wwPDB X-ray Structure Validation Summary Report (i)

Mar 4, 2024 – 11:04 PM EST

PDB ID	:	1Y1V
Title	:	Refined RNA Polymerase II-TFIIS complex
Authors	:	Kettenberger, H.; Armache, K.-J.; Cramer, P.
Deposited on	:	2004-11-19
Resolution	:	3.80 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:

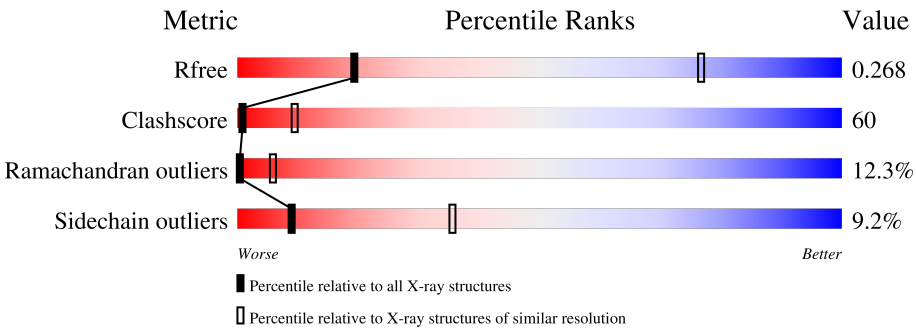
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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 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%

Mol	Chain	Length	Quality of chain
1	A	1733	21% 47% 13% • 18%
2	B	1224	24% 52% 13% • 9%
3	C	318	22% 48% 12% • 16%
4	D	221	33% 40% 6% 20%
5	E	215	34% 55% 11%
6	F	155	15% 30% 8% 46%
7	G	171	33% 59% 8%

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Mol	Chain	Length	Quality of chain
8	H	146	30% 53% 8% 9%
9	I	122	31% 48% 13% 5% •
10	J	70	23% 51% 17% • 7%
11	K	120	37% 52% 5% • 5%
12	L	70	6% 41% 19% 34%
13	S	179	62% 28% • • •

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 31803 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
			Total	C	N	O	S			
1	A	1426	11214	7069	1959	2124	62	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1112	8837	5594	1548	1640	55	58	0	0

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

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

- Molecule 4 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	177	1356	840	241	273	2	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

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

- 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
			Total	C	N	O	S			
8	H	133	1068	673	180	211	4	0	0	0

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

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

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

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- 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
			Total	C	N	O	S			
12	L	46	364	224	72	64	4	0	0	0

- Molecule 13 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	S	174	666	454	99	108	5	0	0	104

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

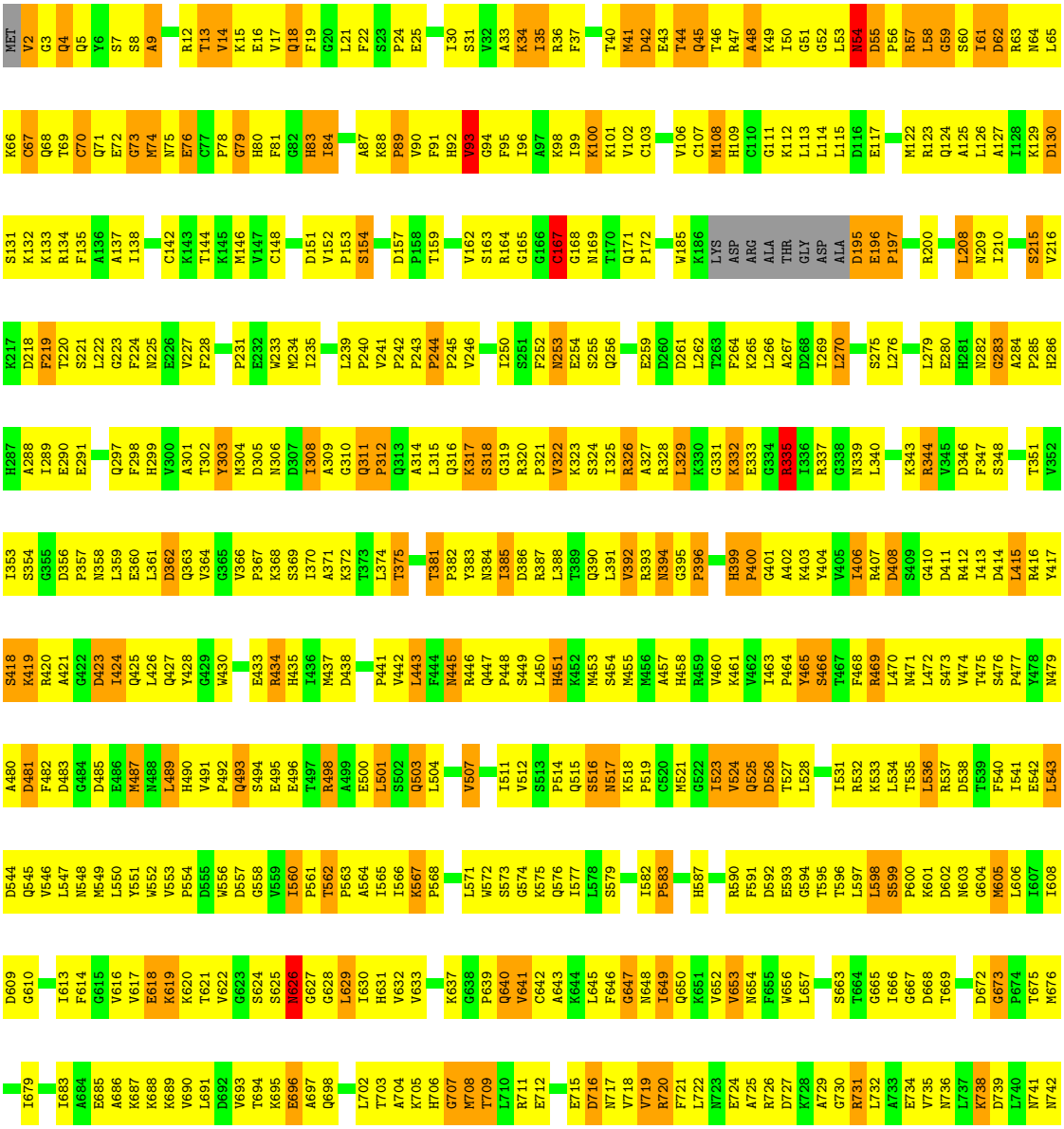
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	S	1	1	1	0	0

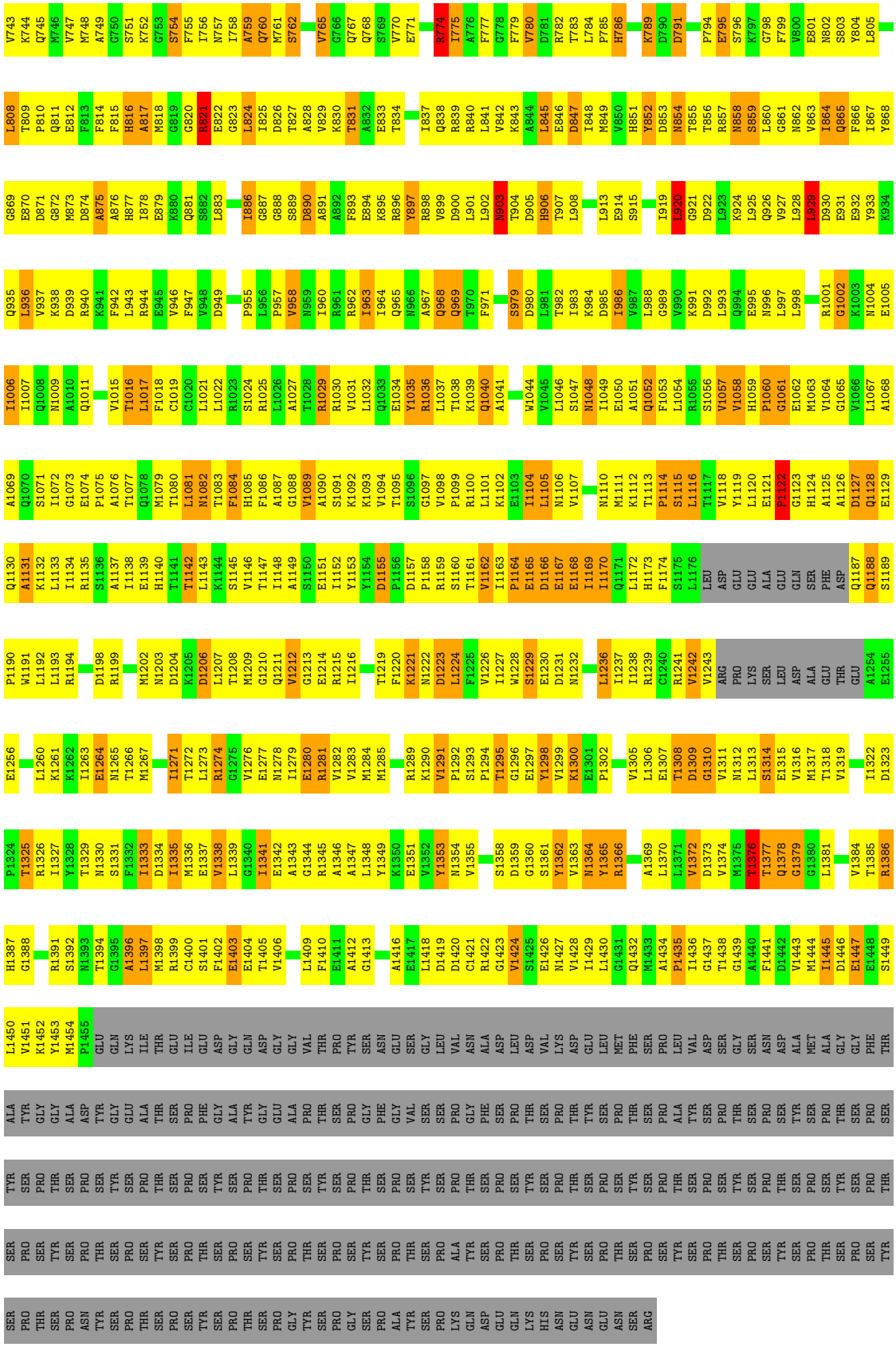
3 Residue-property plots (i)

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. 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. 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

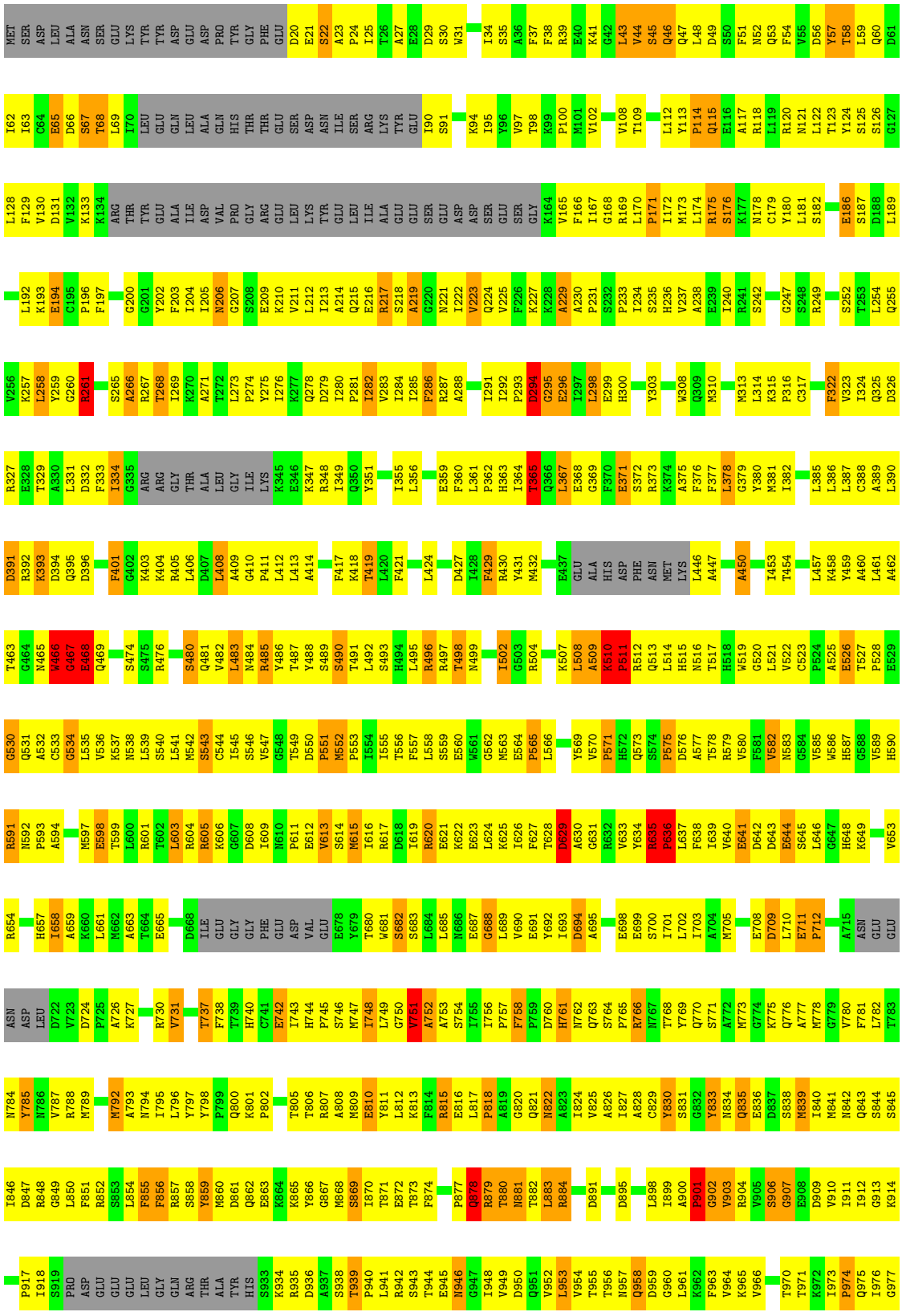
Chain A: 21% 47% 13% • 18%

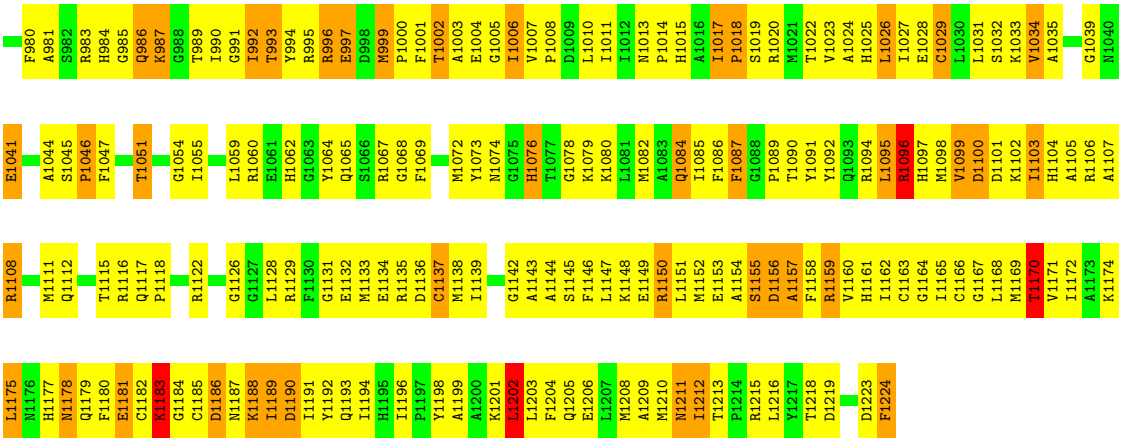




- Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

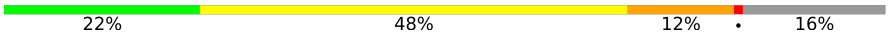
Chain B: 24% 52% 13% • 9%

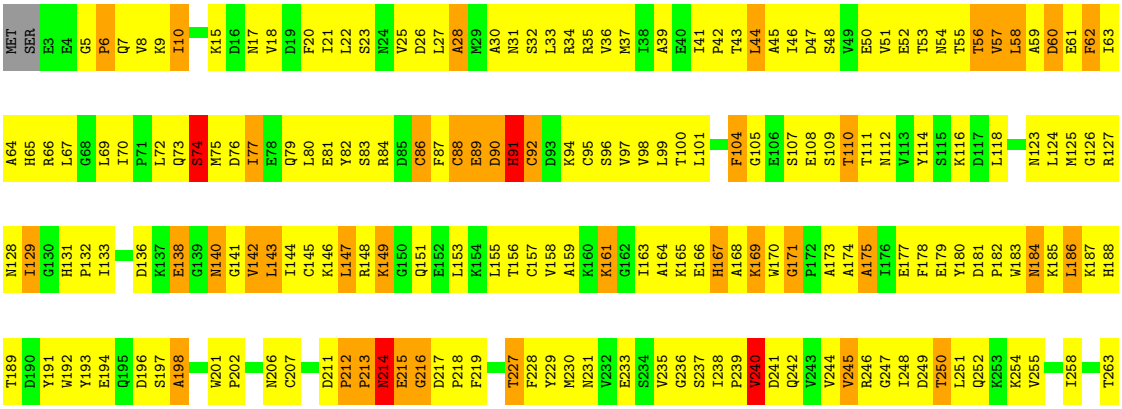




• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

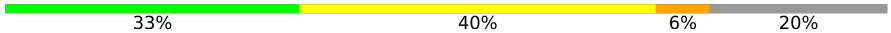
Chain C:

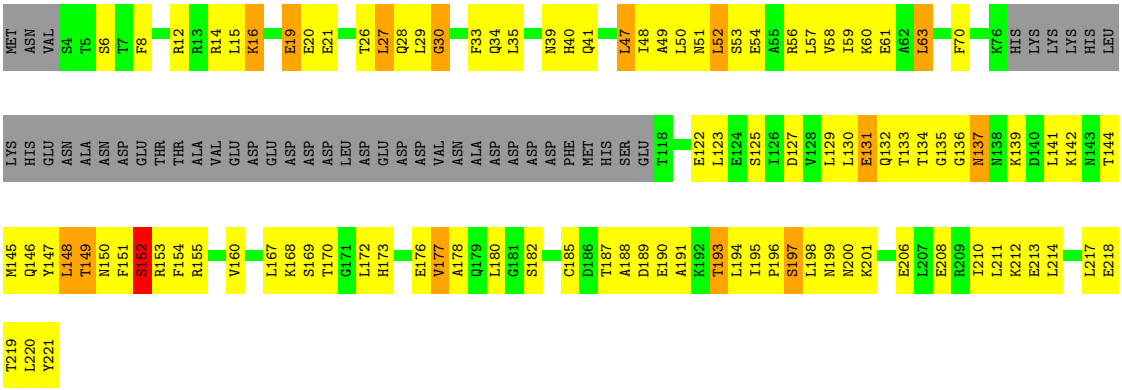




• Molecule 4: DNA-directed RNA polymerase II 32 kDa polypeptide

Chain D:





• Molecule 5: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E: 34% 55% 11%

MET D2 Q3 E4 R7 N8 I9 S10 R11 L12 W13 F16 R17 T18 V19 K20 E21 M22 V23 K24 D25 R26 G27 Y28 F29 I30 T31 Q32 E33 E34 V35 E36 L37 P38 L39 E40 D41 F42 K43 A44 K45 Y46 C47 D48 S49 R52 R55 K56 M57 M58 S59 F60 E66 I69

F72 P73 D74 L78 W79 V80 E81 F82 C83 D84 E85 P86 V90 K91 T92 N93 K94 T95 F96 V97 I98 H99 I100 N104 F105 Q106 Y112 Q113 N114 N115 I116 T117 P118 S119 A120 V124 P125 P129 A130 T131 I132 F135 N136 E137 A138 A139 L140 V141 V142 N143 I144 T145

H146 H147 E148 L149 V150 H153 I154 R155 L156 S157 S158 D159 E160 K161 R162 E163 L164 L165 K166 R167 Y168 R169 L170 K171 E172 S173 Q174 L175 P176 R177 I178 D182 P183 V184 A185 L186 Y187 L188 G189 L190 K191 R192 V196 K197 I198 I199 S202 E203 T204 S205 G206 R207 Y208 A209 S210 Y211

R212 I213 C214 M215

- Molecule 6: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F: 15% 30% 8% 46%

MET SER ASP TYR GLU GLU ALA PHE ASN ASP GLY ASN GLU ASN PHE GLU ASP PHE ASP VAL GLU HIS PHE SER ASP GLU GLU THR TYR GLU GLU LYS PRO GLN PHE LYS ASP GLY GLU THR THR ASP ALA ASN GLY LYS THR ILE VAL THR GLY GLY ASN GLY PRO GLU ASP PHE GLN GLN

HIS GLU GLN ILE ARG ARG LYS THR LEU LYS GLU K72 A73 I74 P75 K76 D77 Q78 R79 A80 T81 T82 P83 Y84 M85 T86 K87 Y88 E89 R90 A91 R92 I93 L94 G95 T96 R97 A98 L99 Q100 M103 N104 F108 V109 D110 L111 E112 G113 D116 R119 I120 K123 E124 L125 A126

E127 K128 K129 I130 P131 L132 V133 I134 R135 R136 Y137 L138 P139 D140 G141 S142 F143 E144 D145 W146 S147 V148 E149 E150 L151 I152 V153 D154 L155

- Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide

Chain G: 33% 59% 8%

M1 F2 F3 I4 K5 D6 L7 S8 L9 N10 L13 H14 P15 S16 F17 F18 G19 P20 R21 M22 K23 Q24 Y25 L26 K27 T28 K29 L30 L31 V34 C38 T39 G40 K41 F42 G43 Y44 I45 L46 C47 V48 L49 I54 D55 I56 Q57 R58 G59 R60 I61 L62 P63 T64 D65 G66 S67

A68 E69 F70 N71 V72 K73 Y74 R75 A76 V77 V78 F79 K80 P81 F82 K83 G84 E85 V86 V87 D88 V91 Q96 H97 V101 Q102 V103 G104 P105 M106 K107 V108 F109 V110 T111 K112 H113 L114 M115 P116 Q117 D118 L119 T120 F121 N122 A123 G124 S125 N126 P127 P128 S129 Y130 Q131 S132 S133

E134 D135 T138 I139 K140 S141 R142 I143 R144 V145 K146 I147 V154 S155 S156 I157 H158 A159 I160 G161 S162 E165 L168 I171

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

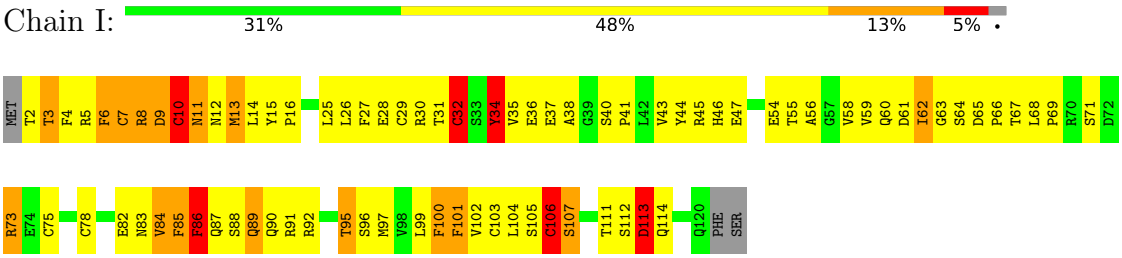
Chain H: 30% 53% 8% 9%

MET S2 N3 T4 L5 F6 D7 D8 I9 F10 Q11 V12 S13 E14 V15 D16 P17 Y20 N21 K22 V23 C24 R25 I26 E27 A28 T31 T32 Q33 D34 Q35 C36 K37 L38 T39 L40 D41 I42 N43 V44 E45 L46 F47 Q52 T56 V57 T58 I59 A60 S61 S62 L63 ASN LEU GLU ASP

THR PRO ALA ASN ASP SER SER ALA T76 R77 S78 W79 R80 P81 P82 Q83 A84 G85 D86 R87 S88 L89 A90 D91 D92 Y93 D94 Y95 V96 M97 Y98 G99 T100 A101 Y102 K103 F104 E105 E106 V107 S108 I112 A113 V114 Y115 Y116 G119 G120 L121 L122 M123 R124 L125 E126 G127 N128 Y129 R130

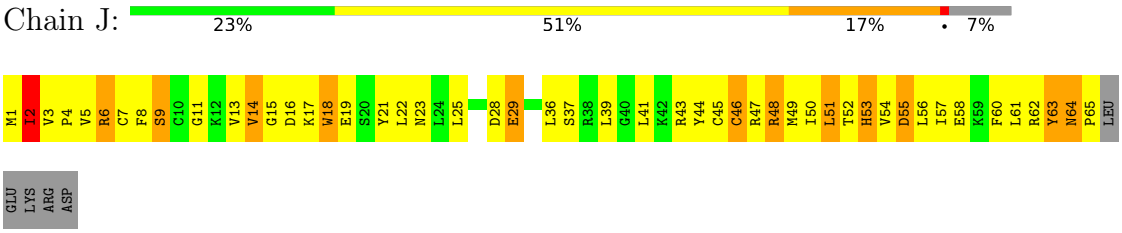
• Molecule 9: DNA-directed RNA polymerase II subunit 9

Chain I:



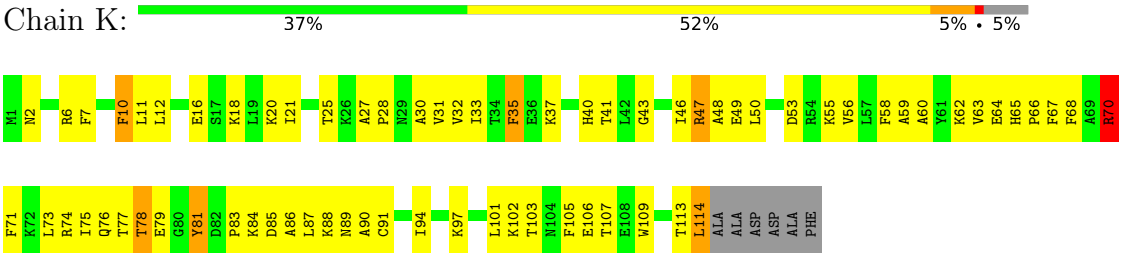
• Molecule 10: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:



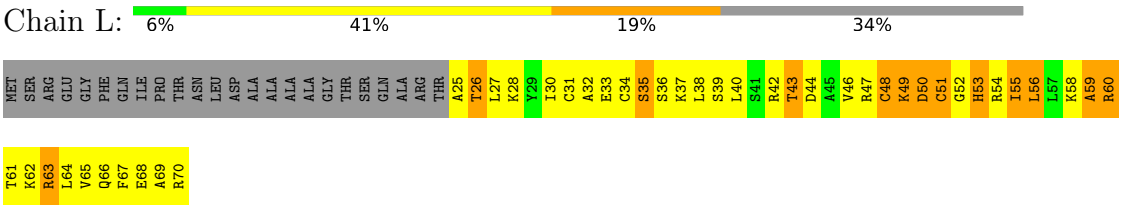
• Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



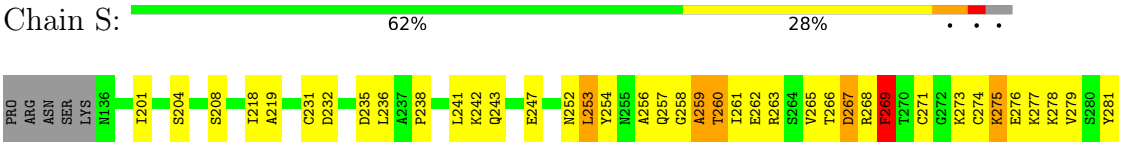
• Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L:



• Molecule 13: Transcription elongation factor S-II

Chain S:



Y282
Q283
L284
Q285
T286
R287
S288
A289
D290
E291
P292
L293
T294
T295
F296
C297
T298
C299
E300
A301
C302
G303
N304
R305
W306
K307
F308
S309

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	218.90Å 395.30Å 281.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 49.41 – 3.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 86.6 (49.41-3.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.294 0.257 , 0.268	Depositor DCC
R_{free} test set	2439 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	68.0	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.13$	Xtriage
Estimated twinning fraction	0.199 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.206 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	31803	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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: 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	0.50	2/11417 (0.0%)	0.78	4/15442 (0.0%)
2	B	0.51	4/9009 (0.0%)	0.76	8/12146 (0.1%)
3	C	0.48	0/2133	0.77	1/2891 (0.0%)
4	D	0.41	0/1365	0.64	0/1837
5	E	0.43	0/1788	0.66	0/2406
6	F	0.52	0/691	0.77	0/933
7	G	0.49	0/1368	0.72	0/1844
8	H	0.38	0/1086	0.65	1/1470 (0.1%)
9	I	0.46	0/989	0.77	1/1331 (0.1%)
10	J	0.48	0/541	0.75	0/727
11	K	0.45	0/937	0.67	0/1265
12	L	0.54	0/366	0.79	0/485
13	S	1.31	4/571 (0.7%)	1.64	7/765 (0.9%)
All	All	0.51	10/32261 (0.0%)	0.77	22/43542 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
13	S	0	2
All	All	0	5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	269	PHE	C-N	-16.91	0.95	1.34
2	B	467	GLY	C-O	-11.91	1.04	1.23
13	S	260	THR	CA-CB	10.48	1.80	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	468	GLU	CB-CG	8.39	1.68	1.52
13	S	268	ARG	CG-CD	6.05	1.67	1.51

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	S	269	PHE	O-C-N	-19.02	92.27	122.70
13	S	269	PHE	C-N-CA	16.73	163.51	121.70
13	S	269	PHE	CA-C-N	16.08	152.57	117.20
1	A	195	ASP	N-CA-C	9.35	136.25	111.00
2	B	510	LYS	CB-CA-C	-7.63	95.14	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	510	LYS	Mainchain
2	B	785	TYR	Sidechain
2	B	833	TYR	Sidechain
13	S	269	PHE	Sidechain,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	11214	0	11281	1514	0
2	B	8837	0	8871	1206	0
3	C	2095	0	2052	260	0
4	D	1356	0	1319	101	0
5	E	1752	0	1776	200	0
6	F	679	0	701	82	0
7	G	1340	0	1357	159	0
8	H	1068	0	1040	115	0
9	I	971	0	929	110	0
10	J	532	0	542	103	0
11	K	919	0	929	96	0
12	L	364	0	387	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	S	666	0	553	105	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
14	S	1	0	0	0	0
15	S	1	0	0	0	0
All	All	31803	0	31737	3774	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 60.

The worst 5 of 3774 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:260:THR:CA	13:S:260:THR:CB	1.80	1.53
13:S:269:PHE:CZ	13:S:297:CYS:SG	2.04	1.50
13:S:269:PHE:CE2	13:S:297:CYS:SG	2.14	1.39
1:A:1230:GLU:OE2	13:S:201:ILE:CA	1.75	1.32
1:A:1283:VAL:CG1	13:S:256:ALA:O	1.78	1.31

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	1418/1733 (82%)	914 (64%)	316 (22%)	188 (13%)	0 4
2	B	1096/1224 (90%)	726 (66%)	223 (20%)	147 (13%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	264/318 (83%)	169 (64%)	62 (24%)	33 (12%)	0 6
4	D	173/221 (78%)	129 (75%)	27 (16%)	17 (10%)	0 10
5	E	212/215 (99%)	141 (66%)	50 (24%)	21 (10%)	0 10
6	F	82/155 (53%)	60 (73%)	15 (18%)	7 (8%)	1 12
7	G	169/171 (99%)	123 (73%)	34 (20%)	12 (7%)	1 17
8	H	129/146 (88%)	93 (72%)	26 (20%)	10 (8%)	1 15
9	I	117/122 (96%)	80 (68%)	22 (19%)	15 (13%)	0 5
10	J	63/70 (90%)	36 (57%)	14 (22%)	13 (21%)	0 2
11	K	112/120 (93%)	82 (73%)	25 (22%)	5 (4%)	2 25
12	L	44/70 (63%)	18 (41%)	14 (32%)	12 (27%)	0 0
13	S	68/179 (38%)	51 (75%)	10 (15%)	7 (10%)	0 9
All	All	3947/4744 (83%)	2622 (66%)	838 (21%)	487 (12%)	0 6

5 of 487 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	55	ASP
1	A	58	LEU
1	A	62	ASP

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	1246/1520 (82%)	1133 (91%)	113 (9%)	9 36
2	B	964/1061 (91%)	880 (91%)	84 (9%)	10 38
3	C	234/274 (85%)	205 (88%)	29 (12%)	4 24
4	D	140/200 (70%)	126 (90%)	14 (10%)	7 32
5	E	196/197 (100%)	184 (94%)	12 (6%)	18 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	74/137 (54%)	63 (85%)	11 (15%)	3	18
7	G	152/152 (100%)	143 (94%)	9 (6%)	19	51
8	H	117/128 (91%)	110 (94%)	7 (6%)	19	50
9	I	113/116 (97%)	97 (86%)	16 (14%)	3	21
10	J	60/65 (92%)	55 (92%)	5 (8%)	11	40
11	K	99/102 (97%)	91 (92%)	8 (8%)	11	41
12	L	40/57 (70%)	33 (82%)	7 (18%)	2	13
13	S	62/156 (40%)	55 (89%)	7 (11%)	6	28
All	All	3497/4165 (84%)	3175 (91%)	322 (9%)	9	35

5 of 322 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	148	LEU
9	I	46	HIS
4	D	197	SER
6	F	143	PHE
11	K	10	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1179	GLN
4	D	137	ASN
3	C	65	HIS
3	C	167	HIS
5	E	143	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	269:PHE	C	270:THR	N	0.95

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.