wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 01:43 AM EST

PDB ID	:	1KQS
Title	:	The Haloarcula marismortui 50S Complexed with a Pretranslocational Intermediate in Protein Synthesis
Authors	:	Schmeing, T.M.; Seila, A.C.; Hansen, J.L.; Freeborn, B.; Soukup, J.K.; Scaringe, S.A.; Strobel, S.A.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2002-01-07
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
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:

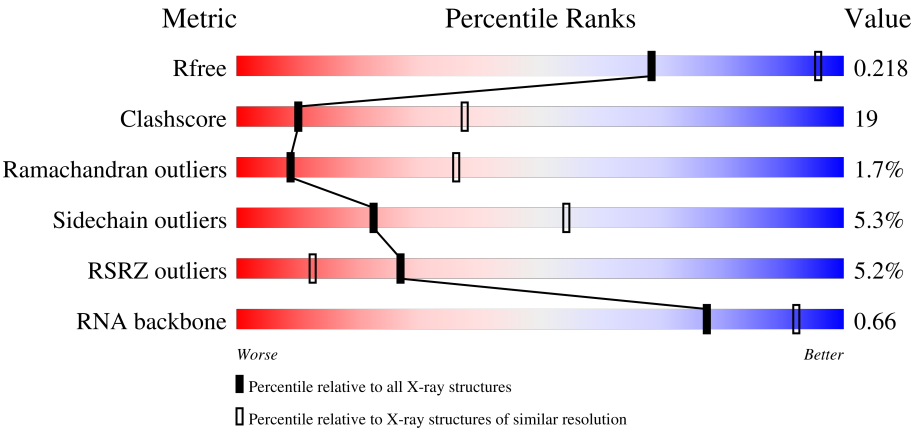
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	2% 57% 32% 5% • 6%
2	9	122	5% 52% 38% 9% •
3	3	3	33% 33% 33%

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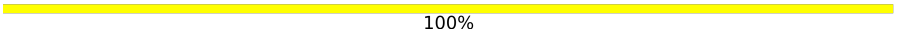
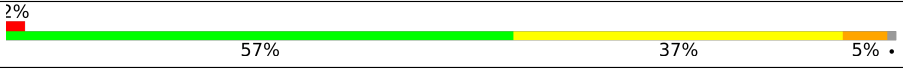
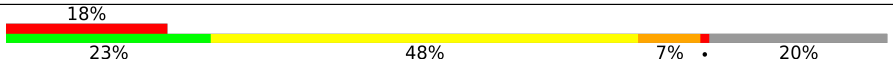
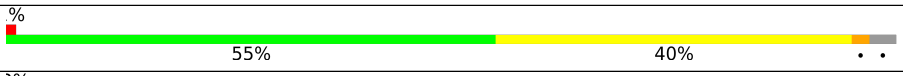
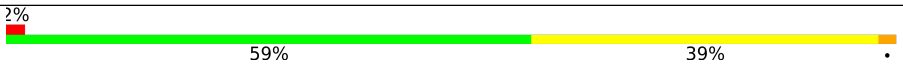
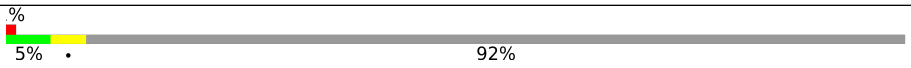
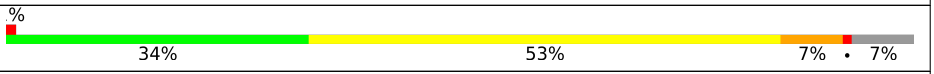
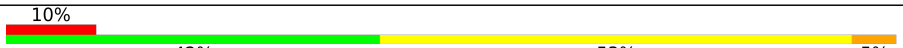
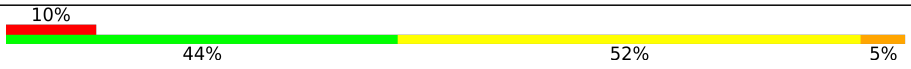
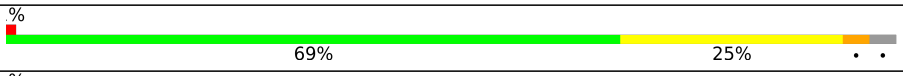
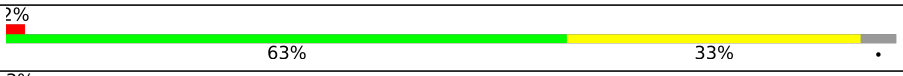
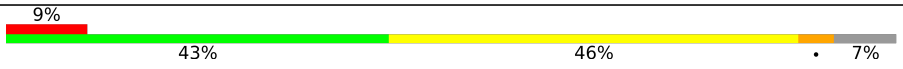
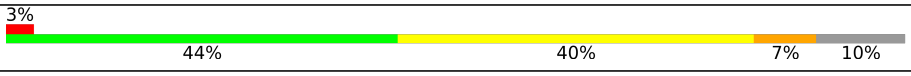
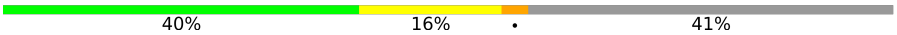
Mol	Chain	Length	Quality of chain
4	4	2	
5	A	239	
6	B	337	
7	C	246	
8	D	176	
9	E	177	
10	F	119	
11	G	348	
12	H	167	
13	I	145	
14	J	132	
15	K	164	
16	L	194	
17	M	186	
18	N	115	
19	O	148	
20	P	95	
21	Q	154	
22	R	84	
23	S	119	
24	T	66	
25	U	70	
26	V	154	
27	W	91	
28	X	240	

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Mol	Chain	Length	Quality of chain
29	Y	73	67% 27% 66% 7%
30	Z	56	68% 32%
31	1	48	65% 29%
32	2	92	100% 42% 53%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8114	-	-	-	X
33	MG	Y	8105	-	-	-	X
35	NA	0	8329	-	-	-	X
35	NA	0	8363	-	-	-	X
35	NA	0	8371	-	-	-	X
35	NA	0	8384	-	-	-	X
35	NA	9	8383	-	-	-	X
35	NA	Q	8386	-	-	-	X
35	NA	R	8312	-	-	-	X
36	CL	2	8504	-	-	-	X
41	CD	2	8404	-	-	-	X

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 98688 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2754	59017	26346	10878	19048	2745	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	conflict	? 3377779

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

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 CCA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	3	3	59	28	11	18	2	0	0	0

- Molecule 4 is a RNA chain called CC-Pmn-pcb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	4	2	37	18	6	12	1	0	0	0

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	A	237	1754	1072	352	325	5	0	0	0

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L3.

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

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 7 is a protein called RIBOSOMAL PROTEIN L4.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L7AE.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L10E.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L15E.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	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 20 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37Ae.

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

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L37E.

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

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	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 32 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	110	Total	Mg	0	0
			110	110		
33	9	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	J	1	Total	Mg	0	0
			1	1		
33	S	1	Total	Mg	0	0
			1	1		
33	X	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	73	Total	Na	0	0
			73	73		
35	9	2	Total	Na	0	0
			2	2		
35	A	1	Total	Na	0	0
			1	1		

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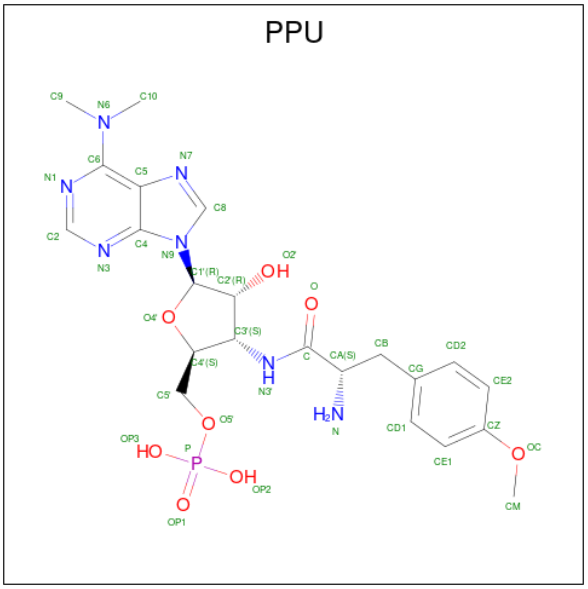
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	I	1	Total Na 1 1	0	0
35	K	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	P	1	Total Na 1 1	0	0
35	Q	3	Total Na 3 3	0	0
35	R	1	Total Na 1 1	0	0

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

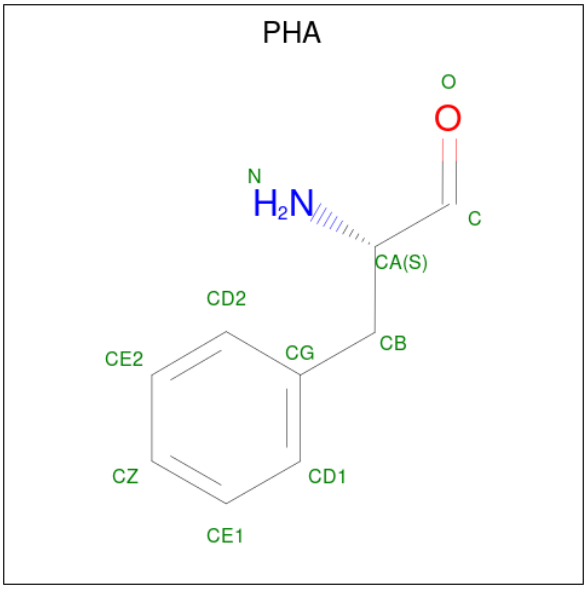
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	I	3	Total Cl 3 3	0	0
36	K	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	Q	1	Total Cl 1 1	0	0
36	X	1	Total Cl 1 1	0	0
36	2	1	Total Cl 1 1	0	0

- Molecule 37 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: $C_{22}H_{30}N_7O_8P$).



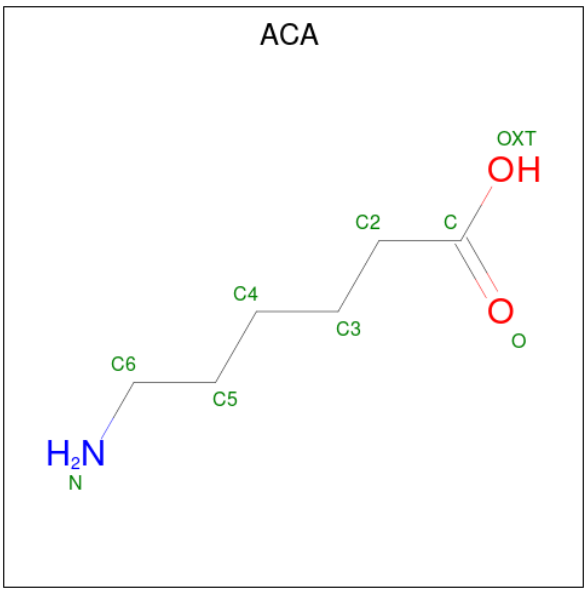
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	4	1	Total	C	N	O	P	0	0
			37	22	7	7	1		

- Molecule 38 is PHENYLALANINAL (three-letter code: PHA) (formula: $C_9H_{11}NO$).



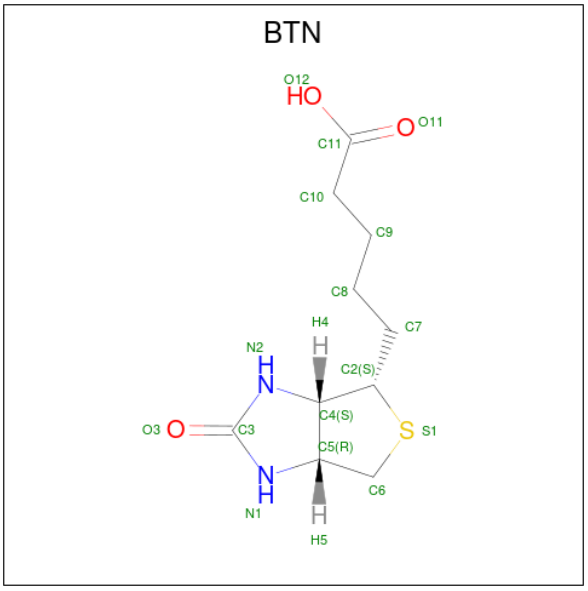
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	4	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 39 is 6-AMINOHEXANOIC ACID (three-letter code: ACA) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
39	4	1	8	6	1	1	0	0

- Molecule 40 is BIOTIN (three-letter code: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
40	4	1	15	10	2	2	1	0	0

- Molecule 41 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	N	1	Total Cd 1 1	0	0
41	T	1	Total Cd 1 1	0	0
41	Y	1	Total Cd 1 1	0	0
41	Z	1	Total Cd 1 1	0	0
41	2	1	Total Cd 1 1	0	0

- Molecule 42 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	0	5873	Total O 5873 5873	0	0
42	9	140	Total O 140 140	0	0
42	3	4	Total O 4 4	0	0
42	4	4	Total O 4 4	0	0
42	A	132	Total O 132 132	0	0
42	B	143	Total O 143 143	0	0
42	C	176	Total O 176 176	0	0
42	D	51	Total O 51 51	0	0
42	E	44	Total O 44 44	0	0
42	F	29	Total O 29 29	0	0
42	G	22	Total O 22 22	0	0
42	H	78	Total O 78 78	0	0
42	I	57	Total O 57 57	0	0
42	J	61	Total O 61 61	0	0
42	K	84	Total O 84 84	0	0

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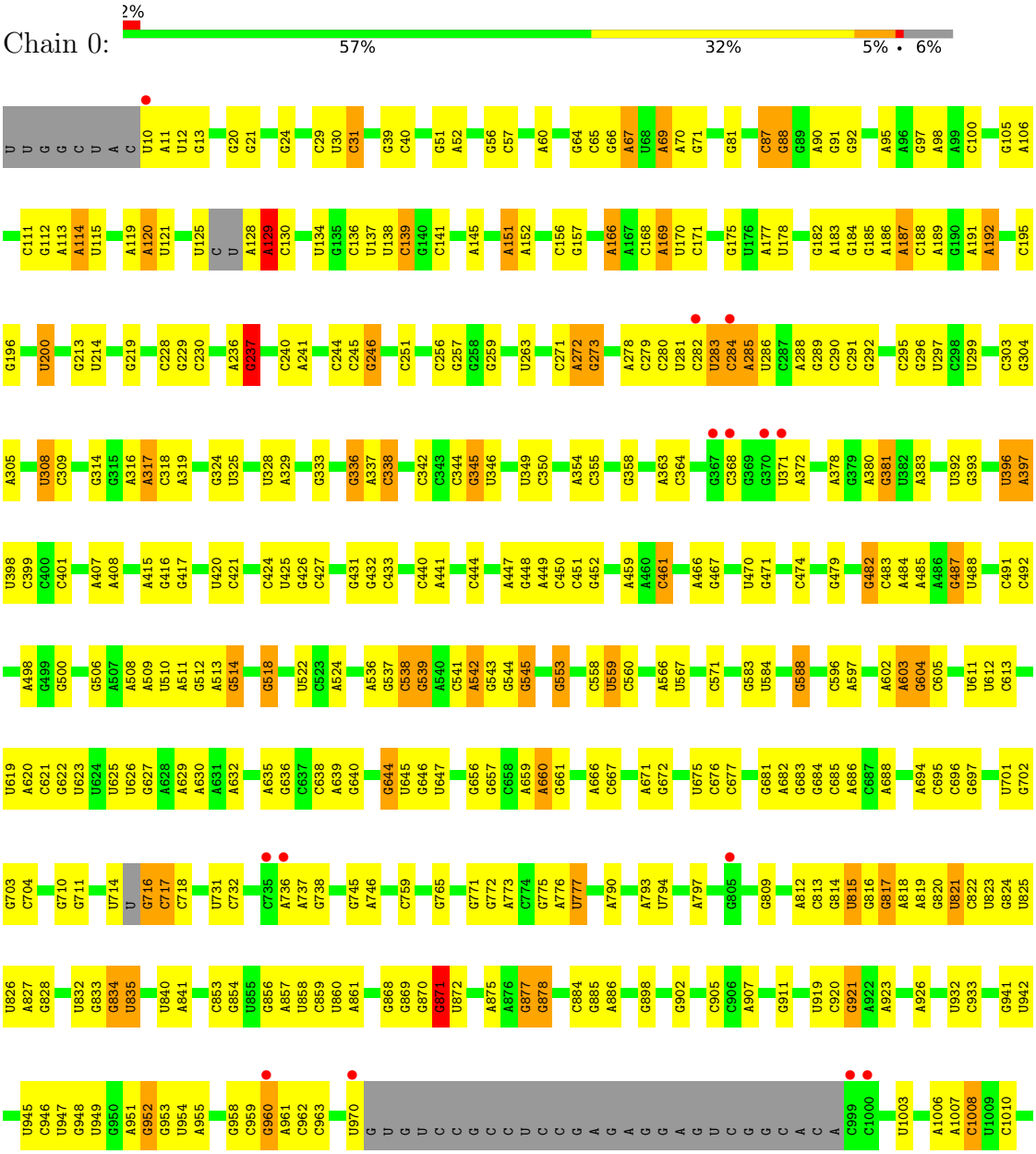
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	L	138	Total O 138 138	0	0
42	M	70	Total O 70 70	0	0
42	N	42	Total O 42 42	0	0
42	O	67	Total O 67 67	0	0
42	P	56	Total O 56 56	0	0
42	Q	87	Total O 87 87	0	0
42	R	36	Total O 36 36	0	0
42	S	37	Total O 37 37	0	0
42	T	26	Total O 26 26	0	0
42	U	16	Total O 16 16	0	0
42	V	66	Total O 66 66	0	0
42	W	30	Total O 30 30	0	0
42	X	96	Total O 96 96	0	0
42	Y	33	Total O 33 33	0	0
42	Z	55	Total O 55 55	0	0
42	1	42	Total O 42 42	0	0
42	2	76	Total O 76 76	0	0

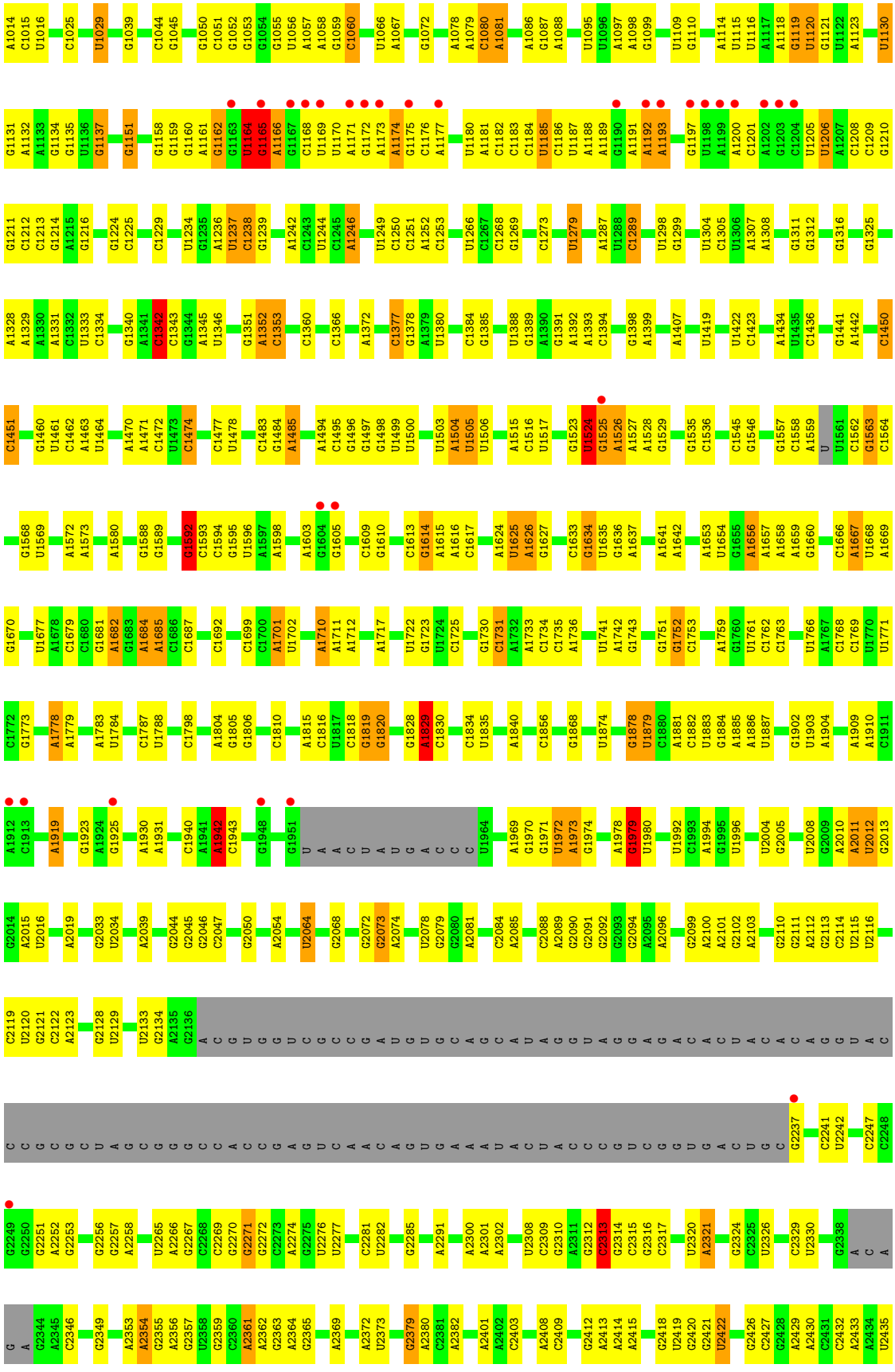
3 Residue-property plots (i)

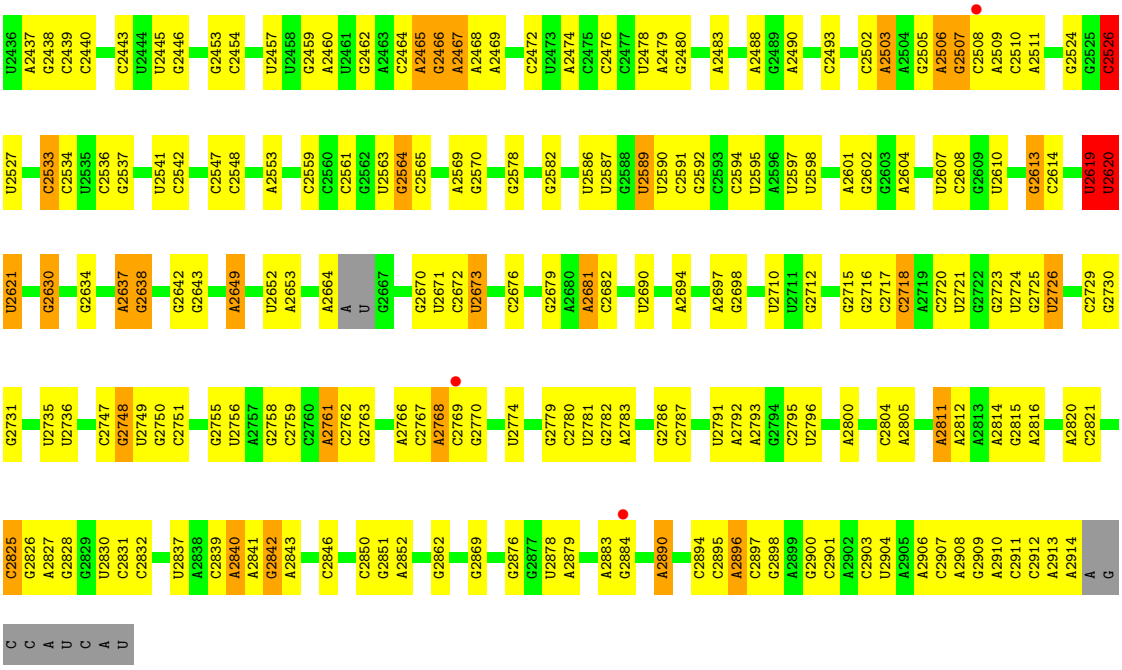
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain 0:

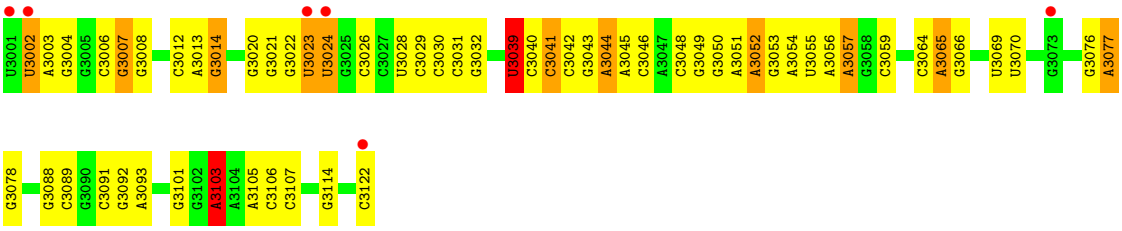






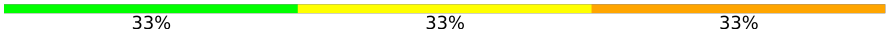
• Molecule 2: 5S RRNA

Chain 9:



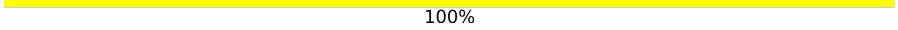
• Molecule 3: CCA

Chain 3:



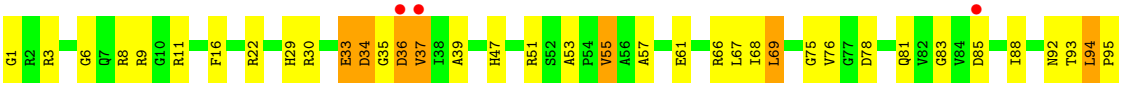
• Molecule 4: CC-Pmn-pcb

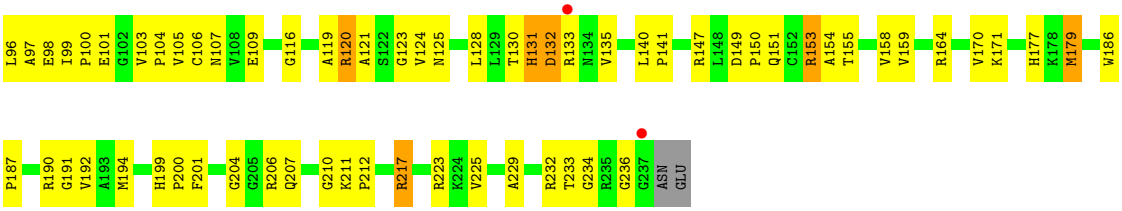
Chain 4:



• Molecule 5: RIBOSOMAL PROTEIN L2

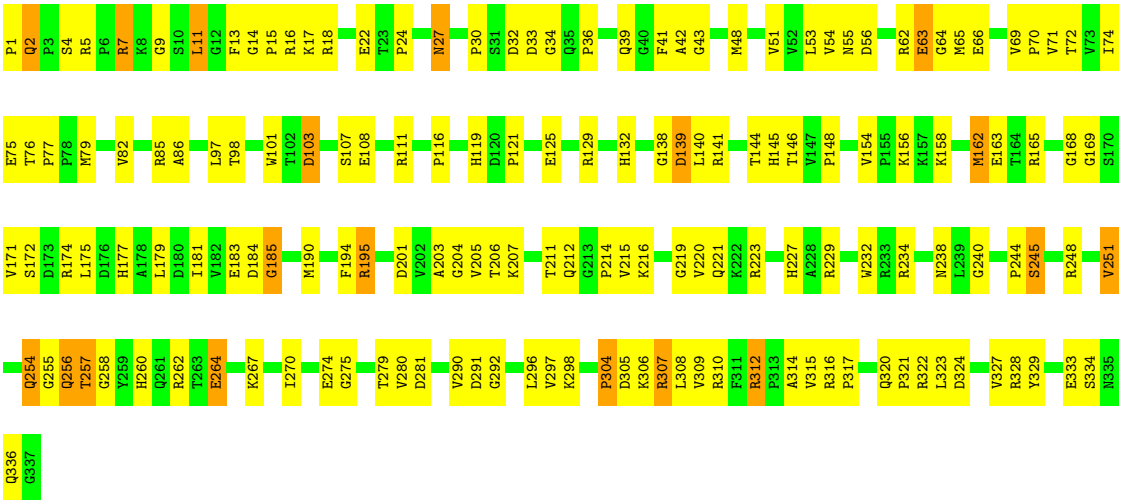
Chain A:





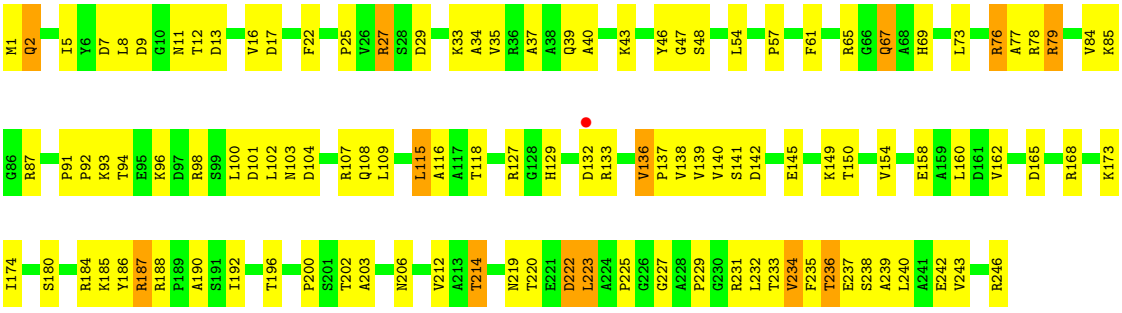
• Molecule 6: RIBOSOMAL PROTEIN L3

Chain B:



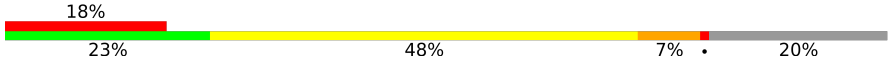
• Molecule 7: RIBOSOMAL PROTEIN L4

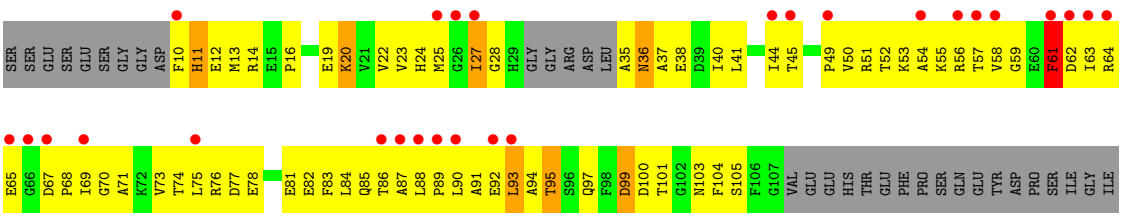
Chain C:

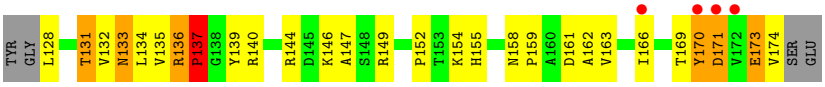


• Molecule 8: RIBOSOMAL PROTEIN L5

Chain D:





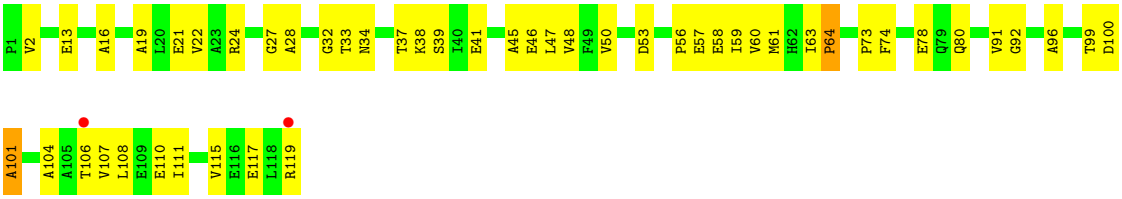


• Molecule 9: RIBOSOMAL PROTEIN L6

Chain E:

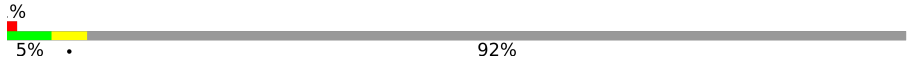
• Molecule 10: RIBOSOMAL PROTEIN L7AE

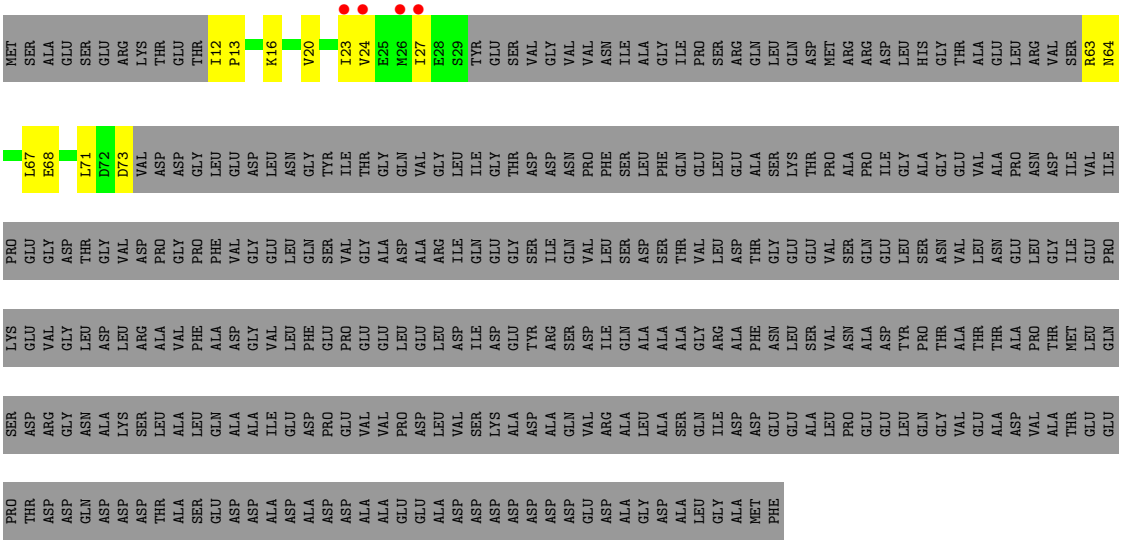
Chain F:



• Molecule 11: RIBOSOMAL PROTEIN L10

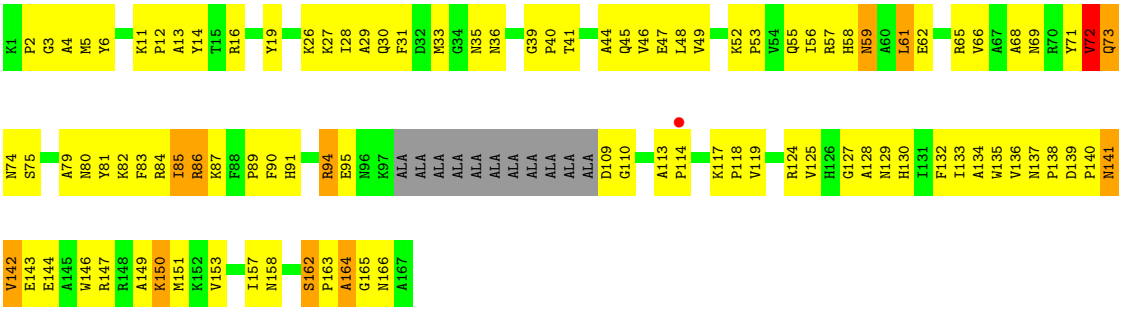
Chain G:





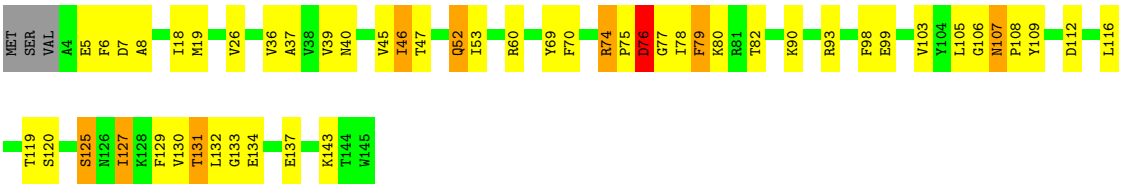
• Molecule 12: RIBOSOMAL PROTEIN L10E

Chain H:



• Molecule 13: RIBOSOMAL PROTEIN L13

Chain I:

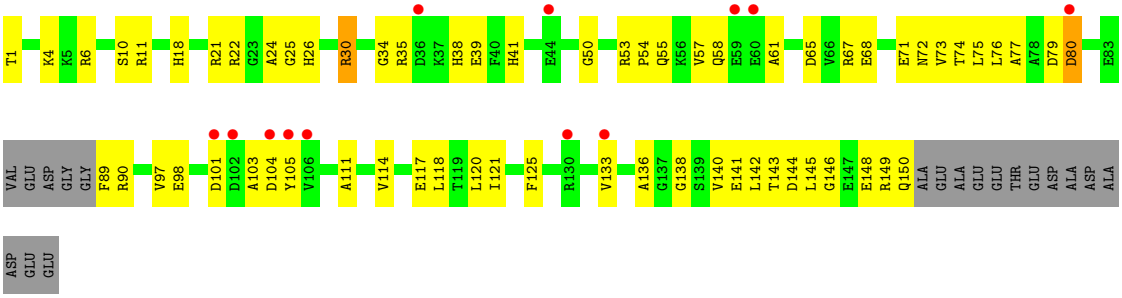


• Molecule 14: RIBOSOMAL PROTEIN L14

Chain J:

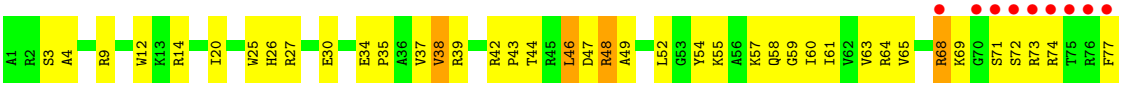
• Molecule 15: RIBOSOMAL PROTEIN L15

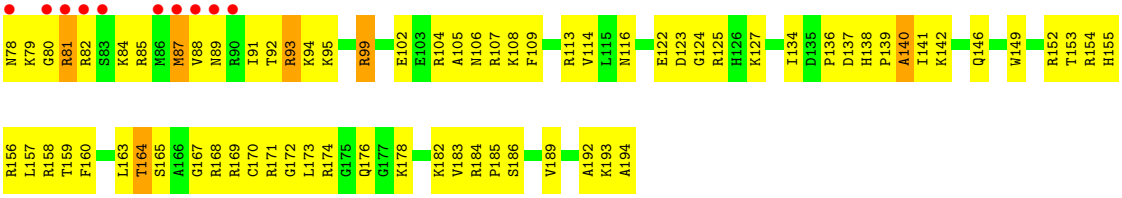
Chain K:



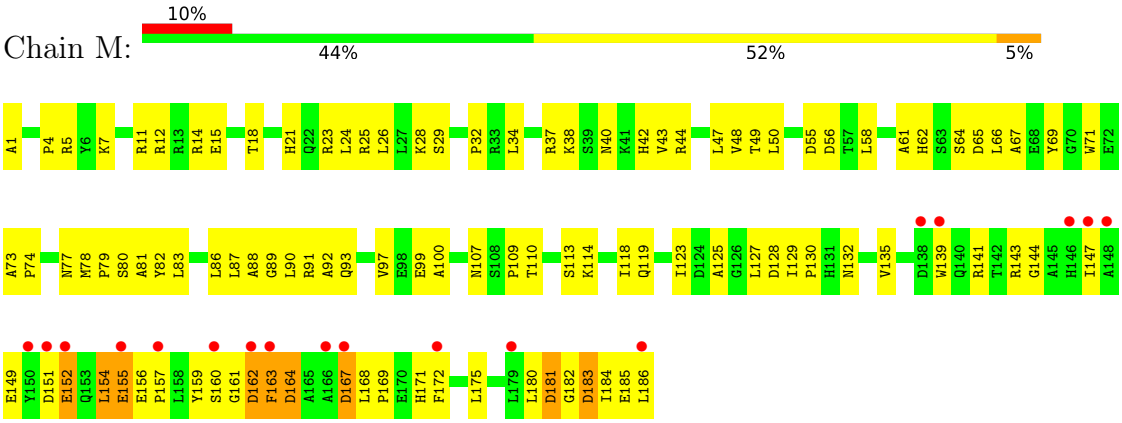
• Molecule 16: RIBOSOMAL PROTEIN L15E

Chain L:

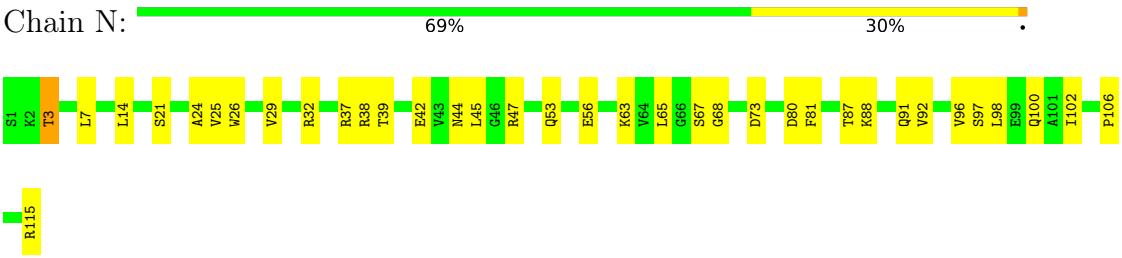




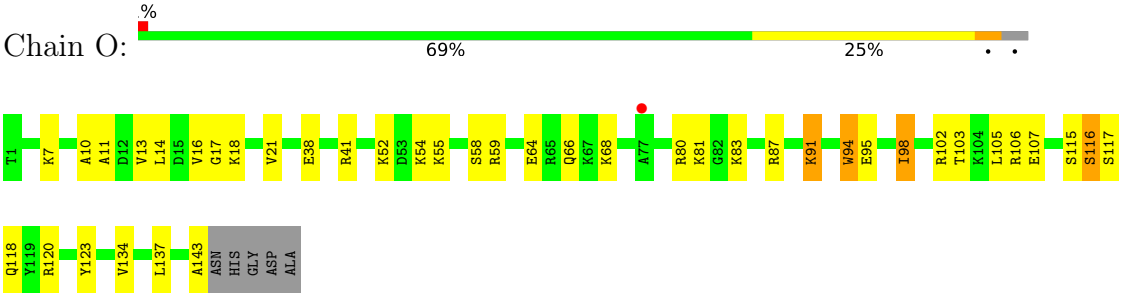
• Molecule 17: RIBOSOMAL PROTEIN L18



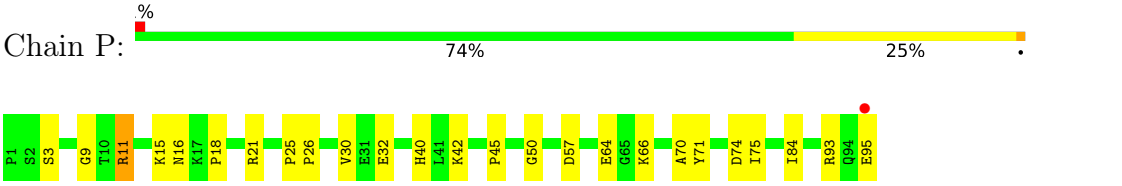
• Molecule 18: RIBOSOMAL PROTEIN L18E



• Molecule 19: RIBOSOMAL PROTEIN L19E

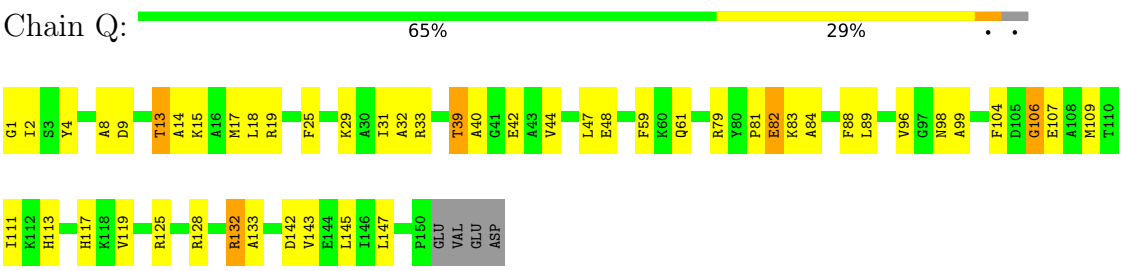


• Molecule 20: RIBOSOMAL PROTEIN L21E



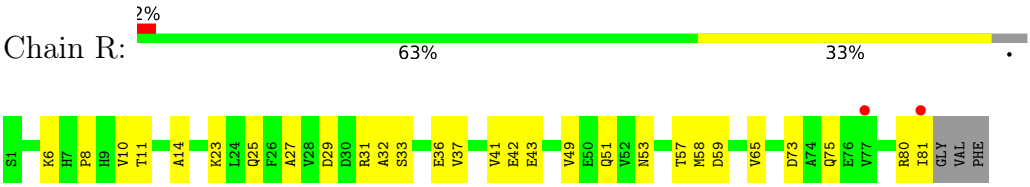
• Molecule 21: RIBOSOMAL PROTEIN L22

Chain Q:



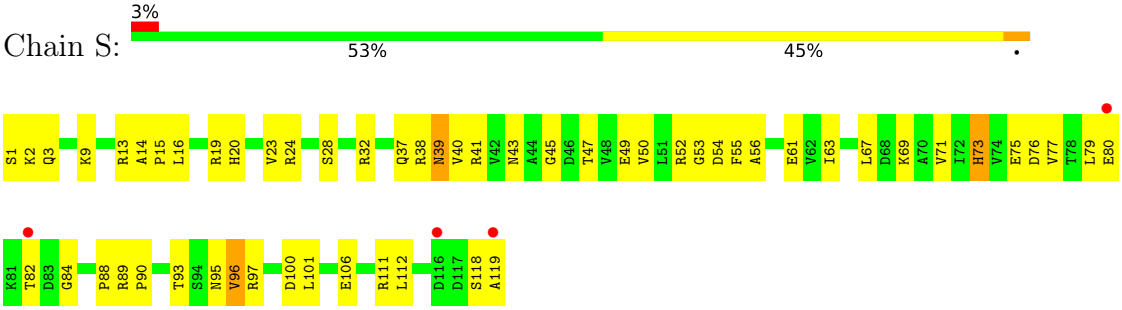
• Molecule 22: RIBOSOMAL PROTEIN L23

Chain R:



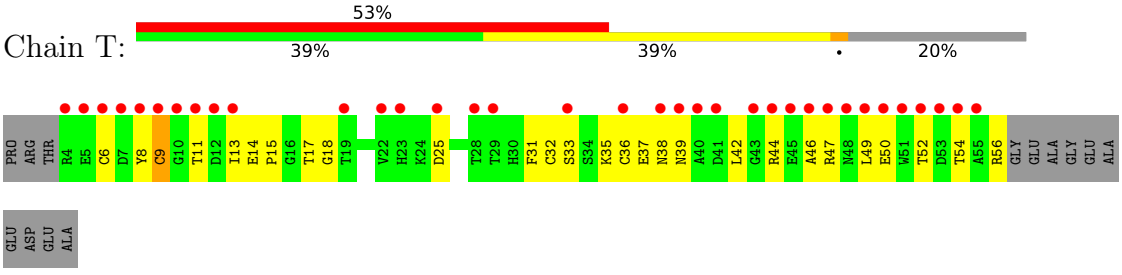
• Molecule 23: RIBOSOMAL PROTEIN L24

Chain S:



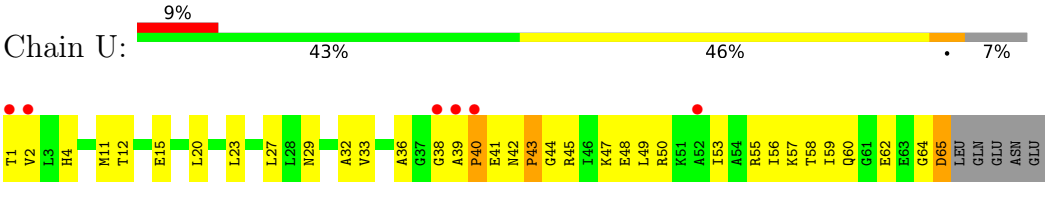
• Molecule 24: RIBOSOMAL PROTEIN L24E

Chain T:



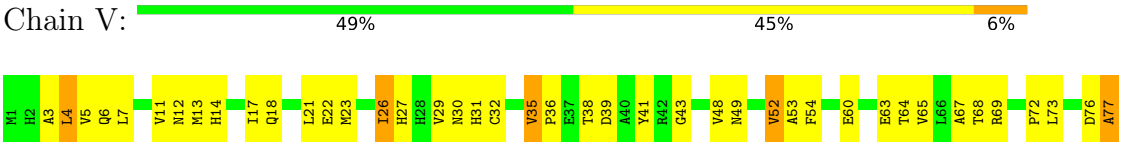
• Molecule 25: RIBOSOMAL PROTEIN L29

Chain U:



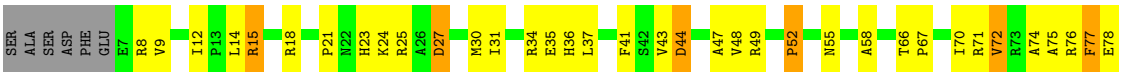
• Molecule 26: RIBOSOMAL PROTEIN L30

Chain V:



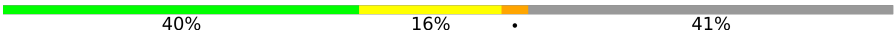
• Molecule 27: RIBOSOMAL PROTEIN L31E

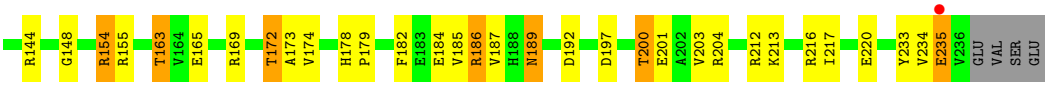
Chain W:



• Molecule 28: RIBOSOMAL PROTEIN L32E

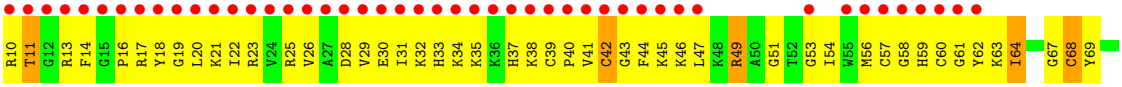
Chain X:

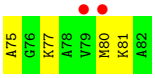




• Molecule 29: RIBOSOMAL PROTEIN L37Ae

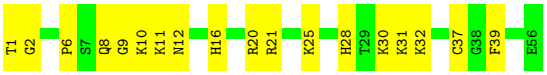
Chain Y:





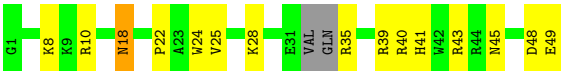
• Molecule 30: RIBOSOMAL PROTEIN L37E

Chain Z:



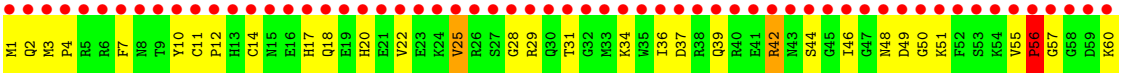
• Molecule 31: RIBOSOMAL PROTEIN L39E

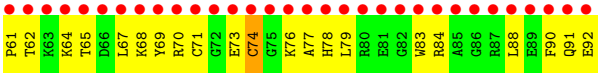
Chain 1:



• Molecule 32: RIBOSOMAL PROTEIN L44E

Chain 2:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	212.78Å 300.35Å 574.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 44.78 – 3.06	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.10) 95.4 (44.78-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.173 , 0.220 0.173 , 0.218	Depositor DCC
R_{free} test set	3329 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 65.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	98688	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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: BTN, ACA, NA, MG, CD, PPU, PHA, CL, K

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	0.41	2/66076 (0.0%)	0.70	27/103052 (0.0%)
2	9	0.39	0/2905	0.75	2/4528 (0.0%)
3	3	0.82	0/65	0.87	0/99
4	4	0.49	0/40	0.62	0/60
5	A	0.34	0/1787	0.66	0/2409
6	B	0.35	0/2689	0.64	0/3652
7	C	0.39	0/1883	0.64	0/2551
8	D	0.32	0/1111	0.59	0/1498
9	E	0.34	0/1382	0.58	0/1880
10	F	0.33	0/896	0.56	0/1219
11	G	0.29	0/241	0.48	0/324
12	H	0.39	0/1246	0.76	2/1686 (0.1%)
13	I	0.38	0/1135	0.62	0/1530
14	J	0.35	0/1003	0.66	0/1351
15	K	0.34	0/1126	0.65	0/1504
16	L	0.41	0/1633	0.71	0/2180
17	M	0.29	0/1473	0.63	0/1999
18	N	0.35	0/873	0.62	0/1181
19	O	0.35	0/1143	0.54	0/1521
20	P	0.36	0/748	0.66	0/1005
21	Q	0.37	0/1172	0.66	0/1578
22	R	0.34	0/648	0.58	0/875
23	S	0.34	0/957	0.64	0/1289
24	T	0.34	0/417	0.56	0/562
25	U	0.30	0/502	0.57	0/675
26	V	0.37	0/1218	0.64	0/1655
27	W	0.35	0/664	0.61	0/895
28	X	0.38	0/1146	0.65	0/1536
29	Y	0.34	0/575	0.66	0/763
30	Z	0.41	0/437	0.64	0/578
31	1	0.32	0/398	0.54	0/527
32	2	0.39	0/771	0.57	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.40	2/98360 (0.0%)	0.69	31/147186 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	37
2	9	0	1
26	V	0	1
All	All	1	39

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	U	O5'-C5'	-7.09	1.31	1.42
1	0	2620	U	C2'-O2'	6.66	1.50	1.41

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1164	U	OP1-P-O3'	-12.07	78.64	105.20
1	0	1164	U	OP2-P-O3'	-10.75	81.56	105.20
1	0	1165	G	O5'-P-OP2	9.72	122.36	110.70
1	0	1563	G	C2'-C3'-O3'	9.36	130.09	109.50
1	0	2619	U	C5'-C4'-C3'	-9.23	101.24	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	171	C	Sidechain
1	0	246	G	Sidechain
1	0	333	G	Sidechain
1	0	393	G	Sidechain
1	0	396	U	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59017	0	29805	983	0
2	9	2600	0	1326	68	0
3	3	59	0	35	4	0
4	4	37	0	23	5	0
5	A	1754	0	1763	130	0
6	B	2624	0	2533	167	0
7	C	1858	0	1816	130	0
8	D	1094	0	1085	133	0
9	E	1357	0	1266	78	0
10	F	885	0	854	63	0
11	G	240	0	231	20	0
12	H	1215	0	1215	162	0
13	I	1119	0	1098	64	0
14	J	993	0	1027	58	0
15	K	1114	0	1072	64	0
16	L	1605	0	1676	164	0
17	M	1444	0	1401	139	0
18	N	864	0	873	33	0
19	O	1133	0	1127	43	0
20	P	734	0	729	23	0
21	Q	1149	0	1122	57	0
22	R	641	0	605	26	0
23	S	949	0	923	53	0
24	T	410	0	366	35	0
25	U	499	0	511	34	0
26	V	1195	0	1137	104	0
27	W	654	0	653	51	0
28	X	1130	0	1133	57	0
29	Y	563	0	601	72	0
30	Z	430	0	426	24	0
31	1	393	0	406	18	0
32	2	755	0	731	63	0
33	0	110	0	0	0	0
33	2	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	S	1	0	0	0	0
33	X	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	73	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	I	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	P	1	0	0	0	0
35	Q	3	0	0	0	0
35	R	1	0	0	0	0
36	0	10	0	0	0	0
36	2	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	I	3	0	0	1	0
36	K	1	0	0	0	0
36	L	1	0	0	1	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	Q	1	0	0	0	0
36	X	1	0	0	0	0
37	4	37	0	26	2	0
38	4	11	0	8	1	0
39	4	8	0	6	0	0
40	4	15	0	15	2	0
41	2	1	0	0	0	0
41	N	1	0	0	0	0
41	T	1	0	0	0	0
41	Y	1	0	0	0	0
41	Z	1	0	0	0	0
42	0	5873	0	0	207	0
42	1	42	0	0	3	0
42	2	76	0	0	7	0
42	3	4	0	0	3	0
42	4	4	0	0	0	0
42	9	140	0	0	11	0
42	A	132	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	B	143	0	0	23	0
42	C	176	0	0	35	0
42	D	51	0	0	19	0
42	E	44	0	0	10	0
42	F	29	0	0	12	0
42	G	22	0	0	5	0
42	H	78	0	0	22	0
42	I	57	0	0	4	0
42	J	61	0	0	9	0
42	K	84	0	0	19	0
42	L	138	0	0	22	0
42	M	70	0	0	15	0
42	N	42	0	0	7	0
42	O	67	0	0	6	0
42	P	56	0	0	3	0
42	Q	87	0	0	9	0
42	R	36	0	0	6	0
42	S	37	0	0	9	0
42	T	26	0	0	4	0
42	U	16	0	0	3	0
42	V	66	0	0	11	0
42	W	30	0	0	5	0
42	X	96	0	0	17	0
42	Y	33	0	0	12	0
42	Z	55	0	0	3	0
All	All	98688	0	59624	2828	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 19.

The worst 5 of 2828 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)
12:H:86:ARG:NH1	12:H:133:ILE:HG13	1.61	1.16
25:U:12:THR:HG22	25:U:15:GLU:HG3	1.34	1.09
7:C:236:THR:HG22	7:C:239:ALA:H	0.97	1.07
1:0:156:C:H5"	16:L:171:ARG:HD3	1.38	1.05
12:H:45:GLN:HB3	12:H:163:PRO:HD2	1.40	1.04

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
5	A	235/239 (98%)	199 (85%)	32 (14%)	4 (2%)	9 36
6	B	335/337 (99%)	299 (89%)	29 (9%)	7 (2%)	7 30
7	C	244/246 (99%)	220 (90%)	22 (9%)	2 (1%)	19 54
8	D	134/176 (76%)	94 (70%)	26 (19%)	14 (10%)	0 3
9	E	170/177 (96%)	159 (94%)	11 (6%)	0	100 100
10	F	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	9 36
11	G	25/348 (7%)	24 (96%)	1 (4%)	0	100 100
12	H	152/167 (91%)	132 (87%)	15 (10%)	5 (3%)	4 21
13	I	140/145 (97%)	127 (91%)	9 (6%)	4 (3%)	4 24
14	J	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	10 39
15	K	141/164 (86%)	124 (88%)	16 (11%)	1 (1%)	22 57
16	L	192/194 (99%)	174 (91%)	17 (9%)	1 (0%)	29 64
17	M	184/186 (99%)	166 (90%)	11 (6%)	7 (4%)	3 19
18	N	113/115 (98%)	108 (96%)	5 (4%)	0	100 100
19	O	141/148 (95%)	138 (98%)	2 (1%)	1 (1%)	22 57
20	P	93/95 (98%)	86 (92%)	7 (8%)	0	100 100
21	Q	148/154 (96%)	136 (92%)	11 (7%)	1 (1%)	22 57
22	R	79/84 (94%)	74 (94%)	5 (6%)	0	100 100
23	S	117/119 (98%)	110 (94%)	7 (6%)	0	100 100
24	T	51/66 (77%)	48 (94%)	3 (6%)	0	100 100
25	U	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4 22
26	V	152/154 (99%)	143 (94%)	7 (5%)	2 (1%)	12 42
27	W	80/91 (88%)	71 (89%)	6 (8%)	3 (4%)	3 19
28	X	140/240 (58%)	140 (100%)	0	0	100 100
29	Y	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	11 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
31	1	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
32	2	90/92 (98%)	84 (93%)	3 (3%)	3 (3%)	4	21
All	All	3633/4235 (86%)	3293 (91%)	278 (8%)	62 (2%)	9	36

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	139	ASP
8	D	93	LEU
8	D	95	THR
8	D	173	GLU
10	F	101	ALA

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	
5	A	179/181 (99%)	166 (93%)	13 (7%)	14	43
6	B	282/282 (100%)	263 (93%)	19 (7%)	16	46
7	C	193/193 (100%)	177 (92%)	16 (8%)	11	38
8	D	117/147 (80%)	108 (92%)	9 (8%)	13	41
9	E	152/155 (98%)	146 (96%)	6 (4%)	32	65
10	F	92/92 (100%)	92 (100%)	0	100	100
11	G	27/283 (10%)	27 (100%)	0	100	100
12	H	122/122 (100%)	111 (91%)	11 (9%)	9	34
13	I	118/121 (98%)	107 (91%)	11 (9%)	9	32
14	J	106/106 (100%)	102 (96%)	4 (4%)	33	66
15	K	112/126 (89%)	108 (96%)	4 (4%)	35	67
16	L	166/166 (100%)	157 (95%)	9 (5%)	22	53
17	M	149/149 (100%)	145 (97%)	4 (3%)	44	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	N	93/93 (100%)	91 (98%)	2 (2%)	52 78
19	O	113/116 (97%)	109 (96%)	4 (4%)	36 68
20	P	79/79 (100%)	76 (96%)	3 (4%)	33 66
21	Q	117/121 (97%)	113 (97%)	4 (3%)	37 69
22	R	71/73 (97%)	71 (100%)	0	100 100
23	S	105/105 (100%)	102 (97%)	3 (3%)	42 72
24	T	44/52 (85%)	43 (98%)	1 (2%)	50 77
25	U	51/56 (91%)	49 (96%)	2 (4%)	32 65
26	V	130/130 (100%)	121 (93%)	9 (7%)	15 45
27	W	66/73 (90%)	61 (92%)	5 (8%)	13 41
28	X	120/195 (62%)	112 (93%)	8 (7%)	16 46
29	Y	56/56 (100%)	49 (88%)	7 (12%)	4 18
30	Z	46/46 (100%)	46 (100%)	0	100 100
31	1	42/44 (96%)	41 (98%)	1 (2%)	49 76
32	2	79/79 (100%)	75 (95%)	4 (5%)	24 56
All	All	3027/3441 (88%)	2868 (95%)	159 (5%)	22 54

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	Q	13	THR
28	X	189	ASN
23	S	39	ASN
26	V	122	ARG
29	Y	49	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
21	Q	61	GLN
26	V	59	GLN
21	Q	98	ASN
23	S	73	HIS
26	V	125	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2747/2922 (94%)	244 (8%)	34 (1%)
2	9	121/122 (99%)	14 (11%)	4 (3%)
3	3	2/3 (66%)	1 (50%)	0
4	4	1/2 (50%)	0	0
All	All	2871/3049 (94%)	259 (9%)	38 (1%)

5 of 259 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 38 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2536	C
2	9	3023	U
1	0	2637	A
1	0	2761	A
2	9	3103	A

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 236 ligands modelled in this entry, 232 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
37	PPU	4	76	4,38	32,40,41	2.50	3 (9%)	33,57,60	0.88	1 (3%)
38	PHA	4	77	37,39	10,11,11	1.01	0	10,13,13	0.56	0
40	BTN	4	79	39	16,16,17	1.83	4 (25%)	21,21,23	1.73	5 (23%)
39	ACA	4	78	38,40	7,7,8	2.02	1 (14%)	6,6,8	1.15	0

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
37	PPU	4	76	4,38	-	1/21/43/44	0/4/4/4
38	PHA	4	77	37,39	-	0/5/6/6	0/1/1/1
40	BTN	4	79	39	-	3/5/27/28	0/2/2/2
39	ACA	4	78	38,40	-	2/4/5/6	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	4	76	PPU	C-N3'	12.24	1.61	1.34
37	4	76	PPU	OC-CM	-5.27	1.26	1.42
39	4	78	ACA	C3-C2	-5.05	1.32	1.52
40	4	79	BTN	C8-C7	-4.33	1.33	1.52
40	4	79	BTN	C9-C10	-3.86	1.36	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	4	79	BTN	C2-C4-N2	4.91	117.52	113.13
40	4	79	BTN	C6-C5-N1	2.64	116.39	113.03
37	4	76	PPU	C-CA-N	2.36	118.52	109.40
40	4	79	BTN	C6-C5-C4	-2.28	106.68	108.66
40	4	79	BTN	C2-C4-C5	2.19	111.48	108.94

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	4	78	ACA	C4-C5-C6-N
40	4	79	BTN	C7-C8-C9-C10
39	4	78	ACA	C3-C4-C5-C6
40	4	79	BTN	C4-C2-C7-C8
37	4	76	PPU	N-CA-CB-CG

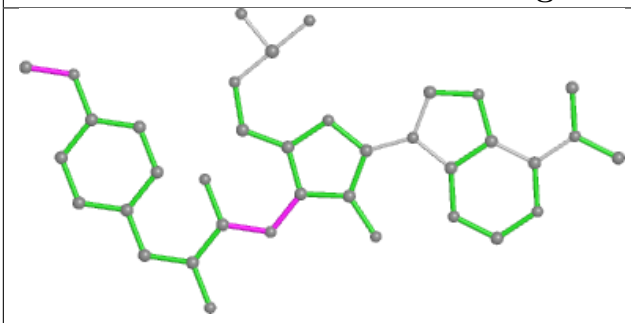
There are no ring outliers.

3 monomers are involved in 5 short contacts:

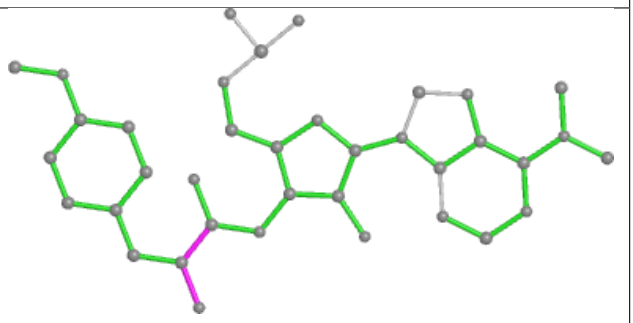
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	4	76	PPU	2	0
38	4	77	PHA	1	0
40	4	79	BTN	2	0

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.

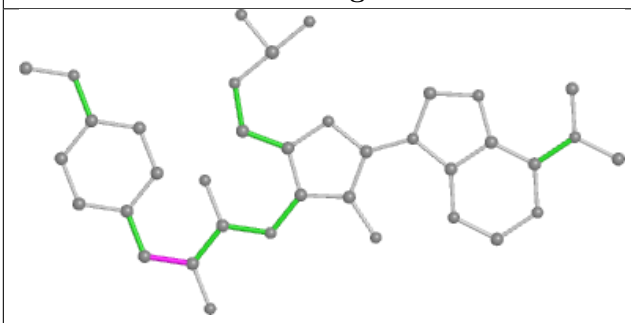
Ligand PPU 4 76



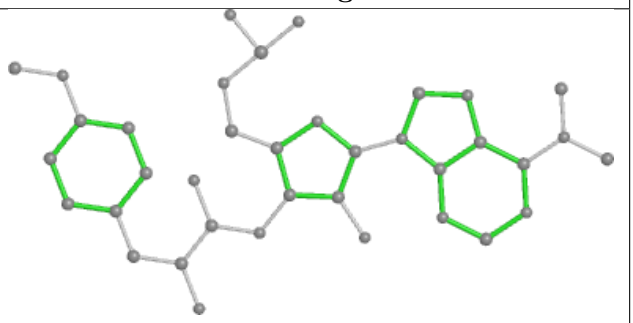
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	0	2754/2922 (94%)	-0.20	47 (1%) 70 49	11, 39, 86, 141	0
2	9	122/122 (100%)	0.25	6 (4%) 29 14	28, 60, 91, 145	0
3	3	3/3 (100%)	1.39	0 100 100	44, 44, 46, 52	3 (100%)
4	4	2/2 (100%)	0.06	0 100 100	48, 48, 48, 56	0
5	A	237/239 (99%)	-0.20	5 (2%) 63 43	21, 53, 94, 113	0
6	B	337/337 (100%)	-0.35	0 100 100	19, 45, 71, 81	0
7	C	246/246 (100%)	-0.41	1 (0%) 92 84	12, 37, 63, 71	0
8	D	140/176 (79%)	1.12	31 (22%) 0 0	55, 94, 120, 127	0
9	E	172/177 (97%)	0.16	2 (1%) 79 61	32, 56, 81, 87	0
10	F	119/119 (100%)	0.10	2 (1%) 70 49	41, 66, 94, 104	0
11	G	29/348 (8%)	1.50	4 (13%) 2 1	60, 79, 84, 89	0
12	H	156/167 (93%)	-0.05	1 (0%) 89 78	30, 48, 74, 81	0
13	I	142/145 (97%)	-0.43	0 100 100	26, 38, 60, 77	0
14	J	132/132 (100%)	-0.34	0 100 100	24, 44, 72, 76	0
15	K	145/164 (88%)	0.30	12 (8%) 11 4	16, 68, 97, 109	0
16	L	194/194 (100%)	0.02	19 (9%) 7 2	23, 39, 118, 128	0
17	M	186/186 (100%)	0.38	18 (9%) 7 2	36, 65, 109, 120	0
18	N	115/115 (100%)	-0.23	0 100 100	31, 47, 65, 69	0
19	O	143/148 (96%)	-0.08	1 (0%) 87 75	27, 47, 67, 77	0
20	P	95/95 (100%)	-0.29	1 (1%) 80 64	27, 40, 57, 79	0
21	Q	150/154 (97%)	-0.54	0 100 100	22, 35, 54, 65	0
22	R	81/84 (96%)	-0.04	2 (2%) 57 34	35, 53, 73, 80	0
23	S	119/119 (100%)	0.07	4 (3%) 45 24	33, 47, 75, 91	0
24	T	53/66 (80%)	2.97	35 (66%) 0 0	101, 113, 122, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	U	65/70 (92%)	0.66	6 (9%) 9 3	45, 69, 106, 112	0
26	V	154/154 (100%)	-0.43	0 100 100	25, 38, 56, 69	0
27	W	82/91 (90%)	0.14	3 (3%) 41 21	32, 49, 69, 89	0
28	X	142/240 (59%)	-0.30	1 (0%) 87 75	17, 36, 58, 77	0
29	Y	73/73 (100%)	3.95	49 (67%) 0 0	89, 118, 129, 133	0
30	Z	56/56 (100%)	-0.75	0 100 100	14, 26, 32, 39	0
31	1	46/48 (95%)	-0.04	0 100 100	23, 52, 84, 96	0
32	2	92/92 (100%)	7.24	92 (100%) 0 0	122, 136, 142, 146	0
All	All	6582/7284 (90%)	0.05	342 (5%) 27 12	11, 45, 105, 146	3 (0%)

The worst 5 of 342 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	2	37	ASP	17.0
32	2	78	HIS	16.8
32	2	82	GLY	16.6
32	2	11	CYS	14.1
29	Y	11	THR	13.3

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 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
35	NA	0	8329	1/1	0.23	0.56	62,62,62,62	0
35	NA	0	8384	1/1	0.34	1.15	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	Q	8386	1/1	0.42	0.79	62,62,62,62	0
35	NA	R	8312	1/1	0.54	0.64	84,84,84,84	0
33	MG	Y	8105	1/1	0.55	0.63	67,67,67,67	0
35	NA	0	8363	1/1	0.65	0.75	40,40,40,40	0
35	NA	0	8385	1/1	0.65	0.39	52,52,52,52	0
35	NA	9	8383	1/1	0.71	0.67	57,57,57,57	0
35	NA	0	8372	1/1	0.74	0.38	73,73,73,73	0
36	CL	2	8504	1/1	0.74	0.43	104,104,104,104	0
35	NA	0	8371	1/1	0.76	0.46	47,47,47,47	0
41	CD	2	8404	1/1	0.76	0.87	200,200,200,200	0
33	MG	0	8114	1/1	0.78	0.73	161,161,161,161	0
35	NA	0	8382	1/1	0.79	0.30	57,57,57,57	0
35	NA	9	8351	1/1	0.81	0.75	112,112,112,112	0
41	CD	T	8401	1/1	0.81	0.77	200,200,200,200	0
35	NA	0	8354	1/1	0.81	0.38	29,29,29,29	0
34	K	0	8202	1/1	0.83	0.46	69,69,69,69	0
35	NA	0	8377	1/1	0.83	0.28	59,59,59,59	0
35	NA	0	8326	1/1	0.83	0.26	38,38,38,38	0
33	MG	2	8078	1/1	0.83	0.42	73,73,73,73	0
33	MG	0	8076	1/1	0.84	0.18	70,70,70,70	0
35	NA	0	8332	1/1	0.84	0.39	57,57,57,57	0
35	NA	0	8352	1/1	0.84	0.26	28,28,28,28	0
36	CL	0	8522	1/1	0.85	0.37	76,76,76,76	0
36	CL	K	8510	1/1	0.85	0.23	70,70,70,70	0
35	NA	0	8373	1/1	0.85	0.23	51,51,51,51	0
33	MG	0	8102	1/1	0.85	1.14	135,135,135,135	0
35	NA	0	8365	1/1	0.85	0.30	42,42,42,42	0
33	MG	0	8024	1/1	0.86	0.69	109,109,109,109	0
35	NA	H	8322	1/1	0.86	0.25	48,48,48,48	0
41	CD	Y	8403	1/1	0.86	0.52	200,200,200,200	0
35	NA	0	8340	1/1	0.86	0.26	48,48,48,48	0
33	MG	0	8049	1/1	0.87	0.29	73,73,73,73	0
35	NA	Q	8337	1/1	0.88	0.18	41,41,41,41	0
35	NA	0	8324	1/1	0.88	0.18	39,39,39,39	0
40	BTN	4	79	15/16	0.88	0.32	91,104,104,105	0
35	NA	0	8369	1/1	0.89	0.36	67,67,67,67	0
35	NA	0	8328	1/1	0.89	0.49	41,41,41,41	0
35	NA	0	8331	1/1	0.89	0.34	69,69,69,69	0
35	NA	0	8310	1/1	0.90	0.31	16,16,16,16	0
33	MG	0	8051	1/1	0.90	0.17	70,70,70,70	0
35	NA	0	8364	1/1	0.90	0.26	47,47,47,47	0
36	CL	A	8509	1/1	0.90	0.25	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8306	1/1	0.90	0.67	21,21,21,21	0
35	NA	0	8374	1/1	0.91	0.52	49,49,49,49	0
33	MG	0	8111	1/1	0.91	0.10	49,49,49,49	0
35	NA	0	8311	1/1	0.91	0.14	38,38,38,38	0
38	PHA	4	77	11/11	0.91	0.27	64,67,71,71	0
35	NA	0	8358	1/1	0.91	0.30	98,98,98,98	0
35	NA	0	8333	1/1	0.91	0.12	25,25,25,25	0
36	CL	0	8515	1/1	0.91	0.69	72,72,72,72	0
33	MG	0	8116	1/1	0.91	0.10	64,64,64,64	0
35	NA	0	8307	1/1	0.92	0.23	40,40,40,40	0
35	NA	0	8308	1/1	0.92	0.22	44,44,44,44	0
33	MG	0	8046	1/1	0.92	0.09	40,40,40,40	0
35	NA	I	8346	1/1	0.92	0.09	20,20,20,20	0
35	NA	0	8366	1/1	0.92	0.17	20,20,20,20	0
35	NA	0	8368	1/1	0.92	0.13	41,41,41,41	0
41	CD	N	8405	1/1	0.92	0.06	111,111,111,111	0
33	MG	0	8103	1/1	0.92	0.20	34,34,34,34	0
33	MG	0	8101	1/1	0.92	0.12	40,40,40,40	0
36	CL	0	8517	1/1	0.92	0.23	57,57,57,57	0
33	MG	9	8095	1/1	0.93	0.14	72,72,72,72	0
36	CL	M	8507	1/1	0.93	0.15	54,54,54,54	0
35	NA	0	8355	1/1	0.93	0.60	60,60,60,60	0
35	NA	0	8336	1/1	0.93	0.08	30,30,30,30	0
36	CL	0	8503	1/1	0.93	0.18	49,49,49,49	0
33	MG	0	8055	1/1	0.93	0.11	82,82,82,82	0
35	NA	0	8379	1/1	0.93	0.23	25,25,25,25	0
33	MG	0	8053	1/1	0.93	0.20	38,38,38,38	0
35	NA	P	8348	1/1	0.93	0.13	45,45,45,45	0
35	NA	0	8314	1/1	0.94	0.16	33,33,33,33	0
33	MG	0	8104	1/1	0.94	0.16	41,41,41,41	0
33	MG	0	8092	1/1	0.94	0.34	71,71,71,71	0
35	NA	0	8357	1/1	0.94	0.11	53,53,53,53	0
35	NA	0	8301	1/1	0.94	0.11	28,28,28,28	0
35	NA	0	8303	1/1	0.94	0.17	33,33,33,33	0
33	MG	0	8099	1/1	0.94	0.18	37,37,37,37	0
33	MG	0	8115	1/1	0.94	0.11	58,58,58,58	0
33	MG	0	8066	1/1	0.94	0.14	60,60,60,60	0
33	MG	0	8082	1/1	0.94	0.13	43,43,43,43	0
35	NA	0	8339	1/1	0.94	0.13	8,8,8,8	0
33	MG	0	8087	1/1	0.94	0.10	36,36,36,36	0
35	NA	0	8341	1/1	0.94	0.14	40,40,40,40	0
35	NA	0	8350	1/1	0.94	0.41	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8378	1/1	0.95	0.18	31,31,31,31	0
36	CL	0	8505	1/1	0.95	0.34	57,57,57,57	0
36	CL	0	8513	1/1	0.95	0.11	52,52,52,52	0
35	NA	0	8362	1/1	0.95	0.27	63,63,63,63	0
35	NA	0	8381	1/1	0.95	0.23	71,71,71,71	0
33	MG	S	8073	1/1	0.95	0.20	36,36,36,36	0
33	MG	0	8088	1/1	0.95	0.09	23,23,23,23	0
36	CL	I	8502	1/1	0.95	0.10	56,56,56,56	0
36	CL	I	8521	1/1	0.95	0.13	39,39,39,39	0
33	MG	0	8106	1/1	0.95	0.09	64,64,64,64	0
33	MG	0	8067	1/1	0.95	0.15	31,31,31,31	0
36	CL	X	8520	1/1	0.95	0.13	35,35,35,35	0
33	MG	0	8041	1/1	0.95	0.29	50,50,50,50	0
35	NA	0	8302	1/1	0.95	0.12	18,18,18,18	0
39	ACA	4	78	8/9	0.95	0.24	67,73,85,88	0
33	MG	0	8059	1/1	0.95	0.13	59,59,59,59	0
33	MG	0	8086	1/1	0.95	0.10	41,41,41,41	0
35	NA	0	8356	1/1	0.95	0.64	59,59,59,59	0
33	MG	0	8050	1/1	0.95	0.22	78,78,78,78	0
33	MG	A	8065	1/1	0.95	0.09	44,44,44,44	0
35	NA	0	8309	1/1	0.96	0.11	24,24,24,24	0
36	CL	0	8511	1/1	0.96	0.22	63,63,63,63	0
34	K	0	8201	1/1	0.96	0.65	80,80,80,80	0
35	NA	0	8360	1/1	0.96	0.65	39,39,39,39	0
36	CL	0	8516	1/1	0.96	0.18	44,44,44,44	0
33	MG	0	8043	1/1	0.96	0.07	34,34,34,34	0
33	MG	0	8058	1/1	0.96	0.06	28,28,28,28	0
35	NA	0	8319	1/1	0.96	0.09	50,50,50,50	0
36	CL	B	8519	1/1	0.96	0.24	51,51,51,51	0
33	MG	0	8100	1/1	0.96	0.10	65,65,65,65	0
35	NA	0	8342	1/1	0.96	0.22	19,19,19,19	0
35	NA	0	8367	1/1	0.96	0.19	36,36,36,36	0
36	CL	L	8518	1/1	0.96	0.12	36,36,36,36	0
35	NA	C	8304	1/1	0.96	0.15	25,25,25,25	0
36	CL	N	8508	1/1	0.96	0.31	82,82,82,82	0
35	NA	0	8349	1/1	0.96	0.14	37,37,37,37	0
35	NA	0	8325	1/1	0.96	0.37	29,29,29,29	0
37	PPU	4	76	37/38	0.96	0.21	48,55,62,63	0
35	NA	K	8380	1/1	0.96	0.17	69,69,69,69	0
35	NA	L	8347	1/1	0.96	0.10	7,7,7,7	0
35	NA	0	8370	1/1	0.96	0.28	48,48,48,48	0
33	MG	0	8074	1/1	0.96	0.05	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	8112	1/1	0.96	0.11	34,34,34,34	0
33	MG	0	8113	1/1	0.96	0.20	36,36,36,36	0
33	MG	0	8025	1/1	0.96	0.08	17,17,17,17	0
35	NA	0	8327	1/1	0.97	0.13	16,16,16,16	0
33	MG	0	8090	1/1	0.97	0.11	65,65,65,65	0
33	MG	0	8036	1/1	0.97	0.10	32,32,32,32	0
33	MG	0	8071	1/1	0.97	0.08	66,66,66,66	0
35	NA	0	8361	1/1	0.97	0.45	40,40,40,40	0
33	MG	0	8072	1/1	0.97	0.10	43,43,43,43	0
33	MG	0	8052	1/1	0.97	0.13	36,36,36,36	0
35	NA	0	8334	1/1	0.97	0.12	29,29,29,29	0
35	NA	A	8345	1/1	0.97	0.11	40,40,40,40	0
33	MG	0	8075	1/1	0.97	0.06	50,50,50,50	0
33	MG	0	8016	1/1	0.97	0.09	25,25,25,25	0
33	MG	0	8008	1/1	0.97	0.06	42,42,42,42	0
35	NA	0	8316	1/1	0.97	0.19	28,28,28,28	0
35	NA	0	8317	1/1	0.97	0.10	23,23,23,23	0
35	NA	0	8344	1/1	0.97	0.06	9,9,9,9	0
33	MG	0	8085	1/1	0.97	0.29	103,103,103,103	0
35	NA	0	8321	1/1	0.97	0.33	58,58,58,58	0
33	MG	0	8010	1/1	0.97	0.05	20,20,20,20	0
33	MG	0	8027	1/1	0.97	0.05	37,37,37,37	0
35	NA	0	8375	1/1	0.97	0.20	40,40,40,40	0
35	NA	0	8376	1/1	0.97	0.23	50,50,50,50	0
33	MG	0	8028	1/1	0.97	0.06	23,23,23,23	0
33	MG	0	8108	1/1	0.98	0.06	61,61,61,61	0
35	NA	0	8330	1/1	0.98	0.19	21,21,21,21	0
33	MG	0	8110	1/1	0.98	0.10	22,22,22,22	0
33	MG	0	8064	1/1	0.98	0.28	17,17,17,17	0
33	MG	0	8040	1/1	0.98	0.09	107,107,107,107	0
33	MG	0	8015	1/1	0.98	0.07	29,29,29,29	0
35	NA	0	8335	1/1	0.98	0.14	47,47,47,47	0
33	MG	0	8068	1/1	0.98	0.07	58,58,58,58	0
33	MG	0	8070	1/1	0.98	0.43	71,71,71,71	0
33	MG	0	8042	1/1	0.98	0.14	40,40,40,40	0
33	MG	0	8006	1/1	0.98	0.09	28,28,28,28	0
33	MG	0	8044	1/1	0.98	0.15	35,35,35,35	0
35	NA	0	8343	1/1	0.98	0.07	17,17,17,17	0
33	MG	J	8069	1/1	0.98	0.08	47,47,47,47	0
33	MG	0	8045	1/1	0.98	0.10	44,44,44,44	0
33	MG	0	8018	1/1	0.98	0.04	32,32,32,32	0
33	MG	0	8081	1/1	0.98	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8353	1/1	0.98	0.07	34,34,34,34	0
33	MG	0	8047	1/1	0.98	0.10	48,48,48,48	0
33	MG	0	8084	1/1	0.98	0.07	38,38,38,38	0
33	MG	0	8048	1/1	0.98	0.08	34,34,34,34	0
36	CL	0	8514	1/1	0.98	0.11	44,44,44,44	0
33	MG	0	8021	1/1	0.98	0.09	26,26,26,26	0
33	MG	0	8022	1/1	0.98	0.05	30,30,30,30	0
35	NA	0	8359	1/1	0.98	0.18	42,42,42,42	0
33	MG	0	8003	1/1	0.98	0.08	22,22,22,22	0
33	MG	0	8089	1/1	0.98	0.12	50,50,50,50	0
33	MG	0	8004	1/1	0.98	0.06	30,30,30,30	0
36	CL	I	8501	1/1	0.98	0.13	60,60,60,60	0
33	MG	0	8091	1/1	0.98	0.06	40,40,40,40	0
33	MG	0	8011	1/1	0.98	0.20	1,1,1,1	0
33	MG	0	8094	1/1	0.98	0.06	54,54,54,54	0
33	MG	0	8096	1/1	0.98	0.05	33,33,33,33	0
35	NA	0	8315	1/1	0.98	0.15	32,32,32,32	0
33	MG	0	8097	1/1	0.98	0.14	30,30,30,30	0
33	MG	0	8098	1/1	0.98	0.29	24,24,24,24	0
33	MG	0	8013	1/1	0.98	0.08	25,25,25,25	0
35	NA	0	8320	1/1	0.98	0.07	15,15,15,15	0
33	MG	0	8056	1/1	0.98	0.06	35,35,35,35	0
35	NA	0	8323	1/1	0.98	0.25	34,34,34,34	0
33	MG	0	8057	1/1	0.98	0.11	30,30,30,30	0
33	MG	0	8035	1/1	0.98	0.05	39,39,39,39	0
33	MG	0	8014	1/1	0.98	0.07	22,22,22,22	0
33	MG	0	8060	1/1	0.98	0.07	32,32,32,32	0
33	MG	0	8062	1/1	0.98	0.04	37,37,37,37	0
33	MG	0	8054	1/1	0.99	0.05	28,28,28,28	0
33	MG	0	8083	1/1	0.99	0.05	38,38,38,38	0
33	MG	0	8012	1/1	0.99	0.08	26,26,26,26	0
33	MG	0	8037	1/1	0.99	0.05	34,34,34,34	0
33	MG	0	8038	1/1	0.99	0.04	23,23,23,23	0
33	MG	0	8117	1/1	0.99	0.09	19,19,19,19	0
33	MG	0	8039	1/1	0.99	0.06	31,31,31,31	0
36	CL	0	8512	1/1	0.99	0.10	34,34,34,34	0
33	MG	0	8007	1/1	0.99	0.05	18,18,18,18	0
33	MG	0	8023	1/1	0.99	0.07	28,28,28,28	0
33	MG	0	8061	1/1	0.99	0.07	28,28,28,28	0
33	MG	X	8109	1/1	0.99	0.20	35,35,35,35	0
33	MG	0	8002	1/1	0.99	0.05	33,33,33,33	0
33	MG	0	8063	1/1	0.99	0.06	68,68,68,68	0

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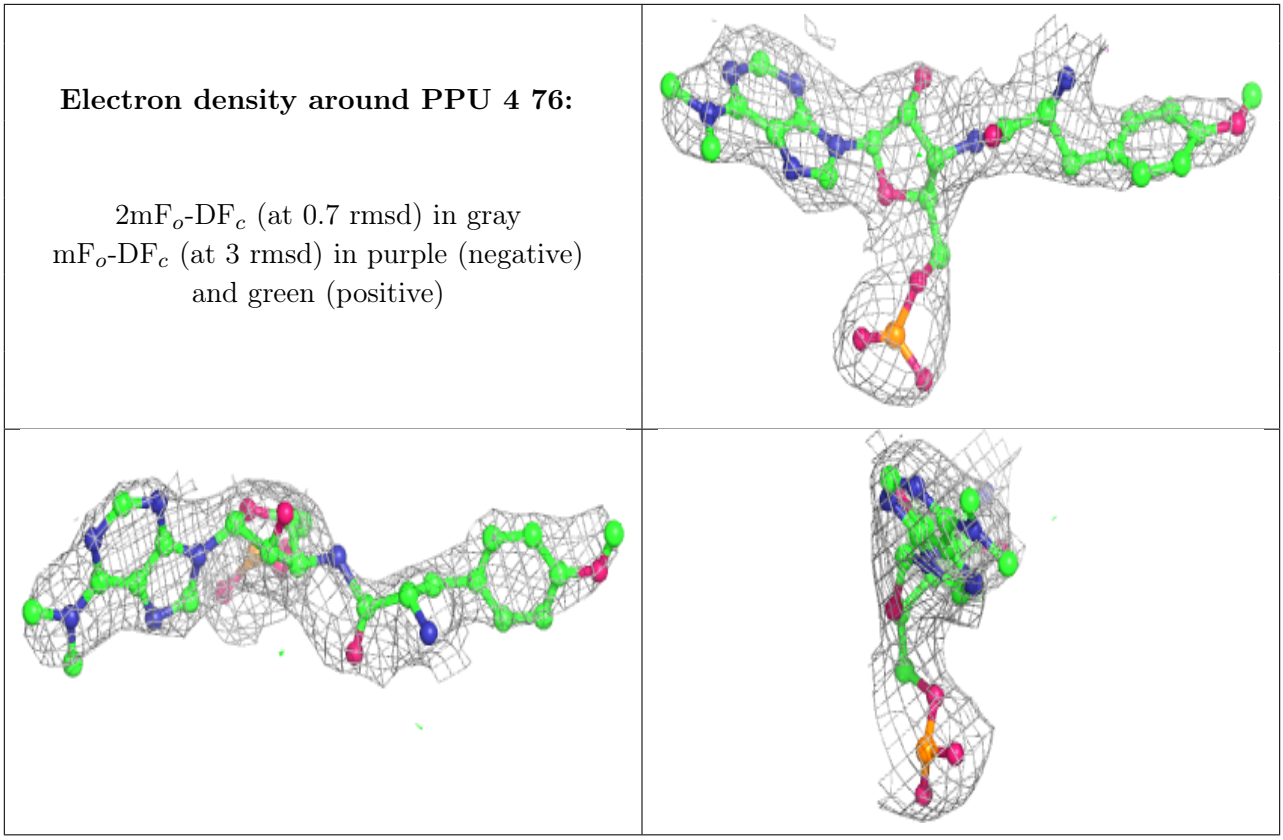
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	8093	1/1	0.99	0.07	43,43,43,43	0
33	MG	0	8009	1/1	0.99	0.04	18,18,18,18	0
33	MG	0	8026	1/1	0.99	0.08	25,25,25,25	0
33	MG	0	8005	1/1	0.99	0.05	26,26,26,26	0
33	MG	0	8017	1/1	0.99	0.03	15,15,15,15	0
35	NA	0	8305	1/1	0.99	0.10	19,19,19,19	0
33	MG	0	8029	1/1	0.99	0.05	23,23,23,23	0
33	MG	0	8030	1/1	0.99	0.11	29,29,29,29	0
33	MG	0	8031	1/1	0.99	0.03	18,18,18,18	0
36	CL	Q	8506	1/1	0.99	0.11	43,43,43,43	0
33	MG	0	8032	1/1	0.99	0.06	29,29,29,29	0
33	MG	0	8033	1/1	0.99	0.10	18,18,18,18	0
33	MG	0	8034	1/1	0.99	0.03	22,22,22,22	0
35	NA	0	8313	1/1	0.99	0.17	59,59,59,59	0
33	MG	0	8077	1/1	0.99	0.06	21,21,21,21	0
33	MG	0	8107	1/1	0.99	0.03	24,24,24,24	0
33	MG	0	8079	1/1	0.99	0.05	27,27,27,27	0
33	MG	0	8080	1/1	0.99	0.06	42,42,42,42	0
35	NA	0	8318	1/1	0.99	0.08	22,22,22,22	0
33	MG	0	8001	1/1	0.99	0.07	21,21,21,21	0
35	NA	Q	8338	1/1	1.00	0.06	57,57,57,57	0
33	MG	0	8019	1/1	1.00	0.03	13,13,13,13	0
41	CD	Z	8402	1/1	1.00	0.06	49,49,49,49	0
33	MG	0	8020	1/1	1.00	0.07	16,16,16,16	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 4 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.