wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2025 – 05:55 AM EDT

PDB ID	:	2NVY / pdb_00002nvy
Title	:	RNA Polymerase II form II in 150 mM Mn+2
Authors	:	Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on	:	2006-11-13
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

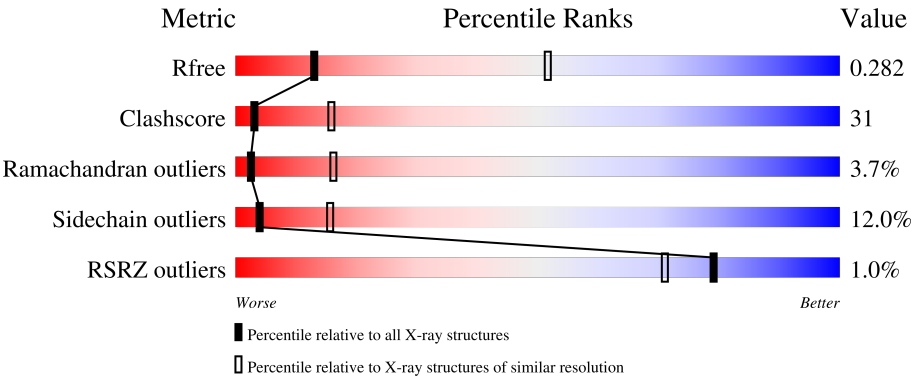
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	% 38% 36% 8% · 18%
2	B	1224	% 41% 42% 6% 11%
3	C	318	34% 39% 10% 16%
4	E	215	53% 40% 7%
5	F	155	21% 32% · 46%

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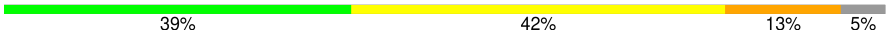
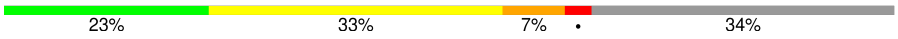
Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 28289 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 largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0	0
			11154	7023	1952	2118	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1094	Total	C	N	O	S	0	0	0
			8711	5525	1519	1614	53			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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 polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

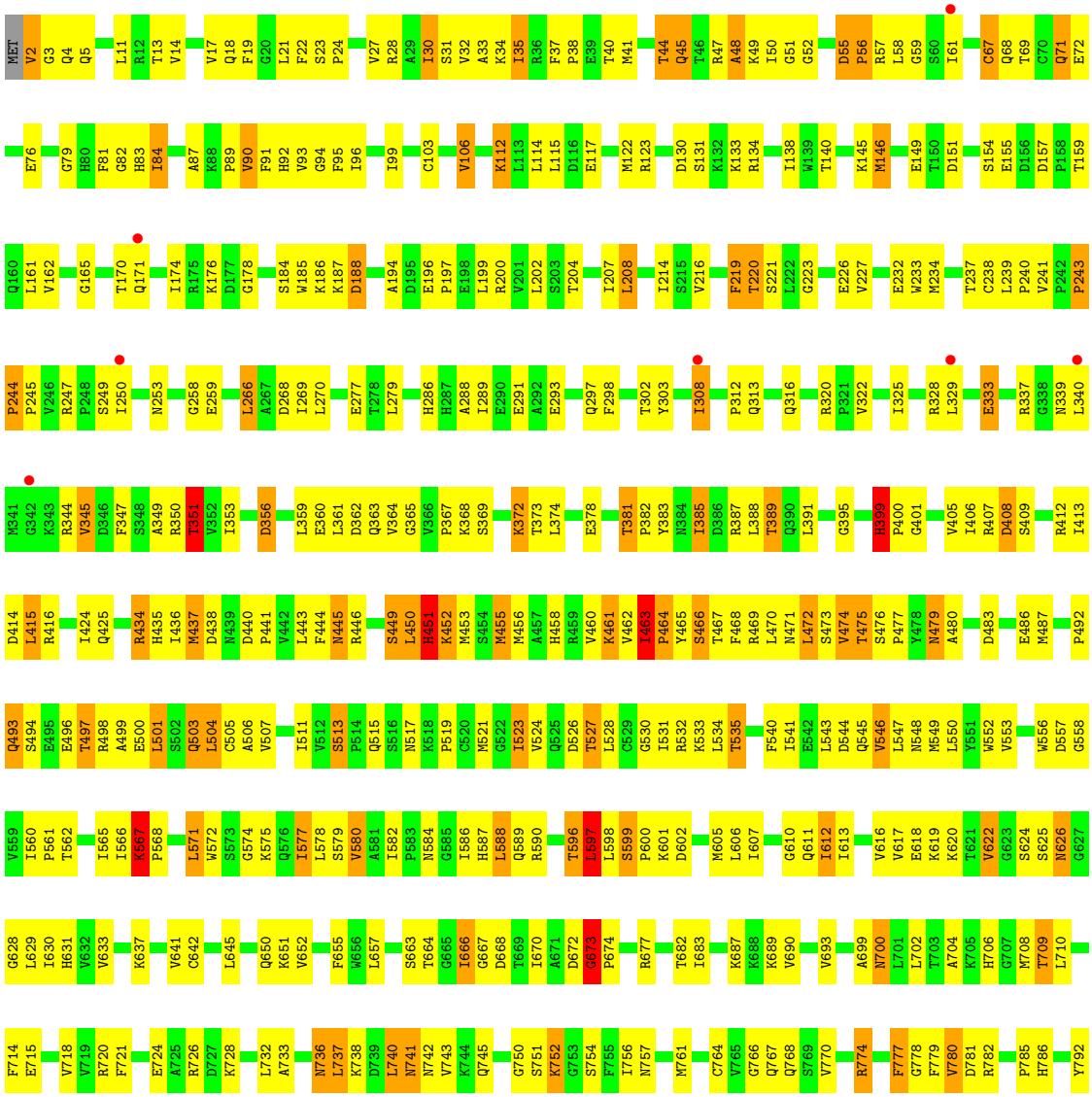
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	2	Total Mn 2 2	0	0

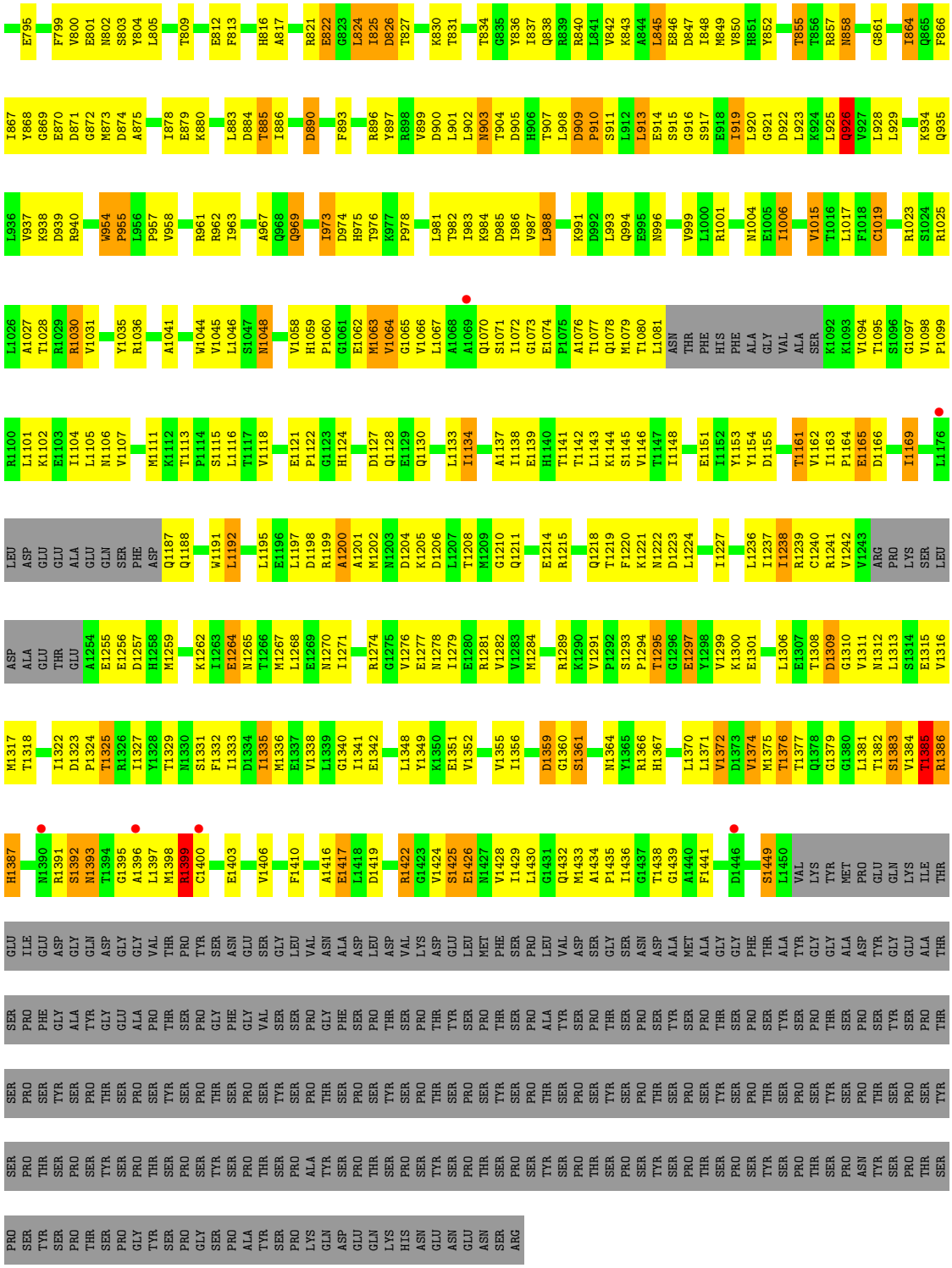
3 Residue-property plots (i)

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

• Molecule 1: DNA-directed RNA polymerase II largest subunit

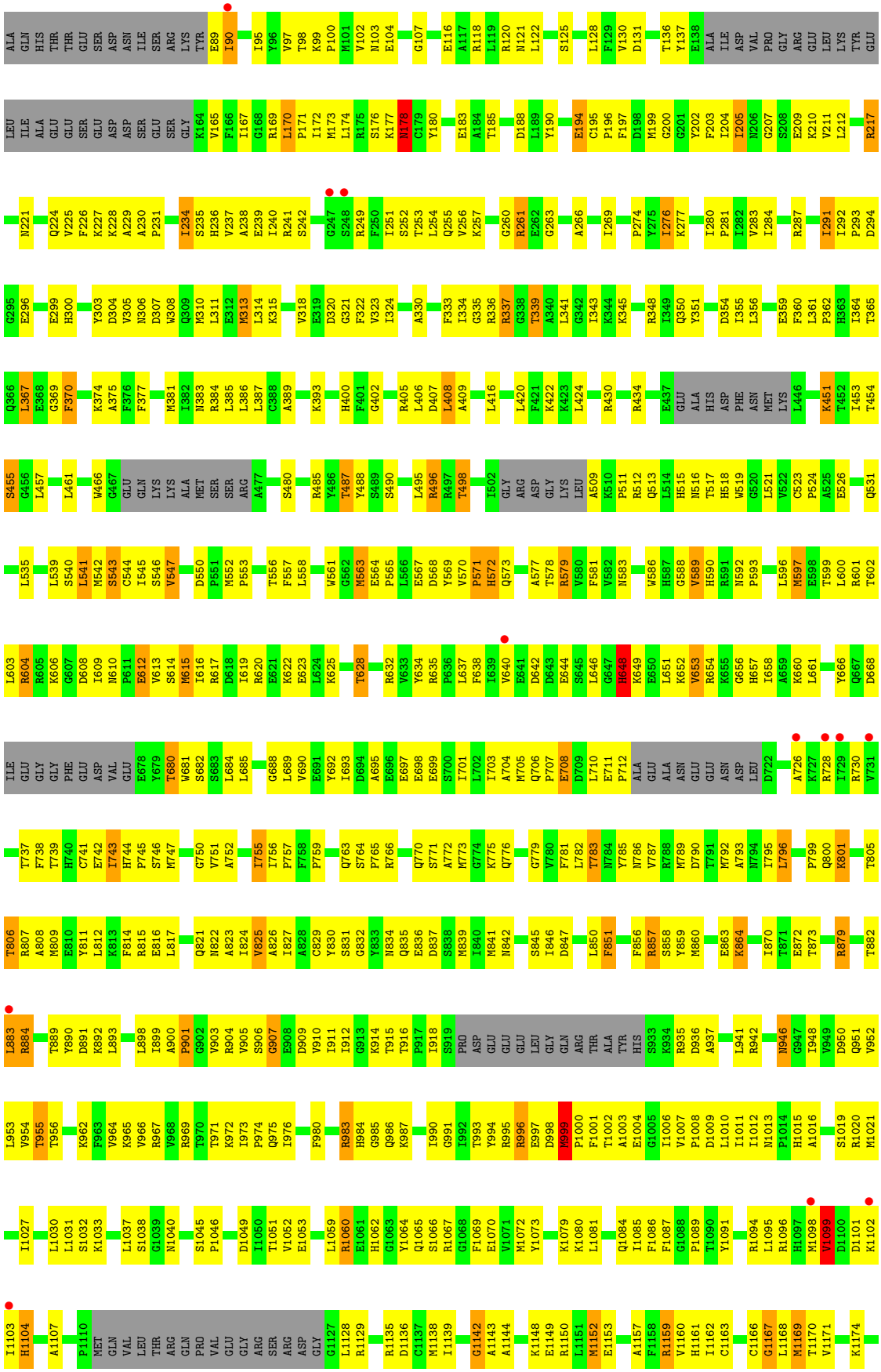
Chain A:

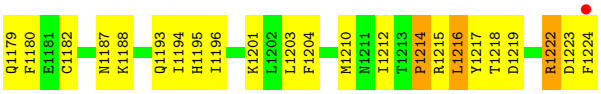




• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

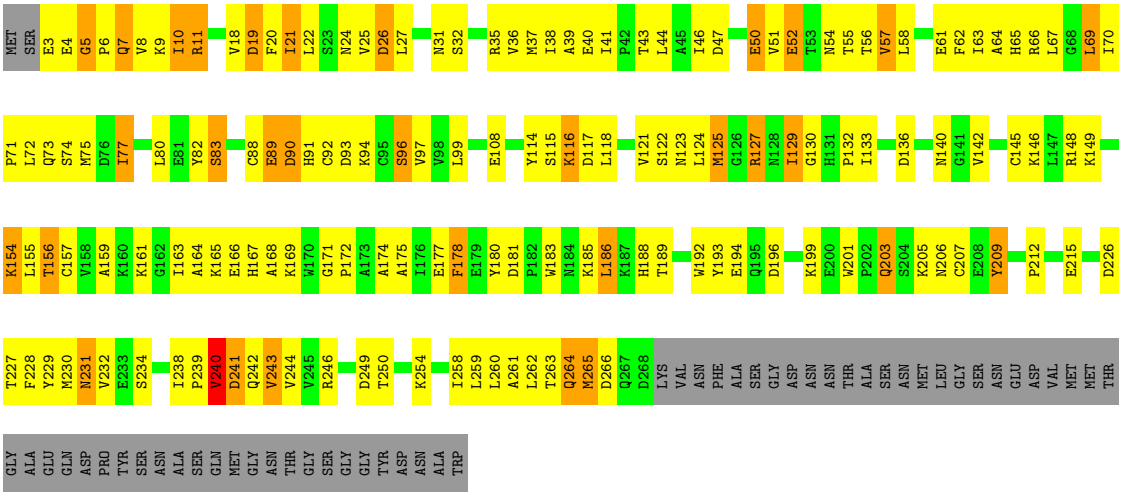
Chain B:


ALA GLN HIS THR THR GLU SER ASP ASN ILE SER ARG LYS TYR
E89 I90 I95 Y96 V97 T98 K99 P100 M101 V102 N103 E104 G107 E116 A117 R118 L119 R120 N121 L122 S125 L128 F129 V130 D131 T136 Y137 E138
LEU ILE ALA GLU GLU SER GLU ASP ASP SER GLU SER GLY
K164 V165 F166 I167 G168 R169 L170 P171 I172 M173 L174 R175 S176 K177 N178 C179 Y180 E183 A184 T185 D188 L189 Y190 E194 C195 P196 F197 D198 M199 G200 G201 Y202 F203 I204 I205 N206 G207 S208 E209 K210 V211 L212 R217
N221 Q224 V225 F226 K227 K228 A229 A230 P231 I234 S235 H236 V237 A238 E239 I240 R241 S242 G247 S248 R249 P250 I251 S252 T253 L254 Q255 V256 K257 G260 R261 E262 G263 A266 I269 P274 Y275 I276 K277 I280 P281 I282 V283 I284 R287 I291 I292 P293 D294
G296 E296 E299 H300 Y303 D304 V305 N306 D307 W308 Q309 M310 L311 E312 M313 L314 K315 V318 E319 D320 G321 F322 V323 I324 A330 F333 I334 G335 R336 R337 G338 T339 A340 L341 G342 I343 K344 K345 R348 I349 Q350 Y351 D354 I355 L356 E359 F360 L361 P362 H363 I364 T365
Q366 L367 E368 G369 F370 K374 A375 F376 F377 M381 I382 N383 R384 L385 L386 L387 C388 A389 K393 H400 F401 G402 R405 L406 D407 L408 A409 L416 L420 F421 K422 K423 L424 R430 R434 E437 GLU ALA HIS ASP PHE ASN MET LYS L446 K451 T452 I453 T454
S455 G456 L457 L461 W466 G467 GLU GLN LYS LYS ALA MET SER SER ARG A477 S480 R485 Y486 T487 Y488 S489 S490 L495 R496 R497 T498 I502 GLY ARG ASP GLY LYS LEU A509 K510 P511 R512 Q513 L514 H515 N516 T517 H518 W519 G520 L521 V522 C523 P524 A525 E526 Q531
L535 L539 S540 L541 M542 S543 C544 I545 S546 V547 D550 P551 M552 P553 T556 F557 L558 W561 G562 M563 E564 P565 L566 E567 D568 Y569 V570 P571 H572 Q573 A577 T578 R579 V580 F581 V582 N583 W586 H587 G588 V589 H590 R591 N592 P593 L596 M597 E598 T599 L600 R601 T602
L603 R604 R605 K606 G607 D608 I609 N610 F611 E612 V613 S614 M615 I616 R617 D618 I619 R620 E621 K622 E623 L624 K625 T628 R632 V633 Y634 R635 P636 L637 F638 I639 V640 E641 D642 D643 E644 S645 L646 G647 H648 K649 E650 L651 K652 V653 R654 K655 G656 H657 I658 A659 K660 L661 Y666 Q667 D668
ILE GLU GLY GLY PHE GLU ASP VAL GLU E678 Y679 T680 W681 S682 S683 L684 L685 G688 L689 V690 E691 Y692 I693 D694 A695 E696 E697 E698 E699 S700 I701 L702 I703 A704 M705 Q706 P707 E708 D709 L710 E711 P712 ALA GLU ALA ASN GLU GLU ASN ASP LEU D722 A726 K727 R728 I729 R730 V731
T737 F738 T739 H740 C741 E742 I743 H744 P745 S746 M747 G750 V751 A752 I755 I756 P757 F758 P759 Q763 S764 P765 R766 Q770 S771 A772 W773 G774 K775 Q776 G779 V780 F781 L782 T783 W784 Y785 N786 V787 R788 W789 D790 T791 W792 A793 W794 I795 L796 P799 Q800 K801 T805
T806 R807 A808 M809 E810 Y811 L812 K813 F814 R815 E816 L817 Q821 N822 A823 I824 V825 A826 I827 A828 C829 Y830 S831 G832 Y833 N834 Q835 E836 D837 S838 M839 I840 M841 N842 S845 I846 D847 L850 F851 F856 R857 S858 Y859 M860 E863 K864 I870 T871 E872 T873 R879 T882
L883 R884 T889 Y890 D891 K892 L893 L898 I899 A900 P901 G902 V903 R904 V905 S906 G907 E908 D909 V910 I911 I912 G913 K914 T915 T916 P917 I918 S919 PRO ASP GLU GLU GLU LEU GLY GLN ARG THR ALA TYR HIS S933 K934 R935 D936 A937 L941 R942 N946 G947 I948 V949 D950 Q951 V952
L953 V954 T955 T956 K962 P963 V964 K965 V966 R967 V968 R969 T970 T971 K972 I973 P974 Q975 I976 F980 R983 H984 G985 Q986 K987 I990 G991 I992 T993 Y994 R995 R996 E997 D998 N999 P1000 F1001 T1002 A1003 E1004 G1005 I1006 V1007 P1008 D1009 L1010 I1011 I1012 N1013 P1014 H1015 A1016 S1019 R1020 M1021
I1027 L1030 L1031 S1032 K1033 L1037 S1038 G1039 N1040 S1045 P1046 D1049 T1050 T1051 V1052 E1053 L1059 R1060 E1061 H1062 G1063 Y1064 Q1065 S1066 R1067 G1068 F1069 E1070 V1071 M1072 Y1073 K1079 K1080 L1081 Q1084 I1085 F1086 F1087 G1088 P1089 T1090 Y1091 R1094 L1095 R1096 H1097 M1098 V1099 D1100 D1101 K1102
I1103 H1104 A1107 P1110 MET GLN VAL LEU THR ARG GLN PRO VAL GLU GLY ARG SER ARG ASP GLY G1127 L1128 R1129 R1135 D1136 C1137 Q1138 I1139 G1142 A1143 A1144 K1148 E1149 R1150 L1151 M1152 E1153 A1157 F1158 R1159 V1160 H1161 I1162 C1163 C1166 G1167 L1168 M1169 T1170 V1171 K1174



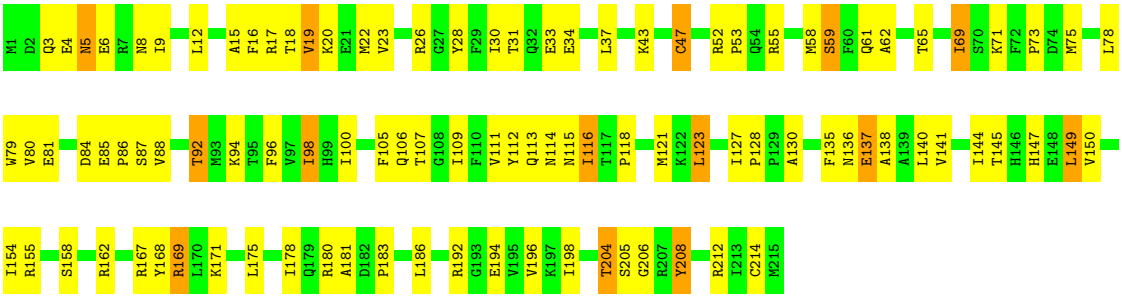
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C:



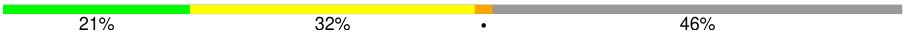
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

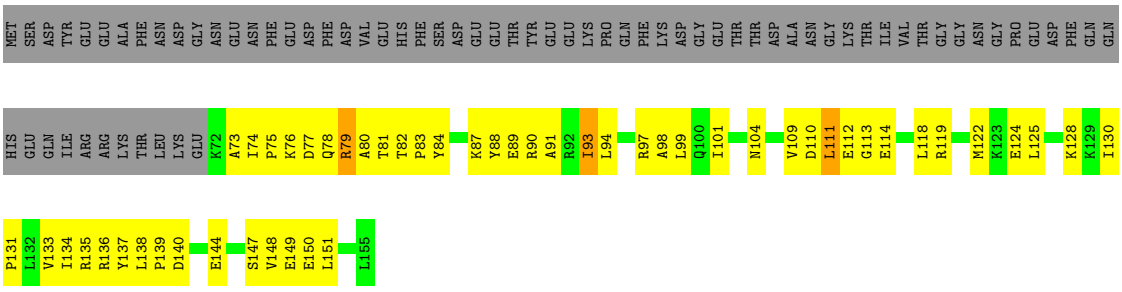
Chain E:



• Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

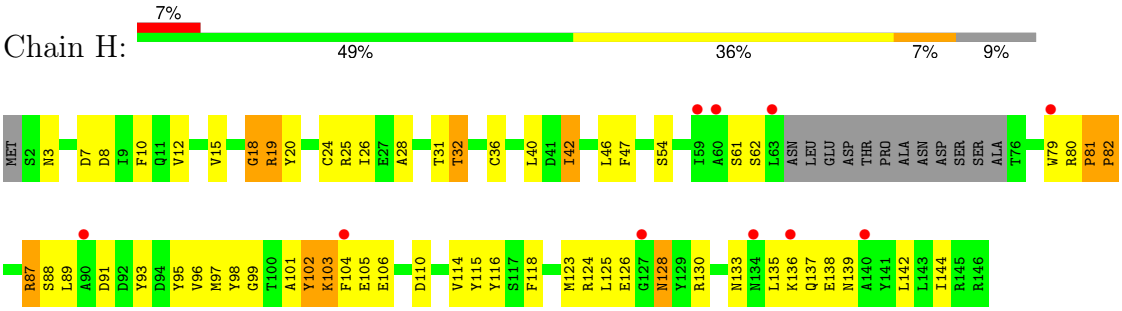
Chain F:





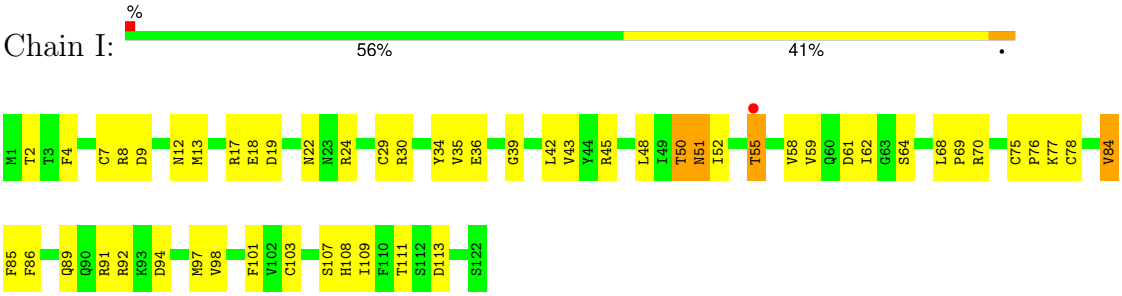
• Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



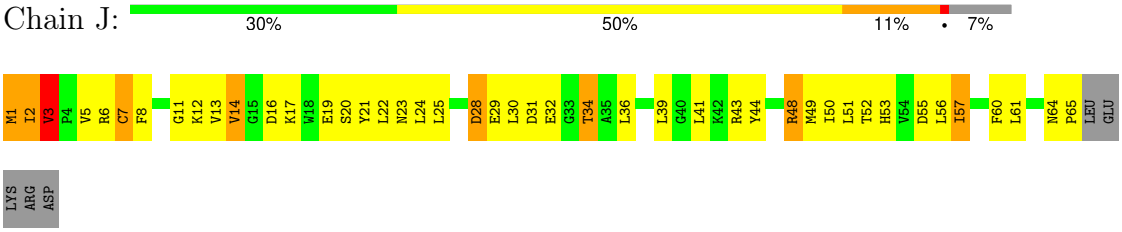
• Molecule 7: DNA-directed RNA polymerase II subunit 9

Chain I:



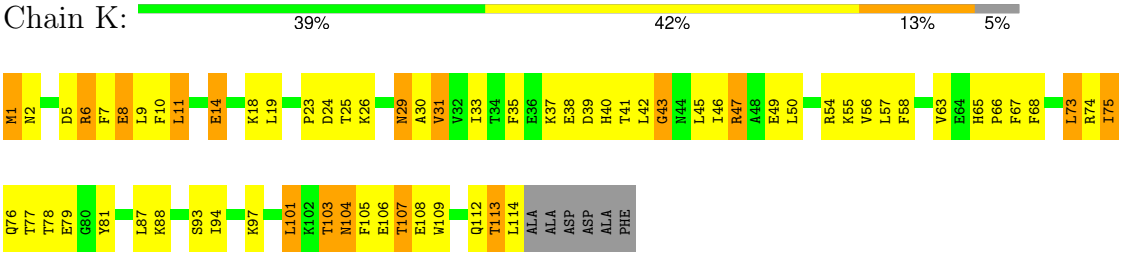
• Molecule 8: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:



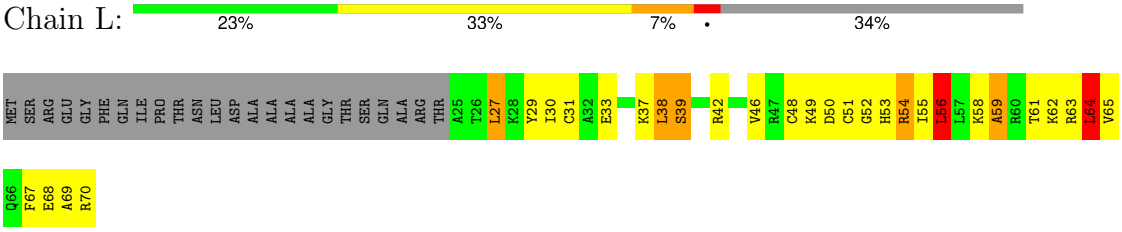
• Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



• Molecule 10: 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	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	118.04Å 218.91Å 369.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 40.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.40) 97.8 (40.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	4.00 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.249 , 0.323 0.229 , 0.282	Depositor DCC
R_{free} test set	1970 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å^2)	89.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	28289	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.74	1/11352 (0.0%)	1.03	34/15352 (0.2%)
2	B	0.72	0/8882	0.96	10/11976 (0.1%)
3	C	0.71	0/2133	0.96	7/2891 (0.2%)
4	E	0.73	1/1796 (0.1%)	1.06	7/2416 (0.3%)
5	F	0.73	0/691	0.99	2/933 (0.2%)
6	H	0.63	1/1086 (0.1%)	0.90	2/1470 (0.1%)
7	I	0.65	0/1016	0.91	1/1365 (0.1%)
8	J	0.73	0/541	1.06	1/727 (0.1%)
9	K	0.65	0/937	0.92	1/1265 (0.1%)
10	L	0.62	0/366	0.91	0/485
All	All	0.72	3/28800 (0.0%)	0.99	65/38880 (0.2%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1449	SER	CB-OG	8.26	1.58	1.42
6	H	87	ARG	CA-C	6.01	1.55	1.52
4	E	128	PRO	CA-C	5.61	1.54	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	673	GLY	CA-C-N	8.26	127.56	118.97
1	A	673	GLY	C-N-CA	8.26	127.56	118.97
1	A	244	PRO	N-CA-C	8.26	120.78	110.70
1	A	463	ILE	CA-C-N	8.11	129.98	119.84
1	A	463	ILE	C-N-CA	8.11	129.98	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	450	LEU	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	11154	0	11225	742	0
2	B	8711	0	8737	588	0
3	C	2095	0	2051	172	0
4	E	1760	0	1788	79	0
5	F	679	0	701	56	0
6	H	1068	0	1040	84	0
7	I	997	0	955	42	0
8	J	532	0	542	65	0
9	K	919	0	929	87	0
10	L	364	0	388	37	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	2	0	0	0	0
All	All	28289	0	28356	1736	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 31.

The worst 5 of 1736 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)
2:B:800:GLN:HB3	8:J:52:THR:CG2	1.63	1.25
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.66	1.21
1:A:672:ASP:HB2	1:A:736:ASN:ND2	1.60	1.15
1:A:855:THR:HG21	1:A:857:ARG:HE	0.98	1.14
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.27	1.14

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	1411/1733 (81%)	1182 (84%)	174 (12%)	55 (4%)	2 15
2	B	1074/1224 (88%)	924 (86%)	122 (11%)	28 (3%)	4 22
3	C	264/318 (83%)	221 (84%)	34 (13%)	9 (3%)	3 17
4	E	213/215 (99%)	179 (84%)	30 (14%)	4 (2%)	6 26
5	F	82/155 (53%)	68 (83%)	11 (13%)	3 (4%)	2 16
6	H	129/146 (88%)	95 (74%)	22 (17%)	12 (9%)	0 3
7	I	120/122 (98%)	96 (80%)	21 (18%)	3 (2%)	4 22
8	J	63/70 (90%)	53 (84%)	8 (13%)	2 (3%)	3 18
9	K	112/120 (93%)	92 (82%)	14 (12%)	6 (5%)	1 10
10	L	44/70 (63%)	25 (57%)	12 (27%)	7 (16%)	0 0
All	All	3512/4173 (84%)	2935 (84%)	448 (13%)	129 (4%)	2 16

5 of 129 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN

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Mol	Chain	Res	Type
1	A	48	ALA
1	A	55	ASP
1	A	415	LEU
1	A	464	PRO

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	1239/1520 (82%)	1077 (87%)	162 (13%)	3 13
2	B	950/1061 (90%)	840 (88%)	110 (12%)	4 17
3	C	234/274 (85%)	202 (86%)	32 (14%)	3 11
4	E	197/197 (100%)	180 (91%)	17 (9%)	8 29
5	F	74/137 (54%)	68 (92%)	6 (8%)	9 31
6	H	117/128 (91%)	115 (98%)	2 (2%)	56 74
7	I	116/116 (100%)	105 (90%)	11 (10%)	7 25
8	J	60/65 (92%)	47 (78%)	13 (22%)	1 2
9	K	99/102 (97%)	84 (85%)	15 (15%)	2 9
10	L	40/57 (70%)	34 (85%)	6 (15%)	2 9
All	All	3126/3657 (86%)	2752 (88%)	374 (12%)	4 16

5 of 374 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	648	HIS
3	C	125	MET
2	B	755	ILE
2	B	1049	ASP
3	C	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1084	GLN
3	C	267	GLN
2	B	1211	ASN
3	C	79	GLN
6	H	11	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 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	A	1419/1733 (81%)	-0.28	13 (0%) 81 73	41, 79, 162, 188	0
2	B	1094/1224 (89%)	-0.28	13 (1%) 76 68	47, 80, 140, 167	0
3	C	266/318 (83%)	-0.34	0 100 100	58, 78, 111, 133	0
4	E	215/215 (100%)	-0.30	0 100 100	51, 98, 130, 145	0
5	F	84/155 (54%)	-0.45	0 100 100	52, 71, 92, 98	0
6	H	133/146 (91%)	0.30	10 (7%) 22 21	103, 119, 147, 149	0
7	I	122/122 (100%)	-0.13	1 (0%) 82 75	75, 107, 129, 150	0
8	J	65/70 (92%)	-0.63	0 100 100	58, 70, 91, 94	0
9	K	114/120 (95%)	-0.42	0 100 100	58, 85, 107, 126	0
10	L	46/70 (65%)	0.24	0 100 100	87, 137, 144, 145	0
All	All	3558/4173 (85%)	-0.27	37 (1%) 79 71	41, 82, 146, 188	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	4.8
7	I	55	THR	3.7
6	H	140	ALA	3.3
1	A	250	ILE	3.3
2	B	247	GLY	3.2

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
12	MN	A	3010	1/1	0.79	0.13	50,50,50,50	0
11	ZN	I	3004	1/1	0.98	0.04	117,117,117,117	0
11	ZN	L	3005	1/1	0.98	0.04	128,128,128,128	0
11	ZN	A	3008	1/1	0.98	0.05	143,143,143,143	0
11	ZN	B	3007	1/1	0.99	0.02	87,87,87,87	0
12	MN	A	3009	1/1	0.99	0.03	49,49,49,49	0
11	ZN	A	3006	1/1	0.99	0.02	95,95,95,95	0
11	ZN	I	3003	1/1	1.00	0.02	97,97,97,97	0
11	ZN	C	3002	1/1	1.00	0.02	79,79,79,79	0
11	ZN	J	3001	1/1	1.00	0.01	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.