



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:54 PM UTC

PDB ID : 4C3I / pdb_00004c3i
Title : Structure of 14-subunit RNA polymerase I at 3.0 Å resolution, crystal form C2-100
Authors : Fernandez-Tornero, C.; Moreno-Morcillo, M.; Rashid, U.J.; Taylor, N.M.I.; Ruiz, F.M.; Gruene, T.; Legrand, P.; Steuerwald, U.; Muller, C.W.
Deposited on : 2013-08-24
Resolution : 3.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

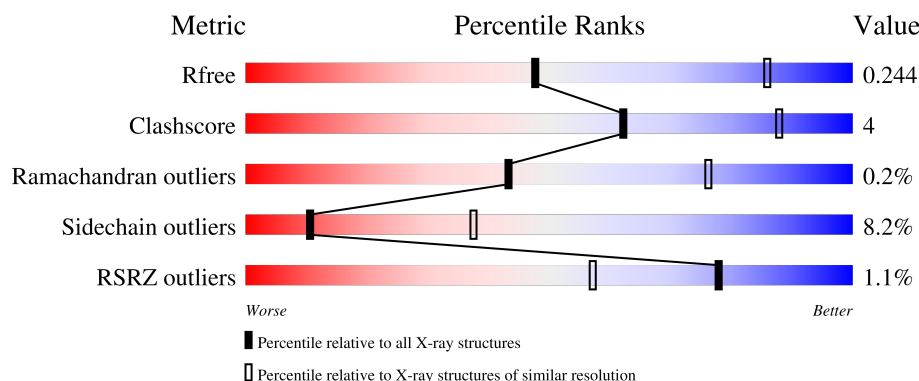
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	1664	% 73% 15% • 11%
2	B	1203	79% 17% • •
3	C	335	% 71% 19% • 9%
4	D	137	36% 7% 57%
5	E	215	87% 13%

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Mol	Chain	Length	Quality of chain
6	F	155	55%9%35%
7	G	326	2% 65%13%21%
8	H	146	% 77%14%8%
9	I	125	10% 77%22%
10	J	70	80%11%7%
11	K	142	58%13%27%
12	L	70	56%9%36%
13	M	415	% 21%75%
14	N	233	2% 52%7%40%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 34252 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 protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1484	Total	C	N	O	S	0	0	0
			11695	7388	2031	2213	63			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1176	Total	C	N	O	S	0	0	0
			9322	5898	1629	1745	50			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	304	Total	C	N	O	S	0	0	0
			2418	1536	414	460	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	59	Total	C	N	O	0	0	0
			466	292	80	94			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	12	SER	THR	conflict	UNP P50106

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	215	Total	C	N	O	S	0	0	0
			1759	1116	310	321	12			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			823	522	144	154	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	259	Total	C	N	O	S	0	0	0
			2052	1301	348	398	5			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1072	676	181	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	124	Total	C	N	O	S	0	0	0
			942	584	160	189	9			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	69	Total	C	N	O	S	0	0	0
			569	362	101	100	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUB-UNIT RPAC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	103	Total	C	N	O	S	0	0	0
			810	506	132	167	5			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	45	Total	C	N	O	S	0	0	0
			359	221	71	63	4			

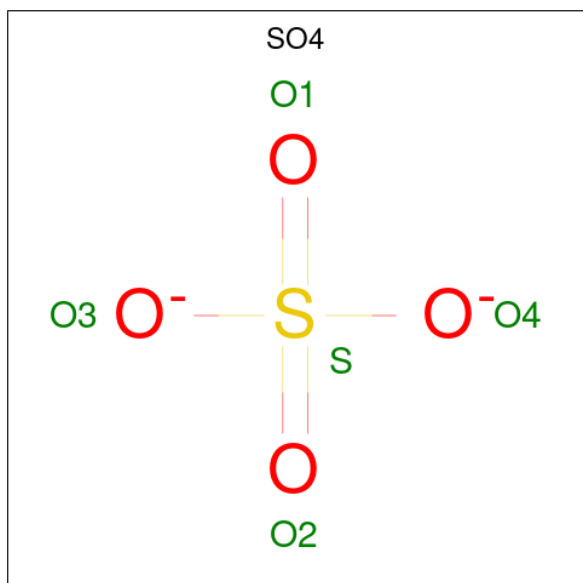
- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	105	Total	C	N	O	0	0	0
			831	528	137	166			

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	139	Total	C	N	O	S	0	0	0
			1103	706	179	214	4			

- Molecule 15 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	O	S	0	0
			5	4	1		
15	A	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		

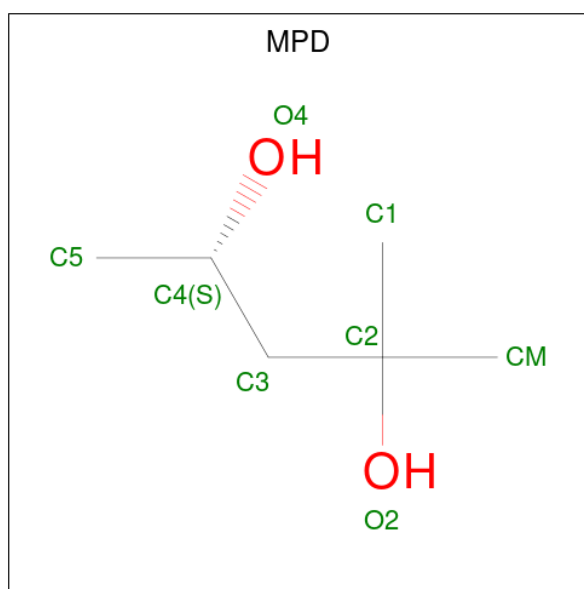
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total	Zn	0	0
			2	2		
16	B	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	J	1	Total	Zn	0	0
			1	1		
16	L	1	Total	Zn	0	0
			1	1		

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	1	Total	Mg	0	0
			1	1		

- Molecule 18 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).

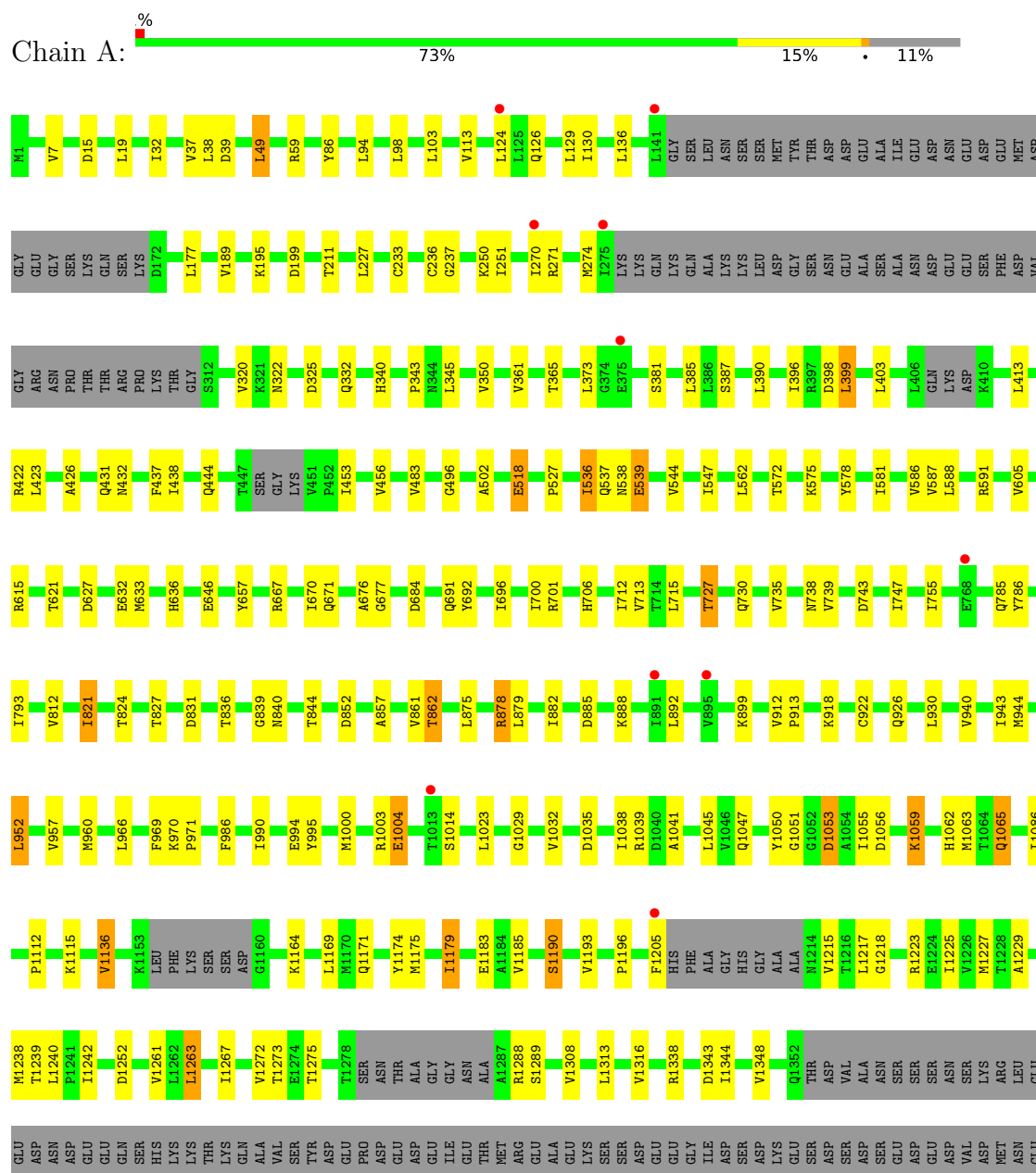


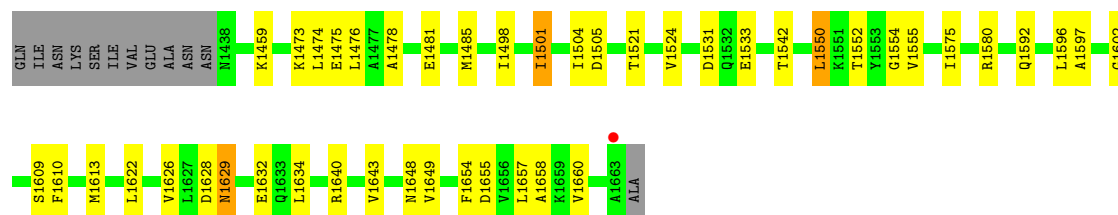
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	G	1	Total	C	O	0	0
			8	6	2		

3 Residue-property plots

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.

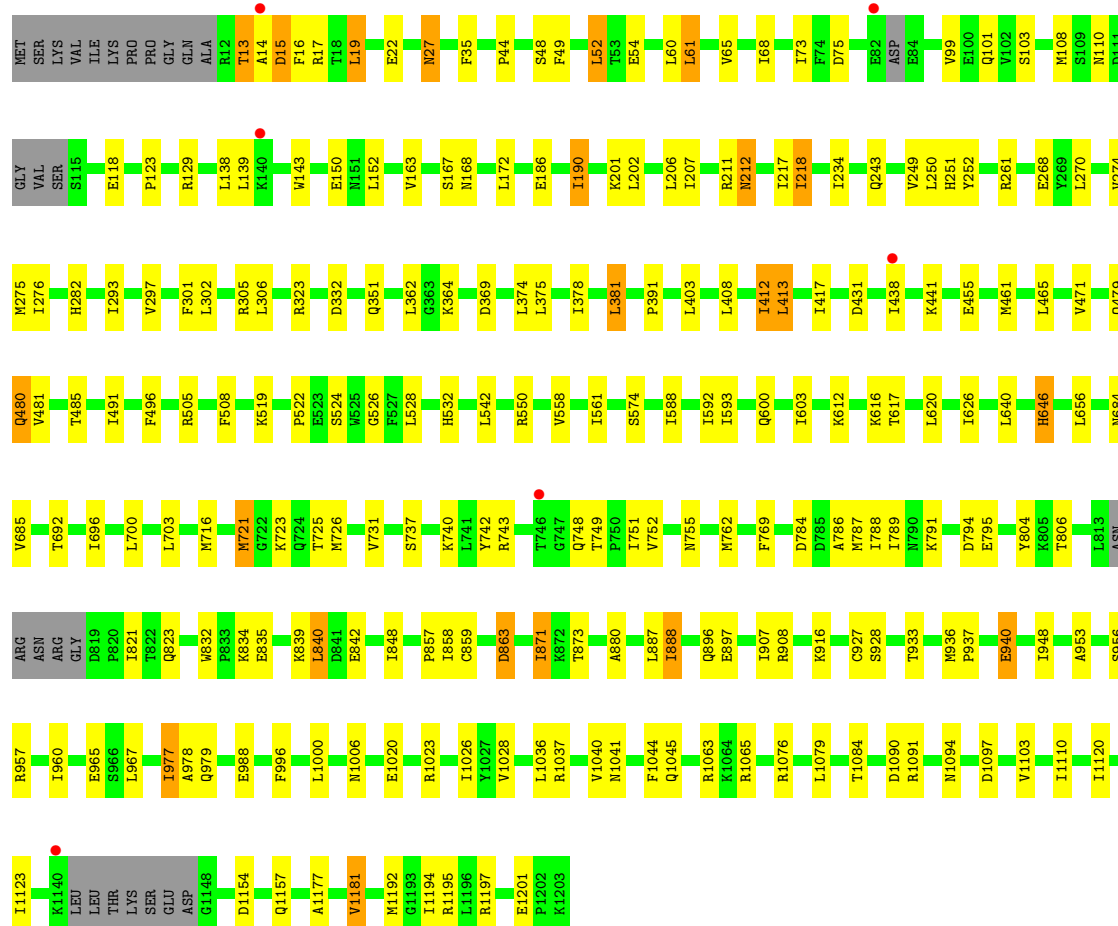
- Molecule 1: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190





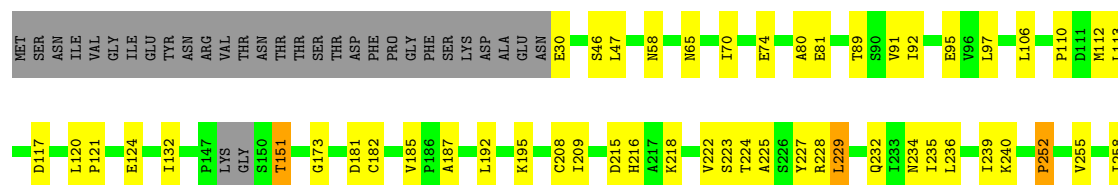
• Molecule 2: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135

Chain B: 79% 17% . .



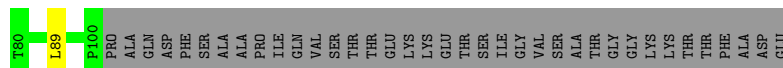
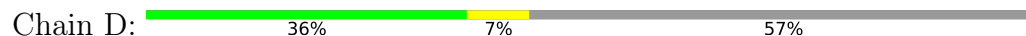
• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

Chain C: 71% 19% 9% . .





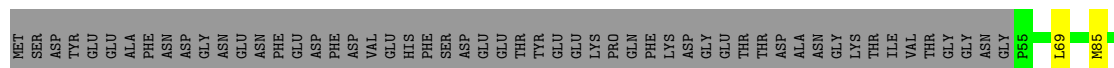
• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14



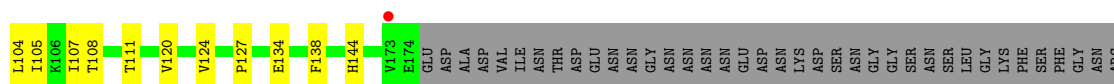
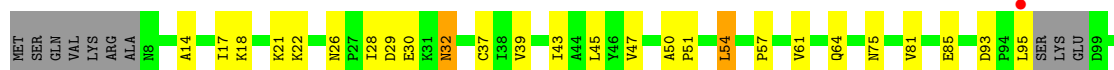
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



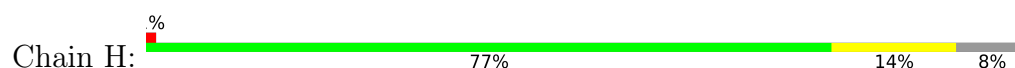
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

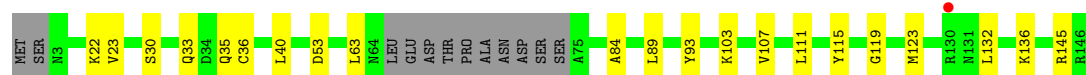


• Molecule 7: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

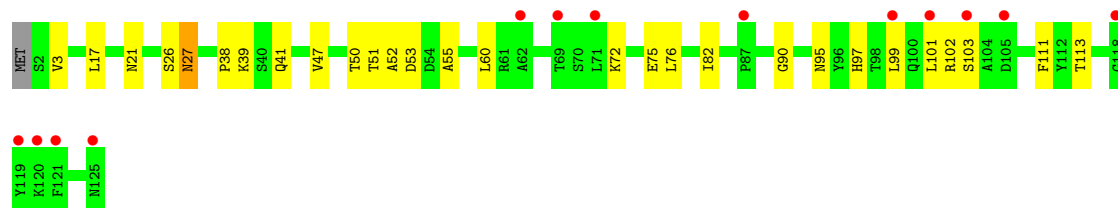
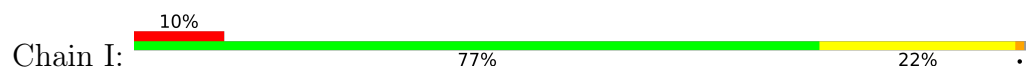


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

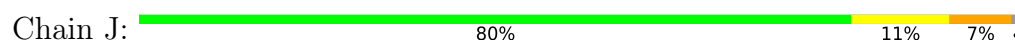




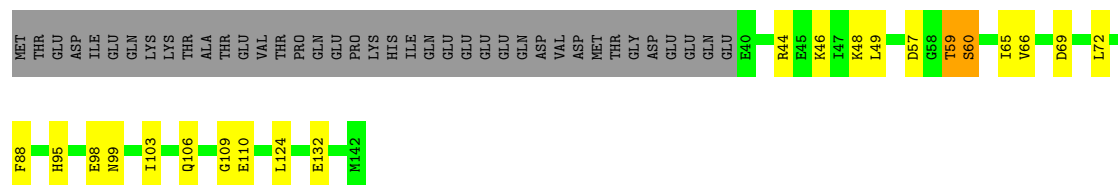
• Molecule 9: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12



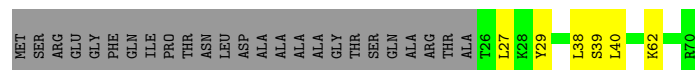
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



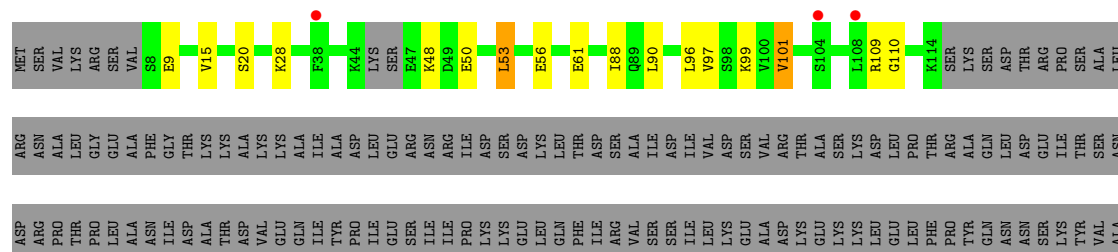
• Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



• Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49



LYS
LYS
LEU
ASP
SER
LEU
THR
GLN
PRO
SER
GLN
MET
THR
LYS
LEU
GLN
LEU
LEU
TYR
TYR
SER
LEU
LEU
LEU
GLY
VAL
TYR
GLU
ASN
ARG
ARG
VAL
MET
HIS
LEU
ASN
LYS
THR
LYS
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LEU
GLU
ARG
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ASN
SER
PRO
HIS
GLU
ILE
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VAL
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ILE
THR
PRO
LEU
ALA
HIS
GLU
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ASN
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ASP
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VAL
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SER
THR
PHE
VAL

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TYR
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LYS
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ALA
THR
MET
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GLY
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● Molecule 14: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34



MET
SER
LYS
LEU
SER
LYS
ASP
TYR
VAL
SER
ASP
SER
ASP
SER
SER
ASP
SER
F23
S24
I25
K36
N44
LYS
LYS
LYS
ALA
K49
M54
L55
L56
L67
L70
P71
F74
I78
D94
ILE
GLU
SER
SER
LEU
THR
GLN
ASP
ASN
SER
SER

N106
H107
S113
E114
E117
A125
LYS
ASP
ASN
ALA
P130
L131
I145
I148
V163
L166
K167
L168
E178
D179
F180
HIS
VAL
ALA
GLU
GLU
VAL
LYS
GLU
ASN
LYS
LYS
LYS
PRO
GLU
LYS
LYS
ARG
SER
HIS
HIS
ASP
ASP
GLU
GLU
GLU
SER
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GLN
LYS
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LYS
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LYS
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GLU
LYS
ARG
GLU
LYS
ARG
GLU
LYS
LYS
ASP
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ASP
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ASP
LYS
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ARG
ASP

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	400.53Å 140.22Å 122.89Å 90.00° 100.14° 90.00°	Depositor
Resolution (Å)	84.00 – 3.00 84.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (84.00-3.00) 99.1 (84.00-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.199 , 0.231 (Not available) , 0.244	Depositor DCC
R_{free} test set	6617 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	93.9	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34252	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, MPD, ZN

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	0.74	0/11907	1.28	29/16088 (0.2%)
2	B	0.73	0/9527	1.24	12/12879 (0.1%)
3	C	0.75	1/2469 (0.0%)	1.22	10/3347 (0.3%)
4	D	0.74	0/472	1.33	0/639
5	E	0.76	0/1795	1.20	8/2416 (0.3%)
6	F	0.72	0/838	1.22	0/1129
7	G	0.76	0/2094	1.20	3/2843 (0.1%)
8	H	0.74	0/1090	1.00	0/1476
9	I	0.79	0/955	1.14	0/1288
10	J	0.76	0/578	1.33	0/775
11	K	0.73	0/821	1.28	1/1108 (0.1%)
12	L	0.69	0/361	1.08	0/478
13	M	0.74	0/846	0.98	0/1136
14	N	0.75	0/1124	1.04	2/1512 (0.1%)
All	All	0.74	1/34877 (0.0%)	1.23	65/47114 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	252	PRO	CA-C	5.78	1.55	1.51

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	670	ILE	N-CA-C	7.61	118.10	111.56
3	C	173	GLY	CA-C-N	6.81	129.71	120.38
3	C	173	GLY	C-N-CA	6.81	129.71	120.38
7	G	138	PHE	CA-CB-CG	6.59	120.39	113.80
1	A	1218	GLY	CA-C-N	6.56	124.37	120.24

There are no chirality outliers.

There are no planarity outliers.

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	11695	0	11764	122	0
2	B	9322	0	9187	99	0
3	C	2418	0	2401	24	0
4	D	466	0	466	3	0
5	E	1759	0	1788	8	0
6	F	823	0	841	7	0
7	G	2052	0	2016	17	0
8	H	1072	0	1042	7	0
9	I	942	0	935	8	0
10	J	569	0	585	12	0
11	K	810	0	801	11	0
12	L	359	0	381	1	0
13	M	831	0	820	10	0
14	N	1103	0	1106	6	0
15	A	10	0	0	0	0
15	K	5	0	0	0	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	B	1	0	0	0	0
18	G	8	0	14	2	0
All	All	34252	0	34147	281	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 4.

The worst 5 of 281 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:712:ILE:H	11:K:106:GLN:HE22	1.22	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:VAL:HG21	2:B:417:ILE:HD11	1.55	0.87
2:B:16:PHE:HD2	2:B:978:ALA:HB2	1.51	0.75
1:A:86:TYR:H	1:A:431:GLN:HE22	1.36	0.72
1:A:824:THR:HG23	2:B:1023:ARG:HB2	1.71	0.71

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	
1	A	1466/1664 (88%)	1393 (95%)	71 (5%)	2 (0%)	48	80
2	B	1166/1203 (97%)	1094 (94%)	70 (6%)	2 (0%)	43	76
3	C	300/335 (90%)	284 (95%)	16 (5%)	0	100	100
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
7	G	251/326 (77%)	234 (93%)	16 (6%)	1 (0%)	30	65
8	H	130/146 (89%)	119 (92%)	10 (8%)	1 (1%)	16	50
9	I	122/125 (98%)	109 (89%)	11 (9%)	2 (2%)	7	34
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	101/142 (71%)	96 (95%)	5 (5%)	0	100	100
12	L	43/70 (61%)	39 (91%)	4 (9%)	0	100	100
13	M	101/415 (24%)	93 (92%)	8 (8%)	0	100	100
14	N	131/233 (56%)	123 (94%)	8 (6%)	0	100	100
All	All	4244/5236 (81%)	3996 (94%)	240 (6%)	8 (0%)	43	76

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	GLY
2	B	532	HIS
2	B	1154	ASP
1	A	1338	ARG
8	H	84	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1306/1465 (89%)	1218 (93%)	88 (7%)	15	46
2	B	1024/1053 (97%)	923 (90%)	101 (10%)	7	30
3	C	269/296 (91%)	242 (90%)	27 (10%)	7	29
4	D	56/116 (48%)	50 (89%)	6 (11%)	6	26
5	E	197/197 (100%)	187 (95%)	10 (5%)	21	55
6	F	90/137 (66%)	85 (94%)	5 (6%)	19	52
7	G	234/291 (80%)	216 (92%)	18 (8%)	12	40
8	H	116/128 (91%)	108 (93%)	8 (7%)	14	45
9	I	109/110 (99%)	97 (89%)	12 (11%)	6	25
10	J	64/65 (98%)	57 (89%)	7 (11%)	6	26
11	K	93/130 (72%)	85 (91%)	8 (9%)	10	36
12	L	40/57 (70%)	36 (90%)	4 (10%)	7	29
13	M	94/371 (25%)	88 (94%)	6 (6%)	16	48
14	N	128/220 (58%)	114 (89%)	14 (11%)	6	26
All	All	3820/4636 (82%)	3506 (92%)	314 (8%)	10	37

5 of 314 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	204	THR
11	K	99	ASN
7	G	28	ILE

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Mol	Chain	Res	Type
8	H	89	LEU
14	N	25	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	912	GLN
7	G	26	ASN
2	B	987	ASN
3	C	248	GLN
7	G	128	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
18	MPD	G	1317	-	7,7,7	0.49	0	9,10,10	0.66	0
15	SO4	K	1143	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SO4	A	2665	-	4,4,4	0.25	0	6,6,6	0.11	0
15	SO4	A	2664	-	4,4,4	0.25	0	6,6,6	0.05	0

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
18	MPD	G	1317	-	-	5/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	G	1317	MPD	C2-C3-C4-C5
18	G	1317	MPD	O2-C2-C3-C4
18	G	1317	MPD	C2-C3-C4-O4
18	G	1317	MPD	C1-C2-C3-C4
18	G	1317	MPD	CM-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	1317	MPD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1484/1664 (89%)	-0.20	11 (0%) 84 66	62, 98, 156, 225	0
2	B	1176/1203 (97%)	-0.11	6 (0%) 87 72	60, 107, 142, 176	0
3	C	304/335 (90%)	-0.07	4 (1%) 75 53	93, 122, 160, 197	0
4	D	59/137 (43%)	-0.26	0 100 100	82, 124, 147, 158	0
5	E	215/215 (100%)	-0.17	1 (0%) 87 72	78, 136, 183, 202	0
6	F	100/155 (64%)	-0.47	0 100 100	69, 86, 125, 142	0
7	G	259/326 (79%)	-0.06	5 (1%) 66 43	71, 121, 196, 231	0
8	H	134/146 (91%)	-0.07	1 (0%) 84 66	94, 123, 152, 165	0
9	I	124/125 (99%)	0.65	13 (10%) 11 6	116, 187, 215, 228	0
10	J	69/70 (98%)	-0.11	0 100 100	94, 112, 141, 161	0
11	K	103/142 (72%)	-0.49	0 100 100	82, 106, 136, 171	0
12	L	45/70 (64%)	-0.24	0 100 100	107, 128, 149, 153	0
13	M	105/415 (25%)	0.31	3 (2%) 53 31	137, 229, 262, 267	0
14	N	139/233 (59%)	0.45	5 (3%) 46 26	111, 249, 267, 276	0
All	All	4316/5236 (82%)	-0.11	49 (1%) 78 57	60, 111, 202, 276	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1205	PHE	4.2
9	I	105	ASP	3.8
7	G	314	THR	3.7
9	I	99	LEU	3.6
14	N	113	SER	3.5

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
15	SO4	A	2664	5/5	0.72	0.08	177,177,178,180	0
17	MG	B	2204	1/1	0.85	0.31	89,89,89,89	0
18	MPD	G	1317	8/8	0.87	0.22	99,101,103,104	0
15	SO4	A	2665	5/5	0.88	0.10	166,167,168,168	0
15	SO4	K	1143	5/5	0.89	0.07	147,147,149,149	0
16	ZN	I	1127	1/1	0.97	0.05	153,153,153,153	0
16	ZN	I	1126	1/1	0.99	0.05	138,138,138,138	0
16	ZN	L	1071	1/1	0.99	0.02	125,125,125,125	0
16	ZN	J	1070	1/1	1.00	0.06	104,104,104,104	0
16	ZN	B	2205	1/1	1.00	0.01	79,79,79,79	0
16	ZN	A	2666	1/1	1.00	0.02	108,108,108,108	0
16	ZN	A	2667	1/1	1.00	0.02	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.