



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 05:08 PM UTC

PDB ID : 1Q7Y / pdb_00001q7y
Title : Crystal Structure of CCdAP-Puromycin bound at the Peptidyl transferase center of the 50S ribosomal subunit
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2003-08-20
Resolution : 3.20 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

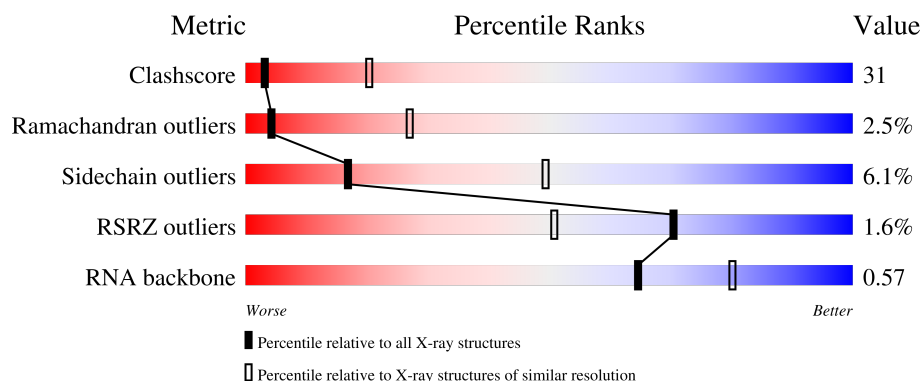
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

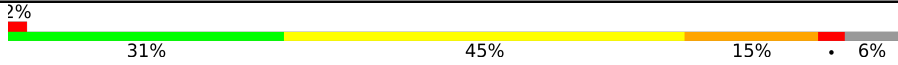
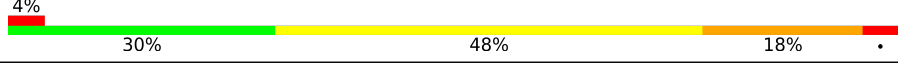
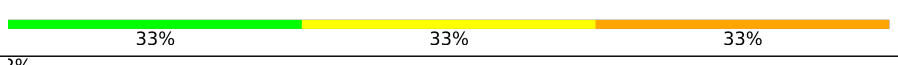
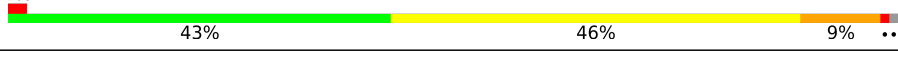
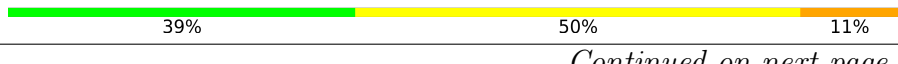
The reported resolution of this entry is 3.20 Å.

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



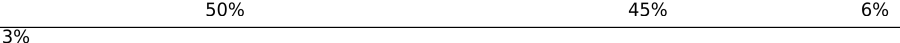
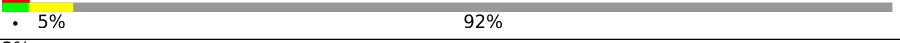
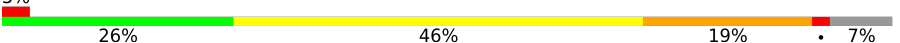
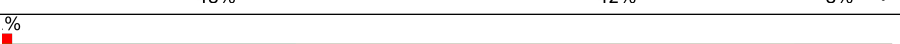
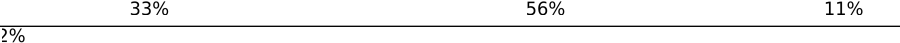
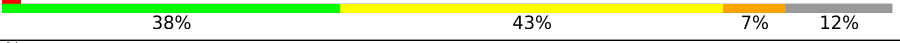
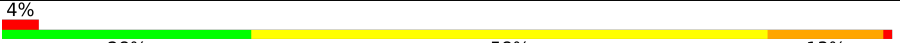
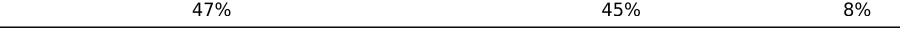
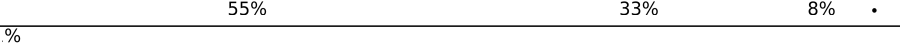
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	A	2922	 2% 31% 45% 15% 6%
2	B	122	 4% 30% 48% 18%
3	5	3	 33% 33% 33%
4	C	239	 2% 43% 46% 9%
5	D	337	 39% 50% 11%

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Mol	Chain	Length	Quality of chain
6	E	246	
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	
30	3	48	

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Mol	Chain	Length	Quality of chain
31	4	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	A	8370	-	-	-	X
34	NA	B	8383	-	-	-	X

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 98616 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal rna.

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

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

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

- Molecule 3 is DNA/RNA hybrid called CCdA-P-Puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	5	3	Total	C	N	O	P	0	0	0
			58	28	11	17	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	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
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

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

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

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

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

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

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

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

- Molecule 15 is a protein called L15 Ribosomal Protein.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	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
Q	71	LYS	TYR	conflict	UNP P14119

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	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
3	?	-	ARG	deletion	UNP P22452

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

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

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	109	Total Mg 109 109	0	0
32	B	1	Total Mg 1 1	0	0
32	5	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	1	1	Total Mg 1 1	0	0
32	4	1	Total Mg 1 1	0	0

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	72	Total Na 72 72	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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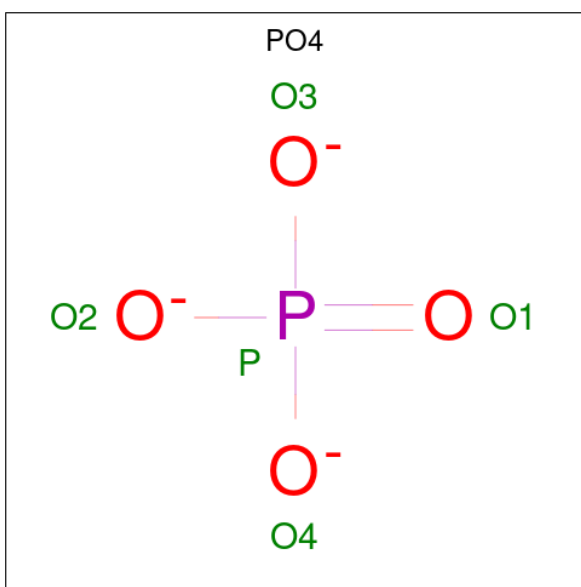
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	R	1	Total 1	Na 1	0	0
34	S	3	Total 3	Na 3	0	0
34	T	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

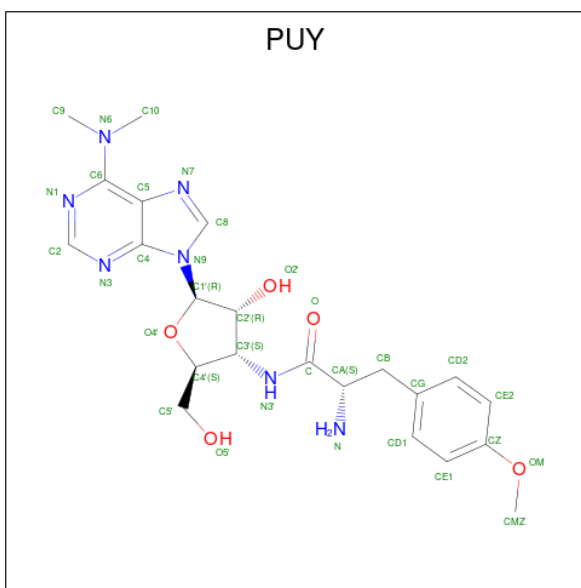
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	11	Total 11	Cl 11	0	0
35	C	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	P	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	Z	1	Total 1	Cl 1	0	0
35	4	1	Total 1	Cl 1	0	0

- Molecule 36 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	5	1	Total	O	P	0	0
			3	2	1		

- Molecule 37 is PUROMYCIN (CCD ID: PUY) (formula: $C_{22}H_{29}N_7O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	5	1	Total	C	N	O	0	0
			34	22	7	5		

- Molecule 38 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	P	1	Total Cd 1 1	0	0
38	V	1	Total Cd 1 1	0	0
38	1	1	Total Cd 1 1	0	0
38	2	1	Total Cd 1 1	0	0
38	4	1	Total Cd 1 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	A	5861	Total O 5861 5861	0	0
39	B	154	Total O 154 154	0	0
39	5	6	Total O 6 6	0	0
39	C	123	Total O 123 123	0	0
39	D	149	Total O 149 149	0	0
39	E	178	Total O 178 178	0	0
39	F	50	Total O 50 50	0	0
39	G	46	Total O 46 46	0	0
39	H	27	Total O 27 27	0	0
39	I	20	Total O 20 20	0	0
39	J	75	Total O 75 75	0	0
39	K	56	Total O 56 56	0	0
39	L	60	Total O 60 60	0	0
39	M	90	Total O 90 90	0	0
39	N	128	Total O 128 128	0	0

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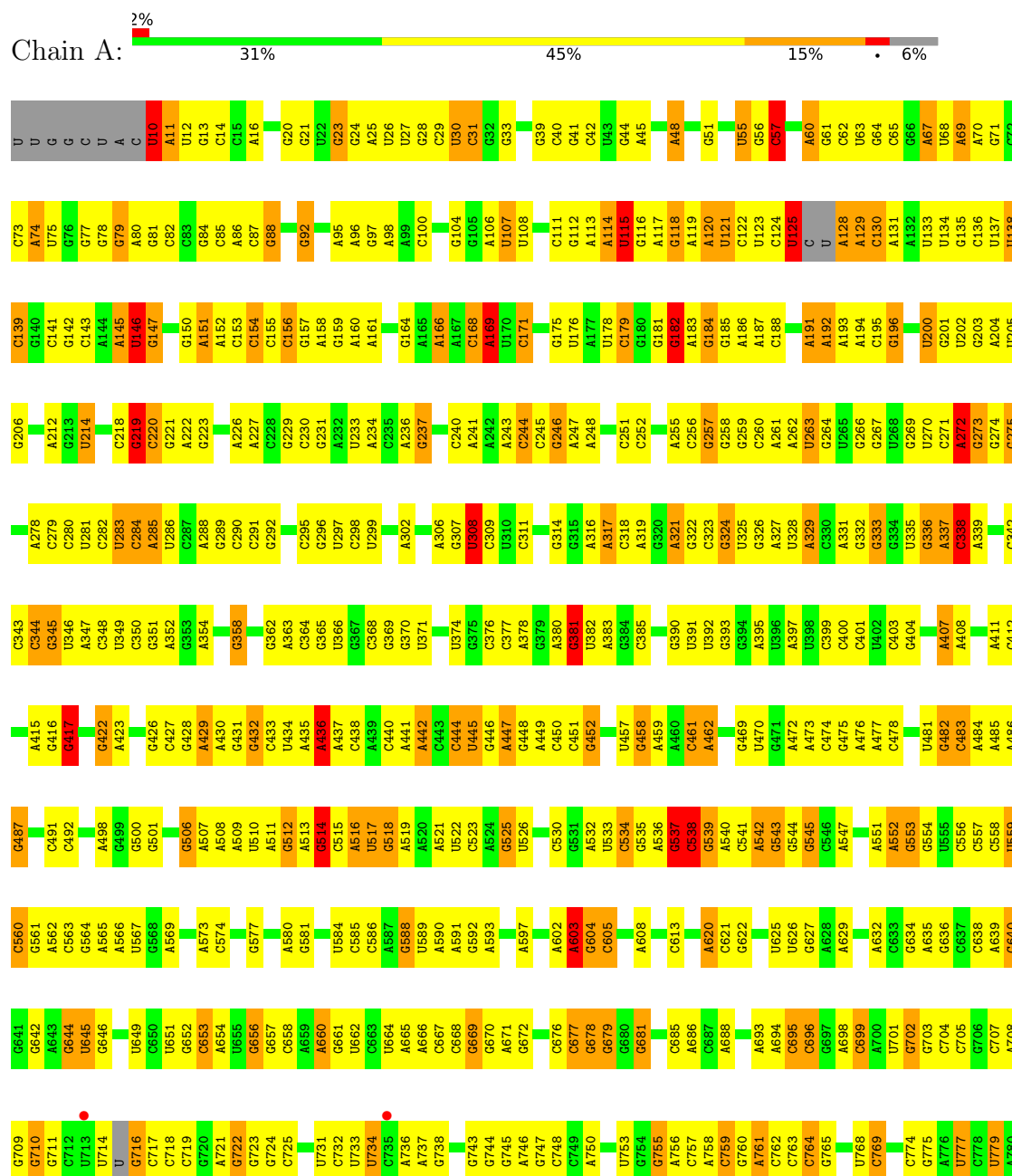
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	63	Total 63	O 63	0	0
39	P	45	Total 45	O 45	0	0
39	Q	62	Total 62	O 62	0	0
39	R	53	Total 53	O 53	0	0
39	S	86	Total 86	O 86	0	0
39	T	36	Total 36	O 36	0	0
39	U	42	Total 42	O 42	0	0
39	V	30	Total 30	O 30	0	0
39	W	15	Total 15	O 15	0	0
39	X	73	Total 73	O 73	0	0
39	Y	30	Total 30	O 30	0	0
39	Z	99	Total 99	O 99	0	0
39	1	36	Total 36	O 36	0	0
39	2	63	Total 63	O 63	0	0
39	3	42	Total 42	O 42	0	0
39	4	73	Total 73	O 73	0	0

3 Residue-property plots

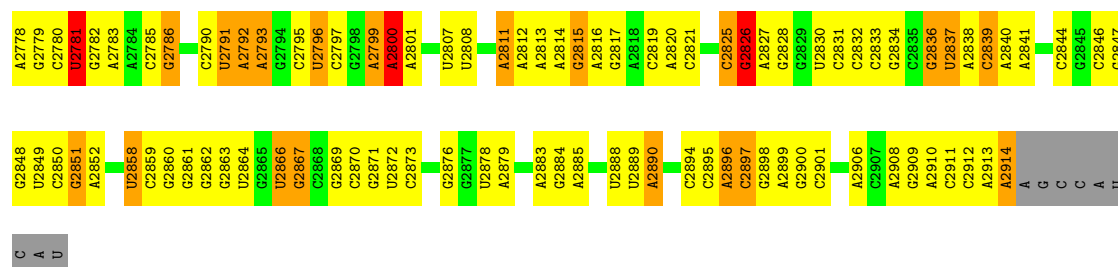
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

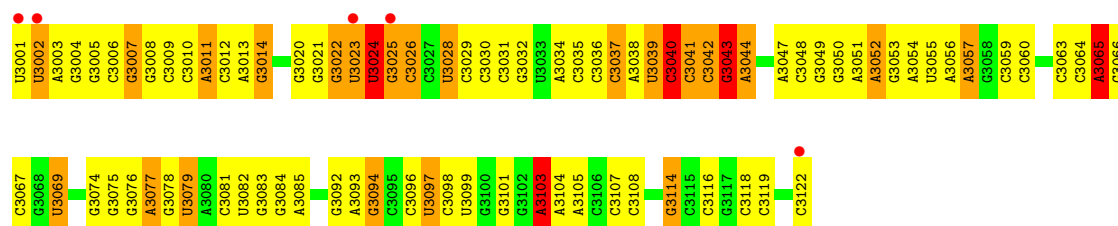


A1669	C1592	C1514	C1450	G1319	A1255	G1195	C1129	A1057	G918	C848	C781
G1672	C1593	A1522	C1451	U1320	C1256	C1196	U1130	A1058	U919	C849	G782
U1673	G1594	G1523	G1452	A1321	U1381	C1197	A1132	C1059	C920	U850	G783
C1674	G1595	U1524	G1453	G1322	A1259	U1198	G1133	C1060	C921	C851	A784
C1675	U1596	G1455	U1454	G1323	G1260	A1199	G1134	C1061	A922	U852	G785
U1676	A1597	G1456	C1456	G1324	A1261	A1200	G1135	U1062	A923	C853	G786
U1677	U1598	U1457	G1457	G1325	C1262	C1201	U1136	G1063	G924	G854	G787
A1678	U1599	A1458	U1458	U1326	G1263	A1202	G1137	U1064	C925	U855	A788
C1679	A1603	A1459	A1459	G1327	U1264	G1203	U1138	A1067	A926	G856	G789
C1680	G1604	G1460	C1460	A1328	U1265	C1204	G1139	U857	A929	U858	A790
G1681	G1605	U1461	C1395	A1329	U1266	U1205	U1140	U859	C930	U860	A791
A1682	A1606	U1462	C1396	A1330	C1267	U1206	C1141	G1071	C931	G861	G792
G1683	C1462	C1397	G1397	C1332	G1268	A1207	U1142	G1072	U932	A861	U794
A1684	G1463	G1398	U1398	U1333	G1269	C1208	A1150	A1073	C933	U862	G795
C1613	U1464	A1399	C1399	C1334	U1270	C1209	G1151	G1074	C934	G863	A796
C1613	A1465	C1400	C1400	U1335	C1272	G1211	C1152	G1075	G935	U864	A797
C1614	G1466	G1401	G1401	C1336	C1273	C1212	A1153	G1076	C936	G798	G798
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A1631	G1481	G1481	G1481	A1347	U1284	G1223	G1163	A1088	U947	G878	A812
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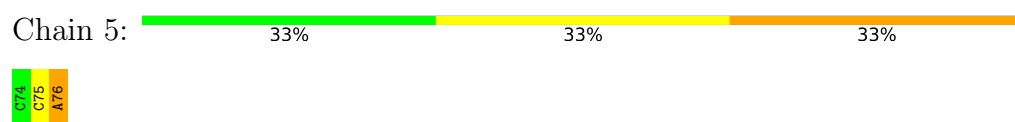
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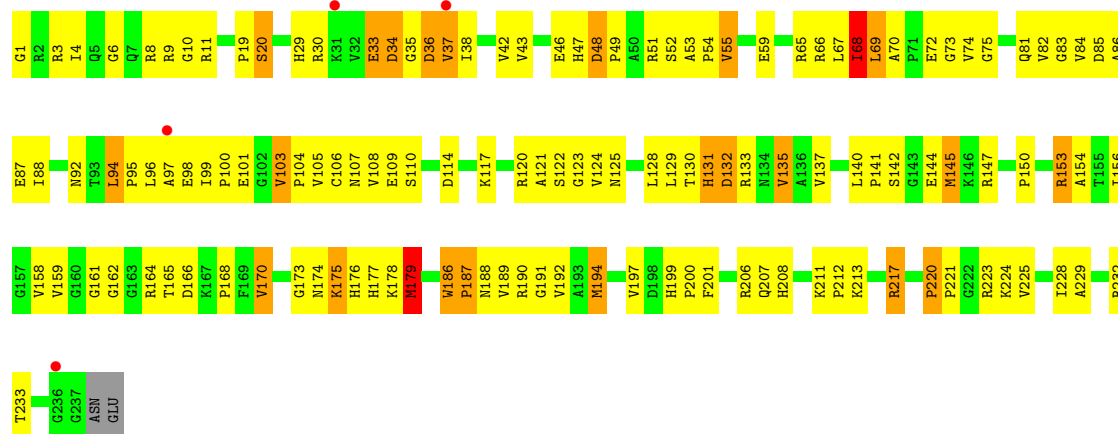
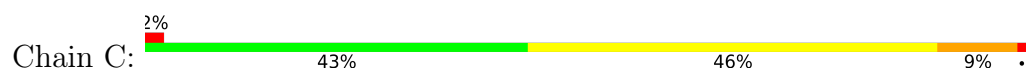
• Molecule 2: 5S ribosomal RNA



• Molecule 3: CCdA-P-Puromycin

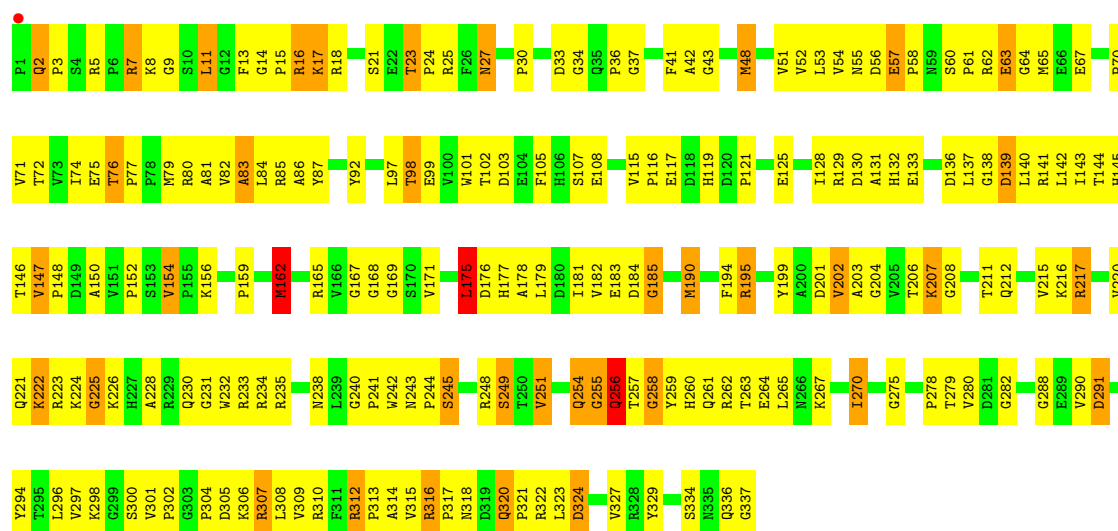


• Molecule 4: 50S ribosomal protein L2P



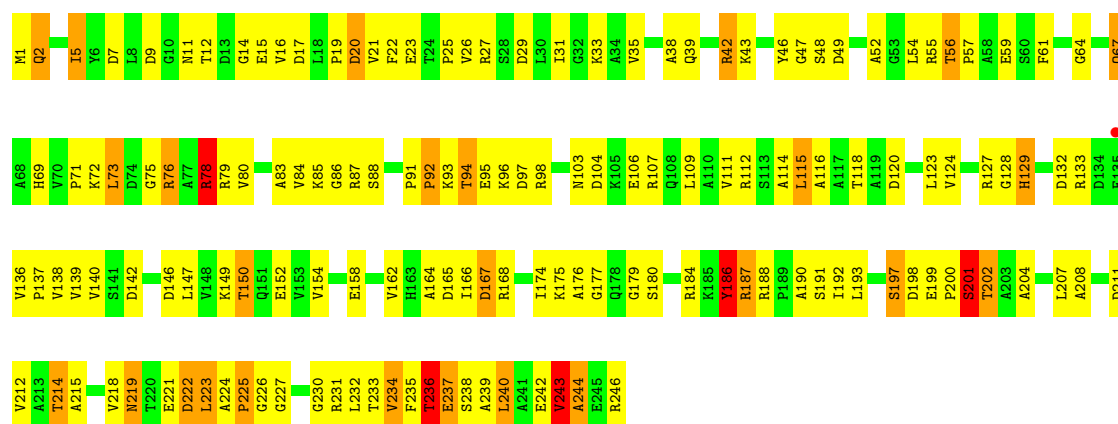
• Molecule 5: 50S ribosomal protein L3P





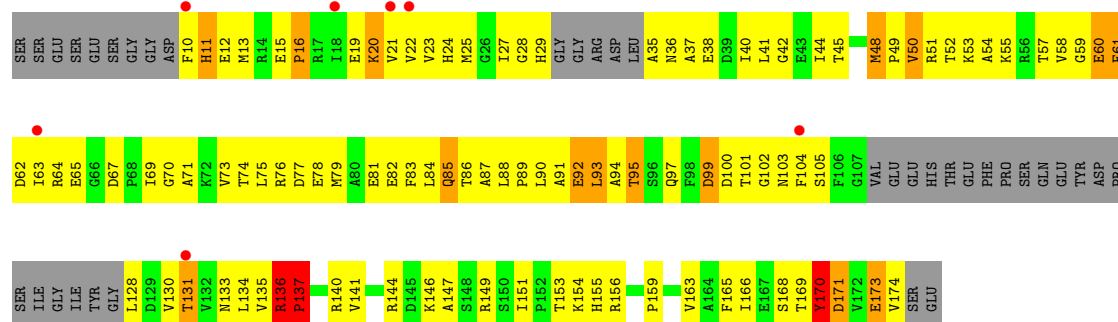
• Molecule 6: 50S ribosomal protein L4E

Chain E: 38% 49% 11%

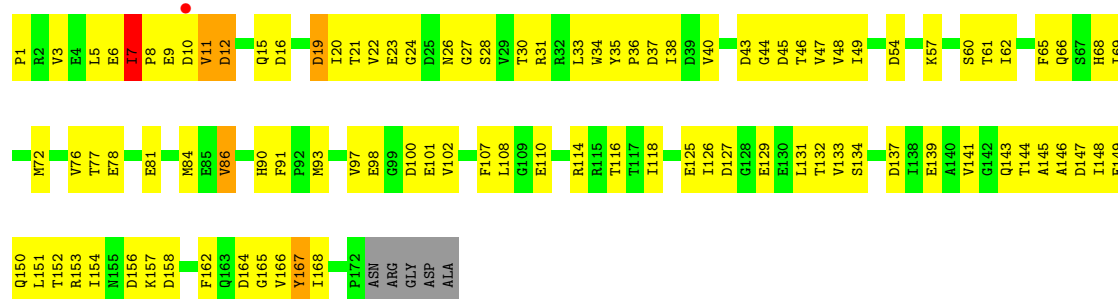
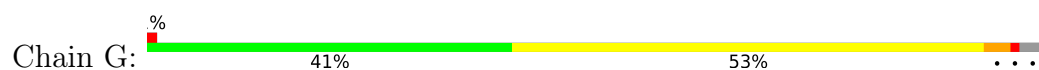


• Molecule 7: 50S ribosomal protein L5P

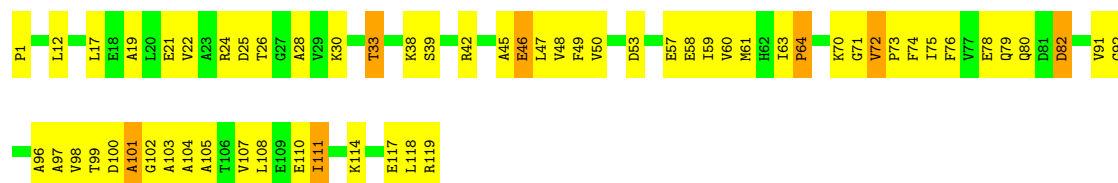
Chain F: 4% 20% 49% 9% 20%



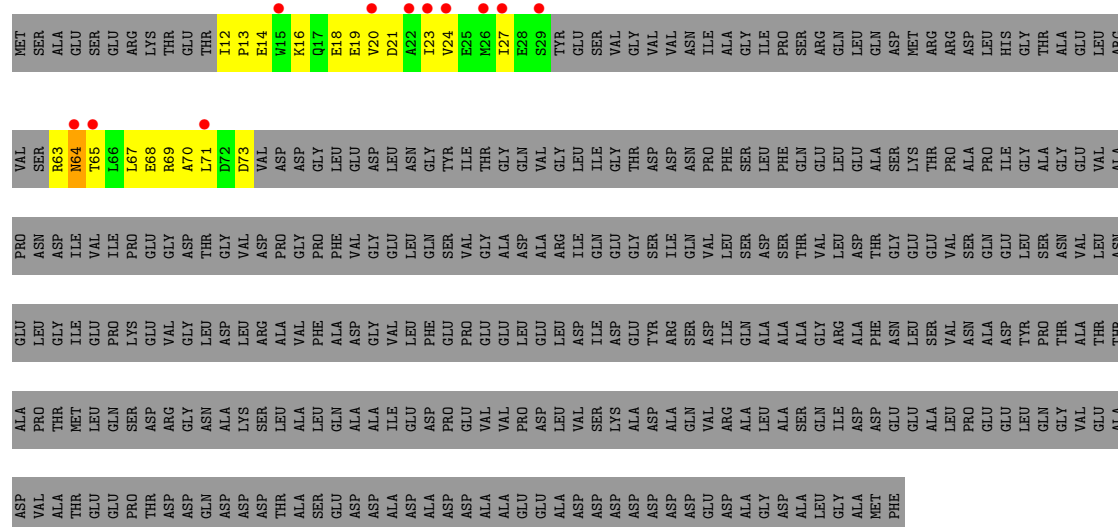
• Molecule 8: 50S ribosomal protein L6P



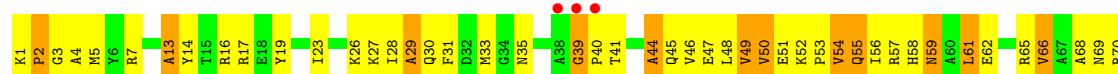
• Molecule 9: 50S ribosomal protein L7Ae

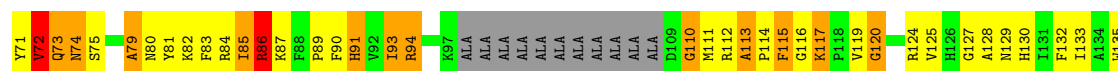


• Molecule 10: Acidic ribosomal protein P0 homolog

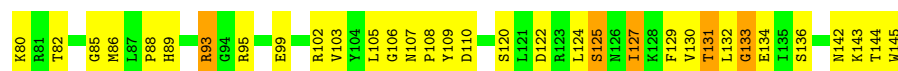


• Molecule 11: L10 Ribosomal Protein

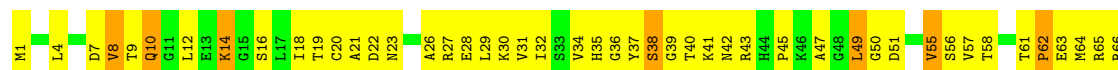




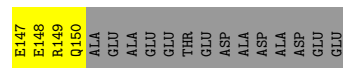
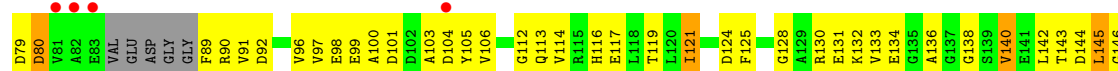
• Molecule 12: 50S ribosomal protein L13P



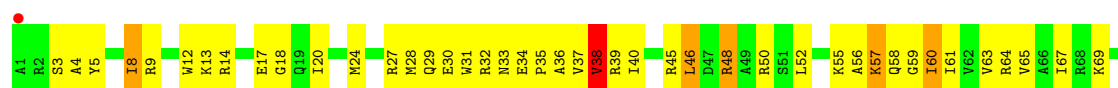
• Molecule 13: 50S ribosomal protein L14P



• Molecule 14: 50S ribosomal protein L15P



• Molecule 15: L15 Ribosomal Protein

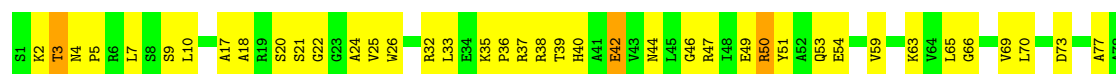




• Molecule 16: 50S ribosomal protein L18P



• Molecule 17: 50S ribosomal protein L18e



• Molecule 18: 50S ribosomal protein L19E

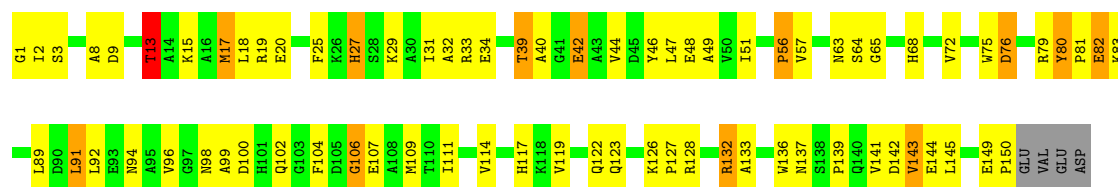


• Molecule 19: 50S ribosomal protein L21e



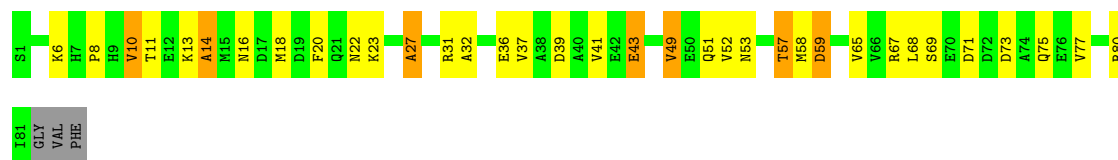
• Molecule 20: 50S ribosomal protein L22P

Chain S:  49% 40% 8% . .



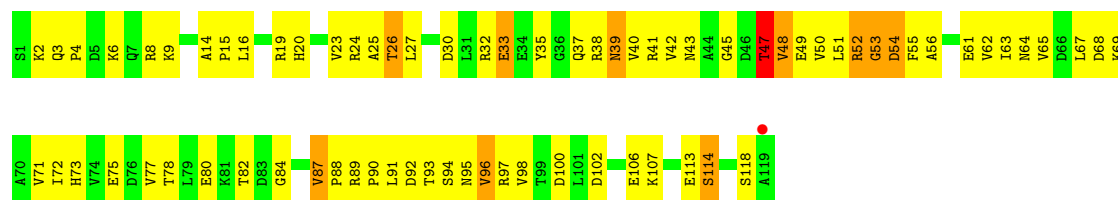
• Molecule 21: 50S ribosomal protein L23P

Chain T:  55% 33% 8% .

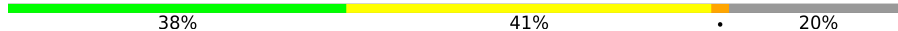


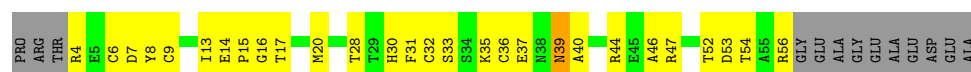
• Molecule 22: 50S ribosomal protein L24P

Chain U:  38% 53% 8% .



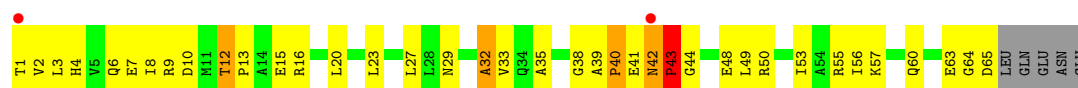
• Molecule 23: 50S ribosomal protein L24E

Chain V:  38% 41% 20%



• Molecule 24: 50S ribosomal protein L29P

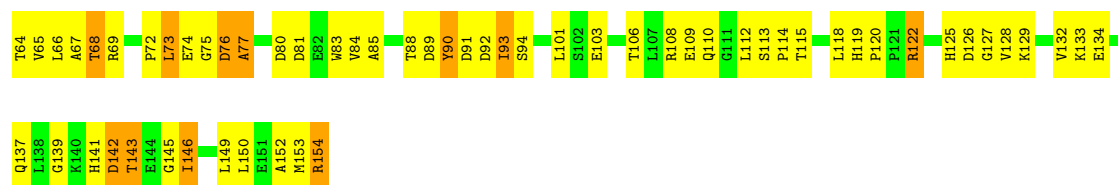
Chain W:  3% 39% 47% 6% 7%



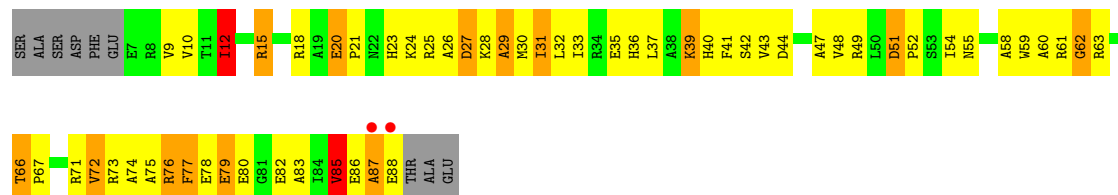
• Molecule 25: 50S ribosomal protein L30P

Chain X:  33% 55% 12%

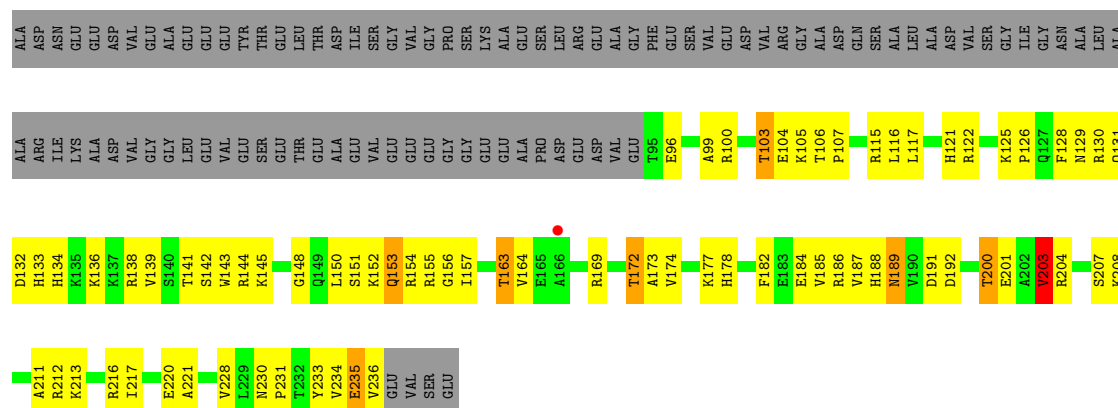
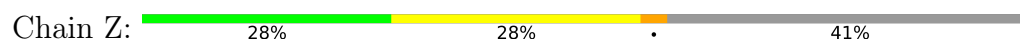




• Molecule 26: 50S ribosomal protein L31e



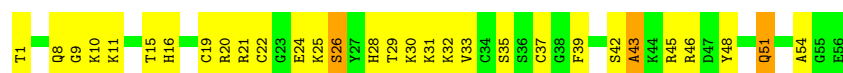
• Molecule 27: 50S ribosomal protein L32E



• Molecule 28: L37Ae 50S ribosomal protein



• Molecule 29: 50S ribosomal protein L37e



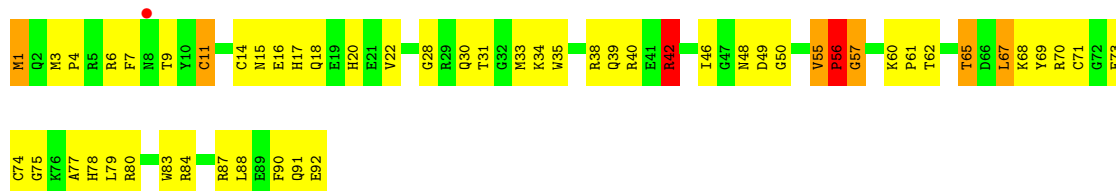
- Molecule 30: 50S ribosomal protein L39e

Chain 3:  44% 50% . .



- Molecule 31: 50S ribosomal protein L44E

Chain 4:  % 41% 50% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.20 19.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.1 (19.99-3.20) 91.7 (19.99-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.280 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	98616	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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: PUY, CD, CL, PO4, MG, K, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.75	21/66076 (0.0%)	0.96	213/103052 (0.2%)
2	B	0.68	0/2905	0.98	11/4528 (0.2%)
3	5	1.18	0/64	1.27	1/97 (1.0%)
4	C	0.97	4/1787 (0.2%)	1.36	16/2409 (0.7%)
5	D	0.94	4/2689 (0.1%)	1.40	37/3652 (1.0%)
6	E	0.96	3/1883 (0.2%)	1.35	24/2551 (0.9%)
7	F	0.75	0/1111	1.12	9/1498 (0.6%)
8	G	0.91	2/1382 (0.1%)	1.22	8/1880 (0.4%)
9	H	0.83	0/896	1.26	6/1219 (0.5%)
10	I	1.23	1/241 (0.4%)	1.27	1/324 (0.3%)
11	J	0.99	0/1246	1.61	34/1686 (2.0%)
12	K	0.97	1/1135 (0.1%)	1.24	7/1530 (0.5%)
13	L	1.00	2/1003 (0.2%)	1.51	16/1351 (1.2%)
14	M	0.91	0/1126	1.42	19/1504 (1.3%)
15	N	1.10	5/1633 (0.3%)	1.44	15/2180 (0.7%)
16	O	0.86	1/1473 (0.1%)	1.47	27/1999 (1.4%)
17	P	0.98	1/873 (0.1%)	1.39	12/1181 (1.0%)
18	Q	0.89	2/1143 (0.2%)	1.31	12/1521 (0.8%)
19	R	0.98	2/748 (0.3%)	1.46	9/1005 (0.9%)
20	S	1.05	1/1172 (0.1%)	1.39	16/1578 (1.0%)
21	T	0.93	1/648 (0.2%)	1.35	8/875 (0.9%)
22	U	0.90	1/957 (0.1%)	1.39	15/1289 (1.2%)
23	V	0.96	0/417	1.27	1/562 (0.2%)
24	W	0.82	1/502 (0.2%)	1.33	5/675 (0.7%)
25	X	0.99	2/1218 (0.2%)	1.36	15/1655 (0.9%)
26	Y	0.96	0/664	1.49	17/895 (1.9%)
27	Z	0.94	1/1146 (0.1%)	1.32	8/1536 (0.5%)
28	1	0.96	0/575	1.35	6/763 (0.8%)
29	2	0.97	0/437	1.41	6/578 (1.0%)
30	3	0.81	0/398	1.16	0/527
31	4	0.89	1/771 (0.1%)	1.33	7/1024 (0.7%)
All	All	0.81	57/98319 (0.1%)	1.09	581/147124 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	386
2	B	1	12
5	D	0	2
6	E	0	1
25	X	0	1
29	2	0	1
All	All	2	403

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2636	C	C3'-O3'	11.13	1.58	1.42
1	A	2638	G	P-OP2	10.90	1.70	1.49
1	A	2619	U	C3'-O3'	9.95	1.57	1.42
1	A	2619	U	C2'-O2'	-9.58	1.28	1.42
25	X	44	MET	SD-CE	-9.22	1.56	1.79

The worst 5 of 581 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-15.25	62.25	108.00
1	A	1563	G	C2'-C3'-O3'	15.06	132.10	109.50
11	J	74	ASN	N-CA-C	-14.21	93.78	114.39
11	J	141	ASN	N-CA-C	-14.10	96.04	113.38
2	B	3024	U	C2'-C3'-O3'	13.97	130.45	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

5 of 403 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	A	Sidechain
1	A	30	U	Sidechain
1	A	44	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	55	U	Sidechain
1	A	57	C	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	A	59017	0	29801	2027	0
2	B	2600	0	1326	129	0
3	5	58	0	34	2	0
4	C	1754	0	1763	164	0
5	D	2624	0	2533	242	0
6	E	1858	0	1816	201	0
7	F	1094	0	1085	182	0
8	G	1357	0	1266	110	0
9	H	885	0	854	79	0
10	I	240	0	231	35	0
11	J	1215	0	1215	197	0
12	K	1119	0	1098	84	0
13	L	993	0	1027	95	0
14	M	1114	0	1072	88	0
15	N	1605	0	1676	211	0
16	O	1444	0	1401	188	0
17	P	864	0	873	68	0
18	Q	1133	0	1127	77	0
19	R	734	0	728	66	0
20	S	1149	0	1122	91	0
21	T	641	0	605	28	0
22	U	949	0	923	91	0
23	V	410	0	364	47	0
24	W	499	0	511	43	0
25	X	1195	0	1137	135	0
26	Y	654	0	653	69	0
27	Z	1130	0	1133	87	0
28	1	563	0	599	77	0
29	2	430	0	427	38	0
30	3	393	0	406	35	0
31	4	755	0	730	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	5	1	0	0	0	0
32	A	109	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	72	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	1	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
35	4	1	0	0	0	0
35	A	11	0	0	2	0
35	C	1	0	0	1	0
35	D	1	0	0	0	0
35	K	3	0	0	2	0
35	N	1	0	0	1	0
35	O	1	0	0	1	0
35	P	1	0	0	1	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	5	3	0	0	1	0
37	5	34	0	28	0	0
38	1	1	0	0	0	0
38	2	1	0	0	0	0
38	4	1	0	0	1	0
38	P	1	0	0	0	0
38	V	1	0	0	0	0
39	1	36	0	0	14	0
39	2	63	0	0	13	0
39	3	42	0	0	7	0
39	4	73	0	0	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	5	6	0	0	0	0
39	A	5861	0	0	566	2
39	B	154	0	0	27	0
39	C	123	0	0	34	0
39	D	149	0	0	37	0
39	E	178	0	0	56	0
39	F	50	0	0	35	0
39	G	46	0	0	17	0
39	H	27	0	0	14	0
39	I	20	0	0	5	0
39	J	75	0	0	35	0
39	K	56	0	0	10	0
39	L	60	0	0	20	0
39	M	90	0	0	27	0
39	N	128	0	0	35	0
39	O	63	0	0	42	0
39	P	45	0	0	22	0
39	Q	62	0	0	12	0
39	R	53	0	0	10	0
39	S	86	0	0	15	0
39	T	36	0	0	6	0
39	U	42	0	0	14	0
39	V	30	0	0	11	0
39	W	15	0	0	5	1
39	X	73	0	0	22	0
39	Y	30	0	0	11	0
39	Z	99	0	0	22	0
All	All	98616	0	59564	4657	2

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 31.

The worst 5 of 4657 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)
1:A:871:G:H5'	1:A:871:G:C8	1.74	1.23
30:3:39:ARG:HG2	39:3:3143:HOH:O	1.36	1.22
2:B:3006:C:H5''	16:O:37:ARG:NH1	1.55	1.19
1:A:1702:U:H5''	39:A:6685:HOH:O	1.35	1.19
5:D:62:ARG:HA	5:D:65:MET:HE3	1.21	1.19

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A:5574:HOH:O	39:W:2786:HOH:O[4_565]	2.14	0.06
39:A:3438:HOH:O	39:A:9956:HOH:O[5_445]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	235/239 (98%)	204 (87%)	23 (10%)	8 (3%)	3	20
5	D	335/337 (99%)	297 (89%)	28 (8%)	10 (3%)	3	23
6	E	244/246 (99%)	206 (84%)	34 (14%)	4 (2%)	7	36
7	F	134/176 (76%)	95 (71%)	26 (19%)	13 (10%)	0	3
8	G	170/177 (96%)	160 (94%)	9 (5%)	1 (1%)	21	56
9	H	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	7	35
10	I	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	J	152/167 (91%)	130 (86%)	13 (9%)	9 (6%)	1	10
12	K	140/145 (97%)	125 (89%)	11 (8%)	4 (3%)	3	24
13	L	130/132 (98%)	110 (85%)	15 (12%)	5 (4%)	2	18
14	M	141/164 (86%)	114 (81%)	25 (18%)	2 (1%)	9	39
15	N	192/194 (99%)	167 (87%)	22 (12%)	3 (2%)	7	36
16	O	184/186 (99%)	153 (83%)	23 (12%)	8 (4%)	2	16
17	P	113/115 (98%)	107 (95%)	4 (4%)	2 (2%)	6	34
18	Q	141/148 (95%)	129 (92%)	12 (8%)	0	100	100
19	R	93/95 (98%)	89 (96%)	3 (3%)	1 (1%)	11	43
20	S	148/154 (96%)	132 (89%)	15 (10%)	1 (1%)	18	52
21	T	79/84 (94%)	75 (95%)	3 (4%)	1 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	U	117/119 (98%)	103 (88%)	11 (9%)	3 (3%)	4	26
23	V	51/66 (77%)	45 (88%)	5 (10%)	1 (2%)	6	31
24	W	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	3	21
25	X	152/154 (99%)	141 (93%)	8 (5%)	3 (2%)	6	31
26	Y	80/91 (88%)	69 (86%)	8 (10%)	3 (4%)	2	18
27	Z	140/240 (58%)	133 (95%)	7 (5%)	0	100	100
28	1	71/73 (97%)	58 (82%)	11 (16%)	2 (3%)	4	25
29	2	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	81 (90%)	7 (8%)	2 (2%)	5	29
All	All	3633/4235 (86%)	3196 (88%)	347 (10%)	90 (2%)	4	27

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	11	HIS
7	F	93	LEU
7	F	95	THR
7	F	173	GLU

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	
4	C	179/181 (99%)	167 (93%)	12 (7%)	15	47
5	D	282/282 (100%)	261 (93%)	21 (7%)	13	43
6	E	193/193 (100%)	173 (90%)	20 (10%)	7	28
7	F	117/147 (80%)	109 (93%)	8 (7%)	14	46
8	G	152/155 (98%)	143 (94%)	9 (6%)	18	50
9	H	92/92 (100%)	89 (97%)	3 (3%)	33	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	I	27/283 (10%)	26 (96%)	1 (4%)	30	63
11	J	122/122 (100%)	109 (89%)	13 (11%)	6	27
12	K	118/121 (98%)	109 (92%)	9 (8%)	12	42
13	L	106/106 (100%)	101 (95%)	5 (5%)	23	57
14	M	112/126 (89%)	108 (96%)	4 (4%)	31	63
15	N	166/166 (100%)	156 (94%)	10 (6%)	17	50
16	O	149/149 (100%)	141 (95%)	8 (5%)	20	53
17	P	93/93 (100%)	88 (95%)	5 (5%)	20	53
18	Q	113/116 (97%)	108 (96%)	5 (4%)	25	59
19	R	79/79 (100%)	74 (94%)	5 (6%)	16	48
20	S	117/121 (97%)	111 (95%)	6 (5%)	21	54
21	T	71/73 (97%)	70 (99%)	1 (1%)	59	77
22	U	105/105 (100%)	100 (95%)	5 (5%)	23	56
23	V	44/52 (85%)	43 (98%)	1 (2%)	44	70
24	W	51/56 (91%)	50 (98%)	1 (2%)	48	72
25	X	130/130 (100%)	120 (92%)	10 (8%)	12	41
26	Y	66/73 (90%)	59 (89%)	7 (11%)	6	27
27	Z	120/195 (62%)	112 (93%)	8 (7%)	15	47
28	1	56/56 (100%)	52 (93%)	4 (7%)	13	44
29	2	46/46 (100%)	45 (98%)	1 (2%)	45	71
30	3	42/44 (96%)	41 (98%)	1 (2%)	43	70
31	4	79/79 (100%)	76 (96%)	3 (4%)	29	62
All	All	3027/3441 (88%)	2841 (94%)	186 (6%)	17	49

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	O	26	LEU
20	S	143	VAL
16	O	128	ASP
18	Q	94	TRP
23	V	28	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	66	GLN
22	U	73	HIS
18	Q	118	GLN
20	S	98	ASN
25	X	2	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	273 (9%)	44 (1%)
2	B	121/122 (99%)	19 (15%)	5 (4%)
3	5	1/3 (33%)	0	0
All	All	2869/3047 (94%)	292 (10%)	49 (1%)

5 of 292 RNA backbone outliers are listed below:

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

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1504	A
1	A	1979	G
1	A	1563	G
1	A	1738	C
1	A	2011	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 234 ligands modelled in this entry, 232 are monoatomic - leaving 2 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	PUY	5	78	36	37,37,37	3.01	13 (35%)	48,53,53	1.79	10 (20%)
36	PO4	5	77	37,3	0,2,4	-	-	0,1,6	-	-

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	PUY	5	78	36	-	4/24/40/40	0/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	5	78	PUY	CE2-CZ	8.28	1.54	1.38
37	5	78	PUY	CD1-CG	7.25	1.53	1.38
37	5	78	PUY	CD2-CG	6.60	1.51	1.38
37	5	78	PUY	C-N3'	6.18	1.47	1.34
37	5	78	PUY	OM-CMZ	-5.09	1.28	1.42

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	5	78	PUY	CG-CB-CA	-5.35	103.18	114.13
37	5	78	PUY	CMZ-OM-CZ	5.15	128.54	117.50
37	5	78	PUY	O-C-N3'	-4.35	115.18	122.96
37	5	78	PUY	C2-N1-C6	3.24	119.75	111.83
37	5	78	PUY	CB-CA-C	-3.14	101.63	108.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

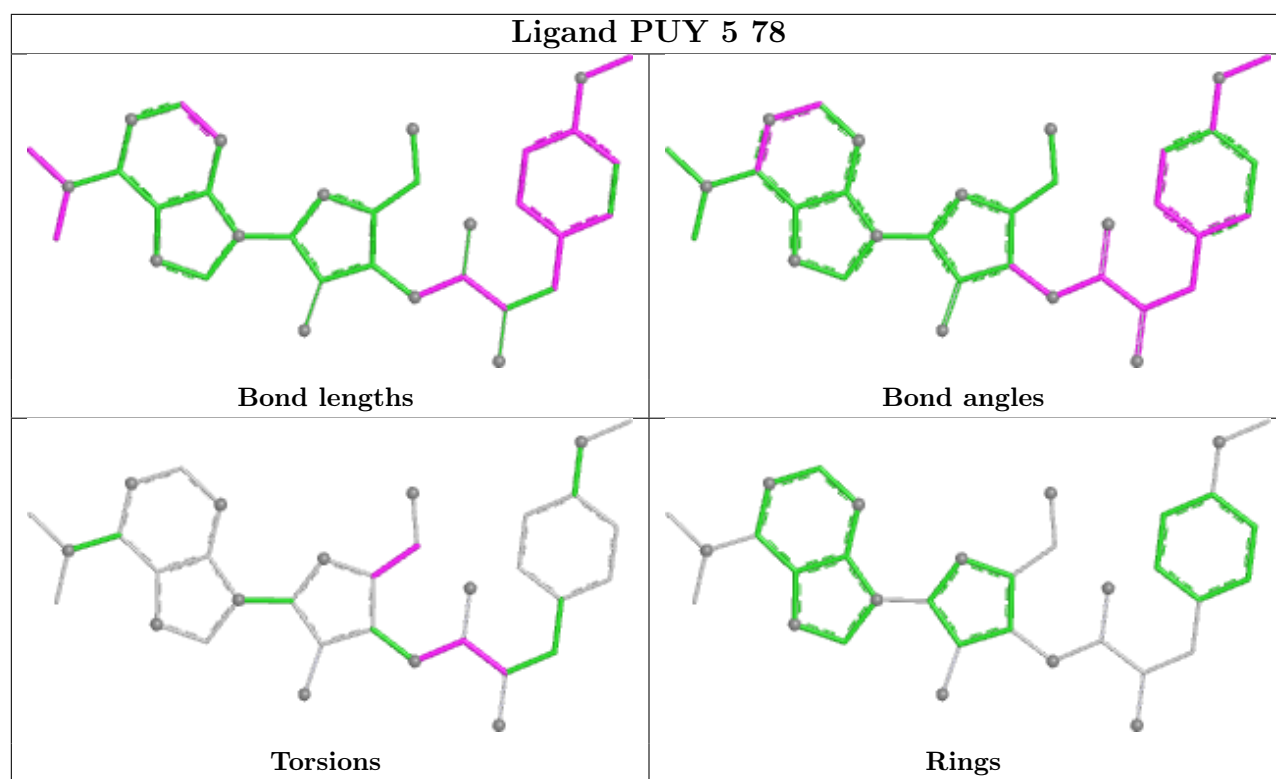
Mol	Chain	Res	Type	Atoms
37	5	78	PUY	N3'-C-CA-CB
37	5	78	PUY	C3'-C4'-C5'-O5'
37	5	78	PUY	O-C-N3'-C3'
37	5	78	PUY	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	77	PO4	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	A	2754/2922 (94%)	-0.32	48 (1%) 69 49	24, 50, 96, 142	0
2	B	122/122 (100%)	0.06	5 (4%) 41 25	36, 65, 94, 147	0
3	5	3/3 (100%)	0.06	0 100 100	53, 53, 56, 62	0
4	C	237/239 (99%)	-0.13	4 (1%) 69 49	29, 59, 91, 111	0
5	D	337/337 (100%)	-0.14	1 (0%) 90 81	23, 55, 83, 90	0
6	E	246/246 (100%)	-0.20	1 (0%) 88 79	29, 54, 76, 85	0
7	F	140/176 (79%)	0.63	7 (5%) 34 22	62, 101, 118, 131	0
8	G	172/177 (97%)	0.11	1 (0%) 85 73	40, 69, 91, 96	0
9	H	119/119 (100%)	0.20	0 100 100	58, 81, 101, 106	0
10	I	29/348 (8%)	1.62	11 (37%) 1 1	82, 96, 102, 103	0
11	J	156/167 (93%)	0.04	5 (3%) 50 31	33, 54, 85, 93	0
12	K	142/145 (97%)	-0.27	0 100 100	32, 48, 71, 87	0
13	L	132/132 (100%)	-0.23	1 (0%) 82 67	28, 51, 73, 82	0
14	M	145/164 (88%)	0.20	4 (2%) 55 35	24, 76, 110, 119	0
15	N	194/194 (100%)	-0.15	2 (1%) 79 63	37, 52, 69, 78	0
16	O	186/186 (100%)	0.42	7 (3%) 44 27	43, 70, 109, 120	0
17	P	115/115 (100%)	-0.02	0 100 100	48, 61, 81, 85	0
18	Q	143/148 (96%)	-0.07	0 100 100	40, 62, 75, 80	0
19	R	95/95 (100%)	-0.31	0 100 100	29, 49, 59, 74	0
20	S	150/154 (97%)	-0.32	0 100 100	31, 47, 66, 72	0
21	T	81/84 (96%)	0.04	0 100 100	53, 70, 85, 90	0
22	U	119/119 (100%)	0.15	1 (0%) 82 67	48, 63, 85, 94	0
23	V	53/66 (80%)	-0.07	0 100 100	43, 57, 74, 81	0
24	W	65/70 (92%)	0.28	2 (3%) 51 32	61, 81, 110, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	154/154 (100%)	-0.36	0 100 100	37, 49, 67, 76	0
26	Y	82/91 (90%)	0.07	2 (2%) 59 40	38, 62, 81, 97	0
27	Z	142/240 (59%)	-0.26	1 (0%) 84 69	30, 51, 74, 89	0
28	1	73/73 (100%)	0.17	1 (1%) 73 54	52, 66, 80, 84	0
29	2	56/56 (100%)	-0.44	0 100 100	25, 40, 46, 48	0
30	3	46/48 (95%)	0.06	0 100 100	43, 65, 86, 95	0
31	4	92/92 (100%)	-0.08	1 (1%) 78 61	36, 62, 72, 78	0
All	All	6580/7282 (90%)	-0.15	105 (1%) 70 51	23, 56, 97, 147	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1175	G	5.8
1	A	1173	A	5.2
1	A	1176	C	4.8
24	W	1	THR	4.3
10	I	27	ILE	4.2

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
34	NA	A	8332	1/1	0.53	0.22	37,37,37,37	0
34	NA	A	8384	1/1	0.55	0.29	103,103,103,103	0
34	NA	B	8383	1/1	0.60	0.46	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8066	1/1	0.65	0.12	84,84,84,84	0
34	NA	A	8323	1/1	0.68	0.18	62,62,62,62	0
34	NA	A	8360	1/1	0.68	0.23	37,37,37,37	0
32	MG	A	8087	1/1	0.69	0.16	41,41,41,41	0
34	NA	A	8357	1/1	0.73	0.16	43,43,43,43	0
34	NA	A	8341	1/1	0.74	0.15	40,40,40,40	0
34	NA	A	8372	1/1	0.75	0.08	25,25,25,25	0
35	CL	A	8513	1/1	0.75	0.20	81,81,81,81	0
32	MG	A	8046	1/1	0.76	0.17	62,62,62,62	0
32	MG	A	8050	1/1	0.76	0.09	41,41,41,41	0
34	NA	A	8334	1/1	0.76	0.13	30,30,30,30	0
34	NA	A	8366	1/1	0.76	0.12	58,58,58,58	0
34	NA	T	8312	1/1	0.77	0.19	122,122,122,122	0
34	NA	A	8370	1/1	0.77	0.59	93,93,93,93	0
35	CL	O	8507	1/1	0.77	0.11	102,102,102,102	0
32	MG	A	8044	1/1	0.78	0.13	68,68,68,68	0
34	NA	A	8355	1/1	0.79	0.15	60,60,60,60	0
35	CL	A	8517	1/1	0.81	0.10	61,61,61,61	0
32	MG	A	8102	1/1	0.82	0.14	83,83,83,83	0
32	MG	A	8103	1/1	0.82	0.21	57,57,57,57	0
35	CL	A	8505	1/1	0.83	0.09	65,65,65,65	0
34	NA	B	8351	1/1	0.83	0.08	67,67,67,67	0
34	NA	A	8303	1/1	0.83	0.28	42,42,42,42	0
34	NA	A	8363	1/1	0.83	0.49	100,100,100,100	0
35	CL	A	8522	1/1	0.84	0.27	57,57,57,57	0
35	CL	C	8509	1/1	0.84	0.14	66,66,66,66	0
32	MG	A	8089	1/1	0.84	0.11	104,104,104,104	0
35	CL	A	8515	1/1	0.85	0.32	131,131,131,131	0
34	NA	A	8307	1/1	0.85	0.16	34,34,34,34	0
34	NA	A	8316	1/1	0.85	0.12	42,42,42,42	0
34	NA	A	8385	1/1	0.85	0.14	22,22,22,22	0
32	MG	A	8070	1/1	0.85	0.42	101,101,101,101	0
34	NA	A	8371	1/1	0.87	0.19	32,32,32,32	0
32	MG	B	8095	1/1	0.87	0.21	85,85,85,85	0
32	MG	A	8024	1/1	0.88	0.83	108,108,108,108	0
32	MG	A	8067	1/1	0.88	0.10	22,22,22,22	0
34	NA	A	8375	1/1	0.88	0.26	42,42,42,42	0
34	NA	A	8382	1/1	0.88	0.34	52,52,52,52	0
34	NA	A	8328	1/1	0.88	0.12	52,52,52,52	0
35	CL	A	8511	1/1	0.88	0.27	92,92,92,92	0
35	CL	P	8508	1/1	0.88	0.14	113,113,113,113	0
37	PUY	5	78	34/34	0.88	0.15	66,69,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	A	8326	1/1	0.89	0.11	35,35,35,35	0
32	MG	A	8053	1/1	0.89	0.09	85,85,85,85	0
38	CD	P	8405	1/1	0.89	0.17	196,196,196,196	0
34	NA	A	8365	1/1	0.90	0.11	29,29,29,29	0
32	MG	A	8104	1/1	0.90	0.08	31,31,31,31	0
35	CL	A	8510	1/1	0.90	0.15	101,101,101,101	0
32	MG	A	8108	1/1	0.90	0.13	50,50,50,50	0
32	MG	A	8042	1/1	0.90	0.08	25,25,25,25	0
34	NA	A	8350	1/1	0.90	0.16	18,18,18,18	0
34	NA	A	8324	1/1	0.90	0.27	32,32,32,32	0
34	NA	A	8356	1/1	0.90	0.25	86,86,86,86	0
32	MG	1	8105	1/1	0.90	0.07	32,32,32,32	0
34	NA	A	8359	1/1	0.90	0.13	47,47,47,47	0
32	MG	A	8039	1/1	0.90	0.13	57,57,57,57	0
35	CL	4	8504	1/1	0.90	0.11	69,69,69,69	0
34	NA	A	8329	1/1	0.90	0.13	40,40,40,40	0
34	NA	S	8337	1/1	0.90	0.09	70,70,70,70	0
34	NA	S	8386	1/1	0.91	0.19	48,48,48,48	0
34	NA	A	8314	1/1	0.91	0.08	29,29,29,29	0
32	MG	A	8116	1/1	0.91	0.10	95,95,95,95	0
33	K	A	8202	1/1	0.91	0.07	56,56,56,56	0
34	NA	A	8336	1/1	0.91	0.07	51,51,51,51	0
34	NA	A	8367	1/1	0.92	0.11	22,22,22,22	0
34	NA	A	8361	1/1	0.92	0.07	35,35,35,35	0
34	NA	A	8362	1/1	0.92	0.15	38,38,38,38	0
32	MG	A	8045	1/1	0.92	0.07	63,63,63,63	0
34	NA	J	8322	1/1	0.92	0.11	26,26,26,26	0
32	MG	A	8041	1/1	0.92	0.10	80,80,80,80	0
34	NA	A	8349	1/1	0.92	0.11	25,25,25,25	0
35	CL	K	8502	1/1	0.93	0.08	91,91,91,91	0
32	MG	A	8052	1/1	0.93	0.06	24,24,24,24	0
32	MG	A	8072	1/1	0.93	0.07	55,55,55,55	0
35	CL	Z	8520	1/1	0.93	0.08	64,64,64,64	0
32	MG	A	8076	1/1	0.93	0.13	134,134,134,134	0
34	NA	A	8335	1/1	0.93	0.12	43,43,43,43	0
32	MG	A	8115	1/1	0.93	0.04	51,51,51,51	0
34	NA	C	8345	1/1	0.94	0.08	68,68,68,68	0
32	MG	A	8111	1/1	0.94	0.06	82,82,82,82	0
34	NA	A	8305	1/1	0.94	0.06	10,10,10,10	0
32	MG	A	8097	1/1	0.94	0.11	64,64,64,64	0
34	NA	A	8377	1/1	0.94	0.39	70,70,70,70	0
32	MG	A	8098	1/1	0.94	0.18	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	CL	S	8506	1/1	0.94	0.14	77,77,77,77	0
34	NA	A	8327	1/1	0.94	0.14	24,24,24,24	0
34	NA	A	8340	1/1	0.94	0.13	29,29,29,29	0
34	NA	A	8368	1/1	0.94	0.14	35,35,35,35	0
34	NA	A	8315	1/1	0.94	0.07	25,25,25,25	0
34	NA	K	8346	1/1	0.95	0.04	7,7,7,7	0
34	NA	A	8330	1/1	0.95	0.09	36,36,36,36	0
32	MG	A	8027	1/1	0.95	0.04	60,60,60,60	0
34	NA	A	8306	1/1	0.95	0.10	35,35,35,35	0
32	MG	A	8051	1/1	0.95	0.11	93,93,93,93	0
34	NA	A	8311	1/1	0.95	0.08	43,43,43,43	0
32	MG	A	8047	1/1	0.95	0.09	62,62,62,62	0
32	MG	A	8049	1/1	0.95	0.07	49,49,49,49	0
32	MG	A	8101	1/1	0.95	0.09	49,49,49,49	0
34	NA	A	8373	1/1	0.95	0.09	36,36,36,36	0
34	NA	A	8319	1/1	0.95	0.13	43,43,43,43	0
34	NA	A	8354	1/1	0.95	0.06	16,16,16,16	0
35	CL	K	8501	1/1	0.95	0.07	55,55,55,55	0
34	NA	A	8378	1/1	0.95	0.07	18,18,18,18	0
32	MG	5	8114	1/1	0.95	0.14	44,44,44,44	0
32	MG	A	8063	1/1	0.95	0.06	64,64,64,64	0
34	NA	A	8325	1/1	0.95	0.07	48,48,48,48	0
32	MG	A	8085	1/1	0.95	0.04	39,39,39,39	0
34	NA	A	8301	1/1	0.95	0.06	22,22,22,22	0
34	NA	A	8302	1/1	0.95	0.09	25,25,25,25	0
32	MG	A	8086	1/1	0.95	0.06	75,75,75,75	0
32	MG	A	8112	1/1	0.96	0.09	58,58,58,58	0
34	NA	A	8381	1/1	0.96	0.15	51,51,51,51	0
35	CL	A	8512	1/1	0.96	0.11	30,30,30,30	0
32	MG	A	8032	1/1	0.96	0.04	23,23,23,23	0
34	NA	A	8352	1/1	0.96	0.09	17,17,17,17	0
35	CL	A	8516	1/1	0.96	0.09	37,37,37,37	0
32	MG	A	8092	1/1	0.96	0.07	58,58,58,58	0
32	MG	A	8117	1/1	0.96	0.06	1,1,1,1	0
34	NA	A	8369	1/1	0.96	0.15	49,49,49,49	0
35	CL	D	8519	1/1	0.96	0.07	55,55,55,55	0
34	NA	A	8320	1/1	0.96	0.07	29,29,29,29	0
34	NA	A	8321	1/1	0.96	0.11	52,52,52,52	0
34	NA	A	8308	1/1	0.96	0.06	40,40,40,40	0
34	NA	M	8380	1/1	0.96	0.10	73,73,73,73	0
34	NA	A	8310	1/1	0.96	0.15	22,22,22,22	0
34	NA	A	8374	1/1	0.96	0.13	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8100	1/1	0.96	0.08	51,51,51,51	0
36	PO4	5	77	3/5	0.96	0.08	67,67,68,68	0
35	CL	A	8503	1/1	0.96	0.08	62,62,62,62	0
34	NA	A	8313	1/1	0.96	0.05	47,47,47,47	0
34	NA	A	8358	1/1	0.97	0.23	109,109,109,109	0
32	MG	A	8090	1/1	0.97	0.09	46,46,46,46	0
32	MG	A	8075	1/1	0.97	0.06	42,42,42,42	0
33	K	A	8201	1/1	0.97	0.07	76,76,76,76	0
35	CL	K	8521	1/1	0.97	0.07	47,47,47,47	0
35	CL	N	8518	1/1	0.97	0.06	50,50,50,50	0
32	MG	A	8113	1/1	0.97	0.07	29,29,29,29	0
32	MG	A	8094	1/1	0.97	0.07	50,50,50,50	0
34	NA	E	8304	1/1	0.97	0.10	4,4,4,4	0
34	NA	J	8309	1/1	0.97	0.10	21,21,21,21	0
34	NA	A	8333	1/1	0.97	0.05	14,14,14,14	0
32	MG	A	8057	1/1	0.97	0.05	15,15,15,15	0
32	MG	A	8023	1/1	0.97	0.05	35,35,35,35	0
32	MG	A	8099	1/1	0.97	0.09	43,43,43,43	0
32	MG	A	8088	1/1	0.98	0.04	12,12,12,12	0
34	NA	A	8331	1/1	0.98	0.09	35,35,35,35	0
35	CL	A	8514	1/1	0.98	0.04	45,45,45,45	0
32	MG	A	8001	1/1	0.98	0.03	31,31,31,31	0
32	MG	A	8068	1/1	0.98	0.04	44,44,44,44	0
34	NA	A	8318	1/1	0.98	0.09	65,65,65,65	0
32	MG	A	8014	1/1	0.98	0.03	18,18,18,18	0
32	MG	A	8110	1/1	0.98	0.08	54,54,54,54	0
34	NA	A	8364	1/1	0.98	0.06	12,12,12,12	0
34	NA	A	8339	1/1	0.98	0.03	30,30,30,30	0
32	MG	A	8093	1/1	0.98	0.04	16,16,16,16	0
32	MG	A	8055	1/1	0.98	0.04	29,29,29,29	0
34	NA	A	8343	1/1	0.98	0.06	9,9,9,9	0
34	NA	A	8344	1/1	0.98	0.03	11,11,11,11	0
32	MG	A	8096	1/1	0.98	0.05	33,33,33,33	0
32	MG	A	8017	1/1	0.98	0.04	40,40,40,40	0
32	MG	A	8059	1/1	0.98	0.07	119,119,119,119	0
34	NA	A	8353	1/1	0.98	0.04	13,13,13,13	0
32	MG	A	8028	1/1	0.98	0.05	75,75,75,75	0
32	MG	A	8064	1/1	0.98	0.09	31,31,31,31	0
32	MG	A	8019	1/1	0.98	0.08	31,31,31,31	0
32	MG	4	8078	1/1	0.99	0.02	23,23,23,23	0
32	MG	A	8030	1/1	0.99	0.04	68,68,68,68	0
32	MG	A	8005	1/1	0.99	0.04	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	A	8342	1/1	0.99	0.09	30,30,30,30	0
32	MG	A	8033	1/1	0.99	0.03	42,42,42,42	0
32	MG	A	8035	1/1	0.99	0.03	70,70,70,70	0
32	MG	A	8054	1/1	0.99	0.04	46,46,46,46	0
32	MG	A	8036	1/1	0.99	0.03	29,29,29,29	0
32	MG	A	8056	1/1	0.99	0.05	75,75,75,75	0
32	MG	A	8037	1/1	0.99	0.03	41,41,41,41	0
34	NA	N	8347	1/1	0.99	0.03	19,19,19,19	0
34	NA	R	8348	1/1	0.99	0.04	18,18,18,18	0
32	MG	A	8018	1/1	0.99	0.04	24,24,24,24	0
34	NA	S	8338	1/1	0.99	0.05	65,65,65,65	0
32	MG	A	8060	1/1	0.99	0.05	43,43,43,43	0
32	MG	A	8061	1/1	0.99	0.04	33,33,33,33	0
32	MG	A	8062	1/1	0.99	0.02	38,38,38,38	0
32	MG	A	8040	1/1	0.99	0.10	33,33,33,33	0
32	MG	A	8006	1/1	0.99	0.03	33,33,33,33	0
32	MG	A	8022	1/1	0.99	0.04	22,22,22,22	0
34	NA	A	8317	1/1	0.99	0.02	25,25,25,25	0
32	MG	A	8043	1/1	0.99	0.04	50,50,50,50	0
32	MG	A	8008	1/1	0.99	0.08	40,40,40,40	0
32	MG	A	8106	1/1	0.99	0.04	69,69,69,69	0
32	MG	A	8107	1/1	0.99	0.02	46,46,46,46	0
32	MG	A	8011	1/1	0.99	0.03	27,27,27,27	0
32	MG	A	8071	1/1	0.99	0.04	52,52,52,52	0
32	MG	A	8025	1/1	0.99	0.05	12,12,12,12	0
32	MG	A	8003	1/1	0.99	0.04	30,30,30,30	0
32	MG	A	8048	1/1	0.99	0.02	33,33,33,33	0
32	MG	A	8079	1/1	0.99	0.03	25,25,25,25	0
32	MG	A	8080	1/1	0.99	0.03	38,38,38,38	0
32	MG	A	8081	1/1	0.99	0.04	29,29,29,29	0
32	MG	A	8082	1/1	0.99	0.03	16,16,16,16	0
32	MG	A	8084	1/1	0.99	0.09	34,34,34,34	0
34	NA	A	8376	1/1	0.99	0.04	27,27,27,27	0
32	MG	C	8065	1/1	0.99	0.03	85,85,85,85	0
32	MG	U	8073	1/1	0.99	0.07	21,21,21,21	0
34	NA	A	8379	1/1	0.99	0.08	33,33,33,33	0
32	MG	Z	8109	1/1	0.99	0.03	32,32,32,32	0
32	MG	A	8016	1/1	0.99	0.06	23,23,23,23	0
38	CD	V	8401	1/1	0.99	0.02	70,70,70,70	0
38	CD	2	8402	1/1	0.99	0.03	72,72,72,72	0
38	CD	4	8404	1/1	0.99	0.02	67,67,67,67	0
32	MG	A	8013	1/1	1.00	0.02	21,21,21,21	0

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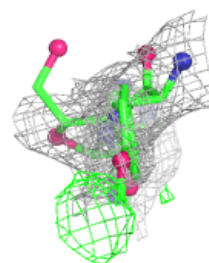
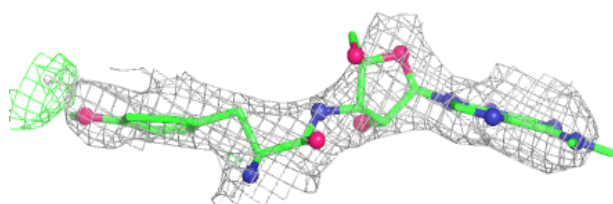
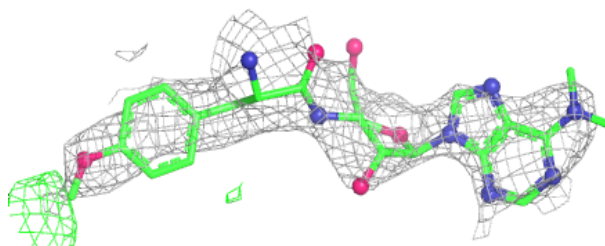
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8038	1/1	1.00	0.01	43,43,43,43	0
32	MG	A	8007	1/1	1.00	0.02	9,9,9,9	0
32	MG	A	8074	1/1	1.00	0.04	16,16,16,16	0
32	MG	A	8015	1/1	1.00	0.01	66,66,66,66	0
32	MG	L	8069	1/1	1.00	0.03	105,105,105,105	0
32	MG	A	8026	1/1	1.00	0.02	45,45,45,45	0
32	MG	A	8077	1/1	1.00	0.03	39,39,39,39	0
32	MG	A	8002	1/1	1.00	0.06	15,15,15,15	0
32	MG	A	8058	1/1	1.00	0.01	33,33,33,33	0
32	MG	A	8009	1/1	1.00	0.03	14,14,14,14	0
32	MG	A	8029	1/1	1.00	0.03	34,34,34,34	0
32	MG	A	8083	1/1	1.00	0.02	32,32,32,32	0
32	MG	A	8010	1/1	1.00	0.02	26,26,26,26	0
32	MG	A	8031	1/1	1.00	0.01	29,29,29,29	0
32	MG	A	8004	1/1	1.00	0.02	43,43,43,43	0
32	MG	A	8020	1/1	1.00	0.02	36,36,36,36	0
32	MG	A	8034	1/1	1.00	0.02	50,50,50,50	0
32	MG	A	8021	1/1	1.00	0.02	46,46,46,46	0
38	CD	1	8403	1/1	1.00	0.01	88,88,88,88	0
32	MG	A	8012	1/1	1.00	0.03	35,35,35,35	0
32	MG	A	8091	1/1	1.00	0.03	65,65,65,65	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 PUY 5 78:

$2mF_o - DF_c$ (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.