



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:55 AM GMT

PDB ID : 1HNX  
Title : STRUCTURE OF THE THERMUS THERMOPHILUS 30S RIBOSOMAL  
SUBUNIT IN COMPLEX WITH PACTAMYCIN  
Authors : Brodersen, D.E.; Clemons Jr., W.M.; Carter, A.P.; Morgan-Warren, R.; Wim-  
berly, B.T.; Ramakrishnan, V.  
Deposited on : 2000-12-08  
Resolution : 3.40 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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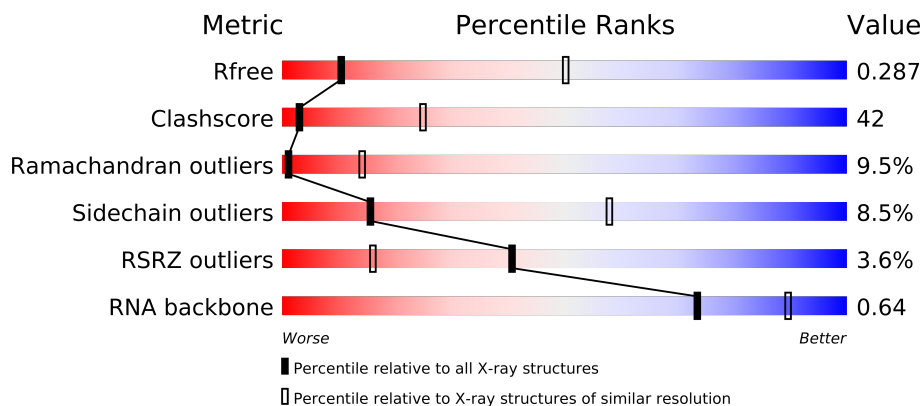
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.40 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.




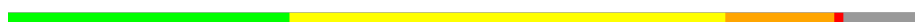


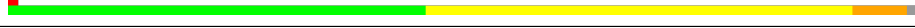



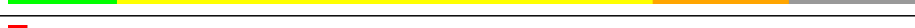


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)
RNA backbone	1838	1002 (4.02-2.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	X	6	
3	B	256	
4	C	239	
5	D	209	
6	E	162	
7	F	101	
8	G	156	
9	H	138	
10	I	128	
11	J	105	

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Mol	Chain	Length	Quality of chain
12	K	129	
13	L	135	
14	M	126	
15	N	61	
16	O	89	
17	P	88	
18	Q	105	
19	R	88	
20	S	93	
21	T	106	
22	V	26	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 51910 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1507	Total	C	N	O	P	22	0	0
			32391	14418	6002	10465	1506			

- Molecule 2 is a RNA chain called FRAGMENT OF MESSENGER RNA.

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

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	88	Total	C	N	O	S	0	0	0
			735	462	147	125	1			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

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

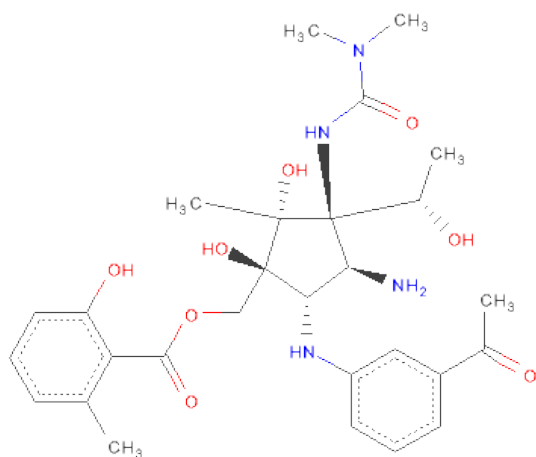
- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	H	1	Total	Mg	0	0
			1	1		
23	A	94	Total	Mg	0	0
			94	94		
23	D	1	Total	Mg	0	0
			1	1		

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 25 is DE-6-MSA-PACTAMYCIN (three-letter code: PCY) (formula: C<sub>28</sub>H<sub>38</sub>N<sub>4</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
25	A	1	40	28	4	8	0	0

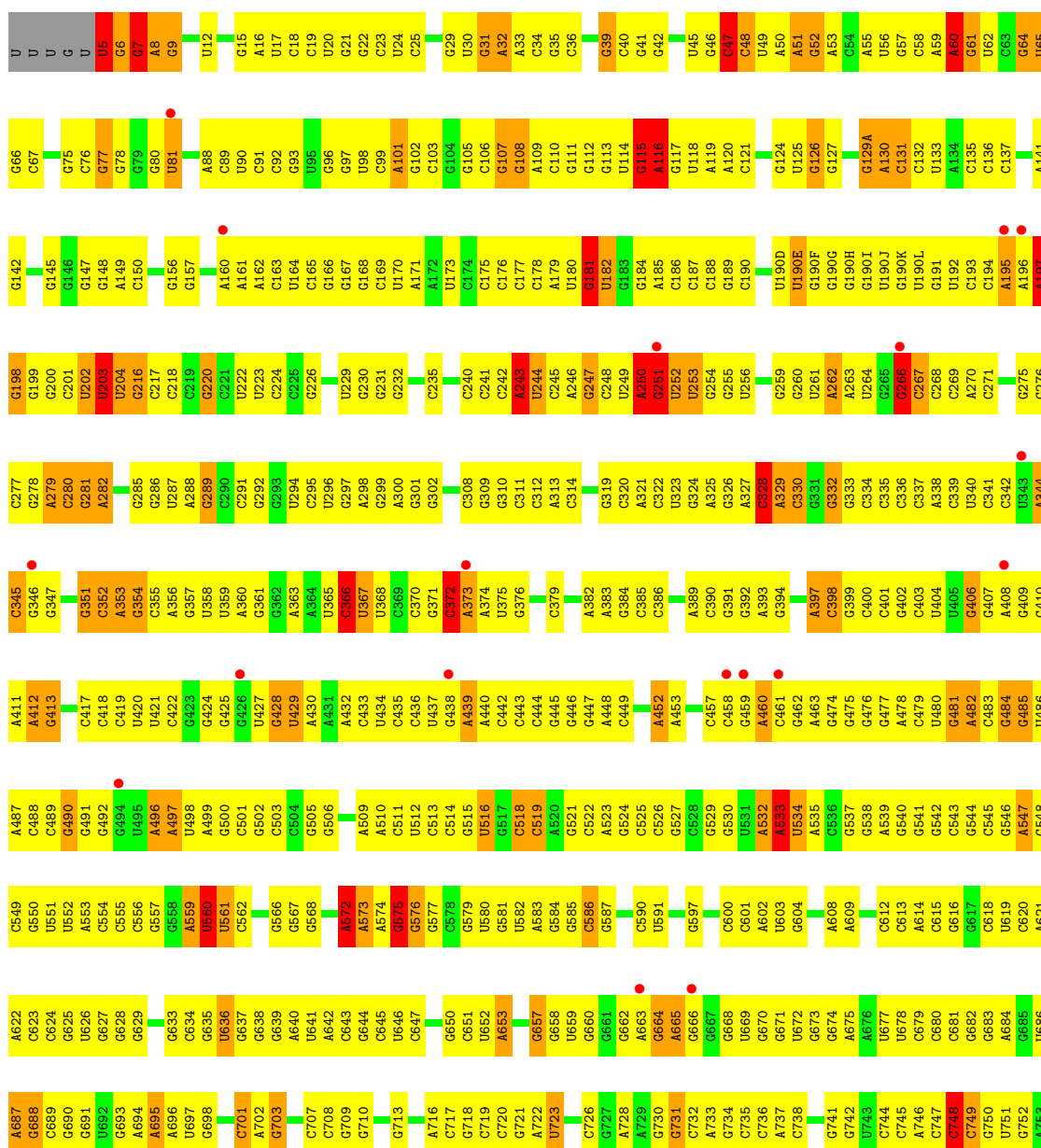


### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

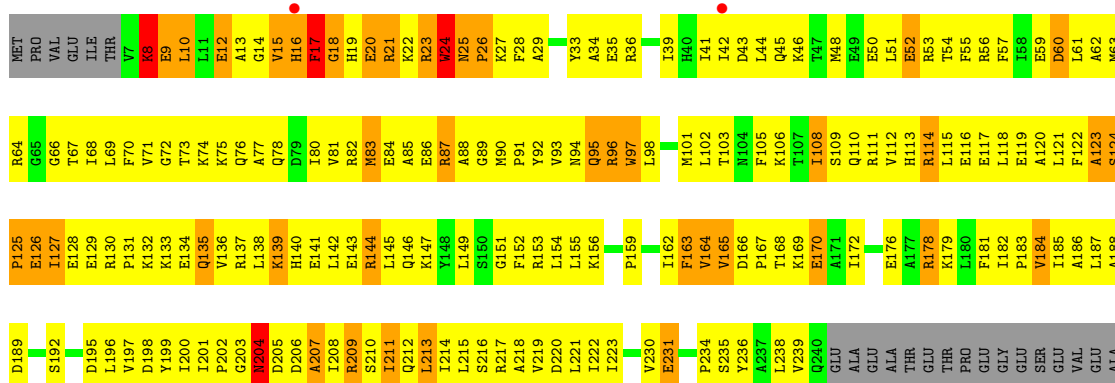
Chain A: 





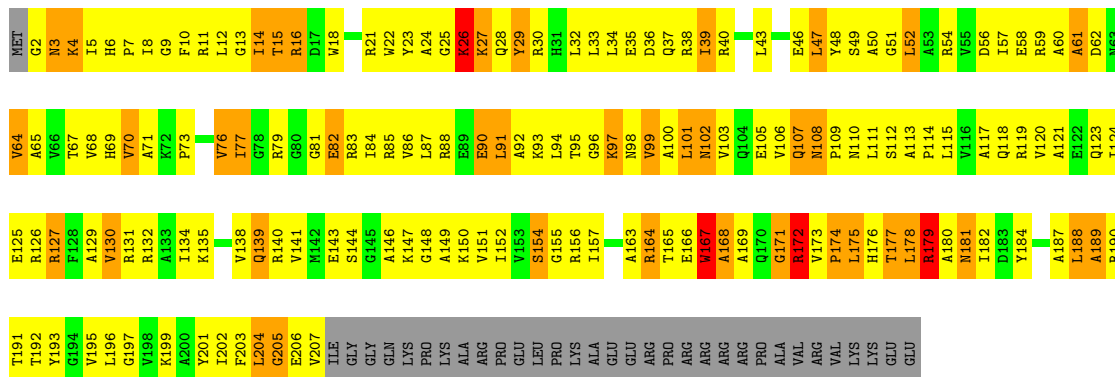
• Molecule 3: 30S RIBOSOMAL PROTEIN S2

Chain B:



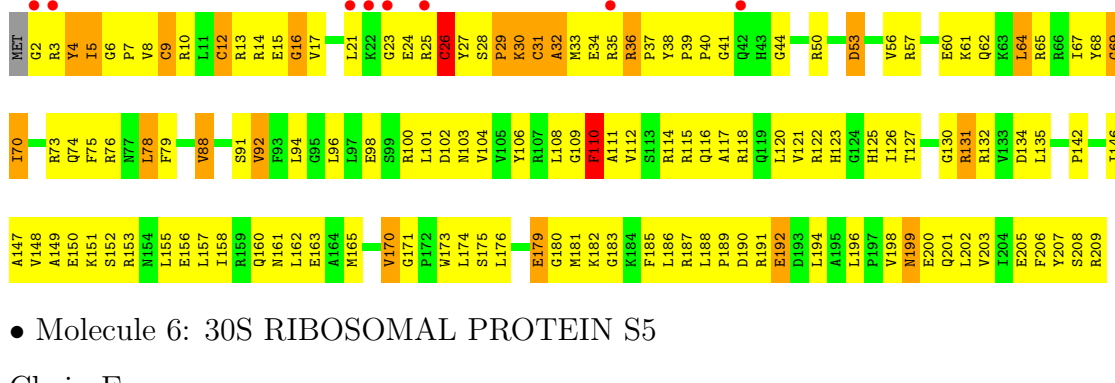
- Molecule 4: 30S RIBOSOMAL PROTEIN S3

Chain C:



- Molecule 5: 30S RIBOSOMAL PROTEIN S4

Chain D:



- Molecule 6: 30S RIBOSOMAL PROTEIN S5

Chain E:

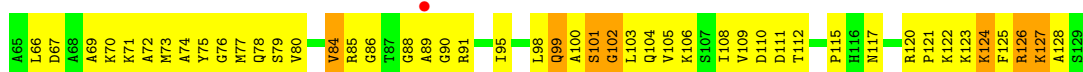
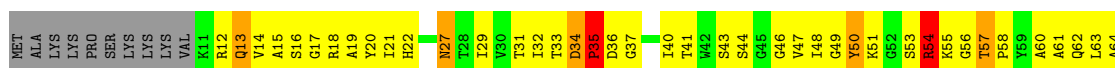






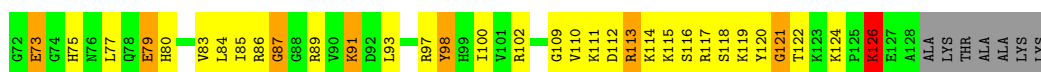
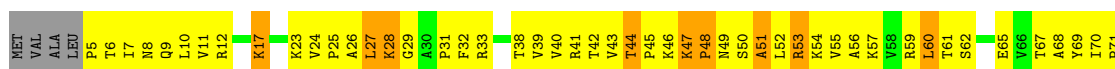
• Molecule 12: 30S RIBOSOMAL PROTEIN S11

Chain K:



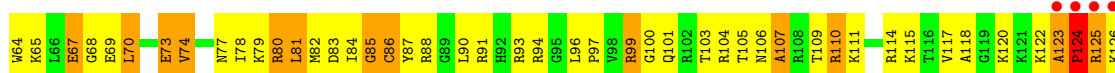
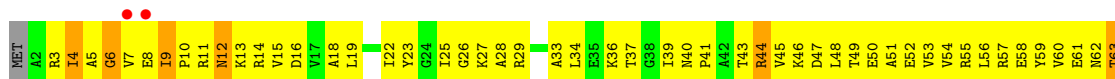
• Molecule 13: 30S RIBOSOMAL PROTEIN S12

Chain L:



• Molecule 14: 30S RIBOSOMAL PROTEIN S13

Chain M:



• Molecule 15: 30S RIBOSOMAL PROTEIN S14

Chain N:



• Molecule 16: 30S RIBOSOMAL PROTEIN S15

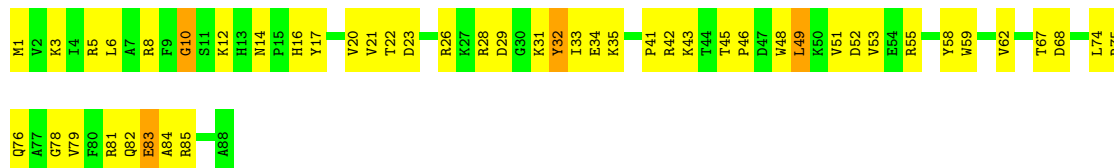
Chain O:





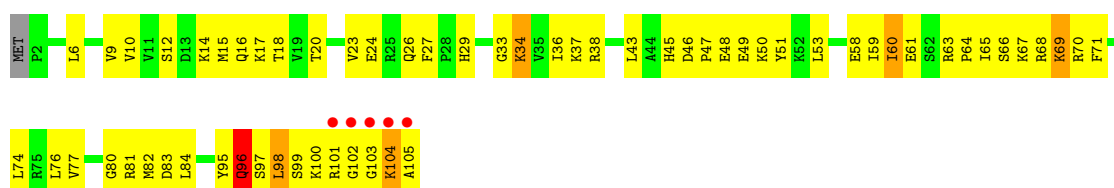
- Molecule 17: 30S RIBOSOMAL PROTEIN S16

Chain P:



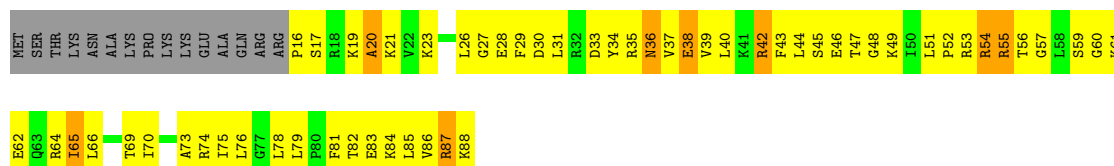
- Molecule 18: 30S RIBOSOMAL PROTEIN S17

Chain Q:



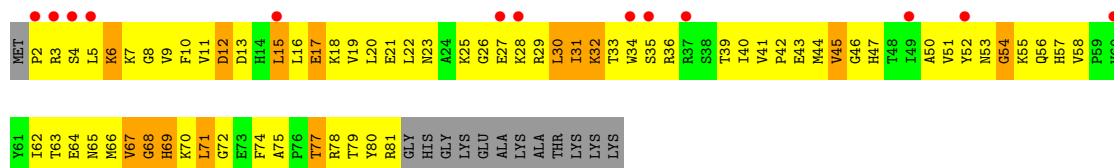
- Molecule 19: 30S RIBOSOMAL PROTEIN S18

Chain R:



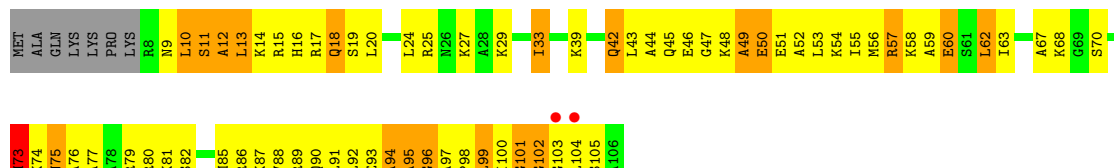
- Molecule 20: 30S RIBOSOMAL PROTEIN S19

Chain S:



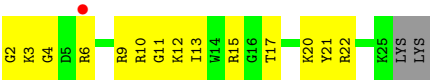
- Molecule 21: 30S RIBOSOMAL PROTEIN S20

Chain T:



- Molecule 22: 30S RIBOSOMAL PROTEIN THX

Chain V: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.72Å 401.72Å 177.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.34 – 3.40 94.29 – 3.11	Depositor EDS
% Data completeness (in resolution range)	88.9 (95.34-3.40) 83.7 (94.29-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.13Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.280 0.241 , 0.287	Depositor DCC
$R_{free}$ test set	10844 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.5	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 66.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	4 of 215677 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	51910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PCY, 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	0.53	0/36259	0.75	42/56593 (0.1%)
2	X	0.56	0/128	0.71	0/196
3	B	0.39	0/1935	0.69	0/2609
4	C	0.38	0/1636	0.65	0/2205
5	D	0.43	0/1733	0.71	1/2318 (0.0%)
6	E	0.49	0/1162	0.80	2/1564 (0.1%)
7	F	0.35	0/856	0.65	0/1154
8	G	0.36	0/1276	0.64	0/1709
9	H	0.47	0/1136	0.78	0/1527
10	I	0.35	0/1029	0.66	0/1378
11	J	0.37	0/805	0.68	0/1082
12	K	0.40	0/900	0.75	0/1213
13	L	0.43	0/986	0.75	0/1320
14	M	0.35	0/1008	0.68	0/1347
15	N	0.41	0/501	0.78	0/664
16	O	0.39	0/745	0.64	0/992
17	P	0.46	0/751	0.76	0/1008
18	Q	0.50	0/870	0.78	0/1159
19	R	0.38	0/603	0.65	0/799
20	S	0.35	0/661	0.68	1/890 (0.1%)
21	T	0.38	0/764	0.73	0/1006
22	V	0.50	0/212	0.64	0/277
All	All	0.49	0/55956	0.74	46/83010 (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	2	47

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	9.79	131.03	109.50
1	A	1085	U	C2'-C3'-O3'	9.22	129.78	109.50
1	A	60	A	C2'-C3'-O3'	8.05	127.22	109.50
1	A	484	G	C2'-C3'-O3'	7.86	126.78	109.50
1	A	181	G	C2'-C3'-O3'	7.65	126.34	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1085	U	C3'
1	A	1498	U	C3'

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	A	Sidechain
1	A	126	G	Sidechain
1	A	47	C	Sidechain
1	A	5	U	Sidechain
1	A	77	G	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32391	0	16349	1512	0
2	X	117	0	64	3	0
3	B	1900	0	1951	289	0
4	C	1612	0	1677	276	0
5	D	1703	0	1764	182	0
6	E	1146	0	1207	120	0
7	F	843	0	857	83	0
8	G	1257	0	1296	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	1116	0	1177	96	0
10	I	1011	0	1043	151	0
11	J	792	0	835	158	0
12	K	885	0	904	100	0
13	L	970	0	1057	125	0
14	M	997	0	1072	142	0
15	N	492	0	529	87	0
16	O	734	0	771	63	0
17	P	735	0	752	67	0
18	Q	857	0	930	104	0
19	R	597	0	668	106	0
20	S	647	0	673	105	0
21	T	762	0	859	106	0
22	V	208	0	221	20	0
23	A	94	0	0	0	0
23	D	1	0	0	0	0
23	H	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	40	0	38	10	0
All	All	51910	0	36694	3662	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 42.

The worst 5 of 3662 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:A:1632:PCY:C3	25:A:1632:PCY:N2	1.69	1.49
13:L:28:LYS:HD2	13:L:33:ARG:HH22	1.01	1.16
12:K:110:ASP:HB2	19:R:88:LYS:HD2	1.28	1.15
6:E:110:LEU:HD13	6:E:118:ILE:HD12	1.28	1.15
4:C:58:GLU:HB3	11:J:92:THR:HG21	1.29	1.15

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	
3	B	232/256 (91%)	155 (67%)	49 (21%)	28 (12%)	1	8
4	C	204/239 (85%)	120 (59%)	52 (26%)	32 (16%)	0	4
5	D	206/209 (99%)	146 (71%)	41 (20%)	19 (9%)	1	15
6	E	148/162 (91%)	126 (85%)	18 (12%)	4 (3%)	8	55
7	F	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	2	28
8	G	153/156 (98%)	114 (74%)	24 (16%)	15 (10%)	1	13
9	H	136/138 (99%)	122 (90%)	10 (7%)	4 (3%)	7	54
10	I	125/128 (98%)	90 (72%)	28 (22%)	7 (6%)	3	30
11	J	96/105 (91%)	58 (60%)	20 (21%)	18 (19%)	0	2
12	K	117/129 (91%)	87 (74%)	16 (14%)	14 (12%)	1	9
13	L	122/135 (90%)	91 (75%)	19 (16%)	12 (10%)	1	13
14	M	123/126 (98%)	84 (68%)	23 (19%)	16 (13%)	0	7
15	N	58/61 (95%)	40 (69%)	10 (17%)	8 (14%)	0	6
16	O	86/89 (97%)	63 (73%)	20 (23%)	3 (4%)	6	48
17	P	86/88 (98%)	66 (77%)	17 (20%)	3 (4%)	6	48
18	Q	102/105 (97%)	84 (82%)	13 (13%)	5 (5%)	3	35
19	R	71/88 (81%)	51 (72%)	18 (25%)	2 (3%)	8	54
20	S	78/93 (84%)	52 (67%)	15 (19%)	11 (14%)	0	5
21	T	97/106 (92%)	61 (63%)	19 (20%)	17 (18%)	0	3
22	V	22/26 (85%)	17 (77%)	4 (18%)	1 (4%)	4	38
All	All	2361/2540 (93%)	1702 (72%)	434 (18%)	225 (10%)	1	14

5 of 225 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	8	LYS
3	B	9	GLU
3	B	15	VAL
3	B	16	HIS
3	B	17	PHE

### 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	
3	B	202/220 (92%)	181 (90%)	21 (10%)	10	45
4	C	160/188 (85%)	136 (85%)	24 (15%)	4	25
5	D	180/181 (99%)	168 (93%)	12 (7%)	23	70
6	E	115/123 (94%)	102 (89%)	13 (11%)	9	39
7	F	90/90 (100%)	87 (97%)	3 (3%)	50	88
8	G	126/127 (99%)	119 (94%)	7 (6%)	30	75
9	H	119/119 (100%)	105 (88%)	14 (12%)	8	36
10	I	98/99 (99%)	86 (88%)	12 (12%)	7	34
11	J	87/92 (95%)	76 (87%)	11 (13%)	7	33
12	K	90/99 (91%)	85 (94%)	5 (6%)	30	75
13	L	104/111 (94%)	96 (92%)	8 (8%)	18	63
14	M	100/101 (99%)	93 (93%)	7 (7%)	21	68
15	N	49/50 (98%)	45 (92%)	4 (8%)	17	60
16	O	79/80 (99%)	77 (98%)	2 (2%)	60	92
17	P	74/74 (100%)	70 (95%)	4 (5%)	31	77
18	Q	96/97 (99%)	92 (96%)	4 (4%)	40	83
19	R	64/77 (83%)	57 (89%)	7 (11%)	9	42
20	S	71/80 (89%)	67 (94%)	4 (6%)	30	75
21	T	76/82 (93%)	68 (90%)	8 (10%)	10	44
22	V	19/21 (90%)	19 (100%)	0	100	100
All	All	1999/2111 (95%)	1829 (92%)	170 (8%)	15	58

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	G	24	THR
10	I	23	ASN
19	R	65	ILE
8	G	126	ASP
9	H	91	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
7	F	57	GLN
8	G	56	GLN
20	S	53	ASN
7	F	94	GLN
8	G	106	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	220 (14%)	85 (5%)
2	X	5/6 (83%)	1 (20%)	0
All	All	1512/1528 (98%)	221 (14%)	85 (5%)

5 of 221 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A

5 of 85 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	687	A
1	A	975	A
1	A	1380	U
1	A	701	C
1	A	840	C

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 99 ligands modelled in this entry, 98 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
25	PCY	A	1632	-	42,42,42	8.47	42 (100%)	65,65,65	1.71	17 (26%)

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
25	PCY	A	1632	-	-	0/33/67/67	0/3/3/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1632	PCY	C3-N2	26.25	1.69	1.48
25	A	1632	PCY	C1-N4	13.63	1.54	1.35
25	A	1632	PCY	C17-N20	12.18	1.59	1.45
25	A	1632	PCY	C13-C7	10.53	1.69	1.52
25	A	1632	PCY	O14-C7	10.46	1.59	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1632	PCY	C22-N20-C17	-5.02	112.19	122.81
25	A	1632	PCY	C11-C6-C3	-3.87	107.95	114.10
25	A	1632	PCY	N2-C1-N4	3.68	121.74	117.00
25	A	1632	PCY	C31-C27-C30	3.30	122.01	117.92
25	A	1632	PCY	C8-C3-N2	-3.25	106.39	112.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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	1506/1522 (98%)	0.70	97 (6%) 19 7	37, 70, 161, 199	0
2	X	6/6 (100%)	0.79	1 (16%) 2 2	62, 79, 117, 151	0
3	B	234/256 (91%)	0.01	2 (0%) 81 47	34, 87, 162, 199	0
4	C	206/239 (86%)	-0.03	0 100 100	41, 91, 153, 179	0
5	D	208/209 (99%)	0.05	8 (3%) 38 15	35, 71, 128, 191	0
6	E	150/162 (92%)	-0.13	0 100 100	34, 58, 111, 168	0
7	F	101/101 (100%)	0.21	0 100 100	56, 95, 147, 167	0
8	G	155/156 (99%)	-0.02	0 100 100	47, 85, 147, 175	0
9	H	138/138 (100%)	-0.14	1 (0%) 84 52	21, 52, 92, 139	0
10	I	127/128 (99%)	0.23	0 100 100	37, 96, 140, 181	0
11	J	98/105 (93%)	0.33	3 (3%) 47 19	50, 119, 184, 199	0
12	K	119/129 (92%)	0.16	1 (0%) 83 49	41, 73, 137, 178	0
13	L	124/135 (91%)	0.07	0 100 100	30, 72, 131, 180	0
14	M	125/126 (99%)	0.37	6 (4%) 29 12	56, 89, 153, 188	0
15	N	60/61 (98%)	0.14	0 100 100	50, 86, 157, 170	0
16	O	88/89 (98%)	0.03	1 (1%) 77 40	38, 70, 136, 186	0
17	P	88/88 (100%)	0.01	0 100 100	35, 63, 164, 198	0
18	Q	104/105 (99%)	0.35	5 (4%) 29 12	35, 62, 137, 199	0
19	R	73/88 (82%)	0.06	0 100 100	43, 75, 154, 194	0
20	S	80/93 (86%)	0.92	13 (16%) 2 2	66, 110, 158, 199	0
21	T	99/106 (93%)	0.17	2 (2%) 62 28	44, 72, 133, 194	0
22	V	24/26 (92%)	0.43	1 (4%) 35 13	44, 79, 128, 149	0
All	All	3913/4068 (96%)	0.34	141 (3%) 41 16	21, 75, 155, 199	0

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	S	3	ARG	10.5
18	Q	105	ALA	8.3
1	A	1129	C	8.1
18	Q	104	LYS	6.9
14	M	124	PRO	6.9

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	MG	A	1602	1/1	0.35	-	45,45,45,45	0
23	MG	A	1609	1/1	0.15	-	45,45,45,45	0
23	MG	A	1575	1/1	0.12	-	45,45,45,45	1
23	MG	A	1605	1/1	0.07	-	45,45,45,45	0
23	MG	A	1562	1/1	0.58	-	45,45,45,45	0
23	MG	A	86	1/1	0.35	-	45,45,45,45	0
23	MG	A	1631	1/1	0.53	-	45,45,45,45	1
23	MG	A	1613	1/1	0.37	-	45,45,45,45	1
24	ZN	D	300	1/1	0.32	-	53,53,53,53	0
23	MG	A	1570	1/1	0.39	-	45,45,45,45	1
23	MG	A	1601	1/1	0.27	-	45,45,45,45	0
23	MG	A	214	1/1	0.18	-	45,45,45,45	0
23	MG	A	1630	1/1	0.99	-	45,45,45,45	1
25	PCY	A	1632	40/40	0.30	-	28,28,28,28	0
23	MG	A	1556	1/1	0.21	-	45,45,45,45	1
23	MG	A	1576	1/1	0.23	-	45,45,45,45	0
23	MG	A	1610	1/1	0.15	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1550	1/1	0.65	-	45,45,45,45	1
23	MG	A	1578	1/1	0.33	-	45,45,45,45	0
23	MG	A	1574	1/1	0.31	-	45,45,45,45	0
23	MG	A	1598	1/1	0.16	-	45,45,45,45	1
23	MG	A	1549	1/1	0.16	-	45,45,45,45	1
23	MG	A	1628	1/1	0.25	-	45,45,45,45	1
23	MG	A	71	1/1	0.47	-	45,45,45,45	0
23	MG	A	1596	1/1	0.45	-	45,45,45,45	1
23	MG	A	1623	1/1	0.49	-	45,45,45,45	1
23	MG	A	1591	1/1	0.45	-	45,45,45,45	0
23	MG	A	1607	1/1	0.23	-	45,45,45,45	0
23	MG	A	1603	1/1	0.17	-	45,45,45,45	0
23	MG	A	1587	1/1	0.24	-	45,45,45,45	0
23	MG	D	215	1/1	0.23	-	45,45,45,45	0
23	MG	A	1625	1/1	0.17	-	45,45,45,45	1
23	MG	A	1545	1/1	0.09	-	45,45,45,45	0
23	MG	H	213	1/1	0.87	-	45,45,45,45	1
23	MG	A	1554	1/1	0.46	-	45,45,45,45	0
23	MG	A	1615	1/1	0.51	-	45,45,45,45	1
23	MG	A	1577	1/1	0.26	-	45,45,45,45	0
24	ZN	N	190	1/1	0.21	-	53,53,53,53	1
23	MG	A	1627	1/1	0.36	-	45,45,45,45	1
23	MG	A	1612	1/1	0.30	-	45,45,45,45	0
23	MG	A	1621	1/1	0.49	-	45,45,45,45	1
23	MG	A	1584	1/1	0.47	-	45,45,45,45	0
23	MG	A	1599	1/1	0.34	-	45,45,45,45	0
23	MG	A	1608	1/1	0.13	-	45,45,45,45	0
23	MG	A	1563	1/1	0.19	-	45,45,45,45	0
23	MG	A	1616	1/1	0.12	-	45,45,45,45	0
23	MG	A	1618	1/1	0.74	-	45,45,45,45	1
23	MG	A	1552	1/1	0.21	-	45,45,45,45	0
23	MG	A	1611	1/1	0.17	-	45,45,45,45	1
23	MG	A	1593	1/1	0.29	-	45,45,45,45	0
23	MG	A	1579	1/1	0.25	-	45,45,45,45	0
23	MG	A	1590	1/1	0.35	-	45,45,45,45	0
23	MG	A	1565	1/1	0.57	-	45,45,45,45	0
23	MG	A	1561	1/1	0.68	-	45,45,45,45	0
23	MG	A	1547	1/1	0.52	-	45,45,45,45	0
23	MG	A	1629	1/1	0.58	-	45,45,45,45	1
23	MG	A	1560	1/1	0.44	-	45,45,45,45	0
23	MG	A	1558	1/1	0.32	-	45,45,45,45	0
23	MG	A	1597	1/1	0.11	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1567	1/1	0.60	-	45,45,45,45	0
23	MG	A	1594	1/1	0.32	-	45,45,45,45	0
23	MG	A	211	1/1	0.24	-	45,45,45,45	0
23	MG	A	1606	1/1	0.50	-	45,45,45,45	0
23	MG	A	1568	1/1	0.66	-	45,45,45,45	0
23	MG	A	1581	1/1	0.24	-	45,45,45,45	1
23	MG	A	1546	1/1	0.34	-	45,45,45,45	0
23	MG	A	1586	1/1	0.45	-	45,45,45,45	0
23	MG	A	1569	1/1	0.74	-	45,45,45,45	1
23	MG	A	1571	1/1	0.22	-	45,45,45,45	0
23	MG	A	1624	1/1	0.49	-	45,45,45,45	1
23	MG	A	1572	1/1	0.49	-	45,45,45,45	0
23	MG	A	1622	1/1	0.64	-	45,45,45,45	1
23	MG	A	1614	1/1	0.32	-	45,45,45,45	0
23	MG	A	1573	1/1	0.50	-	45,45,45,45	0
23	MG	A	1604	1/1	0.15	-	45,45,45,45	1
23	MG	A	1617	1/1	0.19	-	45,45,45,45	1
23	MG	A	1582	1/1	0.23	-	45,45,45,45	1
23	MG	A	1585	1/1	0.30	-	45,45,45,45	1
23	MG	A	1564	1/1	0.20	-	45,45,45,45	0
23	MG	A	1551	1/1	0.36	-	45,45,45,45	0
23	MG	A	1619	1/1	0.17	-	45,45,45,45	1
23	MG	A	210	1/1	0.30	-	45,45,45,45	1
23	MG	A	1588	1/1	0.25	-	45,45,45,45	0
23	MG	A	1595	1/1	0.33	-	45,45,45,45	0
23	MG	A	212	1/1	0.54	-	45,45,45,45	1
23	MG	A	1600	1/1	0.40	-	45,45,45,45	0
23	MG	A	1559	1/1	0.37	-	45,45,45,45	0
23	MG	A	87	1/1	0.18	-	45,45,45,45	1
23	MG	A	1557	1/1	0.44	-	45,45,45,45	0
23	MG	A	1589	1/1	0.40	-	45,45,45,45	0
23	MG	A	1626	1/1	0.30	-	45,45,45,45	1
23	MG	A	1555	1/1	0.26	-	45,45,45,45	0
23	MG	A	1566	1/1	0.36	-	45,45,45,45	0
23	MG	A	1553	1/1	0.39	-	45,45,45,45	0
23	MG	A	1548	1/1	0.28	-	45,45,45,45	0
23	MG	A	1580	1/1	0.17	-	45,45,45,45	0
23	MG	A	1592	1/1	0.12	-	45,45,45,45	0
23	MG	A	1583	1/1	0.10	-	45,45,45,45	0
23	MG	A	1620	1/1	0.22	-	45,45,45,45	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.