



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 06:59 am BST

PDB ID : 5N9J
Title : Core Mediator of transcriptional regulation
Authors : Nozawa, K.; Schneider, T.R.; Cramer, P.
Deposited on : 2017-02-25
Resolution : 3.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

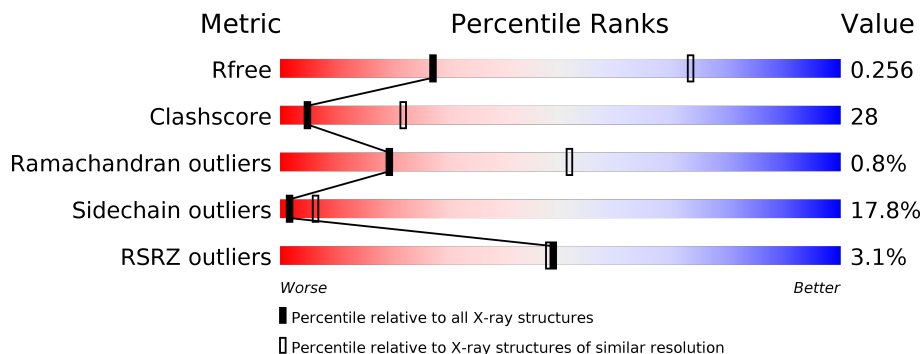
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 ≥ 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	591	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 41%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 40% 41% 13% . .</p>
2	B	144	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 47%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 47% 40% 5% 8%</p>
3	C	138	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 40% 35% 6% 20%</p>
4	D	138	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 51%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 51% 39% 7% . .</p>
5	E	376	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 47%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 30% 19% 5% . 47%</p>
6	F	121	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 35% 25% 6% 35%</p>

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Mol	Chain	Length	Quality of chain
7	G	239	<p>% 32% 28% 8% 32%</p>
8	R	139	<p>9% 22% 39% 10% 29%</p>
9	S	216	<p>3% 36% 35% 8% 21%</p>
10	U	200	<p>5% 59% 31% 9%</p>
11	V	112	<p>46% 35% 7% 12%</p>
12	W	545	<p>2% 42% 34% 8% 15%</p>
13	X	210	<p>2% 48% 38% 12%</p>
14	Y	193	<p>2% 40% 42% 12%</p>
15	Z	136	<p>2% 44% 38% 6% 13%</p>

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 23721 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 Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	566	4597	2979	791	814	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q9P7Y4
A	-9	GLY	-	expression tag	UNP Q9P7Y4
A	-8	HIS	-	expression tag	UNP Q9P7Y4
A	-7	HIS	-	expression tag	UNP Q9P7Y4
A	-6	HIS	-	expression tag	UNP Q9P7Y4
A	-5	HIS	-	expression tag	UNP Q9P7Y4
A	-4	HIS	-	expression tag	UNP Q9P7Y4
A	-3	HIS	-	expression tag	UNP Q9P7Y4
A	-2	HIS	-	expression tag	UNP Q9P7Y4
A	-1	HIS	-	expression tag	UNP Q9P7Y4
A	0	HIS	-	expression tag	UNP Q9P7Y4
A	1	HIS	-	expression tag	UNP Q9P7Y4

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	133	1066	673	172	220	1	0	0	0

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	111	917	592	158	166	1	0	0	0

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	135	1088	684	187	213	4	0	0	0

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	201	1548	982	271	287	8	0	0	0

- Molecule 6 is a protein called Mediator Complex Subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	79	632	405	108	116	3	0	0	0

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	163	1319	826	221	265	7	0	0	0

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	R	99	873	576	134	159	4	0	0	0

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	S	171	1410	905	236	260	9	0	0	0

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	U	198	1628	1022	281	322	3	0	0	0

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	V	99	Total	C	N	O	S	0	0	0
			783	494	130	157	2			

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	463	Total	C	N	O	S	0	0	0
			3692	2347	619	707	19			

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	X	207	Total	C	N	O	S	0	0	0
			1694	1082	288	316	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	MET	-	initiating methionine	UNP O14198
X	-1	ALA	-	expression tag	UNP O14198
X	0	SER	-	expression tag	UNP O14198

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Y	185	Total	C	N	O	S	0	0	0
			1515	989	250	271	5			

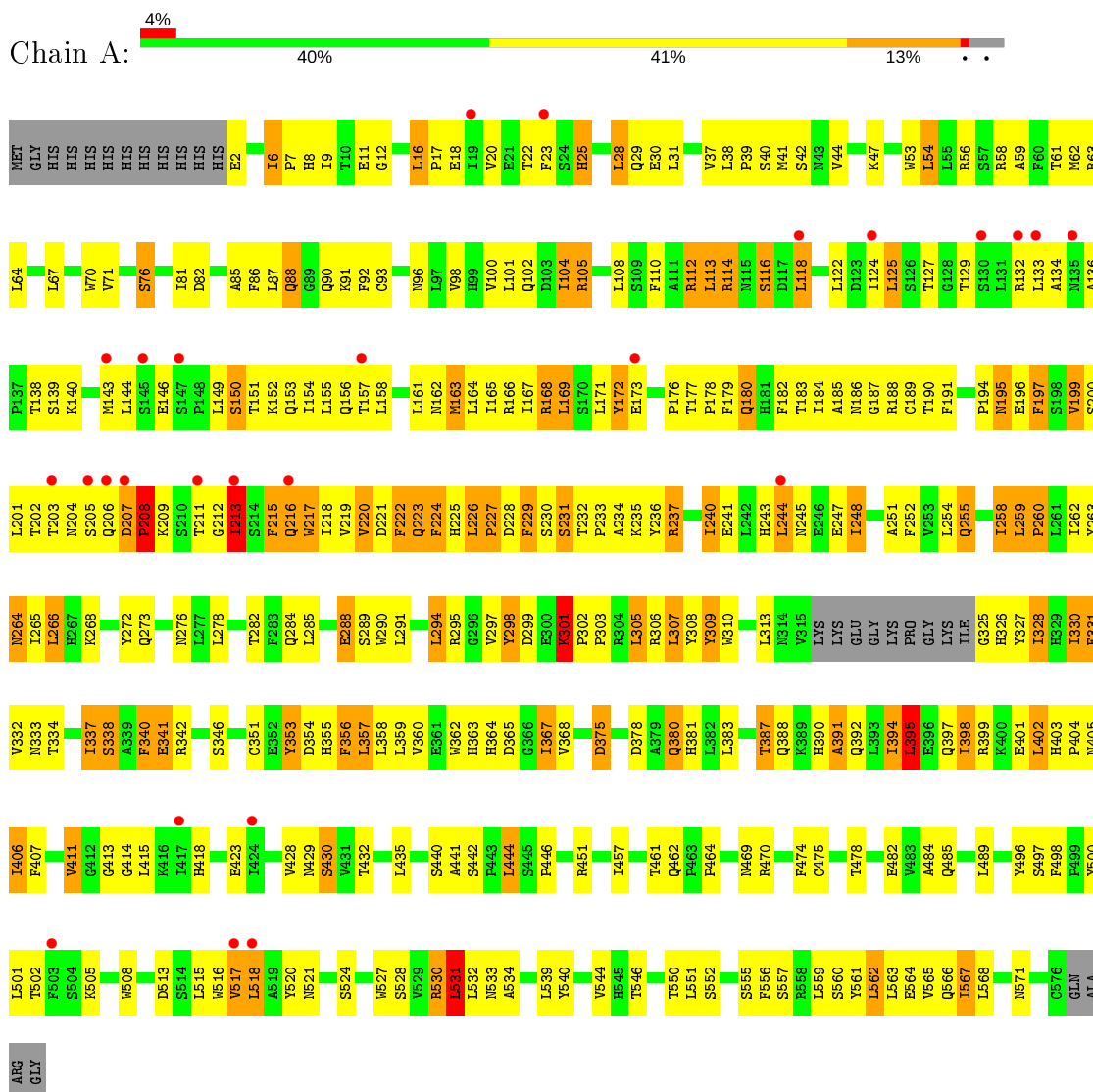
- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	Z	119	Total	C	N	O	S	0	0	0
			959	602	162	193	2			

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

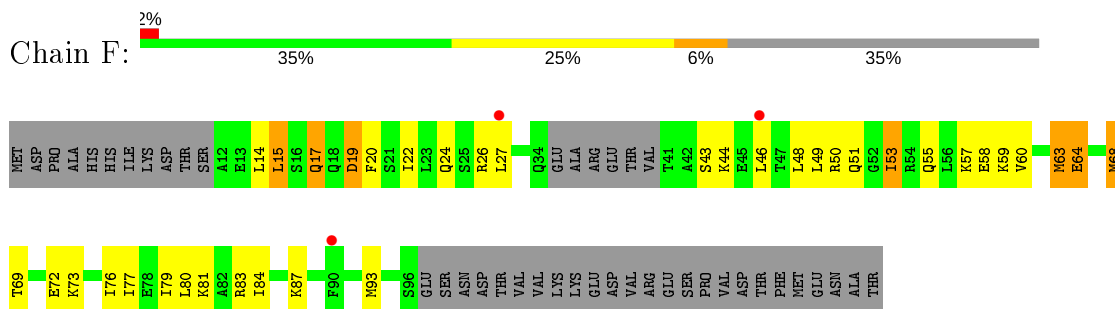
- Molecule 1: Mediator of RNA polymerase II transcription subunit 14



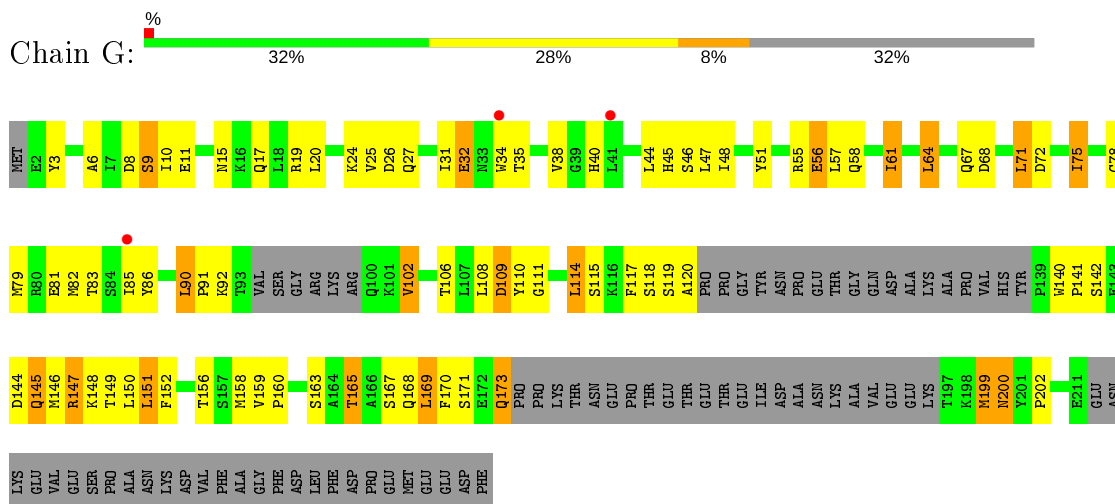
- Molecule 2: Mediator of RNA polymerase II transcription subunit 10



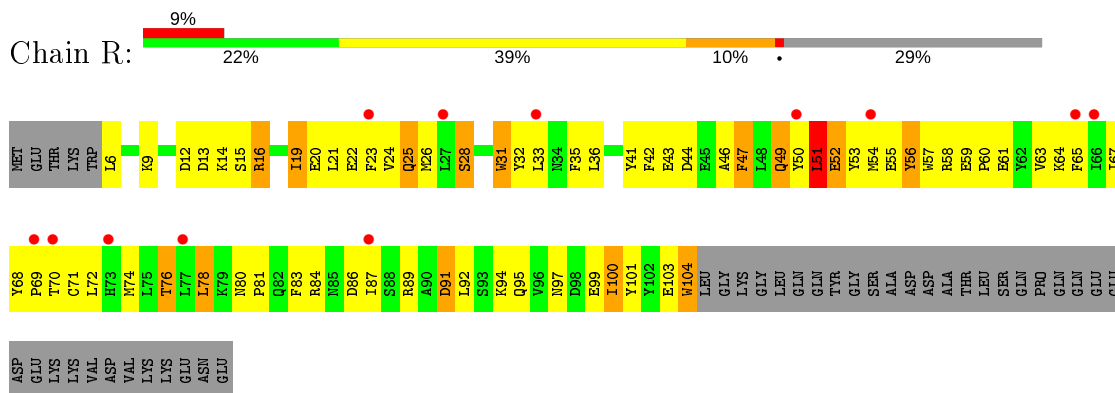
- Molecule 6: Mediator Complex Subunit 9



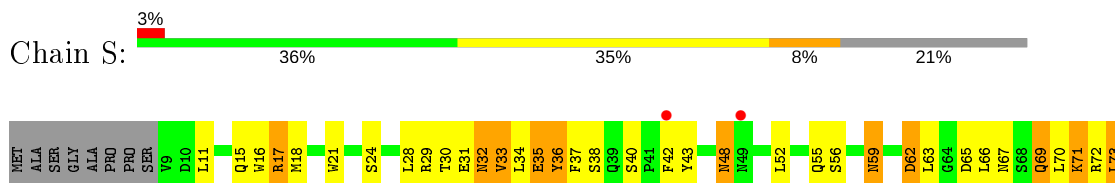
- Molecule 7: Mediator of RNA polymerase II transcription subunit 4

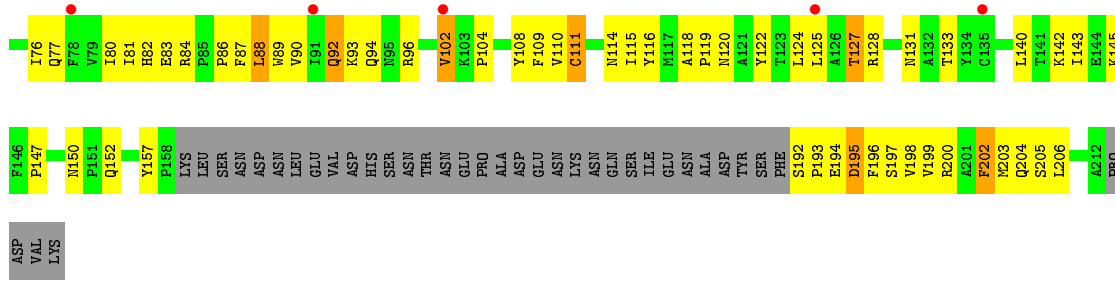


- Molecule 8: Mediator of RNA polymerase II transcription subunit 31

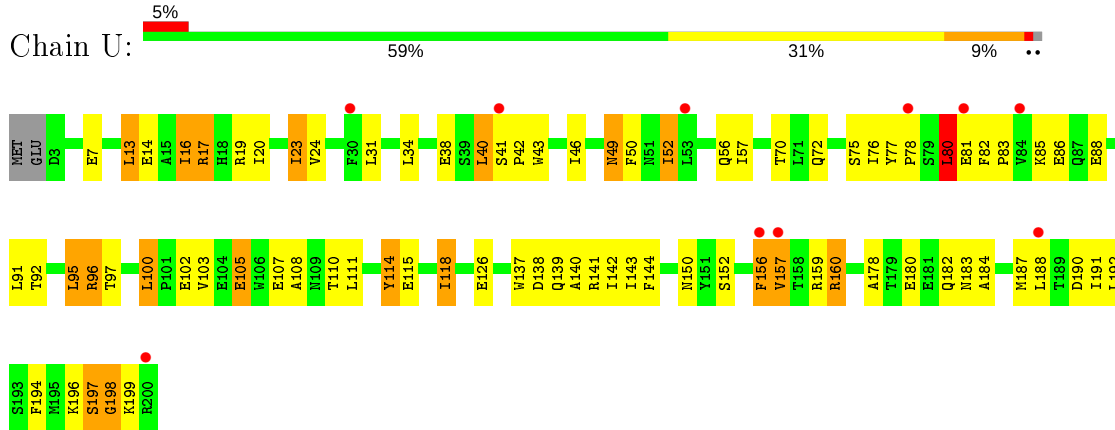


- Molecule 9: Mediator of RNA polymerase II transcription subunit 6

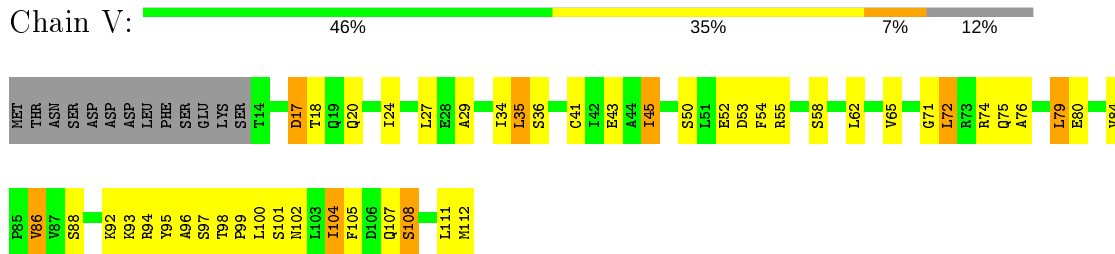




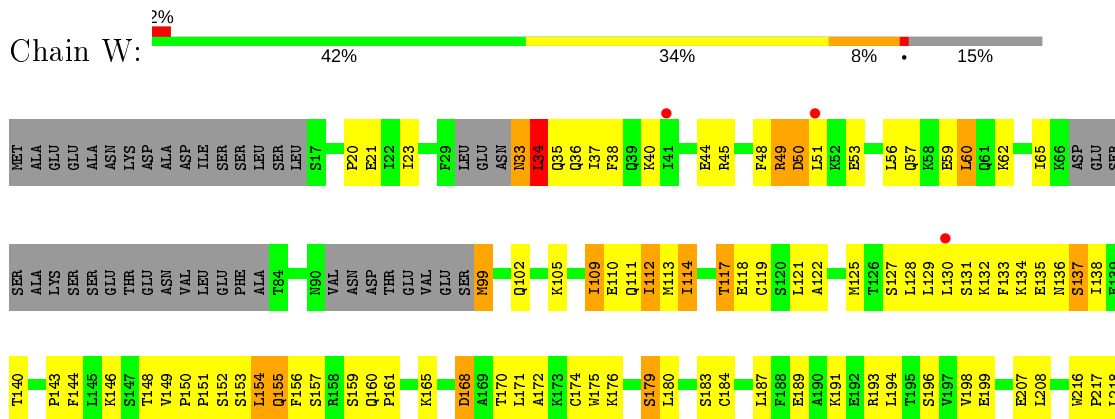
- Molecule 10: Mediator of RNA polymerase II transcription subunit 8

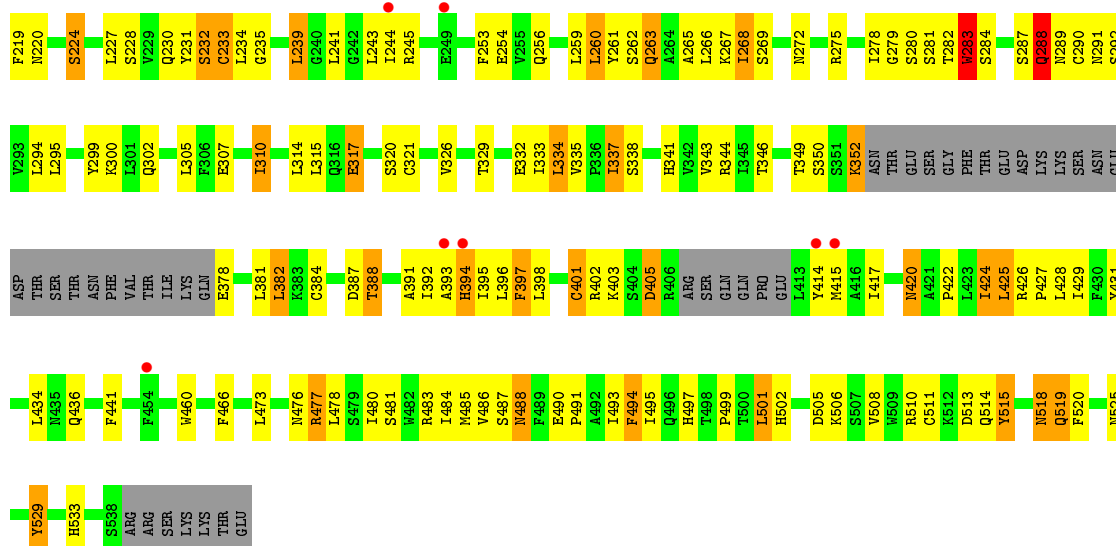


- Molecule 11: Mediator of RNA polymerase II transcription subunit 11

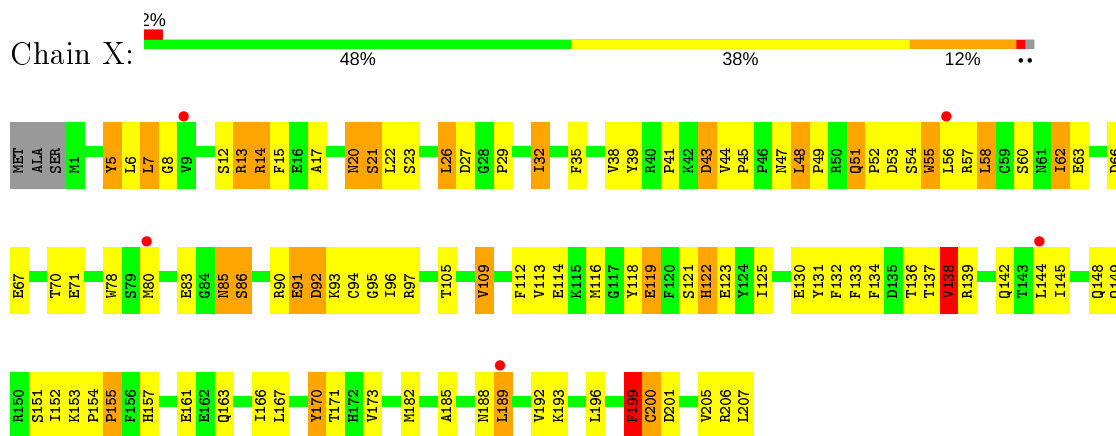


- Molecule 12: Mediator of RNA polymerase II transcription subunit 17

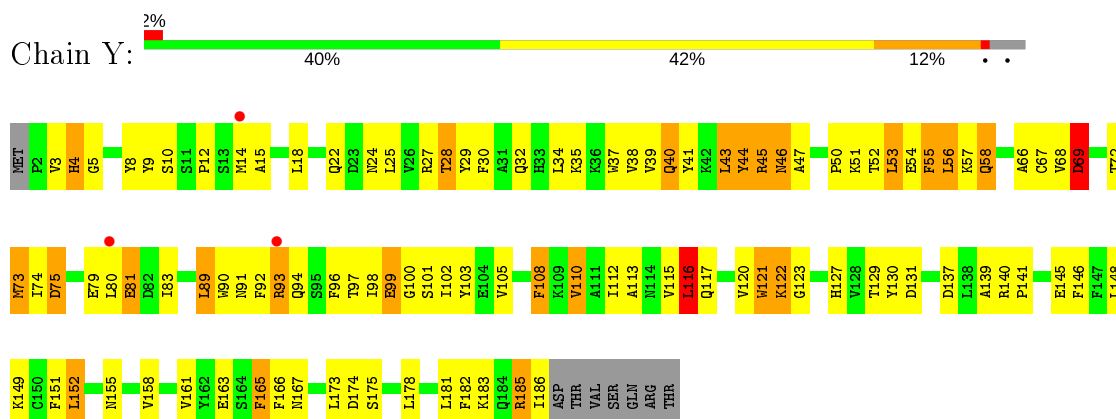




• Molecule 13: Mediator of RNA polymerase II transcription subunit 18

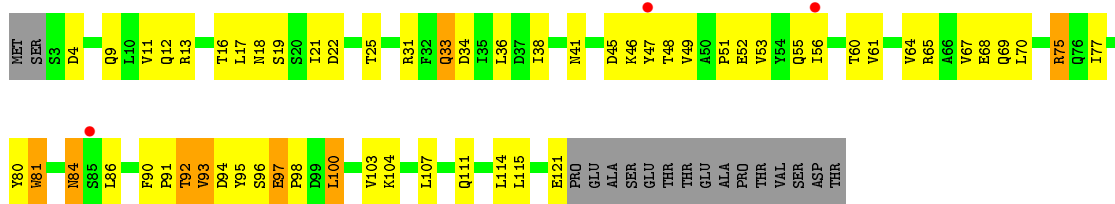


• Molecule 14: Mediator of RNA polymerase II transcription subunit 20



• Molecule 15: Mediator of RNA polymerase II transcription subunit 22





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.86Å 211.77Å 267.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.49 – 3.40 98.49 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (98.49-3.40) 99.2 (98.49-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.33Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.256 0.233 , 0.256	Depositor DCC
R_{free} test set	6194 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	153.1	Xtrriage
Anisotropy	0.161	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 130.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23721	wwPDB-VP
Average B, all atoms (Å ²)	159.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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

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	0.44	1/4718 (0.0%)	0.67	4/6423 (0.1%)
2	B	0.39	0/1082	0.55	0/1467
3	C	0.38	0/943	0.56	0/1278
4	D	0.40	1/1104 (0.1%)	0.57	1/1486 (0.1%)
5	E	0.33	0/1574	0.59	2/2120 (0.1%)
6	F	0.34	0/634	0.54	0/840
7	G	0.32	0/1339	0.57	0/1804
8	R	0.39	0/901	0.61	1/1222 (0.1%)
9	S	0.35	0/1446	0.54	1/1959 (0.1%)
10	U	0.34	0/1661	0.53	0/2248
11	V	0.41	0/792	0.70	2/1067 (0.2%)
12	W	0.52	6/3761 (0.2%)	0.64	3/5072 (0.1%)
13	X	0.46	1/1739 (0.1%)	0.65	0/2362
14	Y	0.43	0/1554	0.63	1/2108 (0.0%)
15	Z	0.62	2/972 (0.2%)	0.75	4/1320 (0.3%)
All	All	0.43	11/24220 (0.0%)	0.62	19/32776 (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
12	W	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	W	283	TRP	CB-CG	-13.47	1.26	1.50
13	X	199	PHE	CB-CG	-8.11	1.37	1.51
15	Z	96	SER	CA-CB	-7.13	1.42	1.52
12	W	401	CYS	CB-SG	-6.81	1.70	1.82
12	W	283	TRP	CE3-CZ3	-6.18	1.27	1.38

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Z	93	VAL	CA-CB-CG2	-7.58	99.54	110.90
8	R	51	LEU	CA-CB-CG	7.51	132.59	115.30
11	V	104	ILE	CG1-CB-CG2	7.00	126.80	111.40
1	A	217	TRP	CA-CB-CG	-6.99	100.42	113.70
4	D	35	LEU	CA-CB-CG	6.99	131.38	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	W	288	GLN	Mainchain

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	4597	0	4636	347	1
2	B	1066	0	1050	63	1
3	C	917	0	905	52	1
4	D	1088	0	1099	82	0
5	E	1548	0	1484	107	0
6	F	632	0	697	39	0
7	G	1319	0	1302	83	0
8	R	873	0	832	77	0
9	S	1410	0	1378	96	0
10	U	1628	0	1588	84	0
11	V	783	0	803	77	0
12	W	3692	0	3633	237	0
13	X	1694	0	1670	91	0
14	Y	1515	0	1527	108	1
15	Z	959	0	965	81	0
All	All	23721	0	23569	1307	2

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 28.

The worst 5 of 1307 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)
13:X:21:SER:HB3	13:X:199:PHE:CZ	1.89	1.08
1:A:150:SER:HB2	1:A:153:GLN:HB2	1.39	1.03
14:Y:51:LYS:HB3	14:Y:69:ASP:HA	1.38	1.02
10:U:83:PRO:HA	10:U:86:GLU:HB2	1.40	1.00
1:A:208:PRO:HD3	1:A:226:LEU:HG	1.43	0.99

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ASP:OD2	14:Y:130:TYR:OH[2_554]	2.03	0.17
1:A:497:SER:OG	3:C:33:THR:OG1[3_654]	2.14	0.06

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	562/591 (95%)	517 (92%)	36 (6%)	9 (2%)	9	34
2	B	131/144 (91%)	126 (96%)	4 (3%)	1 (1%)	19	51
3	C	109/138 (79%)	101 (93%)	8 (7%)	0	100	100
4	D	133/138 (96%)	125 (94%)	6 (4%)	2 (2%)	10	36
5	E	195/376 (52%)	184 (94%)	9 (5%)	2 (1%)	15	46
6	F	75/121 (62%)	73 (97%)	2 (3%)	0	100	100
7	G	155/239 (65%)	150 (97%)	5 (3%)	0	100	100
8	R	97/139 (70%)	94 (97%)	3 (3%)	0	100	100
9	S	167/216 (77%)	159 (95%)	8 (5%)	0	100	100
10	U	196/200 (98%)	187 (95%)	7 (4%)	2 (1%)	15	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	V	97/112 (87%)	91 (94%)	5 (5%)	1 (1%)	15	46
12	W	451/545 (83%)	436 (97%)	13 (3%)	2 (0%)	34	67
13	X	205/210 (98%)	190 (93%)	12 (6%)	3 (2%)	10	36
14	Y	183/193 (95%)	166 (91%)	16 (9%)	1 (0%)	29	61
15	Z	117/136 (86%)	110 (94%)	7 (6%)	0	100	100
All	All	2873/3498 (82%)	2709 (94%)	141 (5%)	23 (1%)	19	51

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	TRP
1	A	301	LYS
4	D	35	LEU
5	E	67	SER
1	A	213	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	518/538 (96%)	407 (79%)	111 (21%)	1	3
2	B	120/131 (92%)	104 (87%)	16 (13%)	4	15
3	C	100/124 (81%)	85 (85%)	15 (15%)	3	12
4	D	126/128 (98%)	113 (90%)	13 (10%)	7	26
5	E	157/350 (45%)	129 (82%)	28 (18%)	2	6
6	F	71/110 (64%)	59 (83%)	12 (17%)	2	8
7	G	154/220 (70%)	125 (81%)	29 (19%)	1	4
8	R	96/131 (73%)	72 (75%)	24 (25%)	0	2
9	S	158/198 (80%)	132 (84%)	26 (16%)	2	9
10	U	183/185 (99%)	158 (86%)	25 (14%)	3	14
11	V	91/104 (88%)	81 (89%)	10 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	W	415/509 (82%)	336 (81%)	79 (19%)	1	4
13	X	191/193 (99%)	158 (83%)	33 (17%)	2	7
14	Y	170/178 (96%)	131 (77%)	39 (23%)	1	2
15	Z	114/129 (88%)	100 (88%)	14 (12%)	4	17
All	All	2664/3228 (82%)	2190 (82%)	474 (18%)	2	6

5 of 474 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	147	ARG
9	S	102	VAL
14	Y	79	GLU
7	G	170	PHE
8	R	65	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	145	GLN
10	U	109	ASN
14	Y	58	GLN
9	S	59	ASN
11	V	75	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	566/591 (95%)	0.50	26 (4%) 32 32	88, 132, 207, 337	0
2	B	133/144 (92%)	0.33	3 (2%) 60 59	91, 128, 188, 241	0
3	C	111/138 (80%)	0.19	1 (0%) 84 83	93, 137, 190, 276	0
4	D	135/138 (97%)	0.11	2 (1%) 73 72	120, 174, 212, 295	0
5	E	201/376 (53%)	0.03	3 (1%) 73 72	112, 185, 256, 300	0
6	F	79/121 (65%)	0.04	3 (3%) 40 39	131, 183, 232, 264	0
7	G	163/239 (68%)	0.21	3 (1%) 68 67	104, 178, 237, 269	0
8	R	99/139 (71%)	0.52	12 (12%) 4 5	133, 172, 214, 246	0
9	S	171/216 (79%)	0.32	7 (4%) 37 36	118, 192, 242, 315	0
10	U	198/200 (99%)	0.15	10 (5%) 28 28	117, 170, 240, 327	0
11	V	99/112 (88%)	0.37	0 100 100	105, 126, 165, 211	0
12	W	463/545 (84%)	0.21	10 (2%) 62 60	93, 142, 230, 288	0
13	X	207/210 (98%)	0.15	5 (2%) 59 57	109, 160, 244, 299	0
14	Y	185/193 (95%)	0.27	3 (1%) 72 70	103, 149, 202, 237	0
15	Z	119/136 (87%)	0.36	3 (2%) 57 55	111, 130, 199, 225	0
All	All	2929/3498 (83%)	0.27	91 (3%) 49 48	88, 155, 231, 337	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	ARG	5.9
1	A	173	GLU	5.4
10	U	156	PHE	4.7
9	S	49	ASN	4.4
1	A	216	GLN	4.3

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.