



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 19, 2016 – 12:19 PM EST

PDB ID : 5M5W
EMDB ID: : EMD-3446
Title : RNA Polymerase I open complex
Authors : Tafur, L.; Sadian, Y.; Hoffmann, N.A.; Jakobi, A.J.; Wetzel, R.; Hagen, W.J.H.; Sachse, C.; Muller, C.W.
Deposited on : 2016-10-23
Resolution : 3.80 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
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) : rb-20028442

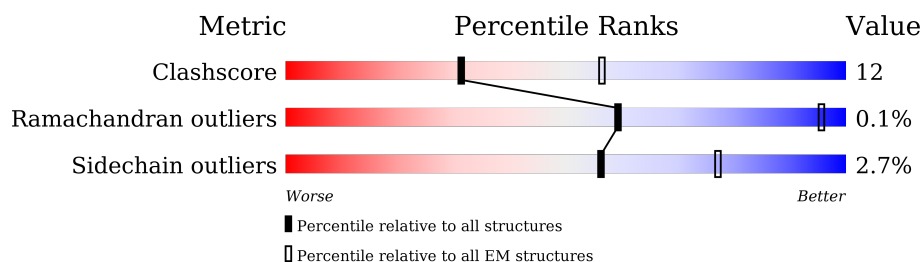
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	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	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	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	S	70	
16	T	70	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 34780 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	1493	Total	C	N	O	S	0	0
			11760	7424	2048	2226	62		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1183	Total	C	N	O	S	0	0
			9389	5936	1642	1760	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	304	Total	C	N	O	S	0	0
			2418	1536	414	460	8		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	59	Total	C	N	O	0	0
			467	293	80	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1751	1111	309	320	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	205	Total	C	N	O	S	0	0
			1624	1040	280	299	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	134	Total	C	N	O	S	0	0
			1075	677	182	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			869	541	146	173	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	100	Total	C	N	O	S	0	0
			785	491	129	160	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	43	Total	C	N	O	S	0	0
			344	211	69	60	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	107	Total	C	N	O		0	0
			850	540	141	169			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1164	743	188	229	4		

- Molecule 15 is a DNA chain called Non-template strand.

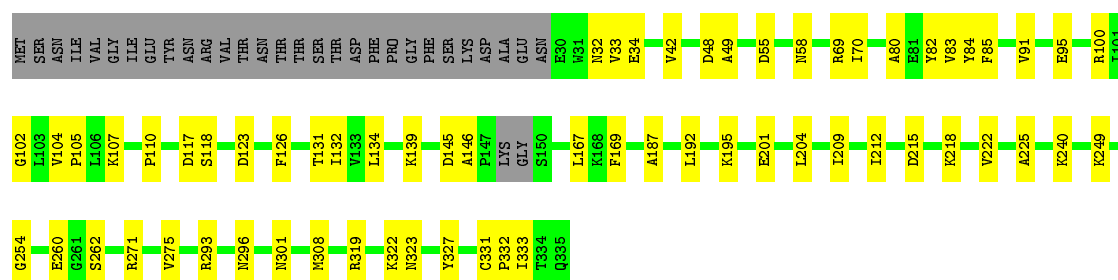
Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	18	Total	C	N	O	P	0	0
			376	178	77	103	18		

- Molecule 16 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	25	Total	C	N	O	P	0	0
			509	244	86	154	25		

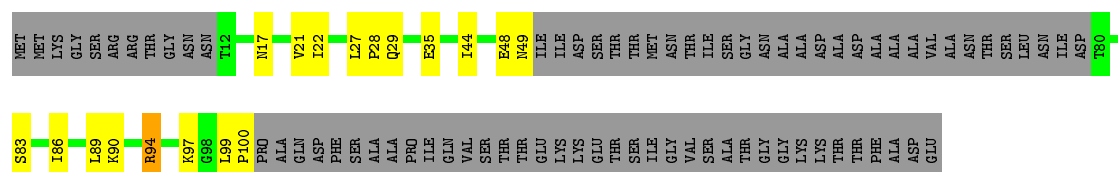
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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



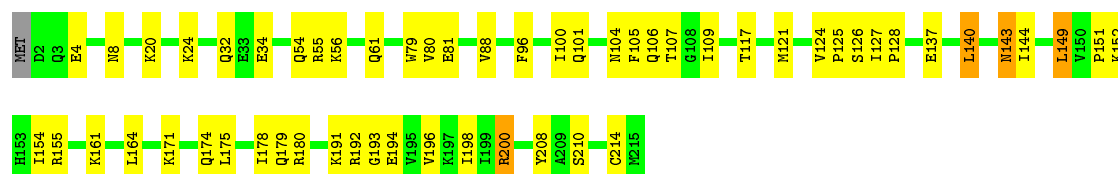
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14

Chain D: 30% 12% 57%



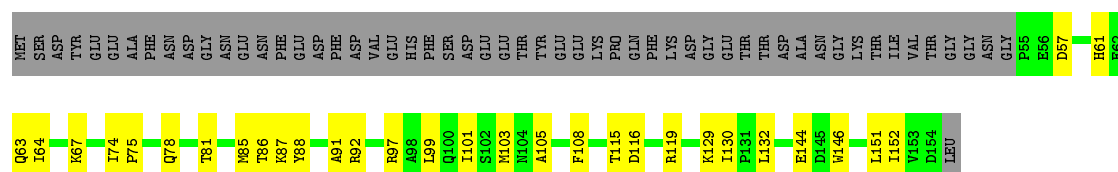
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 73% 24%



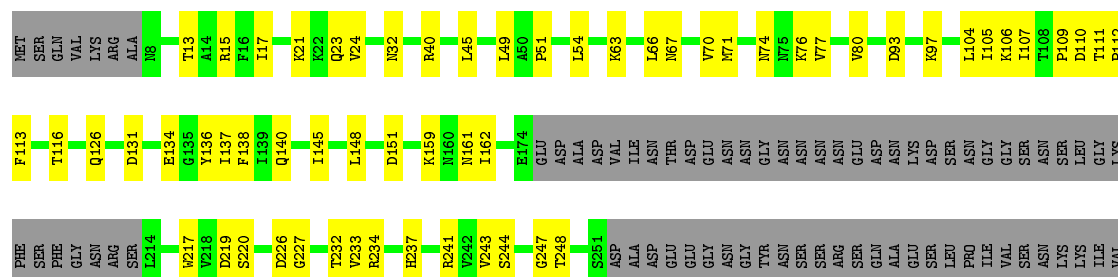
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 45% 20% 35%



- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

Chain G: 44% 18% 37%



PHE
 ASP
 ASP
 GLU
 VAL
 SER
 ILE
 GLU
 ASN
 LYS
 GLU
 SER
 HIS
 LYS
 GLU
 LEU
 ASP
 LEU
 PRO
 GLU
 VAL
 LYS
 GLU
 ASP
 ASN
 GLY
 SER
 GLU
 ILE
 VAL
 TYR
 GLU
 GLU
 ASN
 THR
 SER
 SER
 GLU
 SER
 ASN
 ASP
 GLY
 SER
 SER
 SER
 ASP
 SER
 ASP

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

Chain H: 

MET
 SER
 R3
 F6
 D7
 D8
 I9
 D16
 R25
 Q83
 D94
 Q85
 L38
 N43
 L46
 V49
 D53
 S54
 L55
 T56
 I59
 N64
 LEU
 GLU
 ASP
 THR
 THR
 PRO
 ALA
 ASN
 ASP
 SER
 SER
 A75
 T76
 R77
 R87
 D92
 Y93
 G99
 Y102
 V107
 S108
 K109
 D110

L111
 F118
 R124
 L125
 E126
 Y129
 R130
 N133
 N134
 L143
 I144
 R145
 R146

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

Chain I: 

MET
 S2
 L7
 I8
 F9
 C10
 L11
 G14
 N19
 P20
 N21
 A22
 V28
 P33
 N44
 L60
 R61
 A62
 V67
 R68
 T69
 K72
 E75
 A80
 T81
 I82
 Q88
 Y96
 R97
 T98
 LEU
 GLN
 LEU
 ARG
 SER
 ALA
 ALA
 GLY
 GLY
 ALA
 T109
 V110
 F111
 Y112
 F121
 R122

T123
 N124
 N125

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

Chain J: 

V4
 V5
 S9
 C10
 G11
 G15
 Y21
 D28
 E29
 L30
 L36
 L39
 Y44
 C45
 C46
 R47
 R48
 L51
 T52
 H53
 V54
 D55
 L56
 K59
 F60
 L61
 R62
 Y63
 M64
 P65
 L66
 R69
 ASP

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

Chain K: 

MET
 THR
 GLU
 ASP
 ILE
 GLU
 GLN
 LYS
 LYS
 THR
 THR
 THR
 THR
 VAL
 VAL
 THR
 PRO
 GLU
 GLN
 THR
 LYS
 HIS
 ILE
 ILE
 ARG
 THR
 THR
 THR
 GLU
 GLN
 GLN
 ASP
 MET
 THR
 THR
 GLY
 ASP
 ASP
 GLU
 GLN
 GLN
 GLU
 GLU
 PRO
 D43
 R44
 E45
 K46
 I47
 T54
 D57
 G58
 A61
 S62
 F63
 T71
 I80

F88
 S97
 E98
 R104
 I105
 Q106
 G109
 E110
 A116
 G120
 M125
 D126
 E132
 K138
 H142

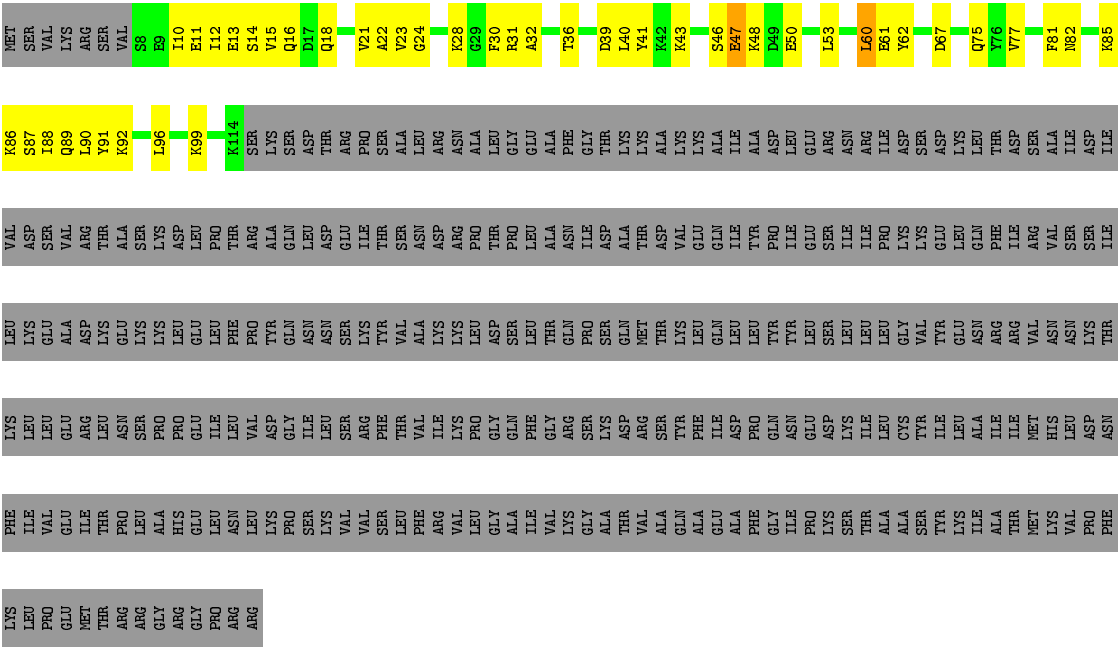
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 

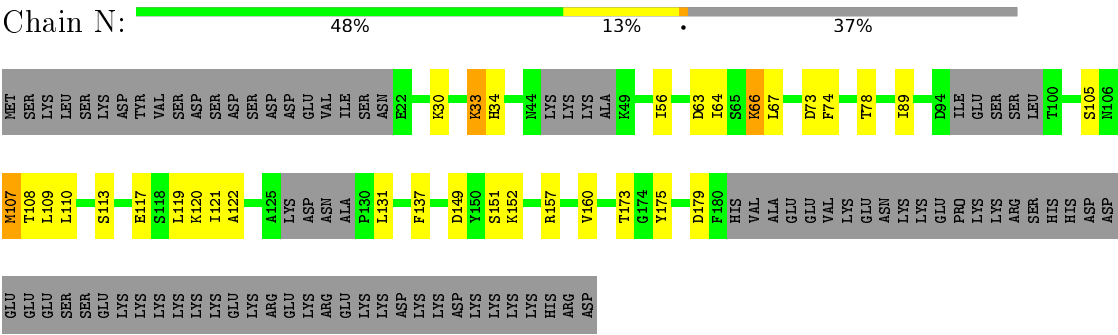
MET
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 PHE
 GLN
 ILE
 PRO
 THR
 THR
 ASN
 LEU
 ASP
 ALA
 ALA
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 GLY
 THR
 THR
 SER
 GLN
 ALA
 ARG
 THR
 THR
 THR
 LEU
 R28
 C31
 A32
 E33
 C34
 R42
 R47
 G52
 K58
 L64
 A69
 F70

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

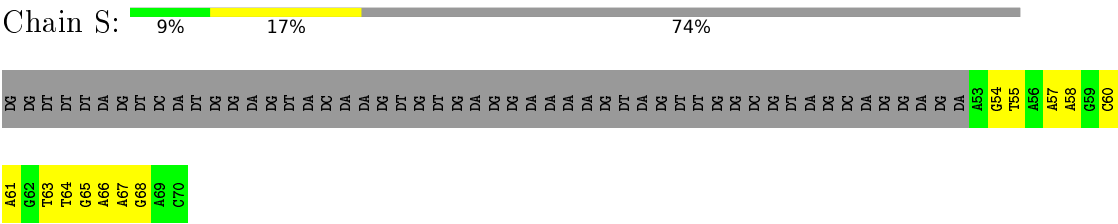
Chain M: 



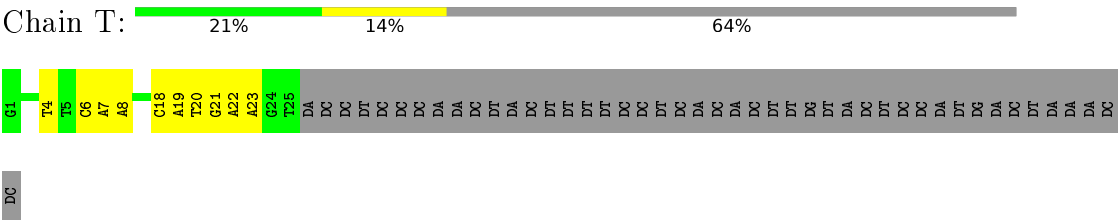
• Molecule 14: DNA-directed RNA polymerase I subunit RPA34



• Molecule 15: Non-template strand



• Molecule 16: Template strand



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	98430	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	0.25	1/11976 (0.0%)	0.43	3/16180 (0.0%)
10	J	0.22	0/578	0.40	0/775
11	K	0.50	3/795 (0.4%)	0.81	5/1072 (0.5%)
12	L	0.22	0/346	0.45	0/457
13	M	0.24	0/866	0.46	0/1162
14	N	0.24	0/1186	0.44	0/1596
15	S	0.47	0/424	0.81	0/653
16	T	0.48	0/568	0.94	0/874
2	B	0.24	0/9596	0.46	4/12971 (0.0%)
3	C	0.24	0/2469	0.41	0/3347
4	D	0.23	0/473	0.44	0/641
5	E	0.24	0/1787	0.41	0/2406
6	F	0.22	0/838	0.38	0/1129
7	G	0.24	0/1662	0.44	0/2260
8	H	0.24	0/1093	0.48	0/1480
9	I	0.24	0/881	0.47	0/1187
All	All	0.26	4/35538 (0.0%)	0.47	12/48190 (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
11	K	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	57	ASP	N-CA	10.18	1.66	1.46
1	A	250	LYS	CA-C	-5.97	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	57	ASP	CA-CB	5.24	1.65	1.53
11	K	58	GLY	CA-C	-5.23	1.43	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	57	ASP	N-CA-C	-14.03	73.12	111.00
11	K	57	ASP	CB-CA-C	-11.85	86.70	110.40
2	B	1064	LYS	N-CA-C	-11.72	79.37	111.00
1	A	444	GLN	C-N-CA	-8.56	104.32	122.30
2	B	359	LEU	CA-CB-CG	8.24	134.25	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	58	GLY	Mainchain

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	11760	0	11838	303	0
2	B	9389	0	9269	280	0
3	C	2418	0	2401	47	0
4	D	467	0	468	13	0
5	E	1751	0	1776	37	0
6	F	823	0	841	23	0
7	G	1624	0	1625	52	0
8	H	1075	0	1045	23	0
9	I	869	0	862	22	0
10	J	569	0	585	20	0
11	K	785	0	782	18	0
12	L	344	0	363	9	0
13	M	850	0	850	34	0
14	N	1164	0	1160	27	0
15	S	376	0	202	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	T	509	0	285	12	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
All	All	34780	0	34352	796	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 12.

The worst 5 of 796 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1140:LYS:HE2	7:G:17:ILE:CD1	1.46	1.44
1:A:248:PHE:CE1	1:A:442:LYS:NZ	2.04	1.26
2:B:1140:LYS:CE	7:G:17:ILE:HD11	1.75	1.15
1:A:248:PHE:CD1	1:A:442:LYS:NZ	2.17	1.10
10:J:10:CYS:HB3	10:J:45:CYS:SG	1.94	1.07

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	A	1479/1664 (89%)	1413 (96%)	62 (4%)	4 (0%)	46	83
2	B	1177/1203 (98%)	1118 (95%)	59 (5%)	0	100	100
3	C	300/335 (90%)	292 (97%)	8 (3%)	0	100	100
4	D	55/137 (40%)	55 (100%)	0	0	100	100
5	E	212/215 (99%)	206 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
7	G	201/326 (62%)	193 (96%)	8 (4%)	0	100	100
8	H	130/146 (89%)	125 (96%)	5 (4%)	0	100	100
9	I	110/125 (88%)	105 (96%)	5 (4%)	0	100	100
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	98/142 (69%)	92 (94%)	6 (6%)	0	100	100
12	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
13	M	105/415 (25%)	99 (94%)	5 (5%)	1 (1%)	19	66
14	N	138/233 (59%)	129 (94%)	9 (6%)	0	100	100
All	All	4211/5236 (80%)	4026 (96%)	180 (4%)	5 (0%)	59	90

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	765	LEU
1	A	250	LYS
1	A	319	GLU
13	M	47	GLU
1	A	445	GLY

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	1313/1465 (90%)	1276 (97%)	37 (3%)	51	81
2	B	1034/1053 (98%)	1008 (98%)	26 (2%)	55	83
3	C	269/296 (91%)	266 (99%)	3 (1%)	80	92
4	D	56/116 (48%)	52 (93%)	4 (7%)	18	59
5	E	196/197 (100%)	189 (96%)	7 (4%)	42	77
6	F	90/137 (66%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	183/291 (63%)	176 (96%)	7 (4%)	40	76
8	H	117/128 (91%)	111 (95%)	6 (5%)	29	69
9	I	102/110 (93%)	100 (98%)	2 (2%)	63	87
10	J	64/65 (98%)	61 (95%)	3 (5%)	32	72
11	K	90/130 (69%)	89 (99%)	1 (1%)	80	92
12	L	38/57 (67%)	37 (97%)	1 (3%)	54	82
13	M	97/371 (26%)	95 (98%)	2 (2%)	61	86
14	N	136/220 (62%)	132 (97%)	4 (3%)	50	81
All	All	3785/4636 (82%)	3682 (97%)	103 (3%)	56	82

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	441	LYS
2	B	946	ASP
11	K	98	GLU
2	B	478	LEU
2	B	721	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	423	ASN
2	B	718	GLN
11	K	106	GLN
2	B	532	HIS
2	B	702	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.