



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:02 PM GMT

PDB ID : 4GWP  
Title : Structure of the Mediator Head Module from *S. cerevisiae*  
Authors : Robinson, P.J.J.; Bushnell, D.A.; Trnka, M.J.; Burlingame, A.L.; Kornberg, R.D.  
Deposited on : 2012-09-03  
Resolution : 4.20 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

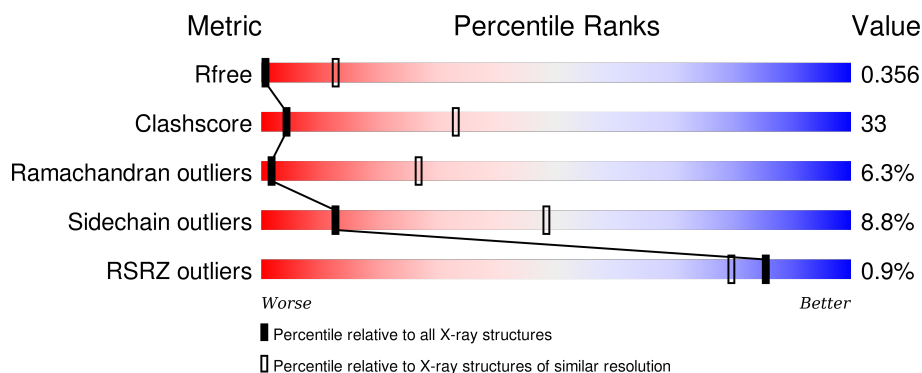
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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	115	<div> <div>89%</div> <div>8%</div> <div>••</div> </div>
2	B	687	<div> <div>53%</div> <div>16%</div> <div>•</div> <div>28%</div> </div>
3	C	407	<div> <div>33%</div> <div>11%</div> <div>55%</div> </div>
4	D	121	<div> <div>%</div> <div>84%</div> <div>14%</div> <div>•</div> </div>
5	E	307	<div> <div>42%</div> <div>35%</div> <div>6%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	210	<div><div></div><div>4%</div><div>56%</div><div>39%</div><div>5%</div></div>
7	G	295	<div><div></div><div>38%</div><div>18%</div><div>•</div><div>42%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9033 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 11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	0	0	0
			556	332	112	112			

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	492	Total	C	N	O	0	0	0
			2446	1462	492	492			

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	184	Total	C	N	O	0	0	0
			1004	611	194	199			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	224	SER	-	EXPRESSION TAG	UNP P38304
C	225	MET	-	EXPRESSION TAG	UNP P38304
C	226	GLU	-	EXPRESSION TAG	UNP P38304
C	227	LYS	-	EXPRESSION TAG	UNP P38304
C	228	ARG	-	EXPRESSION TAG	UNP P38304
C	229	ARG	-	EXPRESSION TAG	UNP P38304
C	230	TRP	-	EXPRESSION TAG	UNP P38304
C	231	LYS	-	EXPRESSION TAG	UNP P38304
C	232	LYS	-	EXPRESSION TAG	UNP P38304
C	233	ASN	-	EXPRESSION TAG	UNP P38304
C	234	PHE	-	EXPRESSION TAG	UNP P38304
C	235	ILE	-	EXPRESSION TAG	UNP P38304
C	236	ALA	-	EXPRESSION TAG	UNP P38304
C	237	VAL	-	EXPRESSION TAG	UNP P38304

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Chain	Residue	Modelled	Actual	Comment	Reference
C	238	SER	-	EXPRESSION TAG	UNP P38304
C	239	ALA	-	EXPRESSION TAG	UNP P38304
C	240	ALA	-	EXPRESSION TAG	UNP P38304
C	241	ASN	-	EXPRESSION TAG	UNP P38304
C	242	ARG	-	EXPRESSION TAG	UNP P38304
C	243	PHE	-	EXPRESSION TAG	UNP P38304
C	244	LYS	-	EXPRESSION TAG	UNP P38304
C	245	LYS	-	EXPRESSION TAG	UNP P38304
C	246	ILE	-	EXPRESSION TAG	UNP P38304
C	247	SER	-	EXPRESSION TAG	UNP P38304
C	248	SER	-	EXPRESSION TAG	UNP P38304
C	249	SER	-	EXPRESSION TAG	UNP P38304
C	250	GLY	-	EXPRESSION TAG	UNP P38304
C	251	ALA	-	EXPRESSION TAG	UNP P38304
C	252	LEU	-	EXPRESSION TAG	UNP P38304
C	253	ASP	-	EXPRESSION TAG	UNP P38304
C	254	TYR	-	EXPRESSION TAG	UNP P38304
C	255	ASP	-	EXPRESSION TAG	UNP P38304
C	256	ILE	-	EXPRESSION TAG	UNP P38304
C	257	PRO	-	EXPRESSION TAG	UNP P38304
C	258	THR	-	EXPRESSION TAG	UNP P38304
C	259	THR	-	EXPRESSION TAG	UNP P38304
C	260	ALA	-	EXPRESSION TAG	UNP P38304
C	261	SER	-	EXPRESSION TAG	UNP P38304
C	262	GLU	-	EXPRESSION TAG	UNP P38304
C	263	ASN	-	EXPRESSION TAG	UNP P38304
C	264	LEU	-	EXPRESSION TAG	UNP P38304
C	265	TYR	-	EXPRESSION TAG	UNP P38304
C	266	PHE	-	EXPRESSION TAG	UNP P38304
C	267	GLN	-	EXPRESSION TAG	UNP P38304
C	268	GLY	-	EXPRESSION TAG	UNP P38304
C	269	GLU	-	EXPRESSION TAG	UNP P38304
C	270	LEU	-	EXPRESSION TAG	UNP P38304
C	271	LYS	-	EXPRESSION TAG	UNP P38304
C	272	THR	-	EXPRESSION TAG	UNP P38304
C	273	ALA	-	EXPRESSION TAG	UNP P38304
C	274	ALA	-	EXPRESSION TAG	UNP P38304
C	275	LEU	-	EXPRESSION TAG	UNP P38304
C	276	ALA	-	EXPRESSION TAG	UNP P38304
C	277	GLN	-	EXPRESSION TAG	UNP P38304
C	278	HIS	-	EXPRESSION TAG	UNP P38304
C	279	ASP	-	EXPRESSION TAG	UNP P38304

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Chain	Residue	Modelled	Actual	Comment	Reference
C	280	GLU	-	EXPRESSION TAG	UNP P38304
C	281	ALA	-	EXPRESSION TAG	UNP P38304
C	282	VAL	-	EXPRESSION TAG	UNP P38304
C	283	ASP	-	EXPRESSION TAG	UNP P38304
C	284	ASN	-	EXPRESSION TAG	UNP P38304
C	285	LYS	-	EXPRESSION TAG	UNP P38304
C	286	PHE	-	EXPRESSION TAG	UNP P38304
C	287	ASN	-	EXPRESSION TAG	UNP P38304
C	288	LYS	-	EXPRESSION TAG	UNP P38304
C	289	GLU	-	EXPRESSION TAG	UNP P38304
C	290	GLN	-	EXPRESSION TAG	UNP P38304
C	291	GLN	-	EXPRESSION TAG	UNP P38304
C	292	ASN	-	EXPRESSION TAG	UNP P38304
C	293	ALA	-	EXPRESSION TAG	UNP P38304
C	294	PHE	-	EXPRESSION TAG	UNP P38304
C	295	TYR	-	EXPRESSION TAG	UNP P38304
C	296	GLU	-	EXPRESSION TAG	UNP P38304
C	297	ILE	-	EXPRESSION TAG	UNP P38304
C	298	LEU	-	EXPRESSION TAG	UNP P38304
C	299	HIS	-	EXPRESSION TAG	UNP P38304
C	300	LEU	-	EXPRESSION TAG	UNP P38304
C	301	PRO	-	EXPRESSION TAG	UNP P38304
C	302	ASN	-	EXPRESSION TAG	UNP P38304
C	303	LEU	-	EXPRESSION TAG	UNP P38304
C	304	ASN	-	EXPRESSION TAG	UNP P38304
C	305	GLU	-	EXPRESSION TAG	UNP P38304
C	306	GLU	-	EXPRESSION TAG	UNP P38304
C	307	GLN	-	EXPRESSION TAG	UNP P38304
C	308	ARG	-	EXPRESSION TAG	UNP P38304
C	309	ASN	-	EXPRESSION TAG	UNP P38304
C	310	ALA	-	EXPRESSION TAG	UNP P38304
C	311	PHE	-	EXPRESSION TAG	UNP P38304
C	312	ILE	-	EXPRESSION TAG	UNP P38304
C	313	GLN	-	EXPRESSION TAG	UNP P38304
C	314	SER	-	EXPRESSION TAG	UNP P38304
C	315	LEU	-	EXPRESSION TAG	UNP P38304
C	316	LYS	-	EXPRESSION TAG	UNP P38304
C	317	ASP	-	EXPRESSION TAG	UNP P38304
C	318	ASP	-	EXPRESSION TAG	UNP P38304
C	319	PRO	-	EXPRESSION TAG	UNP P38304
C	320	SER	-	EXPRESSION TAG	UNP P38304
C	321	GLN	-	EXPRESSION TAG	UNP P38304

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Chain	Residue	Modelled	Actual	Comment	Reference
C	322	SER	-	EXPRESSION TAG	UNP P38304
C	323	ALA	-	EXPRESSION TAG	UNP P38304
C	324	ASN	-	EXPRESSION TAG	UNP P38304
C	325	LEU	-	EXPRESSION TAG	UNP P38304
C	326	LEU	-	EXPRESSION TAG	UNP P38304
C	327	ALA	-	EXPRESSION TAG	UNP P38304
C	328	GLU	-	EXPRESSION TAG	UNP P38304
C	329	ALA	-	EXPRESSION TAG	UNP P38304
C	330	LYS	-	EXPRESSION TAG	UNP P38304
C	331	LYS	-	EXPRESSION TAG	UNP P38304
C	332	LEU	-	EXPRESSION TAG	UNP P38304
C	333	ASN	-	EXPRESSION TAG	UNP P38304
C	334	ASP	-	EXPRESSION TAG	UNP P38304
C	335	ALA	-	EXPRESSION TAG	UNP P38304
C	336	GLN	-	EXPRESSION TAG	UNP P38304
C	337	ALA	-	EXPRESSION TAG	UNP P38304
C	338	PRO	-	EXPRESSION TAG	UNP P38304
C	339	LYS	-	EXPRESSION TAG	UNP P38304
C	340	VAL	-	EXPRESSION TAG	UNP P38304
C	341	ASP	-	EXPRESSION TAG	UNP P38304
C	342	ASN	-	EXPRESSION TAG	UNP P38304
C	343	LYS	-	EXPRESSION TAG	UNP P38304
C	344	PHE	-	EXPRESSION TAG	UNP P38304
C	345	ASN	-	EXPRESSION TAG	UNP P38304
C	346	LYS	-	EXPRESSION TAG	UNP P38304
C	347	GLU	-	EXPRESSION TAG	UNP P38304
C	348	GLN	-	EXPRESSION TAG	UNP P38304
C	349	GLN	-	EXPRESSION TAG	UNP P38304
C	350	ASN	-	EXPRESSION TAG	UNP P38304
C	351	ALA	-	EXPRESSION TAG	UNP P38304
C	352	PHE	-	EXPRESSION TAG	UNP P38304
C	353	TYR	-	EXPRESSION TAG	UNP P38304
C	354	GLU	-	EXPRESSION TAG	UNP P38304
C	355	ILE	-	EXPRESSION TAG	UNP P38304
C	356	LEU	-	EXPRESSION TAG	UNP P38304
C	357	HIS	-	EXPRESSION TAG	UNP P38304
C	358	LEU	-	EXPRESSION TAG	UNP P38304
C	359	PRO	-	EXPRESSION TAG	UNP P38304
C	360	ASN	-	EXPRESSION TAG	UNP P38304
C	361	LEU	-	EXPRESSION TAG	UNP P38304
C	362	ASN	-	EXPRESSION TAG	UNP P38304
C	363	GLU	-	EXPRESSION TAG	UNP P38304

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Chain	Residue	Modelled	Actual	Comment	Reference
C	364	GLU	-	EXPRESSION TAG	UNP P38304
C	365	GLN	-	EXPRESSION TAG	UNP P38304
C	366	ARG	-	EXPRESSION TAG	UNP P38304
C	367	ASN	-	EXPRESSION TAG	UNP P38304
C	368	ALA	-	EXPRESSION TAG	UNP P38304
C	369	PHE	-	EXPRESSION TAG	UNP P38304
C	370	ILE	-	EXPRESSION TAG	UNP P38304
C	371	GLN	-	EXPRESSION TAG	UNP P38304
C	372	SER	-	EXPRESSION TAG	UNP P38304
C	373	LEU	-	EXPRESSION TAG	UNP P38304
C	374	LYS	-	EXPRESSION TAG	UNP P38304
C	375	ASP	-	EXPRESSION TAG	UNP P38304
C	376	ASP	-	EXPRESSION TAG	UNP P38304
C	377	PRO	-	EXPRESSION TAG	UNP P38304
C	378	SER	-	EXPRESSION TAG	UNP P38304
C	379	GLN	-	EXPRESSION TAG	UNP P38304
C	380	SER	-	EXPRESSION TAG	UNP P38304
C	381	ALA	-	EXPRESSION TAG	UNP P38304
C	382	ASN	-	EXPRESSION TAG	UNP P38304
C	383	LEU	-	EXPRESSION TAG	UNP P38304
C	384	LEU	-	EXPRESSION TAG	UNP P38304
C	385	ALA	-	EXPRESSION TAG	UNP P38304
C	386	GLU	-	EXPRESSION TAG	UNP P38304
C	387	ALA	-	EXPRESSION TAG	UNP P38304
C	388	LYS	-	EXPRESSION TAG	UNP P38304
C	389	LYS	-	EXPRESSION TAG	UNP P38304
C	390	LEU	-	EXPRESSION TAG	UNP P38304
C	391	ASN	-	EXPRESSION TAG	UNP P38304
C	392	GLY	-	EXPRESSION TAG	UNP P38304
C	393	ALA	-	EXPRESSION TAG	UNP P38304
C	394	GLN	-	EXPRESSION TAG	UNP P38304
C	395	ALA	-	EXPRESSION TAG	UNP P38304
C	396	PRO	-	EXPRESSION TAG	UNP P38304
C	397	LYS	-	EXPRESSION TAG	UNP P38304
C	398	VAL	-	EXPRESSION TAG	UNP P38304
C	399	ASP	-	EXPRESSION TAG	UNP P38304
C	400	ALA	-	EXPRESSION TAG	UNP P38304
C	401	ASN	-	EXPRESSION TAG	UNP P38304
C	402	SER	-	EXPRESSION TAG	UNP P38304
C	403	ALA	-	EXPRESSION TAG	UNP P38304
C	404	GLY	-	EXPRESSION TAG	UNP P38304
C	405	LYS	-	EXPRESSION TAG	UNP P38304

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Chain	Residue	Modelled	Actual	Comment	Reference
C	406	SER	-	EXPRESSION TAG	UNP P38304
C	407	THR	-	EXPRESSION TAG	UNP P38304

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	121	Total	C	N	O	0	0	0
			604	362	121	121			

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	253	Total	C	N	O	S	0	0	0
			1979	1255	330	384	10			

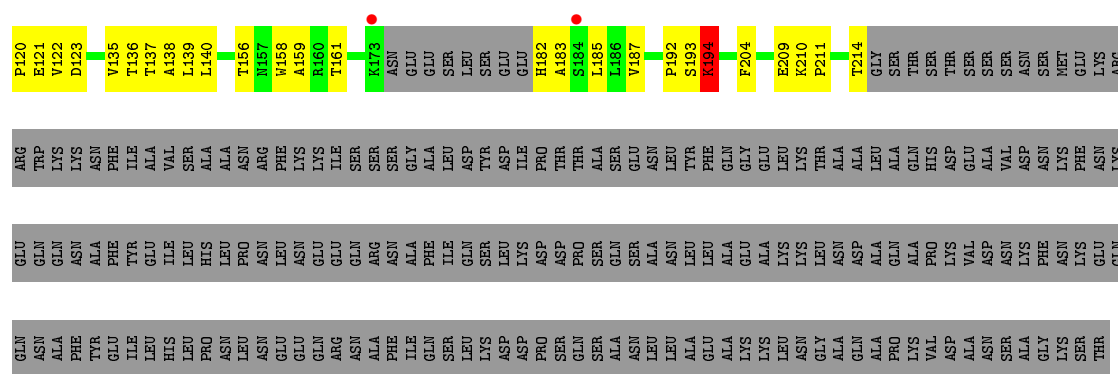
- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	209	Total	C	N	O	S	0	0	0
			1600	1011	269	315	5			

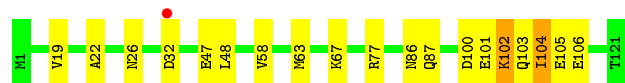
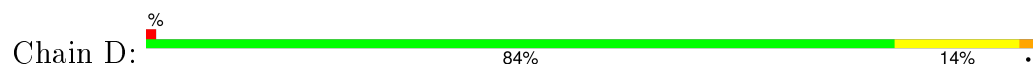
- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	170	Total	C	N	O	0	0	0
			844	504	170	170			

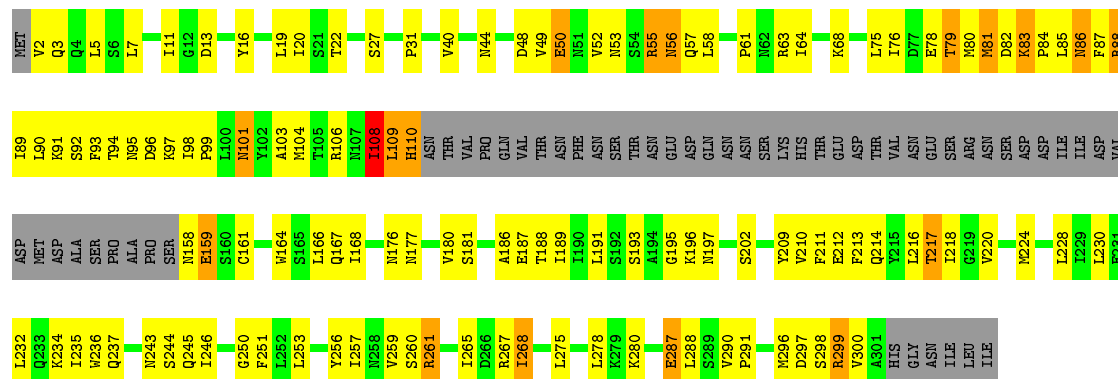




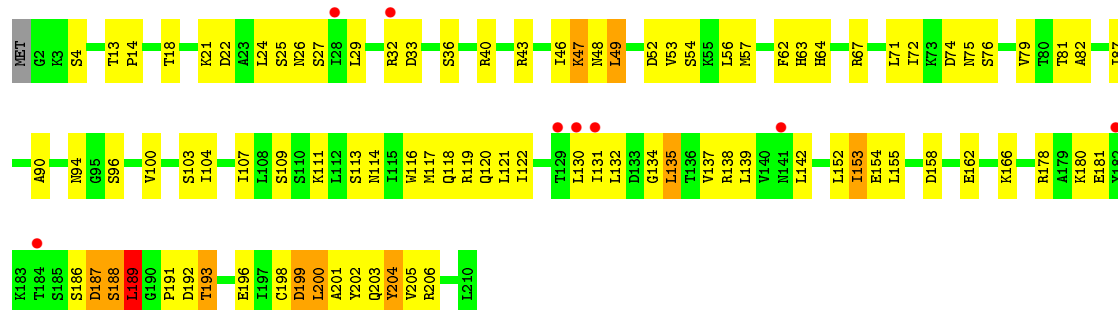
• Molecule 4: Mediator of RNA polymerase II transcription subunit 22



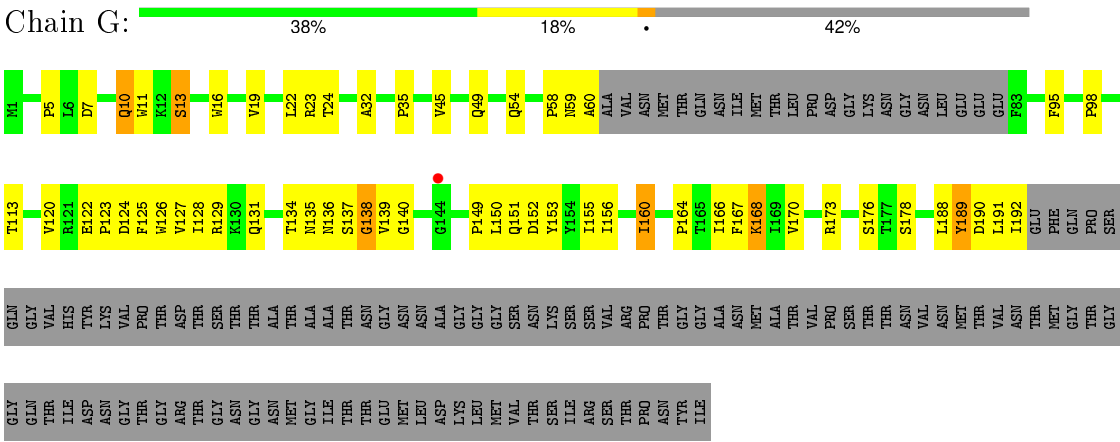
• Molecule 5: Mediator of RNA polymerase II transcription subunit 18



• Molecule 6: Mediator of RNA polymerase II transcription subunit 20



• Molecule 7: Mediator of RNA polymerase II transcription subunit 6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.01Å 142.01Å 305.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.00 – 4.20 44.47 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.00-4.20) 99.3 (44.47-4.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.290 , 0.357 0.289 , 0.356	Depositor DCC
$R_{free}$ test set	1340 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	194.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 340.3	EDS
Estimated twinning fraction	0.086 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 26579 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	222.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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

### 5.1 Standard geometry

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	0.52	0/555	0.69	0/773
2	B	0.58	0/2443	0.78	2/3407 (0.1%)
3	C	0.53	0/1008	0.76	0/1394
4	D	0.55	0/603	0.72	0/842
5	E	0.55	0/2014	0.75	0/2728
6	F	0.50	1/1626 (0.1%)	0.66	0/2205
7	G	0.60	0/842	0.85	0/1172
All	All	0.55	1/9091 (0.0%)	0.75	2/12521 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
5	E	0	1
7	G	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	116	TRP	CD2-CE2	5.06	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	457	VAL	N-CA-C	5.09	124.74	111.00
2	B	342	GLU	N-CA-C	5.08	124.70	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	VAL	Peptide
2	B	471	ASN	Peptide
2	B	532	ASN	Peptide
2	B	626	HIS	Peptide
5	E	101	ASN	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	556	0	233	7	0
2	B	2446	0	1028	97	0
3	C	1004	0	562	25	0
4	D	604	0	265	11	0
5	E	1979	0	1977	248	0
6	F	1600	0	1614	106	0
7	G	844	0	355	38	0
All	All	9033	0	6034	502	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 33.

The worst 5 of 502 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)
5:E:81:MET:CE	5:E:92:SER:HB3	1.20	1.59
5:E:97:LYS:CE	5:E:243:ASN:HB3	1.36	1.54
6:F:72:ILE:HG21	6:F:202:TYR:CE1	1.49	1.44
5:E:97:LYS:HE2	5:E:243:ASN:CB	1.47	1.43
5:E:81:MET:CE	5:E:92:SER:CB	1.95	1.42

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	110/115 (96%)	101 (92%)	5 (4%)	4 (4%)	4	41
2	B	486/687 (71%)	389 (80%)	62 (13%)	35 (7%)	1	22
3	C	180/407 (44%)	146 (81%)	16 (9%)	18 (10%)	1	13
4	D	119/121 (98%)	100 (84%)	11 (9%)	8 (7%)	1	25
5	E	249/307 (81%)	217 (87%)	25 (10%)	7 (3%)	6	46
6	F	207/210 (99%)	190 (92%)	12 (6%)	5 (2%)	7	49
7	G	166/295 (56%)	122 (74%)	25 (15%)	19 (11%)	0	10
All	All	1517/2142 (71%)	1265 (83%)	156 (10%)	96 (6%)	2	27

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	VAL
1	A	94	ASP
2	B	231	SER
2	B	251	PRO
2	B	252	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	28/362 (8%)	25 (89%)	3 (11%)	8	39
5	E	226/280 (81%)	206 (91%)	20 (9%)	12	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	177/178 (99%)	162 (92%)	15 (8%)	13	51
All	All	431/820 (53%)	393 (91%)	38 (9%)	12	48

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	246	ILE
5	E	280	LYS
6	F	193	THR
5	E	268	ILE
5	E	287	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	205	ASN
5	E	243	ASN
6	F	26	ASN
5	E	176	ASN
5	E	269	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	112/115 (97%)	-0.97	0 <span>100</span> <span>100</span>	116, 195, 275, 337	0
2	B	492/687 (71%)	-0.75	2 (0%) <span>93</span> <span>90</span>	114, 203, 354, 469	0
3	C	184/407 (45%)	-0.76	2 (1%) <span>82</span> <span>75</span>	116, 186, 366, 489	0
4	D	121/121 (100%)	-0.81	1 (0%) <span>87</span> <span>82</span>	117, 179, 352, 409	1 (0%)
5	E	253/307 (82%)	-0.43	0 <span>100</span> <span>100</span>	112, 188, 287, 373	0
6	F	209/210 (99%)	0.02	8 (3%) <span>44</span> <span>34</span>	137, 271, 368, 474	0
7	G	170/295 (57%)	-0.66	1 (0%) <span>90</span> <span>86</span>	108, 201, 365, 445	0
All	All	1541/2142 (71%)	-0.61	14 (0%) <span>85</span> <span>80</span>	108, 201, 353, 489	1 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	588	ASN	4.1
6	F	130	LEU	3.2
6	F	129	THR	3.1
4	D	32	ASP	3.0
6	F	182	TYR	2.7

### 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.