wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:12 PM GMT

PDB ID	:	1SFO
Title	:	RNA POLYMERASE II STRAND SEPARATED ELONGATION COMPLEX
Authors	:	Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on	:	2004-02-20
Resolution	:	3.61 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:

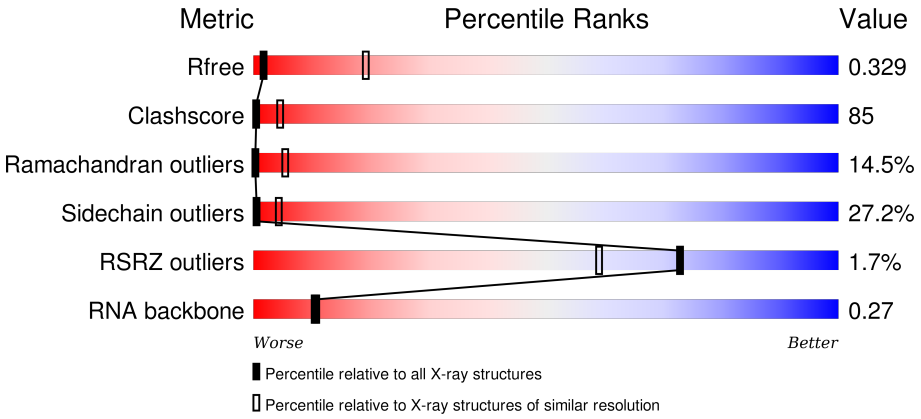
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.61 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	1093 (3.80-3.44)
Clashscore	102246	1043 (3.78-3.46)
Ramachandran outliers	100387	1003 (3.78-3.46)
Sidechain outliers	100360	1003 (3.78-3.46)
RSRZ outliers	91569	1100 (3.80-3.44)
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	R	10	20% 40% 40% 20%
2	T	14	29% 50% 43% 7%
3	A	1733	% 12% 39% 23% 6% 20%
4	B	1224	% 15% 48% 21% 6% 10%

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Mol	Chain	Length	Quality of chain
5	C	318	19% 44% 18% 16%
6	E	215	7% 16% 51% 27% 7%
7	F	155	10% 31% 12% 46%
8	H	146	2% 13% 40% 29% 9% 9%
9	I	122	18% 40% 30% 10%
10	J	70	14% 44% 26% 9% 7%
11	K	120	14% 61% 18% 5%
12	L	70	6% 21% 31% 7% 34%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28647 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

- Molecule 2 is a DNA chain called DNA STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	14	Total	C	N	O	P	0	0	0
			279	135	48	83	13			

- Molecule 3 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1106	Total	C	N	O	S	0	0	0
			8793	5568	1538	1632	55			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

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 8.3 kDa polypeptide.

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 13.6 kDa polypeptide.

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 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

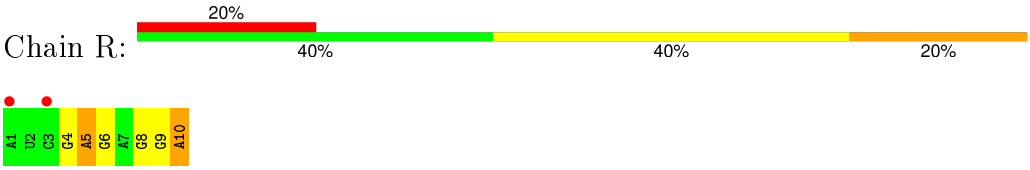
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total Mg 1 1	0	0

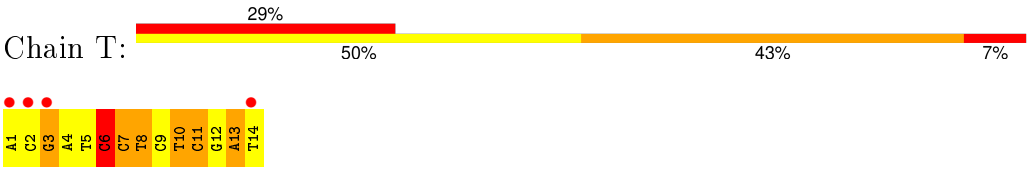
3 Residue-property plots (i)

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.

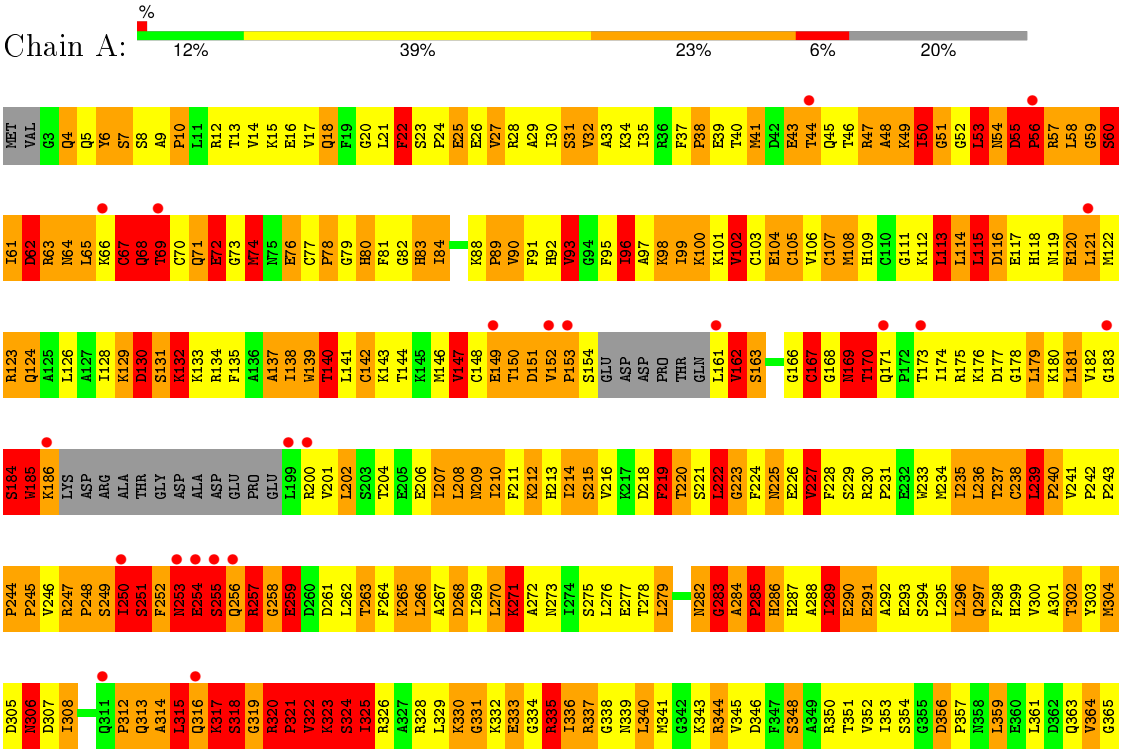
- Molecule 1: RNA STRAND

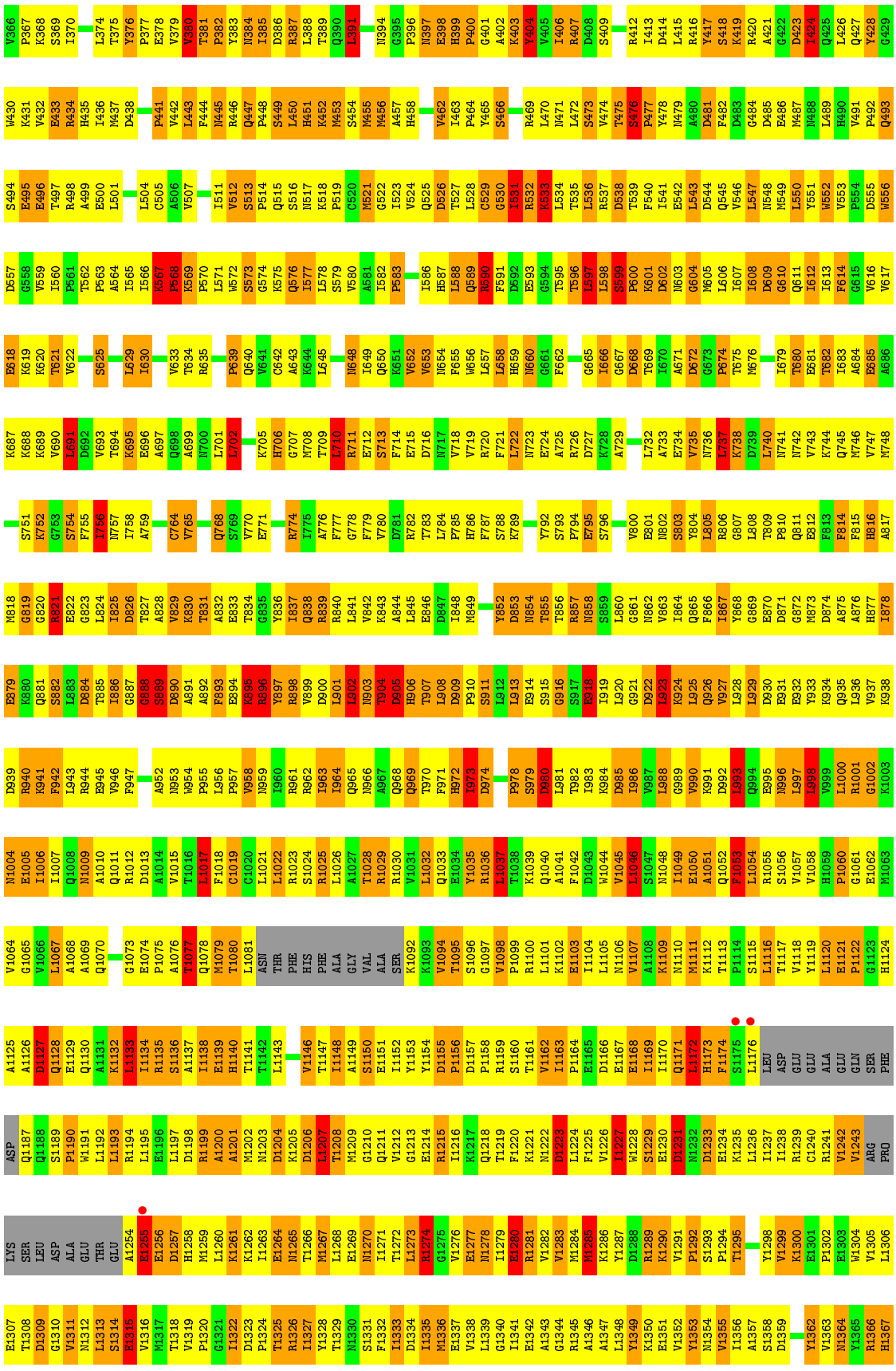


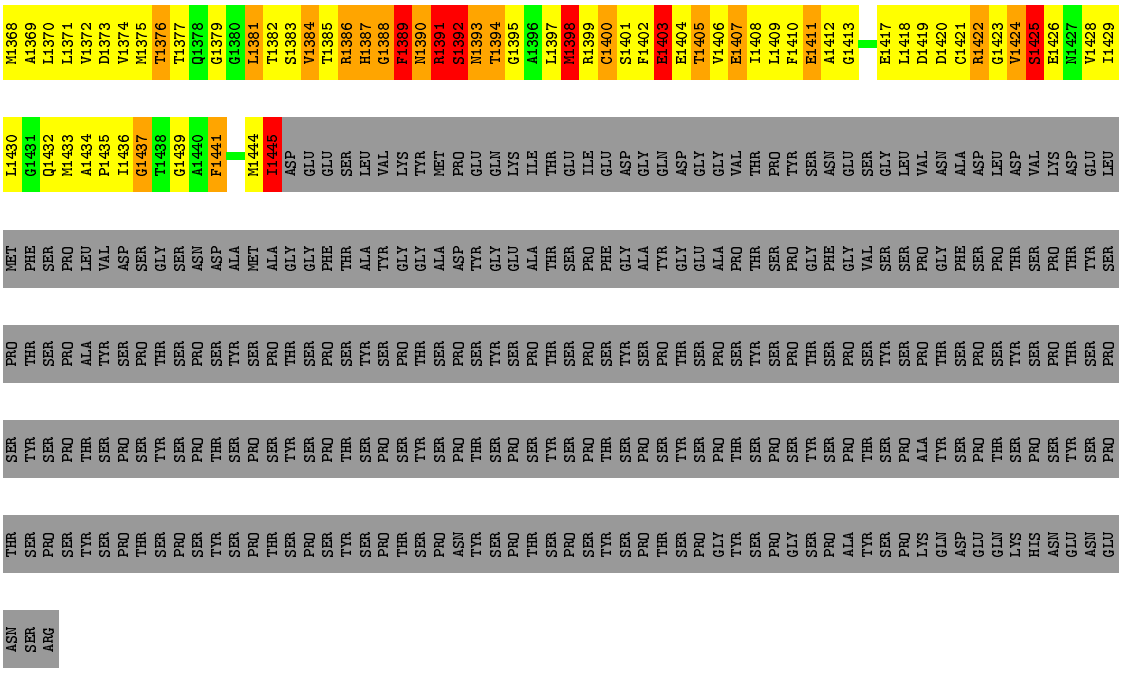
- Molecule 2: DNA STRAND

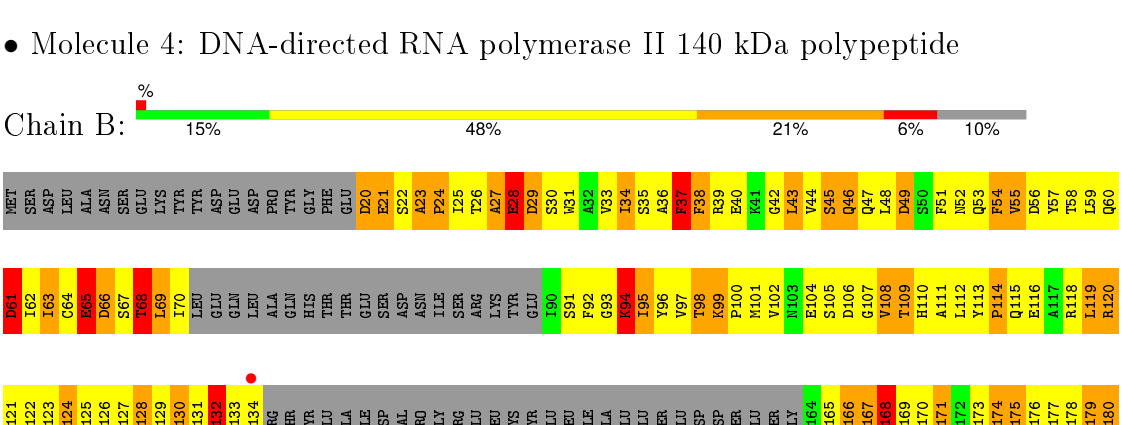


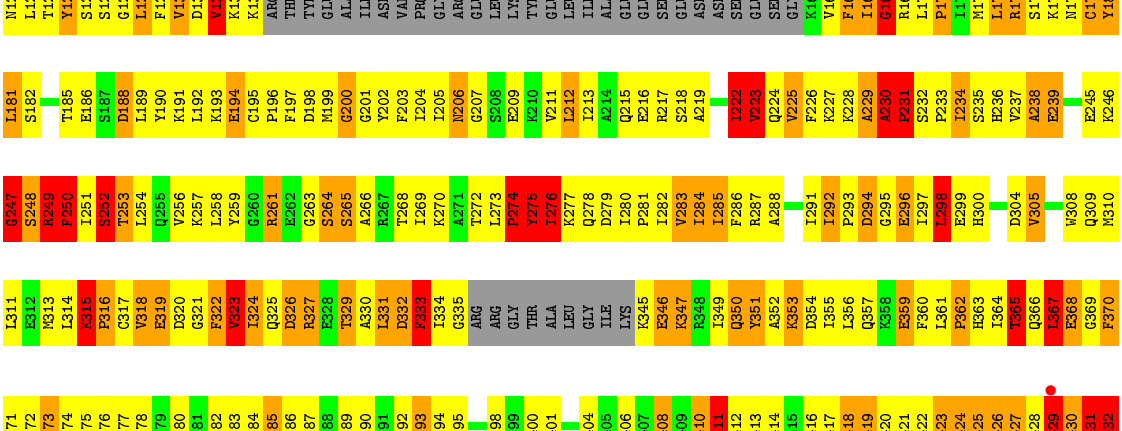
- Molecule 3: DNA-directed RNA polymerase II largest subunit

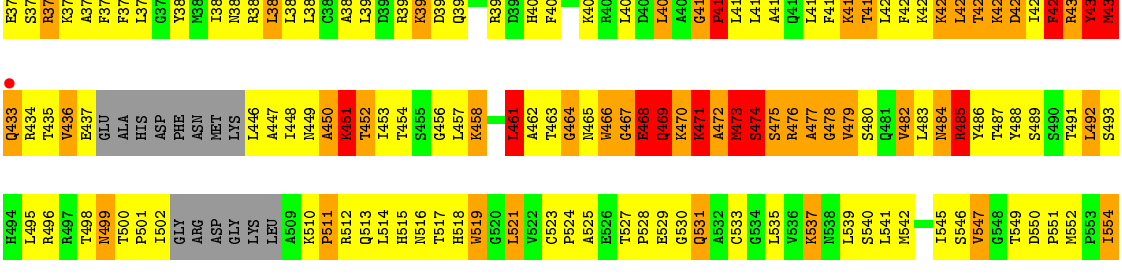






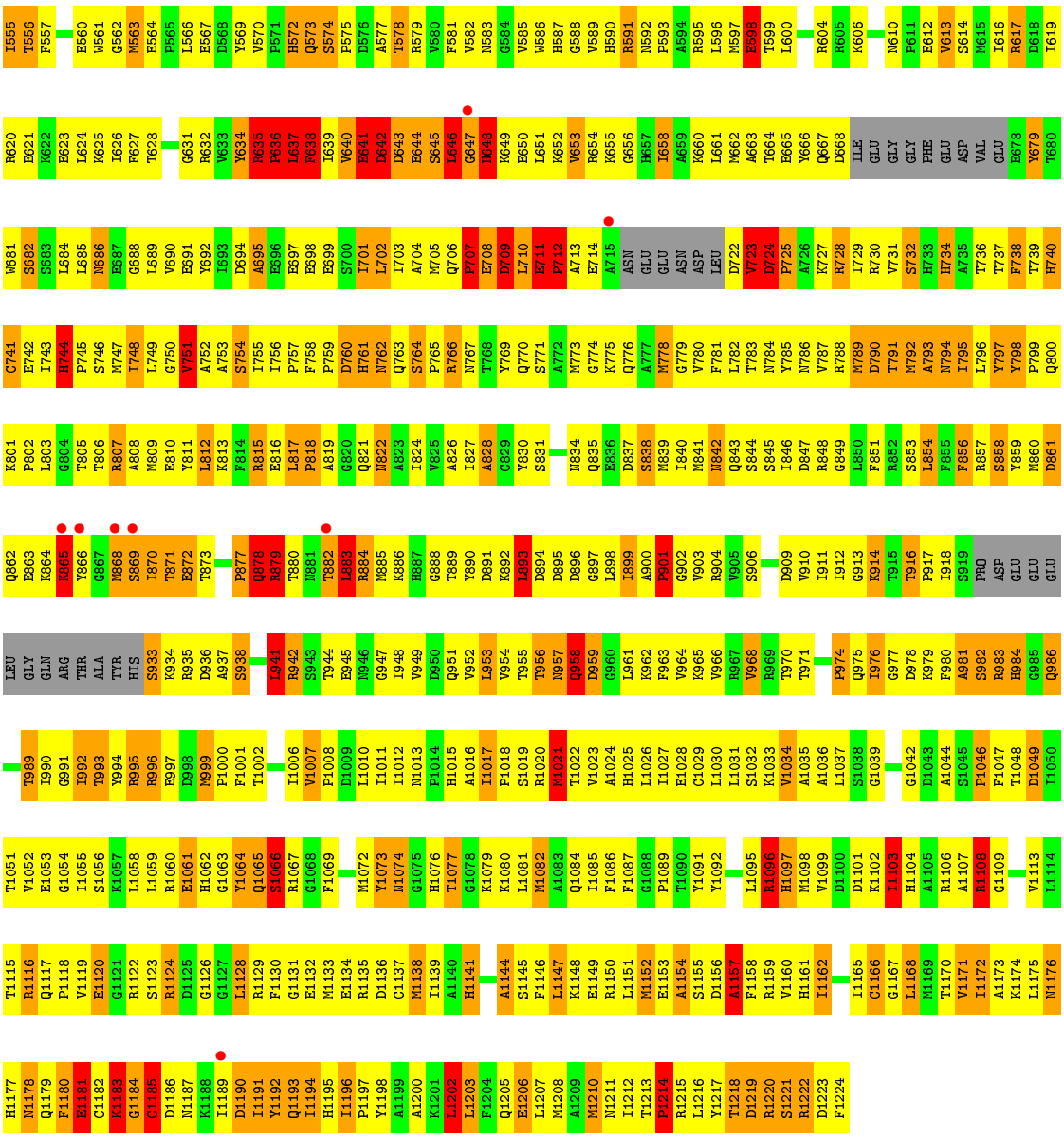






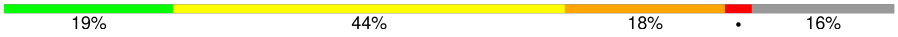
• Molecule 4: DNA-directed RNA polymerase II 140 kDa polypeptide

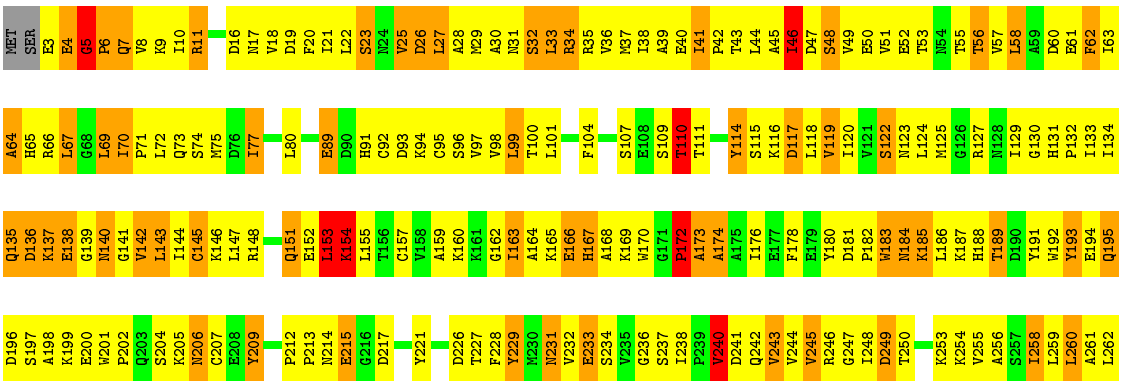
Chain B:



• Molecule 5: DNA-directed RNA polymerase II 45 kDa polypeptide

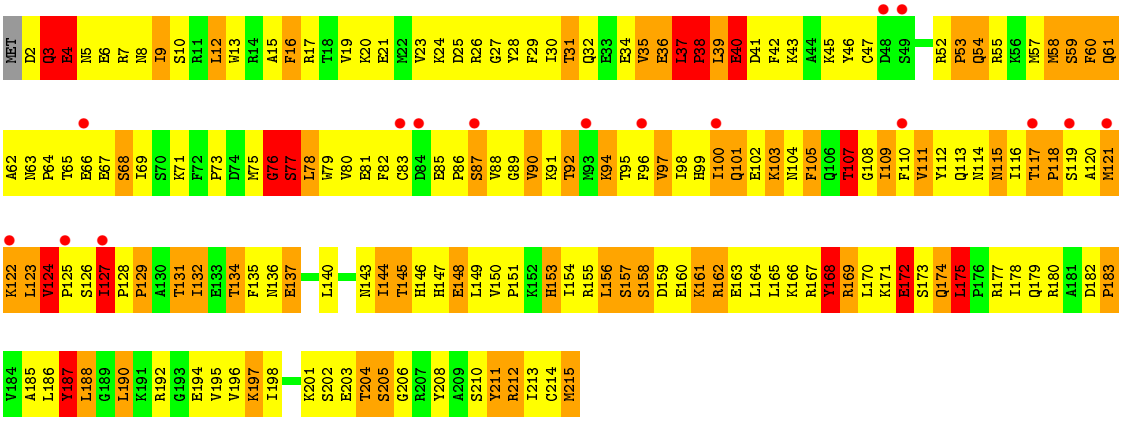
Chain C:





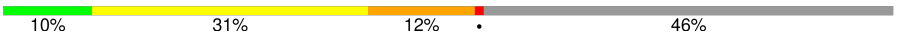
• Molecule 6: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

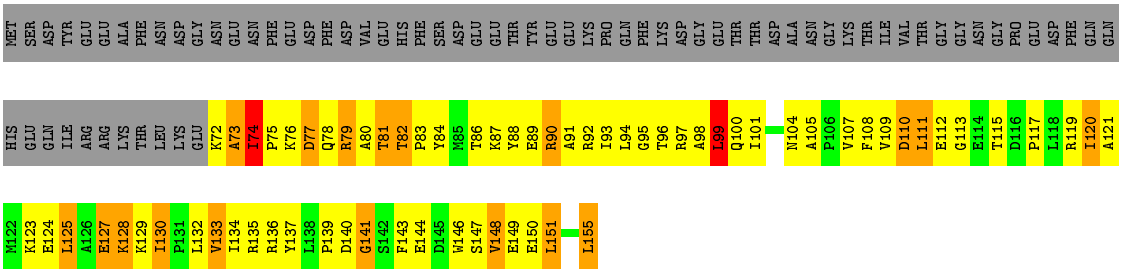
Chain E:



• Molecule 7: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

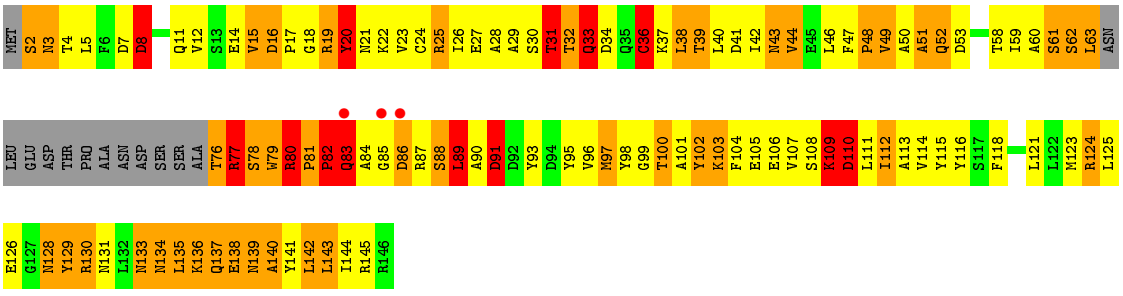
Chain F:





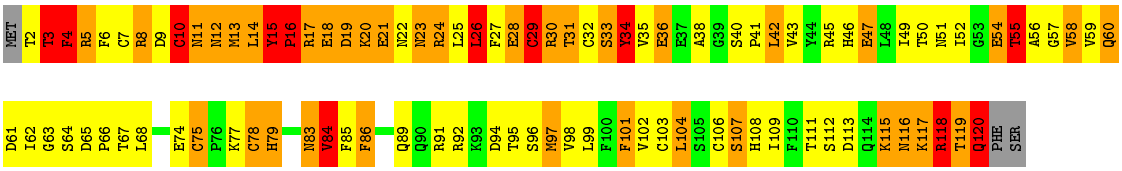
• Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



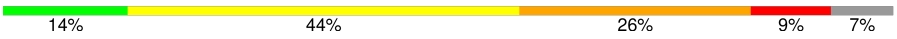
• Molecule 9: DNA-directed RNA polymerase II 14.2 kDa polypeptide

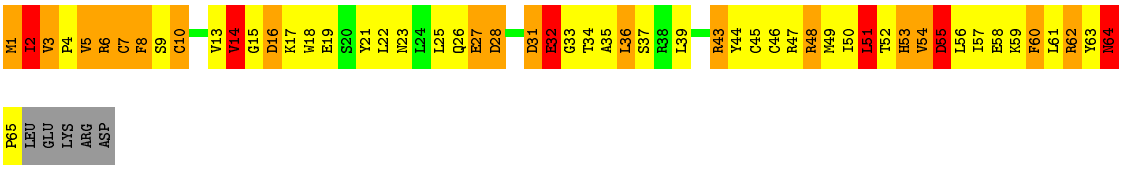
Chain I:



• Molecule 10: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

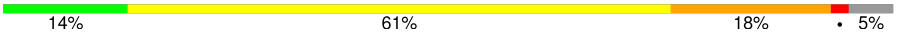
Chain J:





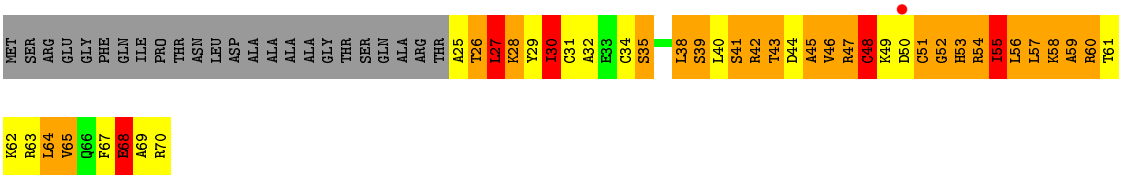
• Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



• Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	167.08Å 221.26Å 193.69Å 90.00° 100.10° 90.00°	Depositor
Resolution (Å)	39.86 – 3.61 39.86 – 3.60	Depositor EDS
% Data completeness (in resolution range)	92.7 (39.86-3.61) 92.7 (39.86-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 3.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.315 , 0.343 0.309 , 0.329	Depositor DCC
R_{free} test set	7393 reflections (10.05%)	DCC
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , -1.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 80020 reflections	Xtriage
F_o,F_c correlation	0.76	EDS
Total number of atoms	28647	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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	R	0.67	0/244	0.83	0/380
2	T	0.75	0/311	1.39	3/477 (0.6%)
3	A	0.88	15/11163 (0.1%)	1.45	167/15091 (1.1%)
4	B	0.84	7/8964 (0.1%)	1.38	114/12086 (0.9%)
5	C	0.78	0/2133	1.24	13/2891 (0.4%)
6	E	0.90	2/1788 (0.1%)	1.40	14/2406 (0.6%)
7	F	0.83	0/691	1.28	7/933 (0.8%)
8	H	0.85	1/1086 (0.1%)	1.59	20/1470 (1.4%)
9	I	1.03	2/989 (0.2%)	1.64	23/1331 (1.7%)
10	J	0.78	0/541	1.44	7/727 (1.0%)
11	K	0.74	0/937	1.20	5/1265 (0.4%)
12	L	0.99	1/366 (0.3%)	1.78	12/485 (2.5%)
All	All	0.86	28/29213 (0.1%)	1.41	385/39542 (1.0%)

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
2	T	0	5
3	A	1	6
4	B	0	7
5	C	0	2
6	E	0	1
9	I	0	1
All	All	1	22

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	319	GLY	C-O	10.97	1.41	1.23
3	A	255	SER	CA-CB	8.59	1.65	1.52
3	A	320	ARG	CA-CB	8.38	1.72	1.53
3	A	320	ARG	CG-CD	7.83	1.71	1.51
4	B	595	ARG	CG-CD	7.49	1.70	1.51

The worst 5 of 385 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	321	PRO	N-CA-C	-18.56	63.84	112.10
3	A	322	VAL	N-CA-C	14.54	150.26	111.00
10	J	10	CYS	CA-CB-SG	12.01	135.61	114.00
3	A	315	LEU	CA-CB-CG	11.82	142.50	115.30
4	B	478	GLY	N-CA-C	-11.76	83.71	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	322	VAL	CA

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	T	10	DT	Sidechain
2	T	11	DC	Sidechain
2	T	13	DA	Sidechain
2	T	6	DC	Sidechain
2	T	8	DT	Sidechain

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	R	217	0	110	18	0
2	T	279	0	160	43	0
3	A	10969	0	11070	2106	0
4	B	8793	0	8823	1592	0
5	C	2095	0	2051	337	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1752	0	1776	303	0
7	F	679	0	701	127	0
8	H	1068	0	1040	193	0
9	I	971	0	929	162	0
10	J	532	0	542	125	0
11	K	919	0	929	175	0
12	L	364	0	387	65	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	28647	0	28518	4856	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 85.

The worst 5 of 4856 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)
3:A:853:ASP:OD1	3:A:855:THR:HB	1.32	1.25
3:A:90:VAL:HG12	3:A:297:GLN:NE2	1.49	1.24
4:B:635:ARG:HB2	4:B:636:PRO:CD	1.65	1.21
3:A:321:PRO:O	3:A:322:VAL:HG22	1.41	1.18
3:A:351:THR:HG23	4:B:1103:ILE:HD12	1.23	1.18

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
3	A	1383/1733 (80%)	851 (62%)	315 (23%)	217 (16%)	0 4
4	B	1088/1224 (89%)	730 (67%)	214 (20%)	144 (13%)	0 6
5	C	264/318 (83%)	187 (71%)	49 (19%)	28 (11%)	0 10
6	E	212/215 (99%)	142 (67%)	41 (19%)	29 (14%)	0 6
7	F	82/155 (53%)	49 (60%)	26 (32%)	7 (8%)	1 14
8	H	129/146 (88%)	87 (67%)	16 (12%)	26 (20%)	0 2
9	I	117/122 (96%)	74 (63%)	24 (20%)	19 (16%)	0 4
10	J	63/70 (90%)	42 (67%)	11 (18%)	10 (16%)	0 4
11	K	112/120 (93%)	81 (72%)	20 (18%)	11 (10%)	1 12
12	L	44/70 (63%)	20 (46%)	10 (23%)	14 (32%)	0 0
All	All	3494/4173 (84%)	2263 (65%)	726 (21%)	505 (14%)	0 5

5 of 505 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	44	THR
3	A	50	ILE
3	A	55	ASP
3	A	56	PRO
3	A	57	ARG

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
3	A	1218/1520 (80%)	859 (70%)	359 (30%)	0 3
4	B	960/1061 (90%)	718 (75%)	242 (25%)	1 6
5	C	234/274 (85%)	175 (75%)	59 (25%)	1 6
6	E	196/197 (100%)	141 (72%)	55 (28%)	0 4
7	F	74/137 (54%)	57 (77%)	17 (23%)	1 8
8	H	117/128 (91%)	80 (68%)	37 (32%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	I	113/116 (97%)	84 (74%)	29 (26%)	0 5
10	J	60/65 (92%)	42 (70%)	18 (30%)	0 3
11	K	99/102 (97%)	81 (82%)	18 (18%)	2 14
12	L	40/57 (70%)	27 (68%)	13 (32%)	0 2
All	All	3111/3657 (85%)	2264 (73%)	847 (27%)	0 4

5 of 847 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	177	LYS
4	B	635	ARG
9	I	31	THR
4	B	234	ILE
4	B	408	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	46	GLN
4	B	515	HIS
9	I	12	ASN
4	B	121	ASN
4	B	366	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	5	A
1	R	10	A

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 9 ligands modelled in this entry, 9 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	R	10/10 (100%)	1.37	2 (20%) 1 1	30, 82, 200, 200	0
2	T	14/14 (100%)	1.08	4 (28%) 1 1	30, 107, 200, 200	0
3	A	1395/1733 (80%)	-0.12	25 (1%) 71 57	30, 32, 134, 200	0
4	B	1106/1224 (90%)	-0.20	11 (0%) 84 73	30, 30, 118, 198	0
5	C	266/318 (83%)	-0.31	0 100 100	30, 30, 84, 140	0
6	E	214/215 (99%)	0.31	16 (7%) 17 12	30, 67, 153, 200	0
7	F	84/155 (54%)	-0.05	0 100 100	30, 31, 93, 141	0
8	H	133/146 (91%)	-0.05	3 (2%) 64 49	30, 47, 138, 190	0
9	I	119/122 (97%)	-0.06	0 100 100	30, 32, 114, 163	0
10	J	65/70 (92%)	-0.37	0 100 100	30, 30, 96, 141	0
11	K	114/120 (95%)	-0.33	0 100 100	30, 30, 73, 107	0
12	L	46/70 (65%)	-0.21	1 (2%) 65 50	30, 45, 132, 158	0
All	All	3566/4197 (84%)	-0.13	62 (1%) 73 59	30, 31, 130, 200	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	866	TYR	5.8
3	A	316	GLN	4.9
2	T	1	DA	4.9
3	A	1175	SER	4.6
3	A	149	GLU	4.5

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

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
13	ZN	A	1734	1/1	0.84	0.29	-0.48	22,22,22,22	0
13	ZN	I	204	1/1	0.96	0.17	-0.68	22,22,22,22	0
13	ZN	I	203	1/1	0.93	0.21	-0.72	22,22,22,22	0
13	ZN	B	1307	1/1	0.91	0.11	-1.61	22,22,22,22	0
13	ZN	L	105	1/1	0.98	0.06	-1.93	22,22,22,22	0
13	ZN	A	1735	1/1	0.87	0.10	-2.07	22,22,22,22	0
13	ZN	C	319	1/1	0.98	0.06	-2.66	22,22,22,22	0
13	ZN	J	101	1/1	0.94	0.11	-4.98	22,22,22,22	0
14	MG	A	2000	1/1	0.70	0.19	-	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.