



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:17 PM BST

PDB ID : 5FJ9
EMDB ID: : EMD-3179
Title : Cryo-EM structure of yeast apo RNA polymerase III at 4.6 Å
Authors : Hoffmann, N.A.; Jakobi, A.J.; Moreno-Morcillo, M.; Glatt, S.; Kosinski, J.;
Hagen, W.J.; Sachse, C.; Muller, C.W.
Deposited on : 2015-10-06
Resolution : 4.60 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

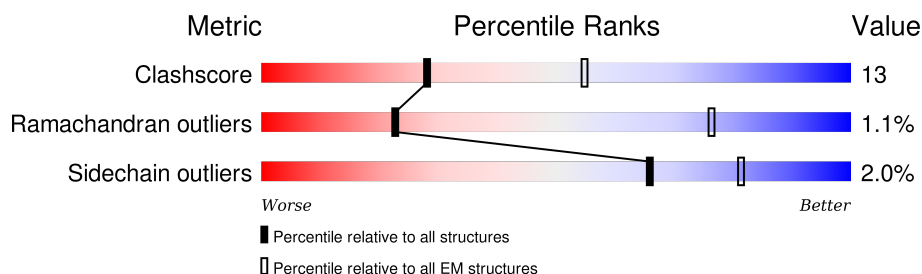
1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	1460	71% 25% ..
2	B	1149	70% 26% ..
3	C	335	75% 24% .
4	D	161	46% 27% . 26%
5	E	215	67% 32% .
6	F	155	46% 6% . 46%
7	G	212	48% 40% . 10%
8	H	146	69% 27% .
9	I	110	65% 18% . 16%

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Mol	Chain	Length	Quality of chain
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	104	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 38680 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 III SUBUNIT RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1412	Total	C	N	O	S	0	0
			11071	6979	1954	2079	59		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1544	1007	250	281	6		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	92	Total	C	N	O	S	0	0
			728	455	117	145	11		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	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
			792	496	130	161	5		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	165	Total	C	N	O	S	0	0
			1347	862	229	255	1		

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	105	Total	C	N	O	S	0	0
			802	508	144	147	3		

- Molecule 15 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	528	Total	C	N	O	S	0	0
			4247	2705	725	798	19		

- Molecule 16 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	98	Total	C	N	O	S	0	0
			820	533	126	157	4		

- Molecule 17 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	70	Total	C	N	O	0	0
			446	282	80	84		

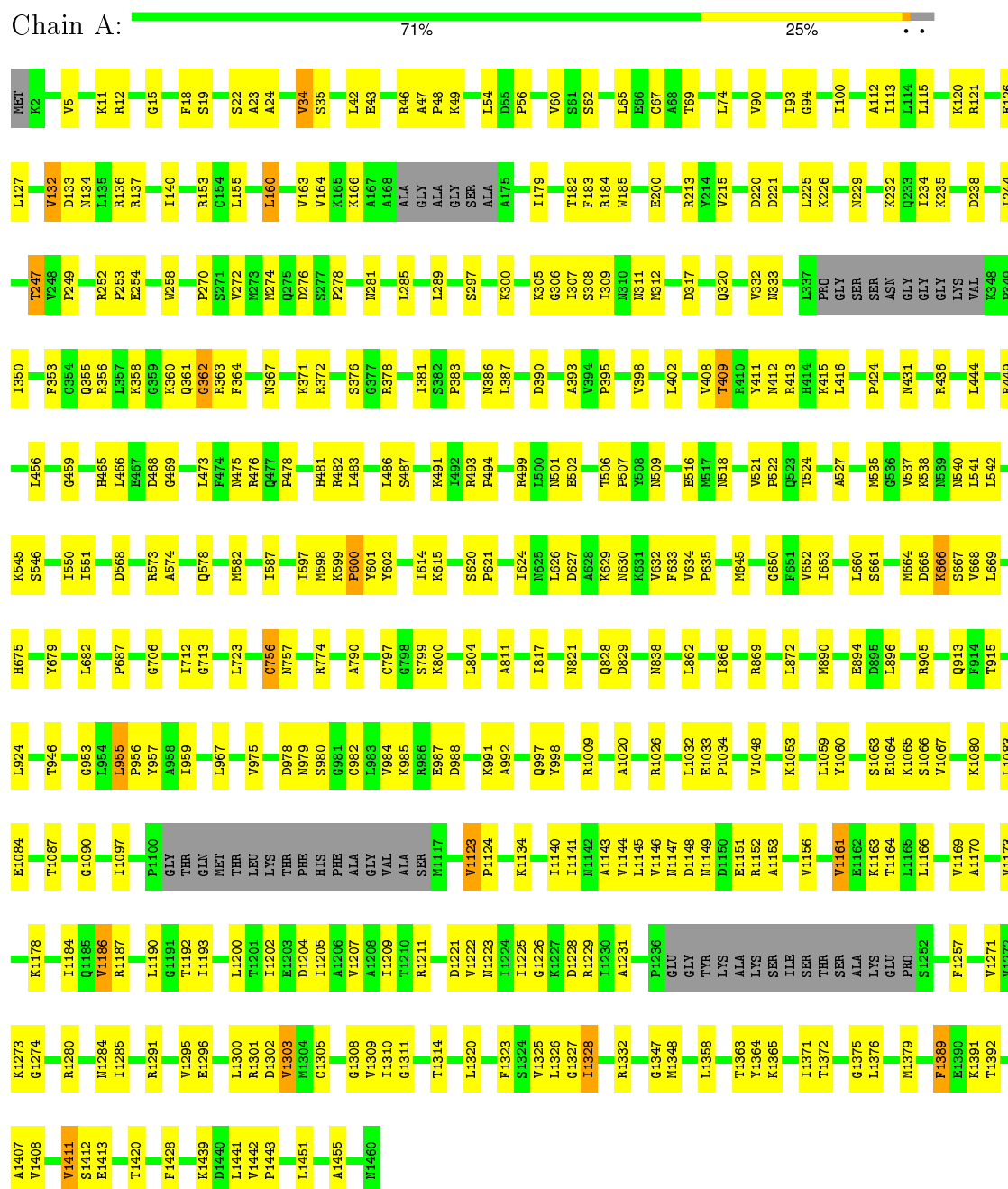
- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	Zn	0
			1	1	
18	A	2	Total	Zn	0
			2	2	
18	L	1	Total	Zn	0
			1	1	
18	J	1	Total	Zn	0
			1	1	
18	I	1	Total	Zn	0
			1	1	

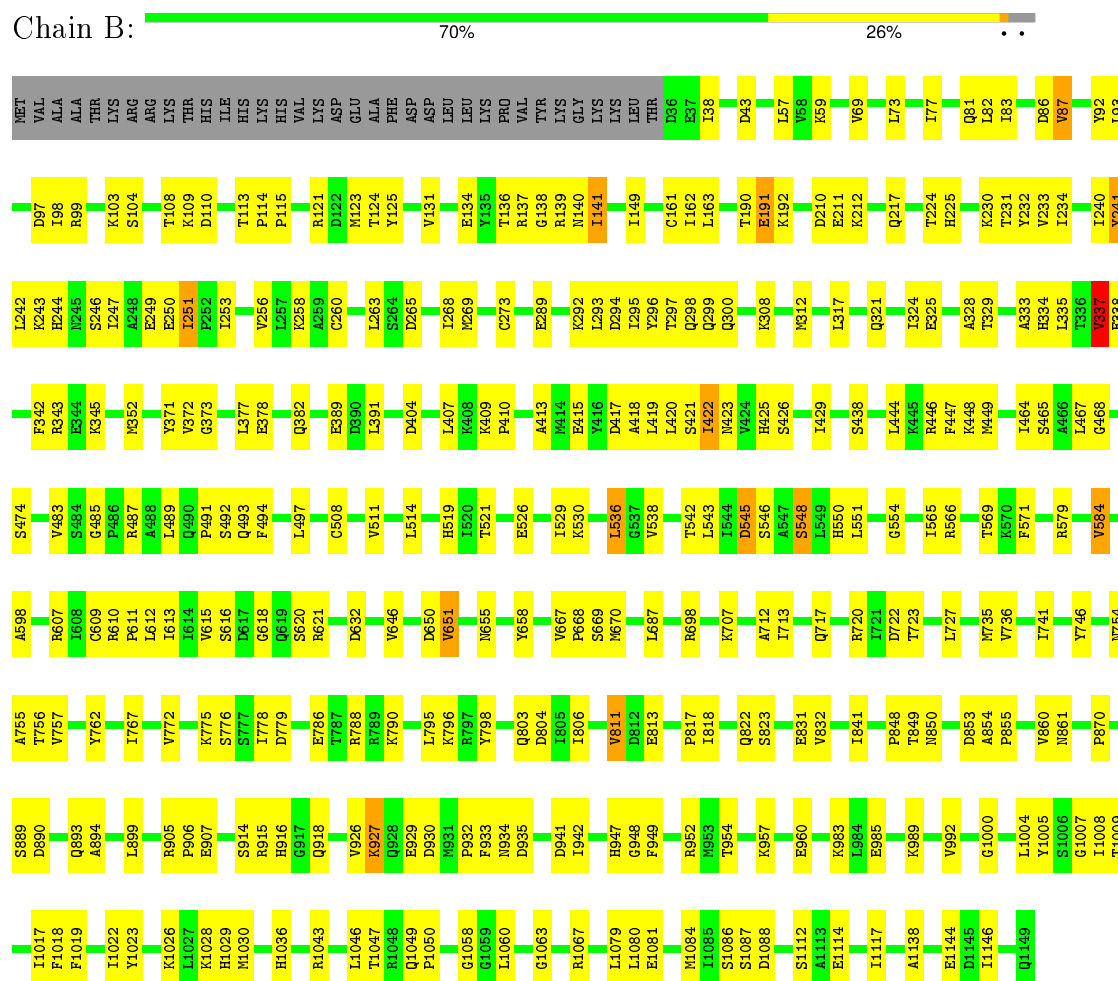
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

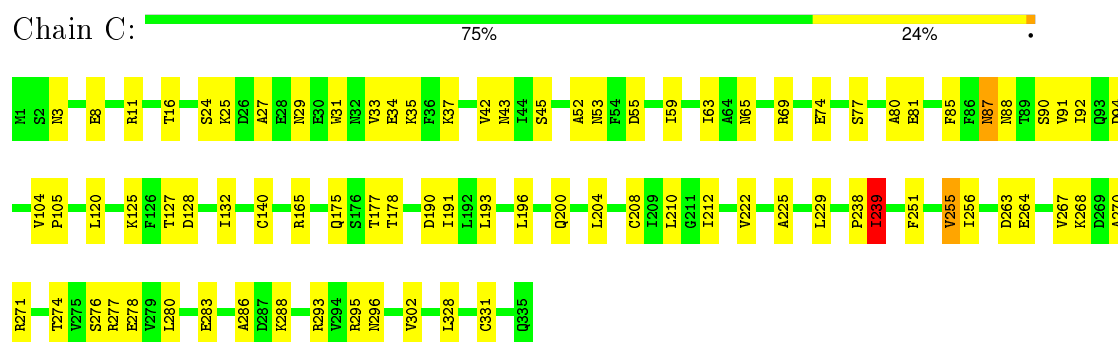
- Molecule 1: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC1



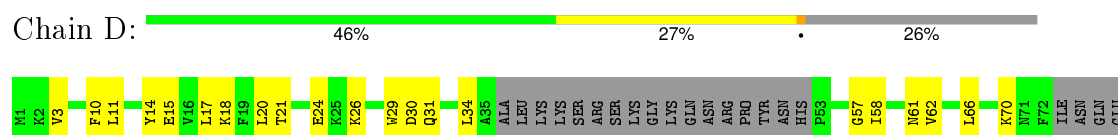
• Molecule 2: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2

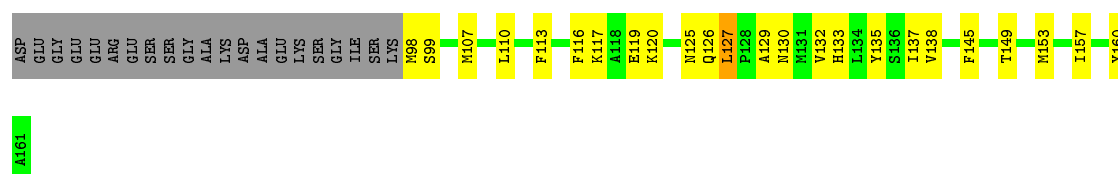


• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1



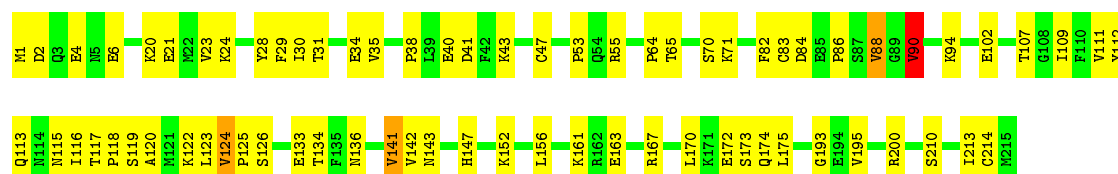
• Molecule 4: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC9





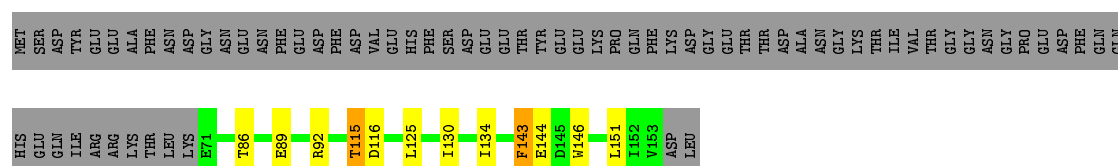
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E: 67% 32%



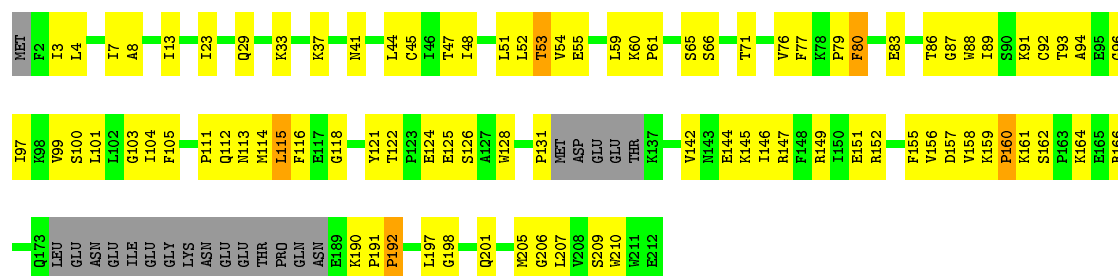
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 46% 6% 46%



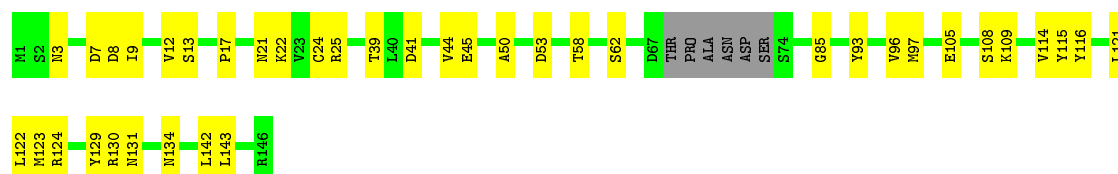
- Molecule 7: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8

Chain G: 48% 40% 10%



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

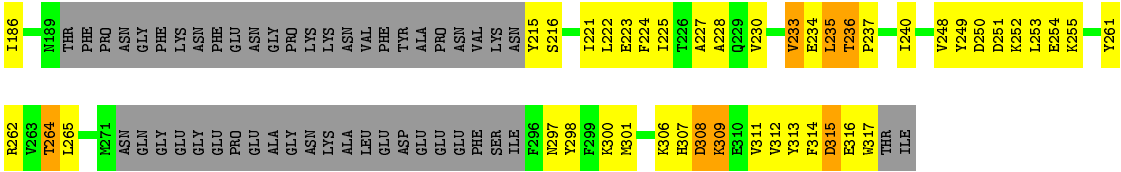
Chain H: 69% 27%



- Molecule 9: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10

Chain I: 65% 18% 16%





• Molecule 17: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

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

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	0.22	0/11267	0.46	0/15220
10	J	0.21	0/558	0.44	0/750
11	K	0.22	0/803	0.45	0/1083
12	L	0.22	0/360	0.48	0/478
13	M	0.23	0/1378	0.46	0/1863
14	N	0.23	0/810	0.52	0/1088
15	O	0.23	0/4310	0.50	0/5813
16	P	0.29	0/837	0.55	0/1134
17	Q	0.24	0/278	0.49	0/377
2	B	0.22	0/8943	0.45	0/12068
3	C	0.23	0/2711	0.45	0/3676
4	D	0.23	0/991	0.52	0/1328
5	E	0.22	0/1795	0.44	0/2416
6	F	0.21	0/683	0.42	0/923
7	G	0.23	0/1583	0.50	0/2146
8	H	0.21	0/1138	0.44	0/1540
9	I	0.22	0/745	0.42	0/1007
All	All	0.22	0/39190	0.47	0/52910

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	11071	0	11200	272	0
2	B	8788	0	8902	221	0
3	C	2655	0	2628	55	0
4	D	977	0	983	33	0
5	E	1759	0	1788	48	0
6	F	671	0	692	9	0
7	G	1544	0	1540	62	0
8	H	1120	0	1089	28	0
9	I	728	0	672	18	0
10	J	549	0	560	8	0
11	K	792	0	790	23	0
12	L	358	0	381	18	0
13	M	1347	0	1315	39	0
14	N	802	0	851	40	0
15	O	4247	0	4413	156	0
16	P	820	0	795	51	0
17	Q	446	0	324	10	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	38680	0	38923	974	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 13.

The worst 5 of 974 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)
15:O:516:LEU:CD2	15:O:567:ARG:HE	1.08	1.58
15:O:516:LEU:HD23	15:O:567:ARG:NE	1.20	1.41
15:O:516:LEU:HD23	15:O:567:ARG:CD	1.60	1.30
1:A:597:ILE:HB	1:A:600:PRO:HG3	1.15	1.15
15:O:516:LEU:HD22	15:O:567:ARG:HE	1.08	1.08

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	1402/1460 (96%)	1157 (82%)	233 (17%)	12 (1%)	21	67
2	B	1112/1149 (97%)	948 (85%)	155 (14%)	9 (1%)	24	69
3	C	333/335 (99%)	282 (85%)	47 (14%)	4 (1%)	16	62
4	D	113/161 (70%)	80 (71%)	33 (29%)	0	100	100
5	E	213/215 (99%)	172 (81%)	38 (18%)	3 (1%)	14	59
6	F	81/155 (52%)	73 (90%)	8 (10%)	0	100	100
7	G	185/212 (87%)	154 (83%)	25 (14%)	6 (3%)	5	43
8	H	136/146 (93%)	116 (85%)	20 (15%)	0	100	100
9	I	88/110 (80%)	77 (88%)	10 (11%)	1 (1%)	17	64
10	J	65/70 (93%)	53 (82%)	11 (17%)	1 (2%)	13	58
11	K	99/142 (70%)	83 (84%)	15 (15%)	1 (1%)	19	65
12	L	43/70 (61%)	33 (77%)	10 (23%)	0	100	100
13	M	161/282 (57%)	135 (84%)	22 (14%)	4 (2%)	7	48
14	N	101/422 (24%)	78 (77%)	22 (22%)	1 (1%)	19	65
15	O	522/654 (80%)	428 (82%)	88 (17%)	6 (1%)	17	64
16	P	92/317 (29%)	60 (65%)	26 (28%)	6 (6%)	1	25
17	Q	33/104 (32%)	29 (88%)	4 (12%)	0	100	100
All	All	4779/6004 (80%)	3958 (83%)	767 (16%)	54 (1%)	23	64

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	587	ILE
1	A	632	VAL
1	A	1371	ILE
9	I	35	ILE
11	K	47	ILE

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	1225/1257 (98%)	1208 (99%)	17 (1%)	74	89
2	B	975/1006 (97%)	958 (98%)	17 (2%)	68	88
3	C	296/296 (100%)	293 (99%)	3 (1%)	82	92
4	D	110/145 (76%)	108 (98%)	2 (2%)	66	87
5	E	197/197 (100%)	192 (98%)	5 (2%)	55	82
6	F	73/137 (53%)	70 (96%)	3 (4%)	37	72
7	G	170/190 (90%)	167 (98%)	3 (2%)	66	87
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	83/98 (85%)	83 (100%)	0	100	100
10	J	62/65 (95%)	60 (97%)	2 (3%)	46	77
11	K	91/130 (70%)	88 (97%)	3 (3%)	45	77
12	L	40/57 (70%)	39 (98%)	1 (2%)	55	82
13	M	143/249 (57%)	140 (98%)	3 (2%)	61	85
14	N	88/360 (24%)	87 (99%)	1 (1%)	80	91
15	O	486/593 (82%)	468 (96%)	18 (4%)	41	75
16	P	94/285 (33%)	89 (95%)	5 (5%)	28	67
17	Q	31/56 (55%)	30 (97%)	1 (3%)	46	77
All	All	4287/5249 (82%)	4203 (98%)	84 (2%)	66	86

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	29	TRP
7	G	53	THR
15	O	645	LEU
5	E	90	VAL
5	E	124	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such

sidechains are listed below:

Mol	Chain	Res	Type
4	D	122	GLN
5	E	174	GLN
15	O	580	ASN
2	B	902	GLN
2	B	936	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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.