



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:06 AM GMT

PDB ID : 2VQE  
Title : MODIFIED URIDINES WITH C5-METHYLENE SUBSTITUENTS AT THE FIRST POSITION OF THE TRNA ANTICODON STABILIZE U-G WOB-  
BLE PAIRING DURING DECODING  
Authors : Kurata, S.; Weixlbaumer, A.; Ohtsuki, T.; Shimazaki, T.; Wada, T.; Kirino, Y.; Takai, K.; Watanabe, K.; Ramakrishnan, V.; Suzuki, T.  
Deposited on : 2008-03-13  
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

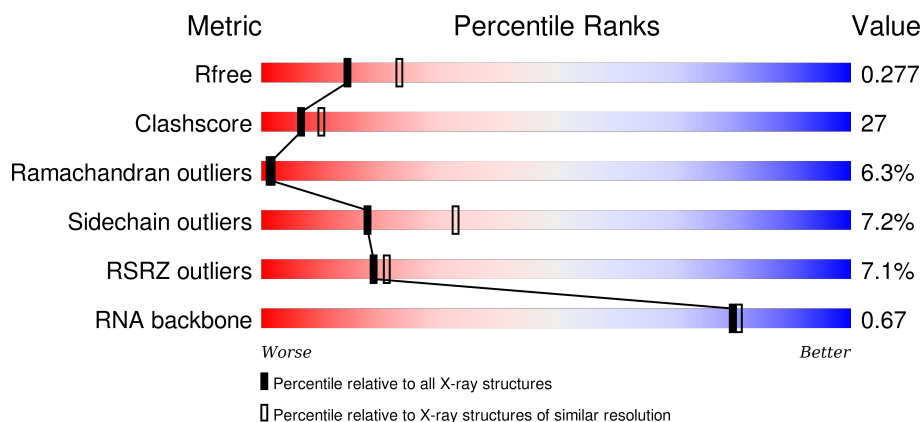
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


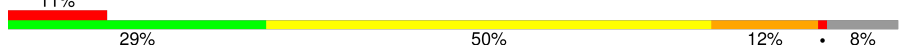
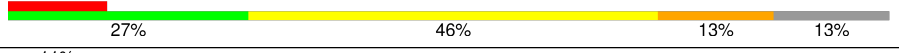

The reported resolution of this entry is 2.50 Å.

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.





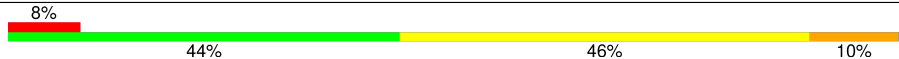

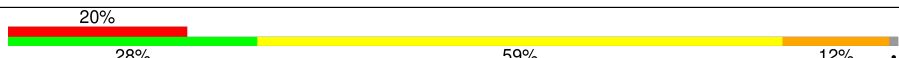
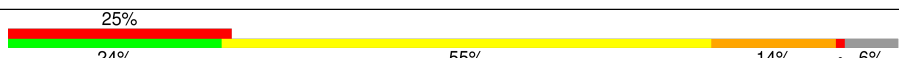

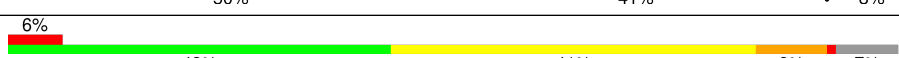
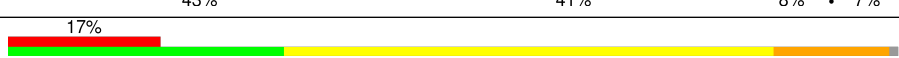
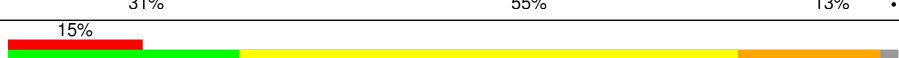
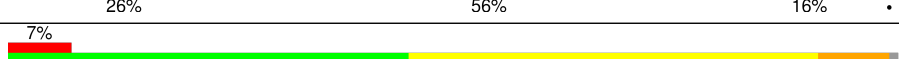
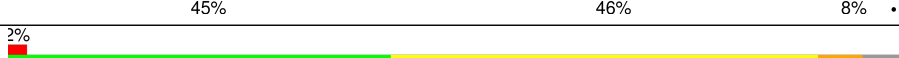
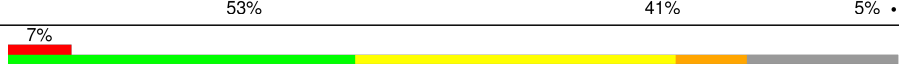
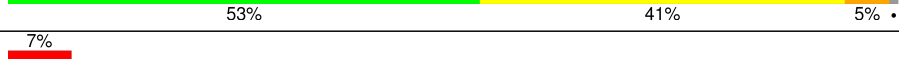

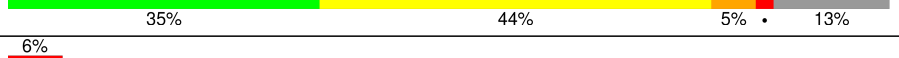


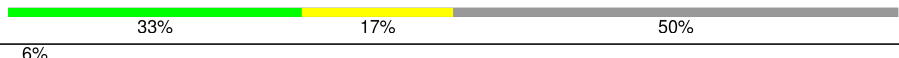
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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. 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	
2	B	256	
3	C	239	
4	D	209	

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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
24	MG	Z	100	-	-	-	X
24	MG	Z	103	-	-	-	X
24	MG	Z	119	-	-	-	X
24	MG	Z	121	-	-	-	X
24	MG	Z	122	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	Z	131	-	-	-	X
24	MG	Z	133	-	-	-	X
24	MG	Z	136	-	-	-	X
24	MG	Z	142	-	-	-	X
24	MG	Z	143	-	-	-	X
24	MG	Z	148	-	-	-	X
24	MG	Z	149	-	-	-	X
24	MG	Z	162	-	-	-	X
24	MG	Z	165	-	-	-	X
24	MG	Z	172	-	-	-	X
24	MG	Z	190	-	-	-	X
24	MG	Z	191	-	-	-	X
24	MG	Z	200	-	-	-	X
24	MG	Z	202	-	-	-	X
24	MG	Z	211	-	-	-	X
24	MG	Z	212	-	-	-	X
24	MG	Z	26	-	-	-	X
24	MG	Z	36	-	-	-	X
24	MG	Z	37	-	-	-	X
24	MG	Z	41	-	-	-	X
24	MG	Z	47	-	-	-	X
24	MG	Z	54	-	-	-	X
24	MG	Z	57	-	-	-	X
24	MG	Z	64	-	-	-	X
24	MG	Z	67	-	-	-	X
24	MG	Z	71	-	-	-	X
24	MG	Z	76	-	-	-	X
24	MG	Z	81	-	-	-	X
24	MG	Z	82	-	-	-	X
24	MG	Z	94	-	-	-	X
25	ZN	Z	140	-	-	-	X
26	K	Z	268	-	-	-	X
26	K	Z	273	-	-	-	X
26	K	Z	287	-	-	-	X
27	PAR	Z	291	-	-	-	X

## 2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52245 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	0	0	0
			32511	14472	6016	10511	1512			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1874	1195	336	338	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
			1011	639	198	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 TYPE Z.

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	161	147	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
			597	380	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
			762	469	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(\*UP\*UP\*AP\*AP\*AP\*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	3	Total	C	N	O	P	0	0	0
			59	28	9	20	2			

- Molecule 23 is a RNA chain called 5'-R(\*GP\*CP\*AP\*UP\*GP\*CP\*UP\*TM2P\*AP\*AP\*AP\*AP\*CP\*AP\*UP\*GP\*CP)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	Y	7	Total	C	N	O	P	S	0	0	0
			153	70	28	48	6	1			

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	Z	206	Total	Mg	0	0
			206	206		

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

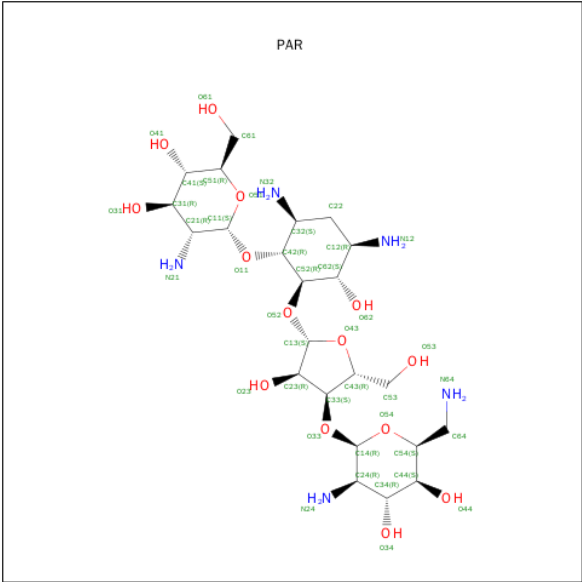
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	Z	2	Total	Zn	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	Z	62	Total	K	0	0
			62	62		

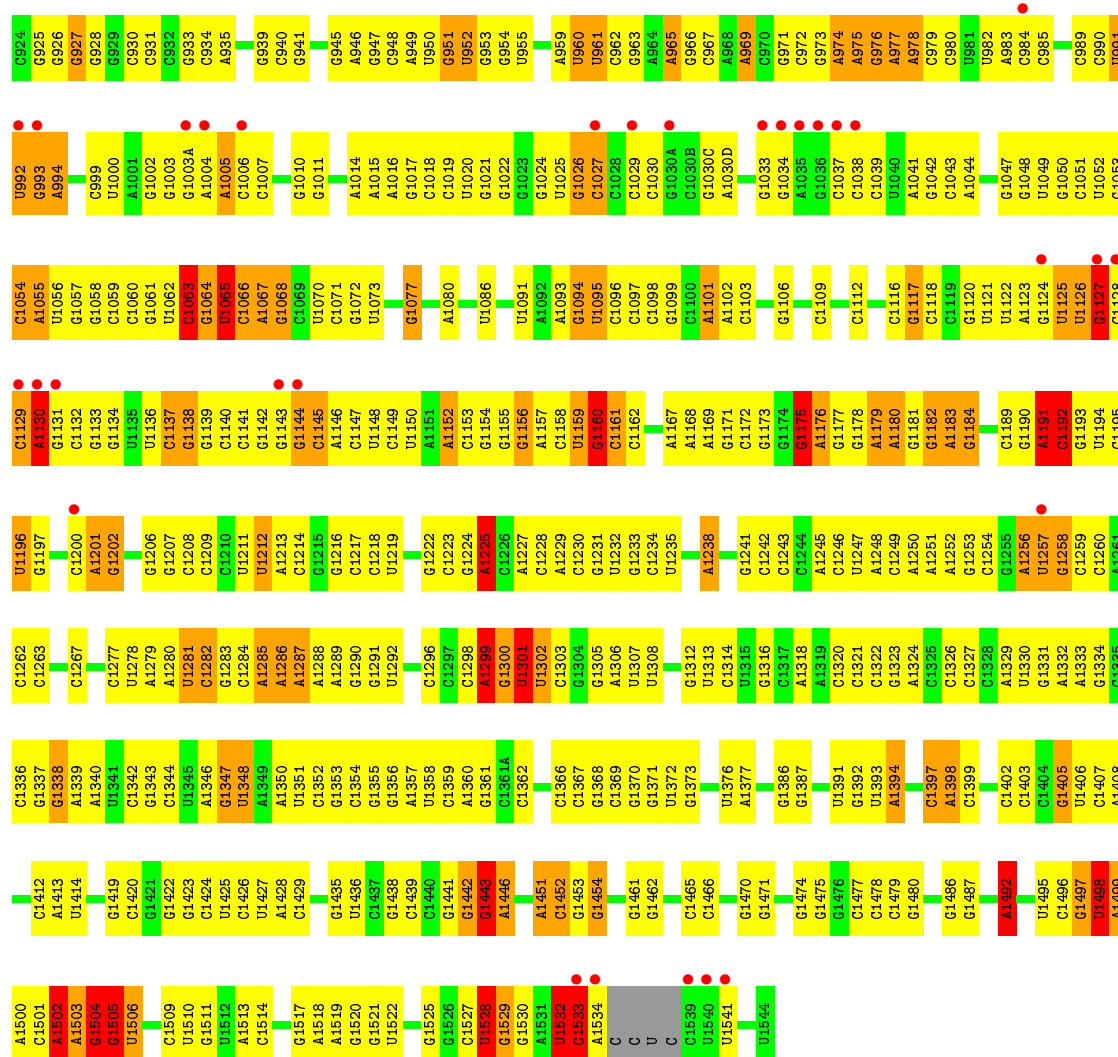
- Molecule 27 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



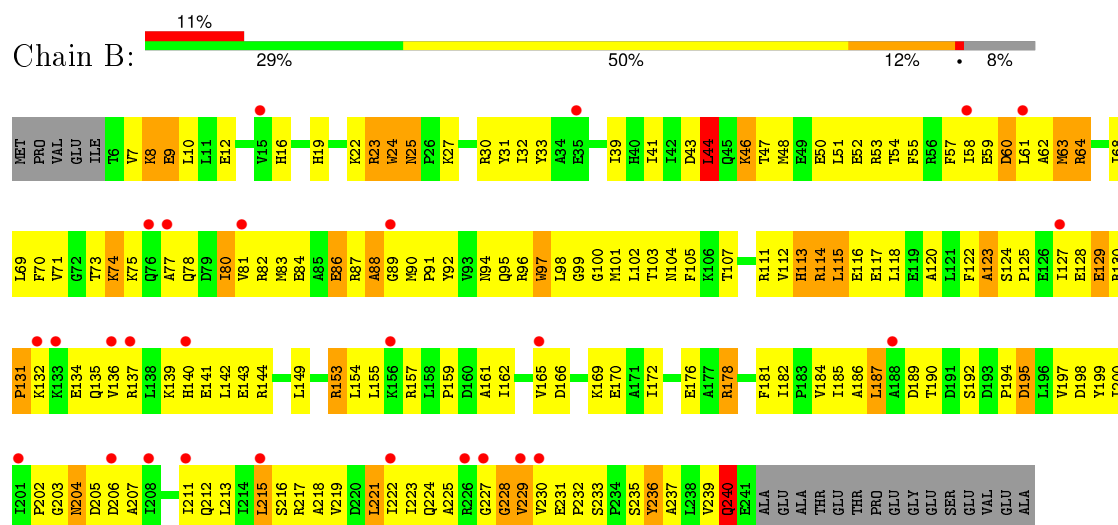


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	Z	1	Total	C	N	O	0	0
			42	23	5	14		

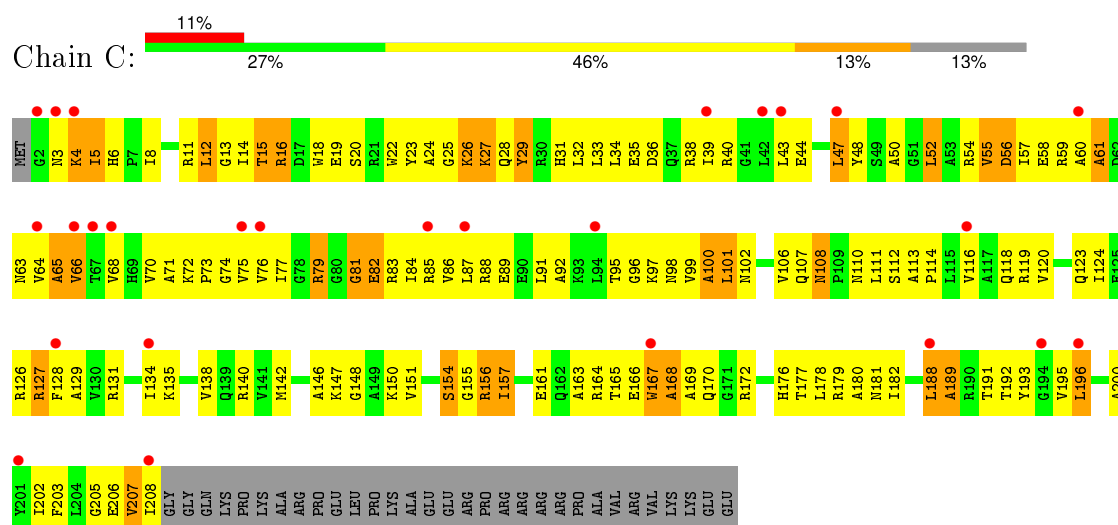




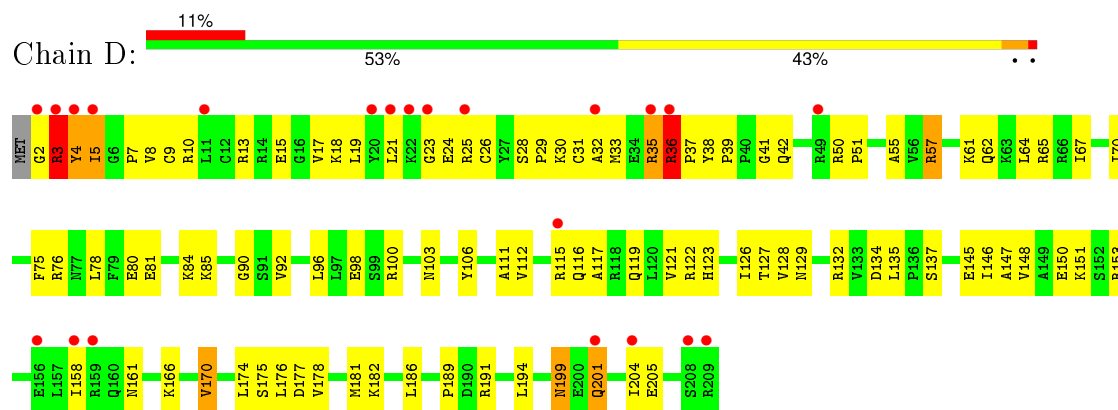
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



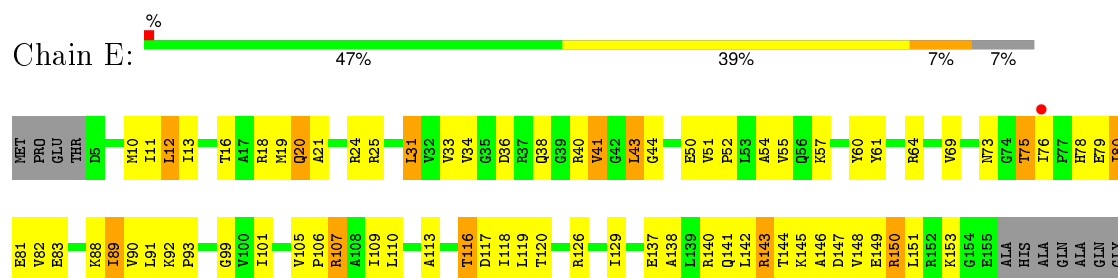
- Molecule 3: 30S RIBOSOMAL PROTEIN S3



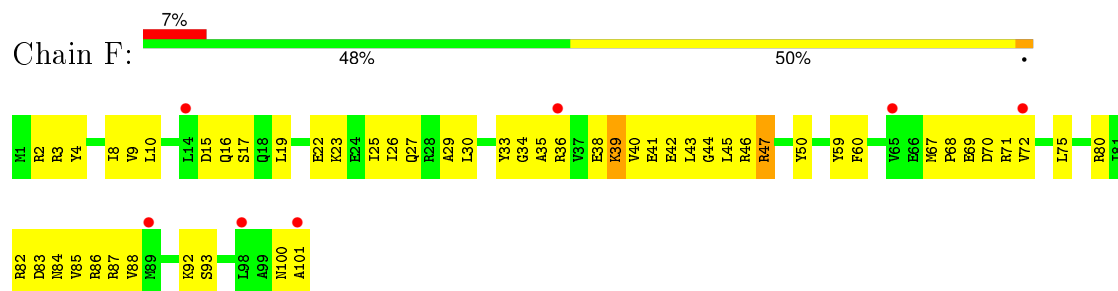
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



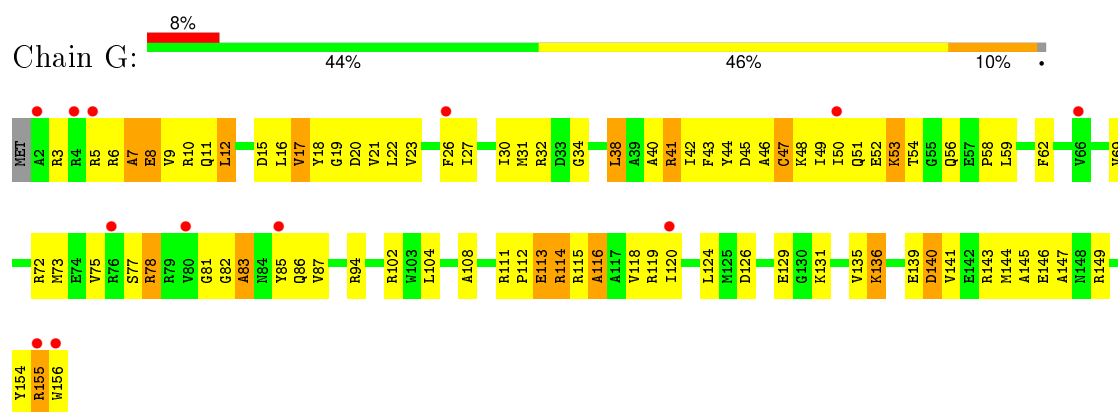
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



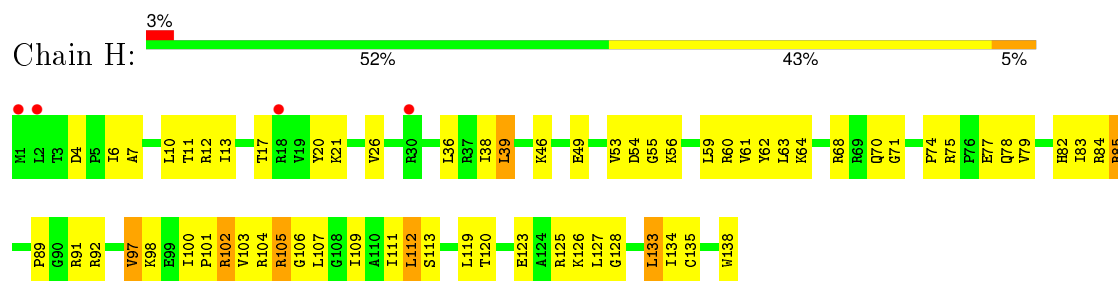
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



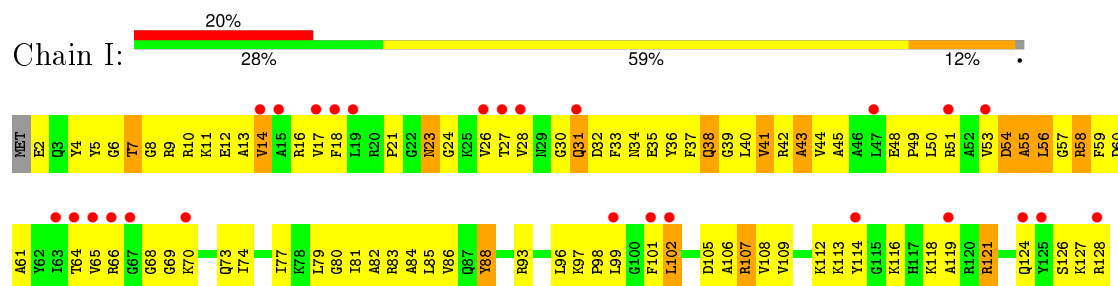
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



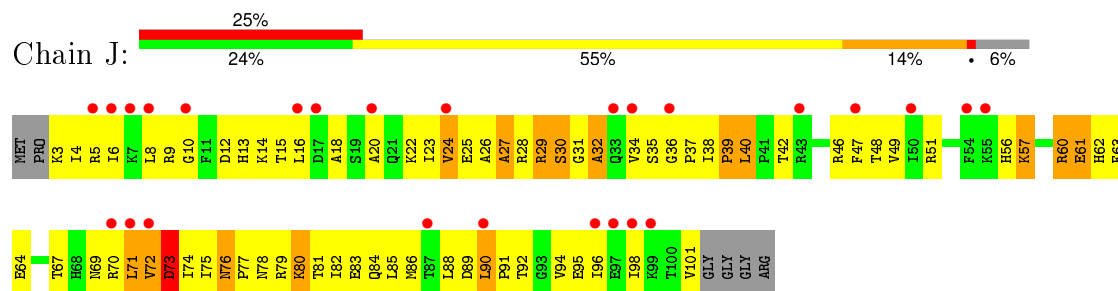
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



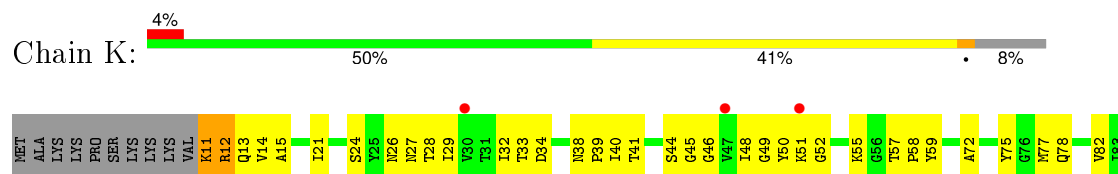
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

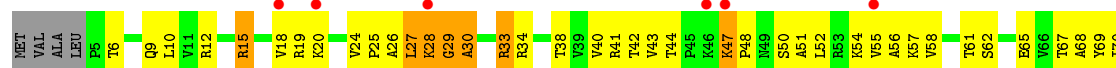


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

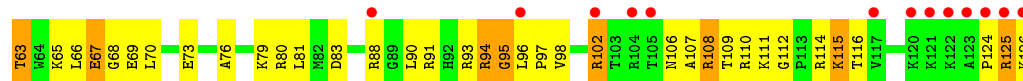
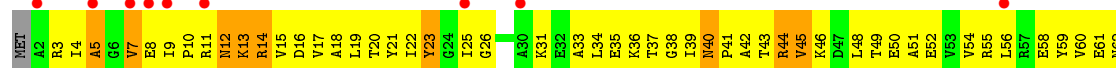




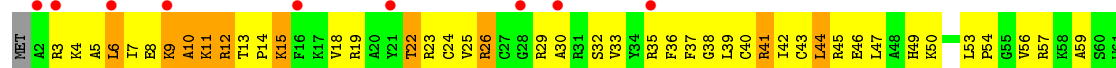
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



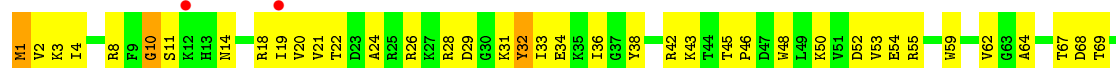
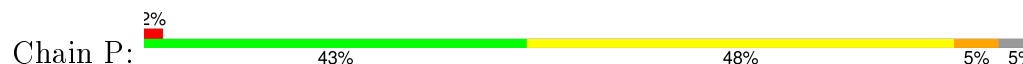
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



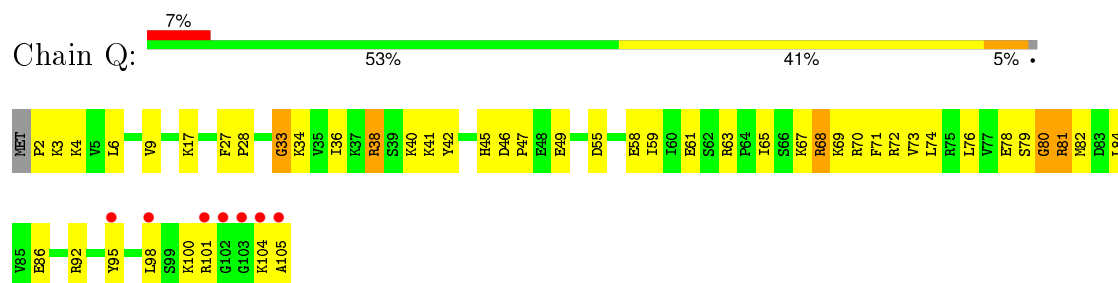
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



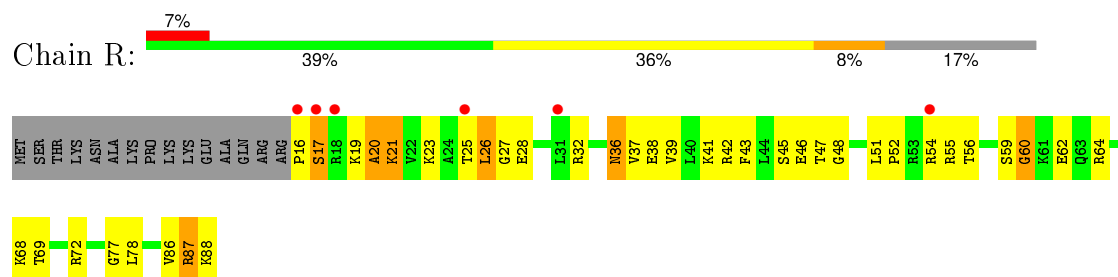
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



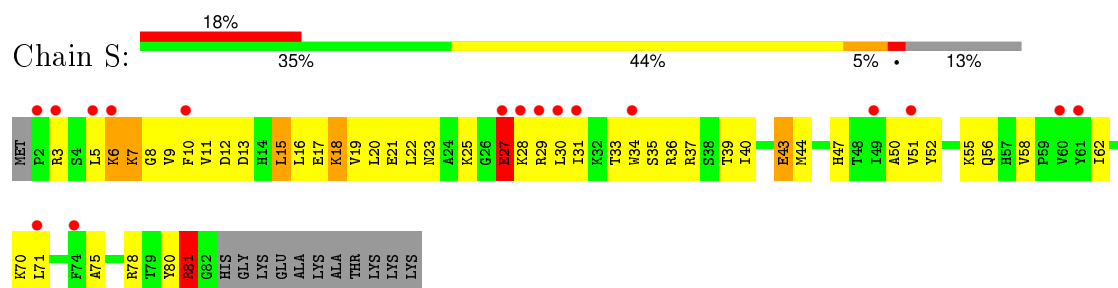
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



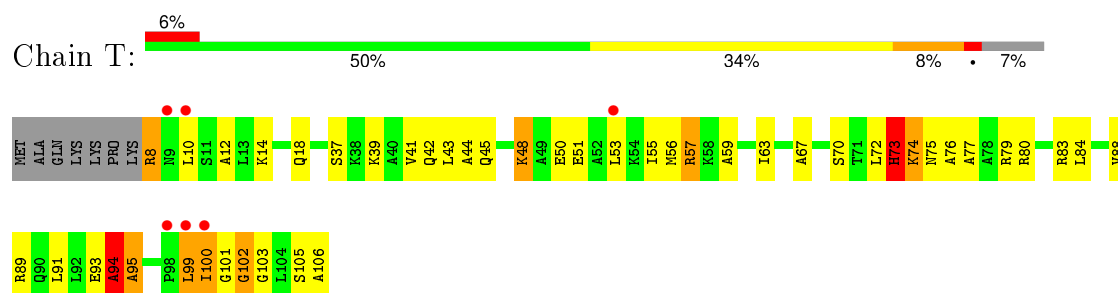
- Molecule 18: 30S RIBOSOMAL PROTEIN S18



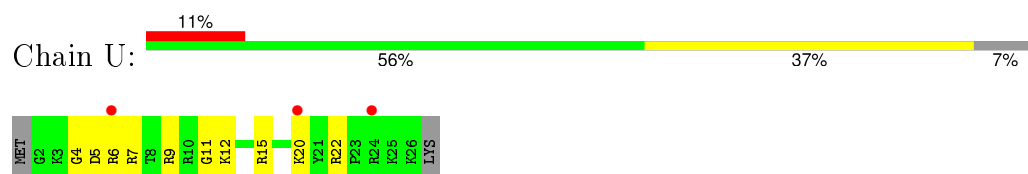
- Molecule 19: 30S RIBOSOMAL PROTEIN S19



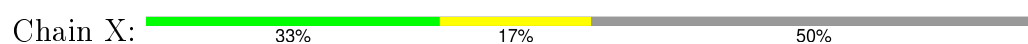
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

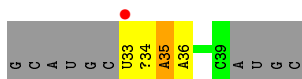
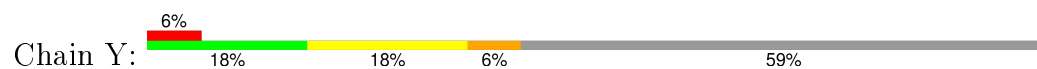


- Molecule 22: 5'-R(\*UP\*UP\*AP\*AP\*AP\*AP)-3'





- Molecule 23: 5'-R(\*GP\*CP\*AP\*UP\*GP\*CP\*UP\*TM2P\*AP\*AP\*AP \*AP\*CP\*AP\*UP\*GP\*CP)-3'





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.00Å 402.00Å 175.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.50 284.26 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.50-2.50) 99.0 (284.26-2.35)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.257 , 0.283 0.253 , 0.277	Depositor DCC
$R_{free}$ test set	24575 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 49.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 587336 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	52245	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, ZN, PAR, MG, TM2

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	1.17	15/36390 (0.0%)	0.88	71/56793 (0.1%)
2	B	29.07	1/1909 (0.1%)	1.16	2/2579 (0.1%)
3	C	0.35	0/1637	0.59	0/2207
4	D	0.34	0/1733	0.57	0/2318
5	E	0.45	0/1163	0.71	0/1566
6	F	0.32	0/856	0.59	0/1154
7	G	0.33	0/1276	0.63	0/1709
8	H	0.43	0/1136	0.75	0/1527
9	I	0.35	0/1029	0.63	0/1378
10	J	0.37	0/806	0.63	0/1084
11	K	0.38	0/900	0.70	0/1213
12	L	0.43	0/987	0.75	0/1322
13	M	0.33	0/1008	0.60	0/1347
14	N	0.35	0/501	0.62	0/664
15	O	0.36	0/745	0.61	1/992 (0.1%)
16	P	0.45	0/717	0.70	0/965
17	Q	0.42	0/870	0.73	1/1159 (0.1%)
18	R	0.37	0/603	0.61	0/799
19	S	0.33	0/662	0.61	0/892
20	T	0.37	0/764	0.72	1/1006 (0.1%)
21	U	0.48	0/213	0.65	0/279
22	X	0.53	0/65	0.60	0/99
23	Y	0.43	0/140	0.65	0/216
All	All	5.45	16/56110 (0.0%)	0.83	76/83268 (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	11	31
2	B	0	1
16	P	0	1
All	All	11	33

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	240	GLN	CD-OE1	1270.14	29.18	1.24
1	A	1127	G	O3'-P	-95.85	0.46	1.61
1	A	1063	C	O3'-P	-75.59	0.70	1.61
1	A	1160	G	O3'-P	-73.55	0.72	1.61
1	A	1532	U	O3'-P	-64.97	0.83	1.61

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	240	GLN	CG-CD-OE1	-49.40	22.81	121.60
1	A	1160	G	P-O3'-C3'	-45.24	65.41	119.70
1	A	1064	G	OP1-P-O3'	-36.76	24.33	105.20
1	A	1192	C	OP2-P-O3'	-35.85	26.34	105.20
1	A	1144	G	P-O3'-C3'	-33.90	79.02	119.70

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	115	G	C3'
1	A	243	A	C3'
1	A	281	G	C3'
1	A	410	G	C3'
1	A	412	A	C1'

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	G	Sidechain
1	A	108	G	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	37	U	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32511	0	16411	951	0
2	B	1874	0	1887	190	0
3	C	1613	0	1677	200	0
4	D	1703	0	1767	93	0
5	E	1147	0	1207	85	0
6	F	843	0	857	58	0
7	G	1257	0	1296	102	0
8	H	1116	0	1177	54	0
9	I	1011	0	1041	120	0
10	J	793	0	835	127	1
11	K	885	0	904	51	0
12	L	971	0	1057	79	0
13	M	997	0	1072	122	0
14	N	492	0	531	66	0
15	O	734	0	771	44	0
16	P	701	0	720	45	0
17	Q	857	0	930	56	0
18	R	597	0	668	47	0
19	S	648	0	673	57	0
20	T	762	0	859	61	0
21	U	209	0	221	15	0
22	X	59	0	33	1	0
23	Y	153	0	83	8	0
24	Z	206	0	0	0	0
25	Z	2	0	0	0	0
26	Z	62	0	0	0	0
27	Z	42	0	45	1	0
All	All	52245	0	36722	2402	1

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 27.

The worst 5 of 2402 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:1192:C:O3'	1:A:1193:G:P	1.10	1.49
1:A:1175:G:O3'	1:A:1176:A:P	0.99	1.39
1:A:1191:A:O3'	1:A:1192:C:P	0.98	1.37
1:A:1175:G:C3'	1:A:1176:A:P	2.14	1.34
1:A:1156:G:C3'	1:A:1157:A:P	2.17	1.32

All (1) 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)
10:J:79:ARG:NH1	10:J:79:ARG:NH1[8_665]	2.06	0.14

## 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	234/256 (91%)	162 (69%)	49 (21%)	23 (10%)	1	0
3	C	205/239 (86%)	139 (68%)	39 (19%)	27 (13%)	0	0
4	D	206/209 (99%)	169 (82%)	29 (14%)	8 (4%)	4	5
5	E	149/162 (92%)	135 (91%)	14 (9%)	0	100	100
6	F	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	5	7
7	G	153/156 (98%)	129 (84%)	14 (9%)	10 (6%)	1	1
8	H	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	26	46
9	I	125/128 (98%)	92 (74%)	23 (18%)	10 (8%)	1	1
10	J	97/105 (92%)	60 (62%)	21 (22%)	16 (16%)	0	0
11	K	117/129 (91%)	100 (86%)	15 (13%)	2 (2%)	11	19
12	L	123/135 (91%)	89 (72%)	26 (21%)	8 (6%)	1	1
13	M	123/126 (98%)	94 (76%)	18 (15%)	11 (9%)	1	1
14	N	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	5	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	86/89 (97%)	71 (83%)	11 (13%)	4 (5%)	3	3
16	P	82/88 (93%)	74 (90%)	6 (7%)	2 (2%)	7	11
17	Q	102/105 (97%)	88 (86%)	10 (10%)	4 (4%)	4	5
18	R	71/88 (81%)	55 (78%)	10 (14%)	6 (8%)	1	1
19	S	79/93 (85%)	58 (73%)	14 (18%)	7 (9%)	1	1
20	T	97/106 (92%)	81 (84%)	10 (10%)	6 (6%)	2	1
21	U	23/27 (85%)	17 (74%)	6 (26%)	0	100	100
All	All	2365/2541 (93%)	1867 (79%)	348 (15%)	150 (6%)	2	1

5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	88	ALA
2	B	123	ALA
2	B	129	GLU
2	B	229	VAL
3	C	15	THR

### 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	194/220 (88%)	176 (91%)	18 (9%)	11	21
3	C	160/188 (85%)	152 (95%)	8 (5%)	30	53
4	D	180/181 (99%)	171 (95%)	9 (5%)	30	53
5	E	115/123 (94%)	101 (88%)	14 (12%)	6	11
6	F	90/90 (100%)	88 (98%)	2 (2%)	60	84
7	G	126/127 (99%)	116 (92%)	10 (8%)	15	28
8	H	119/119 (100%)	109 (92%)	10 (8%)	14	25
9	I	98/99 (99%)	91 (93%)	7 (7%)	18	34
10	J	87/92 (95%)	81 (93%)	6 (7%)	19	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	90/99 (91%)	87 (97%)	3 (3%)	45	73
12	L	104/111 (94%)	96 (92%)	8 (8%)	16	30
13	M	100/101 (99%)	89 (89%)	11 (11%)	8	14
14	N	49/50 (98%)	41 (84%)	8 (16%)	3	5
15	O	79/80 (99%)	71 (90%)	8 (10%)	9	17
16	P	72/74 (97%)	69 (96%)	3 (4%)	36	62
17	Q	96/97 (99%)	93 (97%)	3 (3%)	47	75
18	R	64/77 (83%)	63 (98%)	1 (2%)	70	90
19	S	71/80 (89%)	65 (92%)	6 (8%)	13	25
20	T	76/82 (93%)	68 (90%)	8 (10%)	8	16
21	U	19/22 (86%)	18 (95%)	1 (5%)	28	50
All	All	1989/2112 (94%)	1845 (93%)	144 (7%)	18	33

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	91	ARG
10	J	71	LEU
19	S	27	GLU
8	H	97	VAL
9	I	23	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	100	ASN
9	I	73	GLN
17	Q	96	GLN
7	G	37	ASN
7	G	106	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	196 (12%)	72 (4%)
22	X	2/6 (33%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	Y	6/17 (35%)	1 (16%)	0
All	All	1519/1545 (98%)	197 (12%)	72 (4%)

5 of 197 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 72 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C
1	A	992	U
1	A	1498	U
1	A	748	C
1	A	819	A

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

1 non-standard protein/DNA/RNA residue is 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	TM2	Y	34	23	18,29,30	1.88	4 (22%)	24,42,45	4.35	10 (41%)

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	TM2	Y	34	23	-	0/11/33/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	34	TM2	O4'-C1'	2.15	1.43	1.41
23	Y	34	TM2	C7-N8	2.85	1.59	1.45
23	Y	34	TM2	C4-N3	4.17	1.40	1.33
23	Y	34	TM2	C6-N1	4.65	1.41	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	34	TM2	C5-C4-N3	-8.95	114.90	125.04
23	Y	34	TM2	C11-C9-N8	-4.95	96.71	111.32
23	Y	34	TM2	C7-C5-C6	-2.51	112.91	121.12
23	Y	34	TM2	O2S-S12-O1S	-2.07	105.94	113.48
23	Y	34	TM2	C7-N8-C9	-2.01	106.08	113.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Y	34	TM2	8	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 271 ligands modelled in this entry, 270 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	$\# Z  > 2$
27	PAR	Z	291	-	45,45,45	1.34	7 (15%)	59,67,67	1.27	4 (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
27	PAR	Z	291	-	-	0/18/94/94	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Z	291	PAR	O51-C51	2.04	1.49	1.44
27	Z	291	PAR	C52-C42	2.13	1.56	1.52
27	Z	291	PAR	C11-C21	2.43	1.57	1.52
27	Z	291	PAR	O51-C11	2.46	1.48	1.41
27	Z	291	PAR	C64-C54	2.57	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	291	PAR	O52-C13-C23	2.92	113.82	107.75
27	Z	291	PAR	O54-C54-C64	3.69	113.30	106.10
27	Z	291	PAR	C14-O54-C54	3.81	121.15	113.75
27	Z	291	PAR	O33-C14-C24	4.65	116.56	107.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	Z	291	PAR	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	1513/1522 (99%)	0.10	35 (2%) 64 67	18, 47, 115, 201	0
2	B	236/256 (92%)	0.80	27 (11%) 7 6	41, 79, 129, 136	0
3	C	207/239 (86%)	0.81	26 (12%) 5 5	48, 74, 118, 125	0
4	D	208/209 (99%)	0.72	22 (10%) 8 8	39, 59, 84, 92	0
5	E	151/162 (93%)	0.34	1 (0%) 89 90	25, 41, 69, 84	0
6	F	101/101 (100%)	0.59	7 (6%) 20 22	49, 77, 92, 96	0
7	G	155/156 (99%)	0.61	12 (7%) 16 18	40, 68, 102, 114	0
8	H	138/138 (100%)	0.29	4 (2%) 55 60	21, 38, 55, 65	0
9	I	127/128 (99%)	1.12	26 (20%) 1 1	39, 82, 103, 112	0
10	J	99/105 (94%)	1.37	26 (26%) 1 1	42, 112, 146, 150	0
11	K	119/129 (92%)	0.62	5 (4%) 40 45	23, 50, 79, 96	0
12	L	125/135 (92%)	0.63	8 (6%) 23 25	17, 52, 74, 109	0
13	M	125/126 (99%)	1.99	22 (17%) 2 2	50, 67, 122, 152	0
14	N	60/61 (98%)	1.14	9 (15%) 3 3	47, 66, 101, 107	0
15	O	88/89 (98%)	0.63	6 (6%) 20 23	36, 54, 82, 109	0
16	P	84/88 (95%)	0.33	2 (2%) 62 66	28, 40, 57, 80	0
17	Q	104/105 (99%)	0.80	7 (6%) 21 23	23, 42, 93, 146	0
18	R	73/88 (82%)	0.63	6 (8%) 14 15	43, 60, 107, 139	0
19	S	81/93 (87%)	1.35	17 (20%) 1 1	56, 90, 123, 134	0
20	T	99/106 (93%)	0.51	6 (6%) 25 27	25, 46, 81, 86	0
21	U	25/27 (92%)	1.23	3 (12%) 6 6	44, 53, 88, 94	0
22	X	3/6 (50%)	0.46	0 100 100	83, 83, 83, 88	0
23	Y	6/17 (35%)	0.99	1 (16%) 2 2	97, 105, 124, 134	0
All	All	3927/4086 (96%)	0.53	278 (7%) 19 21	17, 56, 115, 201	0

The worst 5 of 278 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	121	LYS	31.2
13	M	124	PRO	28.3
13	M	123	ALA	27.8
17	Q	105	ALA	26.5
19	S	3	ARG	25.3

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	TM2	Y	34	28/29	0.82	0.24	0.24	108,113,122,123	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
24	MG	Z	41	1/1	0.73	0.49	45.10	77,77,77,77	0
24	MG	Z	142	1/1	0.92	0.45	41.39	69,69,69,69	0
24	MG	Z	122	1/1	0.85	0.55	38.32	83,83,83,83	0
24	MG	Z	37	1/1	0.84	0.42	26.50	71,71,71,71	0
24	MG	Z	36	1/1	0.82	0.50	24.56	70,70,70,70	0
24	MG	Z	26	1/1	0.79	0.44	24.05	79,79,79,79	0
24	MG	Z	64	1/1	0.85	0.36	23.05	107,107,107,107	0
24	MG	Z	143	1/1	0.93	0.42	21.28	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	Z	131	1/1	0.79	0.43	20.24	73,73,73,73	0
24	MG	Z	67	1/1	0.94	0.32	19.42	40,40,40,40	0
26	K	Z	287	1/1	0.85	0.34	16.70	94,94,94,94	0
24	MG	Z	200	1/1	0.94	0.38	15.84	65,65,65,65	0
26	K	Z	268	1/1	0.86	0.73	15.18	111,111,111,111	0
24	MG	Z	47	1/1	0.93	0.42	14.58	72,72,72,72	0
24	MG	Z	81	1/1	0.95	0.25	14.50	39,39,39,39	0
24	MG	Z	211	1/1	0.93	0.48	13.83	91,91,91,91	0
24	MG	Z	136	1/1	0.88	0.49	12.36	35,35,35,35	0
24	MG	Z	100	1/1	0.94	0.29	10.75	56,56,56,56	0
24	MG	Z	212	1/1	0.89	0.87	9.53	62,62,62,62	0
24	MG	Z	54	1/1	0.98	0.50	9.19	85,85,85,85	0
24	MG	Z	76	1/1	0.32	0.21	8.31	103,103,103,103	0
24	MG	Z	103	1/1	0.93	0.26	7.74	44,44,44,44	0
24	MG	Z	149	1/1	0.97	0.30	7.73	66,66,66,66	0
24	MG	Z	71	1/1	0.88	0.54	7.62	88,88,88,88	0
25	ZN	Z	140	1/1	0.88	0.68	6.80	126,126,126,126	0
24	MG	Z	121	1/1	0.91	0.39	6.62	89,89,89,89	0
24	MG	Z	190	1/1	0.88	0.20	5.95	64,64,64,64	0
27	PAR	Z	291	42/42	0.91	0.23	5.54	34,38,57,61	0
26	K	Z	273	1/1	0.65	0.20	5.44	111,111,111,111	0
24	MG	Z	57	1/1	0.86	0.23	5.32	56,56,56,56	0
24	MG	Z	148	1/1	0.98	0.27	4.97	54,54,54,54	0
24	MG	Z	172	1/1	0.98	0.24	4.76	59,59,59,59	0
24	MG	Z	162	1/1	0.85	0.48	4.35	72,72,72,72	0
24	MG	Z	94	1/1	0.86	0.31	4.12	71,71,71,71	0
24	MG	Z	82	1/1	0.87	0.22	3.96	74,74,74,74	0
24	MG	Z	202	1/1	0.88	0.30	3.90	69,69,69,69	0
24	MG	Z	165	1/1	0.82	0.34	3.34	80,80,80,80	0
24	MG	Z	119	1/1	0.91	0.16	2.55	50,50,50,50	0
24	MG	Z	133	1/1	0.90	0.40	2.35	56,56,56,56	0
24	MG	Z	191	1/1	0.72	0.19	2.22	78,78,78,78	0
24	MG	Z	173	1/1	0.78	0.32	1.85	77,77,77,77	0
24	MG	Z	153	1/1	0.98	0.18	1.72	52,52,52,52	0
26	K	Z	236	1/1	0.91	0.20	1.29	107,107,107,107	0
24	MG	Z	174	1/1	0.82	0.19	1.07	69,69,69,69	0
24	MG	Z	176	1/1	0.94	0.18	0.98	60,60,60,60	0
24	MG	Z	51	1/1	0.82	0.16	0.82	72,72,72,72	0
25	ZN	Z	141	1/1	0.98	0.24	0.66	73,73,73,73	0
24	MG	Z	167	1/1	0.88	0.23	0.52	81,81,81,81	0
26	K	Z	222	1/1	0.77	0.16	0.37	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	K	Z	284	1/1	0.05	0.20	0.30	144,144,144,144	0
26	K	Z	274	1/1	0.61	0.16	0.19	118,118,118,118	0
24	MG	Z	186	1/1	0.92	0.20	-0.38	85,85,85,85	0
26	K	Z	266	1/1	0.79	0.18	-0.53	144,144,144,144	0
24	MG	Z	171	1/1	0.88	0.16	-0.56	73,73,73,73	0
24	MG	Z	49	1/1	0.98	0.16	-0.58	63,63,63,63	0
24	MG	Z	155	1/1	0.97	0.16	-0.82	49,49,49,49	0
24	MG	Z	72	1/1	0.97	0.15	-0.91	55,55,55,55	0
24	MG	Z	92	1/1	0.74	0.16	-0.92	109,109,109,109	0
24	MG	Z	154	1/1	0.94	0.13	-1.47	70,70,70,70	0
24	MG	Z	166	1/1	0.94	0.16	-1.57	57,57,57,57	0
24	MG	Z	16	1/1	0.95	0.11	-1.87	53,53,53,53	0
24	MG	Z	123	1/1	0.95	0.09	-2.07	46,46,46,46	0
24	MG	Z	210	1/1	0.92	0.12	-2.27	46,46,46,46	0
26	K	Z	227	1/1	0.95	0.10	-2.45	118,118,118,118	0
24	MG	Z	134	1/1	0.86	0.15	-2.56	59,59,59,59	0
24	MG	Z	159	1/1	0.92	0.08	-2.59	66,66,66,66	0
24	MG	Z	158	1/1	0.85	0.14	-3.24	80,80,80,80	0
24	MG	Z	145	1/1	0.99	0.11	-3.28	34,34,34,34	0
26	K	Z	229	1/1	0.93	0.11	-3.64	123,123,123,123	0
24	MG	Z	215	1/1	0.95	0.04	-5.44	70,70,70,70	0
24	MG	Z	120	1/1	0.87	0.08	-7.23	52,52,52,52	0
24	MG	Z	101	1/1	0.96	0.07	-8.86	44,44,44,44	0
24	MG	Z	4	1/1	0.99	0.10	-8.92	57,57,57,57	0
26	K	Z	218	1/1	0.96	0.05	-9.32	64,64,64,64	0
24	MG	Z	13	1/1	0.95	0.05	-20.72	35,35,35,35	0
26	K	Z	261	1/1	0.77	0.19	-	94,94,94,94	0
26	K	Z	221	1/1	0.95	0.07	-	97,97,97,97	0
26	K	Z	242	1/1	0.79	0.10	-	118,118,118,118	0
24	MG	Z	213	1/1	0.86	0.27	-	68,68,68,68	0
24	MG	Z	86	1/1	0.97	0.34	-	82,82,82,82	0
26	K	Z	243	1/1	0.93	0.05	-	95,95,95,95	0
24	MG	Z	88	1/1	0.93	0.39	-	76,76,76,76	0
26	K	Z	277	1/1	0.81	0.08	-	119,119,119,119	0
24	MG	Z	28	1/1	0.95	0.12	-	59,59,59,59	0
24	MG	Z	59	1/1	0.85	0.52	-	84,84,84,84	0
24	MG	Z	61	1/1	0.97	0.26	-	57,57,57,57	0
26	K	Z	256	1/1	0.91	0.38	-	66,66,66,66	0
24	MG	Z	78	1/1	0.74	0.49	-	97,97,97,97	0
24	MG	Z	19	1/1	0.75	0.09	-	72,72,72,72	0
24	MG	Z	60	1/1	0.80	0.46	-	83,83,83,83	0
24	MG	Z	27	1/1	0.39	0.35	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	Z	144	1/1	0.96	0.28	-	38,38,38,38	0
26	K	Z	255	1/1	0.80	0.19	-	92,92,92,92	0
24	MG	Z	137	1/1	0.93	0.09	-	43,43,43,43	0
24	MG	Z	192	1/1	0.84	0.15	-	71,71,71,71	0
24	MG	Z	111	1/1	0.83	0.56	-	104,104,104,104	0
26	K	Z	228	1/1	0.82	0.12	-	113,113,113,113	0
24	MG	Z	91	1/1	0.90	0.30	-	68,68,68,68	0
24	MG	Z	35	1/1	0.94	0.45	-	79,79,79,79	0
24	MG	Z	74	1/1	0.93	0.26	-	85,85,85,85	0
24	MG	Z	102	1/1	0.87	0.15	-	83,83,83,83	0
24	MG	Z	3	1/1	0.76	0.44	-	104,104,104,104	0
24	MG	Z	146	1/1	0.98	0.26	-	57,57,57,57	0
24	MG	Z	53	1/1	0.76	0.34	-	69,69,69,69	0
24	MG	Z	66	1/1	0.94	0.51	-	87,87,87,87	0
24	MG	Z	189	1/1	0.86	0.19	-	75,75,75,75	0
24	MG	Z	179	1/1	0.67	0.17	-	89,89,89,89	0
24	MG	Z	139	1/1	0.94	0.08	-	38,38,38,38	0
24	MG	Z	110	1/1	0.73	0.48	-	93,93,93,93	0
24	MG	Z	104	1/1	0.87	0.17	-	57,57,57,57	0
26	K	Z	281	1/1	0.84	0.20	-	136,136,136,136	0
24	MG	Z	23	1/1	0.86	0.37	-	92,92,92,92	0
24	MG	Z	107	1/1	0.85	0.21	-	62,62,62,62	0
24	MG	Z	207	1/1	0.99	0.08	-	24,24,24,24	0
24	MG	Z	30	1/1	0.93	0.45	-	82,82,82,82	0
26	K	Z	225	1/1	0.92	0.10	-	93,93,93,93	0
24	MG	Z	10	1/1	0.68	0.45	-	110,110,110,110	0
24	MG	Z	193	1/1	0.95	0.32	-	61,61,61,61	0
24	MG	Z	106	1/1	0.83	0.25	-	63,63,63,63	0
24	MG	Z	75	1/1	0.79	0.15	-	69,69,69,69	0
24	MG	Z	70	1/1	0.91	0.06	-	66,66,66,66	0
26	K	Z	219	1/1	0.96	0.17	-	76,76,76,76	0
24	MG	Z	7	1/1	0.97	0.46	-	70,70,70,70	0
24	MG	Z	98	1/1	0.76	0.11	-	69,69,69,69	0
26	K	Z	285	1/1	0.88	0.46	-	93,93,93,93	0
24	MG	Z	170	1/1	0.91	0.21	-	50,50,50,50	0
24	MG	Z	46	1/1	0.96	0.47	-	75,75,75,75	0
24	MG	Z	12	1/1	0.91	0.10	-	47,47,47,47	0
26	K	Z	244	1/1	0.59	0.26	-	132,132,132,132	0
26	K	Z	257	1/1	0.81	0.28	-	115,115,115,115	0
24	MG	Z	77	1/1	0.76	0.17	-	95,95,95,95	0
24	MG	Z	50	1/1	0.91	0.26	-	66,66,66,66	0
24	MG	Z	113	1/1	0.79	0.26	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	Z	126	1/1	0.66	0.28	-	102,102,102,102	0
26	K	Z	272	1/1	0.79	0.29	-	107,107,107,107	0
24	MG	Z	183	1/1	0.84	0.53	-	78,78,78,78	0
24	MG	Z	14	1/1	0.77	0.36	-	54,54,54,54	0
24	MG	Z	130	1/1	0.95	0.24	-	84,84,84,84	0
24	MG	Z	32	1/1	0.04	0.59	-	160,160,160,160	0
24	MG	Z	177	1/1	0.87	0.04	-	105,105,105,105	0
24	MG	Z	29	1/1	0.81	0.15	-	68,68,68,68	0
26	K	Z	260	1/1	0.88	0.16	-	122,122,122,122	0
26	K	Z	226	1/1	0.84	0.18	-	90,90,90,90	0
26	K	Z	276	1/1	0.88	0.36	-	93,93,93,93	0
24	MG	Z	195	1/1	0.76	0.16	-	91,91,91,91	0
24	MG	Z	69	1/1	0.91	0.36	-	74,74,74,74	0
26	K	Z	286	1/1	0.77	0.59	-	117,117,117,117	0
24	MG	Z	90	1/1	0.39	0.30	-	91,91,91,91	0
24	MG	Z	116	1/1	0.73	0.36	-	78,78,78,78	0
26	K	Z	252	1/1	0.60	0.13	-	101,101,101,101	0
26	K	Z	238	1/1	0.77	0.80	-	116,116,116,116	0
24	MG	Z	52	1/1	0.71	0.17	-	56,56,56,56	0
24	MG	Z	163	1/1	0.77	0.55	-	103,103,103,103	0
24	MG	Z	198	1/1	0.93	0.06	-	93,93,93,93	0
24	MG	Z	93	1/1	0.97	0.28	-	40,40,40,40	0
26	K	Z	251	1/1	0.83	0.15	-	127,127,127,127	0
26	K	Z	235	1/1	0.69	0.13	-	133,133,133,133	0
24	MG	Z	62	1/1	0.81	0.20	-	91,91,91,91	0
24	MG	Z	56	1/1	0.61	0.17	-	89,89,89,89	0
24	MG	Z	24	1/1	0.93	0.31	-	61,61,61,61	0
26	K	Z	232	1/1	0.82	0.08	-	114,114,114,114	0
26	K	Z	223	1/1	0.82	0.14	-	113,113,113,113	0
26	K	Z	258	1/1	0.83	0.07	-	99,99,99,99	0
26	K	Z	248	1/1	0.77	0.10	-	103,103,103,103	0
26	K	Z	263	1/1	0.78	0.24	-	131,131,131,131	0
26	K	Z	233	1/1	0.57	0.34	-	139,139,139,139	0
24	MG	Z	160	1/1	0.89	0.12	-	52,52,52,52	0
26	K	Z	239	1/1	0.59	0.20	-	102,102,102,102	0
24	MG	Z	48	1/1	0.88	0.51	-	81,81,81,81	0
24	MG	Z	161	1/1	0.85	0.29	-	87,87,87,87	0
24	MG	Z	185	1/1	0.98	0.14	-	40,40,40,40	0
26	K	Z	289	1/1	0.66	0.28	-	120,120,120,120	0
26	K	Z	224	1/1	0.63	0.11	-	101,101,101,101	0
26	K	Z	269	1/1	0.98	0.42	-	43,43,43,43	0
26	K	Z	264	1/1	0.89	0.52	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	Z	199	1/1	0.93	0.39	-	59,59,59,59	0
24	MG	Z	80	1/1	0.48	0.27	-	85,85,85,85	0
26	K	Z	283	1/1	0.88	0.26	-	117,117,117,117	0
24	MG	Z	65	1/1	0.79	0.50	-	90,90,90,90	0
24	MG	Z	97	1/1	0.59	0.28	-	101,101,101,101	0
24	MG	Z	63	1/1	0.88	0.46	-	73,73,73,73	0
24	MG	Z	20	1/1	0.81	0.20	-	73,73,73,73	0
24	MG	Z	129	1/1	0.95	0.19	-	53,53,53,53	0
24	MG	Z	178	1/1	0.82	0.18	-	77,77,77,77	0
24	MG	Z	1	1/1	0.96	0.12	-	56,56,56,56	0
24	MG	Z	85	1/1	0.88	0.32	-	98,98,98,98	0
24	MG	Z	5	1/1	0.97	0.36	-	65,65,65,65	0
26	K	Z	270	1/1	0.83	0.73	-	80,80,80,80	0
24	MG	Z	38	1/1	0.89	0.22	-	90,90,90,90	0
24	MG	Z	2	1/1	0.86	0.12	-	106,106,106,106	0
24	MG	Z	95	1/1	0.80	0.31	-	90,90,90,90	0
24	MG	Z	99	1/1	0.95	0.37	-	31,31,31,31	0
24	MG	Z	127	1/1	0.93	0.12	-	63,63,63,63	0
24	MG	Z	11	1/1	0.73	0.22	-	83,83,83,83	0
24	MG	Z	184	1/1	0.74	0.43	-	96,96,96,96	0
24	MG	Z	196	1/1	0.68	0.19	-	93,93,93,93	0
24	MG	Z	188	1/1	0.96	0.42	-	47,47,47,47	0
24	MG	Z	124	1/1	0.89	0.42	-	78,78,78,78	0
24	MG	Z	44	1/1	0.94	0.29	-	69,69,69,69	0
24	MG	Z	58	1/1	0.79	0.47	-	85,85,85,85	0
26	K	Z	240	1/1	0.60	0.19	-	99,99,99,99	0
24	MG	Z	168	1/1	0.91	0.20	-	81,81,81,81	0
24	MG	Z	150	1/1	0.97	0.30	-	51,51,51,51	0
24	MG	Z	68	1/1	0.85	0.32	-	85,85,85,85	0
24	MG	Z	40	1/1	0.93	0.33	-	83,83,83,83	0
24	MG	Z	89	1/1	0.91	0.53	-	93,93,93,93	0
24	MG	Z	152	1/1	0.88	0.28	-	60,60,60,60	0
24	MG	Z	18	1/1	0.96	0.15	-	40,40,40,40	0
24	MG	Z	138	1/1	0.61	0.14	-	81,81,81,81	0
26	K	Z	246	1/1	0.59	0.20	-	122,122,122,122	0
24	MG	Z	164	1/1	0.82	0.47	-	128,128,128,128	0
24	MG	Z	125	1/1	0.87	0.15	-	83,83,83,83	0
24	MG	Z	84	1/1	0.95	0.11	-	55,55,55,55	0
24	MG	Z	42	1/1	0.98	0.42	-	67,67,67,67	0
26	K	Z	278	1/1	0.83	0.15	-	129,129,129,129	0
24	MG	Z	157	1/1	0.96	0.14	-	45,45,45,45	0
24	MG	Z	45	1/1	0.95	0.35	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	Z	118	1/1	0.85	0.33	-	64,64,64,64	0
24	MG	Z	25	1/1	0.85	0.19	-	93,93,93,93	0
24	MG	Z	34	1/1	0.89	0.24	-	68,68,68,68	0
24	MG	Z	9	1/1	0.97	0.26	-	33,33,33,33	0
24	MG	Z	194	1/1	0.40	0.18	-	132,132,132,132	0
24	MG	Z	112	1/1	0.92	0.07	-	54,54,54,54	0
26	K	Z	290	1/1	0.78	0.20	-	119,119,119,119	0
24	MG	Z	15	1/1	0.86	0.44	-	107,107,107,107	0
24	MG	Z	132	1/1	0.83	0.23	-	80,80,80,80	0
26	K	Z	230	1/1	0.37	0.19	-	120,120,120,120	0
24	MG	Z	105	1/1	0.90	0.35	-	74,74,74,74	0
24	MG	Z	55	1/1	0.88	0.43	-	89,89,89,89	0
24	MG	Z	151	1/1	0.95	0.45	-	79,79,79,79	0
26	K	Z	265	1/1	0.87	0.25	-	96,96,96,96	0
24	MG	Z	8	1/1	0.97	0.28	-	61,61,61,61	0
24	MG	Z	156	1/1	0.88	0.46	-	91,91,91,91	0
24	MG	Z	115	1/1	0.78	0.44	-	97,97,97,97	0
24	MG	Z	22	1/1	0.81	0.27	-	66,66,66,66	0
24	MG	Z	147	1/1	0.91	0.35	-	45,45,45,45	0
24	MG	Z	31	1/1	0.59	0.28	-	100,100,100,100	0
24	MG	Z	43	1/1	0.73	0.51	-	88,88,88,88	0
24	MG	Z	128	1/1	0.88	0.17	-	81,81,81,81	0
24	MG	Z	21	1/1	0.92	0.14	-	33,33,33,33	0
24	MG	Z	109	1/1	0.78	0.49	-	114,114,114,114	0
26	K	Z	241	1/1	0.64	0.13	-	101,101,101,101	0
26	K	Z	245	1/1	0.96	0.12	-	83,83,83,83	0
24	MG	Z	6	1/1	0.90	0.16	-	70,70,70,70	0
24	MG	Z	203	1/1	0.88	0.19	-	121,121,121,121	0
24	MG	Z	135	1/1	0.86	0.20	-	78,78,78,78	0
26	K	Z	259	1/1	0.46	0.27	-	132,132,132,132	0
26	K	Z	253	1/1	0.94	0.28	-	69,69,69,69	0
24	MG	Z	175	1/1	0.96	0.23	-	66,66,66,66	0
26	K	Z	220	1/1	0.98	0.06	-	73,73,73,73	0
24	MG	Z	79	1/1	0.98	0.22	-	19,19,19,19	0
24	MG	Z	114	1/1	0.72	0.32	-	88,88,88,88	0
24	MG	Z	96	1/1	0.85	0.31	-	70,70,70,70	0
24	MG	Z	39	1/1	0.97	0.17	-	65,65,65,65	0
26	K	Z	249	1/1	0.90	0.49	-	93,93,93,93	0
24	MG	Z	209	1/1	0.96	0.08	-	36,36,36,36	0
24	MG	Z	208	1/1	0.94	0.29	-	57,57,57,57	0
24	MG	Z	108	1/1	0.93	0.35	-	54,54,54,54	0
24	MG	Z	117	1/1	0.92	0.07	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	MG	Z	169	1/1	0.85	0.35	-	93,93,93,93	0
24	MG	Z	33	1/1	0.96	0.42	-	86,86,86,86	0
24	MG	Z	83	1/1	0.83	0.45	-	79,79,79,79	0
26	K	Z	247	1/1	0.94	0.41	-	82,82,82,82	0
26	K	Z	231	1/1	0.79	0.25	-	126,126,126,126	0
26	K	Z	234	1/1	0.80	0.16	-	116,116,116,116	0
24	MG	Z	214	1/1	0.58	0.18	-	101,101,101,101	0
24	MG	Z	206	1/1	0.94	0.48	-	55,55,55,55	0
24	MG	Z	87	1/1	0.79	0.12	-	56,56,56,56	0
24	MG	Z	17	1/1	0.94	0.06	-	55,55,55,55	0
24	MG	Z	73	1/1	0.72	0.15	-	83,83,83,83	0
24	MG	Z	217	1/1	0.94	0.23	-	86,86,86,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.