



Full wwPDB EM Validation Report ⓘ

May 10, 2026 – 12:14 AM JST

PDB ID : 9K16 / pdb_00009k16
EMDB ID : EMD-61966
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 5U scaffold at 3.19 Angstrom
Authors : Xie, G.; Du, X.; Du, J.
Deposited on : 2024-10-16
Resolution : 3.19 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

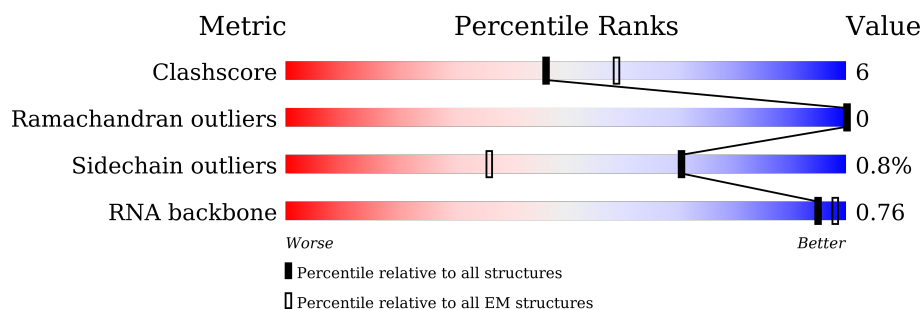
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.19 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	T	34	9% 21% 71%
2	N	34	32% 18% 50%
3	P	20	15% 85%
4	A	2032	34% 7% 59%
5	C	319	80% 10% 10%
6	F	144	42% 12% 44%
7	J	71	85% 11%
8	K	116	85% 8% 7%

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Mol	Chain	Length	Quality of chain
9	L	51	 71% 18% 12%
10	H	146	 73% 23% . .
11	I	114	 68% 18% 15%
12	E	230	 66% 25% 9%
13	B	1169	 76% 7% 17%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23179 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 DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	10	Total	C	N	O	P	0	0
			205	98	40	57	10		

- Molecule 2 is a DNA chain called DNA (34-MER).

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	3	Total	C	N	O	P	0	0
			60	27	6	24	3		

- Molecule 4 is a protein called DNA-directed RNA polymerase V largest subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	843	Total	C	N	O	S	0	0
			6597	4170	1132	1251	44		

- Molecule 5 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	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 6 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	80	Total	C	N	O	S	0	0
			660	420	114	122	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 7 is a protein called DNA-directed RNA polymerase II, IV and V subunit 10.

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

- Molecule 8 is a protein called DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	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 10 is a protein called DNA-directed RNA polymerase II, IV and V subunit 8.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	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 12 is a protein called RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	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 13 is a protein called DNA-directed RNA polymerase IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	967	Total	C	N	O	S	0	0
			7660	4827	1357	1432	44		

- 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



SER
GLN
ILE
GLU
ASP
ILE
GLN
PRO
ILE
GLY
ASN
GLY
GLU
ASP
SER
GLN
THR
GLU
PRO
GLN
ALA

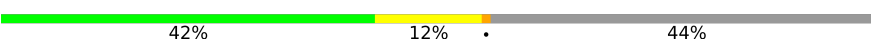
- Molecule 5: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein

Chain C:  80% 10% 10%

MET ASP THR G3 R8 T14 V40 M41 E56 S59 L62 R80 M84 E100 F101 V104 E105 F106 T114 D115 S127 V132 F137 GLY ASP SER SER GLY ALA ASP SER SER SER GLU Q148 V154 R157 E161 D175 T204 D205 D206

R227 Y237 E257 I258 K261 L280 L288 K291 D299 ASP THR VAL ALA ASP ASP GLN PHE GLY LEU GLY ALA HIS MET ARG GLY GLY

- Molecule 6: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein

Chain F:  42% 12% 44%

MET ALA GLU ASP TYR ASN GLU VAL ASP ASP LEU TYR GLU ASP GLU PRO ALA GLU PRO GLU ILE GLU GLY ILE GLU GLY ASP ASP MET LYS ASP ASN ASP ASP ILE ASN GLY GLY PRO LEU GLU THR GLU ASP LYS VAL GLU THR GLU PRO VAL ARG P58 R70

L74 R77 L91 E94 T95 D96 P97 L98 E99 I100 M102 L105 R106 Q107 R108 W126 G127 W137 LYS ARG GLN VAL GLY GLY ASP

- Molecule 7: DNA-directed RNA polymerase II, IV and V subunit 10

Chain J:  85% 11%

H1 I2 C7 M48 R63 THR LEU GLU LYS SER ASP ALA ASN

- Molecule 8: DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein

Chain K:  85% 8% 7%

MET ASN ALA PRO ASP R6 F10 V11 V12 K26 I75 T78 S79 Q80 E97 E108 V109 S113 ASN PRO TYR

- Molecule 9: DNA-directed RNA polymerase II, IV and V subunit 12

Chain L:  71% 18% 12%

MET ASP GLN GLN SER GLU P7 V8 T9 V11 E18 R19 T20 I27 Q28 C29 C32 R35 R43 R51

- Molecule 10: DNA-directed RNA polymerase II, IV and V subunit 8

Chain H:  73% 23%



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59869	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: MG, 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	T	0.19	0/229	0.36	0/348
2	N	0.20	0/391	0.38	0/599
3	P	0.07	0/65	0.19	0/98
4	A	0.15	0/6710	0.41	1/9058 (0.0%)
5	C	0.13	0/2286	0.37	0/3087
6	F	0.15	0/673	0.43	0/905
7	J	0.16	0/515	0.38	0/696
8	K	0.15	0/908	0.33	0/1224
9	L	0.15	0/369	0.40	0/493
10	H	0.15	0/1155	0.44	0/1557
11	I	0.15	0/804	0.41	0/1081
12	E	0.16	0/1732	0.47	0/2332
13	B	0.14	0/7809	0.35	0/10524
All	All	0.15	0/23646	0.39	1/32002 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	1002	MET	CB-CA-C	5.17	117.79	109.51

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	T	205	0	114	7	0
2	N	350	0	193	6	0
3	P	60	0	31	0	0
4	A	6597	0	6648	101	0
5	C	2256	0	2269	23	0
6	F	660	0	669	16	0
7	J	507	0	512	2	0
8	K	890	0	883	5	0
9	L	365	0	364	9	0
10	H	1129	0	1128	29	0
11	I	787	0	736	15	0
12	E	1706	0	1759	41	0
13	B	7660	0	7600	56	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	23179	0	22906	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)
2:N:10:DG:H22	13:B:463:LYS:HD3	1.46	0.81
12:E:100:THR:HA	12:E:129:GLN:HG2	1.70	0.73
4:A:938:HIS:HE2	4:A:1006:MET:HE3	1.54	0.72
11:I:68:LEU:HD11	11:I:87:PHE:HB2	1.73	0.70
4:A:592:LYS:HG3	4:A:596:GLU:HG3	1.74	0.70
4:A:804:SER:HA	12:E:189:GLN:HG2	1.74	0.69
12:E:112:ALA:HA	12:E:115:ILE:HG12	1.74	0.69
6:F:74:LEU:HD21	6:F:105:LEU:HD22	1.74	0.69
10:H:100:ILE:HG22	10:H:135:LEU:HD13	1.75	0.68
6:F:96:ASP:HB3	6:F:99:GLU:HG3	1.76	0.68
12:E:41:ARG:HH21	12:E:61:LEU:HD21	1.58	0.68
13:B:130:VAL:HG11	13:B:435:ILE:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:102:VAL:HB	11:I:111:ARG:HG2	1.75	0.67
4:A:721:MET:HE1	4:A:755:MET:HG2	1.78	0.66
10:H:92:VAL:HG12	10:H:142:LEU:HA	1.78	0.66
13:B:463:LYS:HG2	13:B:464:MET:SD	2.36	0.66
4:A:646:VAL:HG23	4:A:659:LEU:HD11	1.79	0.65
8:K:78:THR:HG23	8:K:80:GLN:H	1.61	0.64
4:A:805:ILE:HG13	12:E:189:GLN:HE22	1.62	0.64
4:A:807:GLN:HE22	12:E:223:TYR:HE1	1.46	0.64
4:A:903:LEU:HD12	4:A:1043:ILE:HG13	1.80	0.64
4:A:909:LYS:HB2	4:A:1033:LEU:HB3	1.78	0.64
4:A:896:ALA:HB1	4:A:1048:ILE:HD13	1.80	0.63
13:B:68:MET:HG2	13:B:415:ARG:HD2	1.80	0.63
12:E:63:LEU:HD21	12:E:67:ARG:HH21	1.63	0.63
4:A:649:LEU:HD12	4:A:656:GLU:HG2	1.79	0.62
10:H:39:MET:HE1	10:H:129:HIS:HD2	1.64	0.62
4:A:650:ARG:HH21	4:A:708:ASP:H	1.47	0.62
13:B:229:SER:HB3	13:B:230:PRO:HD3	1.81	0.61
4:A:1052:SER:HA	4:A:1067:ARG:CZ	2.31	0.61
4:A:1057:THR:H	4:A:1067:ARG:NH1	1.99	0.60
5:C:175:ASP:HA	8:K:10:PHE:HE1	1.66	0.60
10:H:14:VAL:HG13	10:H:55:GLY:H	1.66	0.60
4:A:328:ILE:HD11	4:A:455:VAL:HG22	1.85	0.59
4:A:980:LYS:HG3	4:A:1010:TYR:HB3	1.85	0.59
4:A:545:LEU:HD22	4:A:567:LEU:HD22	1.85	0.58
5:C:114:THR:HG22	5:C:115:ASP:H	1.68	0.58
4:A:805:ILE:HG13	12:E:189:GLN:NE2	2.19	0.57
12:E:133:THR:HG22	12:E:135:LYS:H	1.70	0.57
10:H:61:ALA:HB3	10:H:142:LEU:HB2	1.86	0.57
4:A:992:ARG:HD3	4:A:999:ASP:HA	1.87	0.57
4:A:964:ILE:HD13	4:A:981:MET:HE3	1.87	0.57
11:I:70:ARG:HG2	11:I:85:VAL:HG22	1.87	0.57
11:I:72:LYS:HE3	11:I:72:LYS:HA	1.87	0.56
12:E:174:GLY:HA2	12:E:177:LYS:HD2	1.86	0.56
12:E:195:LYS:HA	12:E:200:VAL:HG11	1.87	0.56
1:T:9:DG:H2''	1:T:10:DT:H5''	1.88	0.56
10:H:8:PHE:HB3	10:H:62:MET:HB2	1.88	0.56
10:H:103:ARG:HH11	10:H:124:ARG:HD2	1.71	0.56
1:T:7:DA:C8	1:T:7:DA:H5'	2.41	0.55
4:A:494:ASP:HB3	4:A:609:MET:HE1	1.88	0.55
4:A:542:PHE:HE1	4:A:570:PHE:HB3	1.71	0.55
13:B:335:ILE:HD11	13:B:346:VAL:HG12	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:822:VAL:HB	13:B:824:GLN:HE22	1.71	0.55
4:A:1099:LEU:HA	4:A:1102:ILE:HG22	1.87	0.55
2:N:12:DG:H4'	13:B:464:MET:HE1	1.88	0.55
4:A:1081:VAL:HG22	4:A:1086:ASP:HB3	1.89	0.55
13:B:165:ILE:HD12	13:B:436:GLU:HG3	1.87	0.55
4:A:953:MET:HA	4:A:956:ILE:HD12	1.88	0.55
10:H:97:LEU:HA	10:H:114:VAL:HG12	1.89	0.55
13:B:120:MET:HE2	13:B:888:ASP:HB2	1.88	0.54
12:E:186:GLU:HG2	12:E:188:LYS:HG2	1.89	0.54
4:A:917:VAL:HG12	11:I:44:TYR:HB3	1.89	0.54
4:A:1023:VAL:HG13	4:A:1024:LEU:HD12	1.90	0.54
13:B:332:GLU:HG2	13:B:346:VAL:HG11	1.88	0.54
11:I:21:GLU:HG2	11:I:22:GLN:HG3	1.90	0.53
11:I:88:GLN:HB2	11:I:97:MET:SD	2.48	0.53
10:H:37:LEU:HD21	10:H:129:HIS:CD2	2.43	0.53
4:A:799:ASN:O	4:A:803:ASN:HA	2.09	0.53
9:L:11:VAL:HG12	9:L:18:GLU:HG2	1.89	0.53
12:E:33:SER:HB3	12:E:74:PRO:HD3	1.91	0.53
5:C:204:THR:HA	5:C:227:ARG:HH22	1.74	0.53
4:A:323:SER:HB3	13:B:1048:ARG:HB2	1.91	0.52
6:F:102:MET:O	6:F:106:ARG:HG2	2.09	0.52
4:A:832:ALA:O	4:A:836:MET:HG2	2.10	0.52
11:I:71:THR:HG21	11:I:74:VAL:HB	1.91	0.52
12:E:50:ARG:HD3	12:E:52:TYR:CZ	2.44	0.52
4:A:1044:ALA:HB2	4:A:1077:GLU:HG2	1.91	0.52
5:C:104:VAL:HG21	5:C:132:VAL:HG21	1.91	0.52
13:B:175:LYS:HB2	13:B:201:GLY:HA3	1.92	0.52
4:A:778:LEU:HD13	4:A:863:LEU:HD21	1.92	0.51
4:A:402:ARG:HH11	4:A:405:MET:HE3	1.75	0.51
10:H:42:HIS:CD2	10:H:122:LEU:HB3	2.46	0.51
12:E:217:GLY:H	12:E:221:GLU:HG3	1.75	0.51
5:C:56:GLU:HG2	9:L:43:ARG:NH1	2.26	0.51
6:F:94:GLU:HB2	6:F:99:GLU:OE2	2.11	0.51
4:A:808:PHE:CE1	12:E:183:PHE:HE2	2.28	0.51
4:A:810:TYR:HE1	4:A:1150:LEU:HD22	1.75	0.51
4:A:960:CYS:O	4:A:964:ILE:HG22	2.10	0.51
4:A:1082:LYS:HD2	4:A:1082:LYS:C	2.36	0.50
4:A:530:VAL:HB	10:H:92:VAL:HG23	1.94	0.50
4:A:941:LEU:HB2	4:A:1003:PRO:HB2	1.94	0.50
9:L:35:ARG:HH21	13:B:103:SER:HB2	1.77	0.50
12:E:22:LEU:HA	12:E:25:TYR:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:99:LYS:HD2	10:H:113:TYR:CD2	2.47	0.50
13:B:459:HIS:CE1	13:B:462:ARG:H	2.30	0.50
7:J:7:CYS:HA	7:J:48:MET:HE2	1.94	0.49
10:H:56:ASP:HB3	10:H:145:LYS:HE2	1.93	0.49
4:A:412:ILE:HG21	4:A:446:LEU:HD21	1.94	0.49
13:B:415:ARG:O	13:B:419:THR:HG23	2.12	0.49
6:F:97:PRO:HA	6:F:100:ILE:HG22	1.94	0.49
4:A:592:LYS:H	6:F:137:TRP:HB2	1.77	0.49
13:B:300:ASP:O	13:B:303:ILE:HG22	2.12	0.49
4:A:1029:TYR:CZ	4:A:1033:LEU:HD21	2.48	0.49
12:E:66:PHE:HA	12:E:69:VAL:HG12	1.95	0.49
9:L:43:ARG:NE	9:L:43:ARG:HA	2.28	0.49
13:B:463:LYS:O	13:B:464:MET:HE2	2.12	0.49
6:F:126:TRP:HD1	6:F:127:GLY:H	1.61	0.48
10:H:99:LYS:HB3	10:H:113:TYR:HB2	1.95	0.48
1:T:8:DA:H2"	1:T:9:DG:C8	2.47	0.48
4:A:895:SER:O	4:A:899:VAL:HG23	2.14	0.48
5:C:56:GLU:HG2	9:L:43:ARG:HH11	1.77	0.48
10:H:43:LEU:HD23	10:H:121:MET:HB2	1.94	0.48
13:B:748:LEU:HB3	13:B:965:ILE:HD11	1.94	0.48
4:A:1076:VAL:HG11	4:A:1090:VAL:HG21	1.94	0.48
5:C:8:ARG:HB2	8:K:97:GLU:OE2	2.13	0.48
5:C:237:TYR:CE2	5:C:258:ILE:HG21	2.49	0.48
12:E:115:ILE:HD12	12:E:124:LEU:HD21	1.95	0.48
4:A:1049:ILE:HG12	4:A:1073:ASP:OD2	2.14	0.48
12:E:111:VAL:O	12:E:115:ILE:HG23	2.13	0.48
13:B:331:VAL:O	13:B:335:ILE:HG12	2.13	0.48
13:B:423:GLN:HA	13:B:426:LEU:HB3	1.95	0.48
13:B:961:LEU:O	13:B:965:ILE:HG23	2.14	0.48
4:A:467:ALA:HB2	6:F:98:LEU:HD21	1.96	0.48
13:B:225:TRP:CG	13:B:236:ARG:HH12	2.32	0.47
4:A:1167:GLY:HA2	4:A:1170:LYS:HE3	1.96	0.47
9:L:29:CYS:SG	9:L:32:CYS:HB2	2.54	0.47
13:B:165:ILE:HG23	13:B:436:GLU:HG3	1.96	0.47
4:A:650:ARG:HD2	4:A:650:ARG:HA	1.63	0.47
4:A:880:TYR:HA	4:A:1071:VAL:HG12	1.96	0.47
5:C:62:LEU:HD12	5:C:154:VAL:HG23	1.96	0.47
1:T:6:DC:H2"	1:T:7:DA:C8	2.49	0.47
4:A:943:LYS:O	4:A:947:GLU:HG2	2.14	0.47
5:C:40:VAL:HG21	5:C:288:LEU:HD13	1.96	0.47
6:F:99:GLU:HA	6:F:102:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:258:LYS:O	13:B:259:ARG:HG3	2.14	0.47
10:H:97:LEU:HD21	10:H:100:ILE:HB	1.96	0.47
4:A:575:ASP:HB2	4:A:687:LYS:HD3	1.97	0.47
5:C:62:LEU:HD11	7:J:2:ILE:HD11	1.96	0.47
13:B:296:PHE:CE2	13:B:303:ILE:HG12	2.50	0.47
4:A:359:ASN:O	4:A:363:LEU:HG	2.16	0.46
4:A:905:LYS:HE2	4:A:1041:PRO:HA	1.97	0.46
4:A:906:VAL:HG11	4:A:949:TRP:CH2	2.50	0.46
5:C:80:ARG:O	5:C:84:MET:HG3	2.15	0.46
9:L:9:THR:HG22	9:L:20:THR:HG22	1.96	0.46
13:B:330:TYR:O	13:B:333:GLN:HG3	2.15	0.46
4:A:885:ARG:HE	12:E:22:LEU:HB2	1.80	0.46
5:C:157:ARG:HA	5:C:157:ARG:HD3	1.75	0.46
13:B:277:VAL:HG11	13:B:330:TYR:HD2	1.80	0.46
4:A:1128:ALA:O	4:A:1132:LEU:HG	2.15	0.46
10:H:109:LYS:HD2	10:H:124:ARG:HE	1.81	0.46
13:B:640:LYS:HA	13:B:640:LYS:HD3	1.70	0.46
11:I:113:ARG:HD2	11:I:114:GLU:H	1.80	0.46
13:B:59:GLN:HE21	13:B:63:GLU:HG3	1.80	0.46
12:E:37:TYR:CE1	12:E:41:ARG:HD3	2.51	0.46
12:E:182:GLN:HG2	12:E:183:PHE:CE1	2.51	0.46
4:A:969:GLN:HA	4:A:972:LYS:HE2	1.98	0.45
10:H:6:ILE:C	10:H:7:MET:HE2	2.41	0.45
13:B:264:LEU:HD12	13:B:275:VAL:HG11	1.98	0.45
12:E:44:LEU:HG	12:E:59:ILE:HG13	1.98	0.45
11:I:99:LEU:HG	11:I:113:ARG:HH12	1.82	0.45
13:B:279:PHE:O	13:B:284:VAL:HG12	2.17	0.45
12:E:34:HIS:HB2	12:E:67:ARG:NH2	2.32	0.45
13:B:215:ALA:HB1	13:B:396:ILE:HG23	1.99	0.45
4:A:786:LEU:HD23	4:A:789:ILE:HD12	1.97	0.45
13:B:475:GLY:HA3	13:B:481:GLN:HE21	1.81	0.45
6:F:58:PRO:HB2	6:F:126:TRP:CZ3	2.52	0.45
10:H:114:VAL:HG22	10:H:121:MET:HE2	1.99	0.45
12:E:181:LYS:HD2	12:E:182:GLN:N	2.32	0.45
6:F:70:ARG:HD2	6:F:105:LEU:HD21	1.98	0.45
13:B:362:THR:HG23	13:B:560:THR:HB	1.98	0.44
4:A:395:LYS:HG3	4:A:398:GLN:NE2	2.32	0.44
4:A:650:ARG:NH2	4:A:707:SER:HB2	2.32	0.44
10:H:114:VAL:CG2	10:H:121:MET:HE2	2.48	0.44
11:I:99:LEU:HG	11:I:113:ARG:NH1	2.32	0.44
12:E:64:GLN:O	12:E:68:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:19:DA:C8	2:N:19:DA:H5'	2.52	0.44
2:N:18:DC:H4'	2:N:19:DA:OP1	2.17	0.44
4:A:728:LYS:HE3	13:B:670:TRP:HE1	1.82	0.44
10:H:109:LYS:HD2	10:H:124:ARG:HB3	1.99	0.44
12:E:135:LYS:HA	12:E:138:LYS:HE2	2.00	0.44
13:B:250:GLU:HG3	13:B:262:LYS:HG3	1.99	0.44
1:T:8:DA:H2''	1:T:9:DG:N7	2.32	0.44
4:A:377:GLN:HG2	4:A:398:GLN:HG2	2.00	0.44
4:A:377:GLN:HG3	4:A:382:TYR:HE1	1.82	0.44
4:A:885:ARG:HE	12:E:22:LEU:N	2.16	0.44
5:C:291:LYS:HB3	5:C:291:LYS:HE2	1.79	0.44
13:B:1046:LYS:HB3	13:B:1046:LYS:HE2	1.70	0.44
4:A:988:CYS:HB2	4:A:1001:ASP:HA	2.00	0.44
4:A:395:LYS:HG3	4:A:398:GLN:HE22	1.83	0.44
6:F:107:GLN:O	6:F:108:ARG:HG2	2.18	0.44
13:B:399:ALA:O	13:B:403:LEU:HB2	2.17	0.44
2:N:17:DG:H2'	13:B:461:PHE:CZ	2.53	0.43
12:E:76:VAL:HB	12:E:97:PHE:HB2	1.99	0.43
13:B:459:HIS:CE1	13:B:462:ARG:HB2	2.53	0.43
4:A:709:LYS:HA	4:A:709:LYS:HD3	1.78	0.43
4:A:885:ARG:NH1	4:A:886:CYS:HB2	2.33	0.43
4:A:1132:LEU:HD11	4:A:1148:ILE:HG23	2.00	0.43
13:B:303:ILE:O	13:B:307:VAL:HG12	2.18	0.43
13:B:626:PRO:HA	13:B:656:GLU:O	2.18	0.43
2:N:12:DG:H2''	2:N:13:DC:C2	2.54	0.43
4:A:643:SER:OG	4:A:644:PRO:HD3	2.18	0.43
4:A:465:ALA:O	4:A:469:VAL:HG22	2.19	0.43
4:A:650:ARG:NH2	4:A:709:LYS:HG2	2.33	0.43
9:L:27:ILE:HD11	13:B:885:SER:C	2.43	0.43
4:A:376:THR:HG22	4:A:399:ILE:HB	1.99	0.43
4:A:787:ARG:HD2	4:A:788:ASP:OD2	2.18	0.43
4:A:916:LEU:HD11	11:I:45:ARG:HG3	2.00	0.43
12:E:158:ASN:HD22	12:E:161:LYS:HD2	1.84	0.43
10:H:98:TYR:CZ	10:H:113:TYR:HB3	2.53	0.43
4:A:940:HIS:CE1	4:A:1004:CYS:HB2	2.54	0.43
4:A:1048:ILE:HG12	4:A:1072:LEU:HG	1.99	0.43
13:B:277:VAL:HG13	13:B:327:ALA:HB1	2.01	0.43
1:T:6:DC:C4	1:T:7:DA:N6	2.87	0.43
4:A:774:GLU:HB3	4:A:775:PRO:HD3	2.01	0.43
4:A:567:LEU:HD12	4:A:567:LEU:HA	1.88	0.42
12:E:135:LYS:HE2	12:E:135:LYS:HB3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:215:TYR:HD2	12:E:223:TYR:HD2	1.66	0.42
1:T:4:DC:H1'	1:T:5:DT:C5	2.55	0.42
4:A:965:ASN:O	4:A:969:GLN:HG2	2.19	0.42
6:F:137:TRP:CE3	6:F:137:TRP:HA	2.55	0.42
10:H:103:ARG:NH1	10:H:124:ARG:HD2	2.35	0.42
12:E:144:THR:HG23	12:E:145:PHE:CD2	2.55	0.42
4:A:788:ASP:HB3	4:A:800:THR:OG1	2.18	0.42
13:B:336:LYS:HD2	13:B:336:LYS:HA	1.86	0.42
13:B:532:LEU:HA	13:B:532:LEU:HD23	1.82	0.42
4:A:405:MET:HE2	4:A:405:MET:HB3	1.97	0.42
4:A:1167:GLY:O	4:A:1170:LYS:HG2	2.20	0.42
10:H:103:ARG:C	10:H:105:GLY:H	2.28	0.42
4:A:412:ILE:HD11	4:A:455:VAL:HG21	2.00	0.42
4:A:1058:TRP:CE2	4:A:1059:ILE:HG23	2.54	0.42
5:C:14:ILE:HD12	8:K:108:GLU:HB3	2.00	0.42
12:E:96:VAL:HB	12:E:126:LEU:HD23	2.01	0.42
13:B:358:LEU:HD23	13:B:358:LEU:HA	1.82	0.42
4:A:938:HIS:HB3	4:A:940:HIS:CD2	2.54	0.42
10:H:57:LYS:HE3	10:H:57:LYS:HB3	1.85	0.42
11:I:88:GLN:O	11:I:88:GLN:HG2	2.20	0.42
13:B:1013:ARG:HD2	13:B:1022:MET:HG2	2.01	0.42
4:A:1019:ARG:O	4:A:1023:VAL:HG12	2.19	0.42
5:C:41:MET:HG2	5:C:280:LEU:HG	2.01	0.42
5:C:100:GLU:HG3	5:C:101:PHE:CE2	2.55	0.42
4:A:725:TYR:HB2	4:A:752:TYR:OH	2.19	0.41
4:A:990:SER:HA	4:A:1002:MET:HE1	2.02	0.41
8:K:26:LYS:N	8:K:26:LYS:HD3	2.35	0.41
4:A:1155:MET:HE3	4:A:1155:MET:HB2	1.89	0.41
4:A:809:LYS:HB3	4:A:809:LYS:HE2	1.94	0.41
11:I:15:TYR:CE1	11:I:30:ARG:HG3	2.55	0.41
4:A:518:MET:HE3	4:A:518:MET:HB3	1.83	0.41
4:A:1081:VAL:HG13	4:A:1086:ASP:HB2	2.02	0.41
12:E:196:LYS:HA	12:E:196:LYS:HD3	1.67	0.41
13:B:946:ALA:O	13:B:950:ARG:HG2	2.20	0.41
4:A:527:PRO:HG3	4:A:539:TRP:CZ2	2.56	0.41
4:A:1159:GLY:HA2	12:E:192:ARG:O	2.21	0.41
13:B:1014:VAL:HG13	13:B:1023:MET:HE3	2.03	0.41
5:C:204:THR:HG23	5:C:206:ASP:OD1	2.21	0.41
10:H:57:LYS:HD2	10:H:57:LYS:O	2.21	0.41
13:B:328:LEU:O	13:B:332:GLU:HG3	2.21	0.41
11:I:97:MET:HE2	11:I:97:MET:HB2	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:59:SER:HB2	5:C:161:GLU:H	1.85	0.41
12:E:217:GLY:O	12:E:221:GLU:HG3	2.20	0.41
4:A:589:MET:O	6:F:137:TRP:HB3	2.21	0.41
6:F:77:ARG:HD2	6:F:77:ARG:HA	1.83	0.41
12:E:93:VAL:HG13	12:E:124:LEU:HA	2.03	0.41
13:B:553:MET:SD	13:B:570:VAL:HG21	2.61	0.41
4:A:917:VAL:HA	4:A:937:GLY:HA2	2.03	0.40
5:C:205:ASP:HB3	5:C:227:ARG:NH1	2.36	0.40
5:C:257:GLU:O	5:C:258:ILE:HD13	2.21	0.40
10:H:17:LEU:HD22	10:H:30:ILE:HG22	2.03	0.40
10:H:43:LEU:HD23	10:H:43:LEU:HA	1.94	0.40
10:H:46:ASN:HB2	10:H:91:TYR:OH	2.21	0.40
12:E:46:MET:HB2	12:E:202:TYR:CE1	2.56	0.40
13:B:332:GLU:HG2	13:B:346:VAL:CG1	2.51	0.40
4:A:807:GLN:CD	4:A:808:PHE:H	2.29	0.40
4:A:1114:GLN:OE1	4:A:1114:GLN:HA	2.21	0.40
9:L:27:ILE:HD12	13:B:884:LEU:HD23	2.04	0.40
12:E:52:TYR:N	12:E:52:TYR:CD1	2.89	0.40
4:A:451:ASP:OD2	4:A:451:ASP:C	2.65	0.40
5:C:261:LYS:HE3	5:C:261:LYS:HB2	1.77	0.40
4:A:698:GLN:HG3	13:B:951:GLN:HG2	2.03	0.40
5:C:106:PHE:CE2	5:C:127:SER:HB3	2.57	0.40
6:F:91:LEU:HD11	6:F:94:GLU:O	2.22	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	
4	A	833/2032 (41%)	805 (97%)	28 (3%)	0	100	100
5	C	283/319 (89%)	271 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	78/144 (54%)	73 (94%)	5 (6%)	0	100	100
7	J	61/71 (86%)	58 (95%)	3 (5%)	0	100	100
8	K	106/116 (91%)	103 (97%)	3 (3%)	0	100	100
9	L	43/51 (84%)	39 (91%)	4 (9%)	0	100	100
10	H	139/146 (95%)	126 (91%)	13 (9%)	0	100	100
11	I	93/114 (82%)	89 (96%)	4 (4%)	0	100	100
12	E	207/230 (90%)	198 (96%)	9 (4%)	0	100	100
13	B	953/1169 (82%)	927 (97%)	26 (3%)	0	100	100
All	All	2796/4392 (64%)	2689 (96%)	107 (4%)	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	
4	A	748/1709 (44%)	741 (99%)	7 (1%)	70	81
5	C	253/276 (92%)	253 (100%)	0	100	100
6	F	72/128 (56%)	71 (99%)	1 (1%)	59	77
7	J	56/63 (89%)	55 (98%)	1 (2%)	51	74
8	K	98/105 (93%)	95 (97%)	3 (3%)	35	66
9	L	40/46 (87%)	40 (100%)	0	100	100
10	H	123/127 (97%)	122 (99%)	1 (1%)	73	82
11	I	85/101 (84%)	85 (100%)	0	100	100
12	E	190/209 (91%)	187 (98%)	3 (2%)	55	75
13	B	846/1026 (82%)	842 (100%)	4 (0%)	81	85
All	All	2511/3790 (66%)	2491 (99%)	20 (1%)	70	82

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	355	VAL
4	A	419	HIS
4	A	574	VAL
4	A	702	LEU
4	A	712	LEU
4	A	732	THR
4	A	1073	ASP
6	F	74	LEU
7	J	2	ILE
8	K	12	VAL
8	K	75	ILE
8	K	109	VAL
10	H	14	VAL
12	E	26	VAL
12	E	203	TYR
12	E	205	LEU
13	B	62	PHE
13	B	279	PHE
13	B	291	VAL
13	B	670	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	682	ASN
4	A	850	ASN
4	A	940	HIS
4	A	1153	ASN
5	C	69	HIS
7	J	52	HIS
8	K	55	ASN
10	H	35	HIS
10	H	106	GLN
10	H	129	HIS
12	E	34	HIS
12	E	42	ASN
12	E	158	ASN
13	B	334	GLN
13	B	473	ASN
13	B	481	GLN
13	B	529	ASN
13	B	648	HIS
13	B	720	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	2/20 (10%)	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.