2%) 57 40	24, 52, 101, 153	0
2	B	122/122 (100%)	0.27	6 (4%) 29 18	42, 71, 102, 149	0
3	5	2/2 (100%)	2.87	2 (100%) 0 0	96, 96, 96, 111	0
4	C	237/239 (99%)	0.52	23 (9%) 7 4	28, 62, 98, 116	0
5	D	337/337 (100%)	0.26	4 (1%) 79 63	29, 60, 88, 96	0
6	E	246/246 (100%)	0.04	3 (1%) 79 63	27, 53, 76, 87	0
7	F	140/176 (79%)	2.24	70 (50%) 0 0	69, 108, 125, 135	0
8	G	172/177 (97%)	1.03	25 (14%) 2 1	50, 75, 99, 106	0
9	H	119/119 (100%)	0.92	21 (17%) 1 1	59, 82, 106, 110	0
10	I	29/348 (8%)	2.95	19 (65%) 0 0	81, 104, 108, 109	0
11	J	156/167 (93%)	0.50	13 (8%) 11 6	40, 61, 92, 97	0
12	K	142/145 (97%)	0.23	3 (2%) 63 46	40, 55, 75, 83	0
13	L	132/132 (100%)	0.12	3 (2%) 60 43	37, 59, 85, 88	0
14	M	145/164 (88%)	1.10	30 (20%) 1 0	27, 83, 118, 124	0
15	N	194/194 (100%)	0.21	6 (3%) 49 32	34, 54, 73, 81	0
16	O	186/186 (100%)	0.95	33 (17%) 1 1	46, 74, 114, 127	0
17	P	115/115 (100%)	0.34	2 (1%) 70 53	47, 63, 86, 91	0
18	Q	143/148 (96%)	0.59	12 (8%) 11 6	43, 63, 82, 90	0
19	R	95/95 (100%)	0.00	1 (1%) 80 65	40, 52, 61, 75	0
20	S	150/154 (97%)	0.04	1 (0%) 87 76	33, 49, 68, 76	0
21	T	81/84 (96%)	0.36	2 (2%) 57 40	55, 69, 88, 92	0
22	U	119/119 (100%)	0.55	9 (7%) 13 7	45, 61, 82, 91	0
23	V	53/66 (80%)	1.55	15 (28%) 0 0	73, 83, 98, 119	0
24	W	65/70 (92%)	1.52	18 (27%) 0 0	58, 84, 111, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	X	154/154 (100%)	0.06	0 100 100	43, 55, 73, 83	0
26	Y	82/91 (90%)	0.48	9 (10%) 5 3	43, 64, 88, 102	0
27	Z	142/240 (59%)	0.21	8 (5%) 24 15	33, 51, 74, 92	0
28	1	73/73 (100%)	3.16	40 (54%) 0 0	76, 107, 118, 119	0
29	2	56/56 (100%)	-0.25	0 100 100	29, 37, 45, 48	0
30	3	46/48 (95%)	0.26	3 (6%) 18 11	41, 62, 83, 97	0
31	4	92/92 (100%)	8.53	92 (100%) 0 0	110, 126, 134, 137	0
All	All	6579/7281 (90%)	0.48	543 (8%) 11 6	24, 59, 111, 153	0

The worst 5 of 543 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	4	82	GLY	21.2
31	4	65	THR	20.2
31	4	83	TRP	18.5
31	4	85	ALA	15.1
31	4	62	THR	14.6

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 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, 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
34	NA	T	8312	1/1	-0.44	0.49	163,163,163,163	0
35	CL	4	8504	1/1	0.34	0.54	114,114,114,114	0
34	NA	B	8351	1/1	0.46	0.43	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	S	8386	1/1	0.51	0.52	77,77,77,77	0
32	MG	A	8076	1/1	0.53	0.37	123,123,123,123	0
32	MG	A	8070	1/1	0.55	1.20	98,98,98,98	0
32	MG	4	8078	1/1	0.55	0.62	117,117,117,117	0
32	MG	A	8024	1/1	0.59	1.06	84,84,84,84	0
35	CL	A	8510	1/1	0.64	0.30	83,83,83,83	0
32	MG	A	8046	1/1	0.64	0.12	74,74,74,74	0
34	NA	A	8384	1/1	0.65	0.74	105,105,105,105	0
35	CL	A	8515	1/1	0.66	0.51	108,108,108,108	0
32	MG	4	8114	1/1	0.68	0.74	111,111,111,111	0
34	NA	A	8363	1/1	0.69	0.36	56,56,56,56	0
32	MG	A	8097	1/1	0.70	0.45	80,80,80,80	0
34	NA	A	8359	1/1	0.71	0.41	53,53,53,53	0
34	NA	A	8382	1/1	0.72	0.24	44,44,44,44	0
32	MG	A	8089	1/1	0.74	0.26	89,89,89,89	0
34	NA	A	8355	1/1	0.74	0.41	88,88,88,88	0
37	CD	P	8405	1/1	0.77	0.45	202,202,202,202	0
37	CD	4	8404	1/1	0.78	0.46	202,202,202,202	0
34	NA	A	8357	1/1	0.79	0.13	43,43,43,43	0
34	NA	A	8377	1/1	0.79	0.55	72,72,72,72	0
34	NA	A	8322	1/1	0.79	0.26	76,76,76,76	0
34	NA	A	8371	1/1	0.80	0.18	35,35,35,35	0
34	NA	A	8370	1/1	0.80	0.39	82,82,82,82	0
32	MG	A	8106	1/1	0.81	0.09	101,101,101,101	0
34	NA	S	8338	1/1	0.83	0.19	84,84,84,84	0
32	MG	A	8044	1/1	0.83	0.21	64,64,64,64	0
32	MG	1	8105	1/1	0.83	0.46	80,80,80,80	0
32	MG	A	8068	1/1	0.83	0.08	59,59,59,59	0
32	MG	A	8092	1/1	0.84	0.28	105,105,105,105	0
35	CL	O	8507	1/1	0.84	0.18	72,72,72,72	0
37	CD	V	8401	1/1	0.84	0.37	202,202,202,202	0
35	CL	P	8508	1/1	0.84	0.16	99,99,99,99	0
36	PPU	5	76	37/38	0.85	0.36	90,95,100,100	0
32	MG	A	8099	1/1	0.85	0.19	55,55,55,55	0
32	MG	A	8116	1/1	0.85	0.32	117,117,117,117	0
34	NA	A	8350	1/1	0.85	0.23	21,21,21,21	0
34	NA	A	8375	1/1	0.86	0.34	44,44,44,44	0
34	NA	E	8304	1/1	0.86	0.12	23,23,23,23	0
32	MG	A	8052	1/1	0.87	0.14	42,42,42,42	0
32	MG	A	8043	1/1	0.87	0.13	67,67,67,67	0
34	NA	A	8344	1/1	0.87	0.09	20,20,20,20	0
32	MG	A	8051	1/1	0.87	0.16	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	CL	A	8514	1/1	0.88	0.19	62,62,62,62	0
34	NA	A	8366	1/1	0.88	0.16	38,38,38,38	0
35	CL	C	8509	1/1	0.88	0.26	92,92,92,92	0
34	NA	A	8369	1/1	0.88	0.15	41,41,41,41	0
32	MG	U	8073	1/1	0.88	0.13	34,34,34,34	0
32	MG	A	8111	1/1	0.88	0.25	69,69,69,69	0
34	NA	A	8333	1/1	0.88	0.09	25,25,25,25	0
34	NA	A	8341	1/1	0.88	0.10	28,28,28,28	0
32	MG	A	8066	1/1	0.88	0.16	76,76,76,76	0
35	CL	A	8511	1/1	0.88	0.21	73,73,73,73	0
34	NA	A	8361	1/1	0.89	0.27	48,48,48,48	0
34	NA	B	8383	1/1	0.89	0.20	52,52,52,52	0
34	NA	A	8319	1/1	0.89	0.11	41,41,41,41	0
35	CL	A	8505	1/1	0.89	0.14	68,68,68,68	0
34	NA	A	8339	1/1	0.90	0.13	15,15,15,15	0
34	NA	A	8356	1/1	0.90	0.37	46,46,46,46	0
32	MG	A	8008	1/1	0.90	0.08	50,50,50,50	0
34	NA	A	8381	1/1	0.90	0.08	35,35,35,35	0
35	CL	S	8506	1/1	0.90	0.16	60,60,60,60	0
34	NA	A	8314	1/1	0.91	0.26	35,35,35,35	0
35	CL	K	8502	1/1	0.91	0.21	83,83,83,83	0
32	MG	A	8040	1/1	0.91	0.17	86,86,86,86	0
32	MG	A	8102	1/1	0.91	0.74	106,106,106,106	0
34	NA	A	8323	1/1	0.91	0.29	55,55,55,55	0
34	NA	A	8331	1/1	0.91	0.19	37,37,37,37	0
32	MG	A	8071	1/1	0.91	0.07	65,65,65,65	0
32	MG	A	8039	1/1	0.91	0.09	66,66,66,66	0
32	MG	A	8112	1/1	0.91	0.26	70,70,70,70	0
34	NA	A	8306	1/1	0.91	0.40	38,38,38,38	0
32	MG	A	8047	1/1	0.92	0.21	76,76,76,76	0
32	MG	A	8062	1/1	0.92	0.08	32,32,32,32	0
34	NA	A	8367	1/1	0.92	0.14	40,40,40,40	0
34	NA	A	8368	1/1	0.92	0.08	22,22,22,22	0
37	CD	2	8402	1/1	0.92	0.11	67,67,67,67	0
35	CL	Z	8520	1/1	0.92	0.15	49,49,49,49	0
34	NA	A	8372	1/1	0.93	0.15	30,30,30,30	0
35	CL	A	8512	1/1	0.93	0.11	43,43,43,43	0
34	NA	A	8317	1/1	0.93	0.12	25,25,25,25	0
32	MG	A	8085	1/1	0.93	0.18	60,60,60,60	0
35	CL	A	8522	1/1	0.93	0.48	72,72,72,72	0
32	MG	A	8049	1/1	0.93	0.17	61,61,61,61	0
32	MG	A	8091	1/1	0.93	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8045	1/1	0.93	0.12	69,69,69,69	0
32	MG	A	8096	1/1	0.93	0.14	55,55,55,55	0
34	NA	A	8365	1/1	0.93	0.12	21,21,21,21	0
32	MG	A	8027	1/1	0.93	0.09	56,56,56,56	0
34	NA	J	8309	1/1	0.93	0.10	23,23,23,23	0
34	NA	A	8340	1/1	0.93	0.38	37,37,37,37	0
32	MG	A	8041	1/1	0.93	0.30	72,72,72,72	0
34	NA	A	8342	1/1	0.93	0.15	31,31,31,31	0
32	MG	A	8063	1/1	0.93	0.09	82,82,82,82	0
32	MG	A	8082	1/1	0.93	0.10	35,35,35,35	0
32	MG	A	8087	1/1	0.94	0.29	42,42,42,42	0
32	MG	A	8101	1/1	0.94	0.09	42,42,42,42	0
32	MG	A	8018	1/1	0.94	0.12	26,26,26,26	0
34	NA	A	8302	1/1	0.94	0.10	36,36,36,36	0
34	NA	A	8305	1/1	0.94	0.14	22,22,22,22	0
32	MG	A	8075	1/1	0.94	0.08	44,44,44,44	0
34	NA	A	8308	1/1	0.94	0.23	61,61,61,61	0
35	CL	D	8519	1/1	0.94	0.32	68,68,68,68	0
32	MG	A	8001	1/1	0.94	0.12	33,33,33,33	0
35	CL	K	8521	1/1	0.94	0.15	49,49,49,49	0
32	MG	A	8058	1/1	0.94	0.12	47,47,47,47	0
32	MG	A	8050	1/1	0.94	0.12	62,62,62,62	0
32	MG	B	8095	1/1	0.94	0.15	90,90,90,90	0
32	MG	D	8055	1/1	0.94	0.08	50,50,50,50	0
34	NA	A	8364	1/1	0.94	0.16	32,32,32,32	0
34	NA	S	8337	1/1	0.94	0.12	57,57,57,57	0
34	NA	A	8325	1/1	0.94	0.17	56,56,56,56	0
32	MG	A	8098	1/1	0.94	0.26	53,53,53,53	0
32	MG	Z	8109	1/1	0.94	0.08	31,31,31,31	0
34	NA	A	8336	1/1	0.94	0.15	72,72,72,72	0
34	NA	A	8329	1/1	0.95	0.08	47,47,47,47	0
32	MG	A	8090	1/1	0.95	0.20	81,81,81,81	0
32	MG	A	8103	1/1	0.95	0.11	45,45,45,45	0
34	NA	A	8335	1/1	0.95	0.15	50,50,50,50	0
32	MG	A	8029	1/1	0.95	0.10	58,58,58,58	0
32	MG	A	8107	1/1	0.95	0.05	64,64,64,64	0
32	MG	A	8059	1/1	0.95	0.12	70,70,70,70	0
32	MG	A	8094	1/1	0.95	0.12	77,77,77,77	0
35	CL	A	8516	1/1	0.95	0.23	57,57,57,57	0
35	CL	A	8517	1/1	0.95	0.29	75,75,75,75	0
34	NA	A	8310	1/1	0.95	0.17	35,35,35,35	0
34	NA	A	8374	1/1	0.95	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	A	8313	1/1	0.95	0.45	76,76,76,76	0
34	NA	A	8349	1/1	0.95	0.18	27,27,27,27	0
34	NA	A	8379	1/1	0.95	0.13	30,30,30,30	0
32	MG	A	8048	1/1	0.95	0.10	51,51,51,51	0
34	NA	A	8354	1/1	0.95	0.13	20,20,20,20	0
32	MG	A	8032	1/1	0.95	0.11	24,24,24,24	0
34	NA	A	8385	1/1	0.95	0.40	29,29,29,29	0
32	MG	A	8037	1/1	0.95	0.07	40,40,40,40	0
34	NA	A	8320	1/1	0.95	0.10	16,16,16,16	0
34	NA	A	8358	1/1	0.95	0.57	75,75,75,75	0
32	MG	A	8013	1/1	0.95	0.15	27,27,27,27	0
32	MG	A	8100	1/1	0.95	0.11	45,45,45,45	0
32	MG	A	8020	1/1	0.95	0.09	38,38,38,38	0
34	NA	A	8328	1/1	0.96	0.13	39,39,39,39	0
32	MG	A	8036	1/1	0.96	0.06	36,36,36,36	0
35	CL	A	8503	1/1	0.96	0.12	65,65,65,65	0
32	MG	A	8056	1/1	0.96	0.12	53,53,53,53	0
34	NA	A	8332	1/1	0.96	0.17	38,38,38,38	0
33	K	A	8201	1/1	0.96	0.09	53,53,53,53	0
33	K	A	8202	1/1	0.96	0.07	43,43,43,43	0
32	MG	A	8072	1/1	0.96	0.22	64,64,64,64	0
34	NA	A	8303	1/1	0.96	0.18	33,33,33,33	0
32	MG	A	8108	1/1	0.96	0.10	44,44,44,44	0
34	NA	A	8373	1/1	0.96	0.07	40,40,40,40	0
32	MG	A	8011	1/1	0.96	0.09	36,36,36,36	0
32	MG	A	8026	1/1	0.96	0.09	19,19,19,19	0
32	MG	A	8115	1/1	0.96	0.09	41,41,41,41	0
34	NA	A	8378	1/1	0.96	0.12	28,28,28,28	0
32	MG	A	8077	1/1	0.96	0.16	37,37,37,37	0
32	MG	A	8006	1/1	0.96	0.09	33,33,33,33	0
34	NA	A	8352	1/1	0.96	0.20	36,36,36,36	0
32	MG	C	8065	1/1	0.96	0.13	62,62,62,62	0
34	NA	A	8318	1/1	0.96	0.22	62,62,62,62	0
32	MG	A	8028	1/1	0.96	0.06	60,60,60,60	0
32	MG	L	8069	1/1	0.96	0.08	65,65,65,65	0
32	MG	A	8005	1/1	0.96	0.12	39,39,39,39	0
32	MG	A	8088	1/1	0.96	0.07	11,11,11,11	0
32	MG	A	8010	1/1	0.96	0.06	37,37,37,37	0
34	NA	A	8326	1/1	0.96	0.10	31,31,31,31	0
32	MG	A	8033	1/1	0.97	0.09	26,26,26,26	0
32	MG	A	8084	1/1	0.97	0.09	65,65,65,65	0
34	NA	A	8343	1/1	0.97	0.09	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8113	1/1	0.97	0.10	40,40,40,40	0
35	CL	A	8513	1/1	0.97	0.13	74,74,74,74	0
32	MG	A	8034	1/1	0.97	0.06	32,32,32,32	0
34	NA	A	8301	1/1	0.97	0.26	27,27,27,27	0
32	MG	A	8004	1/1	0.97	0.08	18,18,18,18	0
34	NA	A	8324	1/1	0.97	0.06	26,26,26,26	0
32	MG	A	8053	1/1	0.97	0.16	86,86,86,86	0
32	MG	A	8023	1/1	0.97	0.07	47,47,47,47	0
34	NA	A	8327	1/1	0.97	0.25	18,18,18,18	0
32	MG	A	8009	1/1	0.97	0.08	15,15,15,15	0
34	NA	A	8307	1/1	0.97	0.11	28,28,28,28	0
34	NA	A	8360	1/1	0.97	0.15	42,42,42,42	0
32	MG	A	8031	1/1	0.97	0.07	14,14,14,14	0
32	MG	A	8061	1/1	0.97	0.07	40,40,40,40	0
34	NA	A	8311	1/1	0.97	0.12	68,68,68,68	0
34	NA	R	8348	1/1	0.97	0.11	20,20,20,20	0
34	NA	A	8334	1/1	0.97	0.05	36,36,36,36	0
32	MG	A	8093	1/1	0.97	0.19	91,91,91,91	0
32	MG	A	8019	1/1	0.97	0.06	27,27,27,27	0
37	CD	1	8403	1/1	0.97	0.14	187,187,187,187	0
34	NA	A	8315	1/1	0.97	0.11	15,15,15,15	0
34	NA	A	8316	1/1	0.97	0.11	31,31,31,31	0
32	MG	A	8083	1/1	0.98	0.07	40,40,40,40	0
32	MG	A	8003	1/1	0.98	0.19	36,36,36,36	0
32	MG	A	8012	1/1	0.98	0.14	41,41,41,41	0
34	NA	A	8321	1/1	0.98	0.23	53,53,53,53	0
32	MG	A	8104	1/1	0.98	0.09	40,40,40,40	0
32	MG	A	8086	1/1	0.98	0.14	49,49,49,49	0
32	MG	A	8030	1/1	0.98	0.13	31,31,31,31	0
34	NA	A	8376	1/1	0.98	0.12	35,35,35,35	0
34	NA	A	8353	1/1	0.98	0.07	15,15,15,15	0
32	MG	A	8022	1/1	0.98	0.05	22,22,22,22	0
32	MG	A	8110	1/1	0.98	0.06	26,26,26,26	0
32	MG	A	8067	1/1	0.98	0.15	41,41,41,41	0
32	MG	A	8002	1/1	0.98	0.11	26,26,26,26	0
32	MG	A	8014	1/1	0.98	0.13	20,20,20,20	0
34	NA	A	8330	1/1	0.98	0.10	37,37,37,37	0
35	CL	N	8518	1/1	0.98	0.08	36,36,36,36	0
32	MG	A	8054	1/1	0.98	0.09	43,43,43,43	0
32	MG	A	8015	1/1	0.98	0.08	35,35,35,35	0
34	NA	C	8345	1/1	0.98	0.15	30,30,30,30	0
34	NA	A	8362	1/1	0.98	0.13	45,45,45,45	0

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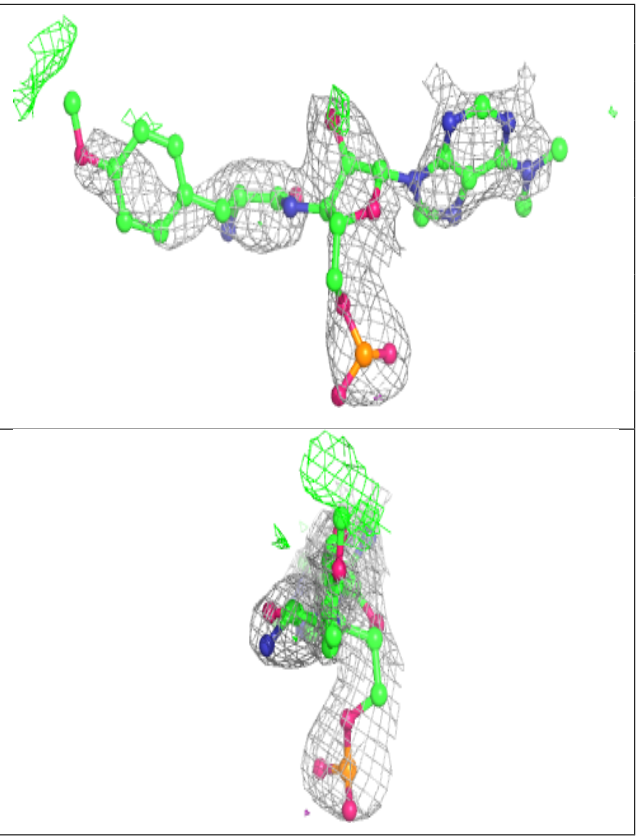
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8057	1/1	0.98	0.10	16,16,16,16	0
34	NA	M	8380	1/1	0.98	0.15	43,43,43,43	0
32	MG	A	8035	1/1	0.98	0.04	64,64,64,64	0
32	MG	A	8007	1/1	0.98	0.09	22,22,22,22	0
32	MG	A	8079	1/1	0.98	0.07	19,19,19,19	0
32	MG	A	8080	1/1	0.98	0.09	35,35,35,35	0
32	MG	A	8060	1/1	0.98	0.12	39,39,39,39	0
32	MG	A	8117	1/1	0.99	0.06	8,8,8,8	0
34	NA	N	8347	1/1	0.99	0.05	21,21,21,21	0
32	MG	A	8017	1/1	0.99	0.05	17,17,17,17	0
32	MG	A	8016	1/1	0.99	0.10	26,26,26,26	0
32	MG	A	8021	1/1	0.99	0.10	45,45,45,45	0
32	MG	A	8042	1/1	0.99	0.05	17,17,17,17	0
32	MG	A	8081	1/1	0.99	0.13	30,30,30,30	0
32	MG	A	8025	1/1	0.99	0.04	57,57,57,57	0
32	MG	A	8038	1/1	0.99	0.10	30,30,30,30	0
35	CL	K	8501	1/1	0.99	0.10	61,61,61,61	0
32	MG	A	8074	1/1	0.99	0.08	24,24,24,24	0
32	MG	A	8064	1/1	0.99	0.11	18,18,18,18	0
34	NA	K	8346	1/1	1.00	0.06	19,19,19,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PPU 5 76:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.