



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 05:00 AM UTC

PDB ID : 1KQS / pdb_00001kqs
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

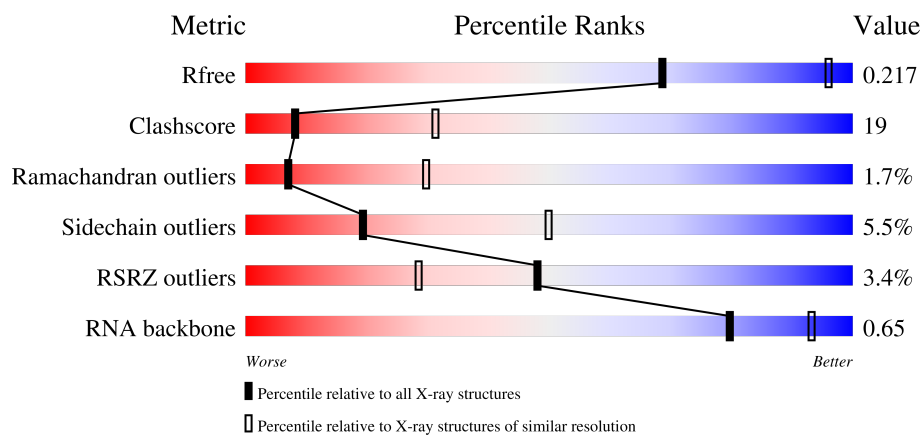
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



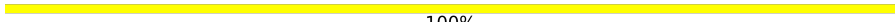
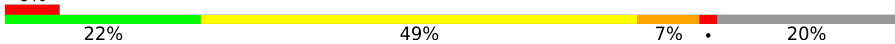
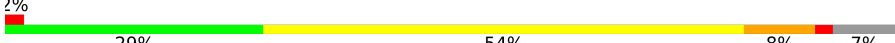
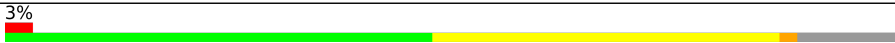
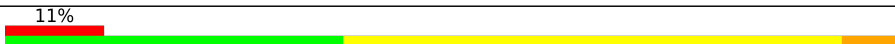
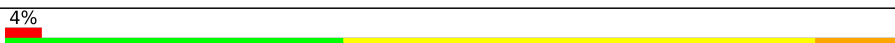
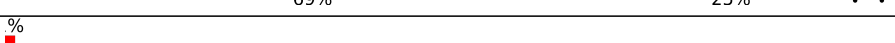
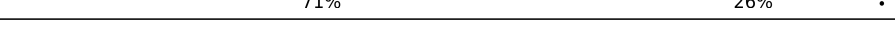
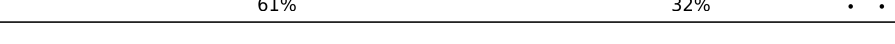
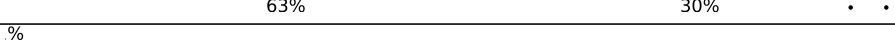
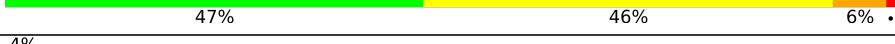
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	57% 31% 5% • 6%
2	9	122	52% 38% 8% •
3	3	3	100% 33% 33% 33%

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Mol	Chain	Length	Quality of chain
4	4	2	 100%
5	A	239	 2% 53% 40% 6%
6	B	337	 50% 44% 6%
7	C	246	 51% 43% 7%
8	D	176	 6% 22% 49% 7% 20%
9	E	177	 55% 40% 5%
10	F	119	 57% 40% 3%
11	G	348	 5% 92%
12	H	167	 2% 29% 54% 8% 7%
13	I	145	 60% 32% 6%
14	J	132	 61% 37% 2%
15	K	164	 3% 48% 39% 12%
16	L	194	 11% 38% 56% 6%
17	M	186	 4% 38% 53% 9%
18	N	115	 62% 36% 2%
19	O	148	 69% 25% 6%
20	P	95	 71% 26% 3%
21	Q	154	 61% 32% 7%
22	R	84	 63% 30% 7%
23	S	119	 49% 47% 4%
24	T	66	 18% 36% 41% 20%
25	U	70	 4% 39% 50% 7%
26	V	154	 47% 46% 6%
27	W	91	 4% 42% 41% 8% 10%
28	X	240	 39% 17% 44%

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Mol	Chain	Length	Quality of chain
29	Y	73	49% 27% 64% 7%
30	Z	56	66% 32%
31	1	48	65% 29%
32	2	92	63% 41% 49% 9%

2 Entry composition

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
1	0	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

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
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called CCA.

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

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

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L2.

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

- 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	S	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	S	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 (CCD ID: 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 (CCD ID: K) (formula: K).

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

- Molecule 35 is SODIUM ION (CCD ID: 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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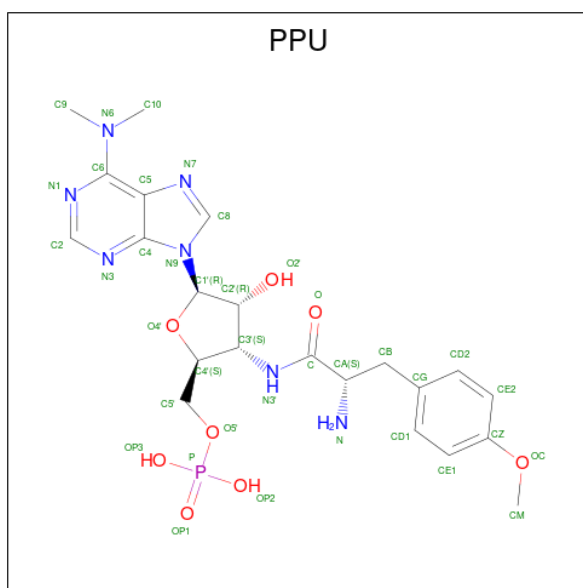
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	C	1	Total 1	Na 1	0	0
35	H	1	Total 1	Na 1	0	0
35	I	1	Total 1	Na 1	0	0
35	K	1	Total 1	Na 1	0	0
35	L	1	Total 1	Na 1	0	0
35	P	1	Total 1	Na 1	0	0
35	Q	3	Total 3	Na 3	0	0
35	R	1	Total 1	Na 1	0	0

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

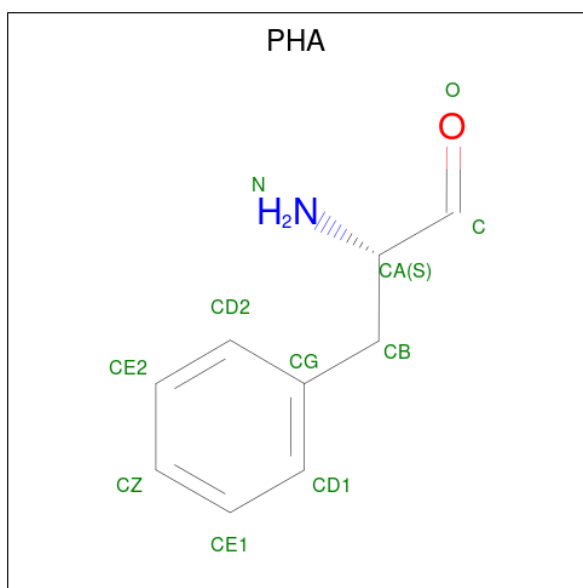
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	0	0
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	I	3	Total 3	Cl 3	0	0
36	K	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	Q	1	Total 1	Cl 1	0	0
36	X	1	Total 1	Cl 1	0	0
36	2	1	Total 1	Cl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

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



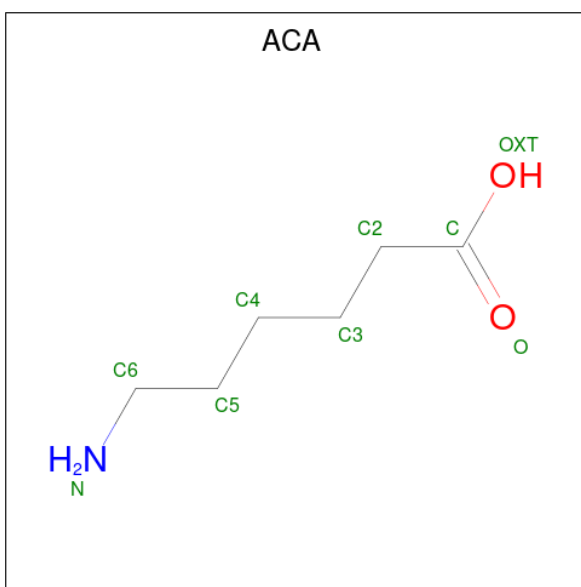
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	4	1	Total	C	N	O	P	0	0
			37	22	7	7	1		

- Molecule 38 is PHENYLALANINAL (CCD ID: PHA) (formula: $C_9H_{11}NO$).



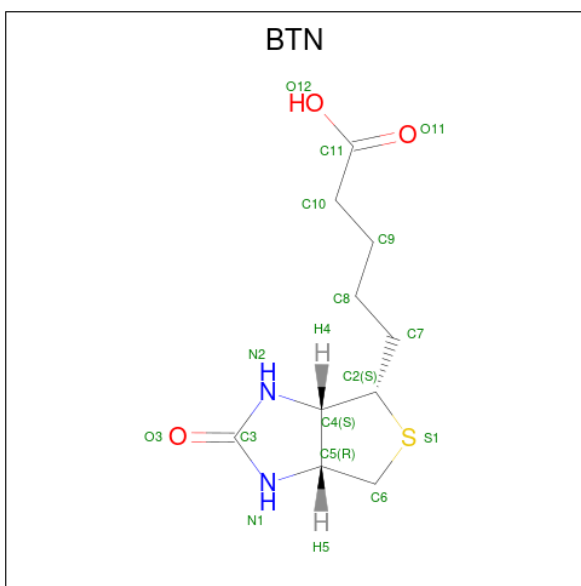
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	4	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 39 is 6-AMINOHEXANOIC ACID (CCD ID: ACA) (formula: $C_6H_{13}NO_2$).



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

- Molecule 40 is BIOTIN (CCD ID: BTN) (formula: C₁₀H₁₆N₂O₃S).



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

- Molecule 41 is CADMIUM ION (CCD ID: 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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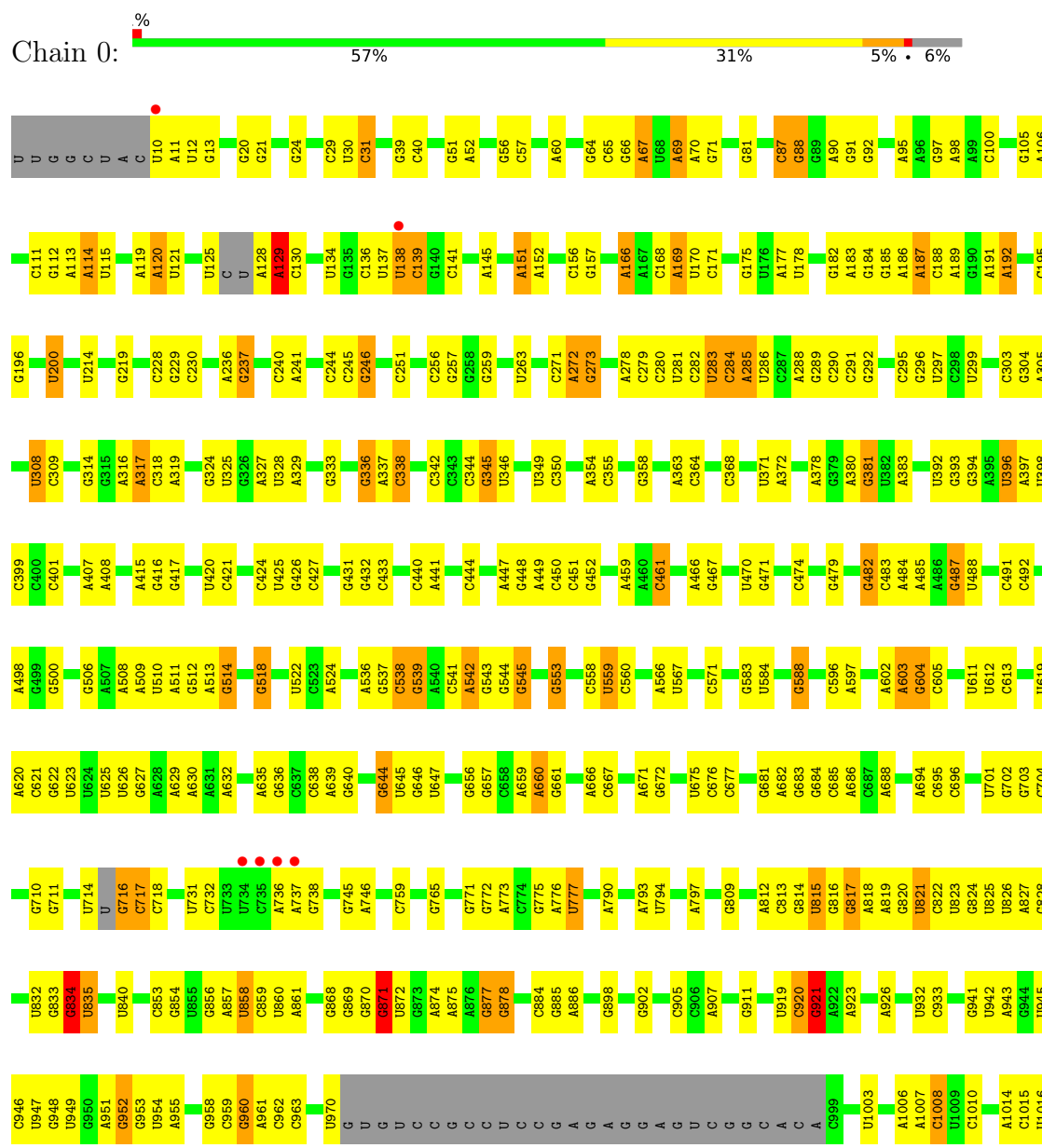
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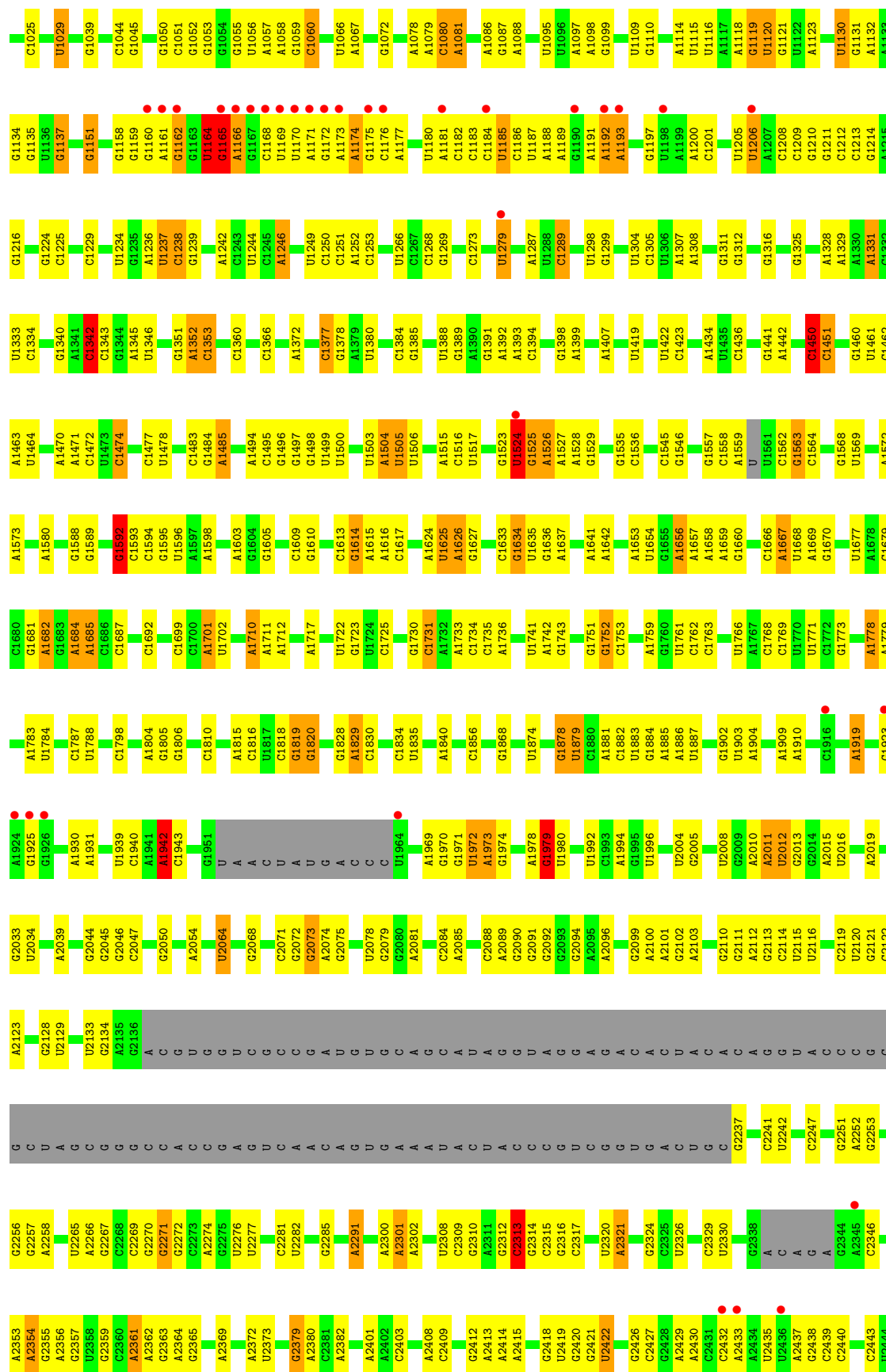
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	L	138	Total 138	O 138	0	0
42	M	70	Total 70	O 70	0	0
42	N	42	Total 42	O 42	0	0
42	O	67	Total 67	O 67	0	0
42	P	56	Total 56	O 56	0	0
42	Q	87	Total 87	O 87	0	0
42	R	36	Total 36	O 36	0	0
42	S	37	Total 37	O 37	0	0
42	T	26	Total 26	O 26	0	0
42	U	16	Total 16	O 16	0	0
42	V	66	Total 66	O 66	0	0
42	W	30	Total 30	O 30	0	0
42	X	96	Total 96	O 96	0	0
42	Y	33	Total 33	O 33	0	0
42	Z	55	Total 55	O 55	0	0
42	1	42	Total 42	O 42	0	0
42	2	76	Total 76	O 76	0	0

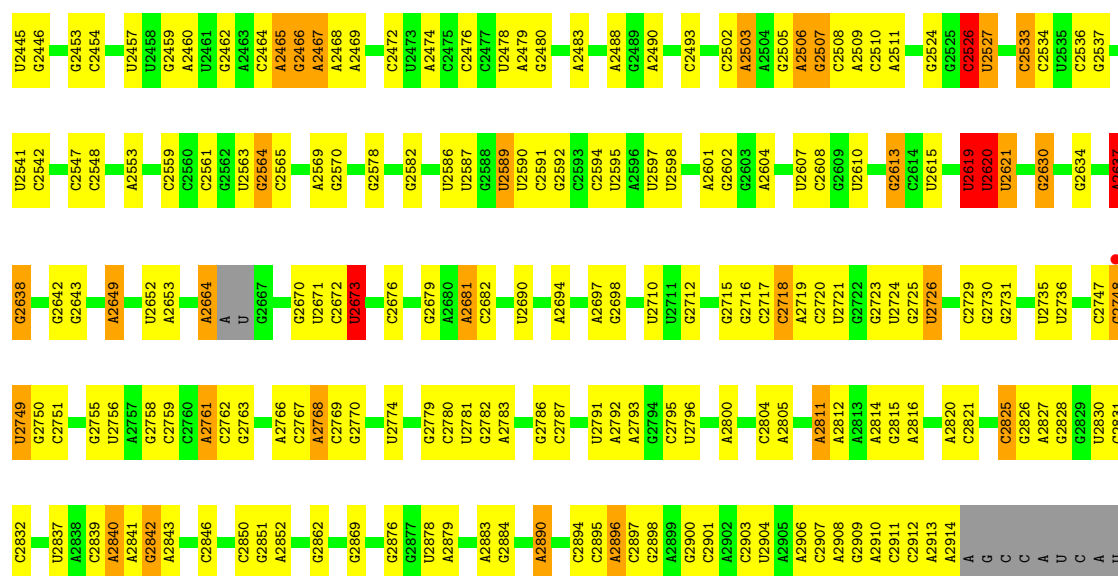
3 Residue-property plots

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.

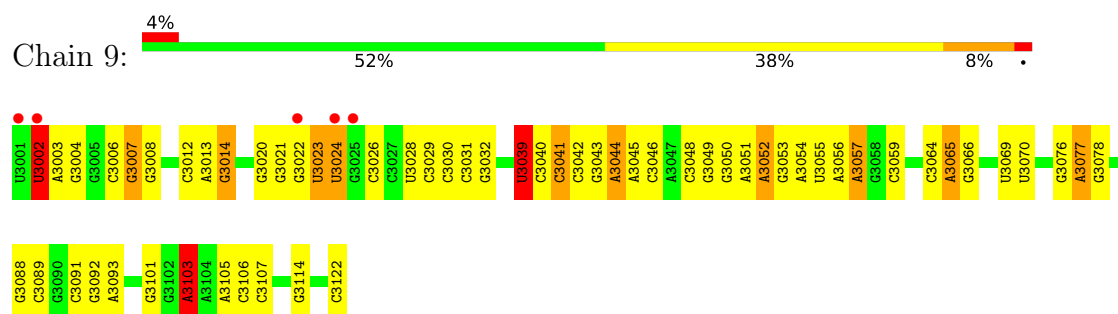
• Molecule 1: 23S rRNA



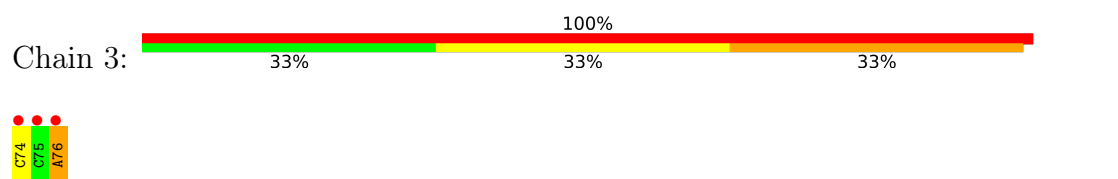




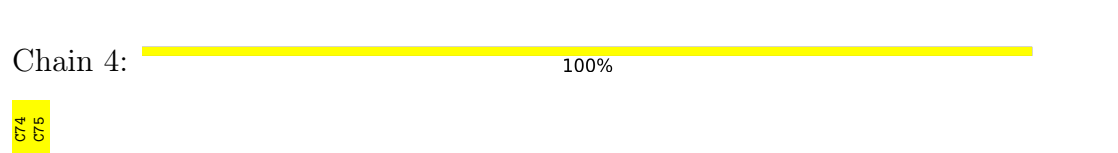
• Molecule 2: 5S RRNA



• Molecule 3: CCA

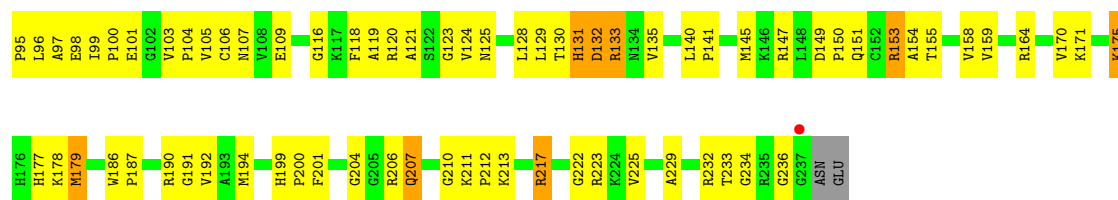


• Molecule 4: CC-Pmn-pcb



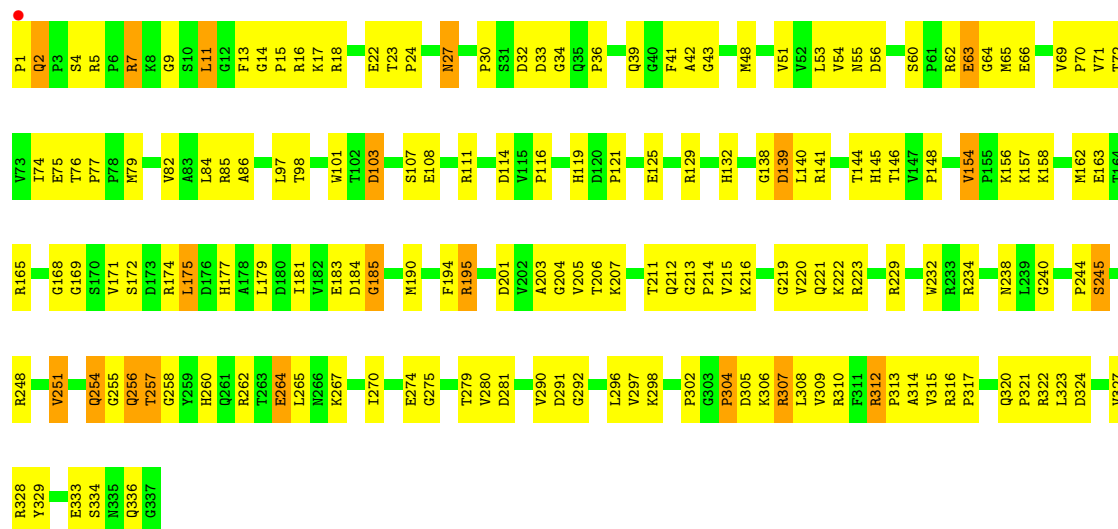
• Molecule 5: RIBOSOMAL PROTEIN L2





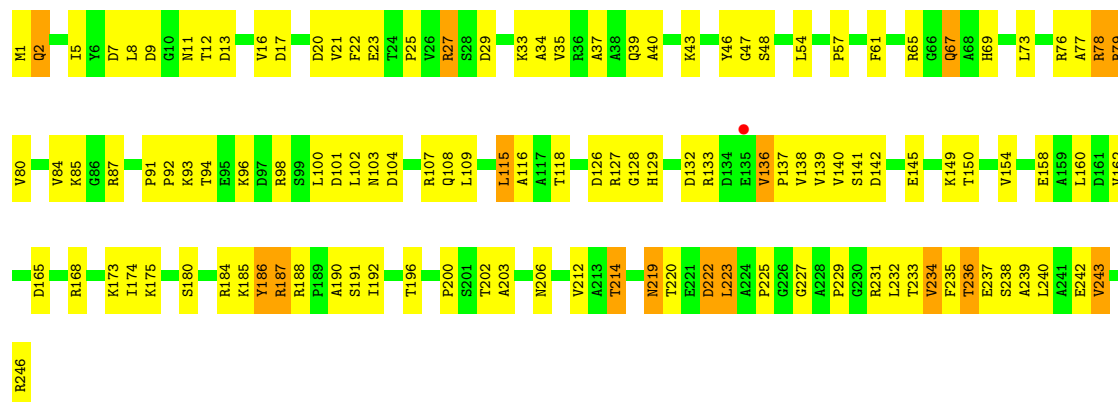
• Molecule 6: RIBOSOMAL PROTEIN L3

Chain B: 50% 44% 6%



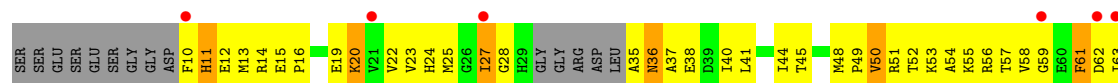
• Molecule 7: RIBOSOMAL PROTEIN L4

Chain C: 51% 43% 7%



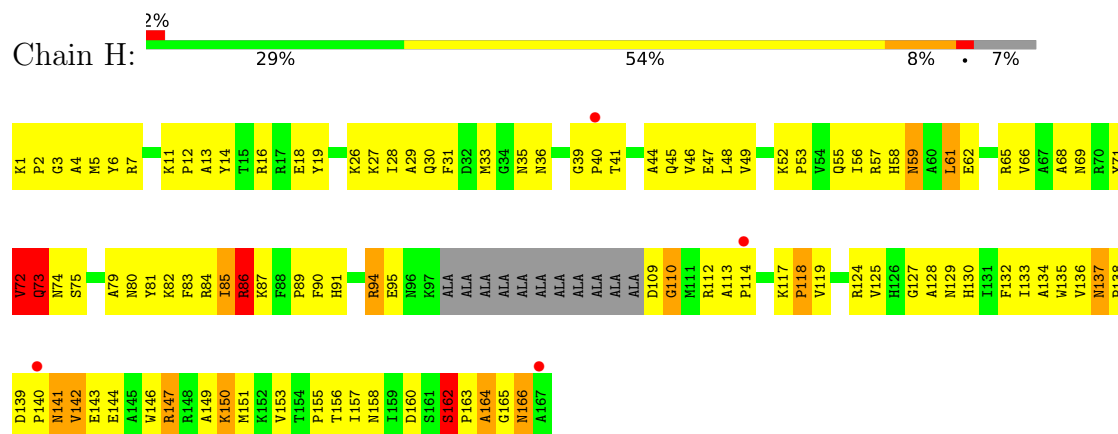
• Molecule 8: RIBOSOMAL PROTEIN L5

Chain D: 6% 22% 49% 7% 20%

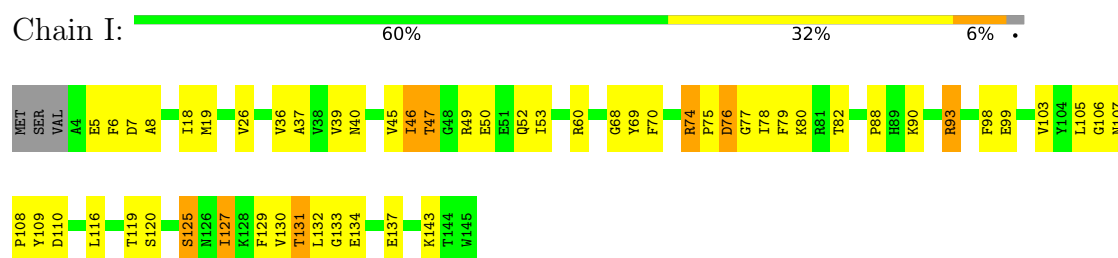




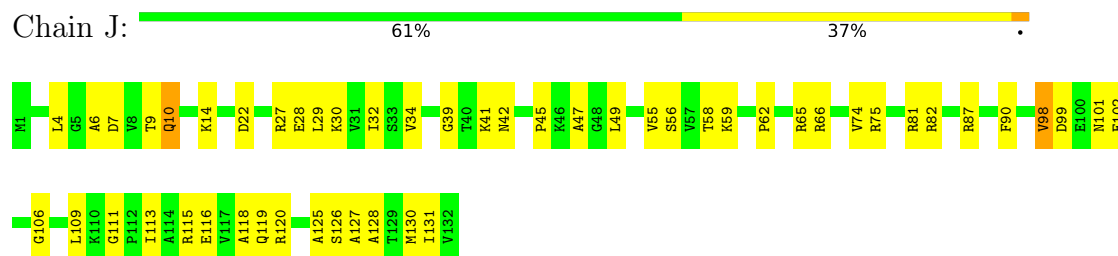
• Molecule 12: RIBOSOMAL PROTEIN L10E



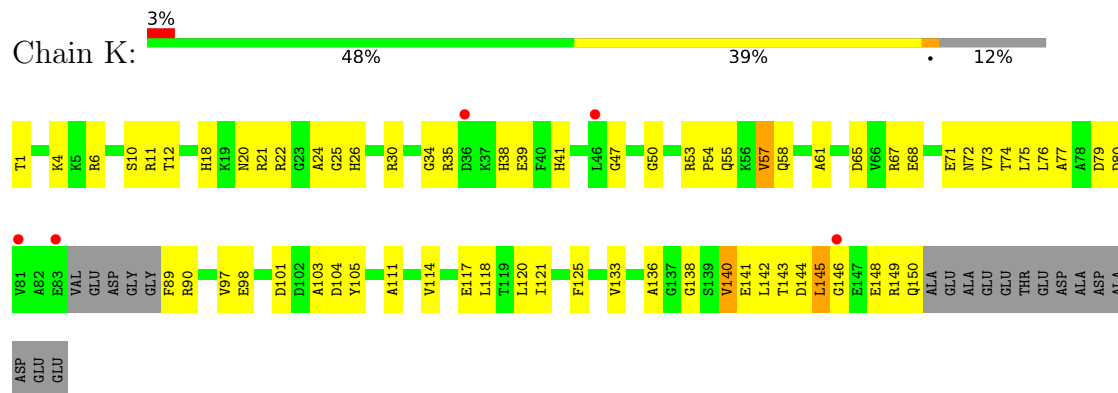
• Molecule 13: RIBOSOMAL PROTEIN L13



• Molecule 14: RIBOSOMAL PROTEIN L14

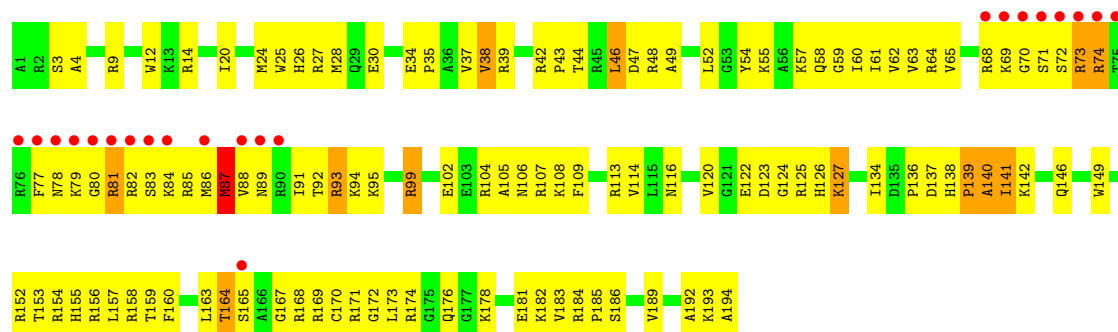


• Molecule 15: RIBOSOMAL PROTEIN L15

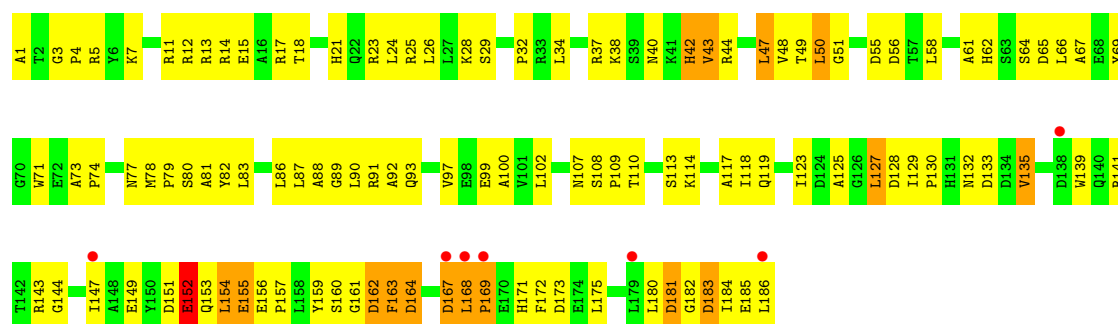


• Molecule 16: RIBOSOMAL PROTEIN L15E

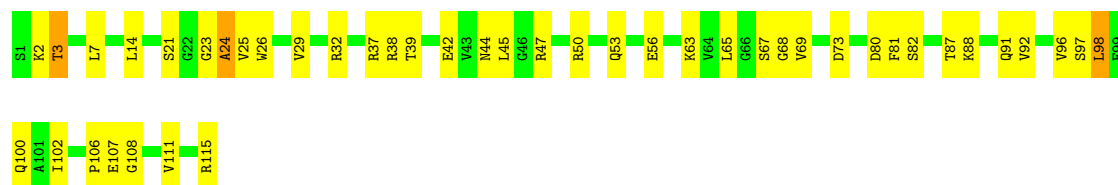




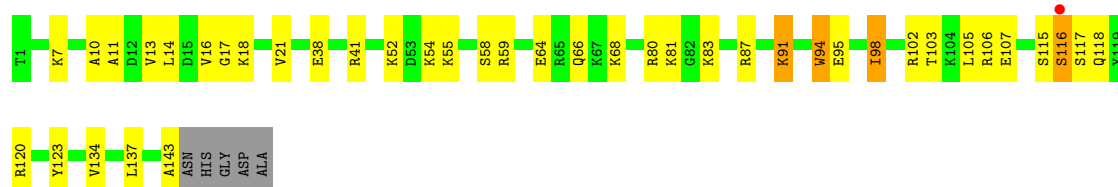
• Molecule 17: RIBOSOMAL PROTEIN L18



• Molecule 18: RIBOSOMAL PROTEIN L18E



• Molecule 19: RIBOSOMAL PROTEIN L19E

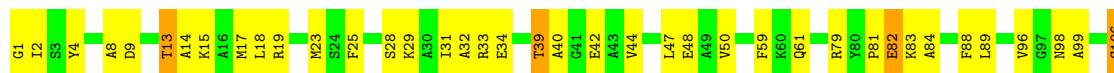


• Molecule 20: RIBOSOMAL PROTEIN L21E

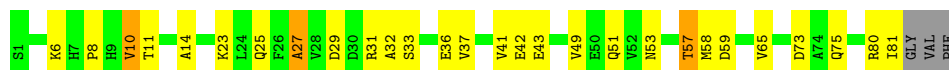




• Molecule 21: RIBOSOMAL PROTEIN L22



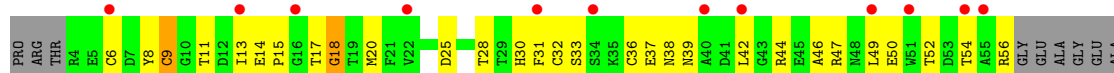
• Molecule 22: RIBOSOMAL PROTEIN L23



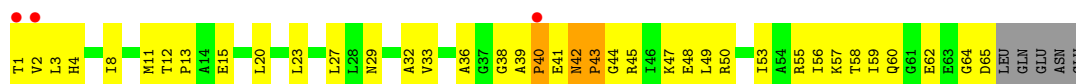
• Molecule 23: RIBOSOMAL PROTEIN L24



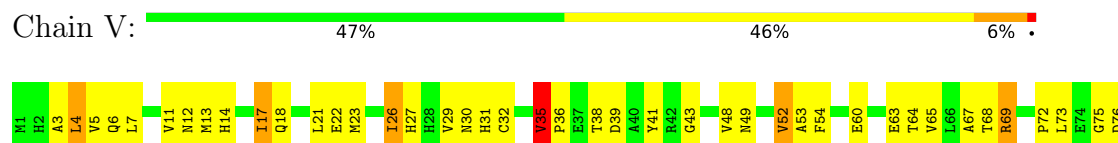
• Molecule 24: RIBOSOMAL PROTEIN L24E



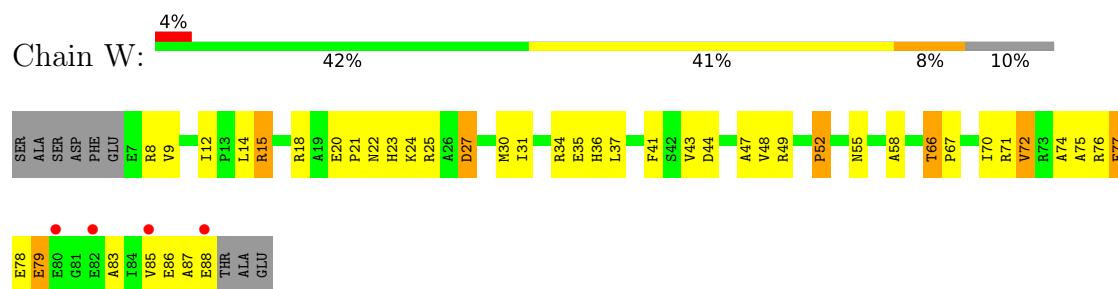
• Molecule 25: RIBOSOMAL PROTEIN L29



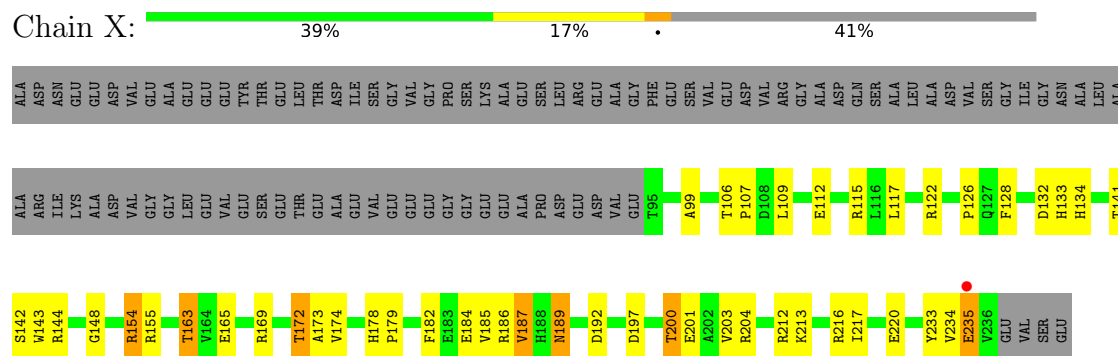
• Molecule 26: RIBOSOMAL PROTEIN L30



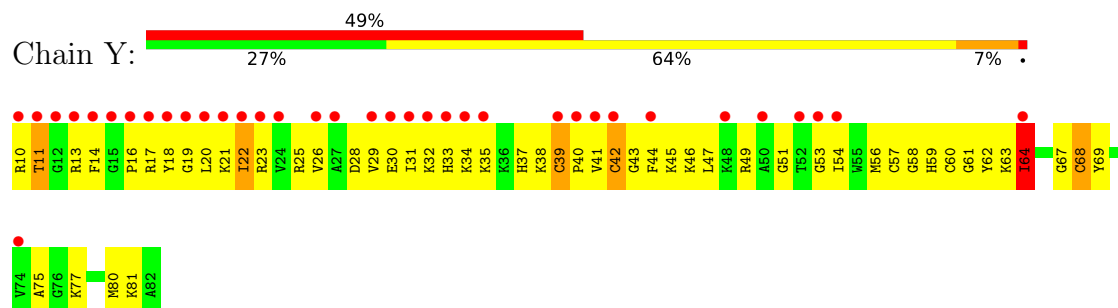
• Molecule 27: RIBOSOMAL PROTEIN L31E



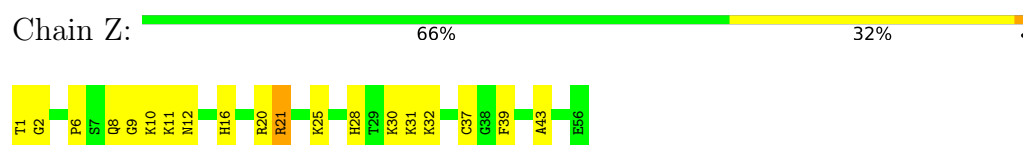
• Molecule 28: RIBOSOMAL PROTEIN L32E



• Molecule 29: RIBOSOMAL PROTEIN L37Ae



• Molecule 30: RIBOSOMAL PROTEIN L37E



• Molecule 31: RIBOSOMAL PROTEIN L39E

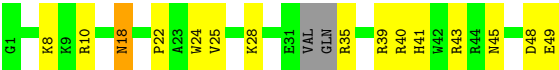
Chain 1:

65%

29%

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● Molecule 32: RIBOSOMAL PROTEIN L44E

Chain 2:

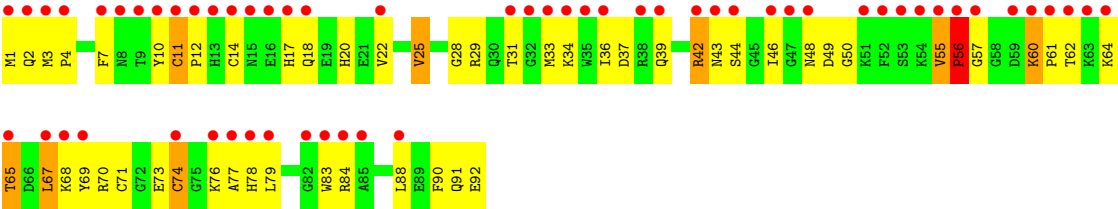
63%

41%

49%

9%

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4 Data and refinement statistics

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 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.10) 95.9 (20.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.173 , 0.220 0.172 , 0.217	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)	0.31 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PPU, CD, CL, K, MG, ACA, BTN, PHA

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	0.40	2/66076 (0.0%)	0.63	37/103052 (0.0%)
2	9	0.41	0/2905	0.67	4/4528 (0.1%)
3	3	0.68	0/65	1.13	0/99
4	4	0.36	0/40	0.64	0/60
5	A	0.45	0/1787	1.01	9/2409 (0.4%)
6	B	0.45	0/2689	1.02	9/3652 (0.2%)
7	C	0.51	0/1883	0.99	8/2551 (0.3%)
8	D	0.38	0/1111	0.94	7/1498 (0.5%)
9	E	0.43	0/1382	0.89	2/1880 (0.1%)
10	F	0.40	0/896	0.88	2/1219 (0.2%)
11	G	0.40	0/241	0.79	0/324
12	H	0.49	0/1246	1.24	14/1686 (0.8%)
13	I	0.46	0/1135	0.96	3/1530 (0.2%)
14	J	0.42	0/1003	1.01	2/1351 (0.1%)
15	K	0.39	0/1126	1.01	5/1504 (0.3%)
16	L	0.52	0/1633	1.07	8/2180 (0.4%)
17	M	0.38	0/1473	1.10	16/1999 (0.8%)
18	N	0.47	0/873	0.97	5/1181 (0.4%)
19	O	0.45	0/1143	0.86	0/1521
20	P	0.44	0/748	1.03	5/1005 (0.5%)
21	Q	0.47	0/1172	0.97	5/1578 (0.3%)
22	R	0.41	0/648	0.90	2/875 (0.2%)
23	S	0.43	0/957	0.97	3/1289 (0.2%)
24	T	0.37	0/417	0.88	1/562 (0.2%)
25	U	0.40	0/502	0.99	2/675 (0.3%)
26	V	0.51	0/1218	1.03	8/1655 (0.5%)
27	W	0.46	0/664	0.99	2/895 (0.2%)
28	X	0.49	0/1146	0.97	2/1536 (0.1%)
29	Y	0.40	0/575	1.01	3/763 (0.4%)
30	Z	0.48	0/437	0.97	2/578 (0.3%)
31	1	0.40	0/398	0.76	0/527
32	2	0.42	0/771	0.95	7/1024 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.41	2/98360 (0.0%)	0.75	173/147186 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	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'	-7.30	1.31	1.42
1	0	2620	U	C2'-O2'	5.77	1.50	1.41

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	13.73	130.09	109.50
16	L	141	ILE	N-CA-C	-13.57	100.91	111.90
12	H	141	ASN	N-CA-C	-13.49	96.91	113.50
1	0	1979	G	C2'-C3'-O3'	12.99	128.98	109.50
12	H	74	ASN	N-CA-C	-11.86	95.15	113.89

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 ⓘ

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	988	0
2	9	2600	0	1326	69	0
3	3	59	0	35	4	0
4	4	37	0	23	5	0
5	A	1754	0	1763	134	0
6	B	2624	0	2533	173	0
7	C	1858	0	1816	135	0
8	D	1094	0	1085	136	0
9	E	1357	0	1266	85	0
10	F	885	0	854	66	0
11	G	240	0	231	21	0
12	H	1215	0	1215	166	0
13	I	1119	0	1098	64	0
14	J	993	0	1027	62	0
15	K	1114	0	1072	64	0
16	L	1605	0	1676	174	0
17	M	1444	0	1401	143	0
18	N	864	0	873	35	0
19	O	1133	0	1127	43	0
20	P	734	0	729	23	0
21	Q	1149	0	1122	59	0
22	R	641	0	605	28	0
23	S	949	0	923	57	0
24	T	410	0	366	36	0
25	U	499	0	511	38	0
26	V	1195	0	1137	108	0
27	W	654	0	653	51	0
28	X	1130	0	1133	60	0
29	Y	563	0	601	72	0
30	Z	430	0	426	24	0
31	1	393	0	406	20	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	1	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	208	0
42	1	42	0	0	4	0
42	2	76	0	0	6	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	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	B	143	0	0	24	0
42	C	176	0	0	36	0
42	D	51	0	0	19	0
42	E	44	0	0	11	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	10	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	8	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	10	0
42	T	26	0	0	3	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	2903	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 2903 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
6:B:162:MET:HE1	6:B:308:LEU:HD21	1.34	1.09
25:U:12:THR:HG22	25:U:15:GLU:HG3	1.34	1.09
8:D:25:MET:HE2	8:D:41:LEU:HG	1.30	1.08
7:C:236:THR:HG22	7:C:239:ALA:H	0.97	1.07

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	235/239 (98%)	199 (85%)	32 (14%)	4 (2%)	7	30
6	B	335/337 (99%)	299 (89%)	29 (9%)	7 (2%)	5	25
7	C	244/246 (99%)	220 (90%)	22 (9%)	2 (1%)	16	47
8	D	134/176 (76%)	94 (70%)	26 (19%)	14 (10%)	0	2
9	E	170/177 (96%)	159 (94%)	11 (6%)	0	100	100
10	F	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	7	30
11	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
12	H	152/167 (91%)	132 (87%)	15 (10%)	5 (3%)	3	17
13	I	140/145 (97%)	127 (91%)	9 (6%)	4 (3%)	3	19
14	J	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	8	32
15	K	141/164 (86%)	124 (88%)	16 (11%)	1 (1%)	18	49
16	L	192/194 (99%)	174 (91%)	17 (9%)	1 (0%)	24	57
17	M	184/186 (99%)	166 (90%)	11 (6%)	7 (4%)	2	15
18	N	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
19	O	141/148 (95%)	138 (98%)	2 (1%)	1 (1%)	18	49
20	P	93/95 (98%)	86 (92%)	7 (8%)	0	100	100
21	Q	148/154 (96%)	136 (92%)	11 (7%)	1 (1%)	18	49
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%)	3	18
26	V	152/154 (99%)	143 (94%)	7 (5%)	2 (1%)	9	35
27	W	80/91 (88%)	71 (89%)	6 (8%)	3 (4%)	2	15
28	X	140/240 (58%)	140 (100%)	0	0	100	100
29	Y	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	9	34

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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%)	3	17
All	All	3633/4235 (86%)	3293 (91%)	278 (8%)	62 (2%)	7	30

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 ⓘ

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%)	167 (93%)	12 (7%)	15	43
6	B	282/282 (100%)	263 (93%)	19 (7%)	15	43
7	C	193/193 (100%)	177 (92%)	16 (8%)	10	35
8	D	117/147 (80%)	109 (93%)	8 (7%)	14	42
9	E	152/155 (98%)	148 (97%)	4 (3%)	40	68
10	F	92/92 (100%)	91 (99%)	1 (1%)	65	78
11	G	27/283 (10%)	26 (96%)	1 (4%)	30	61
12	H	122/122 (100%)	108 (88%)	14 (12%)	5	23
13	I	118/121 (98%)	110 (93%)	8 (7%)	14	42
14	J	106/106 (100%)	102 (96%)	4 (4%)	29	60
15	K	112/126 (89%)	109 (97%)	3 (3%)	39	67
16	L	166/166 (100%)	159 (96%)	7 (4%)	26	58
17	M	149/149 (100%)	140 (94%)	9 (6%)	17	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	N	93/93 (100%)	89 (96%)	4 (4%)	26	57
19	O	113/116 (97%)	109 (96%)	4 (4%)	32	62
20	P	79/79 (100%)	75 (95%)	4 (5%)	21	52
21	Q	117/121 (97%)	112 (96%)	5 (4%)	26	57
22	R	71/73 (97%)	70 (99%)	1 (1%)	59	76
23	S	105/105 (100%)	101 (96%)	4 (4%)	29	60
24	T	44/52 (85%)	42 (96%)	2 (4%)	24	56
25	U	51/56 (91%)	50 (98%)	1 (2%)	48	72
26	V	130/130 (100%)	121 (93%)	9 (7%)	14	41
27	W	66/73 (90%)	61 (92%)	5 (8%)	12	39
28	X	120/195 (62%)	113 (94%)	7 (6%)	18	48
29	Y	56/56 (100%)	49 (88%)	7 (12%)	4	19
30	Z	46/46 (100%)	46 (100%)	0	100	100
31	1	42/44 (96%)	41 (98%)	1 (2%)	43	69
32	2	79/79 (100%)	74 (94%)	5 (6%)	16	45
All	All	3027/3441 (88%)	2862 (94%)	165 (6%)	19	50

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	P	16	ASN
27	W	66	THR
21	Q	39	THR
25	U	43	PRO
28	X	203	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
17	M	140	GLN
31	1	37	HIS
21	Q	140	GLN
31	1	18	ASN
28	X	149	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2747/2922 (94%)	250 (9%)	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%)	265 (9%)	38 (1%)

5 of 265 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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	37,40,41	2.37	3 (8%)	47,57,60	0.88	2 (4%)
40	BTN	4	79	39	15,16,17	1.84	4 (26%)	20,21,23	1.51	3 (15%)
39	ACA	4	78	40,38	6,7,8	2.07	1 (16%)	5,6,8	1.13	0
38	PHA	4	77	39,37	10,11,11	1.10	0	8,13,13	0.63	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	-	1/25/43/44	0/4/4/4
40	BTN	4	79	39	-	3/6/27/28	0/2/2/2
39	ACA	4	78	40,38	-	2/5/5/6	-
38	PHA	4	77	39,37	-	0/5/6/6	0/1/1/1

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'	12.57	1.61	1.34
37	4	76	PPU	OC-CM	-5.70	1.26	1.42
39	4	78	ACA	C3-C2	-4.77	1.32	1.52
40	4	79	BTN	C8-C7	-4.44	1.33	1.52
40	4	79	BTN	C9-C10	-3.65	1.36	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	4	79	BTN	C2-C4-N2	3.95	117.52	113.34
37	4	76	PPU	C2-N1-C6	2.86	118.83	111.83
40	4	79	BTN	C6-C5-N1	2.49	116.39	113.18
37	4	76	PPU	C-CA-N	2.42	118.52	109.37
40	4	79	BTN	C2-C4-C5	2.11	111.48	108.89

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

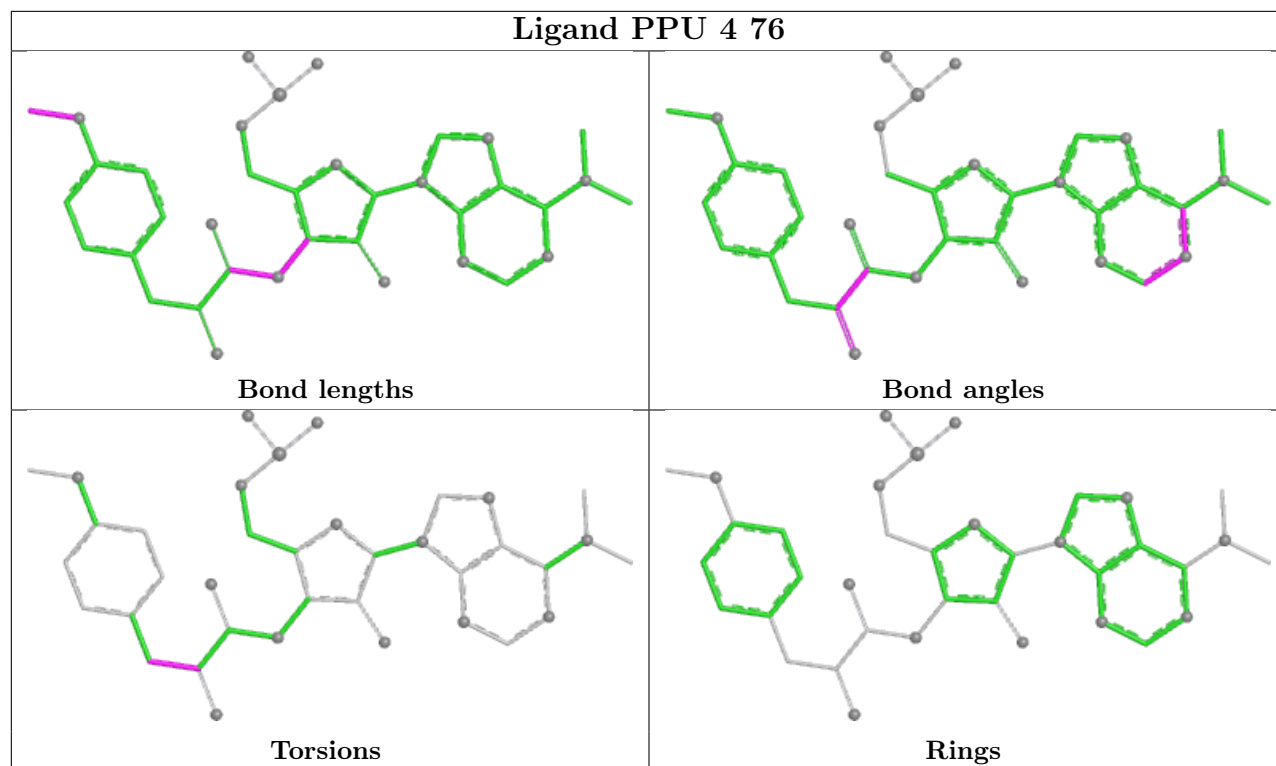
Mol	Chain	Res	Type	Atoms
40	4	79	BTN	C7-C8-C9-C10
39	4	78	ACA	C4-C5-C6-N
39	4	78	ACA	C3-C4-C5-C6
40	4	79	BTN	C4-C2-C7-C8
37	4	76	PPU	N-CA-CB-CG

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
40	4	79	BTN	2	0
38	4	77	PHA	1	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 than 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.



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, 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	0	2754/2922 (94%)	-0.61	40 (1%) 72 52	11, 39, 86, 141	0
2	9	122/122 (100%)	-0.08	5 (4%) 41 23	28, 60, 91, 145	0
3	3	3/3 (100%)	2.74	3 (100%) 0 0	22, 22, 23, 26	3 (100%)
4	4	2/2 (100%)	-0.08	0 100 100	48, 48, 48, 56	0
5	A	237/239 (99%)	-0.15	4 (1%) 69 48	21, 53, 94, 113	0
6	B	337/337 (100%)	-0.36	1 (0%) 90 80	19, 45, 71, 81	0
7	C	246/246 (100%)	-0.46	1 (0%) 88 76	12, 37, 63, 71	0
8	D	140/176 (79%)	0.74	10 (7%) 22 12	55, 94, 120, 127	0
9	E	172/177 (97%)	-0.10	2 (1%) 76 58	32, 56, 81, 87	0
10	F	119/119 (100%)	0.07	1 (0%) 82 65	41, 66, 94, 104	0
11	G	29/348 (8%)	0.69	2 (6%) 23 12	60, 79, 84, 89	0
12	H	156/167 (93%)	-0.07	4 (2%) 57 36	30, 48, 74, 81	0
13	I	142/145 (97%)	-0.46	0 100 100	26, 38, 60, 77	0
14	J	132/132 (100%)	-0.32	0 100 100	24, 44, 72, 76	0
15	K	145/164 (88%)	0.06	5 (3%) 48 28	16, 68, 97, 109	0
16	L	194/194 (100%)	0.13	22 (11%) 10 5	23, 39, 118, 128	0
17	M	186/186 (100%)	0.21	7 (3%) 44 25	36, 65, 109, 120	0
18	N	115/115 (100%)	-0.21	0 100 100	31, 47, 65, 69	0
19	O	143/148 (96%)	-0.28	1 (0%) 84 68	27, 47, 67, 77	0
20	P	95/95 (100%)	-0.40	1 (1%) 78 59	27, 40, 57, 79	0
21	Q	150/154 (97%)	-0.68	0 100 100	22, 35, 54, 65	0
22	R	81/84 (96%)	-0.30	0 100 100	35, 53, 73, 80	0
23	S	119/119 (100%)	-0.21	1 (0%) 82 65	33, 47, 75, 91	0
24	T	53/66 (80%)	1.47	12 (22%) 2 1	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%)	0.17	3 (4%) 37 20	45, 69, 106, 112	0
26	V	154/154 (100%)	-0.42	0 100 100	25, 38, 56, 69	0
27	W	82/91 (90%)	-0.11	4 (4%) 35 18	32, 49, 69, 89	0
28	X	142/240 (59%)	-0.49	1 (0%) 84 68	17, 36, 58, 77	0
29	Y	73/73 (100%)	2.22	36 (49%) 0 0	89, 118, 129, 133	0
30	Z	56/56 (100%)	-0.81	0 100 100	14, 26, 32, 39	0
31	1	46/48 (95%)	-0.11	0 100 100	23, 52, 84, 96	0
32	2	92/92 (100%)	2.65	58 (63%) 0 0	122, 136, 142, 146	0
All	All	6582/7284 (90%)	-0.28	224 (3%) 48 28	11, 45, 105, 146	3 (0%)

The worst 5 of 224 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
16	L	89	ASN	7.7
25	U	1	THR	7.3
16	L	80	GLY	7.1
32	2	12	PRO	6.6
16	L	70	GLY	6.2

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 oligosaccharides 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	8384	1/1	0.41	0.19	87,87,87,87	0
35	NA	0	8329	1/1	0.54	0.33	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	9	8351	1/1	0.58	0.28	112,112,112,112	0
36	CL	2	8504	1/1	0.60	0.11	104,104,104,104	0
41	CD	2	8404	1/1	0.63	0.36	200,200,200,200	0
41	CD	T	8401	1/1	0.65	0.35	200,200,200,200	0
35	NA	R	8312	1/1	0.65	0.17	84,84,84,84	0
35	NA	0	8382	1/1	0.78	0.28	57,57,57,57	0
35	NA	0	8385	1/1	0.81	0.31	52,52,52,52	0
35	NA	9	8383	1/1	0.83	0.21	57,57,57,57	0
35	NA	0	8344	1/1	0.84	0.02	9,9,9,9	0
35	NA	0	8366	1/1	0.85	0.08	20,20,20,20	0
35	NA	0	8371	1/1	0.86	0.29	47,47,47,47	0
33	MG	9	8095	1/1	0.86	0.16	72,72,72,72	0
35	NA	0	8365	1/1	0.87	0.21	42,42,42,42	0
35	NA	0	8333	1/1	0.87	0.18	25,25,25,25	0
35	NA	Q	8386	1/1	0.88	0.23	62,62,62,62	0
35	NA	0	8331	1/1	0.88	0.38	69,69,69,69	0
35	NA	0	8302	1/1	0.88	0.10	18,18,18,18	0
38	PHA	4	77	11/11	0.88	0.15	64,67,71,71	0
35	NA	0	8340	1/1	0.88	0.16	48,48,48,48	0
34	K	0	8202	1/1	0.88	0.18	69,69,69,69	0
33	MG	0	8049	1/1	0.89	0.11	73,73,73,73	0
36	CL	0	8522	1/1	0.89	0.30	76,76,76,76	0
41	CD	Y	8403	1/1	0.89	0.22	200,200,200,200	0
35	NA	0	8372	1/1	0.89	0.23	73,73,73,73	0
35	NA	0	8332	1/1	0.90	0.14	57,57,57,57	0
33	MG	0	8092	1/1	0.90	0.10	71,71,71,71	0
33	MG	0	8055	1/1	0.90	0.09	82,82,82,82	0
35	NA	0	8360	1/1	0.91	0.15	39,39,39,39	0
33	MG	0	8024	1/1	0.91	0.35	109,109,109,109	0
33	MG	0	8094	1/1	0.91	0.12	54,54,54,54	0
33	MG	0	8101	1/1	0.91	0.10	40,40,40,40	0
36	CL	K	8510	1/1	0.91	0.10	70,70,70,70	0
33	MG	0	8102	1/1	0.91	0.61	135,135,135,135	0
33	MG	0	8070	1/1	0.91	0.21	71,71,71,71	0
40	BTN	4	79	15/16	0.91	0.17	91,104,104,105	0
35	NA	0	8334	1/1	0.91	0.17	29,29,29,29	0
33	MG	2	8078	1/1	0.91	0.18	73,73,73,73	0
33	MG	0	8076	1/1	0.91	0.06	70,70,70,70	0
36	CL	I	8502	1/1	0.92	0.06	56,56,56,56	0
35	NA	0	8324	1/1	0.92	0.20	39,39,39,39	0
33	MG	0	8050	1/1	0.92	0.06	78,78,78,78	0
35	NA	0	8355	1/1	0.92	0.24	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8357	1/1	0.92	0.14	53,53,53,53	0
35	NA	0	8373	1/1	0.92	0.09	51,51,51,51	0
35	NA	0	8381	1/1	0.92	0.12	71,71,71,71	0
35	NA	0	8310	1/1	0.92	0.09	16,16,16,16	0
35	NA	0	8307	1/1	0.93	0.09	40,40,40,40	0
35	NA	0	8374	1/1	0.93	0.16	49,49,49,49	0
33	MG	Y	8105	1/1	0.93	0.08	67,67,67,67	0
35	NA	0	8363	1/1	0.93	0.17	40,40,40,40	0
33	MG	0	8044	1/1	0.93	0.09	35,35,35,35	0
35	NA	0	8352	1/1	0.93	0.07	28,28,28,28	0
35	NA	0	8368	1/1	0.93	0.17	41,41,41,41	0
35	NA	0	8326	1/1	0.93	0.09	38,38,38,38	0
35	NA	H	8322	1/1	0.93	0.11	48,48,48,48	0
35	NA	0	8356	1/1	0.93	0.17	59,59,59,59	0
34	K	0	8201	1/1	0.94	0.26	80,80,80,80	0
35	NA	0	8311	1/1	0.94	0.08	38,38,38,38	0
36	CL	0	8515	1/1	0.94	0.15	72,72,72,72	0
35	NA	0	8377	1/1	0.94	0.14	59,59,59,59	0
35	NA	0	8354	1/1	0.94	0.12	29,29,29,29	0
33	MG	0	8053	1/1	0.94	0.09	38,38,38,38	0
33	MG	0	8066	1/1	0.94	0.09	60,60,60,60	0
37	PPU	4	76	37/38	0.94	0.10	48,55,62,63	0
35	NA	0	8369	1/1	0.94	0.25	67,67,67,67	0
39	ACA	4	78	8/9	0.94	0.16	67,73,85,88	0
35	NA	0	8370	1/1	0.94	0.21	48,48,48,48	0
33	MG	0	8114	1/1	0.94	0.30	161,161,161,161	0
35	NA	0	8358	1/1	0.94	0.20	98,98,98,98	0
35	NA	Q	8337	1/1	0.94	0.06	41,41,41,41	0
36	CL	A	8509	1/1	0.95	0.17	76,76,76,76	0
33	MG	0	8090	1/1	0.95	0.19	65,65,65,65	0
35	NA	0	8321	1/1	0.95	0.16	58,58,58,58	0
36	CL	M	8507	1/1	0.95	0.09	54,54,54,54	0
33	MG	0	8045	1/1	0.95	0.07	44,44,44,44	0
33	MG	0	8093	1/1	0.95	0.07	43,43,43,43	0
35	NA	0	8303	1/1	0.95	0.09	33,33,33,33	0
35	NA	0	8378	1/1	0.95	0.11	31,31,31,31	0
35	NA	0	8306	1/1	0.95	0.13	21,21,21,21	0
41	CD	N	8405	1/1	0.95	0.07	111,111,111,111	0
36	CL	0	8514	1/1	0.95	0.05	44,44,44,44	0
33	MG	0	8067	1/1	0.95	0.06	31,31,31,31	0
33	MG	0	8087	1/1	0.95	0.05	36,36,36,36	0
35	NA	0	8349	1/1	0.96	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8350	1/1	0.96	0.11	26,26,26,26	0
33	MG	0	8057	1/1	0.96	0.08	30,30,30,30	0
33	MG	0	8072	1/1	0.96	0.05	43,43,43,43	0
35	NA	0	8325	1/1	0.96	0.10	29,29,29,29	0
36	CL	B	8519	1/1	0.96	0.08	51,51,51,51	0
33	MG	0	8103	1/1	0.96	0.10	34,34,34,34	0
33	MG	0	8104	1/1	0.96	0.04	41,41,41,41	0
33	MG	0	8041	1/1	0.96	0.09	50,50,50,50	0
33	MG	0	8046	1/1	0.96	0.04	40,40,40,40	0
35	NA	0	8362	1/1	0.96	0.15	63,63,63,63	0
35	NA	0	8308	1/1	0.96	0.12	44,44,44,44	0
35	NA	0	8364	1/1	0.96	0.14	47,47,47,47	0
33	MG	0	8099	1/1	0.96	0.09	37,37,37,37	0
35	NA	C	8304	1/1	0.96	0.04	25,25,25,25	0
33	MG	0	8100	1/1	0.96	0.14	65,65,65,65	0
35	NA	0	8341	1/1	0.96	0.14	40,40,40,40	0
35	NA	0	8319	1/1	0.96	0.08	50,50,50,50	0
35	NA	0	8314	1/1	0.97	0.06	33,33,33,33	0
33	MG	0	8047	1/1	0.97	0.11	48,48,48,48	0
33	MG	0	8042	1/1	0.97	0.04	40,40,40,40	0
33	MG	0	8011	1/1	0.97	0.16	1,1,1,1	0
35	NA	0	8353	1/1	0.97	0.05	34,34,34,34	0
36	CL	0	8517	1/1	0.97	0.05	57,57,57,57	0
35	NA	0	8301	1/1	0.97	0.07	28,28,28,28	0
33	MG	0	8051	1/1	0.97	0.04	70,70,70,70	0
35	NA	0	8375	1/1	0.97	0.09	40,40,40,40	0
36	CL	I	8501	1/1	0.97	0.05	60,60,60,60	0
33	MG	0	8106	1/1	0.97	0.05	64,64,64,64	0
36	CL	I	8521	1/1	0.97	0.04	39,39,39,39	0
33	MG	0	8111	1/1	0.97	0.04	49,49,49,49	0
36	CL	L	8518	1/1	0.97	0.08	36,36,36,36	0
33	MG	0	8005	1/1	0.97	0.02	26,26,26,26	0
36	CL	N	8508	1/1	0.97	0.07	82,82,82,82	0
36	CL	X	8520	1/1	0.97	0.05	35,35,35,35	0
33	MG	0	8117	1/1	0.97	0.06	19,19,19,19	0
35	NA	0	8309	1/1	0.97	0.10	24,24,24,24	0
35	NA	0	8335	1/1	0.97	0.09	47,47,47,47	0
35	NA	0	8339	1/1	0.97	0.05	8,8,8,8	0
33	MG	0	8010	1/1	0.97	0.04	20,20,20,20	0
33	MG	0	8082	1/1	0.97	0.07	43,43,43,43	0
35	NA	0	8367	1/1	0.97	0.06	36,36,36,36	0
35	NA	I	8346	1/1	0.97	0.04	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	P	8348	1/1	0.97	0.06	45,45,45,45	0
33	MG	0	8108	1/1	0.98	0.08	61,61,61,61	0
35	NA	0	8327	1/1	0.98	0.04	16,16,16,16	0
35	NA	0	8328	1/1	0.98	0.04	41,41,41,41	0
33	MG	0	8085	1/1	0.98	0.09	103,103,103,103	0
35	NA	0	8330	1/1	0.98	0.04	21,21,21,21	0
36	CL	0	8505	1/1	0.98	0.05	57,57,57,57	0
36	CL	0	8511	1/1	0.98	0.07	63,63,63,63	0
36	CL	0	8513	1/1	0.98	0.08	52,52,52,52	0
35	NA	0	8305	1/1	0.98	0.07	19,19,19,19	0
33	MG	0	8098	1/1	0.98	0.13	24,24,24,24	0
36	CL	0	8516	1/1	0.98	0.12	44,44,44,44	0
33	MG	0	8115	1/1	0.98	0.03	58,58,58,58	0
33	MG	0	8116	1/1	0.98	0.05	64,64,64,64	0
33	MG	0	8086	1/1	0.98	0.04	41,41,41,41	0
35	NA	0	8336	1/1	0.98	0.03	30,30,30,30	0
33	MG	0	8043	1/1	0.98	0.03	34,34,34,34	0
33	MG	S	8073	1/1	0.98	0.03	36,36,36,36	0
35	NA	0	8313	1/1	0.98	0.05	59,59,59,59	0
33	MG	0	8088	1/1	0.98	0.07	23,23,23,23	0
35	NA	0	8376	1/1	0.98	0.11	50,50,50,50	0
35	NA	0	8315	1/1	0.98	0.10	32,32,32,32	0
35	NA	0	8316	1/1	0.98	0.06	28,28,28,28	0
36	CL	Q	8506	1/1	0.98	0.04	43,43,43,43	0
35	NA	0	8379	1/1	0.98	0.05	25,25,25,25	0
35	NA	0	8317	1/1	0.98	0.03	23,23,23,23	0
35	NA	0	8318	1/1	0.98	0.04	22,22,22,22	0
33	MG	0	8075	1/1	0.98	0.06	50,50,50,50	0
35	NA	0	8320	1/1	0.98	0.04	15,15,15,15	0
33	MG	0	8091	1/1	0.98	0.04	40,40,40,40	0
33	MG	0	8059	1/1	0.98	0.04	59,59,59,59	0
35	NA	A	8345	1/1	0.98	0.04	40,40,40,40	0
33	MG	0	8064	1/1	0.98	0.09	17,17,17,17	0
35	NA	0	8359	1/1	0.98	0.10	42,42,42,42	0
33	MG	0	8012	1/1	0.99	0.02	26,26,26,26	0
33	MG	0	8083	1/1	0.99	0.07	38,38,38,38	0
36	CL	0	8503	1/1	0.99	0.04	49,49,49,49	0
33	MG	0	8084	1/1	0.99	0.09	38,38,38,38	0
33	MG	0	8056	1/1	0.99	0.04	35,35,35,35	0
36	CL	0	8512	1/1	0.99	0.04	34,34,34,34	0
33	MG	0	8014	1/1	0.99	0.05	22,22,22,22	0
33	MG	0	8110	1/1	0.99	0.07	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8008	1/1	0.99	0.04	42,42,42,42	0
33	MG	0	8112	1/1	0.99	0.06	34,34,34,34	0
33	MG	0	8113	1/1	0.99	0.04	36,36,36,36	0
35	NA	0	8342	1/1	0.99	0.04	19,19,19,19	0
35	NA	0	8343	1/1	0.99	0.03	17,17,17,17	0
33	MG	0	8060	1/1	0.99	0.05	32,32,32,32	0
33	MG	0	8089	1/1	0.99	0.05	50,50,50,50	0
33	MG	0	8063	1/1	0.99	0.04	68,68,68,68	0
33	MG	0	8025	1/1	0.99	0.03	17,17,17,17	0
33	MG	0	8027	1/1	0.99	0.04	37,37,37,37	0
33	MG	A	8065	1/1	0.99	0.05	44,44,44,44	0
33	MG	0	8036	1/1	0.99	0.03	32,32,32,32	0
35	NA	0	8323	1/1	0.99	0.09	34,34,34,34	0
33	MG	0	8040	1/1	0.99	0.07	107,107,107,107	0
33	MG	0	8096	1/1	0.99	0.06	33,33,33,33	0
33	MG	0	8097	1/1	0.99	0.06	30,30,30,30	0
33	MG	0	8003	1/1	0.99	0.03	22,22,22,22	0
35	NA	0	8361	1/1	0.99	0.06	40,40,40,40	0
33	MG	0	8052	1/1	0.99	0.04	36,36,36,36	0
35	NA	K	8380	1/1	0.99	0.07	69,69,69,69	0
35	NA	L	8347	1/1	0.99	0.03	7,7,7,7	0
33	MG	0	8006	1/1	0.99	0.03	28,28,28,28	0
33	MG	0	8081	1/1	0.99	0.03	36,36,36,36	0
35	NA	Q	8338	1/1	0.99	0.03	57,57,57,57	0
33	MG	J	8069	1/1	1.00	0.02	47,47,47,47	0
33	MG	0	8077	1/1	1.00	0.01	21,21,21,21	0
33	MG	X	8109	1/1	1.00	0.04	35,35,35,35	0
33	MG	0	8079	1/1	1.00	0.03	27,27,27,27	0
33	MG	0	8080	1/1	1.00	0.01	42,42,42,42	0
33	MG	0	8039	1/1	1.00	0.04	31,31,31,31	0
33	MG	0	8013	1/1	1.00	0.02	25,25,25,25	0
33	MG	0	8004	1/1	1.00	0.04	30,30,30,30	0
33	MG	0	8015	1/1	1.00	0.02	29,29,29,29	0
33	MG	0	8016	1/1	1.00	0.02	25,25,25,25	0
33	MG	0	8017	1/1	1.00	0.05	15,15,15,15	0
33	MG	0	8018	1/1	1.00	0.02	32,32,32,32	0
33	MG	0	8019	1/1	1.00	0.04	13,13,13,13	0
33	MG	0	8020	1/1	1.00	0.02	16,16,16,16	0
33	MG	0	8048	1/1	1.00	0.02	34,34,34,34	0
33	MG	0	8021	1/1	1.00	0.02	26,26,26,26	0
33	MG	0	8022	1/1	1.00	0.02	30,30,30,30	0
33	MG	0	8023	1/1	1.00	0.03	28,28,28,28	0

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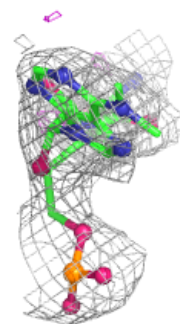
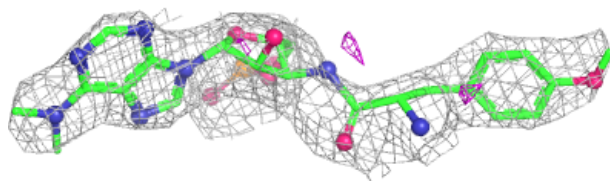
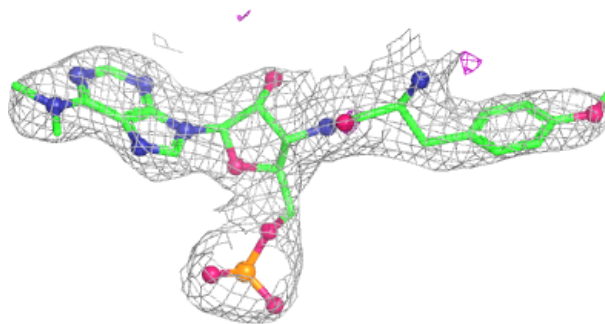
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8009	1/1	1.00	0.05	18,18,18,18	0
33	MG	0	8002	1/1	1.00	0.04	33,33,33,33	0
33	MG	0	8054	1/1	1.00	0.02	28,28,28,28	0
33	MG	0	8026	1/1	1.00	0.02	25,25,25,25	0
33	MG	0	8001	1/1	1.00	0.02	21,21,21,21	0
33	MG	0	8028	1/1	1.00	0.04	23,23,23,23	0
33	MG	0	8058	1/1	1.00	0.05	28,28,28,28	0
33	MG	0	8029	1/1	1.00	0.04	23,23,23,23	0
33	MG	0	8030	1/1	1.00	0.02	29,29,29,29	0
33	MG	0	8061	1/1	1.00	0.02	28,28,28,28	0
33	MG	0	8062	1/1	1.00	0.02	37,37,37,37	0
33	MG	0	8107	1/1	1.00	0.01	24,24,24,24	0
33	MG	0	8031	1/1	1.00	0.04	18,18,18,18	0
33	MG	0	8032	1/1	1.00	0.05	29,29,29,29	0
33	MG	0	8033	1/1	1.00	0.01	18,18,18,18	0
33	MG	0	8034	1/1	1.00	0.03	22,22,22,22	0
33	MG	0	8068	1/1	1.00	0.04	58,58,58,58	0
33	MG	0	8035	1/1	1.00	0.04	39,39,39,39	0
33	MG	0	8071	1/1	1.00	0.04	66,66,66,66	0
33	MG	0	8007	1/1	1.00	0.05	18,18,18,18	0
33	MG	0	8074	1/1	1.00	0.03	27,27,27,27	0
33	MG	0	8037	1/1	1.00	0.02	34,34,34,34	0
41	CD	Z	8402	1/1	1.00	0.04	49,49,49,49	0
33	MG	0	8038	1/1	1.00	0.03	23,23,23,23	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 ⓘ

There are no such residues in this entry.