wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 03:05 PM GMT

PDB ID	:	4BBS
Title	:	Structure of an initially transcribing RNA polymerase II-TFIIB complex
Authors	:	Sainsbury, S.; Niesser, J.; Cramer, P.
Deposited on	:	2012-09-27
Resolution	:	3.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

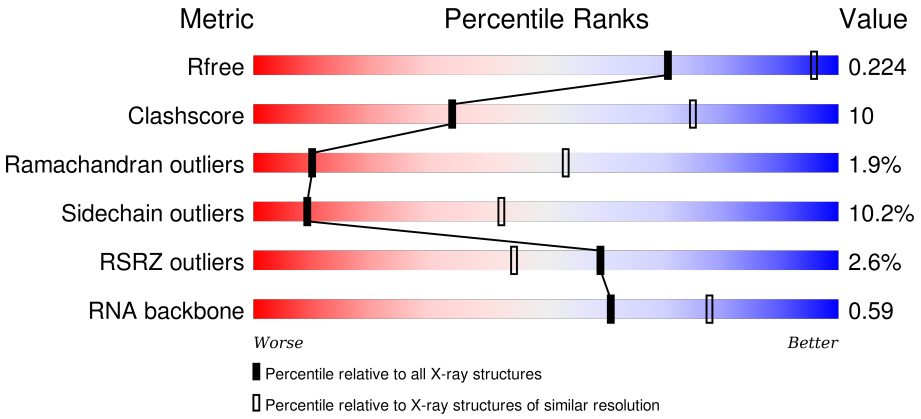
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)
RNA backbone	2183	1058 (4.40-2.80)

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 >=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 <=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	1733	57% 21% • 18%
2	B	1224	65% 26% • 6%
3	C	318	57% 24% • 16%
4	D	221	52% 22% 6% 19%

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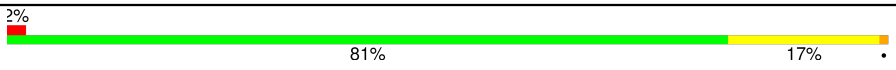
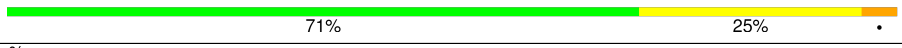
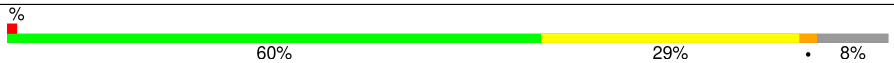
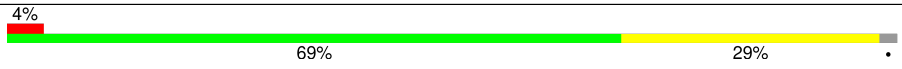
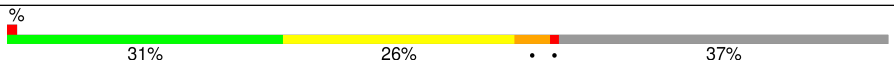
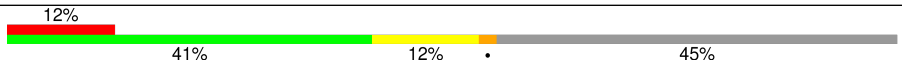
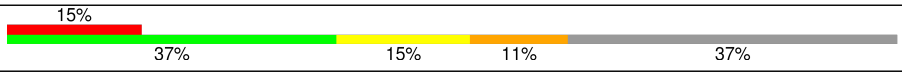
Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	14	
15	P	6	
16	T	27	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 33420 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 II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0	0
			11170	7039	1953	2116	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1150	Total	C	N	O	S	0	0	0
			9095	5751	1598	1690	56			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- 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	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- 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	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- 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	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	189	Total	C	N	O	S	0	0	0
			1357	838	240	267	12			

- Molecule 14 is a DNA chain called 5'-D(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*CP*GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	7	Total	C	N	O	P	0	0	0
			139	67	29	37	6			

- Molecule 15 is a RNA chain called 5'-R(*AP*UP*AP*UP*CP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

- Molecule 16 is a DNA chain called 5'-D(*AP*GP*CP*GP*CP*AP*GP*TP*TP*GP*TP*GP*CP*TP *AP*TP*GP*AP*TP*AP*TP*TP*TP*TP*TP*AP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	17	Total	C	N	O	P	0	0	0
			350	169	56	108	17			

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

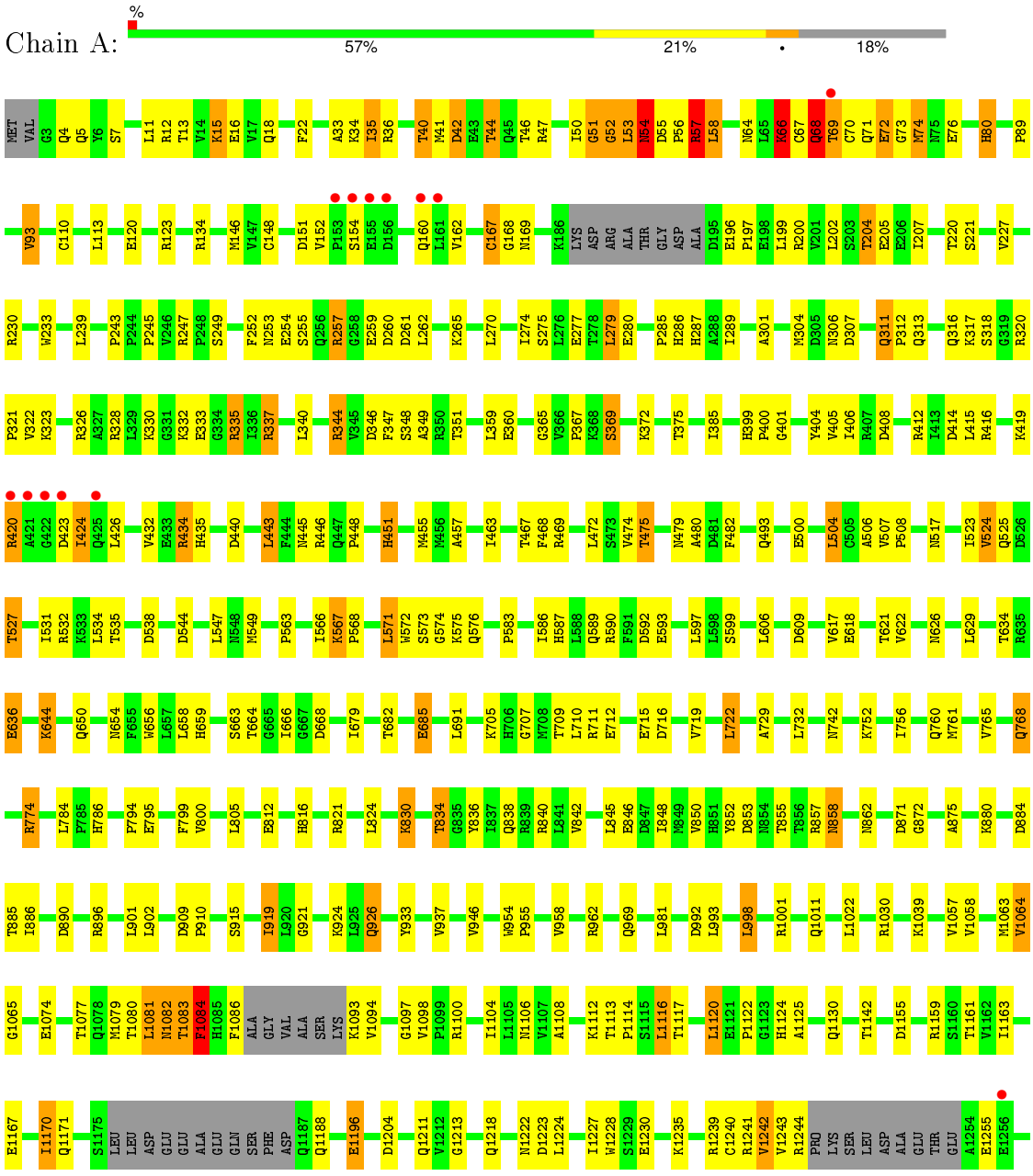
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	2	Total Mg 2 2	0	0

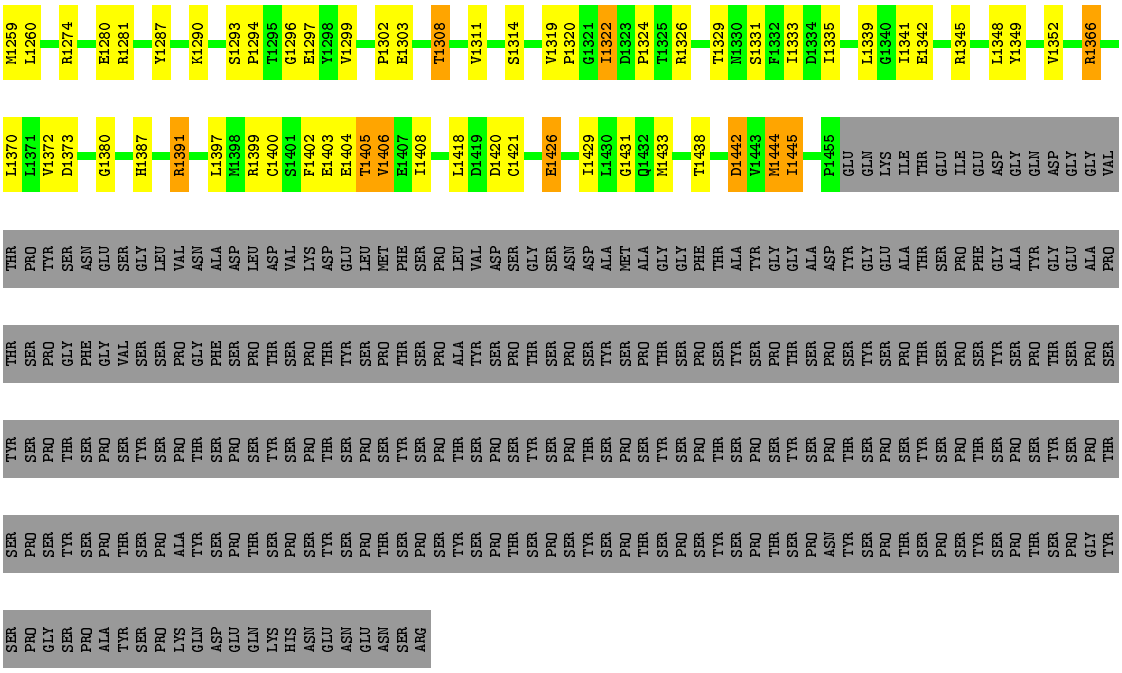
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

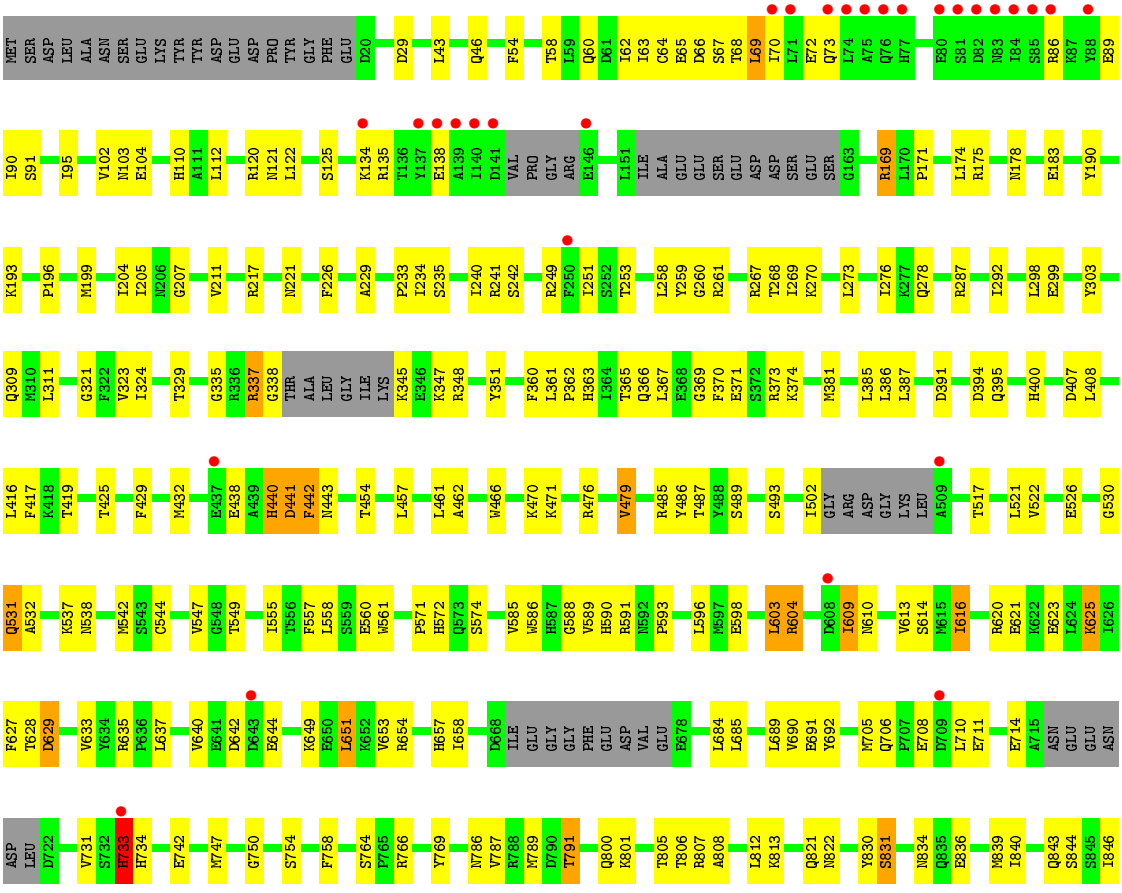
Chain A:

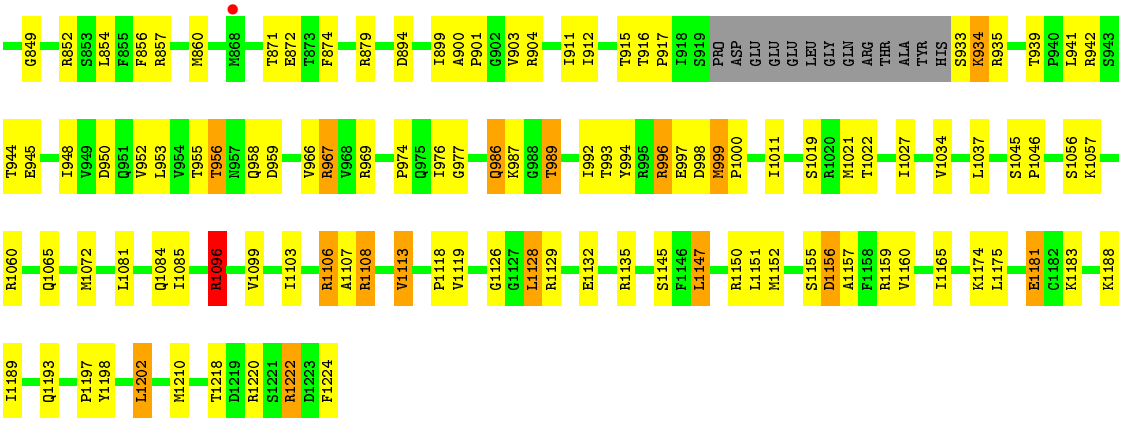




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

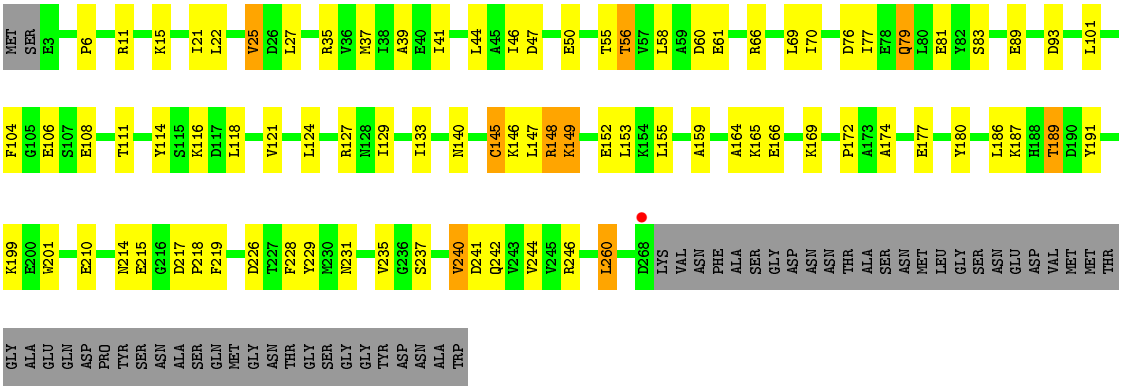
Chain B:





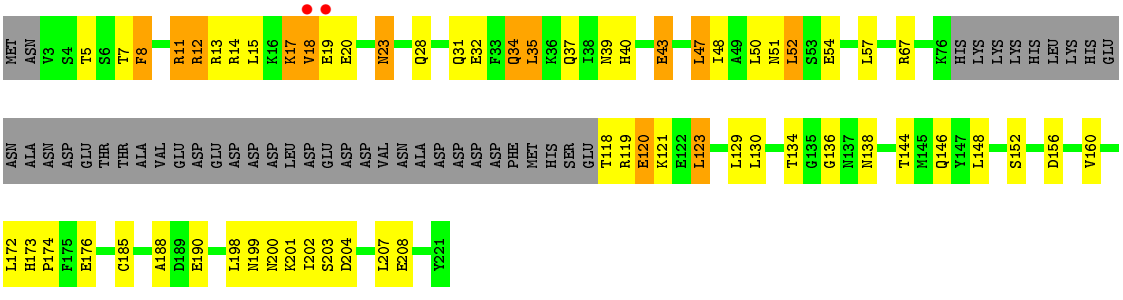
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:



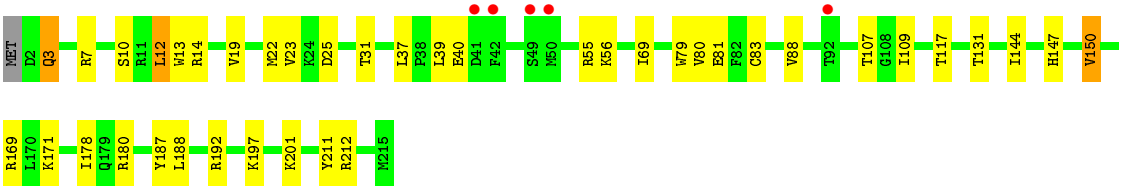
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D:



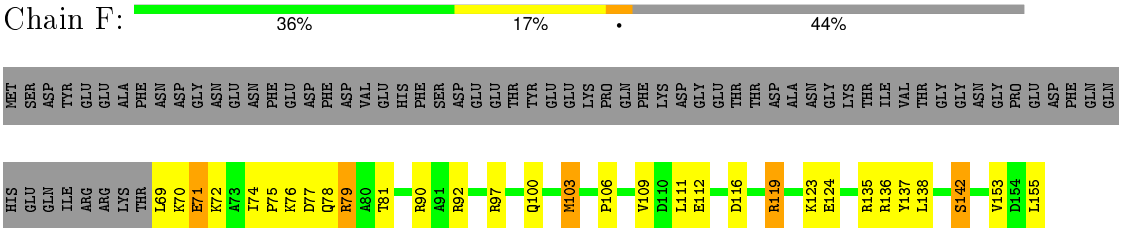
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E:



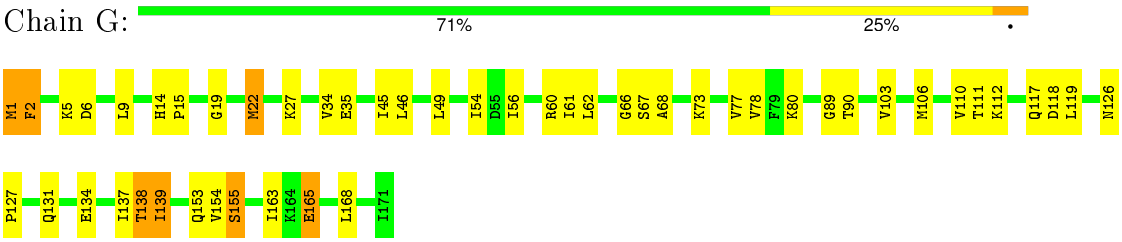
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F:



• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:

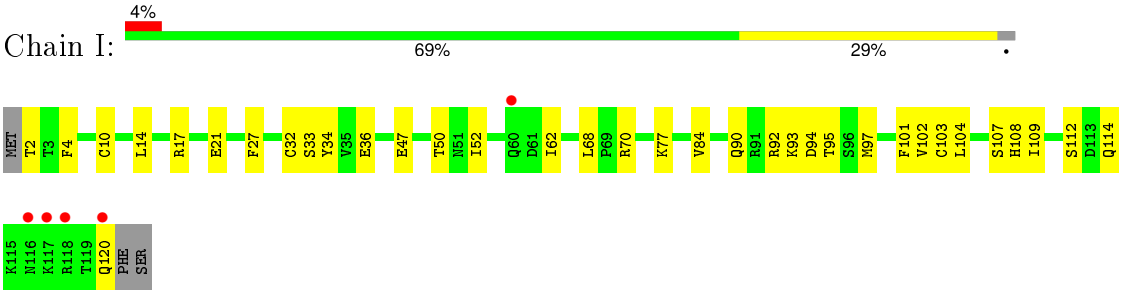


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:

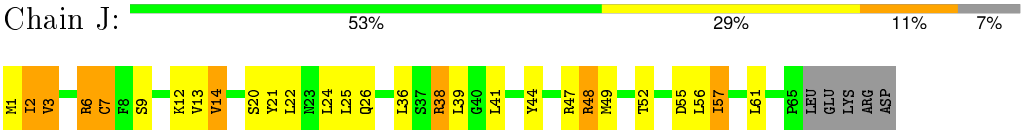
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:



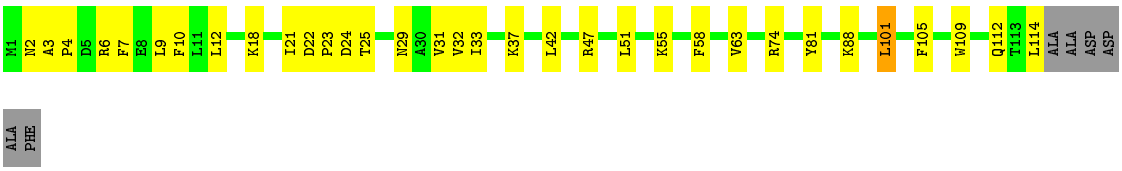
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:



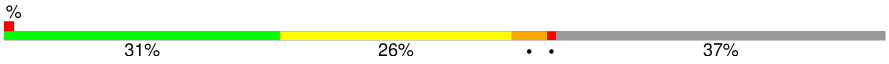
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

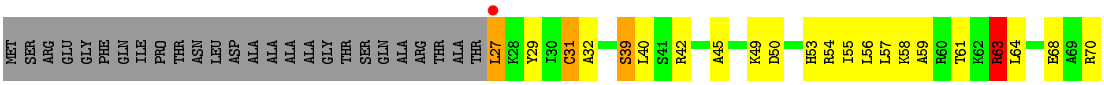
Chain K:



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

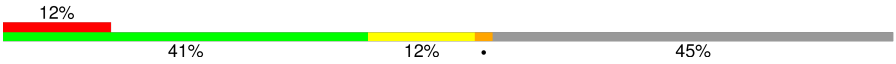
Chain L:

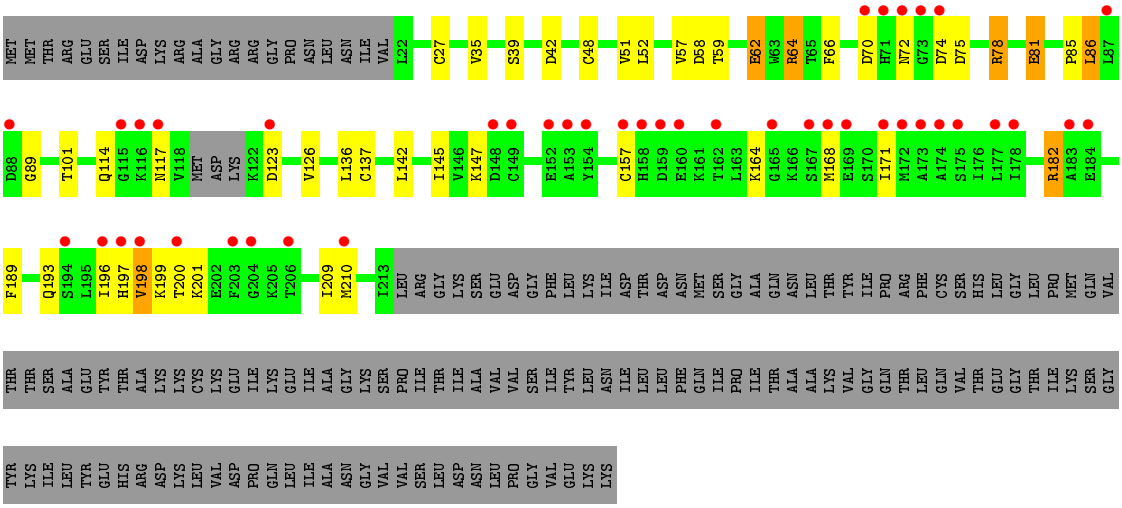




• Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB

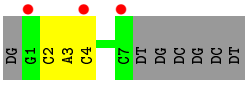
Chain M:





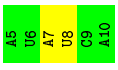
• Molecule 14: 5'-D(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*CP*GP*CP*TP)-3'

Chain N:



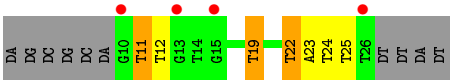
• Molecule 15: 5'-R(*AP*UP*AP*UP*CP*AP)-3'

Chain P:



• Molecule 16: 5'-D(*AP*GP*CP*GP*CP*AP*GP*TP*TP*GP*TP*GP*CP*TP *AP*TP*GP*AP*TP*AP*TP*TP*TP*TP*TP*AP*TP)-3'

Chain T:


DA
DG
DC
DG
DC
DA
G10
T11
T12
G13
T14
G15
T19
T22
A23
T24
T25
T26
DT
DT
DA
DT

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	222.17Å 386.01Å 254.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 3.60 49.33 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-3.60) 100.0 (49.33-3.60)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.185 , 0.225 0.180 , 0.224	Depositor DCC
R_{free} test set	1725 reflections (1.37%)	DCC
Wilson B-factor (Å^2)	87.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 99.0	EDS
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	3 of 252003 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	33420	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.38	0/11372	0.59	1/15380 (0.0%)
2	B	0.36	0/9271	0.56	0/12505
3	C	0.42	0/2133	0.58	0/2891
4	D	0.38	0/1444	0.59	0/1935
5	E	0.32	0/1788	0.51	0/2406
6	F	0.41	0/717	0.63	0/967
7	G	0.43	0/1368	0.61	0/1844
8	H	0.35	0/1094	0.55	0/1481
9	I	0.32	0/989	0.50	0/1331
10	J	0.45	0/541	0.70	1/727 (0.1%)
11	K	0.40	0/937	0.53	0/1265
12	L	0.41	0/353	0.58	0/468
13	M	0.29	0/1373	0.47	0/1863
14	N	0.63	0/156	1.06	0/238
15	P	0.32	0/137	0.81	0/211
16	T	0.62	0/390	1.37	3/601 (0.5%)
All	All	0.38	0/34063	0.59	5/46113 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	T	19	DT	O4'-C4'-C3'	-7.33	101.57	104.50
1	A	58	LEU	CA-CB-CG	5.74	128.51	115.30
16	T	22	DT	O4'-C1'-N1	5.73	112.01	108.00
10	J	3	VAL	CB-CA-C	-5.61	100.74	111.40
16	T	11	DT	N3-C4-O4	5.18	123.01	119.90

There are no chirality outliers.

There are no planarity outliers.

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	11170	0	11222	271	0
2	B	9095	0	9055	196	0
3	C	2095	0	2051	54	0
4	D	1434	0	1460	38	0
5	E	1752	0	1776	21	0
6	F	705	0	731	20	0
7	G	1340	0	1357	35	0
8	H	1076	0	1046	25	0
9	I	971	0	927	15	0
10	J	532	0	542	23	0
11	K	919	0	929	19	0
12	L	351	0	374	17	0
13	M	1357	0	1263	27	0
14	N	139	0	79	2	0
15	P	123	0	66	1	0
16	T	350	0	197	6	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
17	M	1	0	0	0	0
18	A	2	0	0	0	0
All	All	33420	0	33075	674	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 674 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)
7:G:1:MET:HE3	7:G:80:LYS:H	1.15	1.04
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.30	0.95
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG21	1:A:857:ARG:HE	1.36	0.90
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.59	0.84

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	1409/1733 (81%)	1273 (90%)	104 (7%)	32 (2%)	8 50
2	B	1134/1224 (93%)	1016 (90%)	97 (9%)	21 (2%)	10 53
3	C	264/318 (83%)	245 (93%)	17 (6%)	2 (1%)	24 69
4	D	174/221 (79%)	157 (90%)	12 (7%)	5 (3%)	6 44
5	E	212/215 (99%)	200 (94%)	11 (5%)	1 (0%)	34 77
6	F	85/155 (55%)	81 (95%)	4 (5%)	0	100 100
7	G	169/171 (99%)	152 (90%)	15 (9%)	2 (1%)	16 62
8	H	130/146 (89%)	111 (85%)	15 (12%)	4 (3%)	5 43
9	I	117/122 (96%)	99 (85%)	16 (14%)	2 (2%)	11 55
10	J	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	5 42
11	K	112/120 (93%)	107 (96%)	5 (4%)	0	100 100
12	L	42/70 (60%)	29 (69%)	8 (19%)	5 (12%)	0 8
13	M	185/345 (54%)	164 (89%)	19 (10%)	2 (1%)	17 64
All	All	4096/4910 (83%)	3691 (90%)	327 (8%)	78 (2%)	10 53

5 of 78 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	MET

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Mol	Chain	Res	Type
1	A	286	HIS
1	A	317	LYS
1	A	593	GLU
1	A	885	THR

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	1241/1520 (82%)	1112 (90%)	129 (10%)	9 42
2	B	980/1061 (92%)	886 (90%)	94 (10%)	10 45
3	C	234/274 (85%)	211 (90%)	23 (10%)	10 44
4	D	160/200 (80%)	140 (88%)	20 (12%)	6 32
5	E	196/197 (100%)	186 (95%)	10 (5%)	29 70
6	F	77/137 (56%)	67 (87%)	10 (13%)	5 30
7	G	152/152 (100%)	136 (90%)	16 (10%)	8 41
8	H	118/128 (92%)	109 (92%)	9 (8%)	16 56
9	I	113/116 (97%)	101 (89%)	12 (11%)	8 40
10	J	60/65 (92%)	49 (82%)	11 (18%)	2 14
11	K	99/102 (97%)	89 (90%)	10 (10%)	9 43
12	L	39/57 (68%)	35 (90%)	4 (10%)	9 42
13	M	136/299 (46%)	118 (87%)	18 (13%)	5 30
All	All	3605/4308 (84%)	3239 (90%)	366 (10%)	9 42

5 of 366 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	560	GLU
2	B	999	MET
11	K	31	VAL
2	B	609	ILE
2	B	813	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	236	HIS
2	B	325	GLN
5	E	153	HIS
1	A	969	GLN
4	D	51	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 11 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^{th} 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	1419/1733 (81%)	-0.23	13 (0%) 85 75	47, 92, 160, 278	0
2	B	1150/1224 (93%)	-0.24	30 (2%) 59 44	49, 99, 176, 251	0
3	C	266/318 (83%)	-0.25	1 (0%) 93 88	49, 77, 123, 208	0
4	D	178/221 (80%)	-0.14	2 (1%) 82 70	63, 102, 166, 211	0
5	E	214/215 (99%)	0.10	5 (2%) 64 48	73, 130, 188, 213	0
6	F	87/155 (56%)	-0.39	0 100 100	58, 80, 123, 140	0
7	G	171/171 (100%)	-0.31	0 100 100	58, 81, 123, 136	0
8	H	134/146 (91%)	-0.00	2 (1%) 76 64	76, 120, 176, 222	0
9	I	119/122 (97%)	0.06	5 (4%) 40 28	90, 126, 199, 218	0
10	J	65/70 (92%)	-0.45	0 100 100	58, 79, 119, 152	0
11	K	114/120 (95%)	-0.22	0 100 100	57, 80, 129, 153	0
12	L	44/70 (62%)	-0.22	1 (2%) 64 48	80, 128, 181, 210	0
13	M	189/345 (54%)	1.06	43 (22%) 1 1	81, 170, 229, 272	0
14	N	7/14 (50%)	2.07	3 (42%) 0 0	200, 213, 233, 239	0
15	P	6/6 (100%)	1.03	0 100 100	169, 184, 220, 237	0
16	T	17/27 (62%)	1.34	4 (23%) 1 1	163, 197, 261, 274	0
All	All	4180/4957 (84%)	-0.14	109 (2%) 59 44	47, 97, 183, 278	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	72	ASN	5.7
13	M	73	GLY	5.6
1	A	422	GLY	5.2
1	A	69	THR	5.1
2	B	81	SER	4.8

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)

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^{th} 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^2)	Q<0.9
18	MG	A	2458	1/1	0.78	0.26	1.04	109,109,109,109	0
17	ZN	B	2225	1/1	1.00	0.16	-0.55	71,71,71,71	0
17	ZN	I	1121	1/1	1.00	0.10	-1.16	109,109,109,109	0
17	ZN	A	2457	1/1	0.99	0.12	-1.21	94,94,94,94	0
17	ZN	J	1066	1/1	0.99	0.17	-1.32	69,69,69,69	0
17	ZN	L	1071	1/1	0.98	0.07	-1.39	162,162,162,162	0
17	ZN	C	1269	1/1	1.00	0.07	-1.74	86,86,86,86	0
17	ZN	M	1216	1/1	0.98	0.06	-2.05	111,111,111,111	0
17	ZN	I	1122	1/1	0.99	0.04	-2.26	145,145,145,145	0
17	ZN	A	2456	1/1	1.00	0.05	-2.57	118,118,118,118	0
18	MG	A	2459	1/1	0.79	0.75	-	104,104,104,104	0

6.5 Other polymers (i)

There are no such residues in this entry.