



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 27, 2017 – 08:29 AM EDT

PDB ID : 5N5Z
EMDB ID: : EMD-3591
Title : Cryo-EM structure of RNA polymerase I in complex with Rrn3 and Core Factor (Orientation II)
Authors : Engel, C.; Gubbey, T.; Neyer, S.; Sainsbury, S.; Oberthuer, C.; Baejen, C.; Bernecky, C.; Cramer, P.
Deposited on : unknown
Resolution : 7.70 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

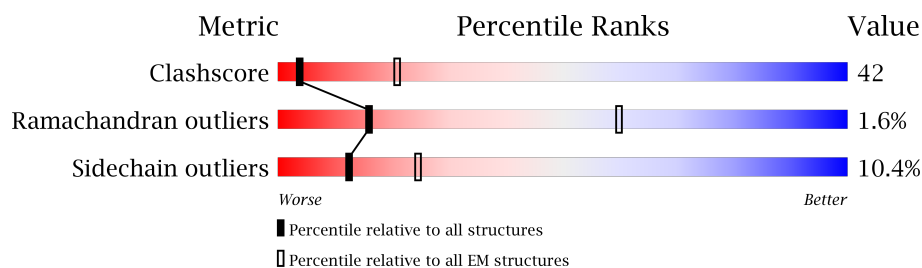
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 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.







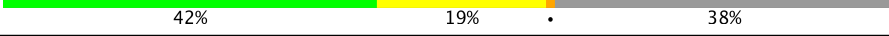
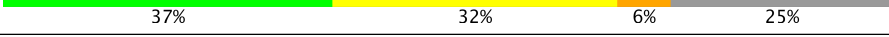
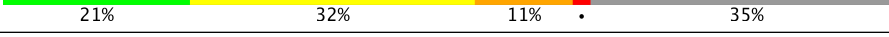
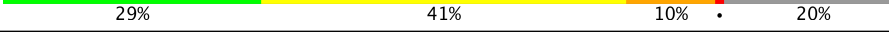

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1664	
2	B	1203	
3	C	335	
4	D	137	
5	E	215	
6	F	155	
7	G	326	
8	H	146	
9	I	125	

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Mol	Chain	Length	Quality of chain
10	J	70	 63%33%...
11	K	142	 48%21%•29%
12	L	70	 34%21%7%37%
13	M	415	 16%9%•74%
14	N	233	 42%19%•38%
15	O	627	 37%32%6%25%
16	P	894	 21%32%11%•35%
17	Q	514	 29%41%10%•20%
18	R	507	 18%32%9%•40%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 48004 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1467	Total	C	N	O	S	0	0
			11598	7327	2017	2193	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1172	Total	C	N	O	S	0	0
			9312	5891	1633	1738	50		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	58	Total	C	N	O	0	0
			459	289	78	92		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	193	Total	C	N	O	S	0	0
			1526	985	262	274	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	99	Total	C	N	O	S	0	0
			755	472	125	149	9		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	108	Total	C	N	O		0	0
			856	543	142	171			

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	145	Total	C	N	O	S	0	0
			1151	735	188	224	4		

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	473	Total	C	N	O	S	0	0
			3907	2533	642	711	21		

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	583	Total	C	N	O	S	0	0
			4729	3010	803	905	11		

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	410	Total	C	N	O	S	0	0
			3421	2219	579	603	20		

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	303	Total	C	N	O	S	0	0
			2535	1634	456	434	11		

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	J	1	Total	Zn	0
			1	1	
19	Q	1	Total	Zn	0
			1	1	
19	B	1	Total	Zn	0
			1	1	
19	I	2	Total	Zn	0
			2	2	

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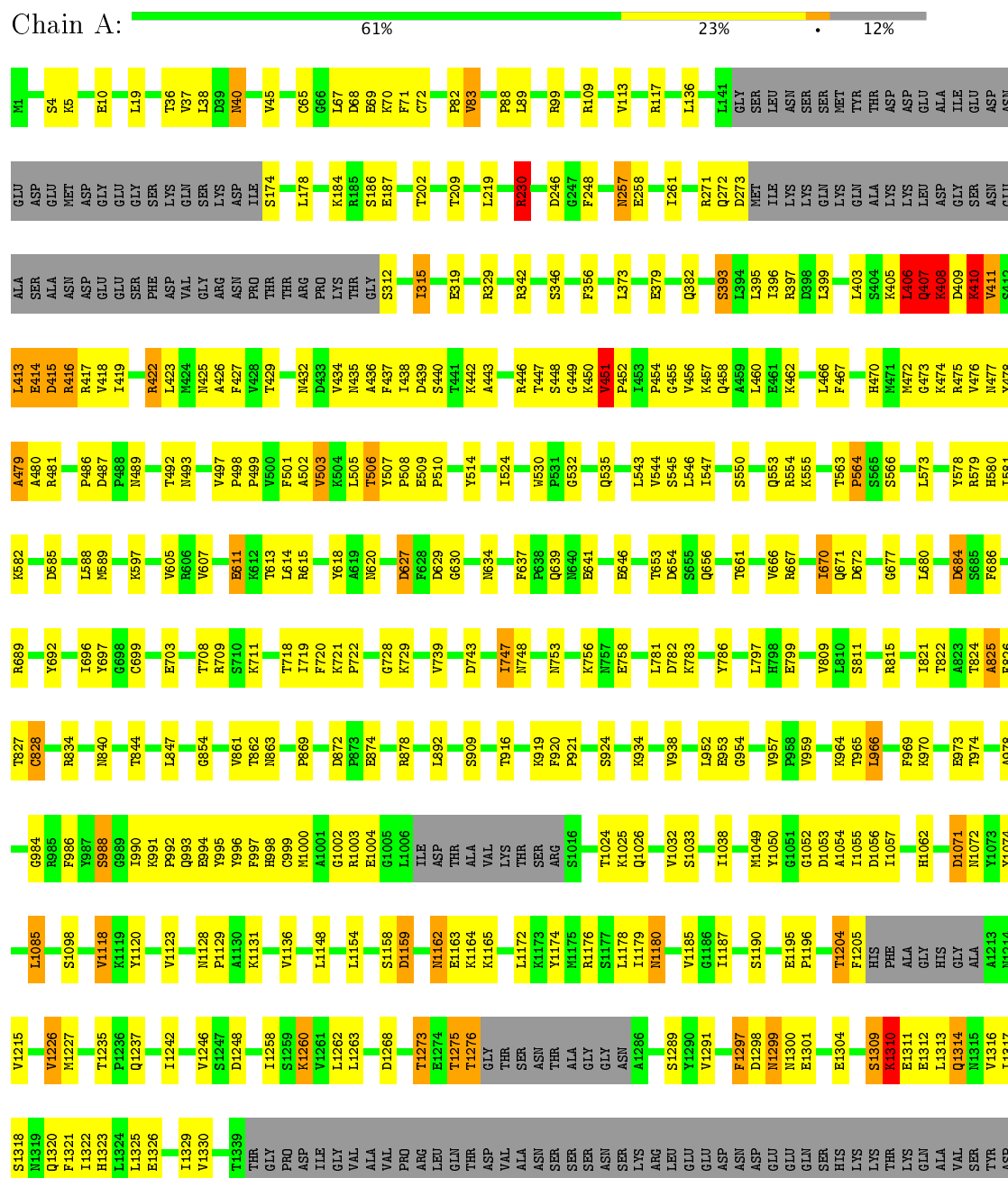
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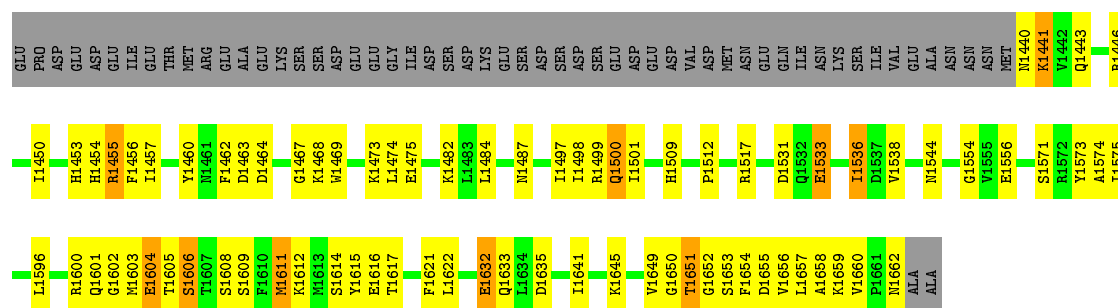
Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total 2	Zn 2	0
19	L	1	Total 1	Zn 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

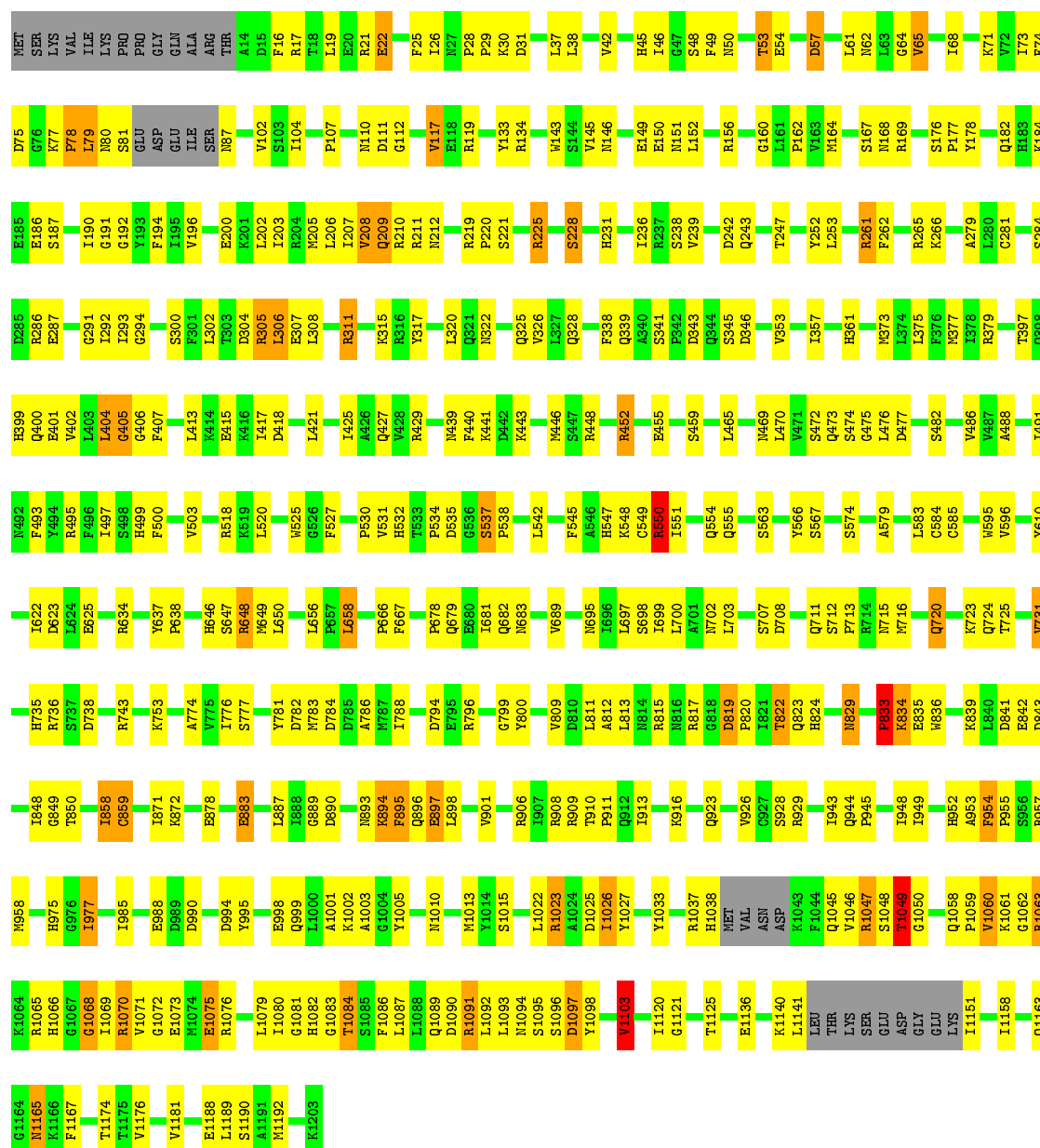
- Molecule 1: DNA-directed RNA polymerase I subunit RPA190





• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

Chain B: 63% 30%



• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

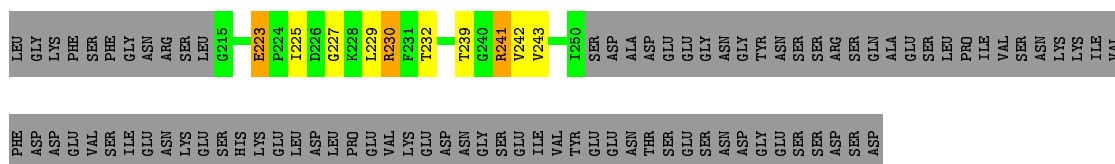
S243	S77	Met
A244	F86	Asn
R245	V91	Ser
R246	L97	Ile
F247	R100	Gly
		Ile
P252		Leu
P253		Thr
G254		Thr
V255		Thr
		Thr
A270	L103	Arg
R271	V104	Val
K272	P105	Thr
D273		Asn
T274	V116	Thr
	D117	Ser
R277	S118	Ser
E278	M119	Thr
V279		Asp
	K125	Phe
V289	F126	Pro
K290	T127	Gly
L291		Phe
G292	M130	Ser
R293		Lys
V294	K139	Asp
R295		Ala
N296		Leu
H297	R142	Asn
F298	Y157	Leu
I299	A160	Asn
		Leu
I313	S176	
F314	D181	N31
F315		N32
		V33
K322		K37
		K38
E326	E201	E41
V327	I202	V42
L328	K205	N43
		T44
		S45
		S46
		L47
		D48
		A49
		R50
		N58
		I59
		D60
		T61
		N65
		A66
		F67
		R68
		G69
		I70
		K71

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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| T145 | H146 | H147 | D159 | R162 | R167 | S173 | R177 | P183 | K191 | K197 | L198 | L199 | T204 | R207 | R212 | M215 | T145 | H146 | H147 | D159 | R162 | R167 | S173 | R177 | P183 | K191 | K197 | L198 | L199 | T204 | R207 | R212 | M215 | T145 | H146 | H147 | D159 | R162 | R167 | S173 | R177 | P183 | K191 | K197 | L198 | L199 | T204 | R207 | R212 | M215 |
| Met | ASP | GLM | E4 | R7 | R11 | K20 | T31 | Q32 | E33 | E34 | L37 | P38 | D41 | D43 | S49 | M50 | R55 | Q61 | E66 | E67 | D74 | M75 | G76 | S77 | L78 | C83 | V90 | K91 | T92 | M93 | F105 | Q106 | T107 | F110 | Q113 | A120 | T131 | N136 | H145 | | | | | | | | | | | |

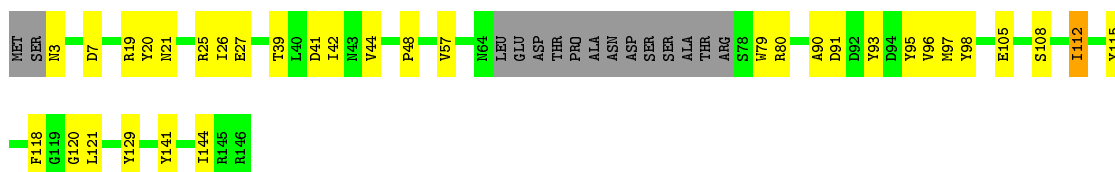
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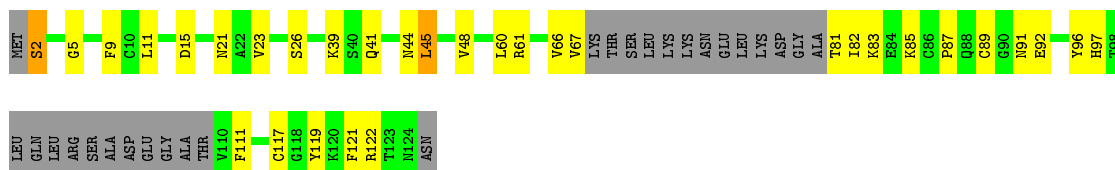
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 67% 22% 10%



- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain I: 54% 24% 21%



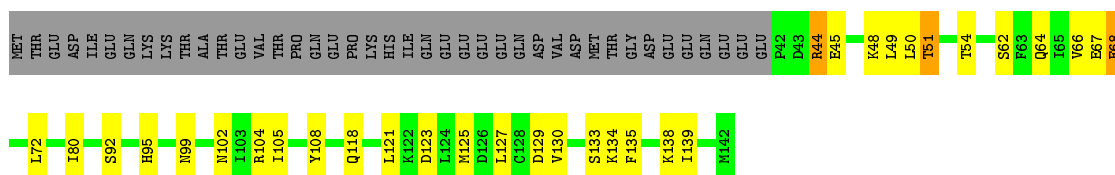
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 63% 33% ...



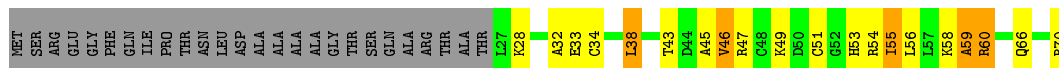
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 48% 21% 29%

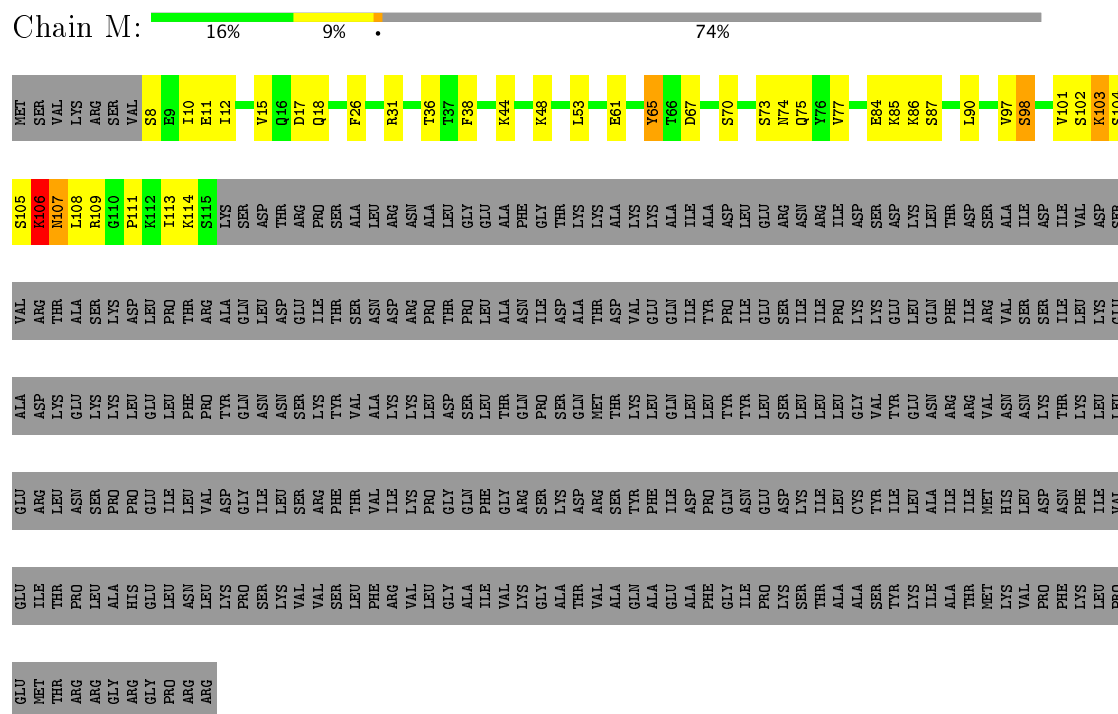


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

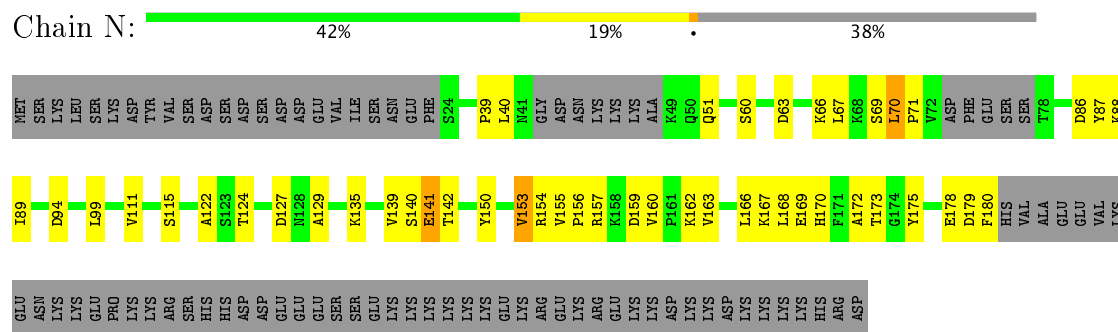
Chain L: 34% 21% 7% 37%



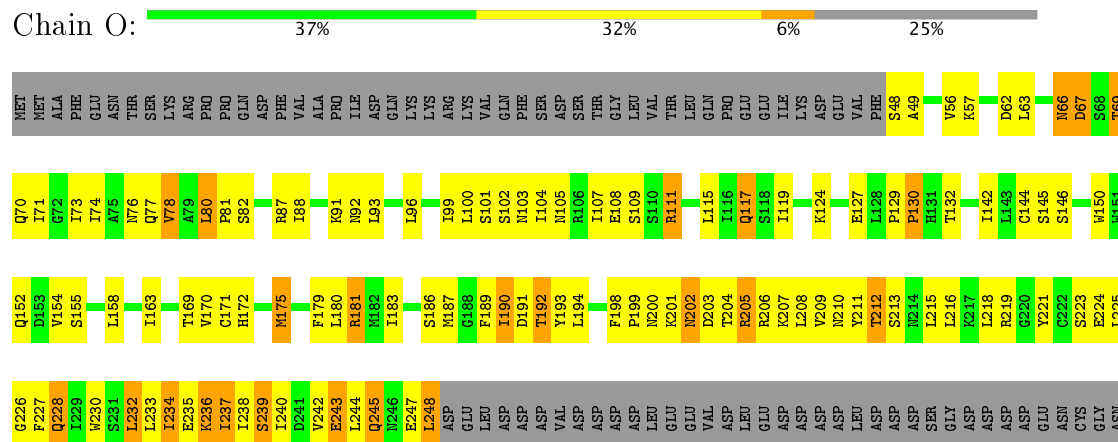
- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

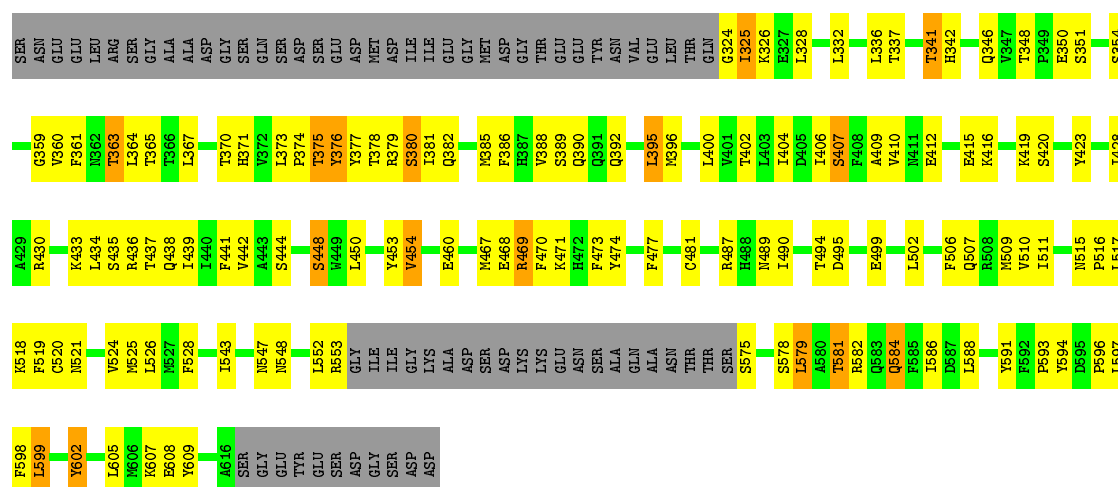


- Molecule 14: DNA-directed RNA polymerase I subunit RPA34



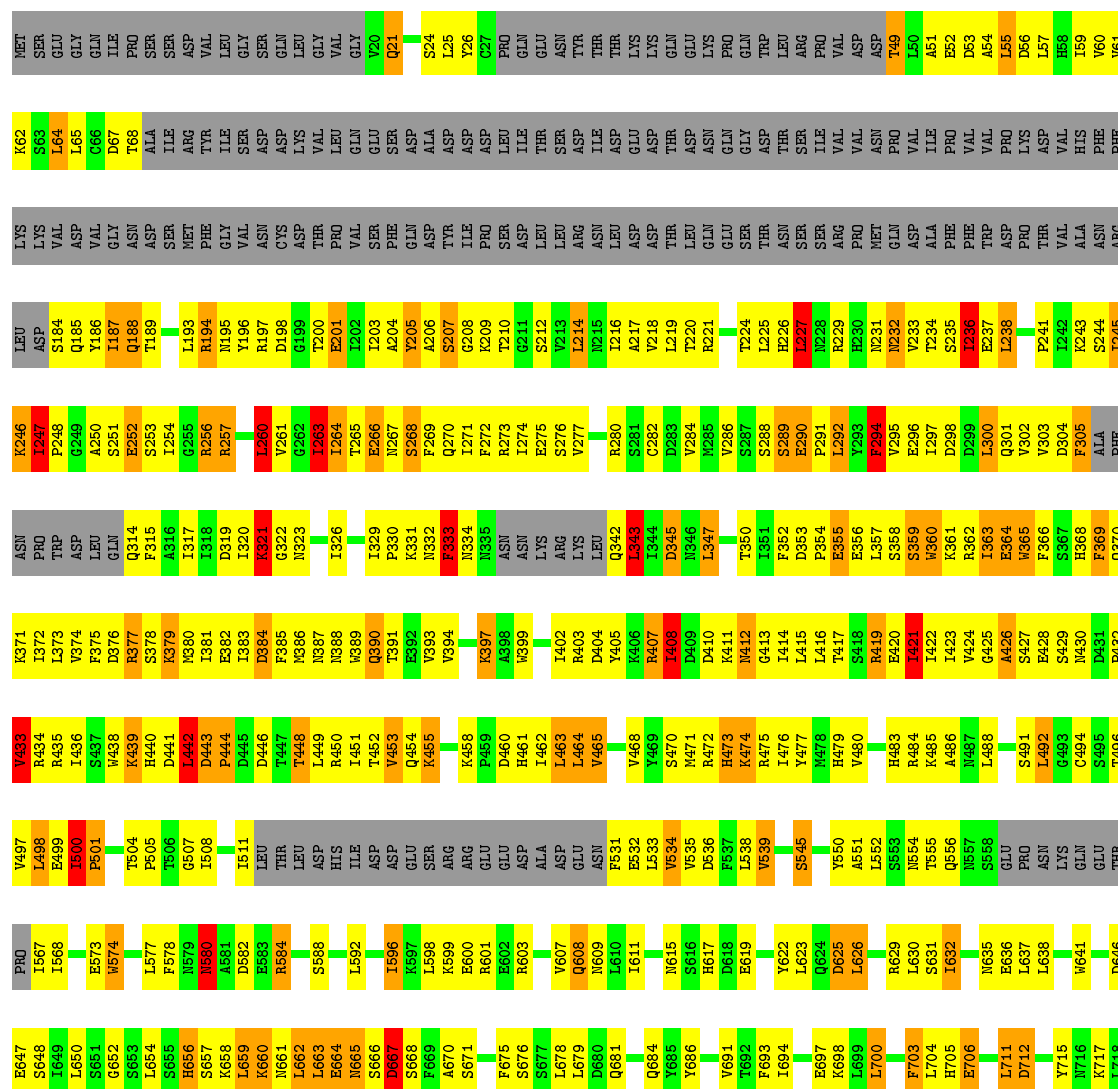
- Molecule 15: RNA polymerase I-specific transcription initiation factor RRN3

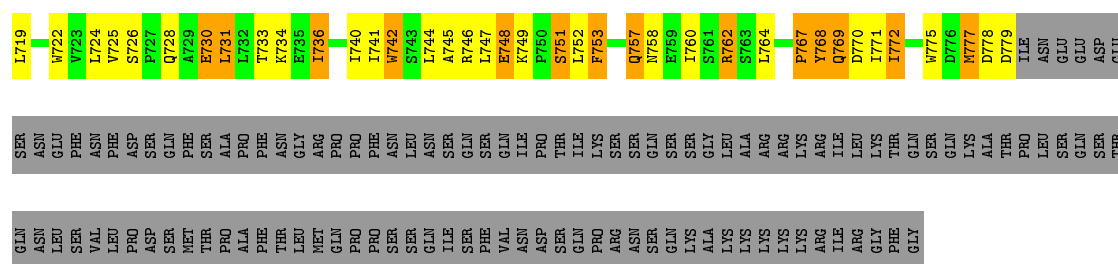




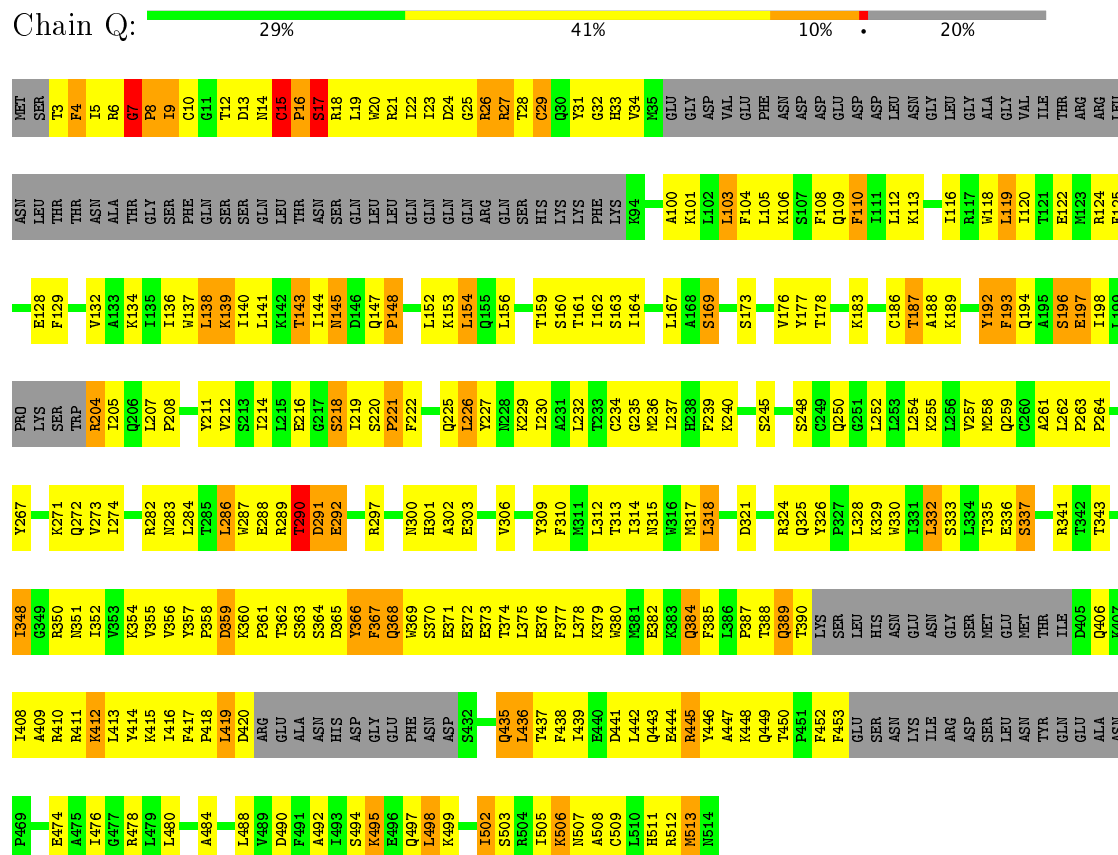
• Molecule 16: RNA polymerase I-specific transcription initiation factor RRN6

Chain P: 21% 32% 11% 35%

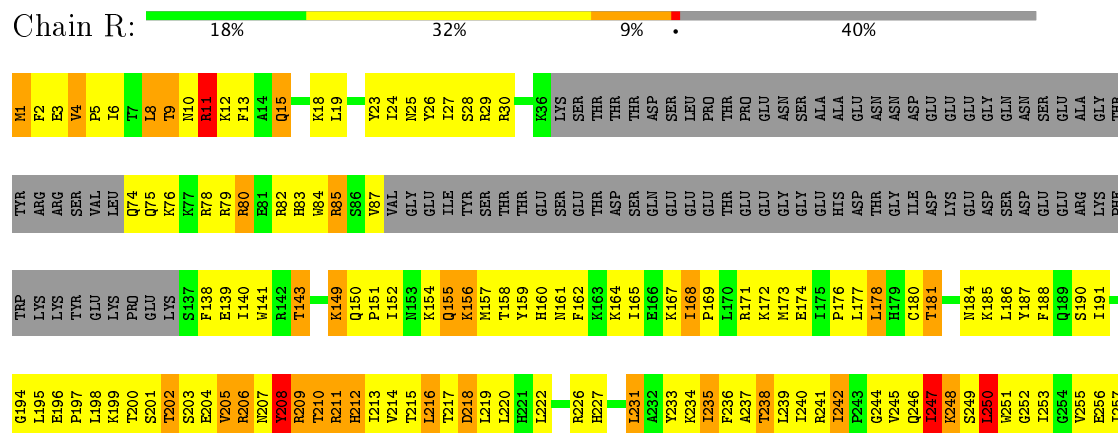




• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN7



• Molecule 18: RNA polymerase I-specific transcription initiation factor RRN11



Tyr	Ile	Ile
Asp	Gly	Leu
Ser	Leu	Lys
Ile	Asp	Pro
Asp	Arg	Phe
Asn	Asp	Asp
Ser	Ile	Thr
Ser	Lys	Glu
Val	I401	Asn
Glu	I402	Asp
Asn		Leu
Ser	I405	Leu
Phe	K406	Gln
Gly	H407	Glu
Asp	I408	L345
Val	H409	L346
Tyr	I410	D347
Glu	V411	K348
Thr	R412	L349
Asn	T413	S350
Ala	F414	E351
		I352
Glu	I417	V353
Phe	C418	L354
Leu	L419	T355
Asp	D420	P356
Thr	K421	
Gln	G422	N359
Leu		F360
Met	A425	D361
Asp	V426	A362
Leu	D427	E363
Ser	R428	V364
Pro	S429	N365
Glu	K430	F366
Asp	I431	L367
Asn		T368
Gly	Q434	A369
Lys	L435	S370
Asp	K436	G371
Glu		R372
Met	E439	L373
His	S440	L374
Tyr	Arg	D377
Ser	Leu	
Asp	Tyr	Leu
Glu	Gly	Ser
Asp	Glu	L317
Ser	Ala	Arg
Ser	Gln	Gln
Glu	Ile	Val
	Gln	Asp
	Glu	Asn
	Arg	Asp
	Val	Asn
	Val	Lys
		Asn
		Ser
		Ser
		Leu
		Trp

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	8317	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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 >2	RMSZ	# Z >2
1	A	0.49	0/11809	0.72	19/15943 (0.1%)
10	J	0.57	1/578 (0.2%)	0.59	0/775
11	K	0.46	0/804	0.79	3/1083 (0.3%)
12	L	0.42	0/354	0.60	0/468
13	M	0.40	0/872	0.55	0/1170
14	N	0.41	0/1172	0.54	0/1580
15	O	0.35	0/3996	0.54	0/5401
16	P	0.41	0/4822	0.68	4/6525 (0.1%)
17	Q	0.38	0/3501	0.64	2/4724 (0.0%)
18	R	0.37	0/2592	0.61	4/3486 (0.1%)
2	B	0.50	2/9518 (0.0%)	0.78	26/12863 (0.2%)
3	C	0.42	0/2475	0.67	3/3354 (0.1%)
4	D	0.40	0/465	0.59	0/630
5	E	0.40	0/1771	0.66	3/2383 (0.1%)
6	F	0.45	0/838	0.58	0/1129
7	G	0.37	0/1563	0.66	3/2124 (0.1%)
8	H	0.42	0/1070	0.61	0/1449
9	I	0.44	0/765	0.58	0/1030
All	All	0.44	3/48965 (0.0%)	0.68	67/66117 (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
1	A	0	15
12	L	0	2
13	M	0	3
14	N	0	1
15	O	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	26
17	Q	0	8
18	R	0	10
2	B	0	4
3	C	0	1
6	F	0	1
All	All	0	75

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	10	CYS	CB-SG	7.64	1.95	1.82
2	B	281	CYS	CB-SG	-6.95	1.70	1.82
2	B	859	CYS	CB-SG	-6.10	1.71	1.82

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	7	GLY	C-N-CD	-15.27	87.00	120.60
2	B	1023	ARG	NE-CZ-NH2	-13.76	113.42	120.30
1	A	397	ARG	NE-CZ-NH1	13.20	126.90	120.30
2	B	452	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	A	329	ARG	NE-CZ-NH2	-13.09	113.76	120.30

There are no chirality outliers.

5 of 75 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	LYS	Peptide
1	A	406	LEU	Peptide
1	A	407	GLN	Peptide
1	A	410	LYS	Peptide
1	A	411	VAL	Peptide

5.2 Too-close contacts ⓘ

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	11598	0	11664	1178	0
2	B	9312	0	9200	990	0
3	C	2423	0	2412	136	0
4	D	459	0	462	7	0
5	E	1735	0	1764	32	0
6	F	823	0	839	90	0
7	G	1526	0	1534	154	0
8	H	1052	0	1021	54	0
9	I	755	0	728	102	0
10	J	569	0	584	55	0
11	K	793	0	790	52	0
12	L	352	0	371	58	0
13	M	856	0	852	60	0
14	N	1151	0	1168	163	0
15	O	3907	0	3902	406	0
16	P	4729	0	4674	589	0
17	Q	3421	0	3459	775	0
18	R	2535	0	2598	606	0
19	A	2	0	0	1	0
19	B	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
19	Q	1	0	0	0	0
All	All	48004	0	48022	4035	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 42.

The worst 5 of 4035 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)
18:R:320:CYS:SG	18:R:374:LEU:HG	1.11	1.67
1:A:995:TYR:CD2	2:B:708:ASP:HA	1.30	1.64
17:Q:20:TRP:CZ3	17:Q:22:ILE:CG2	1.76	1.64
17:Q:186:CYS:HA	18:R:208:TYR:CE1	1.31	1.64
17:Q:326:TYR:CE1	17:Q:452:PHE:CE2	1.87	1.63

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1449/1664 (87%)	1375 (95%)	60 (4%)	14 (1%)	18	61
2	B	1164/1203 (97%)	1095 (94%)	51 (4%)	18 (2%)	12	53
3	C	303/335 (90%)	288 (95%)	12 (4%)	3 (1%)	18	61
4	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	4	33
5	E	210/215 (98%)	197 (94%)	11 (5%)	2 (1%)	18	61
6	F	98/155 (63%)	95 (97%)	2 (2%)	1 (1%)	18	61
7	G	187/326 (57%)	173 (92%)	12 (6%)	2 (1%)	17	60
8	H	127/146 (87%)	121 (95%)	6 (5%)	0	100	100
9	I	91/125 (73%)	80 (88%)	8 (9%)	3 (3%)	4	35
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	42/70 (60%)	36 (86%)	4 (10%)	2 (5%)	2	28
13	M	106/415 (26%)	96 (91%)	8 (8%)	2 (2%)	9	47
14	N	139/233 (60%)	123 (88%)	13 (9%)	3 (2%)	8	44
15	O	467/627 (74%)	426 (91%)	35 (8%)	6 (1%)	14	56
16	P	569/894 (64%)	473 (83%)	76 (13%)	20 (4%)	4	34
17	Q	396/514 (77%)	345 (87%)	41 (10%)	10 (2%)	6	41
18	R	291/507 (57%)	245 (84%)	40 (14%)	6 (2%)	8	45
All	All	5859/7778 (75%)	5373 (92%)	392 (7%)	94 (2%)	16	51

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	LYS
1	A	479	ALA
1	A	1651	THR
2	B	111	ASP

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Mol	Chain	Res	Type
2	B	895	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1297/1465 (88%)	1215 (94%)	82 (6%)	21	53
2	B	1025/1053 (97%)	960 (94%)	65 (6%)	21	53
3	C	269/296 (91%)	253 (94%)	16 (6%)	23	55
4	D	55/116 (47%)	49 (89%)	6 (11%)	7	30
5	E	194/197 (98%)	180 (93%)	14 (7%)	17	49
6	F	90/137 (66%)	86 (96%)	4 (4%)	33	63
7	G	171/291 (59%)	159 (93%)	12 (7%)	18	50
8	H	115/128 (90%)	111 (96%)	4 (4%)	41	69
9	I	89/110 (81%)	84 (94%)	5 (6%)	25	57
10	J	64/65 (98%)	57 (89%)	7 (11%)	7	30
11	K	91/130 (70%)	84 (92%)	7 (8%)	15	47
12	L	39/57 (68%)	36 (92%)	3 (8%)	15	47
13	M	98/371 (26%)	85 (87%)	13 (13%)	4	24
14	N	135/220 (61%)	129 (96%)	6 (4%)	33	63
15	O	439/576 (76%)	387 (88%)	52 (12%)	6	27
16	P	539/828 (65%)	396 (74%)	143 (26%)	0	4
17	Q	383/476 (80%)	318 (83%)	65 (17%)	2	15
18	R	286/474 (60%)	228 (80%)	58 (20%)	1	9
All	All	5379/6990 (77%)	4817 (90%)	562 (10%)	12	32

5 of 562 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	175	MET

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Mol	Chain	Res	Type
16	P	246	LYS
18	R	155	GLN
15	O	204	THR
15	O	454	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	105	ASN
15	O	342	HIS
17	Q	384	GLN
15	O	117	GLN
15	O	228	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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
1	A	2
7	G	1
17	Q	1
9	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	24:VAL	C	25:THR	N	4.53
1	I	45:LEU	C	46:LYS	N	3.17
1	Q	369:TRP	C	370:SER	N	3.11
1	A	438:ILE	C	439:ASP	N	2.97
1	A	991:LYS	C	992:PRO	N	2.87