



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 19, 2016 – 07:05 PM EST

PDB ID : 5M64
EMDB ID: : EMD-3449
Title : RNA Polymerase I elongation complex with A49 tandem winged helix domain
Authors : Tafur, L.; Sadian, Y.; Hoffmann, N.A.; Jakobi, A.J.; Wetzel, R.; Hagen, W.J.H.; Sachse, C.; Muller, C.W.
Deposited on : 2016-10-24
Resolution : 4.60 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

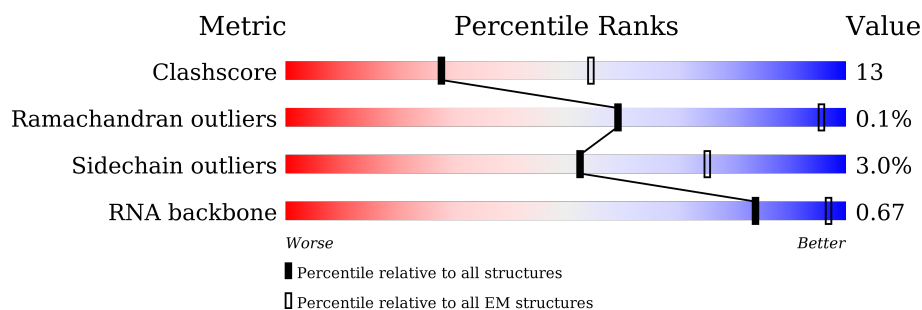
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.






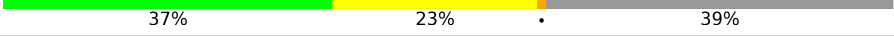

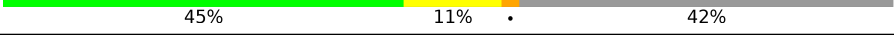


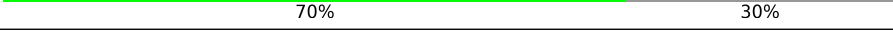
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	59% 27% • 12%
2	B	1203	68% 28% • •
3	C	335	64% 26% • 9%
4	D	137	31% 12% 57%
5	E	215	72% 26% •
6	F	155	50% 13% • 35%
7	G	326	41% 20% 38%
8	H	146	67% 22% • 8%

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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	S	70	
16	T	70	
17	R	10	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 35876 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	1466	Total	C	N	O	S	0	0
			11571	7309	2012	2188	62		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1170	Total	C	N	O	S	0	0
			9301	5888	1625	1737	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	202	Total	C	N	O	S	0	0
			1600	1026	276	293	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	64	Total	C	N	O	S	0	0
			472	295	78	95	4		

- 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	323	Total	C	N	O	S	0	0
			2573	1656	427	486	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	135	Total	C	N	O	S	0	0
			1070	685	175	206	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	19	Total	C	N	O	P	0	0
			397	188	82	108	19		

- Molecule 16 is a DNA chain called Template DNA.

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

- Molecule 17 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	7	Total	C	N	O	P	0	0
			145	65	22	51	7		

- 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	

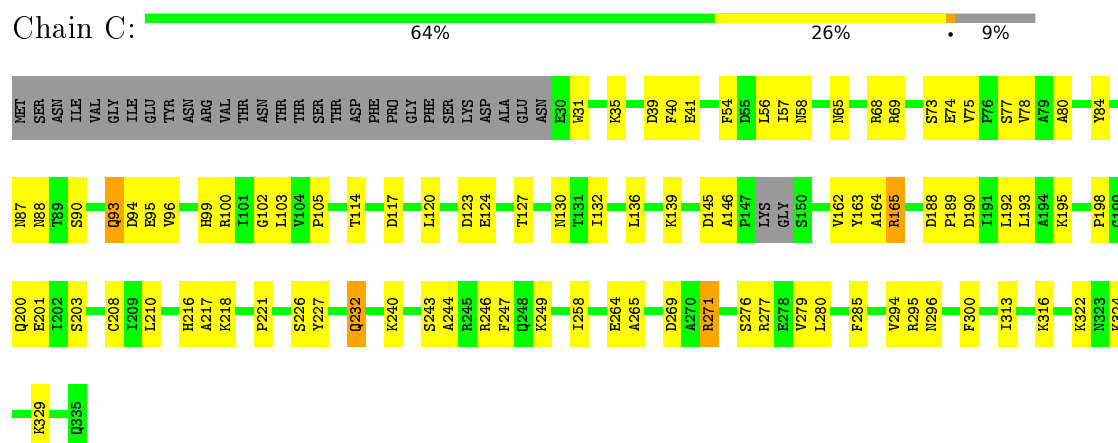
M1227	T1228	P1236	Q1237	M1238	D1248	E1249	Q1250	T1253	K1260	S1264	V1272	T1273	E1274	T1275	T1276	G1277	THR	SER	ASN	THR	GLY	GLY	ASN	ALA	A1287	R1288	I1292	D1298	S1309	K1310	E1311	E1312	L1313	Q1314	M1315	V1316	I1317	E1326	I1329	R1338	THR	THR	GLY	SER	PRO	ASP	ASP	ILE					
GLY	VAL	ALA	ASP	VAL	PRO	ARG	LEU	GLN	THR	THR	ASP	VAL	ALA	ASN	SER	GLU	SER	GLU	GLU	GLN	SER	HIS	LYS	LYS	THR	LYS	GLN	ALA	SER	TYR	ASP	GLU	PRO	ASP	GLU	GLU	ASP	GLU	ILE	GLU	THR	MET	ARG	GLU	ALA	GLU	LYS	SER	SER	PRO	ASP	ASP	ILE
GLU	GLY	ILE	ASP	SER	ASP	LYS	GLU	LYS	SER	ASP	VAL	ASP	MET	ASN	GLU	GLN	ILE	ASN	ASN	LYS	ILE	V1433	M1437	N1438	Q1443	H1454	I1457	T1458	K1459	Y1460	H1461	F1462	E1471	F1472	K1473	L1474	D1479	E1490	C1493	R1494	I1498	R1499	Q1500	T1503									
P1502	H1503	I1504	D1505	R1506	P1510	R1517	V1520	G1523	V1524	M1525	D1531	Q1532	V1538	S1543	N1544	V1549	Y1553	E1556	R1559	I1562	V1563	I1566	M1567	M1568	R1572	A1586	D1587	M1588	M1589	T1590	R1591	Q1592	L1596	A1597	F1598	N1599	R1600	Q1601	G1602	I1603	F1610	M1611	Q1612										
H1613	S1614	Y1615	E1616	G1619	Q1620	F1621	T1622	V1626	E1632	Q1633	L1634	D1635	R1640	V1643	G1644	L1646	D1655	V1656	L1657	A1658	K1659	V1660	A1663	ALA																													

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

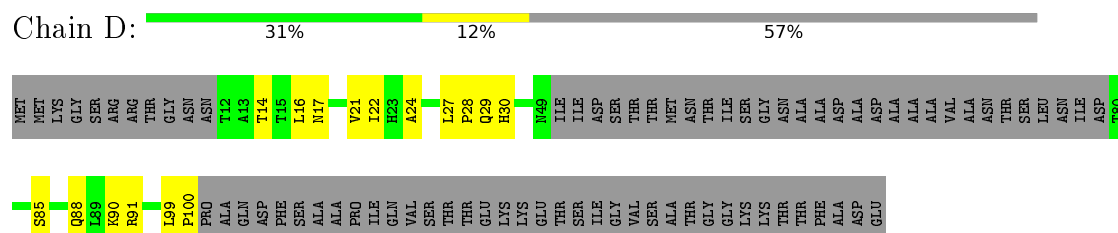
Chain B:

<

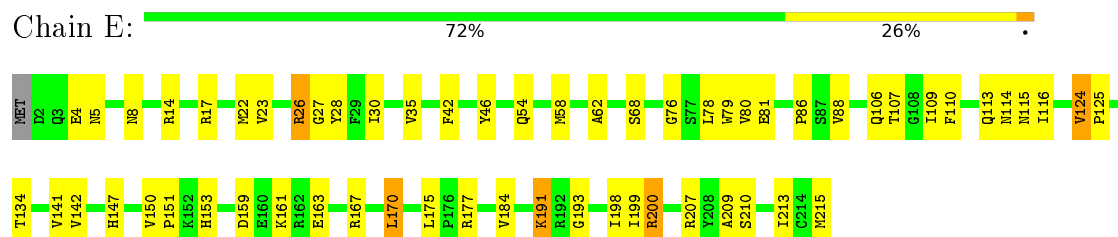
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPA1



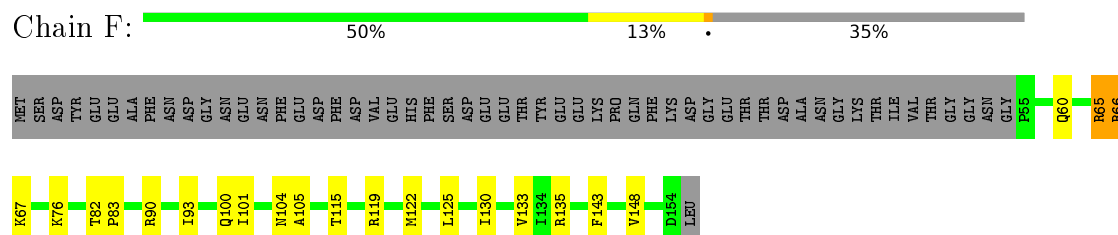
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14



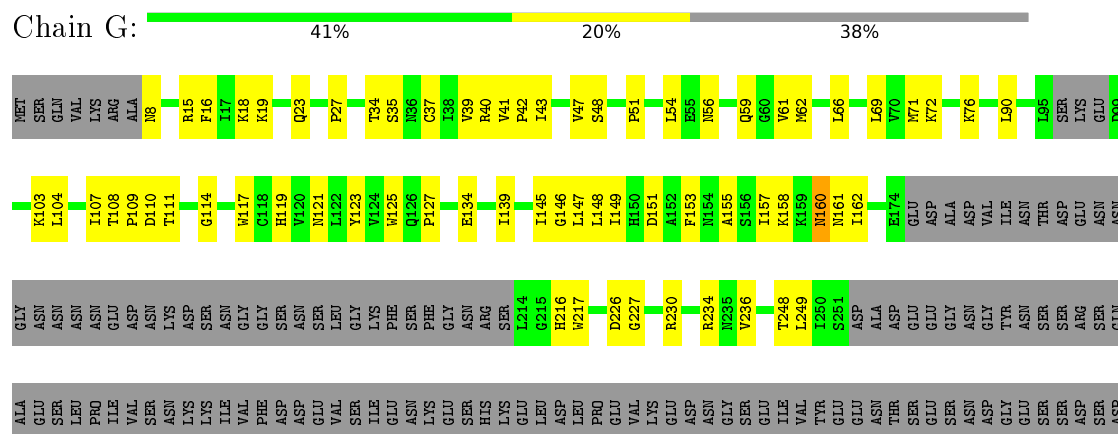
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



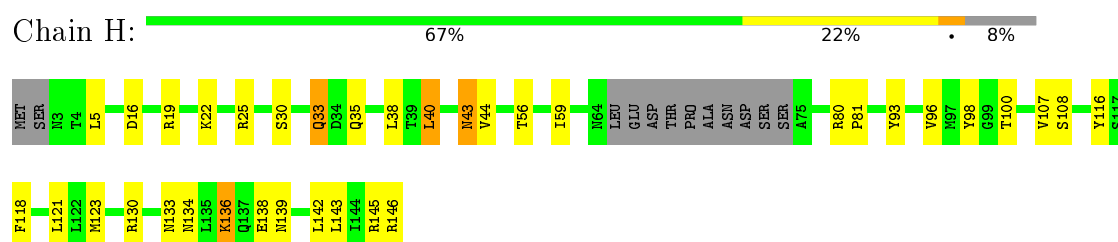
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



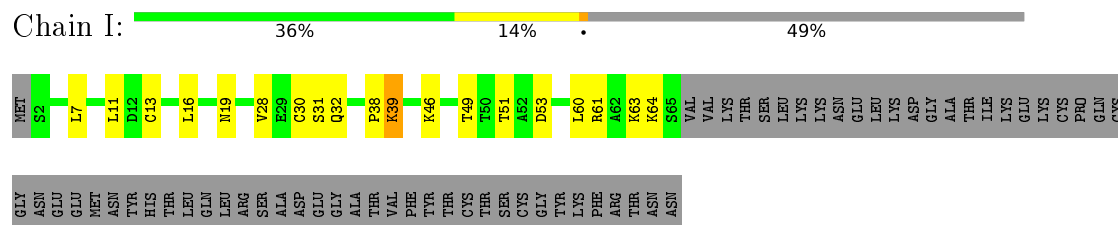
- Molecule 7: DNA-directed RNA polymerase I subunit RPA43



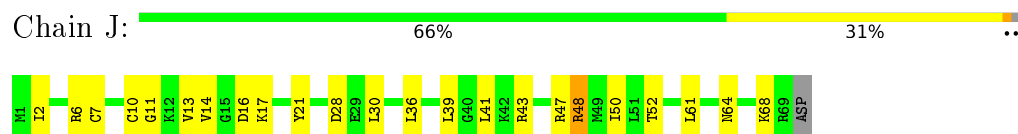
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



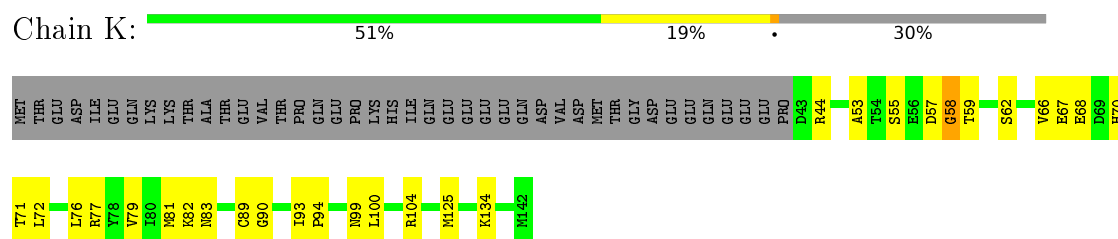
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12



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



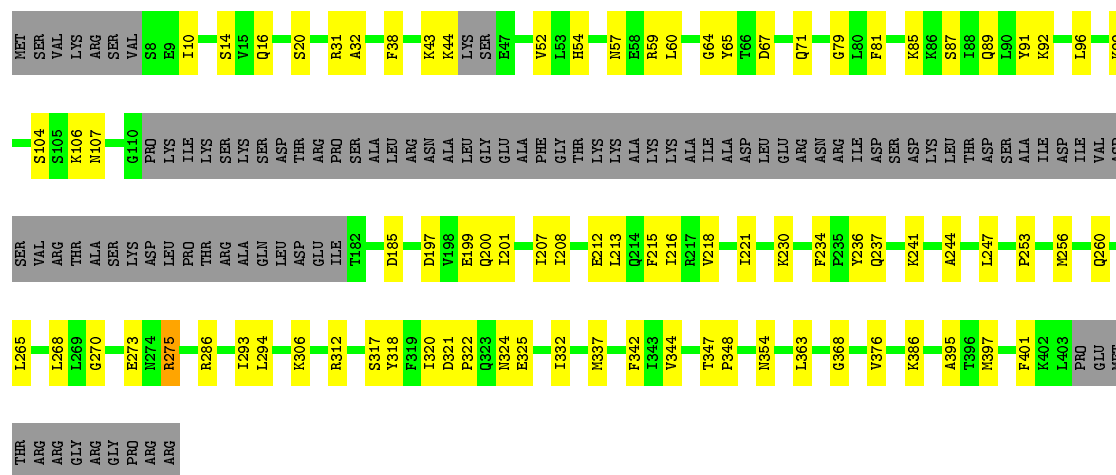
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



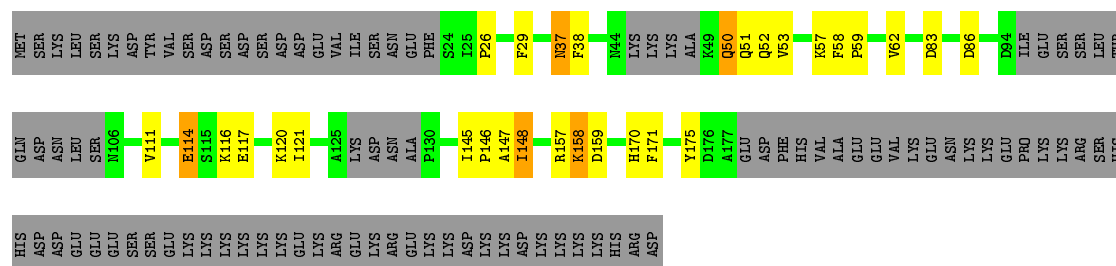
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



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



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

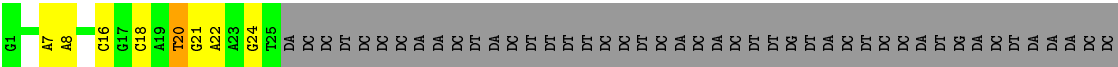


- Molecule 15: Non-template DNA

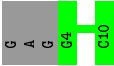


- Molecule 16: Template DNA





● Molecule 17: RNA



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	13412	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	0.28	3/11782 (0.0%)	0.48	7/15913 (0.0%)
10	J	0.23	0/578	0.44	0/775
11	K	0.48	2/795 (0.3%)	0.81	4/1072 (0.4%)
12	L	0.22	0/346	0.43	0/457
13	M	0.24	0/2620	0.44	0/3536
14	N	0.24	0/1090	0.49	0/1466
15	S	0.49	0/448	0.82	0/690
16	T	0.49	0/568	0.96	1/874 (0.1%)
17	R	0.11	0/160	0.69	0/246
2	B	0.25	1/9506 (0.0%)	0.46	3/12847 (0.0%)
3	C	0.24	0/2469	0.42	0/3347
4	D	0.23	0/473	0.46	0/641
5	E	0.24	0/1787	0.41	0/2406
6	F	0.23	0/838	0.40	0/1129
7	G	0.24	0/1637	0.43	0/2226
8	H	0.24	0/1093	0.46	0/1480
9	I	0.25	0/478	0.47	0/647
All	All	0.27	6/36668 (0.0%)	0.49	15/49752 (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
1	A	0	2
11	K	0	1
All	All	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	GLY	CA-C	-10.24	1.35	1.51
11	K	57	ASP	N-CA	9.99	1.66	1.46
1	A	449	GLY	N-CA	9.55	1.60	1.46
1	A	763	GLY	N-CA	6.76	1.56	1.46
2	B	1064	LYS	N-CA	5.39	1.57	1.46

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	57	ASP	N-CA-C	-14.07	73.00	111.00
1	A	449	GLY	N-CA-C	-13.59	79.14	113.10
2	B	1064	LYS	N-CA-C	-11.77	79.22	111.00
11	K	57	ASP	CB-CA-C	-11.66	87.07	110.40
11	K	58	GLY	N-CA-C	-10.02	88.05	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	GLY	Mainchain
1	A	445	GLY	Mainchain
11	K	58	GLY	Mainchain

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	11571	0	11650	379	0
2	B	9301	0	9194	260	0
3	C	2418	0	2401	72	0
4	D	467	0	468	11	0
5	E	1751	0	1776	37	0
6	F	823	0	841	17	0
7	G	1600	0	1600	45	0
8	H	1075	0	1046	30	0
9	I	472	0	473	16	0
10	J	569	0	585	21	0
11	K	785	0	782	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	344	0	363	13	0
13	M	2573	0	2653	58	0
14	N	1070	0	1085	27	0
15	S	397	0	213	9	0
16	T	509	0	285	10	0
17	R	145	0	75	0	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	35876	0	35490	901	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 901 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:811:LEU:HD22	2:B:825:PHE:CZ	1.47	1.47
13:M:197:ASP:OD2	13:M:199:GLU:OE1	1.53	1.26
2:B:811:LEU:CD2	2:B:825:PHE:CZ	2.18	1.25
2:B:1104:CYS:HB3	2:B:1107:CYS:SG	1.90	1.11
13:M:368:GLY:O	13:M:397:MET:HE1	1.52	1.09

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	1450/1664 (87%)	1375 (95%)	71 (5%)	4 (0%)	46 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1160/1203 (96%)	1097 (95%)	63 (5%)	0	100	100
3	C	300/335 (90%)	289 (96%)	11 (4%)	0	100	100
4	D	55/137 (40%)	54 (98%)	1 (2%)	0	100	100
5	E	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
6	F	98/155 (63%)	95 (97%)	3 (3%)	0	100	100
7	G	196/326 (60%)	191 (97%)	5 (3%)	0	100	100
8	H	130/146 (89%)	126 (97%)	4 (3%)	0	100	100
9	I	62/125 (50%)	56 (90%)	6 (10%)	0	100	100
10	J	67/70 (96%)	60 (90%)	7 (10%)	0	100	100
11	K	98/142 (69%)	96 (98%)	2 (2%)	0	100	100
12	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
13	M	317/415 (76%)	304 (96%)	13 (4%)	0	100	100
14	N	127/233 (54%)	106 (84%)	20 (16%)	1 (1%)	24	69
All	All	4313/5236 (82%)	4097 (95%)	211 (5%)	5 (0%)	59	90

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	THR
1	A	248	PHE
1	A	450	LYS
1	A	227	LEU
14	N	148	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	1293/1465 (88%)	1254 (97%)	39 (3%)	48	78
2	B	1025/1053 (97%)	998 (97%)	27 (3%)	54	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	269/296 (91%)	261 (97%)	8 (3%)	48	78
4	D	56/116 (48%)	54 (96%)	2 (4%)	42	75
5	E	196/197 (100%)	189 (96%)	7 (4%)	42	75
6	F	90/137 (66%)	84 (93%)	6 (7%)	20	59
7	G	180/291 (62%)	177 (98%)	3 (2%)	68	88
8	H	117/128 (91%)	111 (95%)	6 (5%)	29	67
9	I	56/110 (51%)	53 (95%)	3 (5%)	27	66
10	J	64/65 (98%)	62 (97%)	2 (3%)	47	78
11	K	90/130 (69%)	87 (97%)	3 (3%)	45	77
12	L	38/57 (67%)	35 (92%)	3 (8%)	15	53
13	M	292/371 (79%)	287 (98%)	5 (2%)	68	88
14	N	125/220 (57%)	121 (97%)	4 (3%)	46	77
All	All	3891/4636 (84%)	3773 (97%)	118 (3%)	52	78

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	528	LEU
3	C	93	GLN
13	M	106	LYS
2	B	595	TRP
2	B	790	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	715	ASN
2	B	1114	GLN
13	M	107	ASN
2	B	745	GLN
2	B	790	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	R	6/10 (60%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.