wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2022 – 09:08 PM EST

PDB ID	:	1IBM
Title	:	STRUCTURE OF THE THERMUS THERMOPHILUS 30S RIBOSOMAL SUBUNIT IN COMPLEX WITH A MESSENGER RNA FRAGMENT AND COGNATE TRANSFER RNA ANTICODON STEM-LOOP BOUND AT THE A SITE
Authors	:	Ogle, J.M.; Brodersen, D.E.; Clemons Jr., W.M.; Tarry, M.J.; Carter, A.P.; Ramakrishnan, V.
Deposited on	:	2001-03-28
Resolution	:	3.31 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

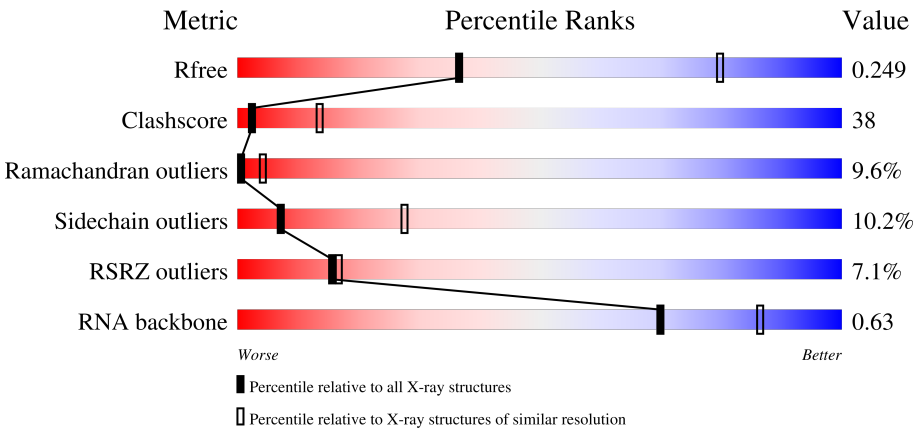
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)
RNA backbone	3102	1125 (3.74-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3%, 27%, 59%, 11%, • •
2	X	6	67%, 67%, 33%
3	Y	15	20%, 33%, 27%, 7%, 7%, 27%

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Mol	Chain	Length	Quality of chain
4	Z	4	25% 50% 25% 25%
5	B	256	6% 18% 57% 14% 9%
6	C	239	3% 20% 50% 14% 14%
7	D	209	8% 36% 51% 11%
8	E	162	8% 28% 51% 12% 7%
9	F	101	2% 38% 61%
10	G	156	2% 32% 58% 9%
11	H	138	2% 42% 48% 8%
12	I	128	8% 18% 66% 15%
13	J	105	13% 15% 59% 17% 7%
14	K	129	5% 28% 48% 14% 8%
15	L	135	13% 36% 43% 13% 8%
16	M	126	7% 20% 58% 16% 6%
17	N	61	46% 26% 56% 15%
18	O	89	3% 36% 52% 10%
19	P	88	16% 38% 49% 8% 6%
20	Q	105	14% 32% 54% 12%
21	R	88	3% 18% 58% 7% 17%
22	S	93	19% 20% 51% 18% 6%
23	T	106	12% 31% 52% 9% 7%
24	V	26	31% 35% 58% 8%

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	1628	-	-	-	X

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 52160 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
			Total	C	N	O	P			
1	A	1507	32391	14418	6002	10465	1506	0	0	0

- Molecule 2 is a RNA chain called P-SITE MESSENGER RNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	X	6	117	54	14	44	5	0	0	0

- Molecule 3 is a RNA chain called ANTICODON STEM-LOOP OF PHENYLALANINE TRANSFER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	Y	11	233	106	44	73	10	0	0	0

- Molecule 4 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	Z	4	77	36	8	30	3	0	0	0

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	234	1900	1213	341	341	5	0	0	0

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	C	206	1612	1016	314	281	1	0	0	0

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	E	150	1146	724	217	201	4	0	0	0

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	I	127	1011	639	198	174	0	0	0

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	J	98	792	498	156	137	1	0	0	0

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	L	124	970	611	195	163	1	0	0	0

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	M	118	937	579	193	163	2	0	0	0

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	P	83	700	443	139	117	1	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	?	-	PHE	conflict	GB 12056104
P	?	-	HIS	conflict	GB 12056104
P	?	-	TYR	conflict	GB 12056104

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	Q	104	857	547	161	147	2	0	0	0

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	R	73	597	380	118	99	0	0	0

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	S	87	697	444	130	121	2	0	0	0

- Molecule 23 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 24 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
24	V	24	208	128	50	30	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
25	A	118	118	118	0	0
			Total	Mg		
25	D	1	1	1	0	0

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

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

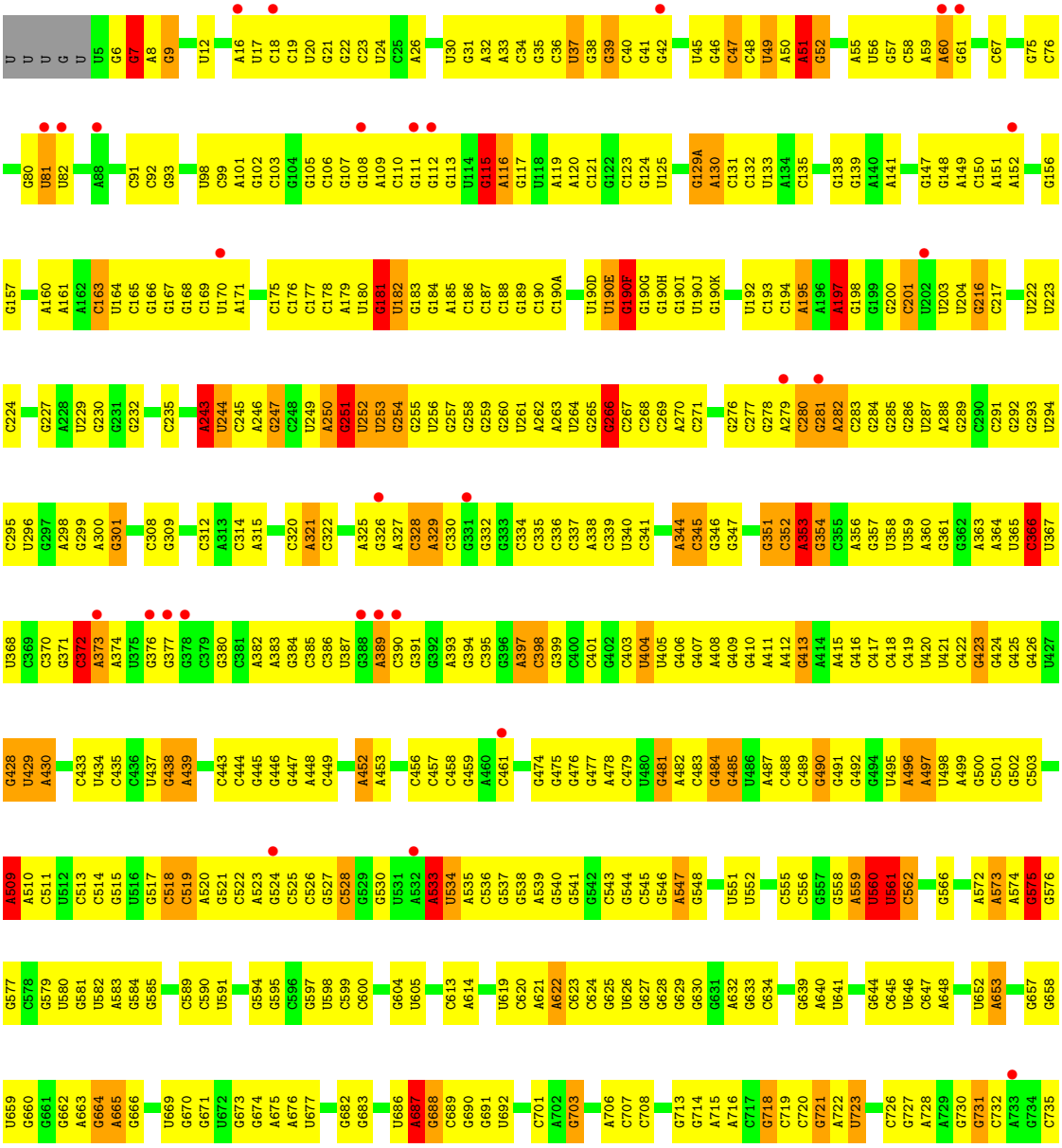
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
26	D	1	1	1	0	0
			Total	Zn		
26	N	1	1	1	0	0

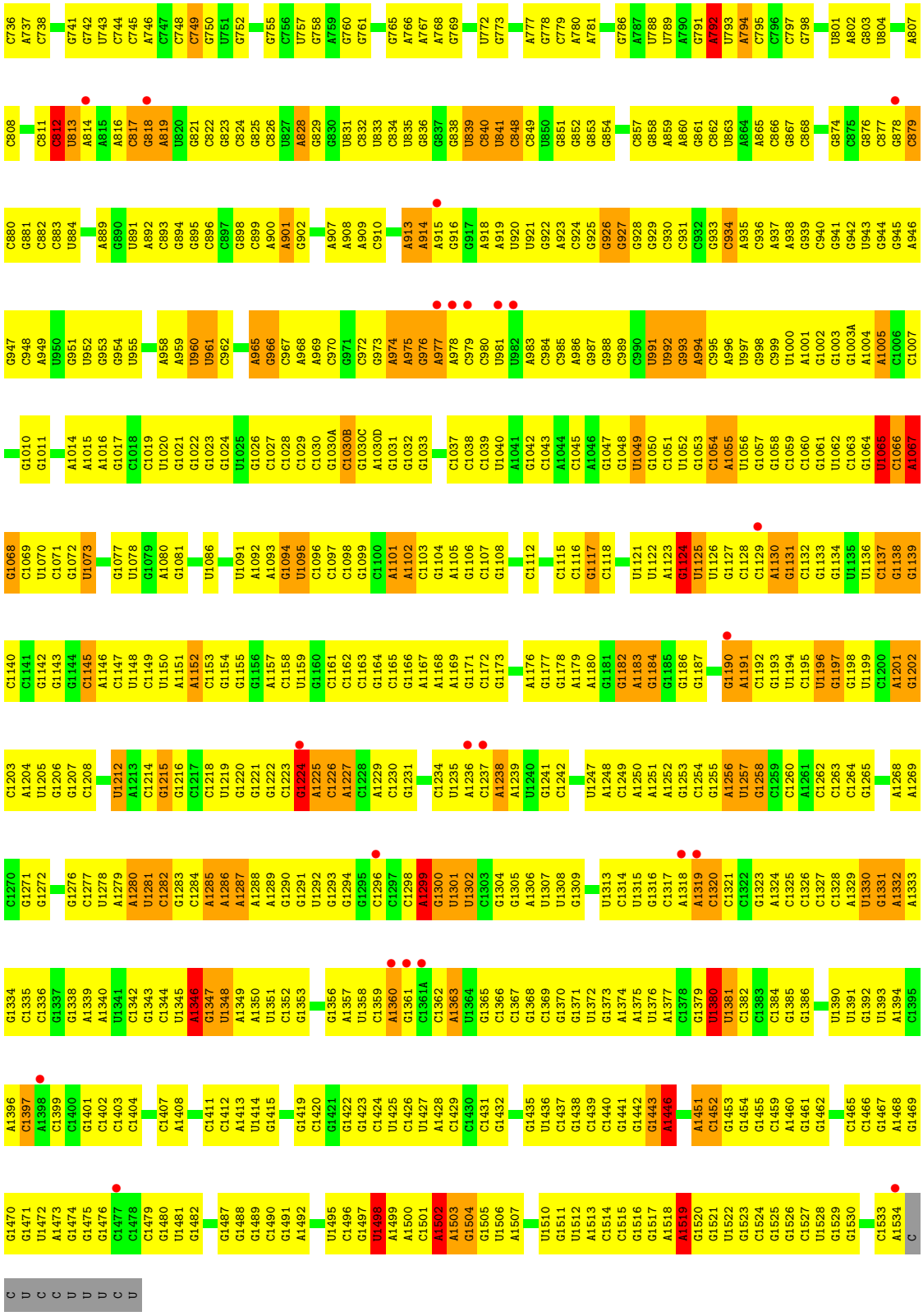
3 Residue-property plots (i)

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

- Molecule 1: 16S RIBOSOMAL RNA

Chain A:



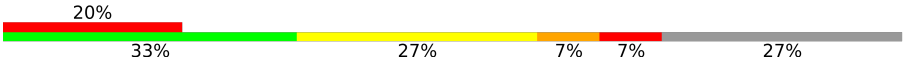


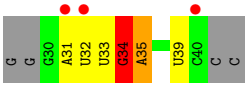
- Molecule 2: P-SITE MESSENGER RNA FRAGMENT

Chain X:

• Molecule 3: ANTICODON STEM-LOOP OF PHENYLALANINE TRANSFER RNA

Chain Y:



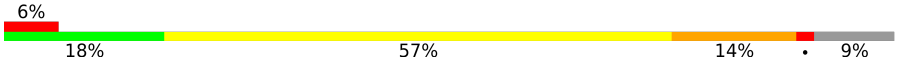


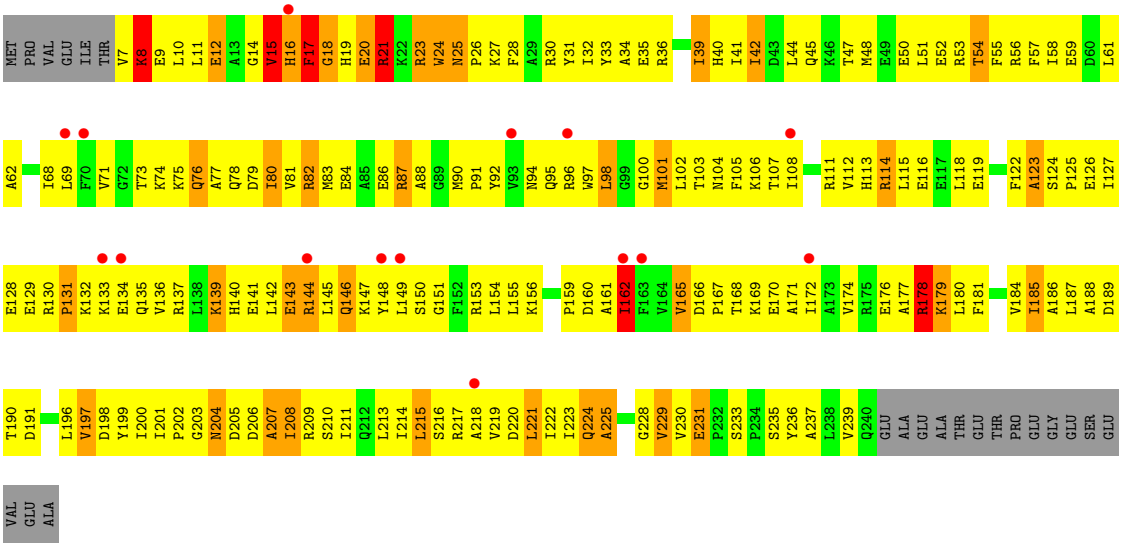
• Molecule 4: A-SITE MESSENGER RNA FRAGMENT

Chain Z:

• Molecule 5: 30S RIBOSOMAL PROTEIN S2

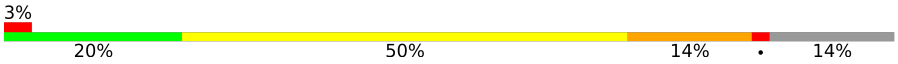
Chain B:

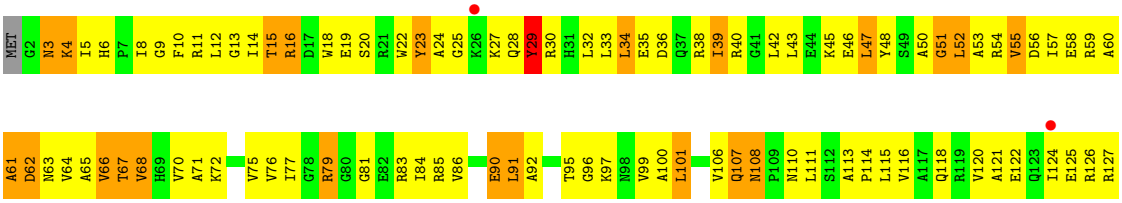


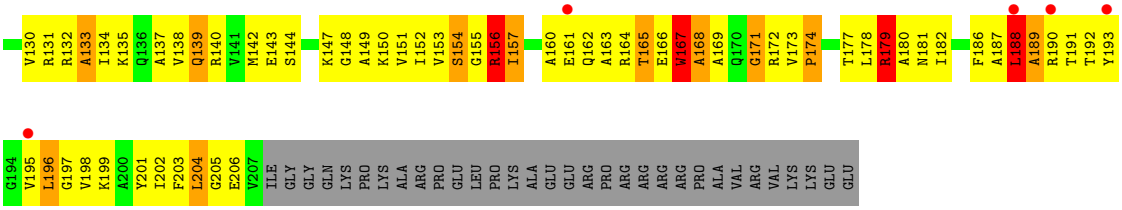


• Molecule 6: 30S RIBOSOMAL PROTEIN S3

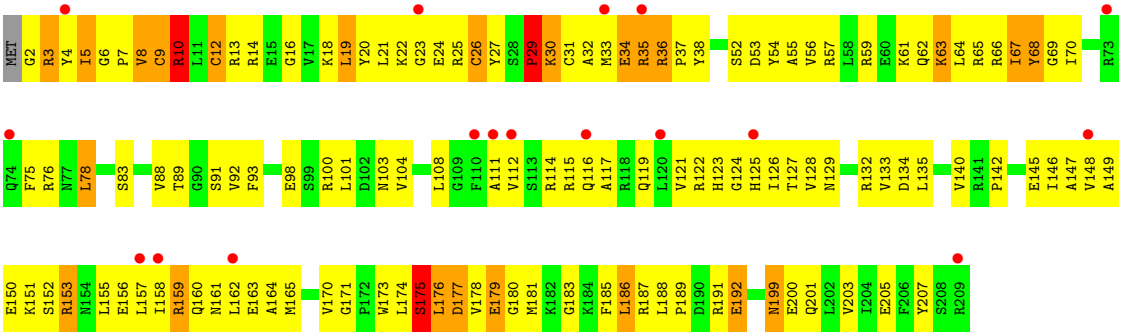
Chain C:



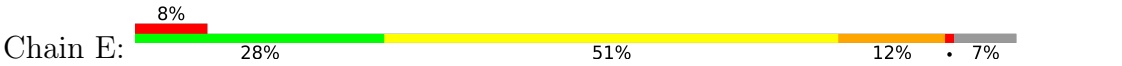


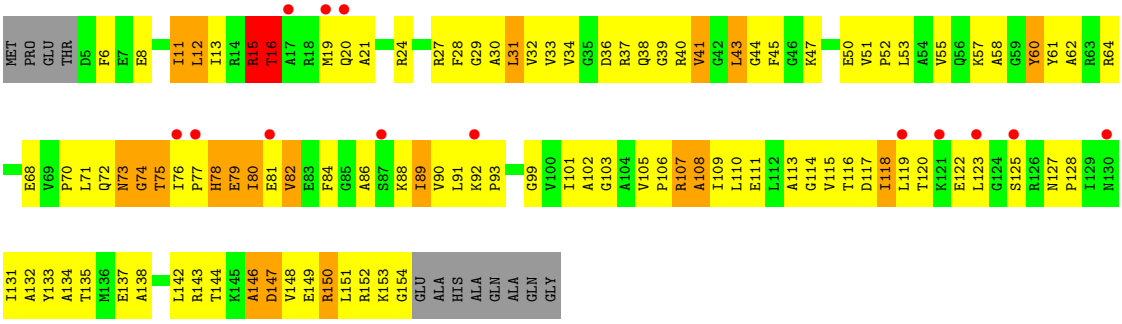


• Molecule 7: 30S RIBOSOMAL PROTEIN S4

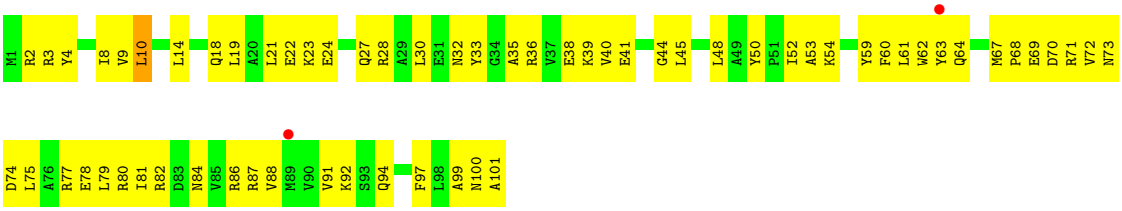


• Molecule 8: 30S RIBOSOMAL PROTEIN S5

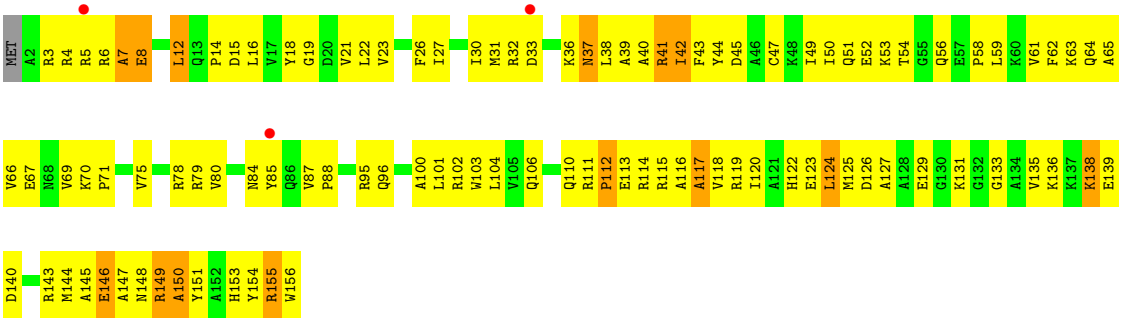




• Molecule 9: 30S RIBOSOMAL PROTEIN S6

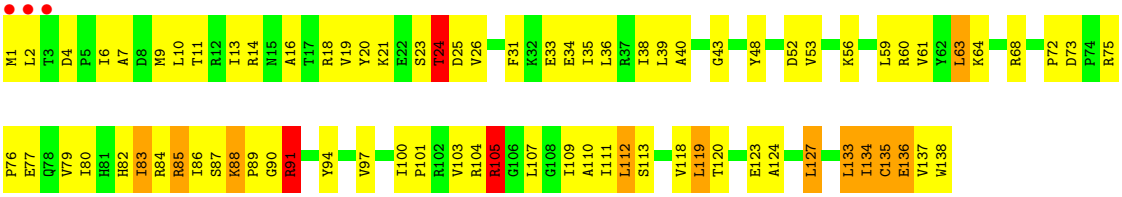


• Molecule 10: 30S RIBOSOMAL PROTEIN S7



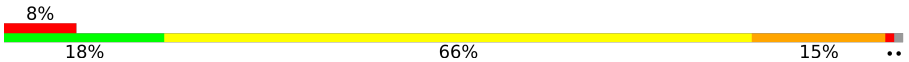
- Molecule 11: 30S RIBOSOMAL PROTEIN S8

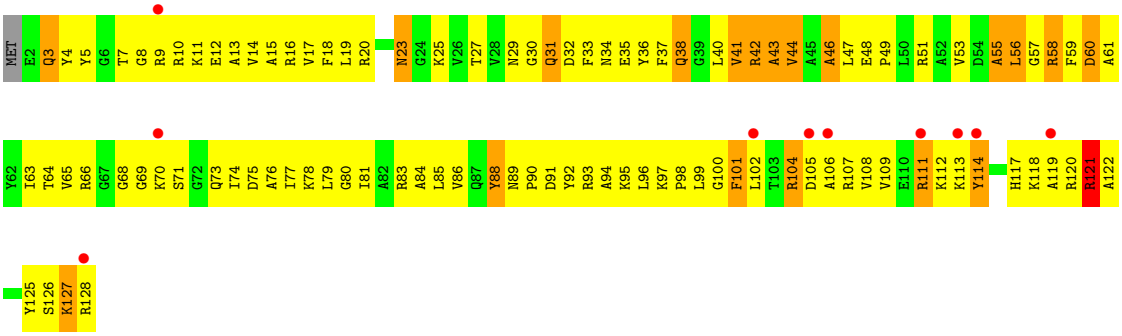
Chain H:



- Molecule 12: 30S RIBOSOMAL PROTEIN S9

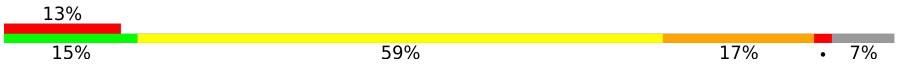
Chain I:

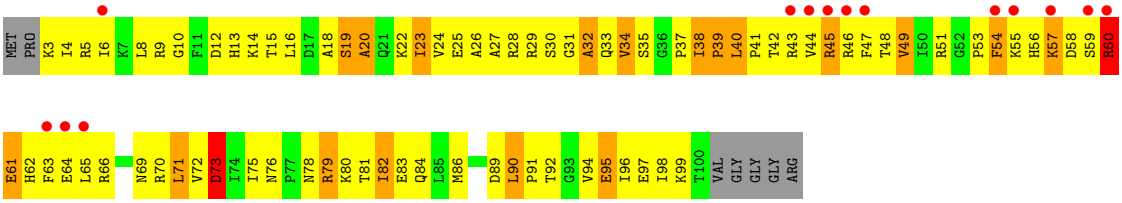




- Molecule 13: 30S RIBOSOMAL PROTEIN S10

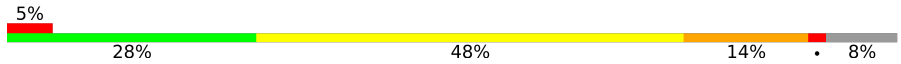
Chain J:

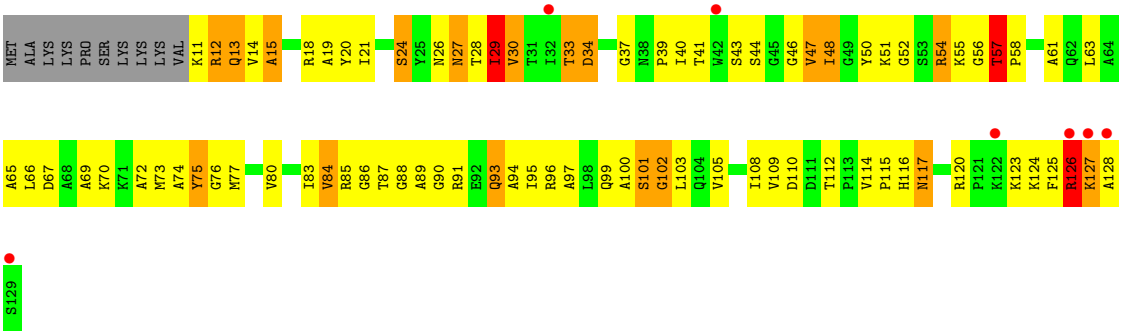




- Molecule 14: 30S RIBOSOMAL PROTEIN S11

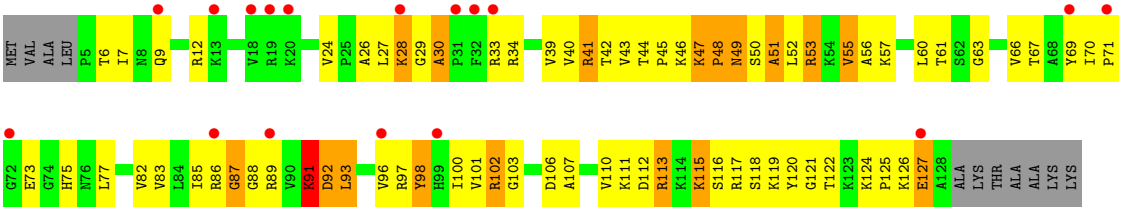
Chain K:





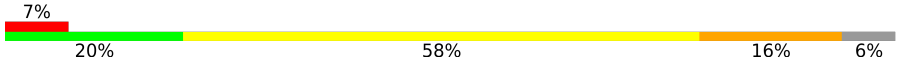
• Molecule 15: 30S RIBOSOMAL PROTEIN S12

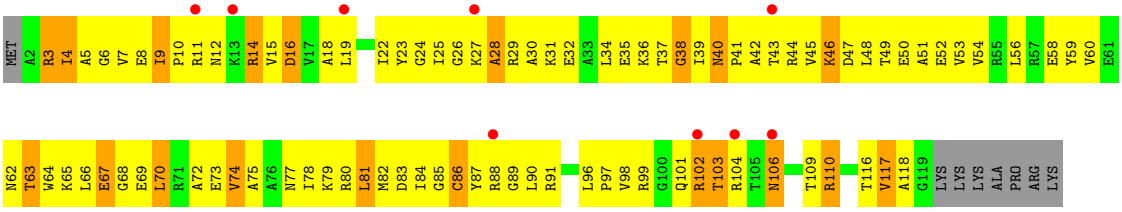
Chain L:



• Molecule 16: 30S RIBOSOMAL PROTEIN S13

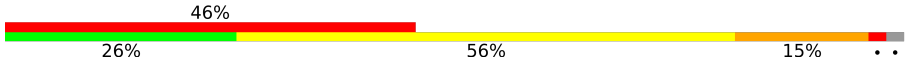
Chain M:

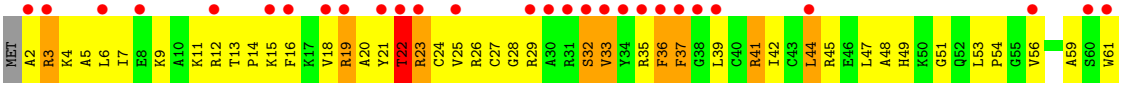




• Molecule 17: 30S RIBOSOMAL PROTEIN S14

Chain N:



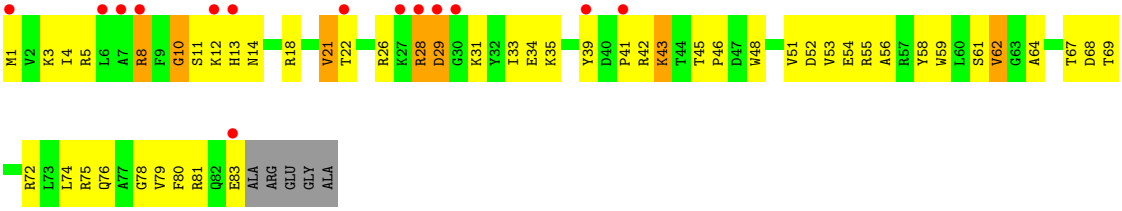


• Molecule 18: 30S RIBOSOMAL PROTEIN S15

Chain O:

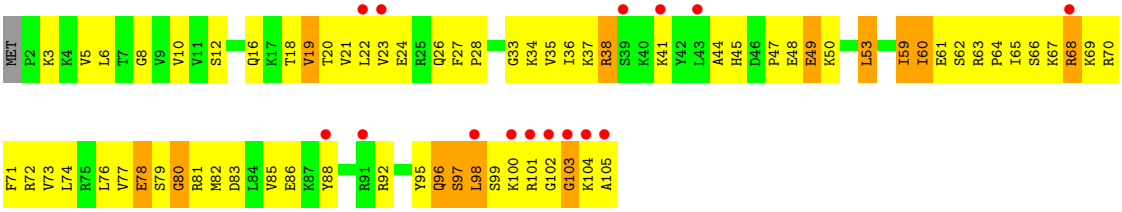
- Molecule 19: 30S RIBOSOMAL PROTEIN S16

Chain P:



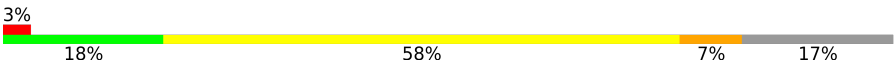
- Molecule 20: 30S RIBOSOMAL PROTEIN S17

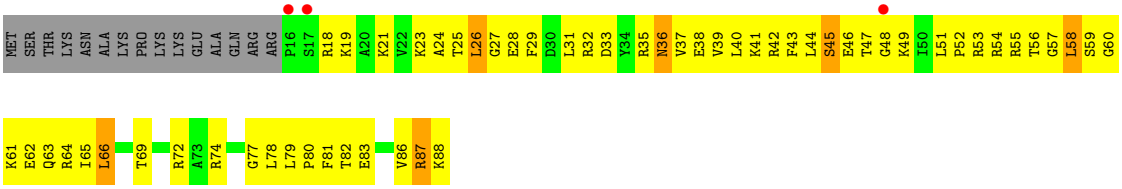
Chain Q:



- Molecule 21: 30S RIBOSOMAL PROTEIN S18

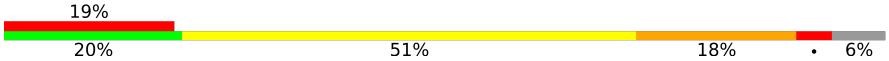
Chain R:

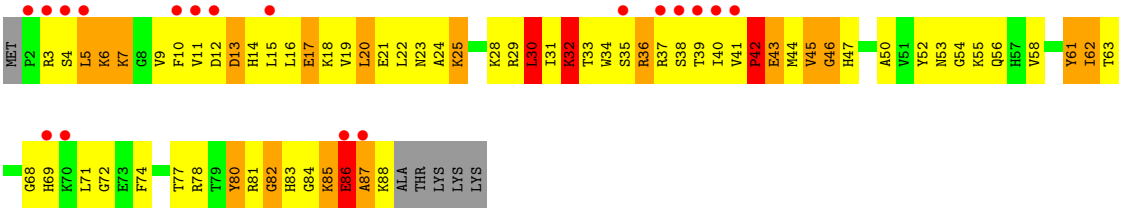




- Molecule 22: 30S RIBOSOMAL PROTEIN S19

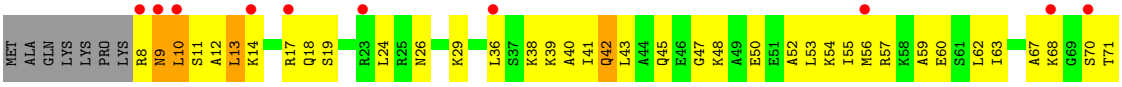
Chain S:

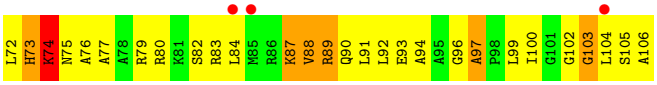




- Molecule 23: 30S RIBOSOMAL PROTEIN S20

Chain T:





• Molecule 24: 30S RIBOSOMAL PROTEIN THX

Chain V:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.57Å 401.57Å 176.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	316.23 – 3.31 200.79 – 3.31	Depositor EDS
% Data completeness (in resolution range)	90.6 (316.23-3.31) 90.6 (200.79-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.34 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.286 0.205 , 0.249	Depositor DCC
R_{free} test set	9648 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	76.8	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 82.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	52160	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.57	0/36259	0.74	36/56593 (0.1%)
2	X	0.58	0/128	0.76	0/196
3	Y	0.33	0/261	0.76	1/405 (0.2%)
4	Z	0.46	0/84	0.81	0/128
5	B	0.34	0/1935	0.66	0/2609
6	C	0.36	0/1636	0.65	0/2205
7	D	0.39	0/1733	0.65	0/2318
8	E	0.46	0/1162	0.79	0/1564
9	F	0.32	0/856	0.61	0/1154
10	G	0.34	0/1276	0.61	0/1709
11	H	0.45	0/1136	0.75	0/1527
12	I	0.34	0/1029	0.67	0/1378
13	J	0.35	0/805	0.67	1/1082 (0.1%)
14	K	0.40	0/900	0.67	0/1213
15	L	0.43	0/986	0.74	0/1320
16	M	0.36	0/947	0.67	0/1270
17	N	0.41	0/501	0.76	0/664
18	O	0.39	0/745	0.62	0/992
19	P	0.46	0/716	0.77	1/963 (0.1%)
20	Q	0.48	0/870	0.76	0/1159
21	R	0.37	0/603	0.67	0/799
22	S	0.35	0/712	0.71	1/956 (0.1%)
23	T	0.39	0/765	0.71	0/1007
24	V	0.45	0/212	0.67	0/277
All	All	0.51	0/56257	0.73	40/83488 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	29

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	G	C2'-C3'-O3'	9.30	129.96	109.50
1	A	559	A	C2'-C3'-O3'	8.99	129.29	109.50
1	A	575	G	C2'-C3'-O3'	8.98	129.25	109.50
1	A	366	C	C2'-C3'-O3'	8.93	129.15	109.50
1	A	243	A	C2'-C3'-O3'	8.21	127.56	109.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	366	C	C3'

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190(F)	G	Sidechain
1	A	197	A	Sidechain
1	A	24	U	Sidechain
1	A	249	U	Sidechain
1	A	37	U	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	32391	0	16349	1272	0
2	X	117	0	64	3	0
3	Y	233	0	120	11	0
4	Z	77	0	42	4	0
5	B	1900	0	1951	279	0
6	C	1612	0	1677	245	0
7	D	1703	0	1764	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	1146	0	1207	124	0
9	F	843	0	857	84	0
10	G	1257	0	1296	124	0
11	H	1116	0	1177	103	0
12	I	1011	0	1043	158	0
13	J	792	0	835	145	0
14	K	885	0	904	88	0
15	L	970	0	1057	119	0
16	M	937	0	995	121	0
17	N	492	0	529	77	0
18	O	734	0	771	60	0
19	P	700	0	720	54	0
20	Q	857	0	930	99	0
21	R	597	0	668	81	0
22	S	697	0	723	120	0
23	T	763	0	861	82	0
24	V	208	0	221	13	0
25	A	118	0	0	0	0
25	D	1	0	0	0	0
25	H	1	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52160	0	36761	3359	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 38.

The worst 5 of 3359 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:1397:C:OP2	8:E:24:ARG:NH2	1.62	1.27
5:B:84:GLU:HB3	5:B:219:VAL:HG21	1.25	1.18
6:C:14:ILE:HG22	6:C:15:THR:H	1.12	1.15
1:A:1443:G:H5"	1:A:1446:A:H5'	1.31	1.11
7:D:36:ARG:H	7:D:37:PRO:HD3	0.95	1.11

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	
5	B	232/256 (91%)	143 (62%)	59 (25%)	30 (13%)	0	1
6	C	204/239 (85%)	125 (61%)	49 (24%)	30 (15%)	0	1
7	D	206/209 (99%)	139 (68%)	49 (24%)	18 (9%)	1	5
8	E	148/162 (91%)	114 (77%)	24 (16%)	10 (7%)	1	9
9	F	99/101 (98%)	81 (82%)	17 (17%)	1 (1%)	15	47
10	G	153/156 (98%)	104 (68%)	37 (24%)	12 (8%)	1	7
11	H	136/138 (99%)	112 (82%)	19 (14%)	5 (4%)	3	21
12	I	125/128 (98%)	85 (68%)	25 (20%)	15 (12%)	0	2
13	J	96/105 (91%)	58 (60%)	23 (24%)	15 (16%)	0	1
14	K	117/129 (91%)	84 (72%)	18 (15%)	15 (13%)	0	2
15	L	122/135 (90%)	84 (69%)	24 (20%)	14 (12%)	0	2
16	M	116/126 (92%)	74 (64%)	28 (24%)	14 (12%)	0	2
17	N	58/61 (95%)	38 (66%)	14 (24%)	6 (10%)	0	3
18	O	86/89 (97%)	58 (67%)	23 (27%)	5 (6%)	1	11
19	P	81/88 (92%)	59 (73%)	20 (25%)	2 (2%)	5	28
20	Q	102/105 (97%)	83 (81%)	12 (12%)	7 (7%)	1	9
21	R	71/88 (81%)	50 (70%)	17 (24%)	4 (6%)	2	12
22	S	85/93 (91%)	55 (65%)	17 (20%)	13 (15%)	0	1
23	T	97/106 (92%)	57 (59%)	30 (31%)	10 (10%)	0	3
24	V	22/26 (85%)	16 (73%)	6 (27%)	0	100	100
All	All	2356/2540 (93%)	1619 (69%)	511 (22%)	226 (10%)	0	4

5 of 226 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	16	HIS

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Mol	Chain	Res	Type
5	B	17	PHE
5	B	20	GLU
5	B	21	ARG
5	B	24	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	B	202/220 (92%)	177 (88%)	25 (12%)	4	19
6	C	160/188 (85%)	143 (89%)	17 (11%)	6	25
7	D	180/181 (99%)	161 (89%)	19 (11%)	6	25
8	E	115/123 (94%)	100 (87%)	15 (13%)	4	18
9	F	90/90 (100%)	88 (98%)	2 (2%)	52	76
10	G	126/127 (99%)	119 (94%)	7 (6%)	21	53
11	H	119/119 (100%)	103 (87%)	16 (13%)	4	17
12	I	98/99 (99%)	89 (91%)	9 (9%)	9	32
13	J	87/92 (95%)	78 (90%)	9 (10%)	7	27
14	K	90/99 (91%)	77 (86%)	13 (14%)	3	15
15	L	104/111 (94%)	96 (92%)	8 (8%)	13	40
16	M	94/101 (93%)	82 (87%)	12 (13%)	4	18
17	N	49/50 (98%)	44 (90%)	5 (10%)	7	27
18	O	79/80 (99%)	70 (89%)	9 (11%)	5	22
19	P	72/74 (97%)	68 (94%)	4 (6%)	21	53
20	Q	96/97 (99%)	88 (92%)	8 (8%)	11	37
21	R	64/77 (83%)	60 (94%)	4 (6%)	18	48
22	S	75/80 (94%)	62 (83%)	13 (17%)	2	9
23	T	76/82 (93%)	69 (91%)	7 (9%)	9	32
24	V	19/21 (90%)	18 (95%)	1 (5%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1995/2111 (94%)	1792 (90%)	203 (10%)	7 27

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	J	71	LEU
16	M	44	ARG
23	T	62	LEU
14	K	24	SER
14	K	125	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
10	G	51	GLN
22	S	69	HIS
12	I	89	ASN
22	S	56	GLN
20	Q	16	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	201 (13%)	70 (4%)
2	X	5/6 (83%)	0	0
3	Y	10/15 (66%)	2 (20%)	1 (10%)
4	Z	3/4 (75%)	1 (33%)	0
All	All	1524/1547 (98%)	204 (13%)	71 (4%)

5 of 204 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 71 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1224	G
1	A	1281	U
1	A	1347	G
1	A	428	G
1	A	372	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 122 ligands modelled in this entry, 122 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1507/1522 (99%)	0.54	52 (3%)	44	42	16, 53, 140, 201	0
2	X	6/6 (100%)	4.90	4 (66%)	0	0	59, 71, 178, 201	0
3	Y	11/15 (73%)	1.54	3 (27%)	0	0	66, 90, 182, 190	0
4	Z	4/4 (100%)	1.33	1 (25%)	0	0	71, 77, 89, 119	0
5	B	234/256 (91%)	0.27	15 (6%)	19	20	19, 87, 173, 201	0
6	C	206/239 (86%)	0.11	7 (3%)	45	43	22, 80, 160, 201	0
7	D	208/209 (99%)	0.50	17 (8%)	11	11	17, 60, 145, 180	0
8	E	150/162 (92%)	0.59	13 (8%)	10	10	17, 48, 107, 201	0
9	F	101/101 (100%)	0.06	2 (1%)	65	64	35, 88, 148, 185	0
10	G	155/156 (99%)	-0.05	3 (1%)	66	65	27, 70, 150, 201	0
11	H	138/138 (100%)	0.32	3 (2%)	62	60	5, 39, 108, 136	0
12	I	127/128 (99%)	0.44	10 (7%)	12	12	19, 82, 144, 184	0
13	J	98/105 (93%)	0.49	14 (14%)	2	2	30, 107, 188, 201	0
14	K	119/129 (92%)	0.56	7 (5%)	22	23	12, 54, 130, 201	0
15	L	124/135 (91%)	0.72	17 (13%)	3	2	16, 57, 144, 187	0
16	M	118/126 (93%)	0.55	9 (7%)	13	14	32, 70, 144, 170	0
17	N	60/61 (98%)	1.88	28 (46%)	0	0	39, 70, 140, 201	0
18	O	88/89 (98%)	0.38	3 (3%)	45	43	7, 56, 145, 201	0
19	P	83/88 (94%)	0.92	14 (16%)	1	1	10, 41, 101, 150	0
20	Q	104/105 (99%)	0.94	15 (14%)	2	2	10, 43, 157, 201	0
21	R	73/88 (82%)	0.48	3 (4%)	37	36	32, 66, 166, 201	0
22	S	87/93 (93%)	0.95	18 (20%)	1	0	54, 99, 176, 201	0
23	T	99/106 (93%)	0.89	13 (13%)	3	3	15, 50, 123, 156	0
24	V	24/26 (92%)	1.63	8 (33%)	0	0	26, 59, 128, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
All	All	3924/4087 (96%)	0.53	279 (7%)	16	17	5, 60, 152, 201	0

The worst 5 of 279 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	K	129	SER	24.9
14	K	128	ALA	18.0
2	X	2	U	13.2
18	O	89	GLY	11.3
22	S	3	ARG	10.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1640	1/1	0.48	0.28	27,27,27,27	1
25	MG	A	1579	1/1	0.54	0.31	27,27,27,27	1
25	MG	A	1655	1/1	0.56	0.26	27,27,27,27	1
25	MG	A	1651	1/1	0.61	0.12	27,27,27,27	0
25	MG	A	1641	1/1	0.66	0.28	27,27,27,27	1
25	MG	A	1607	1/1	0.70	0.23	27,27,27,27	1
25	MG	A	1624	1/1	0.70	0.28	27,27,27,27	1
25	MG	A	1628	1/1	0.72	0.56	27,27,27,27	1
25	MG	A	1636	1/1	0.74	0.15	27,27,27,27	1
25	MG	A	1656	1/1	0.76	0.17	27,27,27,27	0
25	MG	A	1547	1/1	0.77	0.15	27,27,27,27	0
25	MG	A	1620	1/1	0.77	0.33	27,27,27,27	1
25	MG	A	1637	1/1	0.77	0.12	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1606	1/1	0.77	0.23	27,27,27,27	1
25	MG	A	1622	1/1	0.78	0.33	27,27,27,27	0
25	MG	A	87	1/1	0.82	0.41	27,27,27,27	1
25	MG	A	214	1/1	0.83	0.19	27,27,27,27	1
25	MG	A	1626	1/1	0.83	0.14	27,27,27,27	1
25	MG	A	1558	1/1	0.84	0.21	27,27,27,27	0
25	MG	A	1584	1/1	0.85	0.24	27,27,27,27	0
25	MG	A	1654	1/1	0.85	0.06	27,27,27,27	1
25	MG	D	215	1/1	0.85	0.13	27,27,27,27	0
25	MG	A	1556	1/1	0.86	0.43	27,27,27,27	0
25	MG	A	1562	1/1	0.86	0.14	27,27,27,27	1
25	MG	A	1612	1/1	0.87	0.35	27,27,27,27	0
25	MG	A	1653	1/1	0.87	0.18	27,27,27,27	1
25	MG	A	1623	1/1	0.87	0.14	27,27,27,27	0
25	MG	A	210	1/1	0.87	0.14	27,27,27,27	1
25	MG	A	1625	1/1	0.87	0.21	27,27,27,27	0
25	MG	A	1621	1/1	0.87	0.22	27,27,27,27	0
25	MG	A	1618	1/1	0.88	0.15	27,27,27,27	1
25	MG	A	1605	1/1	0.88	0.11	27,27,27,27	0
25	MG	A	1639	1/1	0.88	0.27	27,27,27,27	1
25	MG	A	1627	1/1	0.88	0.16	27,27,27,27	0
25	MG	A	211	1/1	0.88	0.29	27,27,27,27	0
25	MG	A	1647	1/1	0.88	0.15	27,27,27,27	0
25	MG	A	1561	1/1	0.89	0.28	27,27,27,27	0
25	MG	A	1649	1/1	0.89	0.15	27,27,27,27	1
25	MG	A	1590	1/1	0.89	0.20	27,27,27,27	0
25	MG	A	1652	1/1	0.89	0.09	27,27,27,27	0
25	MG	A	1638	1/1	0.89	0.18	27,27,27,27	0
25	MG	A	1548	1/1	0.89	0.32	27,27,27,27	1
25	MG	A	1615	1/1	0.89	0.25	27,27,27,27	0
25	MG	A	1616	1/1	0.89	0.10	27,27,27,27	0
25	MG	A	1644	1/1	0.89	0.25	27,27,27,27	1
25	MG	A	1650	1/1	0.90	0.26	27,27,27,27	1
25	MG	A	1645	1/1	0.90	0.18	27,27,27,27	0
25	MG	A	1643	1/1	0.90	0.16	27,27,27,27	1
25	MG	A	1570	1/1	0.90	0.31	27,27,27,27	0
25	MG	A	1585	1/1	0.91	0.33	27,27,27,27	0
25	MG	A	1569	1/1	0.91	0.34	27,27,27,27	0
25	MG	A	1603	1/1	0.91	0.24	27,27,27,27	0
25	MG	A	1594	1/1	0.91	0.23	27,27,27,27	0
25	MG	A	1634	1/1	0.91	0.14	27,27,27,27	0
25	MG	A	1577	1/1	0.91	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1610	1/1	0.92	0.28	27,27,27,27	1
25	MG	A	1575	1/1	0.92	0.32	27,27,27,27	0
25	MG	A	1629	1/1	0.92	0.13	27,27,27,27	0
25	MG	A	1595	1/1	0.92	0.06	27,27,27,27	0
25	MG	A	1635	1/1	0.92	0.15	27,27,27,27	0
25	MG	A	1545	1/1	0.92	0.09	27,27,27,27	0
25	MG	A	1573	1/1	0.93	0.26	27,27,27,27	0
25	MG	A	1646	1/1	0.93	0.75	27,27,27,27	0
25	MG	A	1564	1/1	0.93	0.13	27,27,27,27	0
25	MG	A	1613	1/1	0.93	0.33	27,27,27,27	0
25	MG	A	1608	1/1	0.93	0.09	27,27,27,27	0
25	MG	A	1633	1/1	0.93	0.32	27,27,27,27	0
25	MG	A	1574	1/1	0.94	0.28	27,27,27,27	0
25	MG	A	1588	1/1	0.94	0.17	27,27,27,27	0
25	MG	A	1631	1/1	0.94	0.31	27,27,27,27	0
25	MG	A	1602	1/1	0.94	0.16	27,27,27,27	0
25	MG	A	1619	1/1	0.94	0.27	27,27,27,27	0
25	MG	A	1589	1/1	0.94	0.28	27,27,27,27	0
25	MG	A	1563	1/1	0.94	0.20	27,27,27,27	0
25	MG	A	1592	1/1	0.94	0.38	27,27,27,27	0
25	MG	A	1559	1/1	0.94	0.26	27,27,27,27	0
25	MG	A	1566	1/1	0.94	0.19	27,27,27,27	0
25	MG	A	1597	1/1	0.94	0.20	27,27,27,27	0
25	MG	A	1599	1/1	0.94	0.18	27,27,27,27	0
25	MG	A	1567	1/1	0.94	0.21	27,27,27,27	1
25	MG	A	1581	1/1	0.95	0.16	27,27,27,27	0
25	MG	A	86	1/1	0.95	0.27	27,27,27,27	0
25	MG	A	1596	1/1	0.95	0.40	27,27,27,27	0
25	MG	A	1551	1/1	0.95	0.28	27,27,27,27	0
25	MG	A	1587	1/1	0.95	0.19	27,27,27,27	0
25	MG	A	1576	1/1	0.95	0.16	27,27,27,27	0
25	MG	A	1571	1/1	0.95	0.26	27,27,27,27	0
25	MG	A	1565	1/1	0.95	0.36	27,27,27,27	0
25	MG	A	1580	1/1	0.95	0.23	27,27,27,27	0
25	MG	A	1642	1/1	0.95	0.23	27,27,27,27	1
25	MG	A	1593	1/1	0.95	0.23	27,27,27,27	0
25	MG	A	1604	1/1	0.95	0.10	27,27,27,27	0
25	MG	H	213	1/1	0.95	0.15	27,27,27,27	0
25	MG	A	1582	1/1	0.96	0.17	27,27,27,27	0
25	MG	A	1611	1/1	0.96	0.16	27,27,27,27	0
25	MG	A	71	1/1	0.96	0.37	27,27,27,27	0
25	MG	A	1568	1/1	0.96	0.30	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1552	1/1	0.96	0.34	27,27,27,27	0
25	MG	A	1549	1/1	0.96	0.33	27,27,27,27	0
25	MG	A	1617	1/1	0.96	0.22	27,27,27,27	0
25	MG	A	1560	1/1	0.96	0.27	27,27,27,27	0
25	MG	A	1609	1/1	0.96	0.24	27,27,27,27	0
25	MG	A	1591	1/1	0.97	0.33	27,27,27,27	0
25	MG	A	1550	1/1	0.97	0.34	27,27,27,27	0
25	MG	A	1586	1/1	0.97	0.16	27,27,27,27	0
25	MG	A	1553	1/1	0.97	0.38	27,27,27,27	0
25	MG	A	1601	1/1	0.97	0.20	27,27,27,27	0
25	MG	A	1578	1/1	0.97	0.24	27,27,27,27	0
25	MG	A	1583	1/1	0.97	0.16	27,27,27,27	0
25	MG	A	1572	1/1	0.97	0.10	27,27,27,27	0
25	MG	A	1614	1/1	0.97	0.20	27,27,27,27	0
25	MG	A	1598	1/1	0.97	0.17	27,27,27,27	0
25	MG	A	1600	1/1	0.98	0.06	27,27,27,27	0
25	MG	A	1555	1/1	0.98	0.26	27,27,27,27	0
25	MG	A	1546	1/1	0.98	0.32	27,27,27,27	0
25	MG	A	1630	1/1	0.98	0.31	27,27,27,27	0
25	MG	A	1557	1/1	0.98	0.26	27,27,27,27	0
25	MG	A	1554	1/1	0.98	0.23	27,27,27,27	0
26	ZN	D	506	1/1	0.98	0.34	27,27,27,27	0
25	MG	A	1648	1/1	0.99	0.08	27,27,27,27	0
25	MG	A	1632	1/1	0.99	0.32	27,27,27,27	0
26	ZN	N	507	1/1	0.99	0.14	27,27,27,27	1

6.5 Other polymers (i)

There are no such residues in this entry.