



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 04:26 pm BST

PDB ID : 2UUC  
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a Valine-ASL with cmo5U in position 34 bound to an mRNA with a GUA-codon in the A-site and paromomycin.  
Authors : Weixlbaumer, A.; Murphy, F.V.; Dziergowska, A.; Malkiewicz, A.; Vendeix, F.A.P.; Agris, P.F.; Ramakrishnan, V.  
Deposited on : 2007-03-01  
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

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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	:	2.11
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)	:	2.11

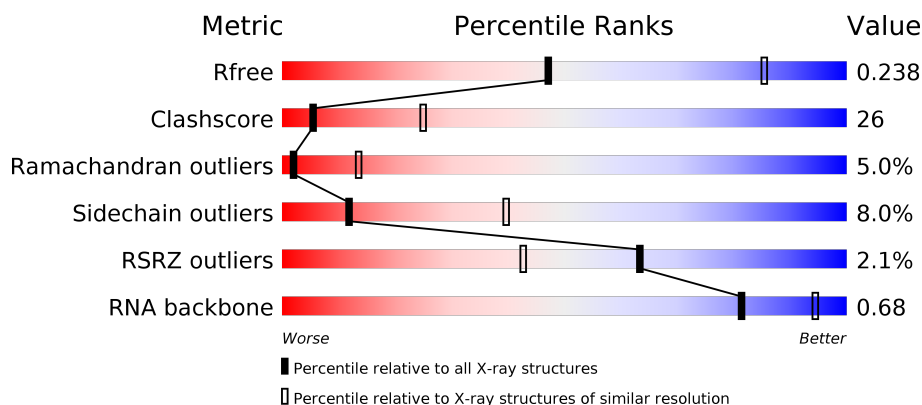
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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




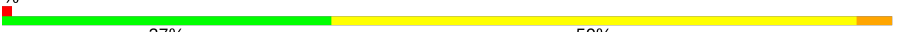

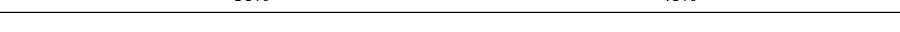
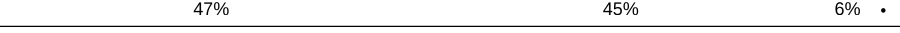
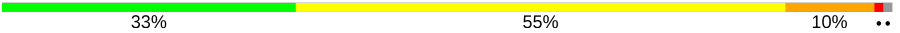
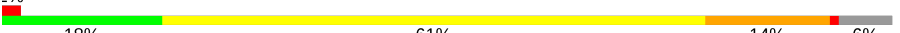


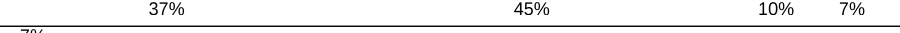
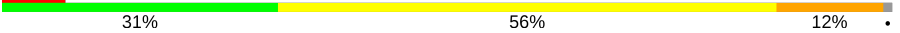
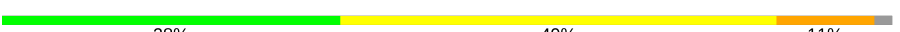

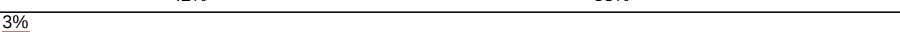

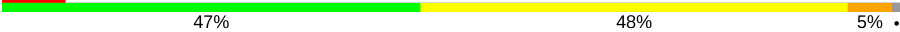



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	1522	<div> <div>2%</div> <div> <div></div> <div>43%</div> <div>46%</div> <div>9%</div> <div>..</div> </div> </div>
2	B	256	<div> <div>3%</div> <div> <div></div> <div>30%</div> <div>51%</div> <div>10%</div> <div>8%</div> </div> </div>
3	C	239	<div> <div></div> <div> <div></div> <div>31%</div> <div>46%</div> <div>9%</div> <div>13%</div> </div> </div>
4	D	209	<div> <div></div> <div> <div></div> <div>54%</div> <div>39%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	X	6	
23	Y	17	

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
25	MG	A	1604	-	-	-	X
25	MG	A	1612	-	-	-	X
25	MG	A	1613	-	-	-	X
25	MG	A	1620	-	-	-	X
25	MG	A	1622	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1623	-	-	-	X
25	MG	A	1626	-	-	-	X
25	MG	A	1630	-	-	-	X
25	MG	A	1665	-	-	-	X
25	MG	A	1667	-	-	-	X
25	MG	A	1672	-	-	-	X
25	MG	A	1673	-	-	-	X
25	MG	A	1680	-	-	-	X
25	MG	A	1700	-	-	-	X
25	MG	A	1709	-	-	-	X
25	MG	A	1716	-	-	-	X
25	MG	A	1735	-	-	-	X
25	MG	A	1737	-	-	-	X
25	MG	A	1742	-	-	-	X
25	MG	A	1749	-	-	-	X
25	MG	A	1758	-	-	-	X
25	MG	A	1773	-	-	-	X
26	K	A	1788	-	-	-	X
26	K	A	1797	-	-	-	X
26	K	A	1806	-	-	-	X
26	K	A	1826	-	-	-	X
26	K	E	203	-	-	-	X
27	ZN	N	101	-	-	X	-

## 2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52372 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 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32489	14462	6011	10505	1511			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	160	148	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			598	381	118	99			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

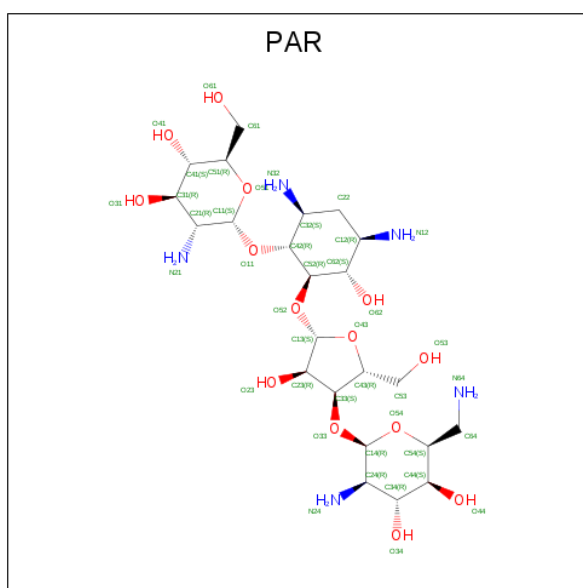
- Molecule 22 is a RNA chain called 5'-R(\*GP\*UP\*AP\*AP\*AP\*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	4	Total	C	N	O	P	0	0	0
			84	39	17	25	3			

- Molecule 23 is a RNA chain called 5'-R(\*CP\*CP\*UP\*CP\*CP\*CP\*UP\*CM0P\*AP\*CP\*6MZP\*AP\*GP\*GP\*AP\*GP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	13	Total	C	N	O	P	0	0	0
			277	126	48	91	12			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	Q	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	D	1	Total 1	Mg 1	0	0
25	K	1	Total 1	Mg 1	0	0
25	E	1	Total 1	Mg 1	0	0
25	B	1	Total 1	Mg 1	0	0
25	I	1	Total 1	Mg 1	0	0
25	A	176	Total 176	Mg 176	0	0
25	N	1	Total 1	Mg 1	0	0
25	M	1	Total 1	Mg 1	0	0

- Molecule 26 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	G	1	Total 1	K 1	0	0
26	Q	1	Total 1	K 1	0	0
26	A	51	Total 51	K 51	0	0
26	E	3	Total 3	K 3	0	0

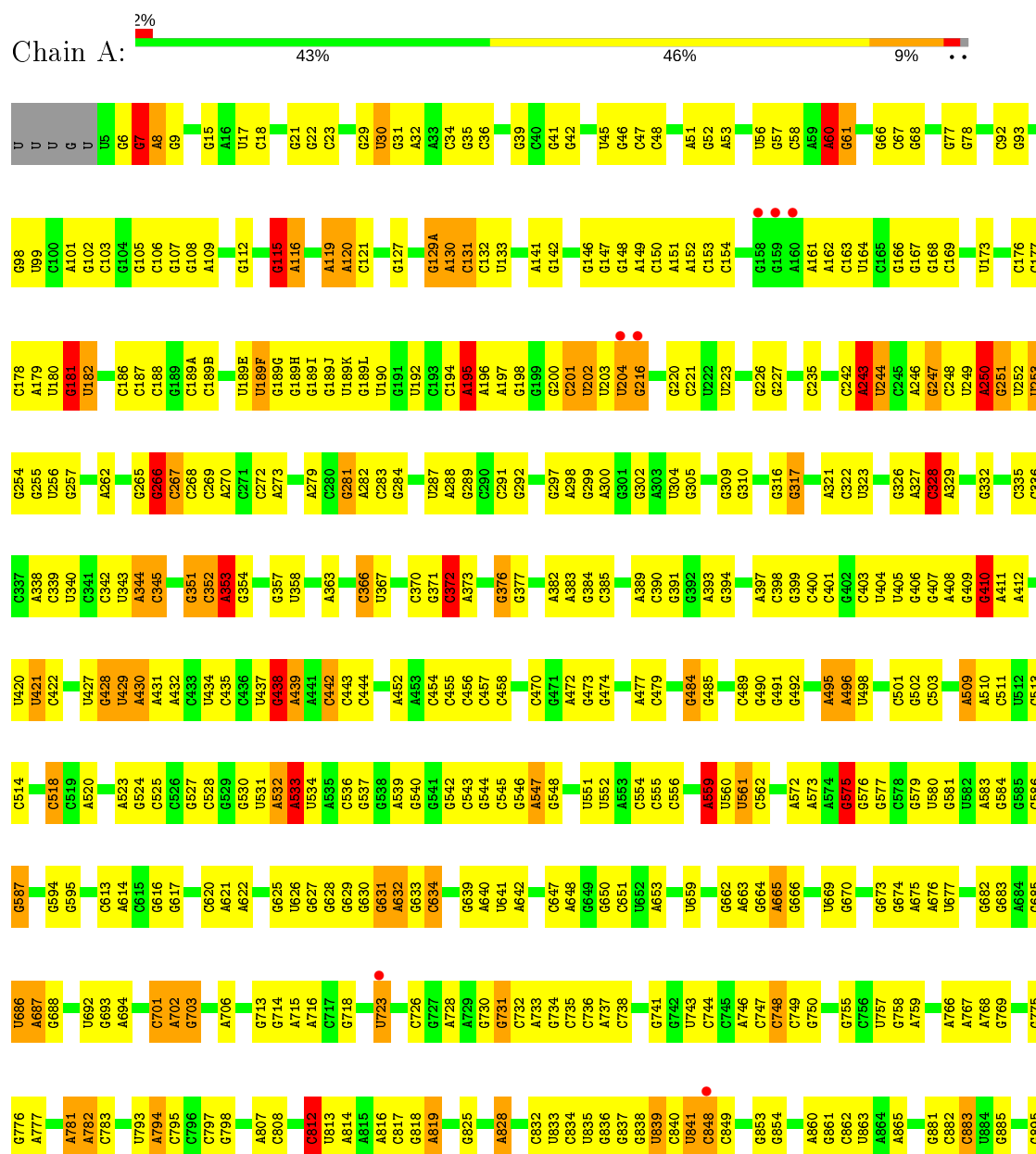
- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

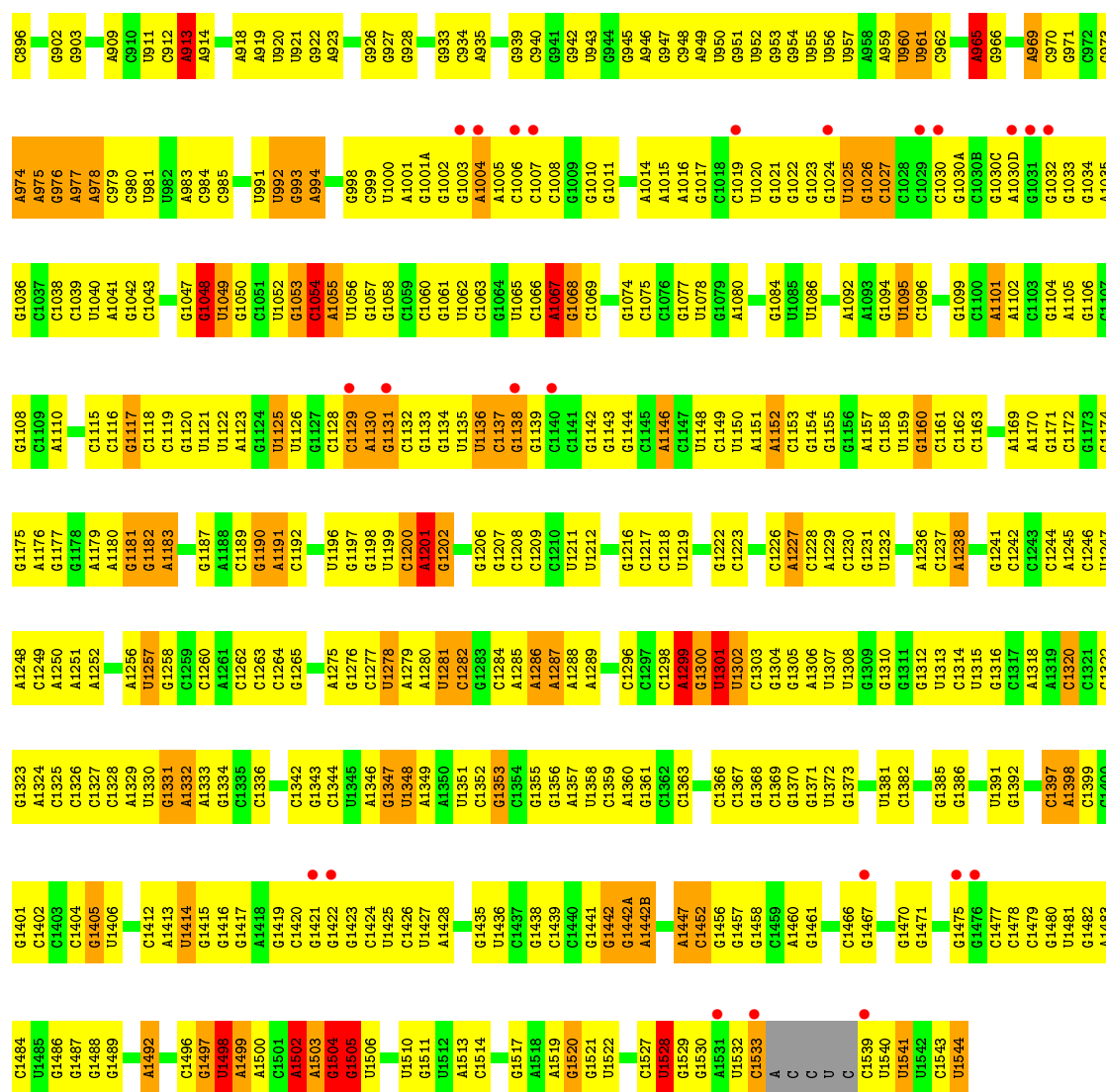
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	D	1	Total 1	Zn 1	0	0
27	N	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

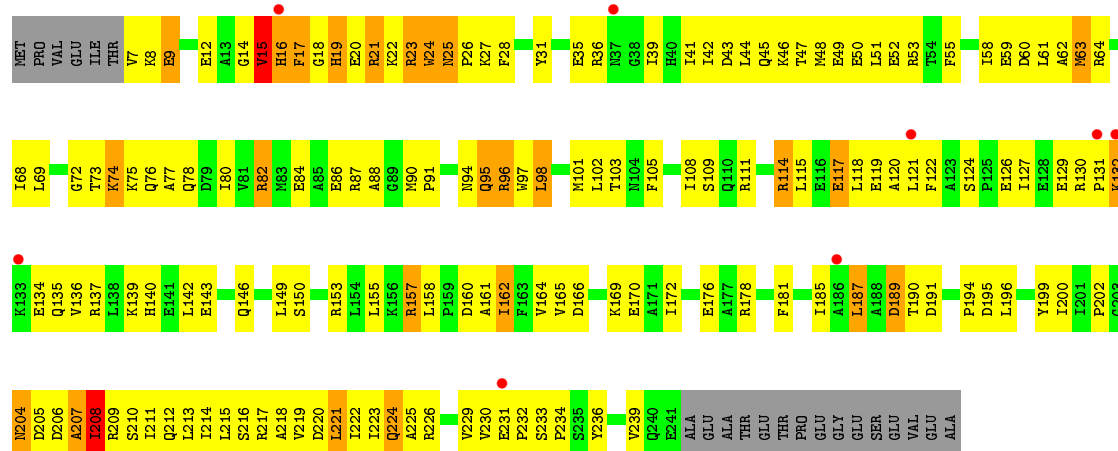
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 16S Ribosomal RNA

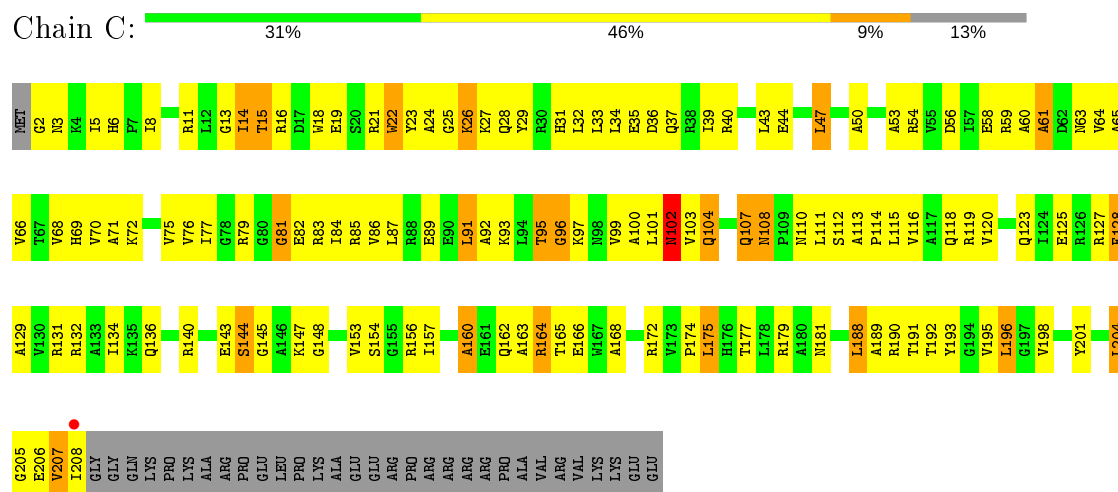




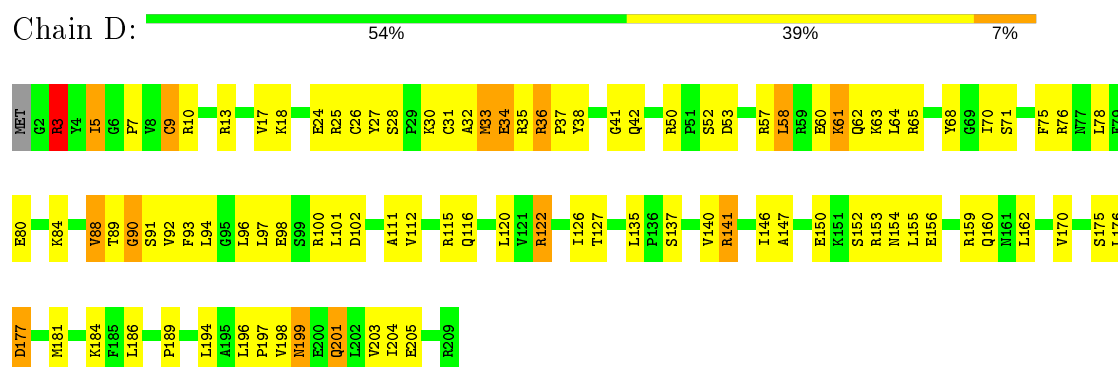
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



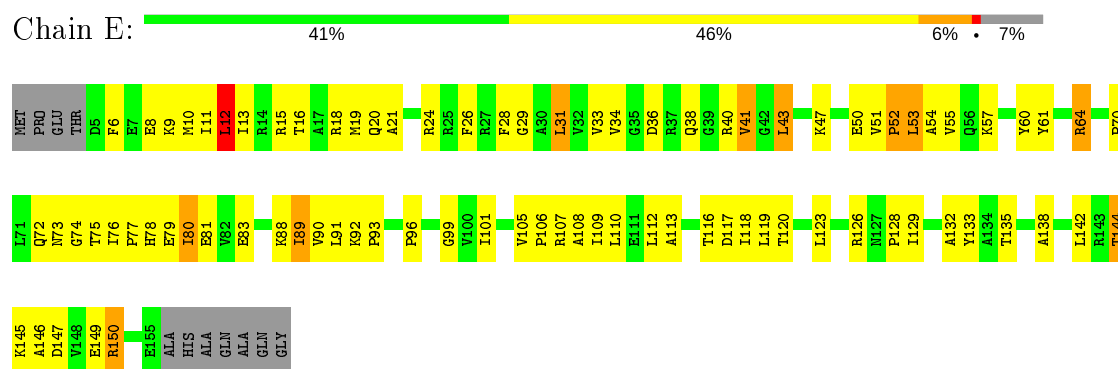
- Molecule 3: 30S RIBOSOMAL PROTEIN S3



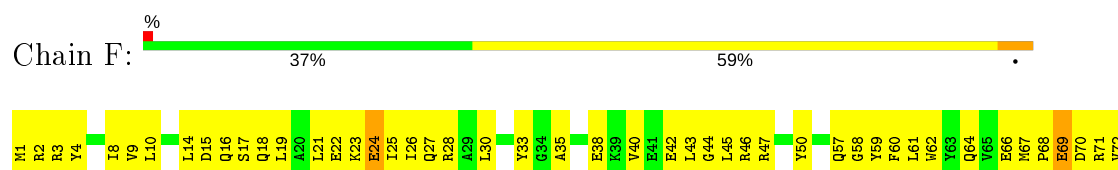
- Molecule 4: 30S RIBOSOMAL PROTEIN S4



- Molecule 5: 30S RIBOSOMAL PROTEIN S5

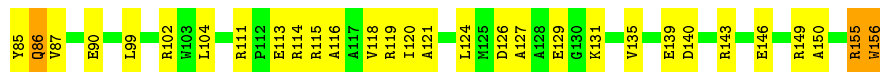
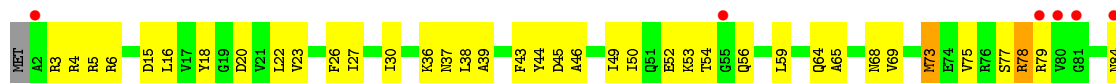


- Molecule 6: 30S RIBOSOMAL PROTEIN S6





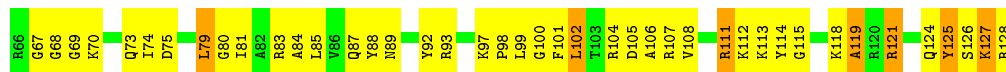
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



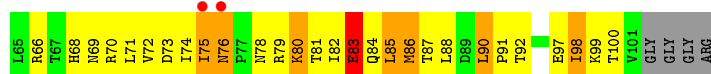
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

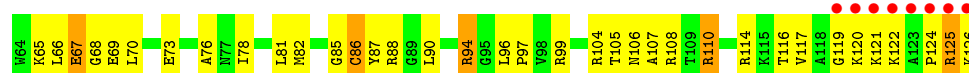
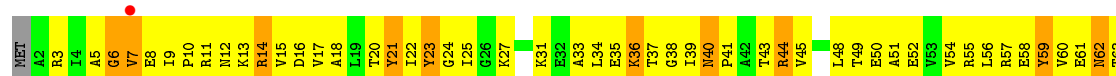




• Molecule 12: 30S RIBOSOMAL PROTEIN S12



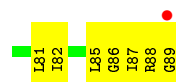
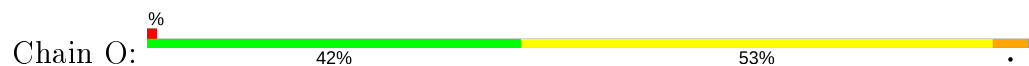
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



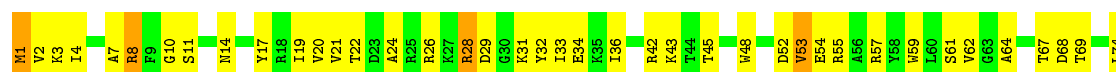
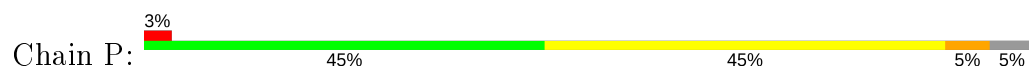
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

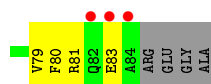


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

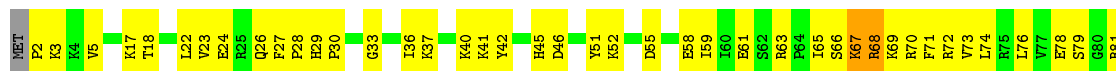


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

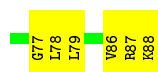
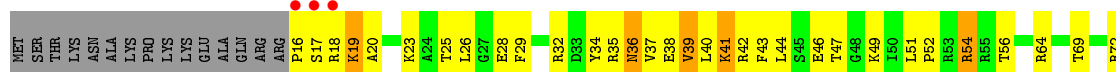




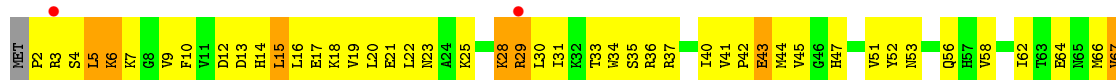
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



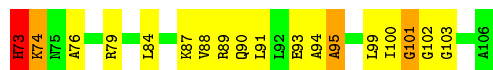
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



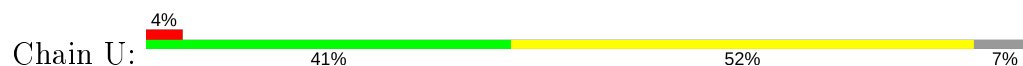
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

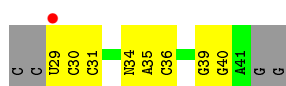




- Molecule 22: 5'-R(\*GP\*UP\*AP\*AP\*AP\*AP)-3'



- Molecule 23: 5'-R(\*CP\*CP\*UP\*CP\*CP\*CP\*UP\*CM0P\*AP\*CP\*6MZP\*AP \*GP\*GP\*AP\*GP\*G)-3'





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	400.96 Å   400.96 Å   174.37 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.89 – 3.10 29.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.89-3.10) 99.5 (29.89-3.10)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 3.11 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.210   ,   0.245 0.204   ,   0.238	Depositor DCC
$R_{free}$ test set	12815 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 71.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	52372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: MG, PAR, K, ZN, 6MZ, CM0

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	0.57	1/36365 (0.0%)	0.72	38/56754 (0.1%)
2	B	0.40	0/1936	0.68	0/2611
3	C	0.42	0/1637	0.65	1/2207 (0.0%)
4	D	0.49	1/1733 (0.1%)	0.66	0/2318
5	E	0.53	0/1163	0.74	1/1566 (0.1%)
6	F	0.40	0/856	0.64	0/1154
7	G	0.41	0/1276	0.60	0/1709
8	H	0.53	0/1136	0.77	0/1527
9	I	0.42	0/1029	0.67	1/1379 (0.1%)
10	J	0.40	0/806	0.67	1/1084 (0.1%)
11	K	0.45	0/900	0.72	0/1213
12	L	0.51	0/987	0.86	3/1322 (0.2%)
13	M	0.40	0/1008	0.66	0/1347
14	N	0.44	0/501	0.65	0/664
15	O	0.45	0/745	0.61	0/992
16	P	0.53	0/717	0.78	0/965
17	Q	0.55	0/870	0.75	1/1159 (0.1%)
18	R	0.45	0/604	0.64	0/801
19	S	0.41	0/662	0.70	0/892
20	T	0.48	0/765	0.76	0/1007
21	U	0.59	0/213	0.67	0/279
22	X	0.60	0/94	0.77	0/145
23	Y	0.56	0/253	0.68	0/387
All	All	0.53	2/56256 (0.0%)	0.71	46/83482 (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	4	21
22	X	0	1
All	All	4	22

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	9	CYS	CB-SG	5.52	1.91	1.82
1	A	438	G	C3'-O3'	5.44	1.49	1.42

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	G	C2'-C3'-O3'	9.87	131.21	109.50
1	A	1498	U	C2'-C3'-O3'	9.85	131.17	109.50
1	A	243	A	C2'-C3'-O3'	9.42	130.23	109.50
1	A	1528	U	C2'-C3'-O3'	9.17	129.67	109.50
1	A	181	G	C2'-C3'-O3'	9.11	129.53	109.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	243	A	C3'
1	A	281	G	C3'
1	A	366	C	C3'
1	A	1528	U	C3'

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	A	Sidechain
1	A	250	A	Sidechain
1	A	253	U	Sidechain
1	A	297	G	Sidechain
1	A	317	G	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	32489	0	16398	785	0
2	B	1901	0	1951	224	0
3	C	1613	0	1677	151	0
4	D	1703	0	1764	103	0
5	E	1147	0	1207	91	0
6	F	843	0	857	73	0
7	G	1257	0	1296	70	0
8	H	1116	0	1177	80	0
9	I	1010	0	1037	103	0
10	J	793	0	835	134	0
11	K	885	0	904	58	0
12	L	971	0	1057	77	0
13	M	997	0	1072	99	0
14	N	492	0	530	57	0
15	O	734	0	771	63	0
16	P	701	0	720	49	0
17	Q	857	0	928	74	0
18	R	598	0	670	51	0
19	S	648	0	673	70	0
20	T	763	0	861	68	0
21	U	209	0	221	26	0
22	X	84	0	45	3	0
23	Y	277	0	145	9	0
24	A	42	0	45	0	0
25	A	176	0	0	0	0
25	B	1	0	0	0	0
25	D	1	0	0	0	0
25	E	1	0	0	0	0
25	I	1	0	0	0	0
25	K	1	0	0	0	0
25	M	1	0	0	0	0
25	N	1	0	0	0	0
25	Q	1	0	0	0	0
26	A	51	0	0	0	0
26	E	3	0	0	0	0
26	G	1	0	0	0	0
26	Q	1	0	0	0	0
27	D	1	0	0	0	0
27	N	1	0	0	2	0
All	All	52372	0	36841	2320	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

The worst 5 of 2320 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:243:A:H4'	1:A:244:U:H5'	1.24	1.16
10:J:32:ALA:HB1	10:J:75:ILE:HG13	1.25	1.13
3:C:14:ILE:HG22	3:C:15:THR:H	1.11	1.13
15:O:87:ILE:HG22	15:O:88:ARG:H	1.07	1.11
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.31	1.07

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/256 (91%)	158 (68%)	61 (26%)	14 (6%)	1	9
3	C	205/239 (86%)	151 (74%)	36 (18%)	18 (9%)	1	4
4	D	206/209 (99%)	168 (82%)	33 (16%)	5 (2%)	6	27
5	E	149/162 (92%)	130 (87%)	16 (11%)	3 (2%)	7	31
6	F	99/101 (98%)	84 (85%)	13 (13%)	2 (2%)	7	31
7	G	153/156 (98%)	123 (80%)	27 (18%)	3 (2%)	7	31
8	H	136/138 (99%)	118 (87%)	12 (9%)	6 (4%)	2	15
9	I	125/128 (98%)	99 (79%)	18 (14%)	8 (6%)	1	8
10	J	97/105 (92%)	69 (71%)	17 (18%)	11 (11%)	0	2
11	K	117/129 (91%)	92 (79%)	21 (18%)	4 (3%)	3	21
12	L	123/135 (91%)	99 (80%)	16 (13%)	8 (6%)	1	8
13	M	123/126 (98%)	90 (73%)	22 (18%)	11 (9%)	1	4
14	N	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	2	12
15	O	86/89 (97%)	71 (83%)	15 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	82/88 (93%)	69 (84%)	12 (15%)	1 (1%)	13	44
17	Q	102/105 (97%)	86 (84%)	13 (13%)	3 (3%)	4	24
18	R	71/88 (81%)	60 (84%)	9 (13%)	2 (3%)	5	25
19	S	79/93 (85%)	65 (82%)	5 (6%)	9 (11%)	0	2
20	T	97/106 (92%)	71 (73%)	20 (21%)	6 (6%)	1	9
21	U	23/27 (85%)	16 (70%)	6 (26%)	1 (4%)	2	16
All	All	2364/2541 (93%)	1865 (79%)	381 (16%)	118 (5%)	2	13

5 of 118 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	74	LYS
2	B	207	ALA
3	C	15	THR
3	C	61	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	181 (90%)	21 (10%)	7	27
3	C	160/188 (85%)	142 (89%)	18 (11%)	6	23
4	D	180/181 (99%)	166 (92%)	14 (8%)	12	40
5	E	115/123 (94%)	101 (88%)	14 (12%)	5	19
6	F	90/90 (100%)	85 (94%)	5 (6%)	21	52
7	G	126/127 (99%)	121 (96%)	5 (4%)	31	65
8	H	119/119 (100%)	106 (89%)	13 (11%)	6	25
9	I	98/99 (99%)	90 (92%)	8 (8%)	11	38
10	J	87/92 (95%)	82 (94%)	5 (6%)	20	52
11	K	90/99 (91%)	83 (92%)	7 (8%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	104/111 (94%)	97 (93%)	7 (7%)	16	46
13	M	100/101 (99%)	90 (90%)	10 (10%)	7	28
14	N	49/50 (98%)	44 (90%)	5 (10%)	7	27
15	O	79/80 (99%)	74 (94%)	5 (6%)	18	48
16	P	72/74 (97%)	65 (90%)	7 (10%)	8	30
17	Q	96/97 (99%)	92 (96%)	4 (4%)	30	62
18	R	64/77 (83%)	61 (95%)	3 (5%)	26	59
19	S	71/80 (89%)	70 (99%)	1 (1%)	67	86
20	T	76/82 (93%)	68 (90%)	8 (10%)	7	26
21	U	19/22 (86%)	19 (100%)	0	100	100
All	All	1997/2112 (95%)	1837 (92%)	160 (8%)	12	40

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	73	MET
8	H	122	ARG
17	Q	101	ARG
7	G	114	ARG
8	H	52	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	37	ASN
9	I	23	ASN
16	P	76	GLN
7	G	56	GLN
7	G	106	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	200 (13%)	62 (4%)
22	X	3/6 (50%)	1 (33%)	0
23	Y	10/17 (58%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	1523/1545 (98%)	201 (13%)	62 (4%)

5 of 201 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	559	A
1	A	793	U
1	A	1498	U
1	A	687	A
1	A	913	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
23	CM0	Y	34	23	16,26,27	1.71	4 (25%)	18,37,40	5.07	6 (33%)
23	6MZ	Y	37	23	18,25,26	0.83	0	16,36,39	1.01	2 (12%)

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
23	CM0	Y	34	23	-	3/8/30/31	0/2/2/2
23	6MZ	Y	37	23	-	0/5/27/28	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	34	CM0	C4-N3	4.04	1.40	1.33
23	Y	34	CM0	O5-C7	3.23	1.54	1.43
23	Y	34	CM0	C4-C5	3.03	1.47	1.40
23	Y	34	CM0	O5-C5	-2.65	1.32	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	34	CM0	C4-N3-C2	15.92	128.58	115.14
23	Y	34	CM0	C7-O5-C5	9.61	136.67	117.76
23	Y	34	CM0	C5-C6-N1	6.03	126.70	120.44
23	Y	34	CM0	C5-C4-N3	-6.00	114.44	122.66
23	Y	34	CM0	O5-C7-C8	5.36	123.01	108.59

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Y	34	CM0	C4-C5-O5-C7
23	Y	34	CM0	C8-C7-O5-C5
23	Y	34	CM0	C6-C5-O5-C7

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Y	34	CM0	5	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 243 ligands modelled in this entry, 242 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PAR	A	1601	-	45,45,45	1.56	6 (13%)	64,67,67	1.26	8 (12%)

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
24	PAR	A	1601	-	-	5/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	C64-C54	4.67	1.58	1.52
24	A	1601	PAR	O54-C14	3.29	1.50	1.41
24	A	1601	PAR	C52-C42	3.01	1.58	1.52
24	A	1601	PAR	C11-C21	2.75	1.57	1.52
24	A	1601	PAR	C31-C21	2.39	1.56	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1601	PAR	O33-C14-C24	4.04	115.17	108.22
24	A	1601	PAR	O54-C54-C64	3.62	112.76	106.01
24	A	1601	PAR	C14-O54-C54	3.33	120.22	113.69
24	A	1601	PAR	O11-C11-C21	2.83	113.09	108.22
24	A	1601	PAR	O52-C13-C23	2.76	113.69	107.96

There are no chirality outliers.

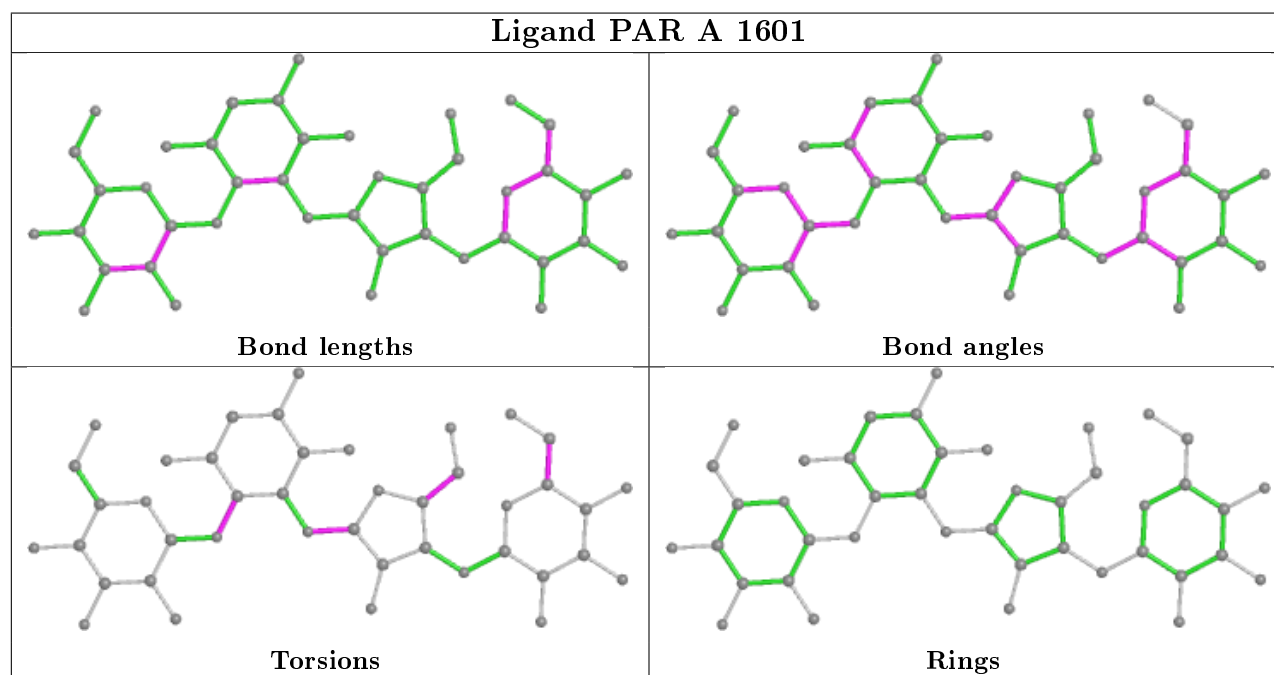
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	C44-C54-C64-N64
24	A	1601	PAR	O54-C54-C64-N64
24	A	1601	PAR	C52-C42-O11-C11
24	A	1601	PAR	C33-C43-C53-O53
24	A	1601	PAR	C23-C13-O52-C52

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	1512/1522 (99%)	0.07	30 (1%) 65 44	32, 58, 130, 183	0
2	B	235/256 (91%)	-0.01	8 (3%) 45 24	50, 84, 126, 147	0
3	C	207/239 (86%)	-0.14	1 (0%) 91 81	48, 74, 109, 117	0
4	D	208/209 (99%)	-0.37	0 100 100	45, 63, 83, 94	0
5	E	151/162 (93%)	-0.40	0 100 100	35, 50, 68, 86	0
6	F	101/101 (100%)	-0.24	1 (0%) 82 67	62, 81, 93, 98	0
7	G	155/156 (99%)	-0.23	6 (3%) 39 20	50, 70, 104, 120	0
8	H	138/138 (100%)	-0.41	0 100 100	33, 50, 65, 70	0
9	I	127/128 (99%)	-0.23	0 100 100	45, 81, 99, 113	0
10	J	99/105 (94%)	0.11	2 (2%) 65 44	46, 102, 141, 147	0
11	K	119/129 (92%)	-0.23	2 (1%) 70 49	39, 58, 81, 96	0
12	L	125/135 (92%)	-0.17	4 (3%) 47 25	23, 54, 71, 104	0
13	M	125/126 (99%)	0.15	9 (7%) 15 6	52, 70, 131, 162	0
14	N	60/61 (98%)	-0.21	0 100 100	50, 65, 88, 100	0
15	O	88/89 (98%)	-0.23	1 (1%) 80 64	46, 64, 82, 102	0
16	P	84/88 (95%)	-0.40	3 (3%) 42 22	39, 50, 62, 89	0
17	Q	104/105 (99%)	-0.01	7 (6%) 17 7	40, 56, 100, 133	0
18	R	73/88 (82%)	-0.07	3 (4%) 37 18	52, 67, 107, 137	0
19	S	81/93 (87%)	-0.14	2 (2%) 57 34	52, 83, 105, 117	0
20	T	99/106 (93%)	-0.27	0 100 100	39, 55, 77, 84	0
21	U	25/27 (92%)	0.03	1 (4%) 38 19	47, 59, 82, 87	0
22	X	4/6 (66%)	-0.15	0 100 100	55, 57, 60, 81	0
23	Y	11/17 (64%)	0.71	1 (9%) 9 3	54, 85, 110, 114	0
All	All	3931/4086 (96%)	-0.09	81 (2%) 63 43	23, 63, 115, 183	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Q	105	ALA	11.3
13	M	123	ALA	9.4
1	A	1129	C	7.0
13	M	124	PRO	6.9
17	Q	103	GLY	6.5

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
23	CM0	Y	34	25/26	0.94	0.16	60,65,68,69	0
23	6MZ	Y	37	23/24	0.95	0.23	56,60,63,66	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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
25	MG	A	1622	1/1	-0.11	1.41	116,116,116,116	0
25	MG	A	1758	1/1	0.29	0.49	79,79,79,79	0
26	K	A	1826	1/1	0.46	1.57	152,152,152,152	0
26	K	A	1788	1/1	0.46	0.51	117,117,117,117	0
25	MG	A	1671	1/1	0.46	0.39	70,70,70,70	0
25	MG	A	1630	1/1	0.47	0.50	87,87,87,87	0
25	MG	A	1673	1/1	0.48	0.54	89,89,89,89	0
25	MG	A	1612	1/1	0.54	0.45	83,83,83,83	0
26	K	A	1820	1/1	0.54	0.23	108,108,108,108	0
26	K	A	1828	1/1	0.54	0.31	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1620	1/1	0.58	0.49	105,105,105,105	0
25	MG	A	1763	1/1	0.60	0.19	96,96,96,96	0
25	MG	A	1680	1/1	0.62	0.60	62,62,62,62	0
26	K	A	1806	1/1	0.62	1.08	129,129,129,129	0
26	K	A	1821	1/1	0.63	0.21	90,90,90,90	0
25	MG	A	1742	1/1	0.63	1.15	88,88,88,88	0
25	MG	A	1653	1/1	0.64	0.39	78,78,78,78	0
25	MG	A	1613	1/1	0.64	0.74	68,68,68,68	0
26	K	A	1785	1/1	0.66	0.16	92,92,92,92	0
26	K	A	1786	1/1	0.68	0.17	94,94,94,94	0
25	MG	A	1672	1/1	0.68	0.46	86,86,86,86	0
25	MG	A	1625	1/1	0.69	0.26	74,74,74,74	0
26	K	A	1787	1/1	0.70	0.20	83,83,83,83	0
25	MG	A	1752	1/1	0.70	0.31	45,45,45,45	0
26	K	A	1814	1/1	0.71	0.32	110,110,110,110	0
25	MG	A	1760	1/1	0.71	0.23	50,50,50,50	0
25	MG	A	1699	1/1	0.71	0.22	50,50,50,50	0
25	MG	A	1602	1/1	0.71	0.19	44,44,44,44	0
26	K	A	1824	1/1	0.72	0.39	115,115,115,115	0
25	MG	A	1667	1/1	0.72	0.95	89,89,89,89	0
25	MG	A	1737	1/1	0.72	0.42	58,58,58,58	0
25	MG	A	1749	1/1	0.73	0.92	85,85,85,85	0
25	MG	A	1773	1/1	0.74	1.29	86,86,86,86	0
26	K	A	1797	1/1	0.75	0.67	94,94,94,94	0
25	MG	A	1687	1/1	0.75	0.24	35,35,35,35	0
25	MG	A	1688	1/1	0.75	0.27	50,50,50,50	0
25	MG	A	1769	1/1	0.75	0.18	35,35,35,35	0
26	K	A	1807	1/1	0.75	0.28	86,86,86,86	0
25	MG	A	1665	1/1	0.75	0.69	67,67,67,67	0
25	MG	A	1716	1/1	0.75	0.78	68,68,68,68	0
25	MG	A	1626	1/1	0.75	0.52	88,88,88,88	0
25	MG	A	1623	1/1	0.76	0.44	98,98,98,98	0
25	MG	A	1669	1/1	0.76	0.25	91,91,91,91	0
25	MG	A	1701	1/1	0.76	0.32	71,71,71,71	0
25	MG	A	1604	1/1	0.76	0.64	59,59,59,59	0
26	K	E	203	1/1	0.76	0.95	115,115,115,115	0
25	MG	A	1648	1/1	0.78	0.36	73,73,73,73	0
25	MG	A	1771	1/1	0.78	0.37	45,45,45,45	0
26	K	A	1781	1/1	0.78	0.32	94,94,94,94	0
25	MG	A	1735	1/1	0.78	0.41	77,77,77,77	0
25	MG	A	1675	1/1	0.78	0.36	91,91,91,91	0
26	K	A	1804	1/1	0.78	0.32	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1678	1/1	0.78	0.37	80,80,80,80	0
26	K	A	1783	1/1	0.79	0.23	82,82,82,82	0
25	MG	A	1614	1/1	0.79	0.17	48,48,48,48	0
25	MG	Q	201	1/1	0.79	0.17	56,56,56,56	0
26	K	A	1780	1/1	0.79	0.25	88,88,88,88	0
25	MG	A	1654	1/1	0.79	0.17	24,24,24,24	0
25	MG	N	102	1/1	0.79	0.27	48,48,48,48	0
25	MG	A	1603	1/1	0.79	0.18	89,89,89,89	0
25	MG	A	1757	1/1	0.80	0.24	82,82,82,82	0
25	MG	A	1700	1/1	0.80	0.44	62,62,62,62	0
25	MG	A	1746	1/1	0.80	0.21	62,62,62,62	0
25	MG	A	1709	1/1	0.80	0.76	48,48,48,48	0
26	K	A	1800	1/1	0.80	0.27	97,97,97,97	0
26	K	A	1803	1/1	0.81	0.13	76,76,76,76	0
26	K	A	1798	1/1	0.81	0.37	93,93,93,93	0
25	MG	A	1681	1/1	0.82	0.25	57,57,57,57	0
25	MG	A	1659	1/1	0.82	0.56	60,60,60,60	0
25	MG	A	1616	1/1	0.82	0.20	31,31,31,31	0
26	K	A	1816	1/1	0.82	0.39	88,88,88,88	0
26	K	E	204	1/1	0.82	0.18	96,96,96,96	0
25	MG	A	1775	1/1	0.82	0.17	48,48,48,48	0
26	K	A	1805	1/1	0.82	0.25	96,96,96,96	0
26	K	A	1811	1/1	0.83	0.33	99,99,99,99	0
26	K	A	1789	1/1	0.83	0.10	103,103,103,103	0
26	K	A	1812	1/1	0.83	0.27	104,104,104,104	0
26	K	A	1792	1/1	0.83	0.35	111,111,111,111	0
25	MG	A	1636	1/1	0.83	0.18	80,80,80,80	0
25	MG	A	1710	1/1	0.83	0.86	61,61,61,61	0
26	K	A	1779	1/1	0.83	0.19	78,78,78,78	0
25	MG	A	1714	1/1	0.83	0.51	57,57,57,57	0
25	MG	A	1730	1/1	0.84	0.53	48,48,48,48	0
26	K	A	1790	1/1	0.84	0.28	85,85,85,85	0
25	MG	A	1754	1/1	0.84	0.26	42,42,42,42	0
25	MG	A	1641	1/1	0.84	0.46	49,49,49,49	0
26	K	A	1794	1/1	0.84	0.26	96,96,96,96	0
25	MG	A	1705	1/1	0.84	0.24	39,39,39,39	0
25	MG	A	1689	1/1	0.84	0.21	46,46,46,46	0
25	MG	A	1718	1/1	0.84	0.27	55,55,55,55	0
25	MG	A	1619	1/1	0.85	0.38	80,80,80,80	0
25	MG	A	1776	1/1	0.85	0.40	52,52,52,52	0
26	K	A	1802	1/1	0.85	0.52	95,95,95,95	0
25	MG	A	1717	1/1	0.85	0.28	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1652	1/1	0.85	0.14	55,55,55,55	0
25	MG	A	1685	1/1	0.85	0.30	64,64,64,64	0
26	K	A	1799	1/1	0.86	0.20	94,94,94,94	0
26	K	A	1796	1/1	0.86	0.32	101,101,101,101	0
25	MG	A	1617	1/1	0.86	0.37	62,62,62,62	0
26	K	A	1808	1/1	0.86	0.22	120,120,120,120	0
25	MG	A	1755	1/1	0.86	0.17	42,42,42,42	0
25	MG	A	1712	1/1	0.86	0.57	68,68,68,68	0
25	MG	A	1615	1/1	0.86	0.15	57,57,57,57	0
25	MG	A	1711	1/1	0.86	0.86	89,89,89,89	0
26	K	A	1810	1/1	0.86	1.01	100,100,100,100	0
25	MG	A	1629	1/1	0.87	0.34	85,85,85,85	0
25	MG	A	1753	1/1	0.87	0.23	56,56,56,56	0
25	MG	A	1618	1/1	0.87	0.21	85,85,85,85	0
25	MG	A	1770	1/1	0.87	0.12	58,58,58,58	0
25	MG	A	1611	1/1	0.87	0.34	65,65,65,65	0
25	MG	A	1644	1/1	0.87	0.25	36,36,36,36	0
25	MG	A	1759	1/1	0.87	0.29	50,50,50,50	0
26	K	A	1822	1/1	0.87	0.15	87,87,87,87	0
26	K	A	1801	1/1	0.87	0.17	82,82,82,82	0
25	MG	A	1624	1/1	0.87	0.40	48,48,48,48	0
25	MG	A	1666	1/1	0.88	0.28	59,59,59,59	0
25	MG	A	1693	1/1	0.88	0.51	65,65,65,65	0
26	K	A	1795	1/1	0.88	0.13	86,86,86,86	0
25	MG	A	1683	1/1	0.88	0.56	56,56,56,56	0
26	K	A	1817	1/1	0.88	0.23	97,97,97,97	0
25	MG	A	1739	1/1	0.88	0.80	74,74,74,74	0
25	MG	A	1676	1/1	0.88	0.11	37,37,37,37	0
26	K	A	1809	1/1	0.88	0.23	93,93,93,93	0
25	MG	A	1719	1/1	0.88	0.37	58,58,58,58	0
25	MG	A	1765	1/1	0.88	0.41	47,47,47,47	0
25	MG	A	1657	1/1	0.88	0.39	50,50,50,50	0
25	MG	A	1635	1/1	0.88	0.48	81,81,81,81	0
25	MG	A	1767	1/1	0.88	0.16	36,36,36,36	0
25	MG	A	1655	1/1	0.88	0.56	46,46,46,46	0
25	MG	A	1713	1/1	0.89	0.31	27,27,27,27	0
25	MG	A	1736	1/1	0.89	0.27	44,44,44,44	0
25	MG	A	1610	1/1	0.89	0.59	106,106,106,106	0
25	MG	A	1608	1/1	0.89	0.27	54,54,54,54	0
25	MG	A	1756	1/1	0.89	0.29	43,43,43,43	0
25	MG	A	1646	1/1	0.89	0.20	51,51,51,51	0
26	K	A	1818	1/1	0.89	0.34	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	K	A	1825	1/1	0.90	0.29	100,100,100,100	0
25	MG	A	1628	1/1	0.90	0.59	39,39,39,39	0
25	MG	A	1637	1/1	0.90	0.39	44,44,44,44	0
25	MG	A	1772	1/1	0.90	0.20	47,47,47,47	0
26	K	A	1827	1/1	0.90	0.14	72,72,72,72	0
26	K	A	1823	1/1	0.90	0.24	109,109,109,109	0
25	MG	A	1731	1/1	0.90	0.33	33,33,33,33	0
26	K	G	201	1/1	0.90	0.19	87,87,87,87	0
25	MG	A	1691	1/1	0.90	0.32	48,48,48,48	0
25	MG	A	1694	1/1	0.90	0.16	28,28,28,28	0
25	MG	A	1645	1/1	0.90	0.30	45,45,45,45	0
25	MG	A	1606	1/1	0.90	0.79	40,40,40,40	0
25	MG	M	201	1/1	0.90	0.23	28,28,28,28	0
26	K	A	1813	1/1	0.90	0.26	127,127,127,127	0
25	MG	A	1663	1/1	0.91	0.48	47,47,47,47	0
25	MG	A	1740	1/1	0.91	0.17	28,28,28,28	0
26	K	A	1815	1/1	0.91	0.10	88,88,88,88	0
25	MG	A	1677	1/1	0.91	0.29	21,21,21,21	0
25	MG	A	1670	1/1	0.91	0.41	67,67,67,67	0
25	MG	A	1751	1/1	0.91	0.20	41,41,41,41	0
25	MG	A	1750	1/1	0.91	0.41	36,36,36,36	0
25	MG	A	1696	1/1	0.91	0.61	50,50,50,50	0
25	MG	D	302	1/1	0.91	0.09	41,41,41,41	0
26	K	A	1793	1/1	0.91	0.21	90,90,90,90	0
25	MG	A	1768	1/1	0.92	0.59	37,37,37,37	0
25	MG	A	1674	1/1	0.92	0.57	51,51,51,51	0
25	MG	A	1632	1/1	0.92	0.90	74,74,74,74	0
25	MG	A	1621	1/1	0.92	0.21	76,76,76,76	0
25	MG	A	1743	1/1	0.92	0.46	51,51,51,51	0
24	PAR	A	1601	42/42	0.92	0.26	48,50,71,74	0
25	MG	A	1703	1/1	0.92	0.30	44,44,44,44	0
25	MG	A	1741	1/1	0.92	0.23	79,79,79,79	0
25	MG	A	1638	1/1	0.92	0.39	30,30,30,30	0
25	MG	A	1633	1/1	0.92	0.47	29,29,29,29	0
25	MG	A	1627	1/1	0.92	0.27	45,45,45,45	0
25	MG	A	1715	1/1	0.93	0.12	24,24,24,24	0
25	MG	A	1662	1/1	0.93	0.51	43,43,43,43	0
25	MG	A	1679	1/1	0.93	0.26	48,48,48,48	0
25	MG	A	1647	1/1	0.93	0.22	38,38,38,38	0
25	MG	A	1722	1/1	0.93	0.70	34,34,34,34	0
25	MG	A	1605	1/1	0.93	0.23	18,18,18,18	0
25	MG	A	1684	1/1	0.93	0.24	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1738	1/1	0.93	0.30	36,36,36,36	0
26	K	A	1782	1/1	0.93	0.17	92,92,92,92	0
25	MG	A	1702	1/1	0.93	0.40	58,58,58,58	0
25	MG	A	1658	1/1	0.93	0.65	47,47,47,47	0
25	MG	A	1692	1/1	0.93	0.20	47,47,47,47	0
25	MG	A	1642	1/1	0.93	0.32	65,65,65,65	0
25	MG	A	1724	1/1	0.93	0.21	35,35,35,35	0
25	MG	A	1609	1/1	0.93	0.39	1,1,1,1	0
25	MG	A	1774	1/1	0.93	0.33	56,56,56,56	0
25	MG	A	1656	1/1	0.94	0.35	31,31,31,31	0
25	MG	A	1762	1/1	0.94	0.28	29,29,29,29	0
25	MG	A	1748	1/1	0.94	0.22	43,43,43,43	0
25	MG	A	1721	1/1	0.94	0.13	26,26,26,26	0
25	MG	A	1682	1/1	0.94	0.24	43,43,43,43	0
25	MG	A	1732	1/1	0.94	0.25	45,45,45,45	0
25	MG	K	201	1/1	0.94	0.16	49,49,49,49	0
26	K	A	1784	1/1	0.94	0.14	76,76,76,76	0
25	MG	A	1661	1/1	0.94	0.53	54,54,54,54	0
26	K	E	202	1/1	0.94	0.34	83,83,83,83	0
26	K	Q	202	1/1	0.94	0.11	95,95,95,95	0
25	MG	A	1698	1/1	0.94	0.13	12,12,12,12	0
25	MG	A	1708	1/1	0.94	0.29	33,33,33,33	0
25	MG	A	1695	1/1	0.95	0.29	47,47,47,47	0
25	MG	A	1734	1/1	0.95	0.26	29,29,29,29	0
25	MG	A	1728	1/1	0.95	0.32	40,40,40,40	0
26	K	A	1778	1/1	0.95	0.07	68,68,68,68	0
25	MG	A	1720	1/1	0.95	0.39	45,45,45,45	0
25	MG	A	1766	1/1	0.95	0.14	28,28,28,28	0
25	MG	A	1747	1/1	0.95	0.24	28,28,28,28	0
25	MG	A	1704	1/1	0.95	0.22	52,52,52,52	0
25	MG	A	1764	1/1	0.95	0.23	26,26,26,26	0
25	MG	A	1631	1/1	0.95	0.22	51,51,51,51	0
25	MG	A	1690	1/1	0.95	0.38	64,64,64,64	0
25	MG	A	1725	1/1	0.95	0.22	36,36,36,36	0
25	MG	A	1723	1/1	0.95	0.07	29,29,29,29	0
25	MG	A	1744	1/1	0.96	0.38	90,90,90,90	0
26	K	A	1791	1/1	0.96	0.17	98,98,98,98	0
25	MG	A	1686	1/1	0.96	0.21	28,28,28,28	0
25	MG	A	1697	1/1	0.96	0.40	48,48,48,48	0
25	MG	A	1706	1/1	0.96	0.75	36,36,36,36	0
25	MG	A	1664	1/1	0.96	0.19	18,18,18,18	0
25	MG	A	1745	1/1	0.96	0.23	25,25,25,25	0

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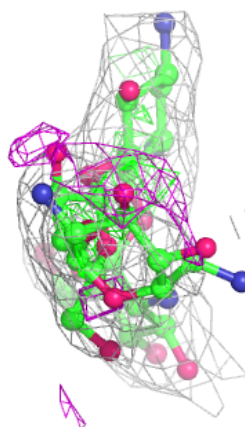
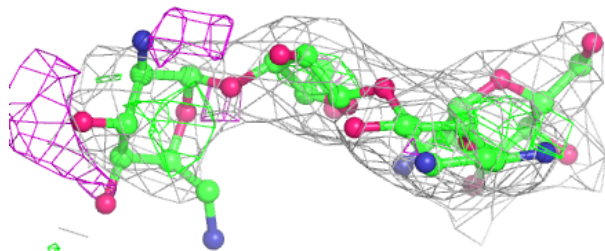
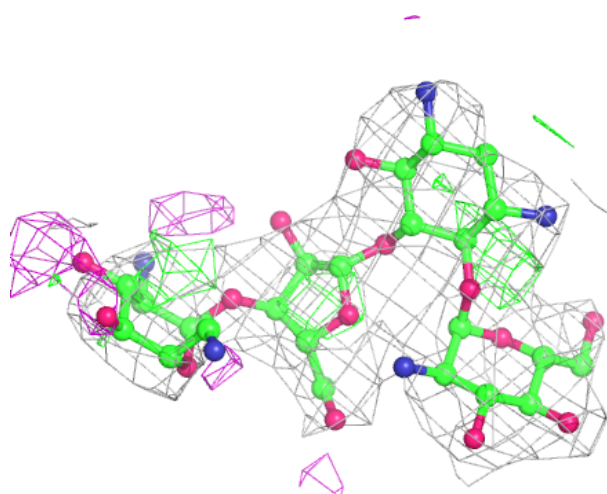
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	I	201	1/1	0.96	0.75	78,78,78,78	0
25	MG	A	1726	1/1	0.96	0.25	28,28,28,28	0
25	MG	A	1651	1/1	0.97	0.53	39,39,39,39	0
25	MG	A	1733	1/1	0.97	0.60	35,35,35,35	0
25	MG	A	1707	1/1	0.97	0.51	33,33,33,33	0
25	MG	A	1640	1/1	0.97	0.34	29,29,29,29	0
25	MG	A	1607	1/1	0.97	0.66	39,39,39,39	0
25	MG	A	1668	1/1	0.97	0.56	38,38,38,38	0
25	MG	A	1650	1/1	0.97	0.37	36,36,36,36	0
25	MG	A	1777	1/1	0.97	0.08	38,38,38,38	0
25	MG	A	1727	1/1	0.97	0.14	27,27,27,27	0
25	MG	A	1729	1/1	0.98	0.60	33,33,33,33	0
25	MG	A	1643	1/1	0.98	0.13	34,34,34,34	0
25	MG	A	1660	1/1	0.98	0.41	28,28,28,28	0
25	MG	A	1634	1/1	0.98	0.58	36,36,36,36	0
25	MG	A	1761	1/1	0.98	0.05	11,11,11,11	0
26	K	A	1819	1/1	0.98	0.73	130,130,130,130	0
25	MG	A	1639	1/1	0.98	0.40	32,32,32,32	0
25	MG	E	201	1/1	0.98	0.39	44,44,44,44	0
25	MG	A	1649	1/1	0.99	0.38	1,1,1,1	0
25	MG	B	301	1/1	0.99	0.26	43,43,43,43	0
27	ZN	D	301	1/1	0.99	0.37	69,69,69,69	0
27	ZN	N	101	1/1	1.00	0.11	64,64,64,64	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 PAR A 1601:**

$2mF_o-DF_c$  (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.