



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2023 – 02:25 PM EDT

PDB ID : 1Q7Y  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

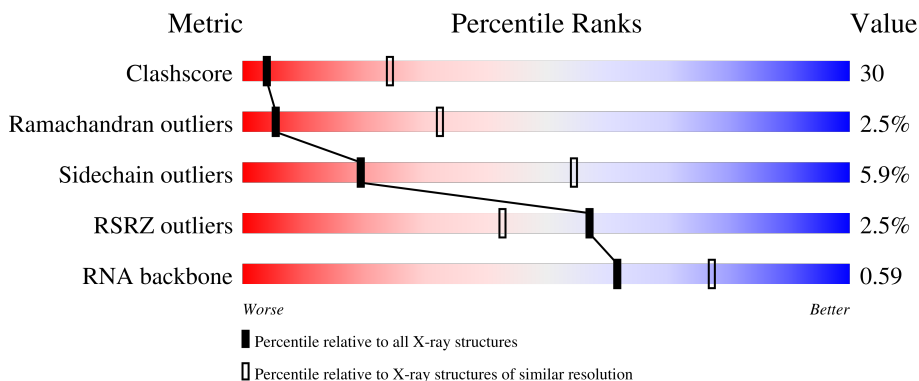
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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.




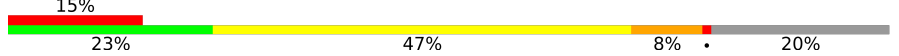


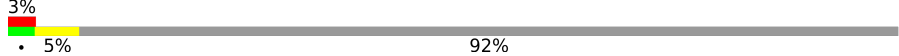


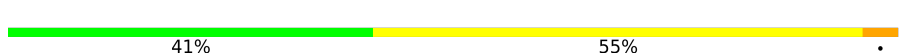




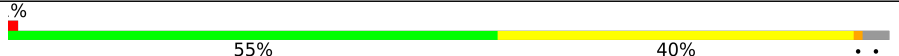
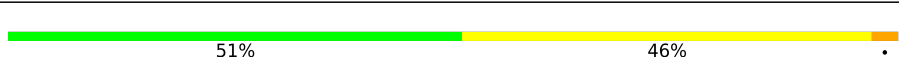
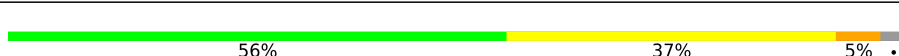

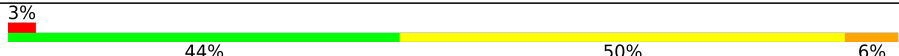
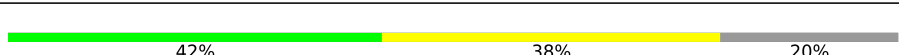
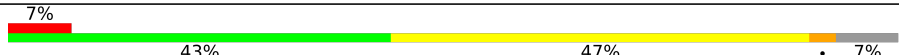
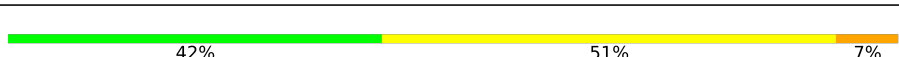
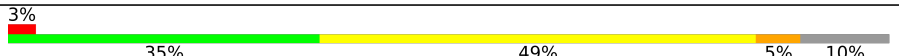
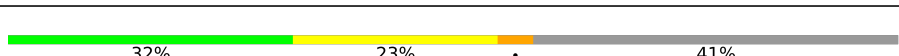
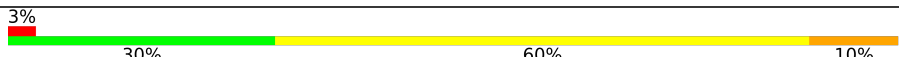

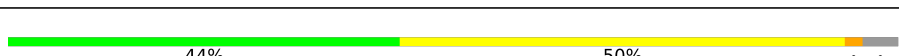
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">32%      45%      15%      6%</p>
2	B	122	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">30%      48%      17%</p>
3	5	3	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">33%      67%</p>
4	C	239	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 46%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 46%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">46%      46%      6%</p>
5	D	337	<div style="display: flex; align-items: center;"> <div style="width: 42%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 52%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">42%      52%      6%</p>

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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	8303	-	-	-	X
34	NA	A	8323	-	-	-	X
34	NA	A	8370	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	S	8386	-	-	-	X
34	NA	T	8312	-	-	-	X
35	CL	A	8511	-	-	-	X
35	CL	O	8507	-	-	-	X
35	CL	P	8508	-	-	-	X
38	CD	4	8404	-	-	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
			Total	C	N	O	P			
1	A	2754	59017	26346	10878	19048	2745	0	0	0

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

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

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

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

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

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

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

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

- Molecule 15 is a protein called L15 Ribosomal Protein.

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	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 (three-letter code: K) (formula: K).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	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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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 (three-letter code: CL) (formula: Cl).

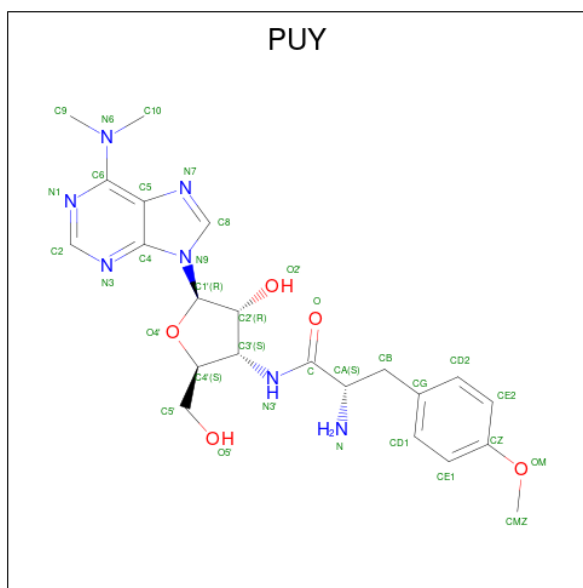
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	11	Total 11	Cl 11	0	0
35	C	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	P	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	Z	1	Total 1	Cl 1	0	0
35	4	1	Total 1	Cl 1	0	0

- Molecule 36 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 37 is PUROMYCIN (three-letter code: PUY) (formula: C<sub>22</sub>H<sub>29</sub>N<sub>7</sub>O<sub>5</sub>).



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

- Molecule 38 is CADMIUM ION (three-letter code: 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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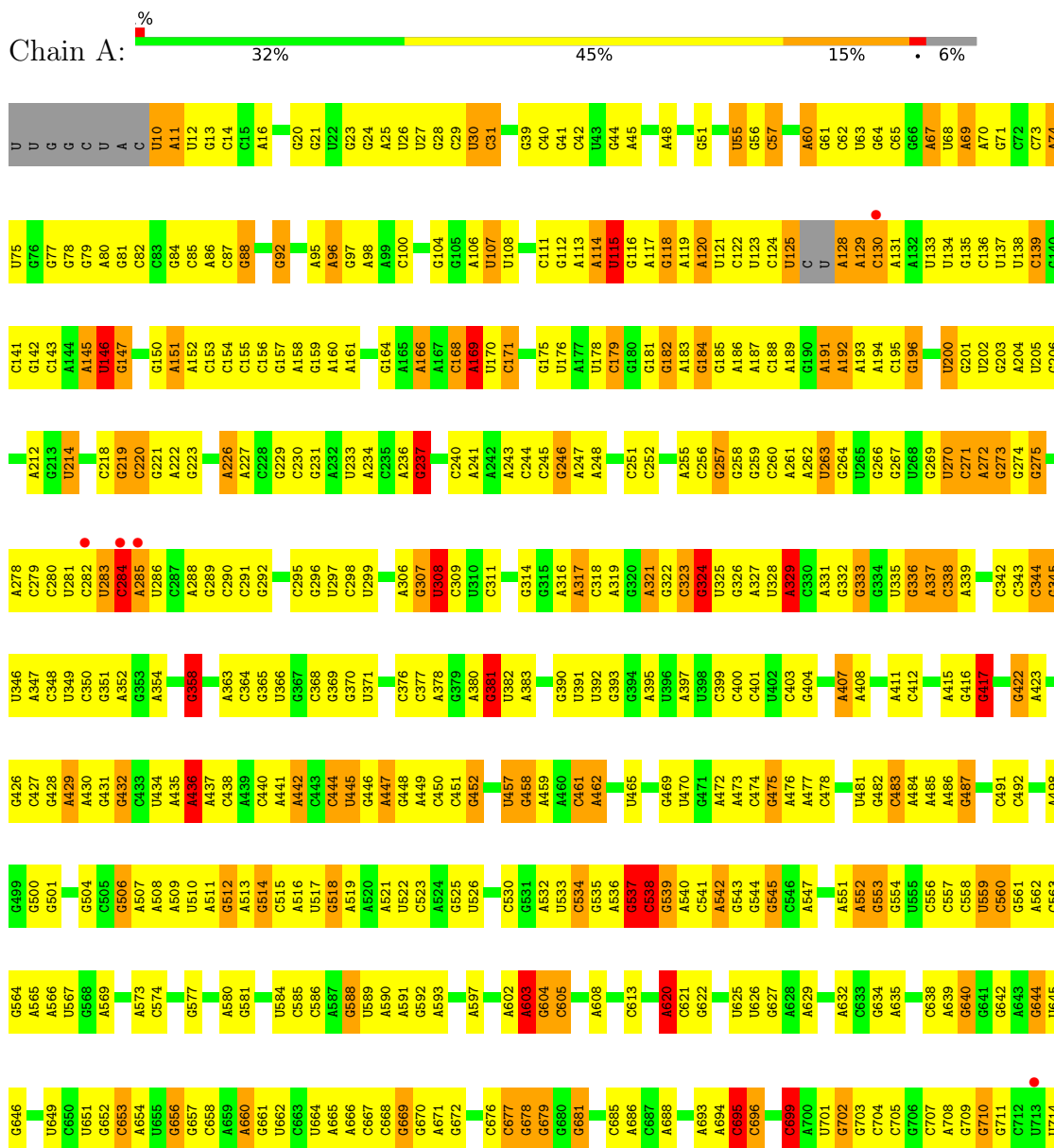
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	63	Total 63	O 63	0	0
39	P	45	Total 45	O 45	0	0
39	Q	62	Total 62	O 62	0	0
39	R	53	Total 53	O 53	0	0
39	S	86	Total 86	O 86	0	0
39	T	36	Total 36	O 36	0	0
39	U	42	Total 42	O 42	0	0
39	V	30	Total 30	O 30	0	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 [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal rna

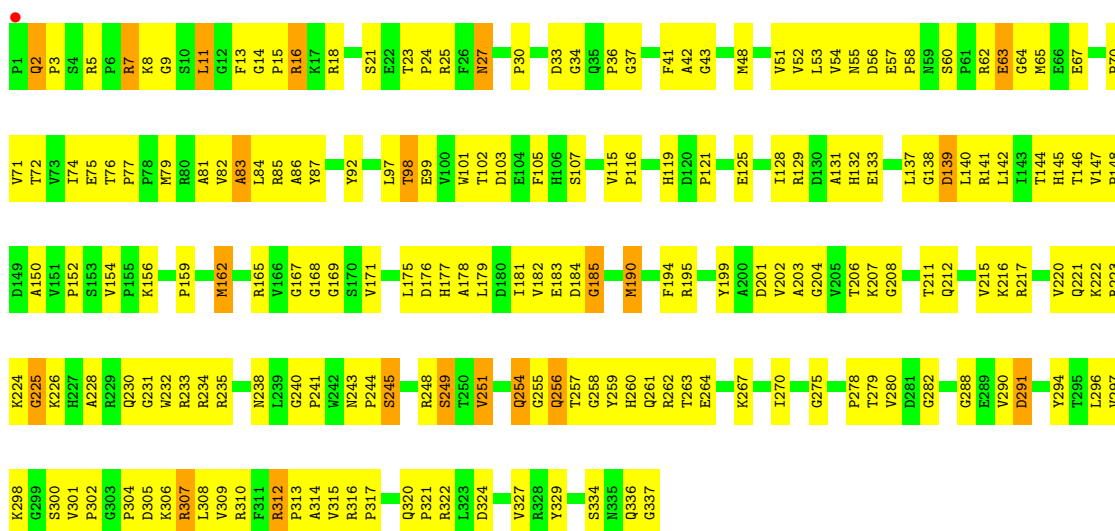
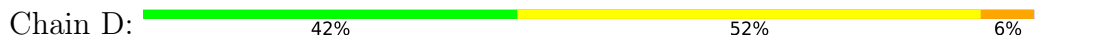




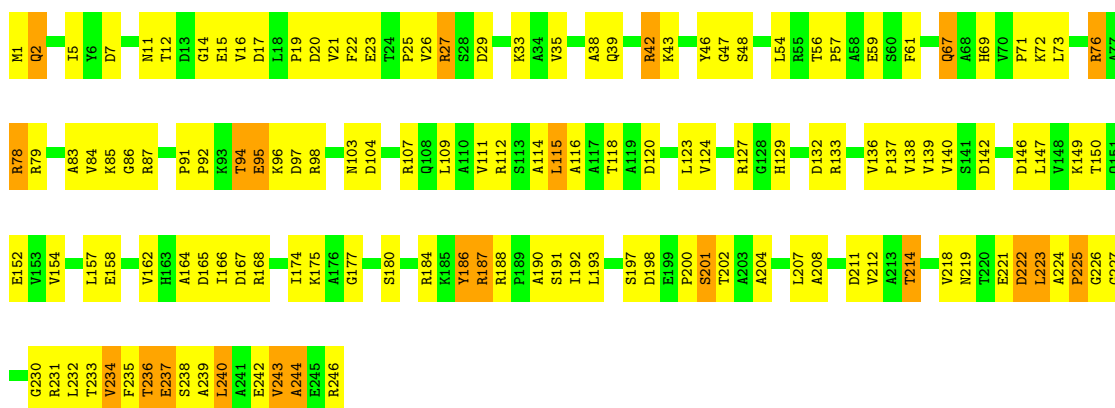




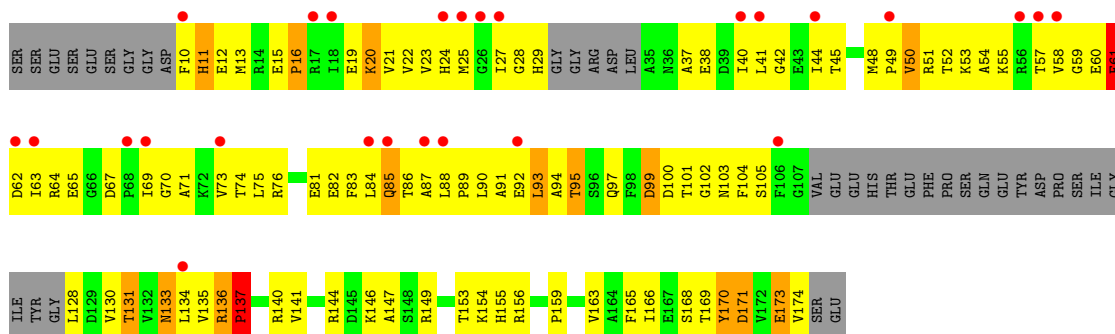
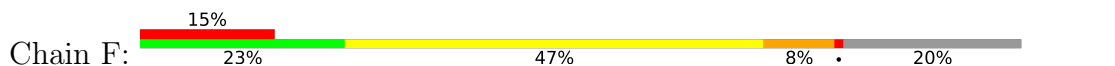




• Molecule 6: 50S ribosomal protein L4E



• Molecule 7: 50S ribosomal protein L5P



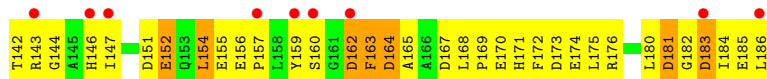
• Molecule 8: 50S ribosomal protein L6P



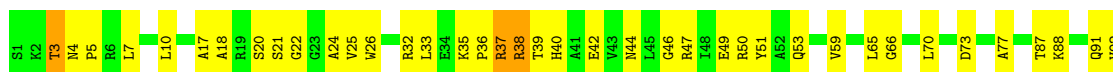




- Molecule 16: 50S ribosomal protein L18P



- Molecule 17: 50S ribosomal protein L18e



- Molecule 18: 50S ribosomal protein L19E

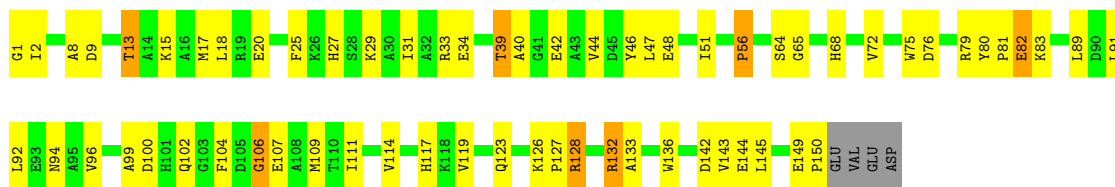


- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P

Chain S:  56% 37% 5%




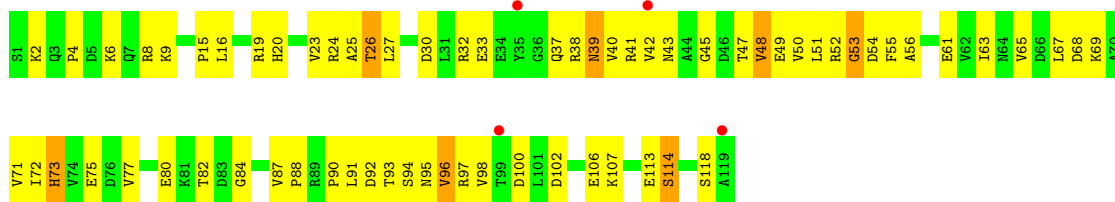
• Molecule 21: 50S ribosomal protein L23P

Chain T:  4% 61% 35%



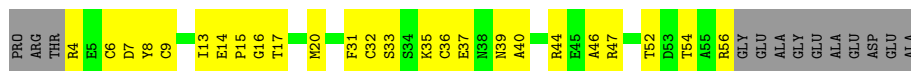
• Molecule 22: 50S ribosomal protein L24P

Chain U:  3% 44% 50% 6%



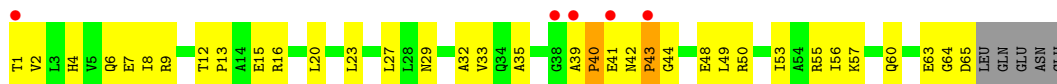
• Molecule 23: 50S ribosomal protein L24E

Chain V:  42% 38% 20%



• Molecule 24: 50S ribosomal protein L29P

Chain W:  7% 43% 47% 7%



• Molecule 25: 50S ribosomal protein L30P

Chain X:  42% 51% 7%







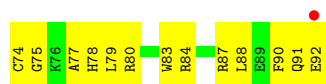
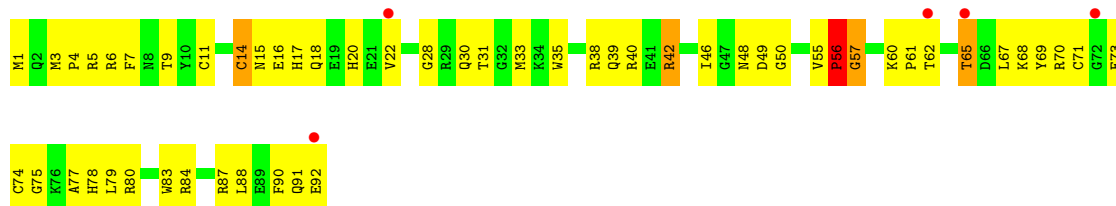
- Molecule 30: 50S ribosomal protein L39e

Chain 3:  44% 50% ..



- Molecule 31: 50S ribosomal protein L44E

Chain 4:  5% 41% 53% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.20 49.89 – 2.98	Depositor EDS
% Data completeness (in resolution range)	92.1 (19.99-3.20) 88.4 (49.89-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.59 (at 2.96Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.225 , 0.280 0.223 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtrriage
Anisotropy	0.673	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	98616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: K, NA, CL, PO4, PUY, CD, MG

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	1.03	52/66076 (0.1%)	0.96	138/103052 (0.1%)
2	B	0.91	0/2905	0.95	10/4528 (0.2%)
3	5	1.87	0/64	1.14	0/97
4	C	0.76	0/1787	0.95	1/2409 (0.0%)
5	D	0.73	0/2689	0.96	1/3652 (0.0%)
6	E	0.77	0/1883	0.97	1/2551 (0.0%)
7	F	0.63	0/1111	0.79	0/1498
8	G	0.71	0/1382	0.85	1/1880 (0.1%)
9	H	0.69	0/896	0.85	0/1219
10	I	0.99	0/241	0.91	0/324
11	J	0.79	0/1246	1.05	4/1686 (0.2%)
12	K	0.76	0/1135	0.89	0/1530
13	L	0.80	1/1003 (0.1%)	1.00	0/1351
14	M	0.75	0/1126	1.00	1/1504 (0.1%)
15	N	0.89	0/1633	1.04	2/2180 (0.1%)
16	O	0.70	0/1473	0.94	0/1999
17	P	0.78	0/873	0.97	2/1181 (0.2%)
18	Q	0.74	0/1143	0.91	0/1521
19	R	0.77	0/748	1.00	2/1005 (0.2%)
20	S	0.81	0/1172	0.99	1/1578 (0.1%)
21	T	0.79	0/648	0.94	0/875
22	U	0.76	0/957	0.95	0/1289
23	V	0.74	0/417	0.88	0/562
24	W	0.66	0/502	0.81	0/675
25	X	0.75	1/1218 (0.1%)	0.94	0/1655
26	Y	0.74	0/664	0.94	0/895
27	Z	0.74	0/1146	0.93	0/1536
28	1	0.79	0/575	0.98	0/763
29	2	0.87	0/437	1.08	0/578
30	3	0.70	0/398	0.86	0/527
31	4	0.81	1/771 (0.1%)	0.97	1/1024 (0.1%)
All	All	0.95	55/98319 (0.1%)	0.96	165/147124 (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	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 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2638	G	P-OP2	12.82	1.70	1.49
1	A	2636	C	C3'-O3'	11.93	1.58	1.42
1	A	2619	U	C3'-O3'	10.66	1.57	1.42
1	A	2620	U	C5'-C4'	-10.62	1.38	1.51
1	A	2619	U	C2'-O2'	-10.44	1.28	1.41

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-19.52	62.25	105.20
1	A	1164	U	OP2-P-O3'	-16.77	68.31	105.20
1	A	1165	G	O5'-P-OP1	-15.53	91.72	105.70
1	A	1563	G	C2'-C3'-O3'	10.27	132.10	109.50
1	A	1942	A	C5'-C4'-C3'	9.66	131.46	116.00

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29801	2017	0
2	B	2600	0	1326	128	0
3	5	58	0	34	2	0
4	C	1754	0	1763	155	0
5	D	2624	0	2533	238	0
6	E	1858	0	1816	194	0
7	F	1094	0	1085	172	0
8	G	1357	0	1266	103	0
9	H	885	0	854	74	0
10	I	240	0	231	33	0
11	J	1215	0	1215	194	0
12	K	1119	0	1098	80	0
13	L	993	0	1027	88	0
14	M	1114	0	1072	85	0
15	N	1605	0	1676	207	0
16	O	1444	0	1401	182	0
17	P	864	0	873	65	0
18	Q	1133	0	1127	74	0
19	R	734	0	728	62	0
20	S	1149	0	1122	87	0
21	T	641	0	605	27	0
22	U	949	0	923	87	0
23	V	410	0	364	44	0
24	W	499	0	511	40	0
25	X	1195	0	1137	120	0
26	Y	654	0	653	64	0
27	Z	1130	0	1133	81	0
28	1	563	0	599	76	0
29	2	430	0	427	38	0
30	3	393	0	406	34	0
31	4	755	0	730	64	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	2	0
38	P	1	0	0	0	0
38	V	1	0	0	0	0
39	1	36	0	0	15	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	35	0
39	E	178	0	0	56	0
39	F	50	0	0	34	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	34	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	41	0
39	P	45	0	0	21	0
39	Q	62	0	0	11	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	10	0
39	W	15	0	0	5	1
39	X	73	0	0	20	0
39	Y	30	0	0	11	0
39	Z	99	0	0	19	0
All	All	98616	0	59564	4529	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 30.

The worst 5 of 4529 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
1:A:871:G:H5'	1:A:871:G:H8	1.02	1.18

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	24
5	D	335/337 (99%)	297 (89%)	28 (8%)	10 (3%)	4	28
6	E	244/246 (99%)	206 (84%)	34 (14%)	4 (2%)	9	43
7	F	134/176 (76%)	95 (71%)	26 (19%)	13 (10%)	0	3
8	G	170/177 (96%)	160 (94%)	9 (5%)	1 (1%)	25	64
9	H	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	9	42
10	I	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	J	152/167 (91%)	130 (86%)	13 (9%)	9 (6%)	1	12
12	K	140/145 (97%)	125 (89%)	11 (8%)	4 (3%)	4	28
13	L	130/132 (98%)	110 (85%)	15 (12%)	5 (4%)	3	22
14	M	141/164 (86%)	114 (81%)	25 (18%)	2 (1%)	11	46
15	N	192/194 (99%)	167 (87%)	22 (12%)	3 (2%)	9	43
16	O	184/186 (99%)	153 (83%)	23 (12%)	8 (4%)	2	20
17	P	113/115 (98%)	107 (95%)	4 (4%)	2 (2%)	8	41
18	Q	141/148 (95%)	129 (92%)	12 (8%)	0	100	100
19	R	93/95 (98%)	89 (96%)	3 (3%)	1 (1%)	14	51
20	S	148/154 (96%)	132 (89%)	15 (10%)	1 (1%)	22	61
21	T	79/84 (94%)	75 (95%)	3 (4%)	1 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	U	117/119 (98%)	103 (88%)	11 (9%)	3 (3%)	5	31
23	V	51/66 (77%)	45 (88%)	5 (10%)	1 (2%)	7	38
24	W	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	4	26
25	X	152/154 (99%)	141 (93%)	8 (5%)	3 (2%)	7	38
26	Y	80/91 (88%)	69 (86%)	8 (10%)	3 (4%)	3	22
27	Z	140/240 (58%)	133 (95%)	7 (5%)	0	100	100
28	1	71/73 (97%)	58 (82%)	11 (16%)	2 (3%)	5	29
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%)	6	35
All	All	3633/4235 (86%)	3196 (88%)	347 (10%)	90 (2%)	5	32

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	179/181 (99%)	167 (93%)	12 (7%)	16	50
5	D	282/282 (100%)	264 (94%)	18 (6%)	17	52
6	E	193/193 (100%)	173 (90%)	20 (10%)	7	28
7	F	117/147 (80%)	107 (92%)	10 (8%)	10	38
8	G	152/155 (98%)	145 (95%)	7 (5%)	27	63
9	H	92/92 (100%)	89 (97%)	3 (3%)	38	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	I	27/283 (10%)	26 (96%)	1 (4%)	34	68
11	J	122/122 (100%)	112 (92%)	10 (8%)	11	41
12	K	118/121 (98%)	107 (91%)	11 (9%)	9	33
13	L	106/106 (100%)	102 (96%)	4 (4%)	33	67
14	M	112/126 (89%)	108 (96%)	4 (4%)	35	69
15	N	166/166 (100%)	156 (94%)	10 (6%)	19	54
16	O	149/149 (100%)	142 (95%)	7 (5%)	26	62
17	P	93/93 (100%)	88 (95%)	5 (5%)	22	58
18	Q	113/116 (97%)	108 (96%)	5 (4%)	28	64
19	R	79/79 (100%)	75 (95%)	4 (5%)	24	60
20	S	117/121 (97%)	112 (96%)	5 (4%)	29	64
21	T	71/73 (97%)	70 (99%)	1 (1%)	67	86
22	U	105/105 (100%)	100 (95%)	5 (5%)	25	61
23	V	44/52 (85%)	44 (100%)	0	100	100
24	W	51/56 (91%)	51 (100%)	0	100	100
25	X	130/130 (100%)	122 (94%)	8 (6%)	18	53
26	Y	66/73 (90%)	61 (92%)	5 (8%)	13	45
27	Z	120/195 (62%)	109 (91%)	11 (9%)	9	33
28	1	56/56 (100%)	50 (89%)	6 (11%)	6	27
29	2	46/46 (100%)	44 (96%)	2 (4%)	29	64
30	3	42/44 (96%)	41 (98%)	1 (2%)	49	77
31	4	79/79 (100%)	76 (96%)	3 (4%)	33	67
All	All	3027/3441 (88%)	2849 (94%)	178 (6%)	19	54

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	O	152	GLU
25	X	26	ILE
17	P	98	LEU
19	R	95	GLU
26	Y	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
19	R	16	ASN
24	W	60	GLN
20	S	61	GLN
20	S	123	GLN
25	X	110	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	259 (9%)	44 (1%)
2	B	121/122 (99%)	19 (15%)	5 (4%)
3	5	1/3 (33%)	0	0
All	All	2869/3047 (94%)	278 (9%)	49 (1%)

5 of 278 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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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	32,37,37	3.07	12 (37%)	33,53,53	2.02	9 (27%)
36	PO4	5	77	3,37	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	-	4/20/40/40	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	5	78	PUY	CE2-CZ	7.77	1.54	1.38
37	5	78	PUY	CD1-CG	6.66	1.53	1.38
37	5	78	PUY	CD2-CG	6.07	1.51	1.38
37	5	78	PUY	C-N3'	6.02	1.47	1.34
37	5	78	PUY	OM-CMZ	-4.70	1.28	1.42

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	5	78	PUY	CG-CB-CA	-5.27	103.18	114.13
37	5	78	PUY	CMZ-OM-CZ	5.08	128.54	117.51
37	5	78	PUY	O-C-N3'	-4.19	115.18	122.93
37	5	78	PUY	CB-CA-C	-3.14	101.63	108.97
37	5	78	PUY	C3'-N3'-C	-2.90	118.83	123.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

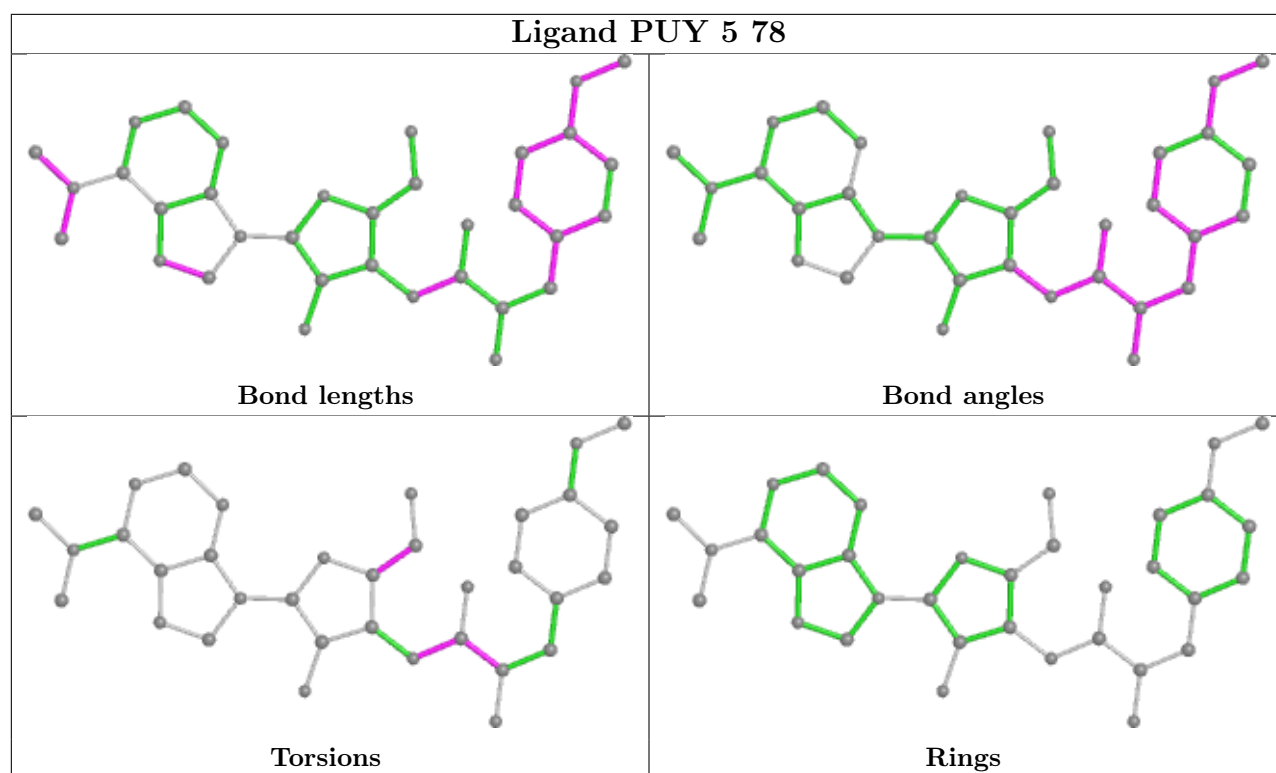
Mol	Chain	Res	Type	Atoms
37	5	78	PUY	N3'-C-CA-CB
37	5	78	PUY	C3'-C4'-C5'-O5'
37	5	78	PUY	O-C-N3'-C3'
37	5	78	PUY	O4'-C4'-C5'-O5'

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	2754/2922 (94%)	-0.20	32 (1%) 79 67	24, 50, 96, 142	0
2	B	122/122 (100%)	0.04	4 (3%) 46 30	36, 65, 94, 147	0
3	5	3/3 (100%)	-0.00	0 100 100	53, 53, 56, 62	0
4	C	237/239 (99%)	0.11	10 (4%) 36 23	29, 59, 91, 111	0
5	D	337/337 (100%)	-0.20	1 (0%) 94 92	23, 55, 83, 90	0
6	E	246/246 (100%)	-0.21	0 100 100	29, 54, 76, 85	0
7	F	140/176 (79%)	1.04	26 (18%) 1 1	62, 101, 118, 131	0
8	G	172/177 (97%)	0.31	4 (2%) 60 47	40, 69, 91, 96	0
9	H	119/119 (100%)	0.55	10 (8%) 11 6	58, 81, 101, 106	0
10	I	29/348 (8%)	1.63	11 (37%) 0 0	82, 96, 102, 103	0
11	J	156/167 (93%)	-0.08	1 (0%) 89 83	33, 54, 85, 93	0
12	K	142/145 (97%)	-0.26	0 100 100	32, 48, 71, 87	0
13	L	132/132 (100%)	-0.28	0 100 100	28, 51, 73, 82	0
14	M	145/164 (88%)	0.66	28 (19%) 1 1	24, 76, 110, 119	0
15	N	194/194 (100%)	-0.23	0 100 100	37, 52, 69, 78	0
16	O	186/186 (100%)	0.37	13 (6%) 16 9	43, 70, 109, 120	0
17	P	115/115 (100%)	-0.11	0 100 100	48, 61, 81, 85	0
18	Q	143/148 (96%)	0.03	1 (0%) 87 81	40, 62, 75, 80	0
19	R	95/95 (100%)	-0.15	0 100 100	29, 49, 59, 74	0
20	S	150/154 (97%)	-0.30	0 100 100	31, 47, 66, 72	0
21	T	81/84 (96%)	0.10	3 (3%) 41 26	53, 70, 85, 90	0
22	U	119/119 (100%)	0.46	4 (3%) 45 29	48, 63, 85, 94	0
23	V	53/66 (80%)	-0.13	0 100 100	43, 57, 74, 81	0
24	W	65/70 (92%)	0.72	5 (7%) 13 7	61, 81, 110, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	154/154 (100%)	-0.40	0 100 100	37, 49, 67, 76	0
26	Y	82/91 (90%)	0.11	3 (3%) 41 26	38, 62, 81, 97	0
27	Z	142/240 (59%)	-0.12	1 (0%) 87 81	30, 51, 74, 89	0
28	1	73/73 (100%)	-0.04	2 (2%) 54 39	52, 66, 80, 84	0
29	2	56/56 (100%)	-0.31	0 100 100	25, 40, 46, 48	0
30	3	46/48 (95%)	0.09	0 100 100	43, 65, 86, 95	0
31	4	92/92 (100%)	0.30	5 (5%) 25 14	36, 62, 72, 78	0
All	All	6580/7282 (90%)	-0.05	164 (2%) 57 43	23, 56, 97, 147	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	M	104	ASP	6.4
16	O	186	LEU	5.4
10	I	27	ILE	5.3
14	M	105	TYR	5.0
10	I	23	ILE	4.5

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
34	NA	A	8384	1/1	0.23	0.79	103,103,103,103	0
34	NA	A	8370	1/1	0.47	0.40	93,93,93,93	0
34	NA	S	8386	1/1	0.51	0.47	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	B	8351	1/1	0.54	0.26	67,67,67,67	0
34	NA	B	8383	1/1	0.60	0.26	63,63,63,63	0
35	CL	A	8505	1/1	0.67	0.30	65,65,65,65	0
34	NA	T	8312	1/1	0.71	0.57	122,122,122,122	0
34	NA	A	8323	1/1	0.71	0.49	62,62,62,62	0
35	CL	O	8507	1/1	0.71	0.51	102,102,102,102	0
35	CL	4	8504	1/1	0.71	0.35	69,69,69,69	0
35	CL	P	8508	1/1	0.72	0.62	113,113,113,113	0
32	MG	A	8103	1/1	0.75	0.39	57,57,57,57	0
32	MG	A	8066	1/1	0.75	0.27	84,84,84,84	0
34	NA	A	8303	1/1	0.76	0.41	42,42,42,42	0
35	CL	A	8511	1/1	0.77	0.42	92,92,92,92	0
34	NA	A	8371	1/1	0.78	0.23	32,32,32,32	0
32	MG	A	8089	1/1	0.79	0.25	104,104,104,104	0
34	NA	A	8382	1/1	0.81	0.46	52,52,52,52	0
35	CL	A	8510	1/1	0.81	0.71	101,101,101,101	0
34	NA	A	8366	1/1	0.82	0.19	58,58,58,58	0
32	MG	A	8070	1/1	0.82	0.79	101,101,101,101	0
32	MG	Z	8109	1/1	0.82	0.12	32,32,32,32	0
34	NA	A	8357	1/1	0.84	0.07	43,43,43,43	0
32	MG	A	8052	1/1	0.84	0.14	24,24,24,24	0
32	MG	A	8100	1/1	0.84	0.13	51,51,51,51	0
34	NA	A	8341	1/1	0.84	0.14	40,40,40,40	0
32	MG	A	8046	1/1	0.85	0.13	62,62,62,62	0
32	MG	1	8105	1/1	0.85	0.33	32,32,32,32	0
35	CL	A	8515	1/1	0.85	0.46	131,131,131,131	0
34	NA	J	8322	1/1	0.86	0.17	26,26,26,26	0
35	CL	A	8513	1/1	0.86	0.35	81,81,81,81	0
34	NA	A	8333	1/1	0.86	0.10	14,14,14,14	0
32	MG	A	8116	1/1	0.86	0.23	95,95,95,95	0
33	K	A	8201	1/1	0.86	0.22	76,76,76,76	0
35	CL	S	8506	1/1	0.86	0.29	77,77,77,77	0
34	NA	A	8375	1/1	0.86	0.56	42,42,42,42	0
34	NA	A	8360	1/1	0.87	0.44	37,37,37,37	0
34	NA	A	8307	1/1	0.87	0.17	34,34,34,34	0
34	NA	A	8359	1/1	0.87	0.46	47,47,47,47	0
32	MG	L	8069	1/1	0.88	0.13	105,105,105,105	0
32	MG	A	8115	1/1	0.88	0.17	51,51,51,51	0
32	MG	A	8102	1/1	0.88	0.19	83,83,83,83	0
34	NA	A	8363	1/1	0.88	0.39	100,100,100,100	0
37	PUY	5	78	34/34	0.88	0.37	66,69,74,75	0
34	NA	A	8326	1/1	0.89	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	A	8503	1/1	0.89	0.24	62,62,62,62	0
34	NA	S	8337	1/1	0.89	0.28	70,70,70,70	0
34	NA	A	8365	1/1	0.89	0.20	29,29,29,29	0
32	MG	A	8018	1/1	0.90	0.13	24,24,24,24	0
34	NA	A	8368	1/1	0.90	0.08	35,35,35,35	0
32	MG	A	8108	1/1	0.90	0.10	50,50,50,50	0
32	MG	A	8064	1/1	0.90	0.17	31,31,31,31	0
32	MG	A	8085	1/1	0.90	0.12	39,39,39,39	0
34	NA	A	8328	1/1	0.90	0.26	52,52,52,52	0
34	NA	A	8329	1/1	0.90	0.10	40,40,40,40	0
34	NA	A	8332	1/1	0.90	0.26	37,37,37,37	0
32	MG	A	8042	1/1	0.91	0.09	25,25,25,25	0
34	NA	A	8355	1/1	0.91	0.23	60,60,60,60	0
32	MG	A	8033	1/1	0.91	0.10	42,42,42,42	0
35	CL	A	8517	1/1	0.91	0.24	61,61,61,61	0
35	CL	K	8502	1/1	0.91	0.27	91,91,91,91	0
32	MG	A	8092	1/1	0.91	0.20	58,58,58,58	0
34	NA	A	8330	1/1	0.91	0.14	36,36,36,36	0
34	NA	A	8362	1/1	0.91	0.27	38,38,38,38	0
34	NA	A	8316	1/1	0.91	0.23	42,42,42,42	0
32	MG	A	8075	1/1	0.91	0.07	42,42,42,42	0
32	MG	A	8044	1/1	0.92	0.23	68,68,68,68	0
35	CL	A	8522	1/1	0.92	0.44	57,57,57,57	0
35	CL	C	8509	1/1	0.92	0.20	66,66,66,66	0
34	NA	A	8385	1/1	0.92	0.25	22,22,22,22	0
34	NA	A	8369	1/1	0.92	0.30	49,49,49,49	0
32	MG	A	8034	1/1	0.92	0.04	50,50,50,50	0
34	NA	A	8356	1/1	0.92	0.60	86,86,86,86	0
32	MG	A	8030	1/1	0.92	0.13	68,68,68,68	0
34	NA	A	8339	1/1	0.92	0.08	30,30,30,30	0
32	MG	A	8104	1/1	0.93	0.11	31,31,31,31	0
34	NA	A	8377	1/1	0.93	0.36	70,70,70,70	0
35	CL	A	8512	1/1	0.93	0.13	30,30,30,30	0
32	MG	A	8024	1/1	0.93	1.03	108,108,108,108	0
33	K	A	8202	1/1	0.93	0.16	56,56,56,56	0
34	NA	A	8302	1/1	0.93	0.17	25,25,25,25	0
32	MG	A	8028	1/1	0.93	0.10	75,75,75,75	0
32	MG	A	8041	1/1	0.93	0.18	80,80,80,80	0
34	NA	A	8336	1/1	0.93	0.09	51,51,51,51	0
34	NA	A	8308	1/1	0.93	0.09	40,40,40,40	0
34	NA	A	8314	1/1	0.93	0.12	29,29,29,29	0
32	MG	A	8001	1/1	0.93	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	Z	8520	1/1	0.93	0.21	64,64,64,64	0
32	MG	A	8087	1/1	0.93	0.19	41,41,41,41	0
34	NA	A	8372	1/1	0.93	0.18	25,25,25,25	0
38	CD	P	8405	1/1	0.93	0.33	196,196,196,196	0
32	MG	A	8099	1/1	0.94	0.14	43,43,43,43	0
34	NA	A	8313	1/1	0.94	0.14	47,47,47,47	0
32	MG	5	8114	1/1	0.94	0.20	44,44,44,44	0
34	NA	A	8343	1/1	0.94	0.07	9,9,9,9	0
34	NA	A	8354	1/1	0.94	0.17	16,16,16,16	0
34	NA	A	8315	1/1	0.94	0.11	25,25,25,25	0
32	MG	A	8076	1/1	0.94	0.43	134,134,134,134	0
32	MG	A	8053	1/1	0.94	0.12	85,85,85,85	0
32	MG	A	8060	1/1	0.94	0.23	43,43,43,43	0
34	NA	A	8327	1/1	0.94	0.19	24,24,24,24	0
35	CL	K	8521	1/1	0.94	0.18	47,47,47,47	0
32	MG	A	8071	1/1	0.94	0.07	52,52,52,52	0
34	NA	E	8304	1/1	0.94	0.09	4,4,4,4	0
32	MG	A	8107	1/1	0.94	0.03	46,46,46,46	0
32	MG	A	8050	1/1	0.94	0.11	41,41,41,41	0
32	MG	A	8113	1/1	0.94	0.10	29,29,29,29	0
34	NA	A	8367	1/1	0.94	0.10	22,22,22,22	0
32	MG	A	8097	1/1	0.94	0.52	64,64,64,64	0
34	NA	A	8353	1/1	0.95	0.07	13,13,13,13	0
34	NA	C	8345	1/1	0.95	0.17	68,68,68,68	0
32	MG	A	8055	1/1	0.95	0.12	29,29,29,29	0
32	MG	A	8094	1/1	0.95	0.09	50,50,50,50	0
34	NA	M	8380	1/1	0.95	0.35	73,73,73,73	0
32	MG	A	8056	1/1	0.95	0.20	75,75,75,75	0
32	MG	B	8095	1/1	0.95	0.17	85,85,85,85	0
32	MG	A	8072	1/1	0.95	0.26	55,55,55,55	0
34	NA	A	8317	1/1	0.95	0.06	25,25,25,25	0
34	NA	A	8319	1/1	0.95	0.11	43,43,43,43	0
32	MG	C	8065	1/1	0.95	0.09	85,85,85,85	0
32	MG	A	8059	1/1	0.95	0.13	119,119,119,119	0
32	MG	U	8073	1/1	0.95	0.14	21,21,21,21	0
32	MG	A	8027	1/1	0.95	0.06	60,60,60,60	0
32	MG	A	8045	1/1	0.95	0.14	63,63,63,63	0
32	MG	4	8078	1/1	0.95	0.07	23,23,23,23	0
32	MG	A	8035	1/1	0.95	0.07	70,70,70,70	0
32	MG	A	8106	1/1	0.95	0.12	69,69,69,69	0
35	CL	D	8519	1/1	0.95	0.33	55,55,55,55	0
35	CL	K	8501	1/1	0.95	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8301	1/1	0.95	0.14	22,22,22,22	0
34	NA	A	8373	1/1	0.95	0.07	36,36,36,36	0
34	NA	A	8374	1/1	0.95	0.29	46,46,46,46	0
32	MG	A	8068	1/1	0.95	0.09	44,44,44,44	0
34	NA	A	8340	1/1	0.95	0.23	29,29,29,29	0
32	MG	A	8090	1/1	0.95	0.22	46,46,46,46	0
32	MG	A	8111	1/1	0.95	0.26	82,82,82,82	0
34	NA	A	8344	1/1	0.95	0.06	11,11,11,11	0
34	NA	A	8350	1/1	0.95	0.22	18,18,18,18	0
32	MG	A	8039	1/1	0.96	0.10	57,57,57,57	0
32	MG	A	8088	1/1	0.96	0.10	12,12,12,12	0
32	MG	A	8051	1/1	0.96	0.10	93,93,93,93	0
34	NA	A	8364	1/1	0.96	0.18	12,12,12,12	0
32	MG	A	8021	1/1	0.96	0.10	46,46,46,46	0
32	MG	A	8032	1/1	0.96	0.07	23,23,23,23	0
32	MG	A	8112	1/1	0.96	0.18	58,58,58,58	0
32	MG	A	8043	1/1	0.96	0.07	50,50,50,50	0
34	NA	A	8334	1/1	0.96	0.06	30,30,30,30	0
34	NA	A	8305	1/1	0.96	0.08	10,10,10,10	0
32	MG	A	8096	1/1	0.96	0.16	33,33,33,33	0
32	MG	A	8006	1/1	0.96	0.05	33,33,33,33	0
34	NA	A	8311	1/1	0.96	0.19	43,43,43,43	0
34	NA	A	8342	1/1	0.96	0.18	30,30,30,30	0
32	MG	A	8117	1/1	0.96	0.08	1,1,1,1	0
32	MG	A	8098	1/1	0.96	0.24	47,47,47,47	0
34	NA	A	8381	1/1	0.96	0.11	51,51,51,51	0
32	MG	A	8057	1/1	0.96	0.11	15,15,15,15	0
32	MG	A	8014	1/1	0.96	0.10	18,18,18,18	0
32	MG	A	8101	1/1	0.96	0.13	49,49,49,49	0
32	MG	A	8081	1/1	0.96	0.15	29,29,29,29	0
34	NA	A	8320	1/1	0.96	0.09	29,29,29,29	0
32	MG	A	8005	1/1	0.96	0.10	68,68,68,68	0
36	PO4	5	77	3/5	0.96	0.12	67,67,68,68	0
34	NA	A	8358	1/1	0.96	0.49	109,109,109,109	0
34	NA	A	8325	1/1	0.96	0.13	48,48,48,48	0
32	MG	A	8015	1/1	0.97	0.07	66,66,66,66	0
34	NA	A	8321	1/1	0.97	0.22	52,52,52,52	0
34	NA	A	8378	1/1	0.97	0.21	18,18,18,18	0
34	NA	A	8379	1/1	0.97	0.14	33,33,33,33	0
34	NA	A	8361	1/1	0.97	0.22	35,35,35,35	0
32	MG	A	8067	1/1	0.97	0.12	22,22,22,22	0
34	NA	A	8324	1/1	0.97	0.10	32,32,32,32	0

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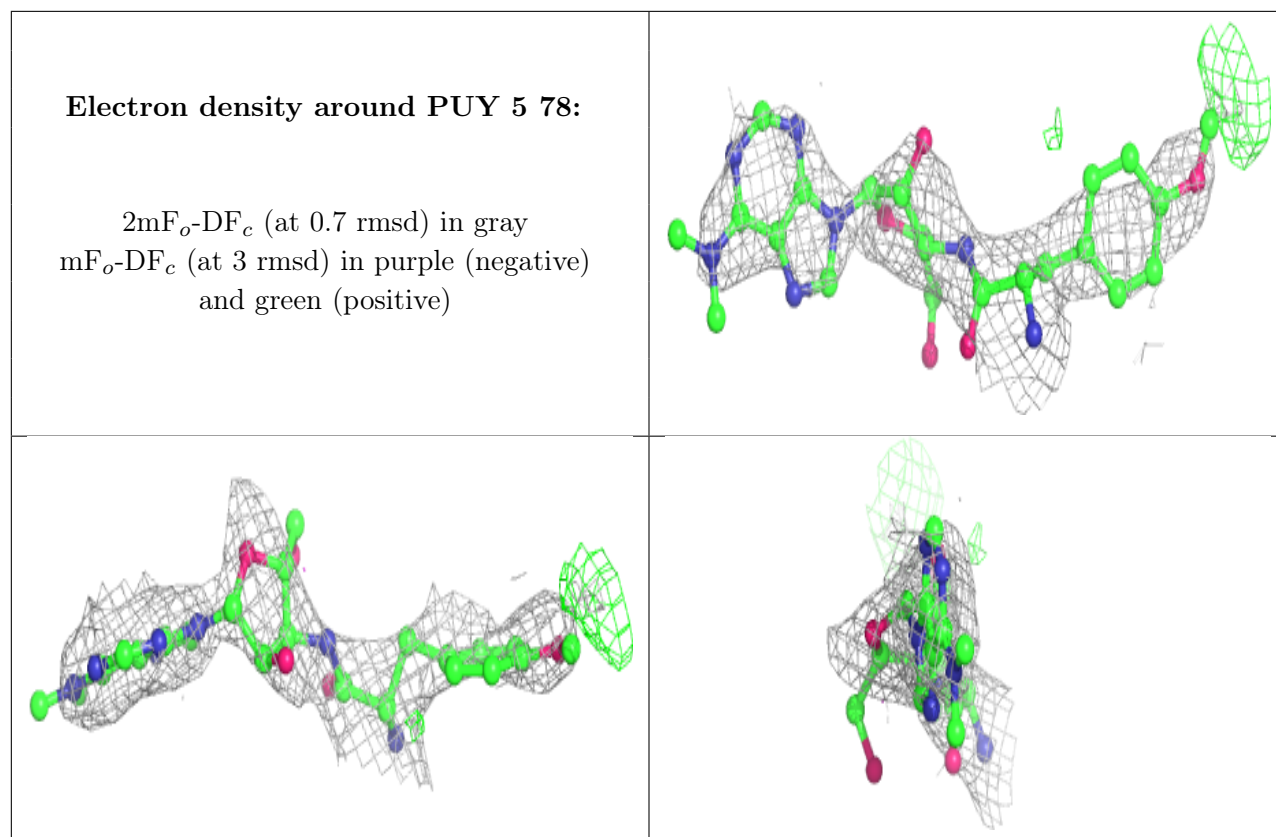
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8310	1/1	0.97	0.15	22,22,22,22	0
32	MG	A	8083	1/1	0.97	0.04	32,32,32,32	0
32	MG	A	8049	1/1	0.97	0.30	49,49,49,49	0
32	MG	A	8017	1/1	0.97	0.04	40,40,40,40	0
34	NA	A	8352	1/1	0.97	0.15	17,17,17,17	0
34	NA	J	8309	1/1	0.97	0.15	21,21,21,21	0
32	MG	A	8011	1/1	0.97	0.05	27,27,27,27	0
34	NA	K	8346	1/1	0.97	0.14	7,7,7,7	0
32	MG	A	8110	1/1	0.97	0.17	54,54,54,54	0
34	NA	N	8347	1/1	0.97	0.10	19,19,19,19	0
34	NA	A	8331	1/1	0.97	0.19	35,35,35,35	0
32	MG	A	8004	1/1	0.97	0.05	43,43,43,43	0
34	NA	A	8318	1/1	0.97	0.15	65,65,65,65	0
32	MG	A	8031	1/1	0.97	0.05	29,29,29,29	0
32	MG	A	8093	1/1	0.98	0.10	16,16,16,16	0
32	MG	A	8061	1/1	0.98	0.05	33,33,33,33	0
32	MG	A	8062	1/1	0.98	0.07	38,38,38,38	0
32	MG	A	8063	1/1	0.98	0.12	64,64,64,64	0
34	NA	R	8348	1/1	0.98	0.07	18,18,18,18	0
32	MG	A	8016	1/1	0.98	0.08	23,23,23,23	0
34	NA	S	8338	1/1	0.98	0.21	65,65,65,65	0
32	MG	A	8029	1/1	0.98	0.12	34,34,34,34	0
32	MG	A	8010	1/1	0.98	0.09	26,26,26,26	0
32	MG	A	8003	1/1	0.98	0.13	30,30,30,30	0
32	MG	A	8048	1/1	0.98	0.09	33,33,33,33	0
32	MG	A	8019	1/1	0.98	0.07	31,31,31,31	0
34	NA	A	8335	1/1	0.98	0.23	43,43,43,43	0
34	NA	A	8306	1/1	0.98	0.39	35,35,35,35	0
32	MG	A	8013	1/1	0.98	0.15	21,21,21,21	0
35	CL	A	8514	1/1	0.98	0.15	45,45,45,45	0
32	MG	A	8022	1/1	0.98	0.05	22,22,22,22	0
32	MG	A	8023	1/1	0.98	0.07	35,35,35,35	0
32	MG	A	8079	1/1	0.98	0.08	25,25,25,25	0
34	NA	A	8376	1/1	0.98	0.12	27,27,27,27	0
32	MG	A	8036	1/1	0.98	0.06	29,29,29,29	0
32	MG	A	8082	1/1	0.98	0.07	16,16,16,16	0
34	NA	A	8349	1/1	0.98	0.21	25,25,25,25	0
32	MG	A	8054	1/1	0.98	0.10	46,46,46,46	0
35	CL	N	8518	1/1	0.98	0.15	50,50,50,50	0
32	MG	A	8037	1/1	0.98	0.09	41,41,41,41	0
32	MG	A	8086	1/1	0.98	0.11	75,75,75,75	0
32	MG	A	8002	1/1	0.98	0.06	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8040	1/1	0.98	0.07	33,33,33,33	0
32	MG	A	8058	1/1	0.98	0.11	33,33,33,33	0
32	MG	A	8025	1/1	0.98	0.05	12,12,12,12	0
32	MG	A	8091	1/1	0.98	0.05	65,65,65,65	0
32	MG	A	8008	1/1	0.98	0.12	40,40,40,40	0
38	CD	V	8401	1/1	0.98	0.11	70,70,70,70	0
32	MG	A	8080	1/1	0.99	0.07	38,38,38,38	0
32	MG	A	8020	1/1	0.99	0.07	36,36,36,36	0
32	MG	A	8047	1/1	0.99	0.09	62,62,62,62	0
32	MG	A	8009	1/1	0.99	0.05	14,14,14,14	0
32	MG	A	8084	1/1	0.99	0.03	34,34,34,34	0
32	MG	A	8026	1/1	0.99	0.13	45,45,45,45	0
35	CL	A	8516	1/1	0.99	0.10	37,37,37,37	0
32	MG	A	8074	1/1	0.99	0.07	16,16,16,16	0
32	MG	A	8012	1/1	0.99	0.10	35,35,35,35	0
32	MG	A	8038	1/1	0.99	0.08	43,43,43,43	0
32	MG	A	8077	1/1	0.99	0.11	39,39,39,39	0
32	MG	A	8007	1/1	0.99	0.08	9,9,9,9	0
38	CD	1	8403	1/1	0.99	0.07	88,88,88,88	0
38	CD	2	8402	1/1	0.99	0.07	72,72,72,72	0
38	CD	4	8404	1/1	0.99	0.08	67,67,67,67	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.