



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:00 PM GMT

PDB ID : 4DUY  
Title : Crystal structure of the Thermus thermophilus 30S ribosomal subunit with a 16S rRNA mutation, U13C  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2012-02-22  
Resolution : 3.39 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.

---

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

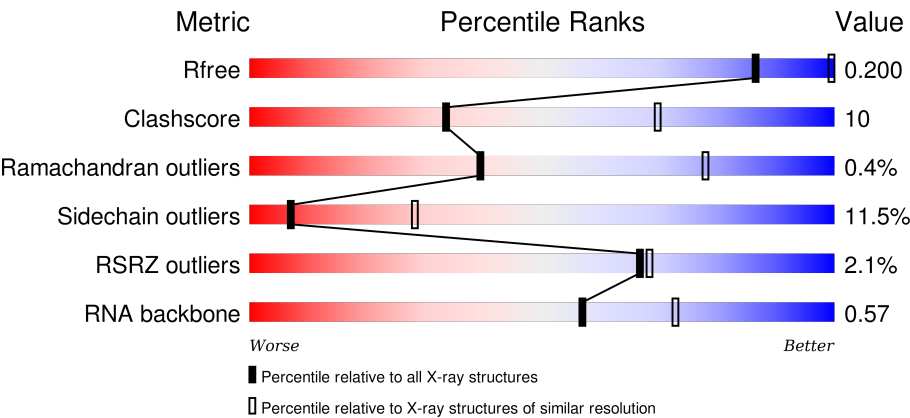
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.39 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.














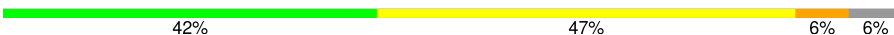





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1084 (3.46-3.30)
Clashscore	102246	1158 (3.46-3.30)
Ramachandran outliers	100387	1139 (3.46-3.30)
Sidechain outliers	100360	1138 (3.46-3.30)
RSRZ outliers	91569	1089 (3.46-3.30)
RNA backbone	2183	1024 (3.96-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	<div><div>1%</div><div>56%33%9%..</div></div>
2	B	256	<div><div>2%</div><div>59%28%.9%</div></div>
3	C	239	<div><div>3%</div><div>50%31%5%14%</div></div>
4	D	209	<div><div>3%</div><div>71%26%. .</div></div>

Continued on next page...

Continued from previous page...

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	

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
22	MG	A	1609	-	-	-	X
22	MG	A	1622	-	-	-	X
22	MG	A	1637	-	-	-	X
22	MG	A	1638	-	-	-	X
22	MG	A	1642	-	-	-	X
22	MG	A	1646	-	-	-	X
22	MG	A	1682	-	-	-	X
22	MG	A	1698	-	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1710	-	-	-	X
22	MG	A	1711	-	-	-	X
22	MG	A	1717	-	-	-	X
22	MG	A	1719	-	-	-	X
22	MG	A	1721	-	-	-	X
22	MG	A	1724	-	-	-	X
22	MG	A	1735	-	-	-	X
22	MG	A	1739	-	-	-	X
22	MG	A	1743	-	-	-	X
22	MG	A	1765	-	-	-	X
22	MG	A	1779	-	-	-	X
22	MG	A	1798	-	-	-	X
22	MG	A	1830	-	-	-	X
22	MG	A	1838	-	-	-	X
22	MG	A	1840	-	-	-	X
22	MG	A	1845	-	-	-	X
22	MG	A	1846	-	-	-	X
22	MG	A	1872	-	-	-	X
22	MG	A	1880	-	-	-	X
22	MG	B	301	-	-	-	X
22	MG	C	301	-	-	-	X
22	MG	D	302	-	-	-	X
22	MG	D	305	-	-	-	X
22	MG	J	201	-	-	-	X
22	MG	P	104	-	-	-	X
22	MG	S	101	-	-	-	X
23	ZN	D	301	-	-	-	X

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52584 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	1512	Total	C	N	O	P	0	6	0
			32644	14540	6040	10546	1518			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	C	U	ENGINEERED MUTATION	GB M26923.1
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

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

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called 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 ribosomal protein S5.

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

- Molecule 6 is a protein called 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 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 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 ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			972	612	195	163	2			

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	CONFLICT	UNP Q5SHP7

- Molecule 18 is a protein called ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called ribosomal protein S19.

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

- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	4	Total	Mg	0	0
			4	4		
22	G	1	Total	Mg	0	0
			1	1		
22	J	1	Total	Mg	0	0
			1	1		
22	Q	2	Total	Mg	0	0
			2	2		
22	D	4	Total	Mg	0	0
			4	4		
22	E	1	Total	Mg	0	0
			1	1		
22	B	2	Total	Mg	0	0
			2	2		
22	C	1	Total	Mg	0	0
			1	1		
22	A	293	Total	Mg	0	0
			293	293		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	N	1	Total 1	Mg 1	0	0
22	S	1	Total 1	Mg 1	0	0
22	F	1	Total 1	Mg 1	0	0

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	501	Total 501	O 501	0	0
24	D	3	Total 3	O 3	0	0
24	E	2	Total 2	O 2	0	0
24	J	3	Total 3	O 3	0	0
24	L	5	Total 5	O 5	0	0
24	M	9	Total 9	O 9	0	0
24	N	3	Total 3	O 3	0	0
24	P	7	Total 7	O 7	0	0
24	Q	1	Total 1	O 1	0	0
24	S	3	Total 3	O 3	0	0
24	T	1	Total 1	O 1	0	0

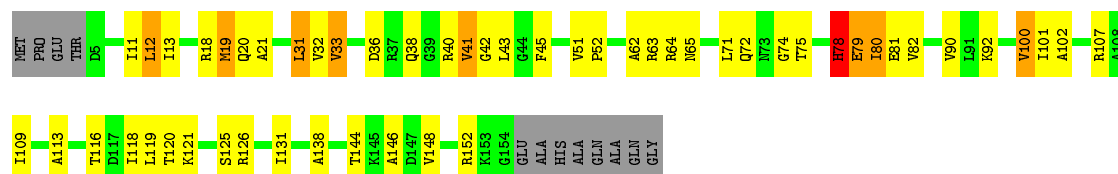






• Molecule 5: ribosomal protein S5

Chain E: 60% 27% 5% 7%



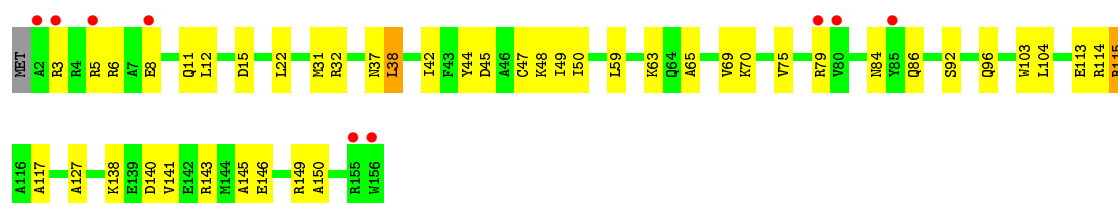
• Molecule 6: ribosomal protein S6

Chain F: 69% 27%



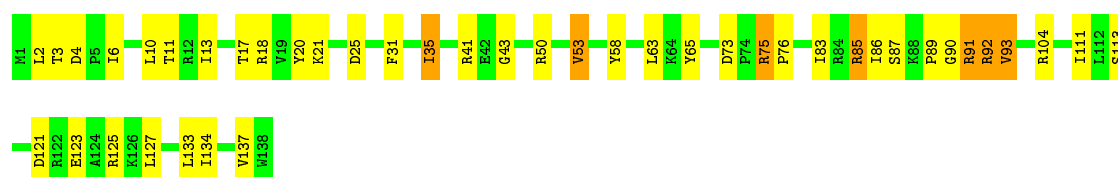
• Molecule 7: ribosomal protein S7

Chain G: 6% 71% 28%



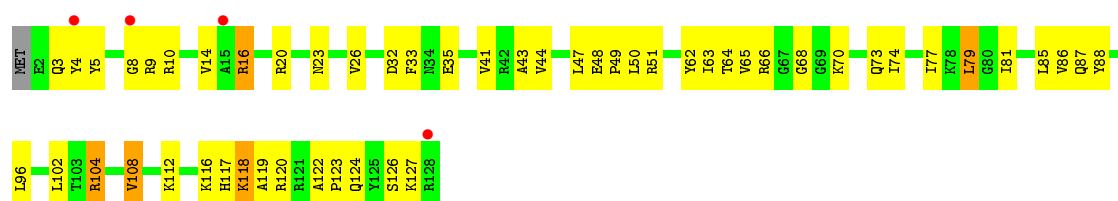
• Molecule 8: ribosomal protein S8

Chain H: 69% 26% 5%

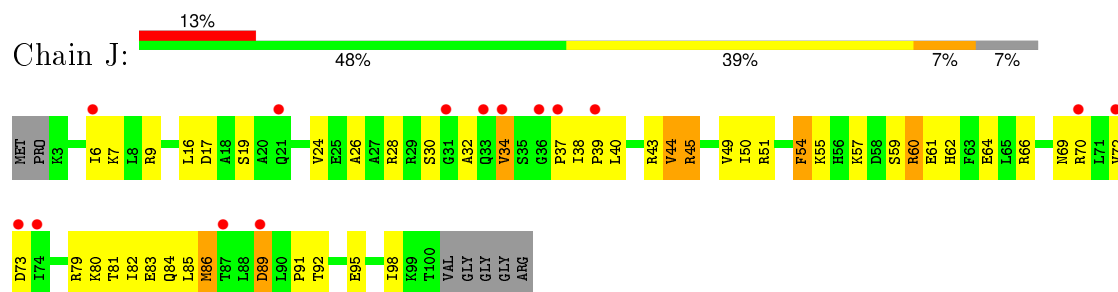


• Molecule 9: ribosomal protein S9

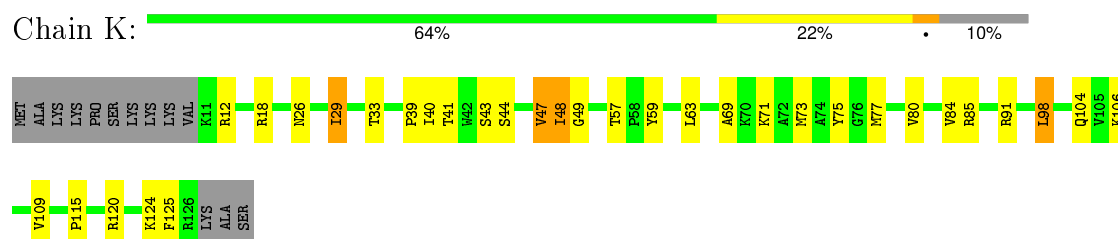
Chain I: 3% 58% 38%



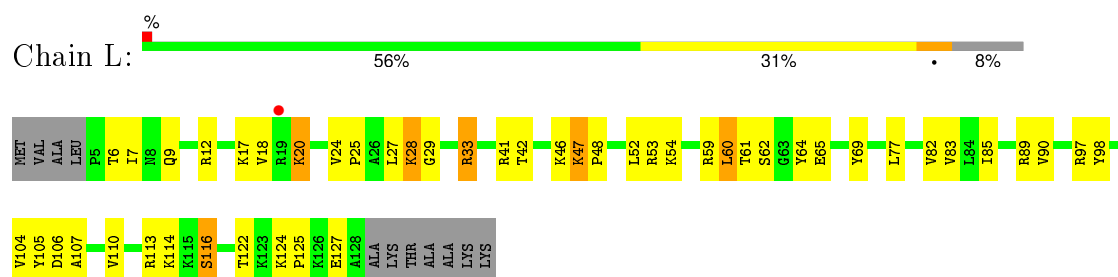
- Molecule 10: ribosomal protein S10



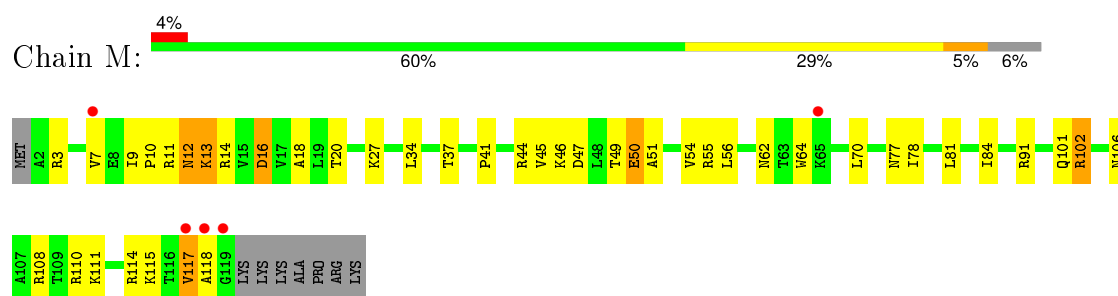
- Molecule 11: ribosomal protein S11



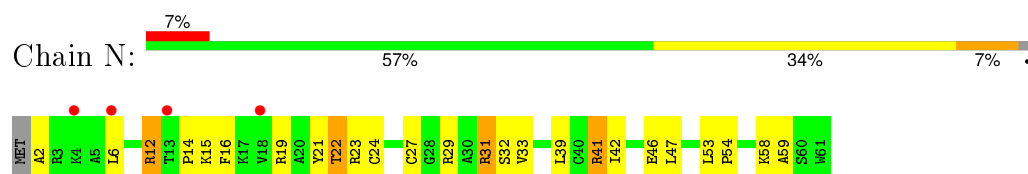
- Molecule 12: ribosomal protein S12



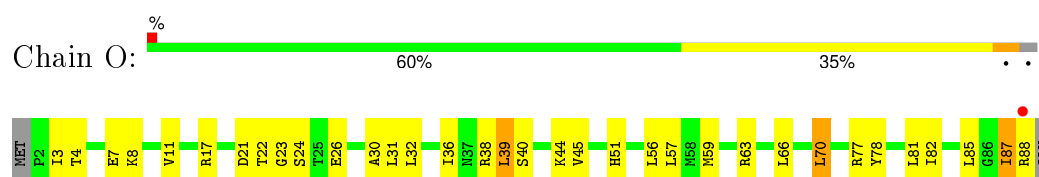
- Molecule 13: ribosomal protein S13



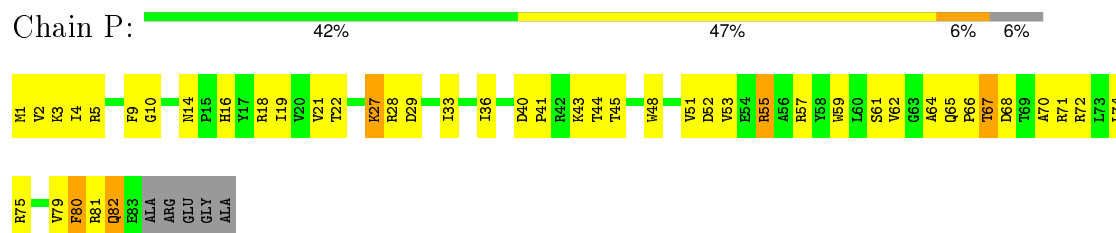
- Molecule 14: ribosomal protein S14



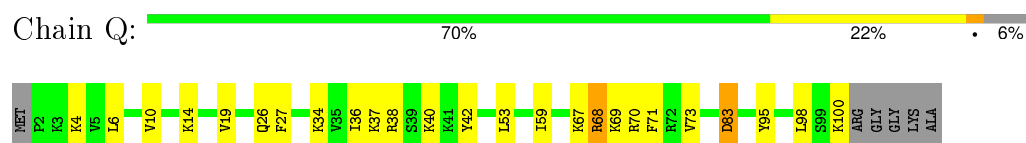
- Molecule 15: ribosomal protein S15



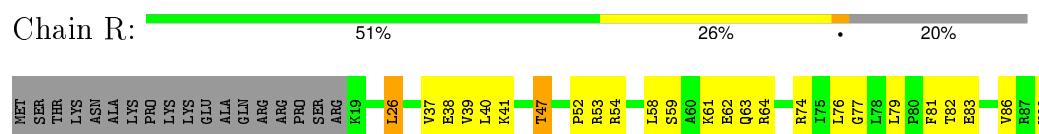
- Molecule 16: ribosomal protein S16



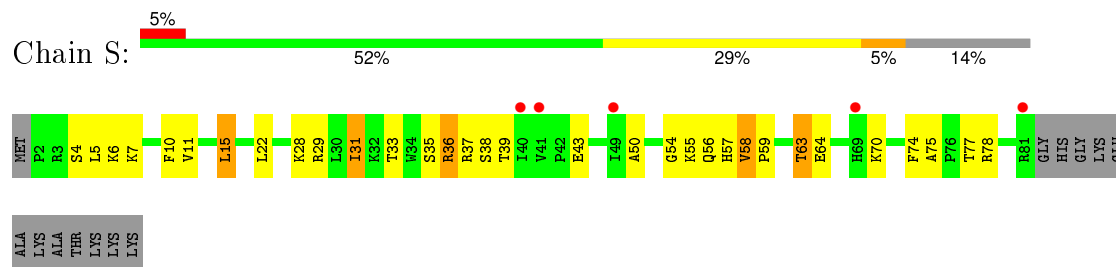
- Molecule 17: ribosomal protein S17



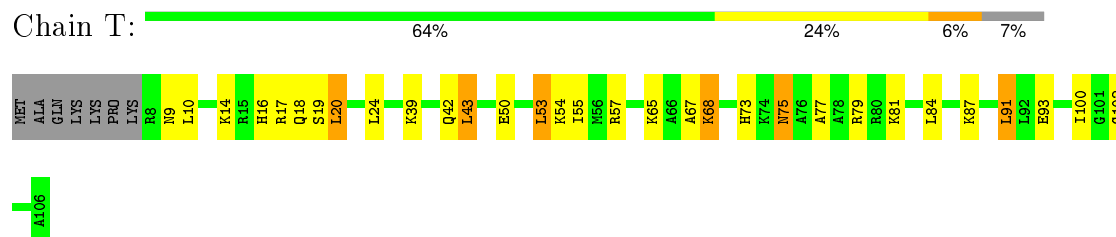
- Molecule 18: ribosomal protein S18



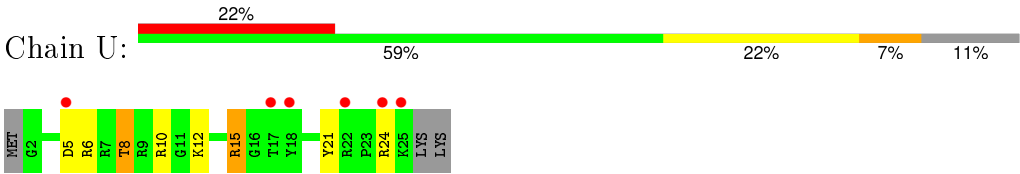
- Molecule 19: ribosomal protein S19



- Molecule 20: ribosomal protein S20



- Molecule 21: ribosomal protein THX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.52Å 402.52Å 175.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.87 – 3.39 34.87 – 3.39	Depositor EDS
% Data completeness (in resolution range)	97.0 (34.87-3.39) 96.8 (34.87-3.39)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 3.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, $R_{free}$	0.159 , 0.202 0.159 , 0.200	Depositor DCC
$R_{free}$ test set	9698 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	124.2	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 101.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 192862 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52584	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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	0.51	1/36139 (0.0%)	0.91	46/56396 (0.1%)
2	B	0.36	0/1935	0.62	0/2609
3	C	0.31	0/1636	0.55	0/2205
4	D	0.41	1/1733 (0.1%)	0.58	1/2318 (0.0%)
5	E	0.48	0/1162	0.72	1/1564 (0.1%)
6	F	0.30	0/856	0.53	0/1154
7	G	0.35	0/1276	0.54	0/1709
8	H	0.46	0/1136	0.66	0/1527
9	I	0.29	0/1029	0.53	0/1379
10	J	0.33	0/805	0.62	0/1082
11	K	0.37	0/879	0.60	0/1187
12	L	0.40	0/977	0.67	0/1306
13	M	0.32	0/947	0.56	0/1270
14	N	0.33	0/501	0.58	0/664
15	O	0.38	0/740	0.57	0/987
16	P	0.40	0/716	0.67	0/963
17	Q	0.43	0/836	0.66	0/1117
18	R	0.37	0/579	0.55	0/768
19	S	0.29	0/661	0.56	0/890
20	T	0.39	0/765	0.66	0/1007
21	U	0.30	0/212	0.53	0/277
All	All	0.47	2/55520 (0.0%)	0.83	48/82379 (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
2	B	0	1
3	C	0	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
8	H	0	1
10	J	0	1
20	T	0	1
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-6.74	1.33	1.37
4	D	12	CYS	CB-SG	5.31	1.91	1.82

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	U	C5-C6-N1	9.14	127.27	122.70
1	A	328	C	N1-C2-O2	8.92	124.25	118.90
1	A	328	C	N3-C2-O2	-8.29	116.10	121.90
1	A	117	G	N1-C6-O6	8.23	124.84	119.90
1	A	1136	U	C2-N1-C1'	8.22	127.57	117.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	HIS	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
5	E	78	HIS	Peptide
8	H	90	GLY	Peptide

## 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	32644	0	16508	437	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1900	0	1951	55	0
3	C	1612	0	1677	67	0
4	D	1703	0	1763	35	0
5	E	1146	0	1207	33	0
6	F	843	0	857	19	0
7	G	1257	0	1296	23	0
8	H	1116	0	1177	29	0
9	I	1010	0	1037	33	0
10	J	792	0	835	33	0
11	K	864	0	881	25	0
12	L	972	0	1058	34	0
13	M	937	0	995	24	0
14	N	492	0	529	20	0
15	O	729	0	768	20	0
16	P	700	0	720	36	0
17	Q	823	0	893	19	0
18	R	574	0	644	14	0
19	S	647	0	673	26	0
20	T	763	0	861	22	0
21	U	208	0	221	8	0
22	A	293	0	0	0	0
22	B	2	0	0	0	0
22	C	1	0	0	0	0
22	D	4	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	G	1	0	0	0	0
22	J	1	0	0	0	0
22	N	1	0	0	0	0
22	P	4	0	0	0	0
22	Q	2	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	501	0	0	12	0
24	D	3	0	0	0	0
24	E	2	0	0	0	0
24	J	3	0	0	1	0
24	L	5	0	0	0	0
24	M	9	0	0	1	0
24	N	3	0	0	0	0
24	P	7	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Q	1	0	0	0	0
24	S	3	0	0	0	0
24	T	1	0	0	0	0
All	All	52584	0	36551	889	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 10.

The worst 5 of 889 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:481:G:HO2'	1:A:482:A:H8	1.07	0.99
20:T:100:ILE:HG22	20:T:102:GLY:H	1.35	0.89
1:A:235:C:H5'	17:Q:70:ARG:HG3	1.54	0.89
1:A:664:G:H22	1:A:741:G:H1	1.20	0.87
1:A:427:U:OP1	4:D:13:ARG:NH2	2.13	0.82

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	208 (90%)	22 (10%)	2 (1%)	21	63
3	C	204/239 (85%)	178 (87%)	26 (13%)	0	100	100
4	D	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
5	E	148/162 (91%)	140 (95%)	8 (5%)	0	100	100
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	H	136/138 (99%)	131 (96%)	5 (4%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	I	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	24 65
10	J	96/105 (91%)	80 (83%)	13 (14%)	3 (3%)	5 35
11	K	114/129 (88%)	105 (92%)	9 (8%)	0	100 100
12	L	121/135 (90%)	108 (89%)	12 (10%)	1 (1%)	24 65
13	M	116/126 (92%)	99 (85%)	17 (15%)	0	100 100
14	N	58/61 (95%)	52 (90%)	6 (10%)	0	100 100
15	O	85/89 (96%)	78 (92%)	7 (8%)	0	100 100
16	P	81/88 (92%)	77 (95%)	4 (5%)	0	100 100
17	Q	97/105 (92%)	91 (94%)	6 (6%)	0	100 100
18	R	68/88 (77%)	65 (96%)	3 (4%)	0	100 100
19	S	78/93 (84%)	72 (92%)	5 (6%)	1 (1%)	15 54
20	T	97/106 (92%)	87 (90%)	10 (10%)	0	100 100
21	U	22/27 (82%)	21 (96%)	0	1 (4%)	3 25
All	All	2336/2541 (92%)	2147 (92%)	180 (8%)	9 (0%)	39 78

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
2	B	21	ARG
10	J	54	PHE
10	J	86	MET

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	202/220 (92%)	177 (88%)	25 (12%)	6 24
3	C	160/188 (85%)	137 (86%)	23 (14%)	4 18
4	D	180/181 (99%)	162 (90%)	18 (10%)	9 36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	115/123 (94%)	101 (88%)	14 (12%)	6	25
6	F	90/90 (100%)	81 (90%)	9 (10%)	9	36
7	G	126/127 (99%)	116 (92%)	10 (8%)	15	50
8	H	119/119 (100%)	109 (92%)	10 (8%)	14	47
9	I	98/99 (99%)	88 (90%)	10 (10%)	9	35
10	J	87/92 (95%)	79 (91%)	8 (9%)	11	40
11	K	88/99 (89%)	79 (90%)	9 (10%)	9	35
12	L	103/110 (94%)	90 (87%)	13 (13%)	5	23
13	M	94/101 (93%)	77 (82%)	17 (18%)	2	9
14	N	49/50 (98%)	44 (90%)	5 (10%)	9	35
15	O	79/80 (99%)	67 (85%)	12 (15%)	3	16
16	P	72/74 (97%)	63 (88%)	9 (12%)	6	24
17	Q	94/97 (97%)	89 (95%)	5 (5%)	28	66
18	R	61/77 (79%)	53 (87%)	8 (13%)	5	22
19	S	71/80 (89%)	63 (89%)	8 (11%)	7	29
20	T	76/82 (93%)	63 (83%)	13 (17%)	2	12
21	U	19/22 (86%)	17 (90%)	2 (10%)	8	33
All	All	1983/2111 (94%)	1755 (88%)	228 (12%)	7	28

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	63	LEU
11	K	18	ARG
19	S	43	GLU
8	H	91	ARG
9	I	108	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	HIS
16	P	82	GLN
3	C	108	ASN
2	B	204	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	O	46	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	258 (17%)	45 (2%)

5 of 258 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	13	C
1	A	14	U
1	A	32	A

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C
1	A	913	A
1	A	1346	A
1	A	792	A
1	A	960	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	2MG	A	1207	1	17,26,27	2.05	3 (17%)	21,38,41	2.16	3 (14%)
1	5MC	A	1400	1	13,22,23	0.97	1 (7%)	15,32,35	0.87	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4OC	A	1402	1	13,23,24	0.71	1 (7%)	18,32,35	0.64	0
1	5MC	A	1404	1	13,22,23	1.15	2 (15%)	15,32,35	0.86	1 (6%)
1	5MC	A	1407	1	13,22,23	1.11	1 (7%)	15,32,35	1.03	2 (13%)
1	UR3	A	1498	1	12,22,23	0.77	0	16,32,35	1.25	1 (6%)
1	MA6	A	1518[A]	1	16,26,27	0.77	0	18,38,41	1.11	2 (11%)
1	MA6	A	1518[B]	1	16,26,27	1.29	2 (12%)	18,38,41	1.08	2 (11%)
1	MA6	A	1519[A]	1	16,26,27	0.60	0	18,38,41	1.37	4 (22%)
1	MA6	A	1519[B]	1	16,26,27	1.31	2 (12%)	18,38,41	1.08	2 (11%)
1	PSU	A	1540	1	13,21,22	1.09	1 (7%)	18,30,33	3.84	6 (33%)
1	PSU	A	1541	1,22	13,21,22	1.09	1 (7%)	18,30,33	3.55	5 (27%)
1	PSU	A	516	1,22	13,21,22	1.11	1 (7%)	18,30,33	3.48	5 (27%)
1	7MG	A	527	1,22	19,26,27	2.40	4 (21%)	24,39,42	2.05	5 (20%)
1	M2G	A	966	1	17,27,28	1.74	4 (23%)	22,40,43	2.06	3 (13%)
1	5MC	A	967	1	13,22,23	1.00	1 (7%)	15,32,35	0.86	1 (6%)
12	0TD	L	92	12	4,9,10	0.89	0	4,11,13	2.64	2 (50%)

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
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	0/3/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/3/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[B]	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1,22	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1,22	-	0/7/37/38	0/3/3/3
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	5MC	A	967	1	-	0/3/25/26	0/2/2/2
12	0TD	L	92	12	-	0/2/12/14	0/0/0/0



The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-6.95	1.35	1.45
1	A	1402	4OC	C5-C4	2.03	1.44	1.39
1	A	967	5MC	C4-N4	2.06	1.39	1.34
1	A	1404	5MC	C6-N1	2.09	1.38	1.35
1	A	1400	5MC	C4-N4	2.22	1.39	1.34

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	N1-C2-N3	-14.01	119.39	128.33
1	A	1541	PSU	N1-C2-N3	-12.76	120.19	128.33
1	A	516	PSU	N1-C2-N3	-12.41	120.41	128.33
1	A	966	M2G	C5-C6-N1	-8.47	112.01	123.59
1	A	1207	2MG	C5-C6-N1	-7.67	113.11	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1400	5MC	1	0
1	A	1402	4OC	2	0
1	A	1498	UR3	4	0
1	A	1518[A]	MA6	2	0
1	A	1518[B]	MA6	4	0
1	A	1519[A]	MA6	3	0
1	A	1519[B]	MA6	3	0
1	A	966	M2G	1	0
1	A	967	5MC	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 314 ligands modelled in this entry, 314 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 ⓘ

### 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	1498/1522 (98%)	-0.29	14 (0%) 85 88	80, 123, 244, 351	0
2	B	234/256 (91%)	-0.21	6 (2%) 59 61	102, 150, 230, 265	0
3	C	206/239 (86%)	0.01	7 (3%) 49 50	131, 174, 221, 266	0
4	D	208/209 (99%)	-0.13	7 (3%) 49 50	94, 131, 181, 214	0
5	E	150/162 (92%)	-0.28	0 100 100	79, 107, 143, 177	0
6	F	101/101 (100%)	-0.49	0 100 100	114, 154, 176, 221	0
7	G	155/156 (99%)	-0.17	9 (5%) 26 28	109, 151, 196, 223	0
8	H	138/138 (100%)	-0.49	0 100 100	74, 99, 133, 155	0
9	I	127/128 (99%)	-0.01	4 (3%) 52 55	126, 180, 210, 231	0
10	J	98/105 (93%)	0.65	14 (14%) 4 4	153, 205, 281, 312	0
11	K	116/129 (89%)	-0.32	0 100 100	98, 123, 161, 180	0
12	L	123/135 (91%)	-0.18	1 (0%) 87 89	75, 130, 163, 197	0
13	M	118/126 (93%)	-0.15	5 (4%) 40 40	125, 155, 185, 290	0
14	N	60/61 (98%)	0.42	4 (6%) 21 22	140, 168, 203, 246	0
15	O	87/89 (97%)	-0.26	1 (1%) 82 84	86, 114, 161, 176	0
16	P	83/88 (94%)	-0.21	0 100 100	96, 124, 155, 205	0
17	Q	99/105 (94%)	-0.30	0 100 100	79, 115, 150, 179	0
18	R	70/88 (79%)	-0.30	0 100 100	95, 128, 181, 202	0
19	S	80/93 (86%)	0.29	5 (6%) 23 25	143, 197, 244, 249	0
20	T	99/106 (93%)	-0.38	0 100 100	96, 125, 168, 200	0
21	U	24/27 (88%)	1.33	6 (25%) 1 1	133, 151, 179, 212	0
All	All	3874/4063 (95%)	-0.20	83 (2%) 67 68	74, 136, 221, 351	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	6.4
4	D	35	ARG	6.2
21	U	18	TYR	5.6
1	A	1001	A	4.5
10	J	33	GLN	4.4

## 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
1	PSU	A	1541	20/21	0.89	0.30	-	157,174,186,187	0
1	PSU	A	516	20/21	0.96	0.10	-	135,141,155,161	0
1	M2G	A	966	25/26	0.96	0.14	-	122,138,155,161	0
1	UR3	A	1498	21/22	0.96	0.20	-	95,109,121,123	0
1	MA6	A	1518[B]	24/25	0.94	0.27	-	97,103,122,125	24
1	7MG	A	527	24/25	0.98	0.14	-	103,114,125,127	0
1	5MC	A	1407	21/22	0.97	0.20	-	111,137,143,147	0
1	5MC	A	1400	21/22	0.95	0.18	-	93,108,127,129	0
1	4OC	A	1402	22/23	0.98	0.17	-	103,111,141,148	0
12	0TD	L	92	10/11	0.97	0.40	-	111,120,126,312	0
1	MA6	A	1518[A]	24/25	0.94	0.27	-	96,100,103,110	24
1	5MC	A	1404	21/22	0.96	0.16	-	104,112,121,126	0
1	PSU	A	1540	20/21	0.85	0.49	-	184,209,213,215	0
1	MA6	A	1519[B]	24/25	0.96	0.28	-	90,98,101,105	24
1	MA6	A	1519[A]	24/25	0.96	0.28	-	91,98,105,112	24
1	2MG	A	1207	24/25	0.95	0.11	-	165,172,180,183	0
1	5MC	A	967	21/22	0.97	0.13	-	117,132,145,150	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
22	MG	A	1719	1/1	0.74	0.59	28.33	105,105,105,105	0
22	MG	A	1880	1/1	0.62	0.51	27.11	104,104,104,104	0
22	MG	A	1739	1/1	0.69	0.47	23.08	95,95,95,95	0
22	MG	A	1622	1/1	0.97	0.81	20.61	67,67,67,67	0
22	MG	A	1798	1/1	0.86	0.54	20.23	297,297,297,297	0
22	MG	A	1845	1/1	0.48	0.73	17.67	389,389,389,389	0
22	MG	A	1717	1/1	0.94	0.42	14.11	72,72,72,72	0
22	MG	A	1642	1/1	0.98	0.54	10.91	130,130,130,130	0
22	MG	A	1638	1/1	0.76	0.87	10.73	106,106,106,106	0
22	MG	A	1840	1/1	0.89	0.82	10.34	200,200,200,200	0
22	MG	A	1765	1/1	0.76	0.23	8.81	193,193,193,193	0
22	MG	A	1830	1/1	0.91	0.36	7.99	297,297,297,297	0
22	MG	A	1724	1/1	0.63	0.39	7.87	99,99,99,99	0
22	MG	D	302	1/1	0.98	0.49	7.80	90,90,90,90	0
22	MG	S	101	1/1	0.85	0.69	6.69	136,136,136,136	0
22	MG	A	1646	1/1	0.93	0.28	6.49	102,102,102,102	0
22	MG	A	1721	1/1	0.97	0.29	6.07	109,109,109,109	0
22	MG	P	104	1/1	0.56	0.63	6.03	136,136,136,136	0
22	MG	A	1711	1/1	0.85	0.33	5.69	117,117,117,117	0
22	MG	J	201	1/1	0.76	0.56	5.67	360,360,360,360	0
22	MG	D	305	1/1	0.77	0.37	5.50	107,107,107,107	0
22	MG	A	1698	1/1	0.79	0.44	5.05	120,120,120,120	0
22	MG	A	1710	1/1	0.93	0.23	4.70	85,85,85,85	0
22	MG	A	1779	1/1	0.97	0.31	4.46	101,101,101,101	0
22	MG	A	1609	1/1	0.99	0.31	4.36	103,103,103,103	0
22	MG	A	1846	1/1	0.96	0.24	4.21	222,222,222,222	0
22	MG	A	1735	1/1	0.90	0.32	3.42	96,96,96,96	0
22	MG	B	301	1/1	0.91	0.24	3.16	117,117,117,117	0
22	MG	A	1872	1/1	0.79	0.24	3.03	91,91,91,91	0
22	MG	A	1743	1/1	0.98	0.50	3.00	92,92,92,92	0
22	MG	A	1682	1/1	0.98	0.24	2.65	122,122,122,122	0
22	MG	C	301	1/1	0.98	0.44	2.38	169,169,169,169	0
22	MG	A	1637	1/1	0.66	0.22	2.26	110,110,110,110	0
22	MG	A	1838	1/1	0.87	0.33	2.01	354,354,354,354	0
22	MG	A	1703	1/1	0.87	0.21	1.65	94,94,94,94	0
22	MG	A	1733	1/1	0.97	0.21	1.57	102,102,102,102	0
22	MG	A	1729	1/1	0.94	0.15	1.47	67,67,67,67	0
22	MG	A	1775	1/1	0.93	0.27	1.45	107,107,107,107	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1725	1/1	0.88	0.34	1.25	128,128,128,128	0
22	MG	N	102	1/1	0.84	0.35	1.21	129,129,129,129	0
22	MG	A	1859	1/1	0.96	0.28	1.21	267,267,267,267	0
22	MG	A	1681	1/1	0.97	0.17	1.16	146,146,146,146	0
22	MG	B	302	1/1	0.89	0.20	1.13	147,147,147,147	0
22	MG	A	1674	1/1	0.89	0.21	1.11	161,161,161,161	0
23	ZN	D	301	1/1	0.99	0.41	1.08	118,118,118,118	0
22	MG	A	1693	1/1	0.97	0.22	0.95	101,101,101,101	0
22	MG	A	1714	1/1	0.96	0.26	0.87	97,97,97,97	0
22	MG	A	1695	1/1	0.94	0.28	0.54	104,104,104,104	0
22	MG	G	201	1/1	0.81	0.21	0.41	121,121,121,121	0
22	MG	A	1843	1/1	0.98	0.20	0.37	401,401,401,401	0
22	MG	A	1773	1/1	0.93	0.33	0.36	151,151,151,151	0
23	ZN	N	101	1/1	0.97	0.19	0.09	160,160,160,160	0
22	MG	A	1818	1/1	0.96	0.20	0.04	242,242,242,242	0
22	MG	A	1639	1/1	0.96	0.15	0.02	204,204,204,204	0
22	MG	A	1704	1/1	0.89	0.17	-0.05	110,110,110,110	0
22	MG	A	1620	1/1	0.97	0.18	-0.25	86,86,86,86	0
22	MG	A	1659	1/1	0.86	0.14	-0.42	168,168,168,168	0
22	MG	A	1772	1/1	0.83	0.12	-0.48	134,134,134,134	0
22	MG	A	1635	1/1	0.98	0.16	-0.49	90,90,90,90	0
22	MG	A	1615	1/1	0.98	0.16	-0.50	72,72,72,72	0
22	MG	A	1763	1/1	0.96	0.18	-0.52	110,110,110,110	0
22	MG	A	1831	1/1	0.95	0.16	-0.61	288,288,288,288	0
22	MG	A	1761	1/1	0.96	0.12	-0.65	98,98,98,98	0
22	MG	A	1752	1/1	0.98	0.13	-0.81	91,91,91,91	0
22	MG	Q	201	1/1	0.96	0.13	-1.00	103,103,103,103	0
22	MG	A	1697	1/1	0.97	0.14	-1.13	101,101,101,101	0
22	MG	A	1688	1/1	0.94	0.10	-1.31	130,130,130,130	0
22	MG	A	1867	1/1	0.97	0.09	-1.32	115,115,115,115	0
22	MG	D	303	1/1	0.98	0.09	-1.54	98,98,98,98	0
22	MG	A	1630	1/1	0.94	0.12	-1.64	103,103,103,103	0
22	MG	A	1634	1/1	0.92	0.14	-1.69	174,174,174,174	0
22	MG	A	1654	1/1	0.99	0.12	-2.17	92,92,92,92	0
22	MG	A	1764	1/1	0.98	0.09	-2.48	113,113,113,113	0
22	MG	A	1742	1/1	0.99	0.07	-4.40	94,94,94,94	0
22	MG	A	1627	1/1	0.99	0.09	-4.64	84,84,84,84	0
22	MG	A	1747	1/1	0.95	0.33	-	100,100,100,100	0
22	MG	A	1866	1/1	0.97	0.26	-	110,110,110,110	0
22	MG	A	1692	1/1	0.96	0.23	-	352,352,352,352	0
22	MG	A	1707	1/1	0.96	0.17	-	69,69,69,69	0
22	MG	A	1796	1/1	0.93	0.33	-	235,235,235,235	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1601	1/1	0.97	0.34	-	112,112,112,112	0
22	MG	A	1832	1/1	0.91	0.35	-	267,267,267,267	0
22	MG	A	1709	1/1	0.83	0.14	-	259,259,259,259	0
22	MG	A	1889	1/1	0.96	0.09	-	100,100,100,100	0
22	MG	A	1855	1/1	0.94	0.18	-	173,173,173,173	0
22	MG	A	1699	1/1	0.84	0.38	-	216,216,216,216	0
22	MG	A	1815	1/1	0.96	0.44	-	147,147,147,147	0
22	MG	A	1804	1/1	0.84	1.23	-	313,313,313,313	0
22	MG	A	1737	1/1	0.95	0.26	-	138,138,138,138	0
22	MG	A	1802	1/1	0.91	0.11	-	324,324,324,324	0
22	MG	A	1667	1/1	0.92	0.25	-	110,110,110,110	0
22	MG	A	1852	1/1	0.94	0.20	-	309,309,309,309	0
22	MG	A	1647	1/1	0.96	0.25	-	92,92,92,92	0
22	MG	A	1886	1/1	0.94	0.17	-	94,94,94,94	0
22	MG	A	1643	1/1	0.94	0.52	-	128,128,128,128	0
22	MG	A	1690	1/1	0.88	0.17	-	126,126,126,126	0
22	MG	E	201	1/1	0.98	0.15	-	118,118,118,118	0
22	MG	A	1661	1/1	0.92	0.21	-	137,137,137,137	0
22	MG	A	1700	1/1	0.90	0.15	-	223,223,223,223	0
22	MG	A	1683	1/1	0.89	0.20	-	111,111,111,111	0
22	MG	A	1727	1/1	0.95	0.47	-	114,114,114,114	0
22	MG	A	1605	1/1	0.99	0.08	-	105,105,105,105	0
22	MG	A	1884	1/1	0.64	1.36	-	113,113,113,113	0
22	MG	A	1645	1/1	0.93	0.19	-	65,65,65,65	0
22	MG	A	1629	1/1	1.00	0.36	-	139,139,139,139	0
22	MG	A	1789	1/1	0.96	0.08	-	229,229,229,229	0
22	MG	A	1810	1/1	0.82	0.37	-	273,273,273,273	0
22	MG	A	1875	1/1	0.93	0.24	-	99,99,99,99	0
22	MG	A	1834	1/1	0.82	0.21	-	315,315,315,315	0
22	MG	A	1691	1/1	0.84	0.26	-	115,115,115,115	0
22	MG	A	1756	1/1	0.72	0.51	-	128,128,128,128	0
22	MG	A	1602	1/1	0.91	0.09	-	108,108,108,108	0
22	MG	A	1806	1/1	0.87	0.23	-	232,232,232,232	0
22	MG	A	1893	1/1	0.89	0.19	-	118,118,118,118	0
22	MG	A	1778	1/1	0.97	0.15	-	135,135,135,135	0
22	MG	A	1788	1/1	0.95	0.21	-	365,365,365,365	0
22	MG	A	1650	1/1	0.99	0.24	-	99,99,99,99	0
22	MG	A	1748	1/1	0.93	0.17	-	114,114,114,114	0
22	MG	A	1633	1/1	0.93	0.46	-	105,105,105,105	0
22	MG	A	1887	1/1	0.50	0.37	-	108,108,108,108	0
22	MG	A	1616	1/1	0.91	0.30	-	125,125,125,125	0
22	MG	A	1797	1/1	0.94	0.24	-	272,272,272,272	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1754	1/1	0.92	0.31	-	151,151,151,151	0
22	MG	A	1663	1/1	0.82	0.17	-	102,102,102,102	0
22	MG	A	1660	1/1	0.99	0.09	-	112,112,112,112	0
22	MG	A	1701	1/1	0.87	0.60	-	134,134,134,134	0
22	MG	Q	202	1/1	0.63	0.76	-	101,101,101,101	0
22	MG	A	1720	1/1	0.94	0.17	-	122,122,122,122	0
22	MG	A	1716	1/1	0.96	0.34	-	80,80,80,80	0
22	MG	A	1873	1/1	0.75	0.60	-	125,125,125,125	0
22	MG	A	1816	1/1	0.99	0.14	-	57,57,57,57	0
22	MG	A	1715	1/1	0.84	0.42	-	116,116,116,116	0
22	MG	A	1628	1/1	0.76	1.20	-	111,111,111,111	0
22	MG	A	1833	1/1	0.94	0.24	-	207,207,207,207	0
22	MG	A	1680	1/1	0.98	0.41	-	144,144,144,144	0
22	MG	A	1822	1/1	0.89	0.19	-	290,290,290,290	0
22	MG	A	1676	1/1	0.98	0.04	-	132,132,132,132	0
22	MG	A	1658	1/1	0.98	0.14	-	134,134,134,134	0
22	MG	A	1617	1/1	0.99	0.26	-	116,116,116,116	0
22	MG	A	1612	1/1	0.94	0.09	-	113,113,113,113	0
22	MG	P	103	1/1	0.97	0.29	-	220,220,220,220	0
22	MG	A	1750	1/1	0.85	0.30	-	119,119,119,119	0
22	MG	A	1824	1/1	0.96	0.08	-	177,177,177,177	0
22	MG	A	1814	1/1	0.84	0.30	-	240,240,240,240	0
22	MG	A	1809	1/1	0.91	0.17	-	169,169,169,169	0
22	MG	A	1758	1/1	0.81	0.81	-	110,110,110,110	0
22	MG	A	1631	1/1	0.99	0.11	-	95,95,95,95	0
22	MG	A	1885	1/1	0.91	0.62	-	124,124,124,124	0
22	MG	A	1745	1/1	0.57	0.88	-	130,130,130,130	0
22	MG	A	1656	1/1	0.79	0.47	-	94,94,94,94	0
22	MG	A	1807	1/1	0.86	0.26	-	200,200,200,200	0
22	MG	A	1856	1/1	0.80	0.40	-	205,205,205,205	0
22	MG	A	1759	1/1	0.89	0.25	-	154,154,154,154	0
22	MG	A	1746	1/1	0.86	0.33	-	107,107,107,107	0
22	MG	A	1678	1/1	0.90	0.28	-	140,140,140,140	0
22	MG	A	1863	1/1	0.69	0.15	-	137,137,137,137	0
22	MG	A	1878	1/1	0.87	0.40	-	107,107,107,107	0
22	MG	A	1864	1/1	0.91	0.15	-	155,155,155,155	0
22	MG	A	1708	1/1	0.98	0.07	-	124,124,124,124	0
22	MG	A	1784	1/1	0.95	0.38	-	324,324,324,324	0
22	MG	A	1664	1/1	0.94	0.07	-	90,90,90,90	0
22	MG	A	1734	1/1	0.97	0.26	-	84,84,84,84	0
22	MG	A	1673	1/1	0.92	0.15	-	208,208,208,208	0
22	MG	A	1762	1/1	0.75	0.21	-	152,152,152,152	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1774	1/1	0.99	0.23	-	190,190,190,190	0
22	MG	A	1610	1/1	0.97	0.16	-	172,172,172,172	0
22	MG	A	1705	1/1	0.84	0.54	-	120,120,120,120	0
22	MG	A	1841	1/1	0.97	0.17	-	278,278,278,278	0
22	MG	A	1621	1/1	0.95	0.22	-	99,99,99,99	0
22	MG	A	1783	1/1	0.88	0.29	-	224,224,224,224	0
22	MG	A	1625	1/1	0.94	0.47	-	120,120,120,120	0
22	MG	A	1741	1/1	0.76	0.35	-	114,114,114,114	0
22	MG	A	1861	1/1	0.96	0.18	-	182,182,182,182	0
22	MG	A	1812	1/1	0.89	0.82	-	401,401,401,401	0
22	MG	A	1844	1/1	0.90	0.19	-	309,309,309,309	0
22	MG	A	1792	1/1	0.96	0.17	-	312,312,312,312	0
22	MG	A	1836	1/1	0.96	0.20	-	228,228,228,228	0
22	MG	A	1648	1/1	0.98	0.30	-	157,157,157,157	0
22	MG	A	1793	1/1	0.97	0.12	-	159,159,159,159	0
22	MG	A	1624	1/1	0.72	0.54	-	114,114,114,114	0
22	MG	A	1821	1/1	0.95	0.24	-	230,230,230,230	0
22	MG	A	1623	1/1	0.98	0.16	-	118,118,118,118	0
22	MG	A	1603	1/1	0.96	0.20	-	109,109,109,109	0
22	MG	A	1768	1/1	0.75	0.74	-	224,224,224,224	0
22	MG	A	1771	1/1	0.77	0.45	-	138,138,138,138	0
22	MG	A	1751	1/1	0.55	0.50	-	116,116,116,116	0
22	MG	A	1675	1/1	0.51	0.33	-	119,119,119,119	0
22	MG	A	1740	1/1	0.89	0.49	-	112,112,112,112	0
22	MG	A	1826	1/1	0.96	0.27	-	235,235,235,235	0
22	MG	A	1882	1/1	0.39	1.16	-	111,111,111,111	0
22	MG	F	201	1/1	0.98	0.43	-	131,131,131,131	0
22	MG	A	1685	1/1	0.98	0.10	-	97,97,97,97	0
22	MG	A	1817	1/1	0.83	0.31	-	264,264,264,264	0
22	MG	A	1881	1/1	0.82	0.38	-	88,88,88,88	0
22	MG	A	1819	1/1	0.94	0.28	-	330,330,330,330	0
22	MG	A	1677	1/1	0.97	0.68	-	185,185,185,185	0
22	MG	A	1870	1/1	0.91	0.10	-	138,138,138,138	0
22	MG	A	1604	1/1	0.94	0.87	-	113,113,113,113	0
22	MG	A	1791	1/1	0.83	0.09	-	313,313,313,313	0
22	MG	A	1644	1/1	0.97	0.32	-	114,114,114,114	0
22	MG	A	1626	1/1	0.93	0.24	-	106,106,106,106	0
22	MG	A	1608	1/1	0.91	0.23	-	93,93,93,93	0
22	MG	A	1757	1/1	0.91	0.24	-	99,99,99,99	0
22	MG	A	1777	1/1	0.91	0.14	-	104,104,104,104	0
22	MG	A	1766	1/1	0.97	0.11	-	195,195,195,195	0
22	MG	A	1636	1/1	0.97	0.14	-	120,120,120,120	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1671	1/1	0.98	0.48	-	108,108,108,108	0
22	MG	A	1876	1/1	0.97	0.58	-	138,138,138,138	0
22	MG	A	1813	1/1	0.95	0.22	-	326,326,326,326	0
22	MG	A	1823	1/1	0.96	0.25	-	246,246,246,246	0
22	MG	A	1749	1/1	0.96	0.26	-	108,108,108,108	0
22	MG	A	1770	1/1	0.95	0.16	-	120,120,120,120	0
22	MG	P	102	1/1	0.87	0.16	-	128,128,128,128	0
22	MG	A	1652	1/1	0.85	0.36	-	122,122,122,122	0
22	MG	A	1871	1/1	0.92	0.65	-	136,136,136,136	0
22	MG	A	1851	1/1	0.97	0.35	-	286,286,286,286	0
22	MG	A	1632	1/1	0.99	0.40	-	88,88,88,88	0
22	MG	A	1614	1/1	0.79	0.38	-	134,134,134,134	0
22	MG	A	1803	1/1	0.95	0.19	-	206,206,206,206	0
22	MG	A	1689	1/1	0.83	0.38	-	118,118,118,118	0
22	MG	A	1795	1/1	0.82	0.38	-	321,321,321,321	0
22	MG	A	1686	1/1	0.78	0.90	-	103,103,103,103	0
22	MG	A	1883	1/1	0.64	0.33	-	117,117,117,117	0
22	MG	A	1839	1/1	0.96	0.30	-	258,258,258,258	0
22	MG	A	1877	1/1	0.96	0.34	-	150,150,150,150	0
22	MG	A	1702	1/1	0.89	0.33	-	101,101,101,101	0
22	MG	A	1736	1/1	0.75	0.54	-	94,94,94,94	0
22	MG	A	1760	1/1	0.80	0.43	-	126,126,126,126	0
22	MG	A	1738	1/1	0.90	0.48	-	112,112,112,112	0
22	MG	A	1892	1/1	0.94	0.47	-	92,92,92,92	0
22	MG	A	1726	1/1	0.70	0.29	-	128,128,128,128	0
22	MG	A	1849	1/1	0.96	0.32	-	174,174,174,174	0
22	MG	A	1874	1/1	0.61	0.20	-	155,155,155,155	0
22	MG	A	1781	1/1	0.95	0.16	-	160,160,160,160	0
22	MG	A	1835	1/1	0.95	0.24	-	148,148,148,148	0
22	MG	A	1858	1/1	0.82	0.57	-	332,332,332,332	0
22	MG	A	1613	1/1	0.94	0.12	-	113,113,113,113	0
22	MG	A	1655	1/1	0.92	0.45	-	96,96,96,96	0
22	MG	A	1782	1/1	0.96	0.22	-	127,127,127,127	0
22	MG	A	1712	1/1	0.77	0.71	-	102,102,102,102	0
22	MG	A	1868	1/1	0.87	0.49	-	100,100,100,100	0
22	MG	A	1640	1/1	0.92	0.31	-	143,143,143,143	0
22	MG	A	1744	1/1	0.89	0.86	-	128,128,128,128	0
22	MG	A	1888	1/1	0.70	0.52	-	105,105,105,105	0
22	MG	A	1805	1/1	0.94	0.09	-	198,198,198,198	0
22	MG	A	1890	1/1	0.52	0.49	-	124,124,124,124	0
22	MG	A	1731	1/1	0.87	0.62	-	92,92,92,92	0
22	MG	A	1801	1/1	0.98	0.18	-	350,350,350,350	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1767	1/1	0.95	0.12	-	193,193,193,193	0
22	MG	A	1728	1/1	0.88	0.32	-	106,106,106,106	0
22	MG	A	1829	1/1	0.98	0.18	-	269,269,269,269	0
22	MG	A	1780	1/1	0.94	0.19	-	131,131,131,131	0
22	MG	A	1679	1/1	0.99	0.13	-	169,169,169,169	0
22	MG	A	1825	1/1	0.96	0.73	-	271,271,271,271	0
22	MG	A	1800	1/1	0.98	0.06	-	297,297,297,297	0
22	MG	P	101	1/1	0.87	0.39	-	90,90,90,90	0
22	MG	A	1649	1/1	0.95	0.37	-	121,121,121,121	0
22	MG	A	1785	1/1	0.92	0.28	-	242,242,242,242	0
22	MG	A	1706	1/1	0.98	0.26	-	128,128,128,128	0
22	MG	A	1879	1/1	0.85	0.28	-	107,107,107,107	0
22	MG	A	1827	1/1	0.96	0.14	-	393,393,393,393	0
22	MG	A	1662	1/1	0.81	0.23	-	109,109,109,109	0
22	MG	A	1786	1/1	0.98	0.39	-	310,310,310,310	0
22	MG	A	1869	1/1	0.94	0.30	-	129,129,129,129	0
22	MG	A	1799	1/1	0.95	0.16	-	185,185,185,185	0
22	MG	A	1653	1/1	0.59	0.27	-	120,120,120,120	0
22	MG	A	1669	1/1	0.84	0.34	-	158,158,158,158	0
22	MG	A	1730	1/1	0.82	0.69	-	117,117,117,117	0
22	MG	A	1696	1/1	0.96	0.70	-	150,150,150,150	0
22	MG	A	1606	1/1	0.87	0.09	-	143,143,143,143	0
22	MG	A	1755	1/1	0.96	0.15	-	96,96,96,96	0
22	MG	A	1776	1/1	0.86	0.13	-	118,118,118,118	0
22	MG	A	1723	1/1	0.98	0.16	-	122,122,122,122	0
22	MG	A	1850	1/1	0.85	0.17	-	333,333,333,333	0
22	MG	A	1651	1/1	0.98	0.27	-	149,149,149,149	0
22	MG	A	1820	1/1	0.91	0.19	-	320,320,320,320	0
22	MG	A	1787	1/1	0.96	0.14	-	260,260,260,260	0
22	MG	A	1847	1/1	0.98	0.12	-	269,269,269,269	0
22	MG	A	1607	1/1	0.98	0.40	-	101,101,101,101	0
22	MG	A	1811	1/1	0.96	0.14	-	325,325,325,325	0
22	MG	A	1808	1/1	0.87	0.61	-	242,242,242,242	0
22	MG	A	1641	1/1	0.99	0.21	-	151,151,151,151	0
22	MG	A	1853	1/1	0.93	0.15	-	333,333,333,333	0
22	MG	A	1790	1/1	0.95	0.09	-	138,138,138,138	0
22	MG	A	1618	1/1	0.96	0.61	-	124,124,124,124	0
22	MG	A	1657	1/1	0.93	0.22	-	124,124,124,124	0
22	MG	A	1794	1/1	0.91	0.24	-	346,346,346,346	0
22	MG	A	1862	1/1	0.96	0.89	-	130,130,130,130	0
22	MG	A	1828	1/1	0.85	0.46	-	310,310,310,310	0
22	MG	A	1865	1/1	0.88	0.31	-	118,118,118,118	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1672	1/1	0.95	0.08	-	147,147,147,147	0
22	MG	A	1684	1/1	0.98	0.15	-	128,128,128,128	0
22	MG	A	1619	1/1	0.90	0.50	-	123,123,123,123	0
22	MG	A	1694	1/1	0.93	0.16	-	152,152,152,152	0
22	MG	A	1769	1/1	0.94	0.18	-	193,193,193,193	0
22	MG	A	1854	1/1	0.97	0.10	-	251,251,251,251	0
22	MG	D	304	1/1	0.84	0.83	-	113,113,113,113	0
22	MG	A	1687	1/1	0.91	0.57	-	146,146,146,146	0
22	MG	A	1842	1/1	0.93	0.47	-	228,228,228,228	0
22	MG	A	1713	1/1	0.85	0.51	-	117,117,117,117	0
22	MG	A	1848	1/1	0.94	0.29	-	233,233,233,233	0
22	MG	A	1670	1/1	0.84	0.38	-	110,110,110,110	0
22	MG	A	1857	1/1	0.92	0.35	-	287,287,287,287	0
22	MG	A	1732	1/1	0.93	0.20	-	104,104,104,104	0
22	MG	A	1722	1/1	0.99	0.05	-	97,97,97,97	0
22	MG	A	1837	1/1	0.95	0.16	-	142,142,142,142	0
22	MG	A	1668	1/1	0.97	0.16	-	130,130,130,130	0
22	MG	A	1666	1/1	0.98	0.34	-	108,108,108,108	0
22	MG	A	1753	1/1	0.97	0.19	-	99,99,99,99	0
22	MG	A	1718	1/1	0.96	0.24	-	108,108,108,108	0
22	MG	A	1891	1/1	0.68	0.36	-	140,140,140,140	0
22	MG	A	1611	1/1	0.98	0.09	-	128,128,128,128	0
22	MG	A	1665	1/1	0.97	0.14	-	253,253,253,253	0
22	MG	A	1860	1/1	0.82	0.79	-	95,95,95,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.