Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Sep 7, 2019 – 11:20 PM EDT

PDB ID	:	6KIW
EMDB ID:	:	EMD-0693
Title	:	Cryo-EM structure of human MLL3-ubNCP complex (4.0 angstrom)
Authors	:	Huang, J.; Xue, H.; Yao, T.
Deposited on	:	2019-07-20
Resolution	:	4.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB 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 (i) symbol.

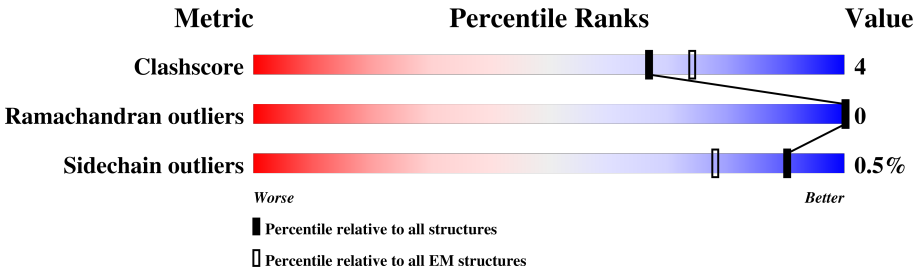
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	135	64% 7% · 28%
1	E	135	64% 7% · 28%
2	B	102	74% 7% 20%
2	F	102	74% 6% 21%
3	C	129	82% · 17%
3	G	129	78% · 19%
4	D	122	72% · 25%
4	H	122	74% · 23%
5	I	144	91% 9%

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Mol	Chain	Length	Quality of chain
6	J	145	90% 10%
7	K	205	61% 15% 24%
8	N	538	53% 11% 36%
9	O	76	76% 24%
10	R	334	68% 22% 10%
11	T	534	25% 8% 67%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 20225 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total 802	C 506	N 155	O 138	S 3	0	0
1	E	97	Total 802	C 506	N 155	O 138	S 3	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	82	Total 657	C 416	N 128	O 112	S 1	0	0
2	F	81	Total 648	C 410	N 126	O 111	S 1	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total 823	C 519	N 161	O 143	0	0
3	G	104	Total 800	C 504	N 156	O 140	0	0

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	92	Total 718	C 451	N 128	O 136	S 3	0	0
4	H	94	Total 733	C 460	N 131	O 139	S 3	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	engineered mutation	UNP P02281

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Chain	Residue	Modelled	Actual	Comment	Reference
D	117	CYS	LYS	engineered mutation	UNP P02281
H	29	THR	SER	engineered mutation	UNP P02281
H	117	CYS	LYS	engineered mutation	UNP P02281

- Molecule 5 is a DNA chain called DNA (144-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	144	Total	C	N	O	P	0	0
			2935	1393	536	862	144		

- Molecule 6 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	145	Total	C	N	O	P	0	0
			2990	1415	559	871	145		

- Molecule 7 is a protein called Histone-lysine N-methyltransferase 2C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	156	Total	C	N	O	S	0	0
			1259	784	235	228	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	4708	SER	CYS	engineered mutation	UNP Q8NEZ4

- Molecule 8 is a protein called Retinoblastoma-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	347	Total	C	N	O	S	0	0
			2724	1715	472	522	15		

- Molecule 9 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	76	Total	C	N	O	S	0	0
			603	379	105	117	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	76	CYS	GLY	engineered mutation	UNP P62979

- Molecule 10 is a protein called WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	300	Total	C	N	O	S	0	0
			2326	1485	388	444	9		

- Molecule 11 is a protein called Set1/Ash2 histone methyltransferase complex subunit ASH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	176	Total	C	N	O	S	0	0
			1404	907	235	256	6		

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	K	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

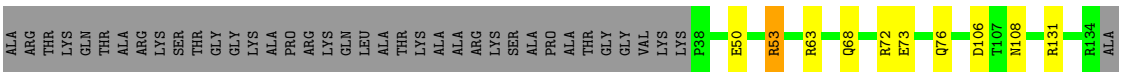
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Histone H3

Chain A:

- Molecule 1: Histone H3

Chain E:



- Molecule 2: Histone H4

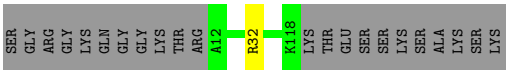
Chain B:

- Molecule 2: Histone H4

Chain F:

- Molecule 3: Histone H2A

Chain C:



- Molecule 3: Histone H2A

Chain G:

• Molecule 4: Histone H2B 1.1

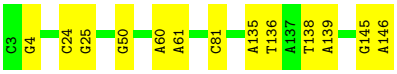
Chain D:

• Molecule 4: Histone H2B 1.1

Chain H:

• Molecule 5: DNA (144-MER)

Chain I:

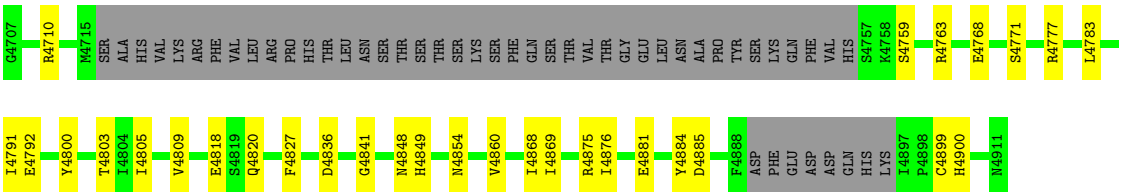


• Molecule 6: DNA (145-MER)

Chain J:

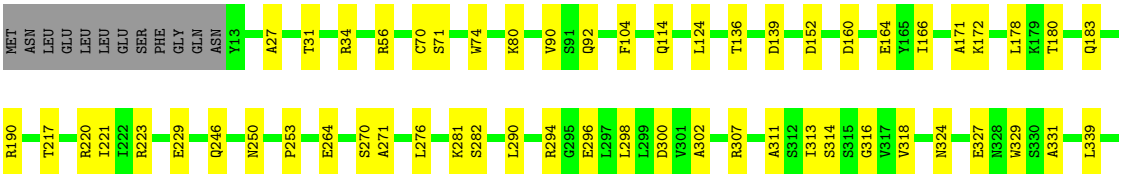
• Molecule 7: Histone-lysine N-methyltransferase 2C

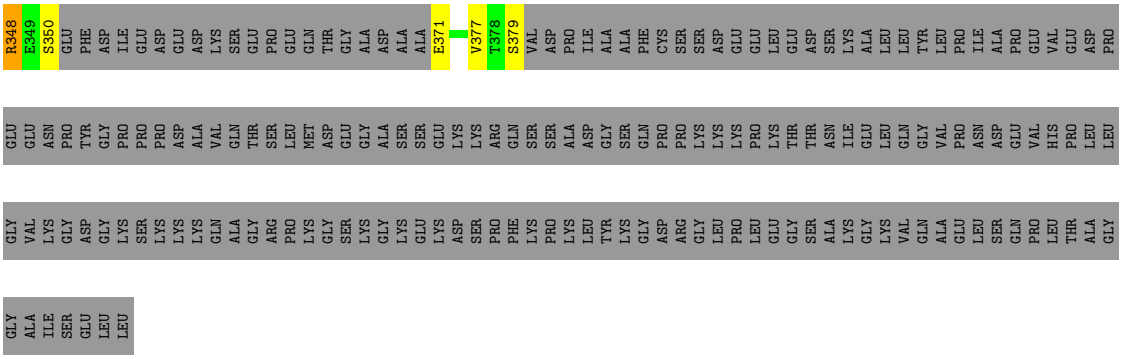
Chain K:



• Molecule 8: Retinoblastoma-binding protein 5

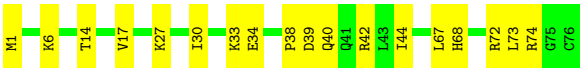
Chain N:





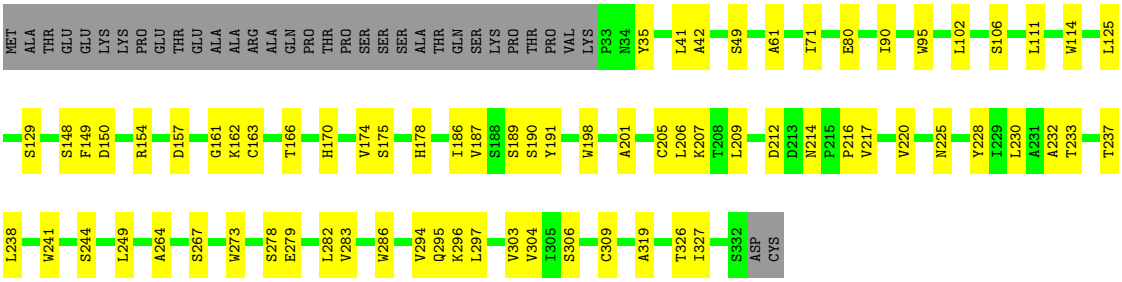
• Molecule 9: Ubiquitin

Chain O:



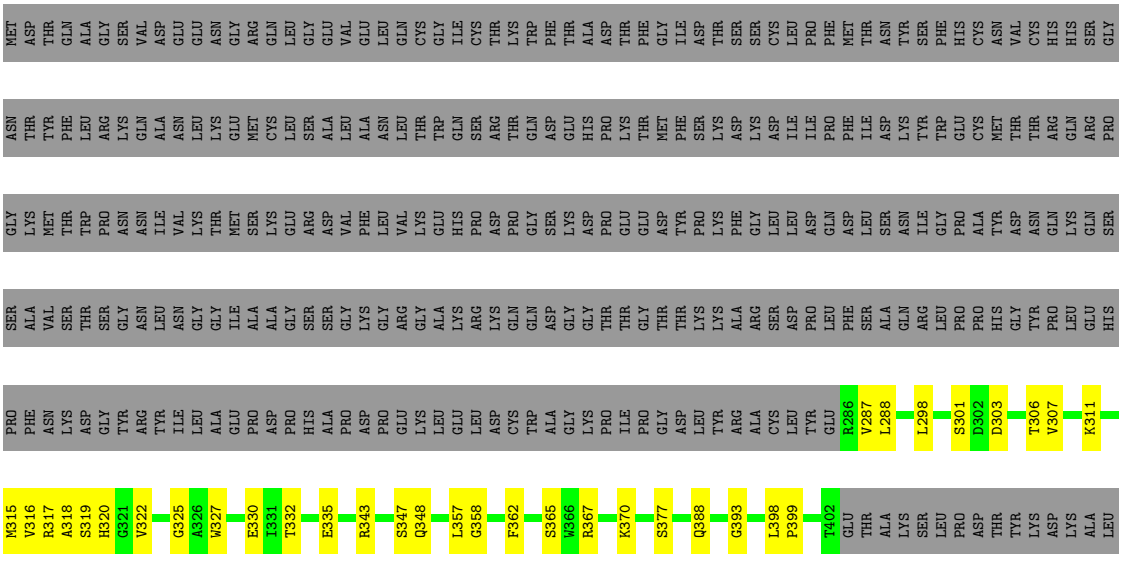
• Molecule 10: WD repeat-containing protein 5

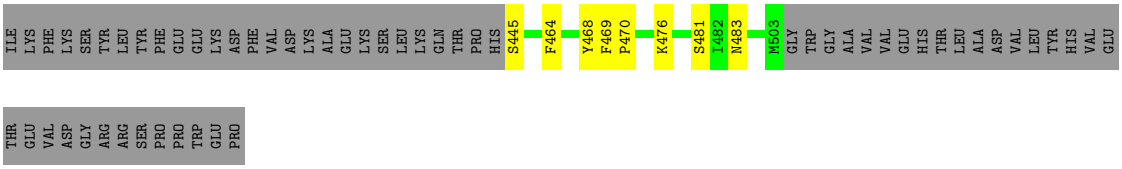
Chain R:



• Molecule 11: Set1/Ash2 histone methyltransferase complex subunit ASH2

Chain T:




ILE LYS PHE LYS SER TYR LEU TYR PHE GLU GLU LYS ASP PHE VAL ASP LYS ALA GLU LYS SER LEU LYS GLN THR PRO HIS S445 F464 Y468 F469 P470 K476 S481 T482 N483 M503 GLY TRP GLY ALA VAL VAL GLU HIS THR LEU ALA ASP VAL LEU TYR HIS VAL GLU
THR GLU VAL ASP GLY ARG ARG SER PRO PRO TRP GLU PRO

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81945	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	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	0.36	0/814	0.59	0/1092
1	E	0.36	0/814	0.59	0/1092
10	R	0.27	0/2382	0.54	1/3231 (0.0%)
11	T	0.28	0/1445	0.55	0/1954
2	B	0.45	0/664	0.63	0/889
2	F	0.45	0/655	0.59	0/878
3	C	0.37	0/833	0.54	0/1124
3	G	0.35	0/810	0.55	0/1095
4	D	0.41	0/729	0.55	0/983
4	H	0.37	0/744	0.55	0/1001
5	I	0.72	0/3289	1.00	1/5069 (0.0%)
6	J	0.71	0/3357	0.98	0/5184
7	K	0.28	0/1281	0.53	0/1715
8	N	0.30	0/2781	0.56	0/3777
9	O	0.26	0/609	0.57	0/819
All	All	0.48	0/21207	0.74	2/29903 (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
8	N	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	4	DG	O4'-C4'-C3'	-6.81	101.78	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	R	309	CYS	C-N-CA	5.75	136.08	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	N	327	GLU	Peptide

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	802	0	841	8	0
1	E	802	0	841	7	0
2	B	657	0	706	6	0
2	F	648	0	693	5	0
3	C	823	0	882	1	0
3	G	800	0	851	2	0
4	D	718	0	734	3	0
4	H	733	0	752	3	0
5	I	2935	0	1615	9	0
6	J	2990	0	1628	10	0
7	K	1259	0	1252	22	0
8	N	2724	0	2677	35	0
9	O	603	0	631	11	0
10	R	2326	0	2309	48	0
11	T	1404	0	1369	24	0
12	K	1	0	0	0	0
All	All	20225	0	17781	163	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 4.

All (163) 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:E:63:ARG:HH21	6:J:60:DA:H5"	1.56	0.71
9:O:44:ILE:HB	9:O:68:HIS:HB2	1.78	0.65
1:E:76:GLN:HE22	2:F:21:VAL:HG23	1.62	0.64
8:N:27:ALA:H	8:N:316:GLY:HA2	1.61	0.63
11:T:315:MET:SD	11:T:317:ARG:NH1	2.73	0.62
10:R:205:CYS:SG	10:R:206:LEU:N	2.73	0.61
10:R:111:LEU:HB2	10:R:125:LEU:HB2	1.83	0.61
10:R:283:VAL:HB	10:R:297:LEU:HB2	1.83	0.60
2:B:64:ASN:OD1	2:B:67:ARG:NH2	2.35	0.59
5:I:25:DG:H1	6:J:123:DC:H42	1.49	0.59
1:E:108:ASN:ND2	2:F:42:GLY:O	2.36	0.59
10:R:267:SER:HB3	10:R:273:TRP:HB2	1.85	0.59
10:R:90:ILE:HA	10:R:106:SER:HA	1.84	0.58
11:T:325:GLY:H	11:T:398:LEU:HB2	1.67	0.58
10:R:230:LEU:HD23	10:R:264:ALA:HB1	1.84	0.58
1:E:106:ASP:OD2	1:E:131:ARG:NH2	2.36	0.58
1:A:106:ASP:OD2	1:A:131:ARG:NH2	2.36	0.58
11:T:307:VAL:HG21	11:T:316:VAL:HG11	1.85	0.58
7:K:4783:LEU:HD11	8:N:329:TRP:HZ2	1.68	0.58
8:N:172:LYS:HB3	8:N:190:ARG:HH22	1.69	0.57
3:C:32:ARG:NH2	4:D:32:GLU:OE2	2.38	0.57
11:T:367:ARG:HH21	11:T:370:LYS:HB2	1.70	0.56
4:D:119:THR:HG21	8:N:246:GLN:HE21	1.71	0.56
10:R:207:LYS:NZ	10:R:244:SER:O	2.39	0.56
1:A:108:ASN:ND2	2:B:42:GLY:O	2.39	0.56
10:R:61:ALA:H	10:R:95:TRP:HH2	1.53	0.56
11:T:318:ALA:HB3	11:T:470:PRO:HD2	1.89	0.55
7:K:4818:GLU:O	10:R:214:ASN:ND2	2.39	0.55
7:K:4768:GLU:HB2	7:K:4771:SER:HB2	1.90	0.54
11:T:464:PHE:O	11:T:468:TYR:OH	2.25	0.54
1:E:73:GLU:HB2	2:F:25:ASN:HD22	1.73	0.53
7:K:4854:ASN:ND2	7:K:4881:GLU:O	2.39	0.53
1:A:57:SER:O	2:B:40:ARG:NH2	2.41	0.53
9:O:39:ASP:HB2	9:O:74:ARG:HB3	1.89	0.53
9:O:33:LYS:HG3	9:O:34:GLU:HG2	1.90	0.53
11:T:330:GLU:HA	11:T:393:GLY:HA2	1.91	0.53
7:K:4805:ILE:HG23	7:K:4809:VAL:HB	1.90	0.52
8:N:31:THR:HG23	8:N:74:TRP:HD1	1.73	0.52
10:R:102:LEU:HB2	10:R:114:TRP:HB2	1.92	0.52
1:A:63:ARG:HH21	5:I:60:DA:H5"	1.74	0.52
10:R:129:SER:OG	10:R:150:ASP:OD2	2.26	0.52
7:K:4710:ARG:HD2	10:R:49:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HB3	2:B:80:THR:HG22	1.93	0.51
10:R:233:THR:OG1	10:R:237:THR:O	2.28	0.51
7:K:4849:HIS:ND1	7:K:4884:TYR:O	2.40	0.51
7:K:4783:LEU:O	7:K:4848:ASN:ND2	2.43	0.51
3:G:32:ARG:NH2	4:H:32:GLU:OE2	2.44	0.51
10:R:295:GLN:HE21	10:R:297:LEU:HD21	1.76	0.50
2:F:39:ARG:NH1	2:F:44:LYS:O	2.41	0.50
2:F:45:ARG:HE	5:I:81:DC:H4'	1.76	0.50
6:J:95:DG:H2'	6:J:96:DT:H71	1.92	0.50
8:N:379:SER:OG	10:R:225:ASN:ND2	2.45	0.50
7:K:4860:VAL:HB	7:K:4869:ILE:HG13	1.94	0.49
8:N:178:LEU:HB3	8:N:183:GLN:HA	1.94	0.49
11:T:347:SER:N	11:T:469:PHE:O	2.43	0.49
8:N:296:GLU:OE1	8:N:314:SER:OG	2.29	0.49
8:N:331:ALA:HB1	10:R:205:CYS:HB3	1.93	0.49
8:N:302:ALA:HB3	8:N:311:ALA:HB3	1.93	0.49
9:O:14:THR:O	9:O:33:LYS:NZ	2.37	0.49
10:R:209:LEU:HD11	10:R:241:TRP:HB3	1.93	0.49
11:T:399:PRO:HD2	11:T:445:SER:HB3	1.94	0.49
7:K:4792:GLU:OE1	7:K:4875:ARG:NE	2.43	0.49
10:R:232:ALA:HA	10:R:238:LEU:HD22	1.93	0.48
11:T:332:THR:N	11:T:481:SER:O	2.45	0.48
7:K:4805:ILE:HD11	7:K:4836:ASP:HB2	1.95	0.48
7:K:4900:HIS:NE2	10:R:150:ASP:OD2	2.47	0.48
8:N:229:GLU:OE2	9:O:72:ARG:NH2	2.44	0.48
10:R:278:SER:H	10:R:304:VAL:HB	1.78	0.48
8:N:217:THR:HG21	8:N:223:ARG:HH11	1.79	0.48
8:N:270:SER:OG	8:N:271:ALA:N	2.47	0.47
7:K:4820:GLN:HE21	10:R:212:ASP:HA	1.79	0.47
11:T:298:LEU:HD13	11:T:316:VAL:HB	1.95	0.47
7:K:4841:GLY:HA2	8:N:339:LEU:HG	1.97	0.47
5:I:135:DA:H2'	5:I:136:DT:H71	1.96	0.47
10:R:186:ILE:O	10:R:198:TRP:N	2.40	0.46
11:T:357:LEU:HG	11:T:365:SER:HB3	1.97	0.46
4:H:30:ARG:HH12	6:J:29:DG:H5'	1.80	0.46
6:J:82:DG:H2'	6:J:83:DT:C6	2.50	0.46
10:R:71:ILE:HB	10:R:80:GLU:HB3	1.98	0.46
11:T:330:GLU:HB2	11:T:483:ASN:HB3	1.96	0.46
11:T:311:LYS:HG2	11:T:476:LYS:HG2	1.97	0.46
7:K:4800:TYR:CZ	7:K:4827:PHE:HB3	2.50	0.46
8:N:217:THR:OG1	8:N:221:ILE:O	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:4759:SER:HB3	7:K:4763:ARG:HH12	1.81	0.46
7:K:4791:ILE:O	7:K:4876:ILE:N	2.49	0.46
8:N:264:GLU:O	8:N:281:LYS:N	2.49	0.46
8:N:377:VAL:HG23	10:R:228:TYR:HB2	1.98	0.46
10:R:286:TRP:HD1	10:R:294:VAL:HG22	1.81	0.46
8:N:313:ILE:HG12	8:N:318:VAL:HG22	1.98	0.45
10:R:186:ILE:HB	10:R:198:TRP:HB2	1.99	0.45
7:K:4803:THR:HB	7:K:4836:ASP:HB3	1.98	0.45
8:N:56:ARG:O	10:R:162:LYS:NZ	2.44	0.45
8:N:282:SER:HB2	9:O:73:LEU:HD22	1.97	0.45
9:O:27:LYS:HB3	9:O:38:PRO:HB3	1.98	0.45
10:R:157:ASP:HB3	10:R:161:GLY:H	1.82	0.45
10:R:279:GLU:HG2	10:R:303:VAL:HG13	1.97	0.45
10:R:41:LEU:HB2	10:R:327:ILE:HB	1.99	0.45
11:T:288:LEU:O	11:T:319:SER:OG	2.32	0.45
10:R:278:SER:OG	10:R:279:GLU:N	2.49	0.45
8:N:307:ARG:NH1	10:R:201:ALA:O	2.50	0.45
7:K:4777:ARG:NH1	10:R:166:THR:O	2.49	0.45
6:J:15:DT:H6	6:J:15:DT:H2'	1.65	0.44
8:N:152:ASP:HB3	8:N:171:ALA:HB3	1.99	0.44
5:I:50:DG:N2	6:J:99:DT:O2	2.50	0.44
11:T:322:VAL:HG21	11:T:327:TRP:CD1	2.51	0.44
8:N:90:VAL:HB	8:N:104:PHE:HB2	1.99	0.44
8:N:166:ILE:HG13	8:N:180:THR:HA	1.98	0.44
8:N:298:LEU:HA	8:N:314:SER:HB3	1.98	0.44
10:R:189:SER:HB3	10:R:220:VAL:HG22	1.99	0.44
8:N:160:ASP:OD1	8:N:164:GLU:N	2.49	0.44
11:T:347:SER:O	11:T:469:PHE:N	2.51	0.44
10:R:175:SER:OG	10:R:189:SER:OG	2.27	0.44
3:G:26:PRO:HG3	3:G:29:ARG:HD3	2.00	0.43
10:R:154:ARG:NH1	10:R:163:CYS:SG	2.91	0.43
5:I:138:DT:H2"	5:I:139:DA:C8	2.53	0.43
10:R:170:HIS:HD2	10:R:174:VAL:HG22	1.83	0.43
10:R:190:SER:OG	10:R:191:TYR:N	2.51	0.43
8:N:371:GLU:N	10:R:249:LEU:O	2.51	0.43
11:T:301:SER:OG	11:T:306:THR:O	2.37	0.43
8:N:70:CYS:SG	8:N:71:SER:N	2.91	0.43
11:T:358:GLY:O	11:T:377:SER:N	2.52	0.43
5:I:145:DG:H2"	5:I:146:DA:C8	2.54	0.43
9:O:1:MET:HB3	9:O:17:VAL:HG23	2.01	0.43
6:J:23:DG:H2"	6:J:24:DT:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:40:GLN:O	9:O:42:ARG:N	2.53	0.42
1:A:50:GLU:HA	1:A:53:ARG:HB3	2.01	0.42
8:N:114:GLN:O	8:N:124:LEU:N	2.48	0.42
1:E:68:GLN:HE21	1:E:72:ARG:HH21	1.68	0.42
6:J:31:DA:H2'	6:J:32:DG:C8	2.55	0.42
8:N:220:ARG:HG2	8:N:253:PRO:HA	2.02	0.42
4:H:119:THR:HA	4:H:122:LYS:HB2	2.02	0.42
8:N:80:LYS:HD2	8:N:92:GLN:HE21	1.84	0.42
11:T:348:GLN:HB2	11:T:362:PHE:HB3	2.02	0.42
11:T:335:GLU:HA	11:T:388:GLN:HG3	2.02	0.42
8:N:136:THR:OG1	8:N:139:ASP:O	2.37	0.41
1:A:68:GLN:HE21	1:A:72:ARG:HH21	1.68	0.41
8:N:300:ASP:HB3	8:N:313:ILE:HD12	2.02	0.41
9:O:6:LYS:N	9:O:67:LEU:O	2.43	0.41
5:I:60:DA:H2"	5:I:61:DA:C8	2.56	0.41
10:R:178:HIS:HB3	10:R:187:VAL:HG12	2.02	0.41
10:R:217:VAL:HA	10:R:232:ALA:HB3	2.03	0.41
10:R:209:LEU:HD21	10:R:241:TRP:CD2	2.56	0.41
10:R:306:SER:HB3	10:R:319:ALA:HB3	2.03	0.41
7:K:4899:CYS:SG	7:K:4900:HIS:N	2.94	0.41
9:O:30:ILE:HA	9:O:33:LYS:HG2	2.03	0.41
11:T:287:VAL:HG13	11:T:320:HIS:HB2	2.03	0.41
11:T:343:ARG:HB3	11:T:365:SER:HB2	2.02	0.41
2:B:47:SER:OG	2:B:48:GLY:N	2.53	0.41
1:E:50:GLU:HA	1:E:53:ARG:HB3	2.02	0.41
10:R:282:LEU:HD13	10:R:296:LYS:HD2	2.03	0.41
5:I:24:DC:H2"	5:I:25:DG:C8	2.56	0.41
7:K:4849:HIS:CE1	7:K:4885:ASP:HA	2.56	0.41
10:R:42:ALA:HB2	10:R:326:THR:HG22	2.02	0.41
10:R:35:TYR:HD2	10:R:295:GLN:HE22	1.69	0.40
1:A:58:THR:HA	2:B:40:ARG:HH22	1.87	0.40
10:R:148:SER:OG	10:R:149:PHE:N	2.55	0.40
10:R:191:TYR:HA	10:R:216:PRO:HA	2.01	0.40
4:D:95:VAL:HG13	4:D:99:LEU:HD12	2.04	0.40
8:N:348:ARG:NH2	8:N:350:SER:OG	2.54	0.40
11:T:301:SER:OG	11:T:303:ASP:OD1	2.34	0.40
6:J:27:DC:H2"	6:J:28:DT:C5	2.57	0.40
7:K:4800:TYR:HB3	7:K:4868:ILE:HB	2.03	0.40
8:N:276:LEU:HB2	8:N:290:LEU:HB2	2.03	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	95/135 (70%)	89 (94%)	6 (6%)	0	100	100
1	E	95/135 (70%)	89 (94%)	6 (6%)	0	100	100
2	B	80/102 (78%)	73 (91%)	7 (9%)	0	100	100
2	F	79/102 (78%)	77 (98%)	2 (2%)	0	100	100
3	C	105/129 (81%)	99 (94%)	6 (6%)	0	100	100
3	G	102/129 (79%)	96 (94%)	6 (6%)	0	100	100
4	D	90/122 (74%)	88 (98%)	2 (2%)	0	100	100
4	H	92/122 (75%)	89 (97%)	3 (3%)	0	100	100
7	K	150/205 (73%)	132 (88%)	18 (12%)	0	100	100
8	N	343/538 (64%)	294 (86%)	49 (14%)	0	100	100
9	O	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
10	R	298/334 (89%)	263 (88%)	35 (12%)	0	100	100
11	T	172/534 (32%)	157 (91%)	15 (9%)	0	100	100
All	All	1775/2663 (67%)	1614 (91%)	161 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	85/110 (77%)	84 (99%)	1 (1%)	74	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	85/110 (77%)	84 (99%)	1 (1%)	74 87
2	B	68/78 (87%)	68 (100%)	0	100 100
2	F	67/78 (86%)	67 (100%)	0	100 100
3	C	84/101 (83%)	84 (100%)	0	100 100
3	G	82/101 (81%)	81 (99%)	1 (1%)	74 87
4	D	79/102 (78%)	79 (100%)	0	100 100
4	H	80/102 (78%)	80 (100%)	0	100 100
7	K	136/182 (75%)	136 (100%)	0	100 100
8	N	304/462 (66%)	299 (98%)	5 (2%)	65 84
9	O	69/69 (100%)	69 (100%)	0	100 100
10	R	262/291 (90%)	262 (100%)	0	100 100
11	T	150/460 (33%)	150 (100%)	0	100 100
All	All	1551/2246 (69%)	1543 (100%)	8 (0%)	90 95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	E	53	ARG
3	G	110	ASN
8	N	34	ARG
8	N	250	ASN
8	N	294	ARG
8	N	324	ASN
8	N	348	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
4	D	81	ASN
1	E	76	GLN
2	F	25	ASN
3	G	110	ASN
4	H	81	ASN
7	K	4794	HIS
7	K	4807	ASN

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Mol	Chain	Res	Type
8	N	246	GLN
8	N	273	GLN
8	N	324	ASN
8	N	328	ASN
10	R	44	HIS
10	R	136	ASN
10	R	295	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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 (i)

There are no chain breaks in this entry.