



Full wwPDB EM Validation Report ⓘ

May 10, 2026 – 12:25 AM JST

PDB ID : 9K15 / pdb_00009k15
EMDB ID : EMD-61965
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 4U scaffold at 3.32 Angstrom
Authors : Xie, G.; Du, X.; Du, J.
Deposited on : 2024-10-16
Resolution : 3.32 Å(reported)

This is a Full wwPDB EM Validation 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 Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

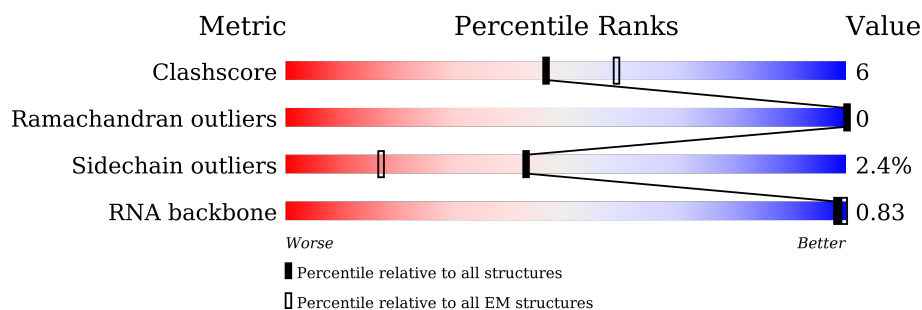
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.32 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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	A	2032	33% 7% 59%
2	C	319	81% 9% 10%
3	F	144	40% 12% 48%
4	J	71	89% 11%
5	K	116	84% 8% 7%
6	L	51	65% 24% 12%
7	H	146	79% 17% ..
8	I	114	66% 19% 15%

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Mol	Chain	Length	Quality of chain
9	E	230	 74% 17% 9%
10	B	1169	 73% 9% 17%
11	T	34	 9% 24% 68%
12	N	34	 38% 12% 50%
13	P	20	 10% 10% 80%

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 23098 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 V largest subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	834	Total	C	N	O	S	0	0
			6530	4124	1125	1237	44		

- Molecule 2 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	287	Total	C	N	O	S	0	0
			2256	1418	380	445	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	THR	SER	conflict	UNP A0A0D3D418

- Molecule 3 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	75	Total	C	N	O	S	0	0
			616	392	108	112	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	51	GLU	ASP	conflict	UNP A0A0D3BZZ8

- Molecule 4 is a protein called DNA-directed RNA polymerase II, IV and V subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	63	Total	C	N	O	S	0	0
			507	324	85	91	7		

- Molecule 5 is a protein called DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	108	Total	C	N	O	S	0	0
			890	565	156	167	2		

- Molecule 6 is a protein called DNA-directed RNA polymerase II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	45	Total	C	N	O	S	0	0
			365	224	70	67	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	18	GLU	LYS	conflict	UNP A0A0D2ZPP3
L	32	CYS	ARG	conflict	UNP A0A0D2ZPP3

- Molecule 7 is a protein called DNA-directed RNA polymerase II, IV and V subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	141	Total	C	N	O	S	0	0
			1129	729	183	208	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			787	482	150	143	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	20	ARG	LYS	conflict	UNP A0A0D3A7P5
I	40	ASP	ASN	conflict	UNP A0A0D3A7P5

- Molecule 9 is a protein called RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	209	Total	C	N	O	S	0	0
			1706	1085	303	316	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	101	GLY	SER	conflict	UNP A0A0D3DTU3
E	182	GLN	HIS	conflict	UNP A0A0D3DTU3
E	210	ILE	VAL	conflict	UNP A0A0D3DTU3

- Molecule 10 is a protein called DNA-directed RNA polymerase IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	965	Total	C	N	O	S	0	0
			7645	4816	1355	1430	44		

- Molecule 11 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	11	Total	C	N	O	P	0	0
			225	107	43	64	11		

- Molecule 12 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	17	Total	C	N	O	P	0	0
			350	166	65	102	17		

- Molecule 13 is a RNA chain called RNA (5'-R(*UP*AP*UP*AP*UP*GP*CP*AP*GP*AP*AP*AP*GP*CP*GP*AP*UP*UP*UP*U)-3').

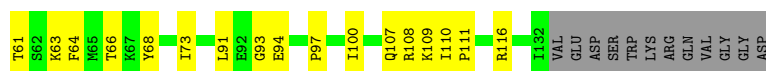
Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	4	Total	C	N	O	P	0	0
			85	38	15	28	4		

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Mg	0
			1	1	

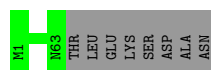
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total 1	Zn 1	0
15	C	1	Total 1	Zn 1	0
15	J	1	Total 1	Zn 1	0
15	L	1	Total 1	Zn 1	0
15	I	2	Total 2	Zn 2	0



- Molecule 4: DNA-directed RNA polymerase II, IV and V subunit 10

Chain J: 89% 11%



- Molecule 5: DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein

Chain K: 84% 8% 7%



- Molecule 6: DNA-directed RNA polymerase II, IV and V subunit 12

Chain L: 65% 24% 12%



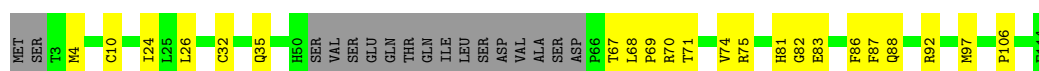
- Molecule 7: DNA-directed RNA polymerase II, IV and V subunit 8

Chain H: 79% 17% 4%



- Molecule 8: DNA-directed RNA polymerase subunit

Chain I: 66% 19% 15%



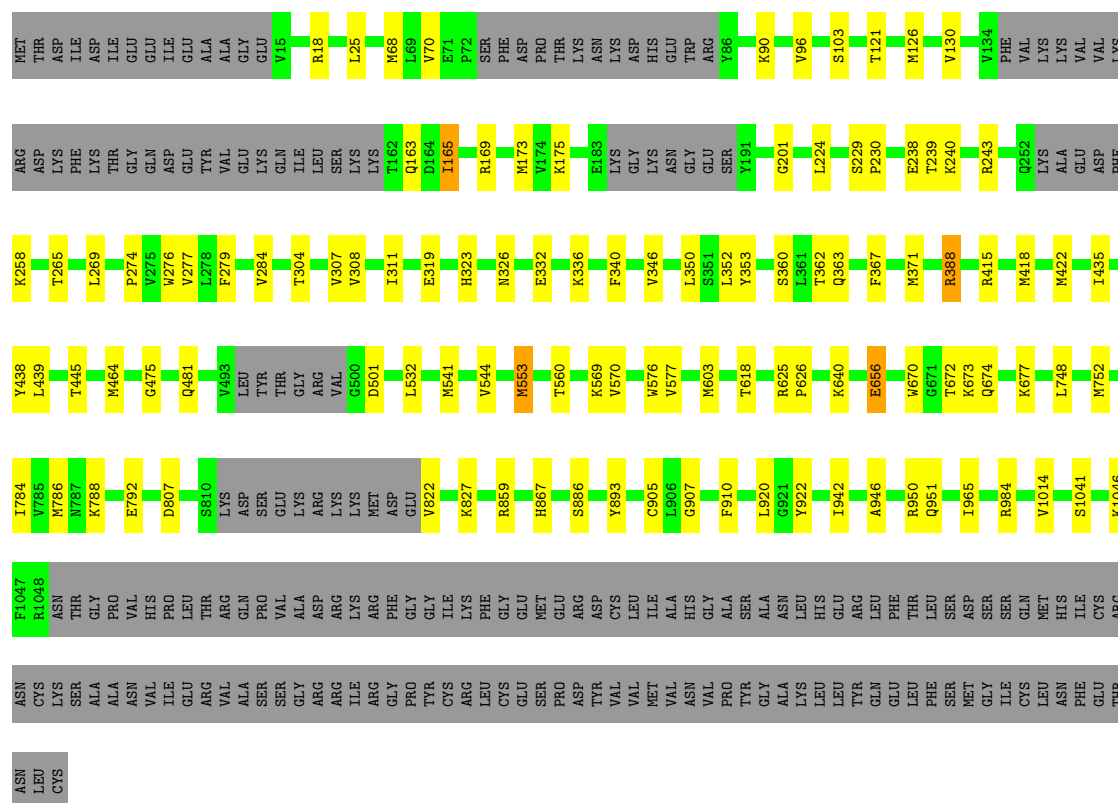
- Molecule 9: RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein

Chain E: 74% 17% 9%



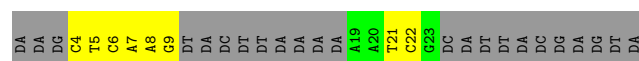
- Molecule 10: DNA-directed RNA polymerase IV and V subunit 2

Chain B:  73% 9% 17%



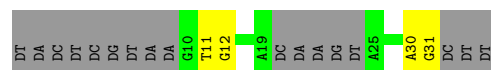
- Molecule 11: DNA (34-MER)

Chain T:  9% 24% 68%



- Molecule 12: DNA (34-MER)

Chain N:  38% 12% 50%



- Molecule 13: RNA (5'-R(*UP*AP*UP*AP*UP*GP*CP*AP*GP*AP*AP*AP*GP*CP*GP*A P*UP*UP*UP*U)-3')

Chain P:  10% 10% 80%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5625	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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, MG

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	A	0.16	0/6640	0.36	0/8961
2	C	0.20	0/2286	0.34	0/3087
3	F	0.15	0/627	0.37	0/841
4	J	0.21	0/515	0.33	0/696
5	K	0.20	0/908	0.29	0/1224
6	L	0.17	0/369	0.33	0/493
7	H	0.15	0/1155	0.36	0/1557
8	I	0.14	0/804	0.34	0/1081
9	E	0.12	0/1732	0.33	0/2332
10	B	0.20	0/7794	0.34	0/10503
11	T	0.20	0/251	0.38	0/382
12	N	0.22	0/391	0.41	0/599
13	P	0.08	0/94	0.21	0/144
All	All	0.18	0/23566	0.34	0/31900

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	6530	0	6583	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2256	0	2269	13	0
3	F	616	0	635	14	0
4	J	507	0	512	0	0
5	K	890	0	883	6	0
6	L	365	0	364	6	0
7	H	1129	0	1128	15	0
8	I	787	0	733	40	0
9	E	1706	0	1759	22	0
10	B	7645	0	7580	74	0
11	T	225	0	125	9	0
12	N	350	0	193	3	0
13	P	85	0	44	1	0
14	A	1	0	0	0	0
15	A	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	23098	0	22808	281	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 6.

All (281) 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)
1:A:947:GLU:HG2	8:I:92:ARG:NH1	1.54	1.13
1:A:897:TYR:CE1	8:I:88:GLN:HB3	1.97	0.99
1:A:897:TYR:CD1	8:I:88:GLN:HB3	2.07	0.89
1:A:656:GLU:HG3	8:I:70:ARG:NH2	1.88	0.88
1:A:947:GLU:HG2	8:I:92:ARG:HH11	1.36	0.84
1:A:1058:TRP:HE3	1:A:1059:ILE:HG13	1.42	0.83
1:A:897:TYR:CD1	8:I:88:GLN:OE1	2.37	0.78
8:I:26:LEU:HD11	8:I:35:GLN:HB3	1.65	0.77
1:A:1057:THR:HB	1:A:1060:ARG:HB2	1.67	0.75
1:A:466:LYS:O	1:A:470:LEU:HD12	1.86	0.74
1:A:1070:TRP:CH2	8:I:86:PHE:HZ	2.06	0.73
3:F:59:ARG:HE	3:F:59:ARG:HA	1.56	0.70
12:N:11:DT:H1'	12:N:12:DG:C8	2.26	0.70
10:B:464:MET:HE2	10:B:464:MET:H	1.57	0.69
1:A:656:GLU:HG3	8:I:70:ARG:CZ	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:748:LEU:HB3	10:B:965:ILE:HD11	1.75	0.68
8:I:4:MET:HE2	10:B:304:THR:HG23	1.76	0.66
1:A:1070:TRP:CH2	8:I:86:PHE:CZ	2.83	0.66
10:B:362:THR:HG23	10:B:560:THR:HB	1.78	0.66
10:B:68:MET:HE1	10:B:415:ARG:HG2	1.78	0.66
3:F:107:GLN:HG2	3:F:109:LYS:HG2	1.77	0.65
1:A:897:TYR:CD2	8:I:88:GLN:HB2	2.32	0.65
9:E:100:THR:HA	9:E:129:GLN:HG2	1.79	0.65
1:A:669:VAL:HG12	1:A:673:PHE:CZ	2.31	0.64
1:A:503:MET:HE1	1:A:577:LEU:HD21	1.77	0.64
1:A:474:SER:HB3	1:A:477:LYS:HD2	1.78	0.64
1:A:897:TYR:CZ	8:I:88:GLN:HB3	2.32	0.64
10:B:169:ARG:H	10:B:445:THR:HG22	1.63	0.64
1:A:1049:ILE:HG22	1:A:1051:ASN:H	1.63	0.63
9:E:34:HIS:HB2	9:E:67:ARG:HH22	1.65	0.62
10:B:672:THR:HB	10:B:674:GLN:OE1	2.00	0.62
1:A:592:LYS:HG3	1:A:596:GLU:HG3	1.81	0.62
1:A:1027:THR:HG22	10:B:258:LYS:HE3	1.82	0.61
1:A:1058:TRP:CE3	1:A:1059:ILE:HG13	2.31	0.61
1:A:965:ASN:O	1:A:969:GLN:HG2	2.01	0.61
10:B:435:ILE:HA	10:B:438:TYR:HD2	1.65	0.61
10:B:332:GLU:HG2	10:B:346:VAL:HG11	1.82	0.61
1:A:941:LEU:HB2	1:A:1003:PRO:HB2	1.82	0.61
1:A:947:GLU:O	8:I:92:ARG:NH2	2.33	0.61
10:B:464:MET:HE2	10:B:464:MET:N	2.15	0.61
10:B:475:GLY:HA3	10:B:481:GLN:HE21	1.66	0.61
1:A:674:MET:HE1	1:A:695:LEU:HD23	1.84	0.60
10:B:96:VAL:HG22	10:B:126:MET:HG2	1.85	0.59
1:A:905:LYS:HE2	1:A:1041:PRO:HA	1.83	0.59
7:H:41:MET:HG2	7:H:123:LEU:HD13	1.84	0.59
9:E:200:VAL:HG23	9:E:205:LEU:HB2	1.84	0.58
1:A:591:GLU:O	1:A:591:GLU:HG2	2.02	0.58
11:T:8:DA:H2"	11:T:9:DG:N7	2.19	0.58
1:A:1022:ASP:O	1:A:1026:ASN:HB2	2.04	0.58
1:A:1123:CYS:O	1:A:1127:GLN:HG2	2.04	0.58
7:H:40:PHE:HB3	7:H:124:ARG:HB2	1.86	0.57
1:A:897:TYR:CE2	8:I:88:GLN:N	2.69	0.57
1:A:1040:ASP:HB3	1:A:1043:ILE:HD13	1.85	0.57
3:F:108:ARG:O	3:F:109:LYS:HD2	2.05	0.57
3:F:97:PRO:HA	3:F:100:ILE:HD12	1.86	0.57
3:F:59:ARG:HA	3:F:59:ARG:NE	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:106:ASN:HA	9:E:109:ARG:NE	2.21	0.56
1:A:897:TYR:CD1	8:I:88:GLN:CB	2.88	0.55
8:I:75:ARG:HH21	8:I:82:GLY:HA3	1.71	0.55
11:T:7:DA:C8	11:T:7:DA:H5'	2.42	0.55
7:H:100:ILE:HG22	7:H:135:LEU:HD13	1.88	0.55
1:A:351:PHE:HE1	1:A:459:TYR:HB3	1.72	0.55
7:H:43:LEU:HB2	7:H:121:MET:HG3	1.88	0.55
7:H:142:LEU:HD22	7:H:142:LEU:H	1.70	0.55
7:H:82:LYS:HZ2	7:H:85:LEU:HB3	1.72	0.54
1:A:605:GLN:HB3	1:A:606:PRO:HD3	1.88	0.54
10:B:18:ARG:HA	10:B:677:LYS:HD3	1.90	0.54
6:L:10:TYR:CE2	6:L:21:LEU:HB3	2.43	0.54
1:A:1108:ILE:HD11	1:A:1115:VAL:HG13	1.91	0.53
8:I:68:LEU:HD21	8:I:87:PHE:HB3	1.90	0.53
10:B:163:GLN:HE21	10:B:165:ILE:HD13	1.73	0.53
10:B:788:LYS:O	10:B:792:GLU:HG3	2.08	0.53
10:B:422:MET:HE3	10:B:422:MET:HA	1.90	0.53
1:A:1070:TRP:HH2	8:I:86:PHE:CZ	2.27	0.53
9:E:76:VAL:HG23	9:E:97:PHE:HB2	1.89	0.52
1:A:865:LYS:NZ	1:A:1163:GLY:HA3	2.24	0.52
1:A:670:ALA:HA	1:A:673:PHE:CD2	2.45	0.52
1:A:805:ILE:HG21	1:A:808:PHE:HE1	1.74	0.52
7:H:42:HIS:CD2	7:H:122:LEU:HB3	2.45	0.52
1:A:875:ARG:NH1	1:A:1078:LYS:HD3	2.25	0.51
11:T:8:DA:H2''	11:T:9:DG:C8	2.46	0.51
1:A:897:TYR:CZ	8:I:88:GLN:CB	2.93	0.51
1:A:947:GLU:O	8:I:92:ARG:CZ	2.59	0.51
13:P:16:A:H2'	13:P:17:U:C6	2.46	0.51
1:A:671:ALA:HA	1:A:674:MET:HG3	1.93	0.51
1:A:865:LYS:HZ1	1:A:1163:GLY:HA3	1.76	0.51
1:A:1070:TRP:CZ2	8:I:86:PHE:HZ	2.28	0.51
1:A:698:GLN:NE2	10:B:951:GLN:HA	2.26	0.50
1:A:1043:ILE:HG23	1:A:1074:VAL:HG13	1.93	0.50
10:B:786:MET:HE1	10:B:910:PHE:CZ	2.47	0.50
6:L:35:ARG:HH21	10:B:103:SER:HB2	1.76	0.50
1:A:648:ARG:NH1	8:I:106:PRO:HB3	2.26	0.50
10:B:603:MET:HG3	10:B:618:THR:HG22	1.94	0.49
10:B:475:GLY:HA3	10:B:481:GLN:NE2	2.27	0.49
10:B:907:GLY:HA3	10:B:1041:SER:HB2	1.95	0.49
1:A:518:MET:HG2	5:K:62:GLN:HB2	1.93	0.49
1:A:897:TYR:CG	8:I:88:GLN:CB	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:TYR:CE1	1:A:1033:LEU:HD21	2.48	0.49
1:A:973:LYS:O	1:A:974:LYS:HG2	2.13	0.49
6:L:42:THR:HG21	6:L:44:ARG:HH21	1.76	0.48
10:B:418:MET:HG3	10:B:439:LEU:HD12	1.95	0.48
9:E:133:THR:HG22	9:E:135:LYS:H	1.78	0.48
3:F:110:ILE:HD12	3:F:111:PRO:HD2	1.94	0.48
1:A:897:TYR:HB3	8:I:88:GLN:OE1	2.13	0.48
7:H:82:LYS:NZ	7:H:85:LEU:HB3	2.29	0.48
2:C:10:PRO:HD3	5:K:97:GLU:OE1	2.14	0.48
2:C:222:PHE:HZ	2:C:227:ARG:HD3	1.79	0.48
10:B:418:MET:HE3	10:B:418:MET:HB3	1.77	0.48
3:F:61:THR:HB	3:F:116:ARG:HH11	1.78	0.48
10:B:25:LEU:HD13	10:B:673:LYS:HZ3	1.79	0.47
1:A:947:GLU:HG3	8:I:92:ARG:HD2	0.79	0.47
1:A:355:VAL:HG21	1:A:394:LEU:HB3	1.96	0.47
5:K:67:LEU:HD21	10:B:922:TYR:HE1	1.79	0.47
1:A:587:GLY:O	1:A:590:VAL:HG12	2.15	0.47
10:B:240:LYS:HD2	10:B:243:ARG:HH12	1.78	0.47
1:A:542:PHE:HE1	1:A:570:PHE:HB3	1.80	0.47
1:A:999:ASP:H	1:A:1002:MET:HE2	1.80	0.47
10:B:68:MET:HE3	10:B:418:MET:HE1	1.95	0.47
10:B:435:ILE:HD12	10:B:438:TYR:HB2	1.96	0.47
1:A:885:ARG:CZ	9:E:23:SER:HA	2.44	0.47
6:L:29:CYS:SG	6:L:32:CYS:HB2	2.54	0.47
10:B:25:LEU:HB3	10:B:673:LYS:HZ2	1.79	0.47
10:B:784:ILE:HG22	10:B:942:ILE:HG22	1.97	0.47
1:A:1018:GLU:HG2	1:A:1019:ARG:N	2.30	0.47
9:E:197:ASP:HB3	9:E:200:VAL:HG12	1.96	0.47
10:B:90:LYS:HB3	10:B:90:LYS:HE2	1.67	0.47
10:B:340:PHE:CD1	10:B:340:PHE:N	2.82	0.47
1:A:517:ALA:HB2	1:A:524:LEU:HD13	1.97	0.47
1:A:662:SER:O	1:A:665:LYS:HG2	2.15	0.46
10:B:229:SER:HB3	10:B:230:PRO:HD3	1.96	0.46
11:T:6:DC:H2"	11:T:7:DA:C8	2.49	0.46
2:C:285:ILE:HG21	5:K:102:LYS:HB2	1.96	0.46
7:H:114:VAL:HG22	7:H:121:MET:HE2	1.98	0.46
1:A:1145:LYS:O	1:A:1148:ILE:HG12	2.15	0.46
9:E:91:ASN:HA	9:E:122:THR:HG21	1.98	0.46
1:A:626:MET:HE3	1:A:699:ILE:HG22	1.96	0.46
6:L:17:GLN:HG3	6:L:31:GLU:OE1	2.16	0.46
1:A:976:GLU:O	1:A:979:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:ILE:HB	1:A:1005:LEU:HB3	1.97	0.46
7:H:88:LYS:HG2	7:H:144:ARG:HH12	1.81	0.46
2:C:80:ARG:O	2:C:84:MET:HG2	2.16	0.46
1:A:897:TYR:CD2	8:I:88:GLN:CB	2.99	0.46
1:A:1089:ARG:HD3	9:E:154:ASP:OD1	2.16	0.46
2:C:297:LEU:HD12	2:C:297:LEU:HA	1.83	0.46
1:A:942:ASN:OD1	1:A:945:LEU:HG	2.16	0.46
10:B:25:LEU:HB3	10:B:673:LYS:NZ	2.31	0.46
1:A:675:LEU:HD22	1:A:675:LEU:HA	1.84	0.46
1:A:527:PRO:HG3	1:A:539:TRP:CZ2	2.52	0.45
1:A:897:TYR:CE2	8:I:88:GLN:CB	2.99	0.45
1:A:1108:ILE:HD12	1:A:1109:PRO:HD2	1.98	0.45
9:E:93:VAL:HG23	9:E:123:GLY:O	2.16	0.45
11:T:21:DT:H2'	11:T:22:DC:H6	1.81	0.45
7:H:21:GLY:C	7:H:22:LYS:HG2	2.41	0.45
1:A:634:ILE:O	1:A:638:ILE:HG12	2.16	0.45
1:A:664:GLN:O	1:A:668:GLU:HG2	2.16	0.45
9:E:84:HIS:HB3	9:E:92:LYS:HD3	1.98	0.45
10:B:965:ILE:HG21	10:B:984:ARG:HB3	1.99	0.45
5:K:87:TYR:O	5:K:91:ILE:HG12	2.16	0.45
11:T:21:DT:H2'	11:T:22:DC:C6	2.51	0.45
1:A:659:LEU:O	1:A:663:ILE:HG12	2.17	0.45
7:H:41:MET:HE3	7:H:41:MET:HB3	1.89	0.45
8:I:88:GLN:CG	8:I:97:MET:HE2	2.46	0.45
10:B:553:MET:HE1	10:B:577:VAL:HG12	1.98	0.45
1:A:674:MET:HE1	1:A:695:LEU:CD2	2.47	0.45
1:A:904:LYS:HD2	1:A:904:LYS:HA	1.65	0.45
1:A:943:LYS:HD3	1:A:1003:PRO:HG3	1.98	0.45
1:A:1043:ILE:HD12	1:A:1043:ILE:N	2.31	0.45
11:T:4:DC:H1'	11:T:5:DT:C5	2.52	0.45
1:A:978:PHE:CE1	1:A:981:MET:HE3	2.52	0.45
10:B:274:PRO:HB2	10:B:277:VAL:HG23	1.99	0.45
1:A:900:ARG:HH22	8:I:68:LEU:CD1	2.30	0.45
11:T:6:DC:C4	11:T:7:DA:N6	2.85	0.45
1:A:836:MET:HE3	1:A:1148:ILE:HG22	1.99	0.44
8:I:4:MET:HE1	10:B:307:VAL:HG11	1.99	0.44
8:I:71:THR:HG21	8:I:74:VAL:HB	1.99	0.44
1:A:897:TYR:CG	8:I:88:GLN:HB2	2.52	0.44
9:E:135:LYS:HE2	9:E:135:LYS:HB3	1.88	0.44
1:A:645:MET:HA	1:A:649:LEU:HD13	2.00	0.44
3:F:91:LEU:HD23	3:F:93:GLY:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:TYR:HB2	1:A:752:TYR:OH	2.18	0.44
3:F:91:LEU:HG	3:F:94:GLU:OE1	2.17	0.44
8:I:68:LEU:HD12	8:I:69:PRO:HD2	1.99	0.44
10:B:371:MET:HE2	10:B:371:MET:HB3	1.91	0.44
8:I:97:MET:HB2	8:I:97:MET:HE3	1.82	0.44
9:E:35:ARG:HG3	9:E:156:LEU:HD21	1.99	0.44
1:A:965:ASN:HA	1:A:968:VAL:HG12	1.99	0.44
1:A:414:ARG:HG3	1:A:415:PRO:HD2	2.00	0.44
1:A:653:TYR:OH	8:I:67:THR:HA	2.17	0.44
1:A:698:GLN:HG3	10:B:951:GLN:HG2	1.99	0.44
6:L:27:ILE:HB	10:B:886:SER:HB3	1.98	0.44
8:I:81:HIS:CE1	8:I:83:GLU:HB3	2.53	0.44
1:A:503:MET:CE	1:A:577:LEU:HD21	2.46	0.43
2:C:287:LEU:O	2:C:291:LYS:HG3	2.18	0.43
7:H:62:MET:HE1	7:H:121:MET:HE1	2.00	0.43
1:A:946:LEU:HD12	1:A:951:ILE:HB	1.99	0.43
12:N:11:DT:H1'	12:N:12:DG:N7	2.33	0.43
1:A:978:PHE:HE1	1:A:981:MET:HE3	1.83	0.43
10:B:279:PHE:O	10:B:284:VAL:HG23	2.19	0.43
11:T:4:DC:H1'	11:T:5:DT:C4	2.53	0.43
1:A:465:ALA:O	1:A:469:VAL:HG23	2.19	0.43
1:A:1147:HIS:O	1:A:1151:VAL:HG23	2.18	0.43
9:E:106:ASN:O	9:E:109:ARG:HG2	2.18	0.43
10:B:276:TRP:CD1	10:B:311:ILE:HD13	2.54	0.43
10:B:352:LEU:HD22	10:B:353:TYR:CE1	2.54	0.43
10:B:243:ARG:NH1	10:B:243:ARG:HB2	2.34	0.43
10:B:336:LYS:HD2	10:B:336:LYS:HA	1.90	0.43
1:A:357:VAL:HG13	1:A:358:HIS:CD2	2.53	0.43
10:B:238:GLU:CD	10:B:239:THR:HG23	2.43	0.43
10:B:367:PHE:O	10:B:371:MET:HG3	2.19	0.43
10:B:946:ALA:O	10:B:950:ARG:HG2	2.18	0.43
2:C:214:SER:OG	2:C:246:LYS:HG2	2.19	0.43
5:K:38:GLU:OE1	5:K:42:ILE:HD12	2.19	0.43
10:B:569:LYS:HG2	10:B:576:TRP:CZ2	2.54	0.42
1:A:590:VAL:HG13	1:A:591:GLU:OE1	2.18	0.42
1:A:1144:LEU:HD23	1:A:1144:LEU:HA	1.84	0.42
2:C:108:LEU:HB2	2:C:125:LEU:HD23	2.01	0.42
1:A:357:VAL:HG22	1:A:358:HIS:H	1.84	0.42
2:C:246:LYS:HE3	2:C:250:MET:HE3	2.00	0.42
3:F:66:THR:HG22	3:F:68:TYR:H	1.84	0.42
10:B:752:MET:HE3	10:B:752:MET:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:108:ARG:C	3:F:109:LYS:HD2	2.44	0.42
7:H:83:LYS:HG3	7:H:83:LYS:O	2.20	0.42
10:B:807:ASP:HB3	10:B:893:TYR:CD1	2.55	0.42
10:B:905:CYS:O	10:B:920:LEU:HD23	2.20	0.42
1:A:863:LEU:HD23	1:A:863:LEU:HA	1.83	0.42
1:A:1037:ILE:HD13	1:A:1037:ILE:HA	1.85	0.42
10:B:308:VAL:HA	10:B:311:ILE:HG22	2.01	0.42
10:B:640:LYS:HA	10:B:640:LYS:HD3	1.64	0.42
1:A:1148:ILE:HD11	9:E:219:LEU:HD23	2.01	0.42
2:C:40:VAL:HG21	2:C:288:LEU:HD13	2.02	0.42
10:B:532:LEU:HA	10:B:532:LEU:HD23	1.81	0.42
10:B:827:LYS:O	10:B:827:LYS:HG3	2.18	0.42
9:E:186:GLU:HG2	9:E:188:LYS:HG2	2.02	0.42
1:A:871:THR:HG22	1:A:872:THR:H	1.85	0.42
1:A:885:ARG:NE	9:E:23:SER:HA	2.35	0.42
1:A:1019:ARG:HA	1:A:1022:ASP:OD2	2.19	0.42
10:B:360:SER:OG	10:B:363:GLN:HG3	2.20	0.42
7:H:109:LYS:HD3	7:H:109:LYS:HA	1.79	0.42
1:A:325:ARG:HA	1:A:455:VAL:O	2.20	0.41
1:A:374:SER:HB3	1:A:401:HIS:HB2	2.02	0.41
1:A:992:ARG:HG2	1:A:1002:MET:HE1	2.02	0.41
1:A:1029:TYR:CE2	1:A:1033:LEU:HD11	2.55	0.41
3:F:63:LYS:HZ3	3:F:64:PHE:HE1	1.67	0.41
3:F:73:ILE:HD13	3:F:73:ILE:HA	1.87	0.41
10:B:224:LEU:HD22	10:B:371:MET:HE3	2.02	0.41
10:B:319:GLU:CD	10:B:319:GLU:H	2.27	0.41
1:A:877:VAL:HG11	1:A:1091:VAL:HG11	2.01	0.41
10:B:323:HIS:HB2	10:B:326:ASN:ND2	2.36	0.41
1:A:689:ASN:O	1:A:692:ILE:HG22	2.20	0.41
1:A:863:LEU:HD13	1:A:1164:PHE:HB2	2.03	0.41
10:B:1046:LYS:HB3	10:B:1046:LYS:HE2	1.84	0.41
1:A:1155:MET:HE2	1:A:1155:MET:HB3	1.82	0.41
10:B:173:MET:HE3	10:B:173:MET:HB2	1.93	0.41
3:F:108:ARG:O	3:F:108:ARG:HG2	2.21	0.41
10:B:350:LEU:HD23	10:B:350:LEU:HA	1.83	0.41
10:B:626:PRO:HA	10:B:656:GLU:O	2.21	0.41
1:A:1127:GLN:O	1:A:1131:ARG:HG3	2.20	0.41
1:A:897:TYR:CG	8:I:88:GLN:OE1	2.73	0.41
10:B:163:GLN:NE2	10:B:165:ILE:HD13	2.36	0.41
1:A:897:TYR:CZ	8:I:88:GLN:N	2.82	0.41
1:A:1053:PRO:O	1:A:1055:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:40:VAL:HG13	2:C:44:GLU:HB2	2.02	0.41
9:E:56:LEU:C	9:E:58:ASP:H	2.28	0.41
9:E:91:ASN:O	9:E:92:LYS:HG2	2.21	0.41
9:E:124:LEU:HD23	9:E:125:ILE:N	2.36	0.41
10:B:388:ARG:H	10:B:388:ARG:HG3	1.59	0.41
1:A:674:MET:SD	1:A:675:LEU:HD23	2.62	0.40
1:A:750:ASP:OD1	1:A:751:PRO:HD2	2.21	0.40
1:A:964:ILE:HD12	1:A:964:ILE:HA	1.94	0.40
2:C:62:LEU:HD12	2:C:154:VAL:HG23	2.03	0.40
10:B:175:LYS:HB2	10:B:201:GLY:HA3	2.04	0.40
2:C:225:VAL:HG23	2:C:226:THR:HG23	2.03	0.40
8:I:10:CYS:HB2	8:I:32:CYS:SG	2.61	0.40
1:A:646:VAL:HG23	1:A:659:LEU:HD11	2.03	0.40
10:B:859:ARG:HB2	10:B:867:HIS:O	2.22	0.40
12:N:30:DA:H2"	12:N:31:DG:C5	2.56	0.40
1:A:635:HIS:O	1:A:639:VAL:HG22	2.21	0.40
1:A:717:LEU:HB2	10:B:501:ASP:OD2	2.20	0.40
10:B:553:MET:SD	10:B:570:VAL:HG21	2.61	0.40
10:B:625:ARG:HA	10:B:626:PRO:HD3	1.93	0.40
9:E:81:ILE:HG12	9:E:94:LYS:HE3	2.04	0.40

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	822/2032 (40%)	776 (94%)	46 (6%)	0	100	100
2	C	283/319 (89%)	274 (97%)	9 (3%)	0	100	100
3	F	73/144 (51%)	69 (94%)	4 (6%)	0	100	100
4	J	61/71 (86%)	58 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K	106/116 (91%)	101 (95%)	5 (5%)	0	100	100
6	L	43/51 (84%)	39 (91%)	4 (9%)	0	100	100
7	H	139/146 (95%)	126 (91%)	13 (9%)	0	100	100
8	I	93/114 (82%)	87 (94%)	6 (6%)	0	100	100
9	E	207/230 (90%)	194 (94%)	13 (6%)	0	100	100
10	B	951/1169 (81%)	904 (95%)	47 (5%)	0	100	100
All	All	2778/4392 (63%)	2628 (95%)	150 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	742/1709 (43%)	722 (97%)	20 (3%)	39	63
2	C	253/276 (92%)	246 (97%)	7 (3%)	38	63
3	F	67/128 (52%)	67 (100%)	0	100	100
4	J	56/63 (89%)	56 (100%)	0	100	100
5	K	98/105 (93%)	95 (97%)	3 (3%)	35	61
6	L	40/46 (87%)	38 (95%)	2 (5%)	22	50
7	H	123/127 (97%)	117 (95%)	6 (5%)	22	51
8	I	85/101 (84%)	84 (99%)	1 (1%)	63	74
9	E	190/209 (91%)	184 (97%)	6 (3%)	34	60
10	B	844/1026 (82%)	830 (98%)	14 (2%)	53	70
All	All	2498/3790 (66%)	2439 (98%)	59 (2%)	43	65

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	SER

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Mol	Chain	Res	Type
1	A	351	PHE
1	A	355	VAL
1	A	419	HIS
1	A	535	SER
1	A	675	LEU
1	A	788	ASP
1	A	790	VAL
1	A	804	SER
1	A	850	ASN
1	A	865	LYS
1	A	871	THR
1	A	962	ASP
1	A	981	MET
1	A	982	ASN
1	A	1058	TRP
1	A	1070	TRP
1	A	1112	ILE
1	A	1136	VAL
1	A	1158	SER
2	C	152	ILE
2	C	184	THR
2	C	194	ILE
2	C	202	THR
2	C	231	VAL
2	C	255	LEU
2	C	295	VAL
5	K	12	VAL
5	K	42	ILE
5	K	56	VAL
6	L	26	VAL
6	L	45	VAL
7	H	36	ASN
7	H	74	THR
7	H	107	THR
7	H	131	SER
7	H	132	HIS
7	H	142	LEU
8	I	24	ILE
9	E	95	VAL
9	E	142	LEU
9	E	152	ILE
9	E	171	LEU

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Mol	Chain	Res	Type
9	E	220	THR
9	E	229	VAL
10	B	70	VAL
10	B	121	THR
10	B	130	VAL
10	B	165	ILE
10	B	265	THR
10	B	269	LEU
10	B	388	ARG
10	B	541	MET
10	B	544	VAL
10	B	553	MET
10	B	656	GLU
10	B	670	TRP
10	B	822	VAL
10	B	1014	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	635	HIS
1	A	682	ASN
1	A	705	GLN
1	A	818	ASN
1	A	870	ASN
1	A	958	GLN
1	A	1100	HIS
1	A	1127	GLN
1	A	1147	HIS
1	A	1226	GLN
2	C	69	HIS
4	J	52	HIS
5	K	88	ASN
6	L	47	GLN
7	H	36	ASN
7	H	129	HIS
8	I	22	GLN
8	I	31	ASN
8	I	41	ASN
8	I	81	HIS
9	E	64	GLN
9	E	130	ASN

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Mol	Chain	Res	Type
10	B	118	GLN
10	B	216	GLN
10	B	326	ASN
10	B	363	GLN
10	B	491	GLN
10	B	529	ASN
10	B	892	ASN
10	B	900	GLN
10	B	934	GLN
10	B	951	GLN
10	B	1000	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	3/20 (15%)	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 [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 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.