



wwPDB EM Validation Summary Report ⓘ

Jun 16, 2025 – 02:53 PM JST

PDB ID : 9VD9 / pdb_00009vd9
EMDB ID : EMD-39339
Title : Cryo-EM structure of the human DSS1-INTAC-PEC complex
Authors : Zheng, H.; Xu, Y.; Cheng, J.
Deposited on : 2025-06-07
Resolution : 4.60 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

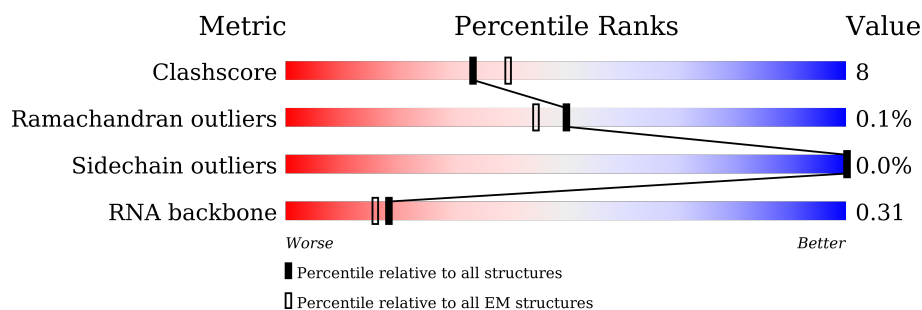
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

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














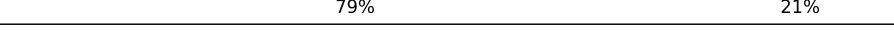






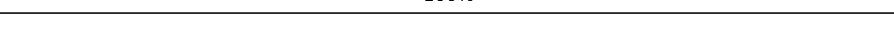
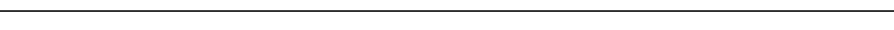

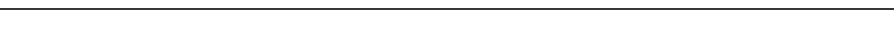
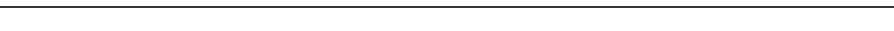


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	70	31% 14% 54%
2	I	658	74% 22% .
3	K	600	79% 19% .
4	c	21	38% 52% 10%
5	B	1204	71% 17% 12%
6	D	963	69% 16% 14%
7	G	962	78% 16% 5%
8	m	14	100%



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Mol	Chain	Length	Quality of chain
9	n	8	
10	P	589	
11	Q	309	
12	1	1970	
13	2	1300	
14	3	275	
15	4	210	
16	5	127	
17	6	150	
18	7	125	
19	8	67	
20	9	117	
21	a	58	
22	b	48	
23	d	45	
24	e	528	
25	f	580	
26	g	590	
27	h	22	
28	i	117	
29	j	1087	
30	k	172	
31	l	142	
32	A	2190	
33	E	1019	

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Mol	Chain	Length	Quality of chain
34	F	887	 50% 14% 36%
35	H	995	 76% 19% 6%
36	M	17	 94% 6%
37	p	4	 100%
38	o	8	 88% 12%

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 113214 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 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	32	Total	C	N	O	S	0	0
			275	169	47	58	1		

- Molecule 2 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	633	Total	C	N	O	S	0	0
			4985	3210	815	926	34		

- Molecule 3 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	590	Total	C	N	O	S	0	0
			4646	2964	806	841	35		

- Molecule 4 is a RNA chain called RNA (5'-R(P*UP*AP*AP*CP*CP*GP*GP*AP*GP*AP*GP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	21	Total	C	N	O	P	0	0
			452	202	87	142	21		

- Molecule 5 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	1061	Total	C	N	O	S	0	0
			8328	5322	1412	1530	64		

- Molecule 6 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	828	Total	C	N	O	S	0	0
			6199	3928	1082	1158	31		

- Molecule 7 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	910	Total	C	N	O	S	0	0
			6914	4373	1211	1289	41		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	m	14	Total	C	N	O	0	0
			102	64	14	24		

- Molecule 9 is a protein called THR-SER-PRO-SER-TYR-SER-PRO-THR.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	n	8	Total	C	N	O	0	0
			58	36	8	14		

- Molecule 10 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	581	Total	C	N	O	S	0	0
			4527	2877	763	860	27		

- Molecule 11 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	293	Total	C	N	O	S	0	0
			2366	1497	405	449	15		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	1417	Total	C	N	O	S	0	0
			11125	6999	1999	2059	68		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit beta,DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2	1113	Total	C	N	O	S	0	0
			8649	5489	1515	1581	64		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	882	GLY	SER	conflict	UNP P30876

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	259	Total	C	N	O	S	0	0
			2047	1289	354	398	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	74	THR	ILE	conflict	UNP P19387
3	140	SER	ASN	conflict	UNP P19387

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	44	PHE	SER	conflict	UNP P19388

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	5	81	Total	C	N	O	S	0	0
			649	413	111	120	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	126	SER	THR	conflict	UNP P61218

- Molecule 17 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	7	117	Total	C	N	O	S	0	0
			950	587	169	183	11		

- Molecule 19 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	8	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 20 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	9	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 21 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	a	46	Total	C	N	O	S	0	0
			389	241	75	67	6		

- Molecule 22 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	36	Total	C	N	O	P	0	0
			752	351	153	212	36		

- Molecule 23 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	45	Total	C	N	O	P	0	0
			909	431	157	276	45		

- Molecule 24 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	183	Total	C	N	O	S	0	0
			1410	895	239	269	7		

- Molecule 25 is a protein called Negative elongation factor B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	480	Total	C	N	O		0	0
			1920	960	480	480			

- Molecule 26 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	534	Total	C	N	O	S	0	0
			3764	2382	653	710	19		

- Molecule 27 is a protein called Negative elongation factor E.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	22	Total	C	N	O		0	0
			110	66	22	22			

- Molecule 28 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	i	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

- Molecule 29 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	j	482	Total	C	N	O	S	0	0
			3854	2448	681	708	17		

- Molecule 30 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	k	171	Total	C	N	O	S	0	0
			1299	849	205	238	7		

- Molecule 31 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	l	129	Total	C	N	O	S	0	1
			998	629	170	195	4		

- Molecule 32 is a protein called Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A	1779	Total	C	N	O	S	0	0
			13054	8226	2322	2432	74		

- Molecule 33 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	E	798	Total	C	N	O	S	0	0
			5244	3284	988	958	14		

- Molecule 34 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	F	564	Total	C	N	O	S	0	0
			4333	2766	745	800	22		

- Molecule 35 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	H	937	Total	C	N	O	S	0	0
			7440	4761	1274	1361	44		

- Molecule 36 is a protein called Unknown2.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	M	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 37 is a protein called SER-PRO-THR-SER.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	p	4	Total	C	N	O	0	0
			20	12	4	4		

- Molecule 38 is a protein called SER-PRO-LYS-TYR-SER-PRO-THR-SER.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	8	Total	C	N	O	0	0
			60	38	9	13		

- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
39	K	2	Total	Zn	0
			2	2	
39	1	2	Total	Zn	0
			2	2	
39	2	1	Total	Zn	0
			1	1	
39	3	1	Total	Zn	0
			1	1	
39	7	2	Total	Zn	0
			2	2	
39	8	1	Total	Zn	0
			1	1	
39	a	1	Total	Zn	0
			1	1	

- Molecule 40 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
40	Q	2	Total	Mn	0
			2	2	

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

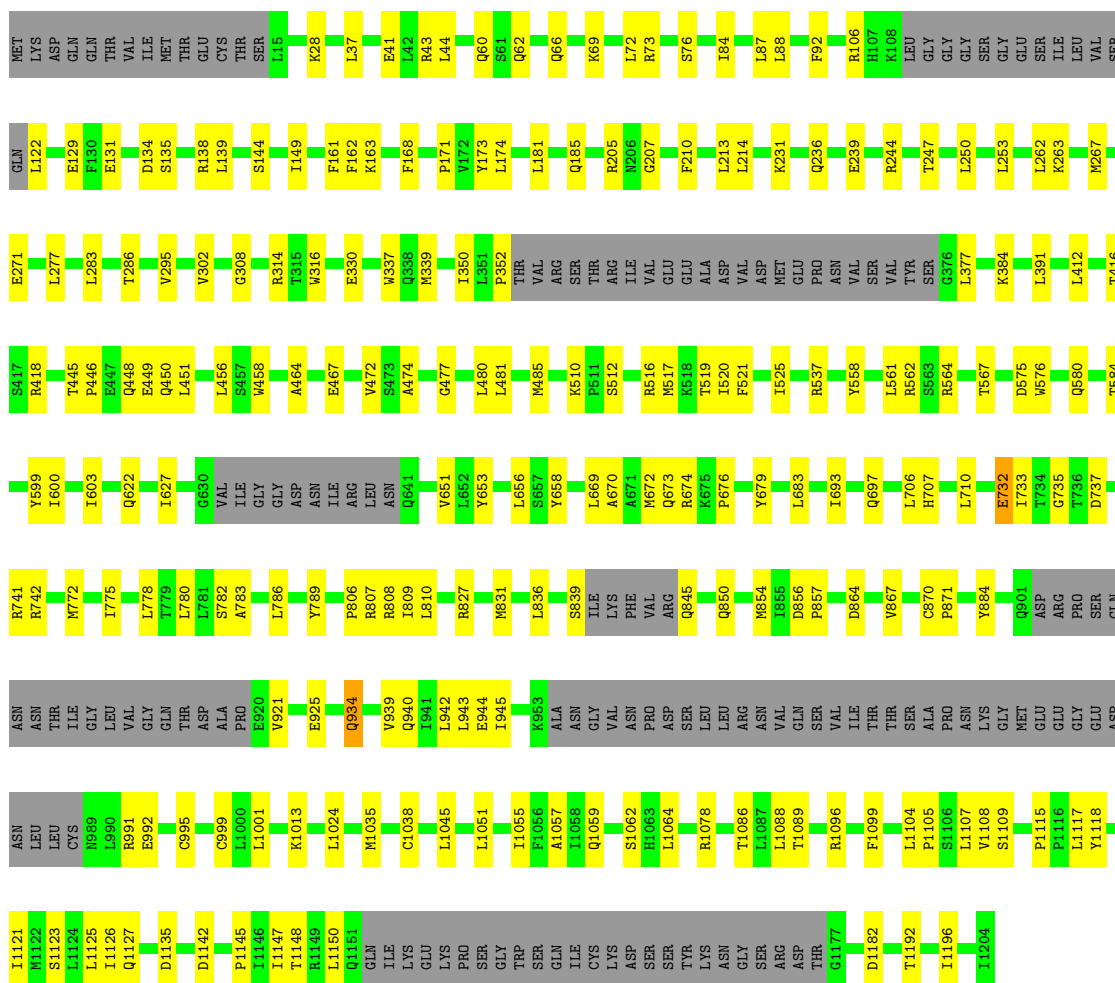
Mol	Chain	Residues	Atoms		AltConf
41	1	1	Total	Mg	0
			1	1	



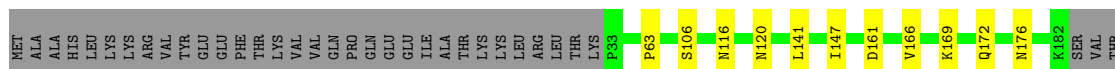
- Molecule 4: RNA (5'-R(P*UP*AP*AP*CP*CP*GP*GP*AP*GP*AP*GP*GP*GP*AP*AP*C
P*CP*CP*AP*CP*U)-3')



- Molecule 5: Integrator complex subunit 2



- Molecule 6: Integrator complex subunit 4

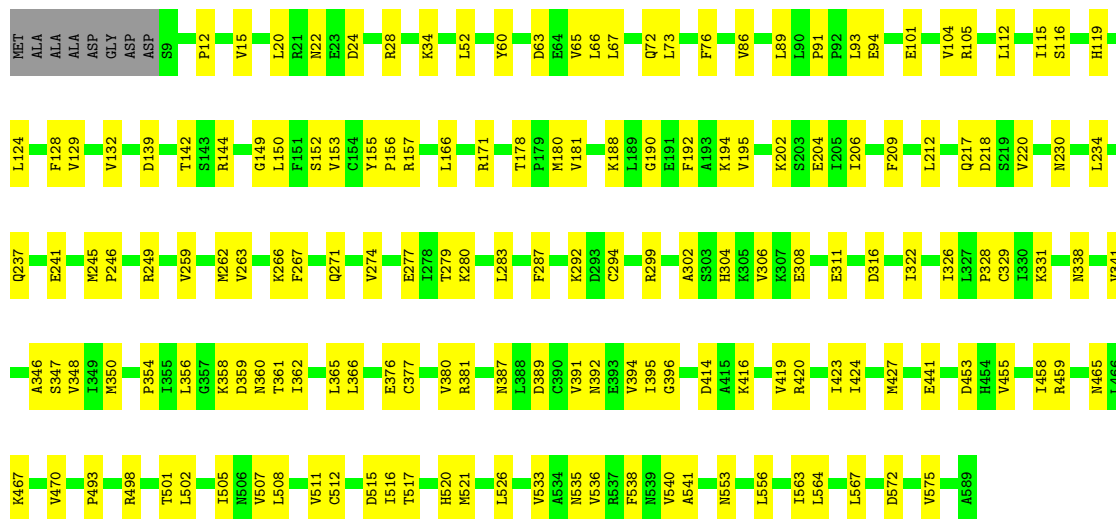






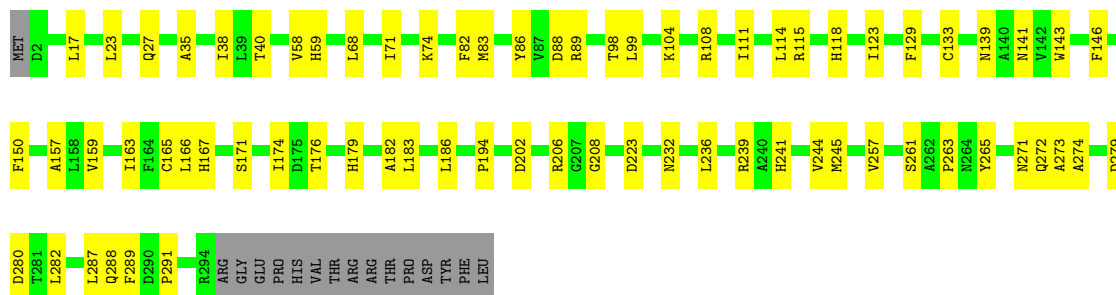
- Molecule 10: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

Chain P: 71% 28%



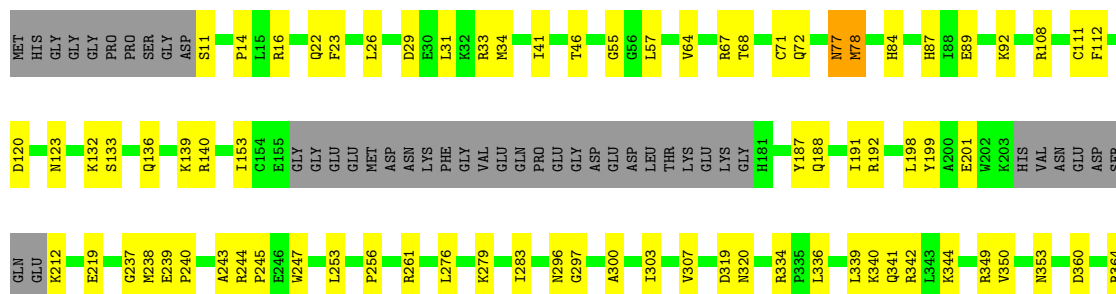
- Molecule 11: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain Q: 72% 23% 5%



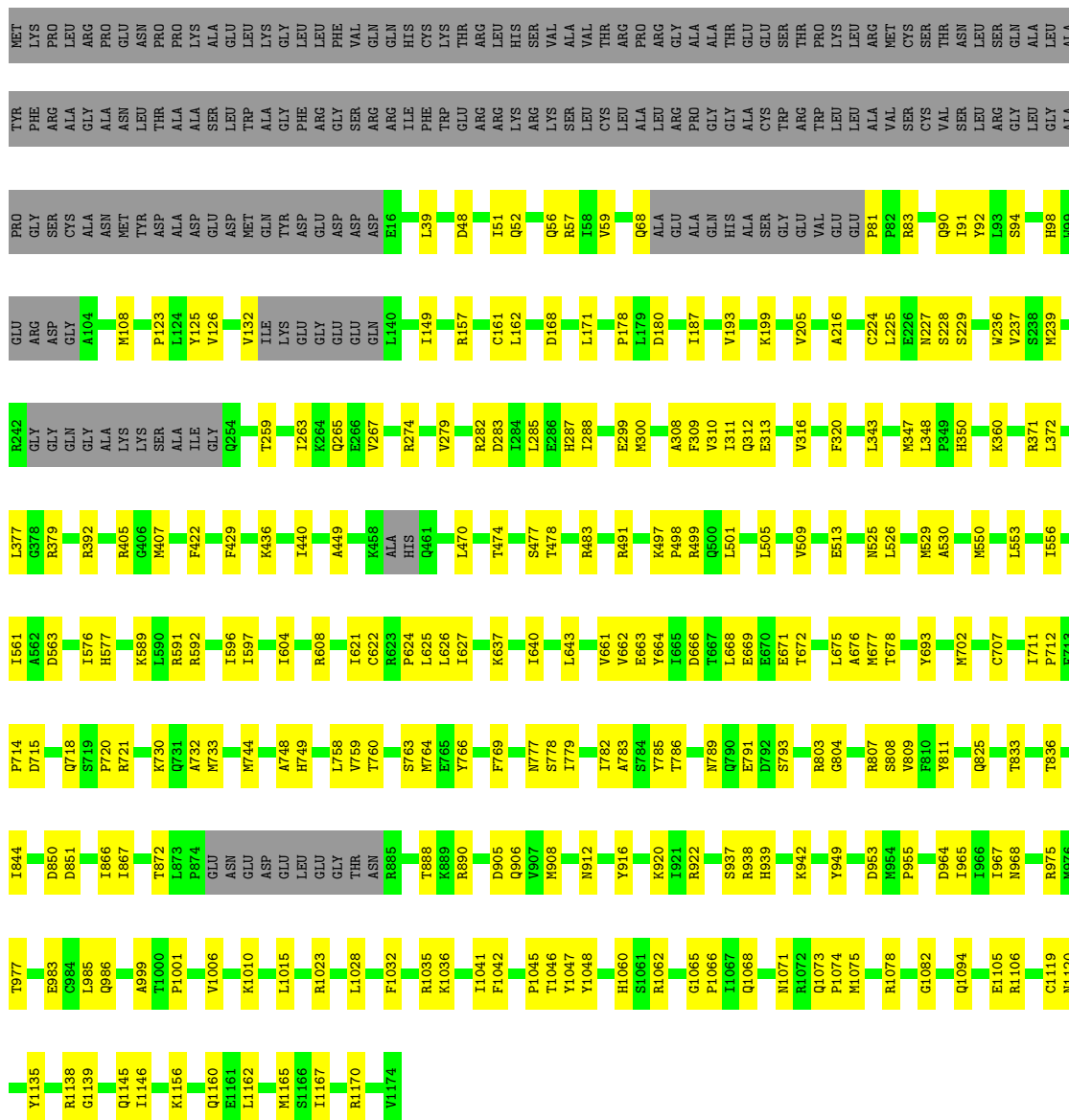
- Molecule 12: DNA-directed RNA polymerase II subunit RPB1

Chain 1: 55% 17% 28%



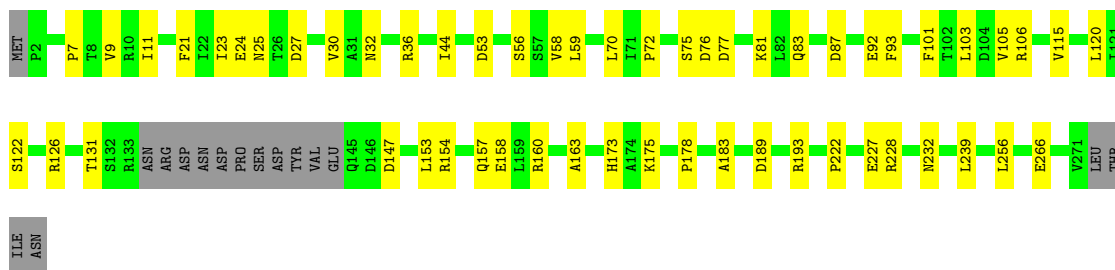
- Molecule 13: DNA-directed RNA polymerase subunit beta,DNA-directed RNA polymerase II subunit RPB2

Response	Percentage
Yes, the U.S. is a democracy	67%
No, the U.S. is not a democracy	19%
Don't know	14%




- Molecule 14: DNA-directed RNA polymerase II subunit RPB3

Digital Tool Type	Percentage of Respondents
Video conferencing tool	74%
Document collaboration tool	20%
Project management tool	6%



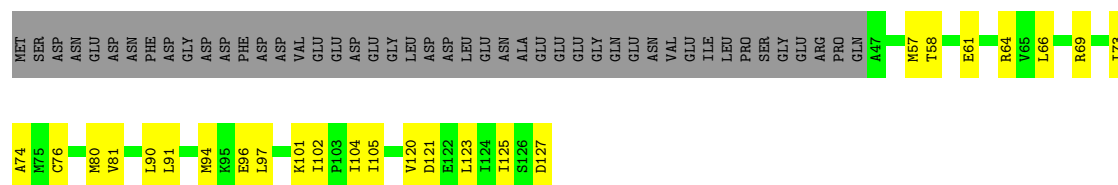
- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain 4:  78% 22%



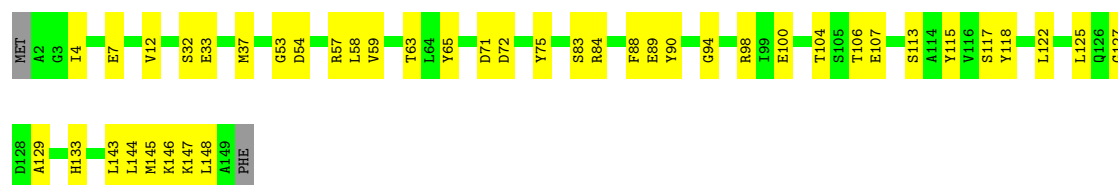
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain 5:  44% 20% 36%



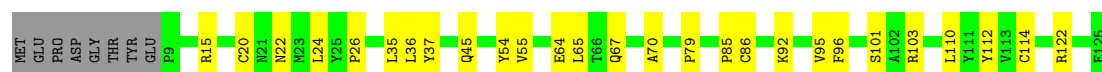
- Molecule 17: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain 6:  71% 28%




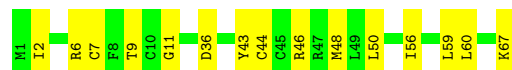
- Molecule 18: DNA-directed RNA polymerase II subunit RPB9

Chain 7:  72% 22% 6%




- Molecule 19: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain 8:  78% 22%



- Molecule 20: DNA-directed RNA polymerase II subunit RPB11-a

Chain 9:  79% 21%



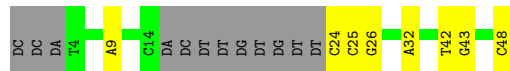
- Molecule 21: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain a: 



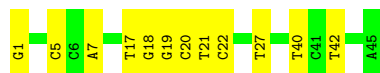
- Molecule 22: DNA (48-MER)

Chain b: 



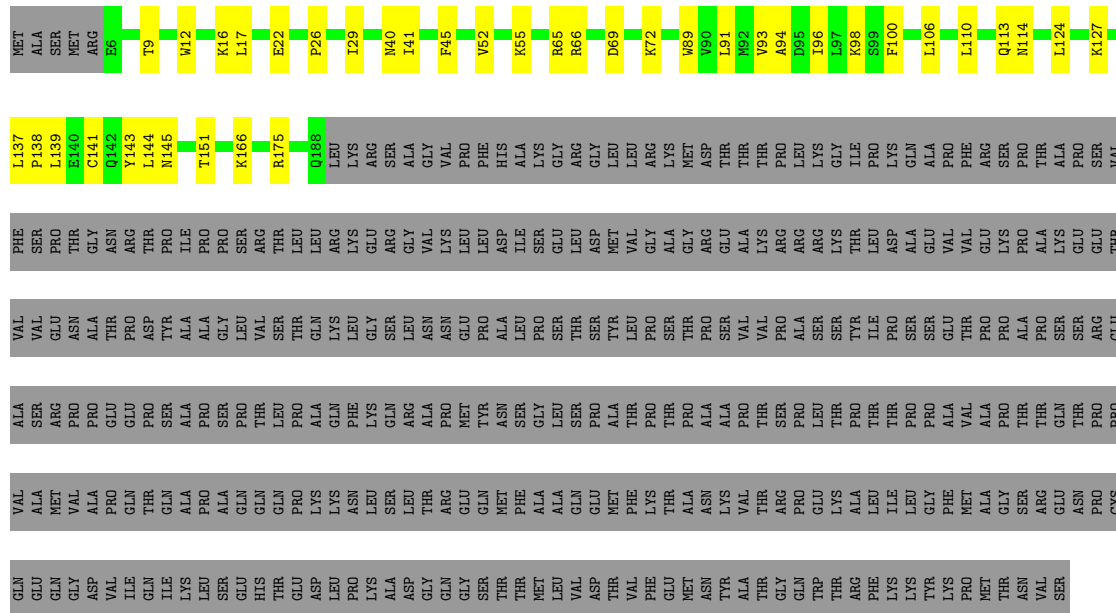
- Molecule 23: DNA (45-MER)

Chain d: 




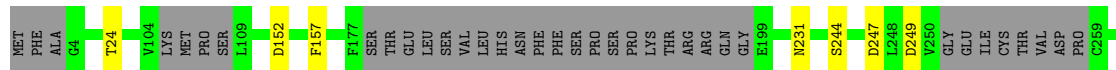
- Molecule 24: Negative elongation factor A

Chain e: 

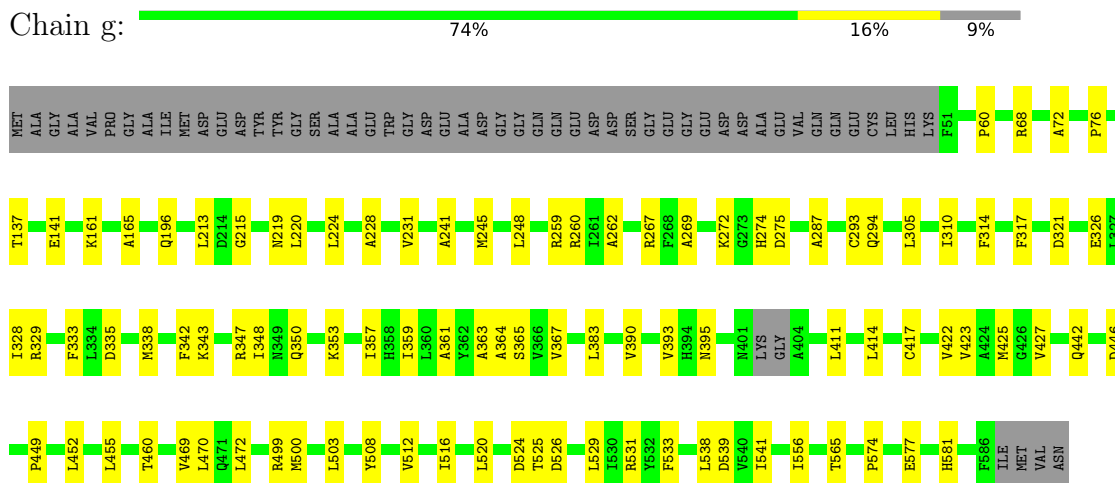


- Molecule 25: Negative elongation factor B

Chain f: 



- Molecule 26: Negative elongation factor C/D

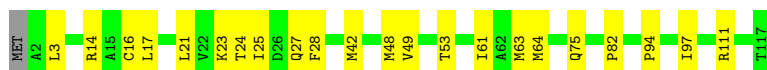
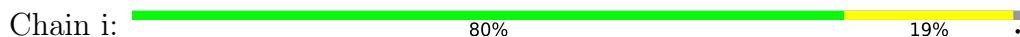


- Molecule 27: Negative elongation factor E

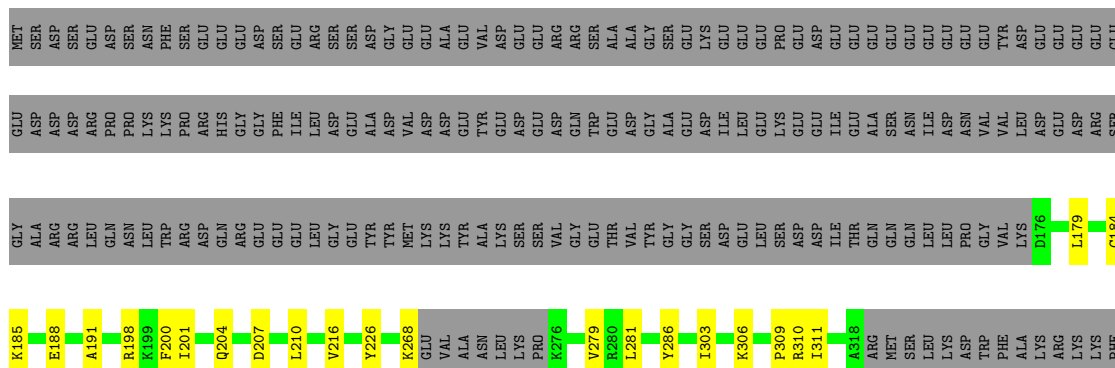
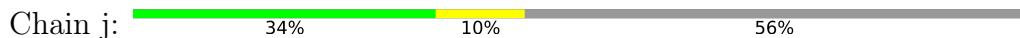


There are no outlier residues recorded for this chain.

- Molecule 28: Transcription elongation factor SPT4

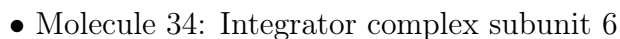
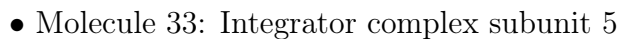


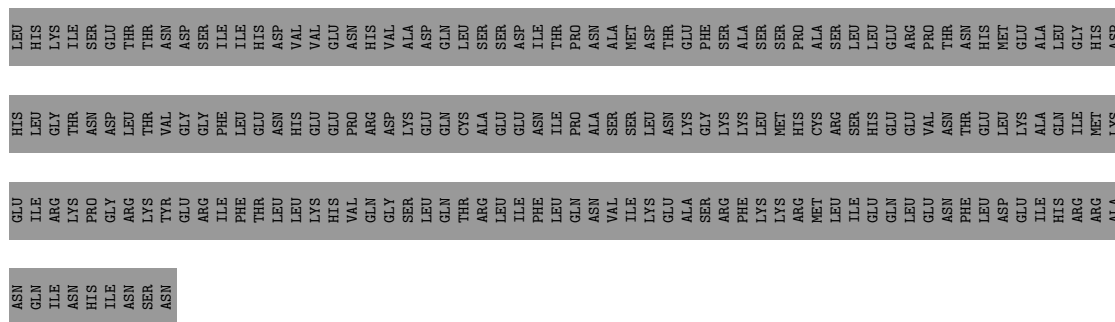
- Molecule 29: Transcription elongation factor SPT5



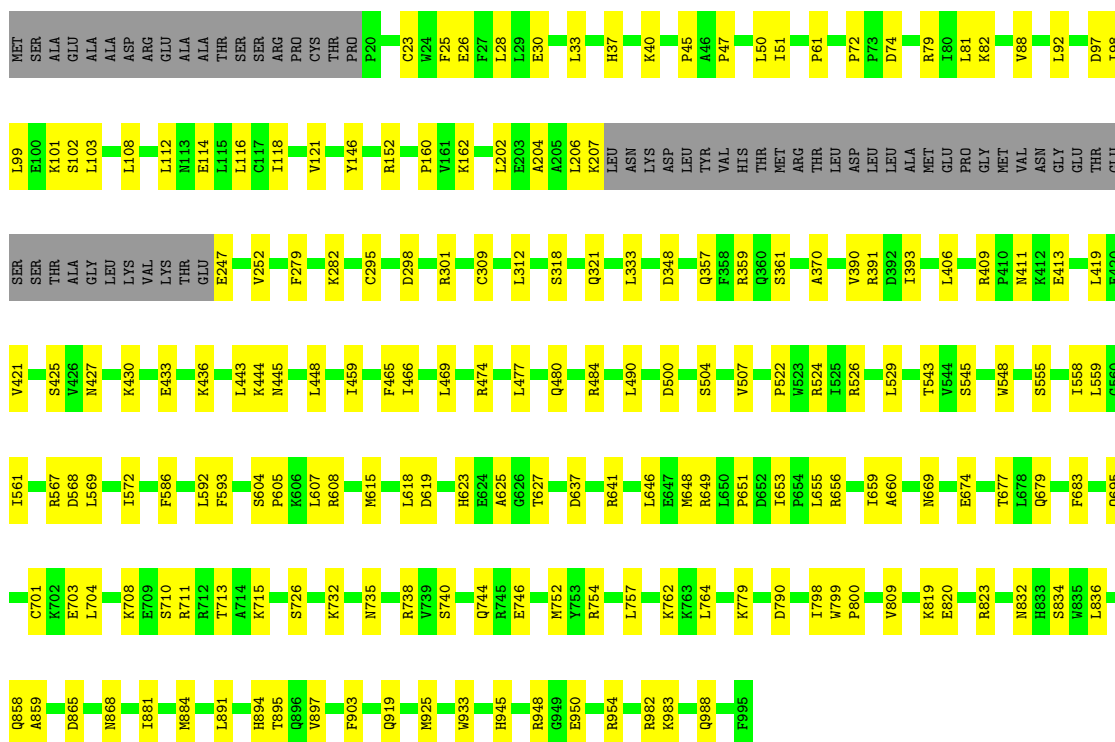
Response	Percentage
Yes, the U.S. is a democracy	69%
No, the U.S. is not a democracy	12%
Don't know	19%







- Molecule 35: Integrator complex subunit 8



- Molecule 36: Unknown2

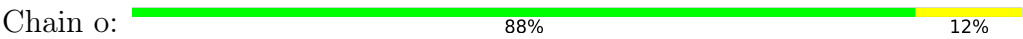


- Molecule 37: SER-PRO-THR-SER



There are no outlier residues recorded for this chain.

- Molecule 38: SER-PRO-LYS-TYR-SER-PRO-THR-SER



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26882	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: MG, 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	0	0.28	0/282	0.68	0/381
2	I	0.25	0/5110	0.58	1/6959 (0.0%)
3	K	0.22	0/4747	0.54	1/6412 (0.0%)
4	c	0.14	0/506	0.35	0/787
5	B	0.29	0/8474	0.57	3/11498 (0.0%)
6	D	0.29	0/6309	0.62	1/8576 (0.0%)
7	G	0.30	0/7023	0.62	2/9512 (0.0%)
8	m	0.29	0/107	0.79	0/149
9	n	0.29	0/60	0.73	0/83
10	P	0.24	0/4601	0.60	2/6246 (0.0%)
11	Q	0.29	0/2423	0.60	0/3285
12	1	0.20	1/11325 (0.0%)	0.53	7/15293 (0.0%)
13	2	0.21	0/8823	0.52	0/11947
14	3	0.22	0/2090	0.47	0/2843
15	4	0.20	0/1752	0.53	0/2366
16	5	0.21	0/659	0.62	0/889
17	6	0.18	0/1207	0.49	0/1628
18	7	0.18	0/973	0.47	0/1316
19	8	0.23	0/542	0.51	0/730
20	9	0.24	0/956	0.64	3/1294 (0.2%)
21	a	0.24	0/395	0.57	0/524
22	b	0.16	0/846	0.28	0/1304
23	d	0.19	0/1014	0.34	0/1560
24	e	0.19	0/1434	0.51	0/1948
25	f	0.13	0/1913	0.36	0/2379
26	g	0.22	0/3830	0.58	2/5236 (0.0%)
28	i	0.14	0/927	0.39	0/1250
29	j	0.16	0/3920	0.41	0/5276
30	k	0.18	0/1330	0.47	1/1813 (0.1%)
31	l	0.17	0/1012	0.43	0/1366
32	A	0.20	0/13264	0.50	2/18049 (0.0%)
33	E	0.22	0/5344	0.53	2/7312 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	F	0.20	0/4441	0.47	0/6045
35	H	0.20	0/7583	0.49	0/10280
37	p	0.13	0/19	0.35	0/25
38	o	0.30	0/62	0.58	0/84
All	All	0.23	1/115303 (0.0%)	0.53	27/156645 (0.0%)

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
35	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1	526	VAL	C-N	5.83	1.42	1.33

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g	76	PRO	N-CA-CB	10.38	109.76	102.81
2	I	396	GLY	N-CA-C	7.09	120.73	112.50
6	D	248	VAL	N-CA-C	-6.54	104.38	110.53
5	B	732	GLU	CB-CA-C	-6.36	107.44	116.34
10	P	441	GLU	CA-C-N	-6.09	112.76	122.08

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	H	543	THR	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	0	275	0	231	8	0
2	I	4985	0	5013	94	0
3	K	4646	0	4663	78	0
4	c	452	0	230	6	0
5	B	8328	0	8566	146	0
6	D	6199	0	5896	105	0
7	G	6914	0	6898	105	0
8	m	102	0	92	0	0
9	n	58	0	54	2	0
10	P	4527	0	4633	104	0
11	Q	2366	0	2269	49	0
12	1	11125	0	11187	226	0
13	2	8649	0	8462	164	0
14	3	2047	0	1985	38	0
15	4	1721	0	1737	31	0
16	5	649	0	676	20	0
17	6	1186	0	1147	34	0
18	7	950	0	879	19	0
19	8	533	0	553	14	0
20	9	937	0	959	18	0
21	a	389	0	393	9	0
22	b	752	0	401	7	0
23	d	909	0	506	11	0
24	e	1410	0	1455	33	0
25	f	1920	0	504	3	0
26	g	3764	0	3378	70	0
27	h	110	0	24	0	0
28	i	911	0	908	13	0
29	j	3854	0	3913	69	0
30	k	1299	0	1258	24	0
31	l	998	0	953	24	0
32	A	13054	0	12233	165	0
33	E	5244	0	4501	64	0
34	F	4333	0	4240	73	0
35	H	7440	0	7530	116	0
36	M	85	0	19	1	0
37	p	20	0	9	0	0
38	o	60	0	60	1	0
39	1	2	0	0	0	0
39	2	1	0	0	0	0
39	3	1	0	0	0	0
39	7	2	0	0	0	0
39	8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	K	2	0	0	0	0
39	a	1	0	0	0	0
40	Q	2	0	0	0	0
41	1	1	0	0	0	0
All	All	113214	0	108415	1768	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 8.

The worst 5 of 1768 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)
29:j:626:CYS:O	29:j:634:GLY:HA3	1.55	1.07
12:1:11:SER:N	13:2:1135:TYR:HH	1.57	1.01
13:2:825:GLN:HA	13:2:872:THR:O	1.61	0.99
10:P:188:LYS:O	10:P:192:PHE:HB2	1.63	0.98
12:1:23:PHE:O	12:1:1446:GLY:HA2	1.68	0.94

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 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	0	30/70 (43%)	28 (93%)	2 (7%)	0	100	100
2	I	629/658 (96%)	598 (95%)	30 (5%)	1 (0%)	44	78
3	K	586/600 (98%)	554 (94%)	32 (6%)	0	100	100
5	B	1045/1204 (87%)	1004 (96%)	41 (4%)	0	100	100
6	D	814/963 (84%)	748 (92%)	61 (8%)	5 (1%)	22	59
7	G	904/962 (94%)	839 (93%)	62 (7%)	3 (0%)	37	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	m	12/14 (86%)	9 (75%)	3 (25%)	0	100	100
9	n	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
10	P	579/589 (98%)	568 (98%)	11 (2%)	0	100	100
11	Q	291/309 (94%)	272 (94%)	19 (6%)	0	100	100
12	1	1407/1970 (71%)	1341 (95%)	63 (4%)	3 (0%)	44	78
13	2	1099/1300 (84%)	1040 (95%)	59 (5%)	0	100	100
14	3	255/275 (93%)	242 (95%)	13 (5%)	0	100	100
15	4	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
16	5	79/127 (62%)	76 (96%)	3 (4%)	0	100	100
17	6	146/150 (97%)	138 (94%)	8 (6%)	0	100	100
18	7	115/125 (92%)	113 (98%)	2 (2%)	0	100	100
19	8	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
20	9	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
21	a	44/58 (76%)	43 (98%)	1 (2%)	0	100	100
24	e	181/528 (34%)	177 (98%)	4 (2%)	0	100	100
25	f	466/580 (80%)	436 (94%)	28 (6%)	2 (0%)	30	68
26	g	530/590 (90%)	490 (92%)	40 (8%)	0	100	100
28	i	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
29	j	470/1087 (43%)	447 (95%)	23 (5%)	0	100	100
30	k	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
31	l	127/142 (89%)	124 (98%)	3 (2%)	0	100	100
32	A	1755/2190 (80%)	1671 (95%)	82 (5%)	2 (0%)	48	83
33	E	794/1019 (78%)	728 (92%)	63 (8%)	3 (0%)	30	68
34	F	560/887 (63%)	539 (96%)	21 (4%)	0	100	100
35	H	933/995 (94%)	888 (95%)	45 (5%)	0	100	100
37	p	2/4 (50%)	2 (100%)	0	0	100	100
38	o	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	14535/18095 (80%)	13773 (95%)	743 (5%)	19 (0%)	50	83

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	358	PRO

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Mol	Chain	Res	Type
6	D	63	PRO
6	D	106	SER
6	D	561	MET
7	G	553	VAL

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	0	29/63 (46%)	29 (100%)	0	100	100
2	I	575/600 (96%)	575 (100%)	0	100	100
3	K	505/520 (97%)	505 (100%)	0	100	100
5	B	946/1072 (88%)	945 (100%)	1 (0%)	92	94
6	D	616/845 (73%)	616 (100%)	0	100	100
7	G	741/840 (88%)	741 (100%)	0	100	100
8	m	14/14 (100%)	14 (100%)	0	100	100
9	n	8/8 (100%)	8 (100%)	0	100	100
10	P	508/512 (99%)	508 (100%)	0	100	100
11	Q	259/274 (94%)	259 (100%)	0	100	100
12	1	1217/1748 (70%)	1216 (100%)	1 (0%)	92	94
13	2	908/1127 (81%)	908 (100%)	0	100	100
14	3	227/252 (90%)	227 (100%)	0	100	100
15	4	191/192 (100%)	191 (100%)	0	100	100
16	5	70/111 (63%)	70 (100%)	0	100	100
17	6	129/131 (98%)	129 (100%)	0	100	100
18	7	105/112 (94%)	105 (100%)	0	100	100
19	8	56/56 (100%)	56 (100%)	0	100	100
20	9	106/106 (100%)	106 (100%)	0	100	100
21	a	43/55 (78%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	e	158/451 (35%)	158 (100%)	0	100	100
26	g	339/513 (66%)	339 (100%)	0	100	100
28	i	102/103 (99%)	102 (100%)	0	100	100
29	j	425/940 (45%)	425 (100%)	0	100	100
30	k	136/153 (89%)	136 (100%)	0	100	100
31	l	104/126 (82%)	104 (100%)	0	100	100
32	A	1253/1907 (66%)	1253 (100%)	0	100	100
33	E	395/812 (49%)	395 (100%)	0	100	100
34	F	466/796 (58%)	466 (100%)	0	100	100
35	H	822/896 (92%)	822 (100%)	0	100	100
38	o	8/8 (100%)	8 (100%)	0	100	100
All	All	11461/15343 (75%)	11459 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	934	GLN
12	1	77	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
12	1	757	GLN
35	H	613	ASN
13	2	1013	ASN
35	H	540	GLN
33	E	708	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	c	20/21 (95%)	8 (40%)	0

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	c	27	A
4	c	28	A
4	c	31	G
4	c	32	G
4	c	33	A

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.