



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 18, 2018 – 09:33 pm GMT

PDB ID : 4A7N  
EMDB ID: : EMD-1990  
Title : Structure of bare F-actin filaments obtained from the same sample as the Actin-Tropomyosin-Myosin Complex  
Authors : Behrmann, E.; Mueller, M.; Penczek, P.A.; Mannherz, H.G.; Manstein, D.J.; Raunser, S.  
Deposited on : 2011-11-14  
Resolution : 8.90 Å (reported)  
Based on PDB ID : 3MFP

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](mailto: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.

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MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
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) : trunk30686

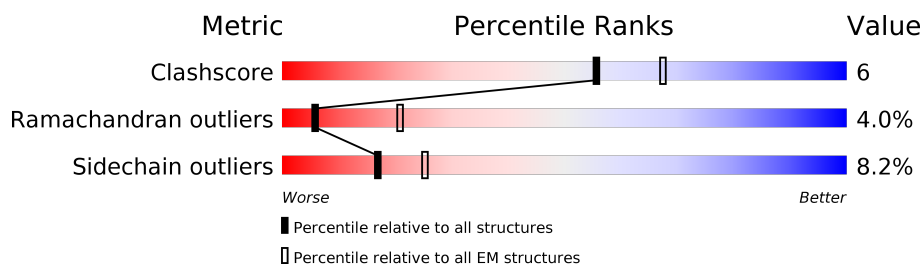
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.90 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	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  $\geq 3$ , 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	375	80% 17% .
1	B	375	80% 17% .
1	C	375	79% 18% .
1	D	375	80% 16% .
1	E	375	79% 18% .

## 2 Entry composition [i](#)

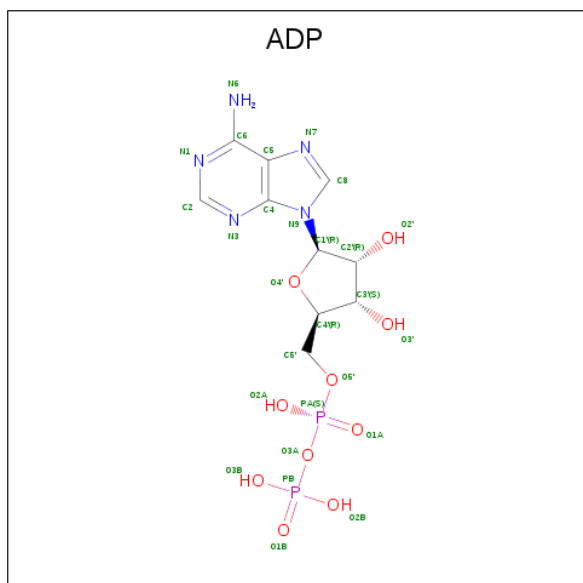
There are 3 unique types of molecules in this entry. The entry contains 14810 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 F-ACTIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

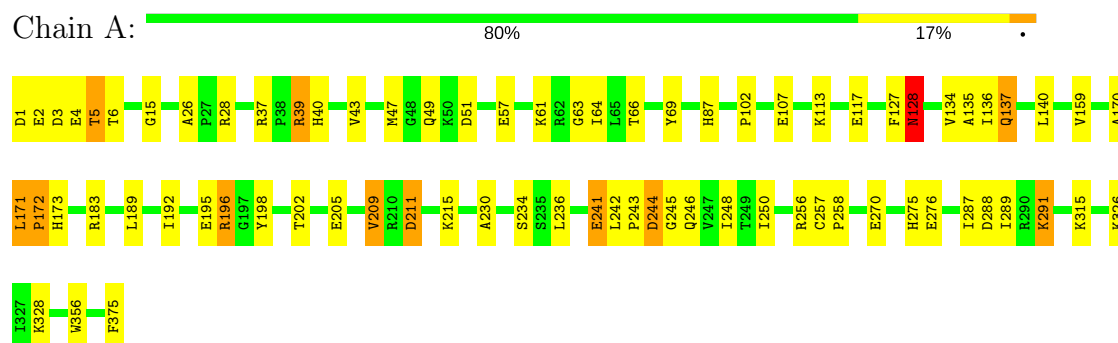
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Ca	0
			1	1	
3	A	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	E	1	Total	Ca	0
			1	1	

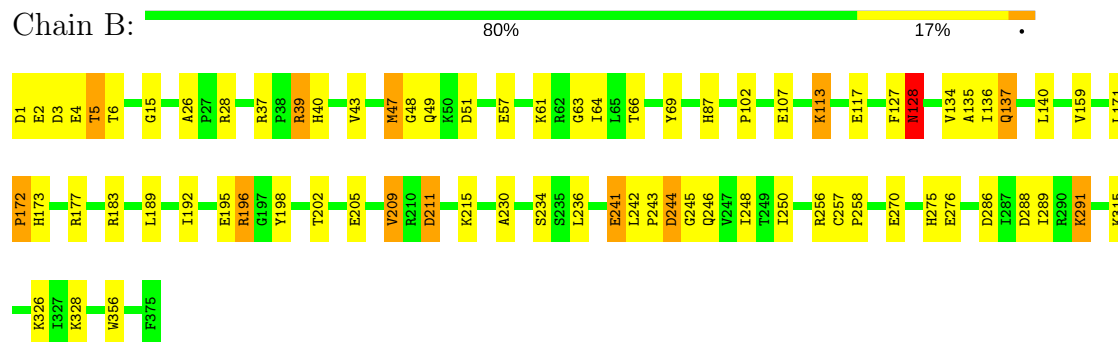
### 3 Residue-property plots

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.

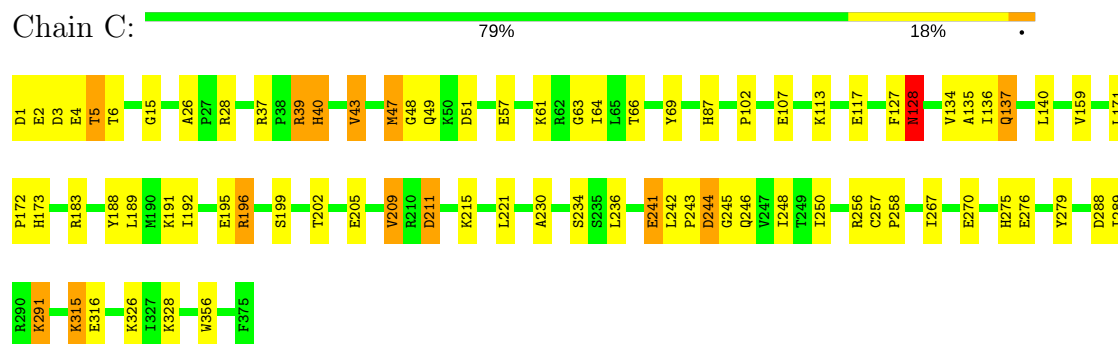
#### • Molecule 1: F-ACTIN



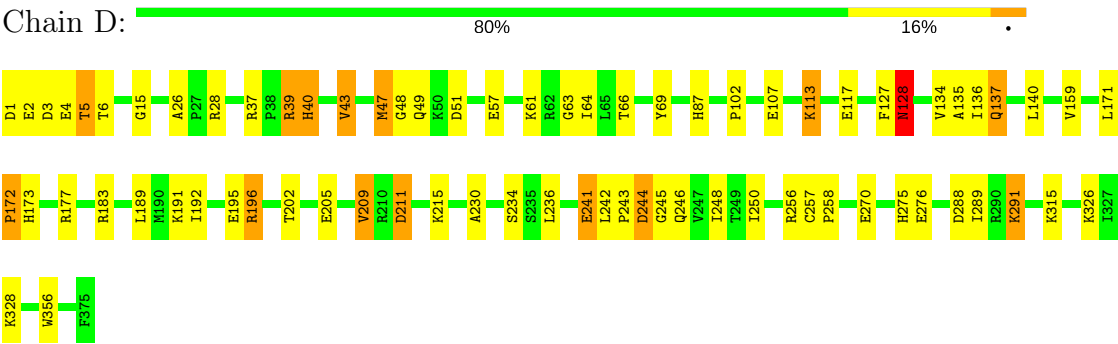
#### • Molecule 1: F-ACTIN



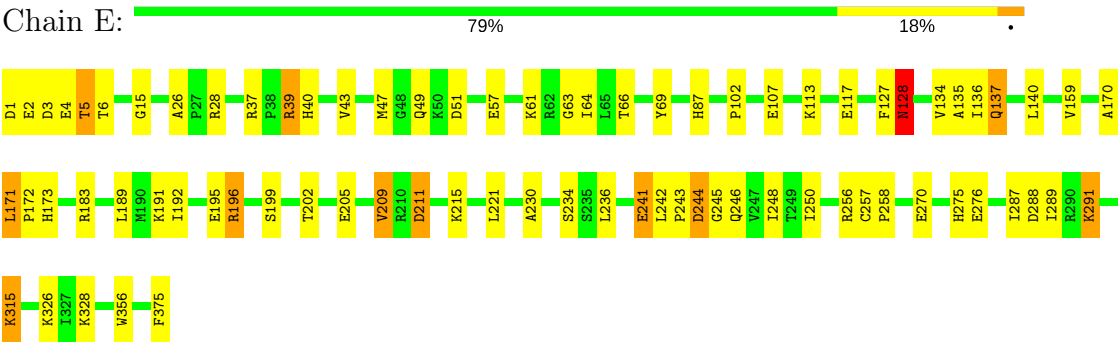
#### • Molecule 1: F-ACTIN



#### • Molecule 1: F-ACTIN



• Molecule 1: F-ACTIN



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of particles used	4626	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	17	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	169644	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	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: CA, HIC, ADP

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	0.21	0/2984	0.37	0/4040
1	B	0.21	0/2984	0.37	0/4040
1	C	0.21	0/2984	0.37	0/4040
1	D	0.21	0/2984	0.37	0/4040
1	E	0.21	0/2984	0.37	0/4040
All	All	0.21	0/14920	0.37	0/20200

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	2934	0	2897	38	0
1	B	2934	0	2897	34	0
1	C	2934	0	2897	41	0
1	D	2934	0	2897	41	0
1	E	2934	0	2897	39	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	27	0	12	0	0
2	E	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
All	All	14810	0	14545	167	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 (167) 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:B:270:GLU:OE2	1:E:39:ARG:NH1	1.87	1.07
1:A:270:GLU:OE2	1:D:39:ARG:NH1	1.89	1.04
1:C:39:ARG:NH1	1:D:270:GLU:OE2	1.94	0.98
1:A:375:PHE:HE1	1:C:43:VAL:HG22	1.30	0.92
1:D:43:VAL:HG22	1:E:375:PHE:HE1	1.46	0.78
1:A:39:ARG:NH1	1:E:270:GLU:OE2	2.18	0.76
1:C:1:ASP:O	1:C:3:ASP:N	2.20	0.75
1:A:1:ASP:O	1:A:3:ASP:N	2.20	0.75
1:B:1:ASP:O	1:B:3:ASP:N	2.20	0.75
1:E:1:ASP:O	1:E:3:ASP:N	2.20	0.73
1:D:1:ASP:O	1:D:3:ASP:N	2.20	0.73
1:A:375:PHE:CE1	1:C:43:VAL:HG22	2.19	0.73
1:A:288:ASP:HA	1:C:244:ASP:OD2	1.92	0.69
1:C:270:GLU:OE1	1:C:270:GLU:N	2.30	0.64
1:A:270:GLU:OE1	1:A:270:GLU:N	2.30	0.64
1:E:270:GLU:OE1	1:E:270:GLU:N	2.30	0.64
1:B:270:GLU:OE1	1:B:270:GLU:N	2.30	0.63
1:D:270:GLU:N	1:D:270:GLU:OE1	2.30	0.62
1:D:288:ASP:OD1	1:D:291:LYS:NZ	2.34	0.61
1:C:288:ASP:OD1	1:C:291:LYS:NZ	2.34	0.61
1:A:288:ASP:OD1	1:A:291:LYS:NZ	2.34	0.60
1:E:288:ASP:OD1	1:E:291:LYS:NZ	2.34	0.60
1:B:288:ASP:OD1	1:B:291:LYS:NZ	2.34	0.60
1:A:171:LEU:HG	1:C:40:HIS:CD2	2.39	0.57
1:E:1:ASP:N	1:E:4:GLU:O	2.30	0.57
1:D:244:ASP:OD2	1:E:288:ASP:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:VAL:HG22	1:E:375:PHE:CE1	2.34	0.56
1:A:1:ASP:N	1:A:4:GLU:O	2.30	0.56
1:C:205:GLU:OE1	1:C:205:GLU:N	2.39	0.56
1:E:205:GLU:OE1	1:E:205:GLU:N	2.39	0.56
1:D:205:GLU:OE1	1:D:205:GLU:N	2.39	0.56
1:B:205:GLU:N	1:B:205:GLU:OE1	2.39	0.56
1:A:205:GLU:OE1	1:A:205:GLU:N	2.39	0.55
1:C:242:LEU:O	1:C:244:ASP:N	2.40	0.55
1:D:242:LEU:O	1:D:244:ASP:N	2.40	0.55
1:B:242:LEU:O	1:B:244:ASP:N	2.40	0.55
1:E:117:GLU:N	1:E:117:GLU:OE1	2.40	0.55
1:B:117:GLU:N	1:B:117:GLU:OE1	2.40	0.55
1:C:1:ASP:N	1:C:4:GLU:O	2.30	0.55
1:A:117:GLU:OE1	1:A:117:GLU:N	2.40	0.55
1:D:117:GLU:OE1	1:D:117:GLU:N	2.40	0.55
1:E:242:LEU:O	1:E:244:ASP:N	2.40	0.55
1:A:242:LEU:O	1:A:244:ASP:N	2.40	0.54
1:C:117:GLU:OE1	1:C:117:GLU:N	2.40	0.54
1:D:57:GLU:OE2	1:D:61:LYS:NZ	2.41	0.54
1:C:57:GLU:OE2	1:C:61:LYS:NZ	2.41	0.54
1:A:57:GLU:OE2	1:A:61:LYS:NZ	2.41	0.53
1:B:172:PRO:HB3	1:E:191:LYS:HD2	1.90	0.53
1:B:57:GLU:OE2	1:B:61:LYS:NZ	2.41	0.53
1:E:57:GLU:OE2	1:E:61:LYS:NZ	2.41	0.53
1:D:107:GLU:HB2	1:D:134:VAL:HG22	1.92	0.52
1:E:107:GLU:HB2	1:E:134:VAL:HG22	1.92	0.52
1:A:287:ILE:O	1:C:244:ASP:OD1	2.27	0.52
1:D:40:HIS:CD2	1:E:171:LEU:HG	2.45	0.52
1:E:37:ARG:NH1	1:E:51:ASP:O	2.43	0.52
1:A:107:GLU:HB2	1:A:134:VAL:HG22	1.92	0.51
1:C:107:GLU:HB2	1:C:134:VAL:HG22	1.92	0.51
1:C:37:ARG:NH1	1:C:51:ASP:O	2.43	0.51
1:D:37:ARG:NH1	1:D:51:ASP:O	2.43	0.51
1:A:170:ALA:HA	1:C:40:HIS:CE1	2.46	0.51
1:A:37:ARG:NH1	1:A:51:ASP:O	2.43	0.51
1:B:37:ARG:NH1	1:B:51:ASP:O	2.43	0.51
1:B:107:GLU:HB2	1:B:134:VAL:HG22	1.92	0.51
1:B:1:ASP:N	1:B:4:GLU:O	2.30	0.50
1:C:275:HIS:NE2	1:C:276:GLU:OE2	2.45	0.50
1:D:1:ASP:N	1:D:4:GLU:O	2.30	0.50
1:E:275:HIS:NE2	1:E:276:GLU:OE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:NE	1:A:196:ARG:O	2.45	0.50
1:B:196:ARG:O	1:B:196:ARG:NE	2.45	0.50
1:D:196:ARG:NE	1:D:196:ARG:O	2.45	0.50
1:D:275:HIS:NE2	1:D:276:GLU:OE2	2.45	0.50
1:E:211:ASP:OD1	1:E:215:LYS:NZ	2.45	0.50
1:A:275:HIS:NE2	1:A:276:GLU:OE2	2.45	0.50
1:B:275:HIS:NE2	1:B:276:GLU:OE2	2.45	0.49
1:C:39:ARG:NH2	1:C:63:GLY:O	2.46	0.49
1:D:39:ARG:NH2	1:D:63:GLY:O	2.46	0.49
1:C:196:ARG:O	1:C:196:ARG:NE	2.45	0.49
1:B:39:ARG:NH2	1:B:63:GLY:O	2.46	0.49
1:C:211:ASP:OD1	1:C:215:LYS:NZ	2.45	0.49
1:A:39:ARG:NH2	1:A:63:GLY:O	2.46	0.49
1:E:39:ARG:NH2	1:E:63:GLY:O	2.46	0.49
1:A:127:PHE:O	1:A:128:ASN:C	2.51	0.49
1:B:211:ASP:OD1	1:B:215:LYS:NZ	2.45	0.48
1:D:127:PHE:O	1:D:128:ASN:C	2.51	0.48
1:B:127:PHE:O	1:B:128:ASN:C	2.51	0.48
1:E:196:ARG:NE	1:E:196:ARG:O	2.45	0.48
1:C:189:LEU:HD23	1:C:209:VAL:HG13	1.95	0.48
1:C:127:PHE:O	1:C:128:ASN:C	2.51	0.48
1:D:244:ASP:OD1	1:E:287:ILE:O	2.31	0.48
1:A:189:LEU:HD23	1:A:209:VAL:HG13	1.95	0.48
1:D:195:GLU:OE2	1:D:256:ARG:NH1	2.47	0.48
1:A:205:GLU:HB3	1:B:286:ASP:OD1	2.14	0.48
1:E:127:PHE:O	1:E:128:ASN:C	2.51	0.48
1:A:195:GLU:OE2	1:A:256:ARG:NH1	2.47	0.48
1:E:195:GLU:OE2	1:E:256:ARG:NH1	2.47	0.48
1:B:195:GLU:OE2	1:B:256:ARG:NH1	2.47	0.47
1:C:195:GLU:OE2	1:C:256:ARG:NH1	2.47	0.47
1:D:189:LEU:HD23	1:D:209:VAL:HG13	1.95	0.47
1:D:211:ASP:OD1	1:D:215:LYS:NZ	2.45	0.47
1:E:189:LEU:HD23	1:E:209:VAL:HG13	1.95	0.47
1:B:189:LEU:HD23	1:B:209:VAL:HG13	1.95	0.47
1:A:248:ILE:HG22	1:A:250:ILE:HG23	1.98	0.46
1:B:177:ARG:NH2	1:E:199:SER:OG	2.49	0.46
1:A:211:ASP:OD1	1:A:215:LYS:NZ	2.45	0.46
1:C:248:ILE:HG22	1:C:250:ILE:HG23	1.98	0.46
1:C:199:SER:OG	1:D:177:ARG:NH2	2.48	0.46
1:B:248:ILE:HG22	1:B:250:ILE:HG23	1.98	0.46
1:E:230:ALA:HA	1:E:236:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:ILE:HG22	1:E:250:ILE:HG23	1.98	0.45
1:B:64:ILE:HG22	1:B:64:ILE:O	2.17	0.45
1:C:47:MET:SD	1:C:48:GLY:N	2.80	0.45
1:E:64:ILE:O	1:E:64:ILE:HG22	2.17	0.45
1:D:47:MET:SD	1:D:48:GLY:N	2.80	0.45
1:E:221:LEU:O	1:E:315:LYS:NZ	2.36	0.45
1:B:230:ALA:HA	1:B:236:LEU:HD22	1.98	0.45
1:A:230:ALA:HA	1:A:236:LEU:HD22	1.98	0.45
1:C:221:LEU:O	1:C:315:LYS:NZ	2.36	0.45
1:C:257:CYS:HB3	1:C:258:PRO:HD3	1.99	0.45
1:C:64:ILE:O	1:C:64:ILE:HG22	2.17	0.45
1:D:248:ILE:HG22	1:D:250:ILE:HG23	1.98	0.45
1:D:136:ILE:HD12	1:D:136:ILE:N	2.32	0.45
1:C:230:ALA:HA	1:C:236:LEU:HD22	1.98	0.45
1:A:136:ILE:HD12	1:A:136:ILE:N	2.32	0.45
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.99	0.45
1:D:230:ALA:HA	1:D:236:LEU:HD22	1.98	0.45
1:B:136:ILE:N	1:B:136:ILE:HD12	2.32	0.44
1:A:64:ILE:HG22	1:A:64:ILE:O	2.17	0.44
1:E:257:CYS:HB3	1:E:258:PRO:HD3	1.99	0.44
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.99	0.44
1:E:136:ILE:N	1:E:136:ILE:HD12	2.32	0.44
1:C:136:ILE:HD12	1:C:136:ILE:N	2.32	0.44
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.99	0.44
1:D:64:ILE:HG22	1:D:64:ILE:O	2.17	0.43
1:B:47:MET:SD	1:B:48:GLY:N	2.80	0.43
1:A:172:PRO:HB3	1:D:191:LYS:HD2	1.99	0.43
1:C:195:GLU:O	1:D:113:LYS:N	2.49	0.43
1:D:40:HIS:CE1	1:E:170:ALA:HA	2.54	0.42
1:C:279:TYR:OH	1:C:316:GLU:O	2.30	0.42
1:B:107:GLU:N	1:B:135:ALA:O	2.53	0.42
1:D:136:ILE:O	1:D:137:GLN:C	2.58	0.42
1:B:136:ILE:O	1:B:137:GLN:C	2.58	0.42
1:C:136:ILE:O	1:C:137:GLN:C	2.58	0.42
1:A:136:ILE:O	1:A:137:GLN:C	2.58	0.41
1:A:26:ALA:O	1:A:28:ARG:NH1	2.53	0.41
1:B:26:ALA:O	1:B:28:ARG:NH1	2.53	0.41
1:A:171:LEU:HD23	1:C:40:HIS:HA	2.01	0.41
1:C:191:LYS:HD2	1:D:172:PRO:HB3	2.01	0.41
1:C:26:ALA:O	1:C:28:ARG:NH1	2.53	0.41
1:E:107:GLU:N	1:E:135:ALA:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ALA:HB1	1:A:140:LEU:HD11	2.02	0.41
1:C:135:ALA:HB1	1:C:140:LEU:HD11	2.02	0.41
1:D:26:ALA:O	1:D:28:ARG:NH1	2.53	0.41
1:E:136:ILE:O	1:E:137:GLN:C	2.58	0.41
1:C:107:GLU:N	1:C:135:ALA:O	2.53	0.41
1:D:135:ALA:HB1	1:D:140:LEU:HD11	2.02	0.41
1:E:26:ALA:O	1:E:28:ARG:NH1	2.53	0.41
1:E:135:ALA:HB1	1:E:140:LEU:HD11	2.02	0.41
1:B:135:ALA:HB1	1:B:140:LEU:HD11	2.02	0.41
1:B:113:LYS:N	1:E:195:GLU:O	2.52	0.41
1:A:107:GLU:N	1:A:135:ALA:O	2.53	0.41
1:D:107:GLU:N	1:D:135:ALA:O	2.53	0.41
1:D:40:HIS:HA	1:E:171:LEU:HD23	2.03	0.41
1:B:134:VAL:O	1:B:134:VAL:HG13	2.22	0.40
1:A:196:ARG:HD3	1:A:198:TYR:CE2	2.56	0.40
1:B:196:ARG:HD3	1:B:198:TYR:CE2	2.56	0.40
1:D:134:VAL:HG13	1:D:134:VAL:O	2.22	0.40
1:C:188:TYR:CE1	1:C:267:ILE:HG12	2.57	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	371/375 (99%)	305 (82%)	51 (14%)	15 (4%)	3	29
1	B	371/375 (99%)	305 (82%)	51 (14%)	15 (4%)	3	29
1	C	371/375 (99%)	305 (82%)	51 (14%)	15 (4%)	3	29
1	D	371/375 (99%)	304 (82%)	52 (14%)	15 (4%)	3	29
1	E	371/375 (99%)	305 (82%)	51 (14%)	15 (4%)	3	29
All	All	1855/1875 (99%)	1524 (82%)	256 (14%)	75 (4%)	6	29

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	137	GLN
1	B	2	GLU
1	B	137	GLN
1	C	2	GLU
1	C	137	GLN
1	D	2	GLU
1	D	137	GLN
1	E	2	GLU
1	E	137	GLN
1	A	5	THR
1	A	128	ASN
1	A	245	GLY
1	B	5	THR
1	B	128	ASN
1	B	245	GLY
1	C	5	THR
1	C	128	ASN
1	C	245	GLY
1	D	5	THR
1	D	128	ASN
1	D	245	GLY
1	E	5	THR
1	E	128	ASN
1	E	245	GLY
1	A	6	THR
1	A	173	HIS
1	A	234	SER
1	A	244	ASP
1	B	6	THR
1	B	173	HIS
1	B	234	SER
1	B	244	ASP
1	C	6	THR
1	C	173	HIS
1	C	234	SER
1	C	244	ASP
1	D	6	THR
1	D	173	HIS
1	D	234	SER
1	D	244	ASP
1	E	6	THR

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Mol	Chain	Res	Type
1	E	173	HIS
1	E	234	SER
1	E	244	ASP
1	A	172	PRO
1	B	172	PRO
1	C	172	PRO
1	D	172	PRO
1	E	172	PRO
1	A	15	GLY
1	A	241	GLU
1	B	15	GLY
1	B	241	GLU
1	C	15	GLY
1	C	241	GLU
1	D	15	GLY
1	D	241	GLU
1	E	15	GLY
1	E	241	GLU
1	A	102	PRO
1	A	243	PRO
1	B	102	PRO
1	B	243	PRO
1	C	102	PRO
1	C	243	PRO
1	D	102	PRO
1	D	243	PRO
1	E	102	PRO
1	E	243	PRO
1	A	289	ILE
1	B	289	ILE
1	C	289	ILE
1	D	289	ILE
1	E	289	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	317/317 (100%)	291 (92%)	26 (8%)	12	41
1	B	317/317 (100%)	291 (92%)	26 (8%)	12	41
1	C	317/317 (100%)	291 (92%)	26 (8%)	12	41
1	D	317/317 (100%)	291 (92%)	26 (8%)	12	41
1	E	317/317 (100%)	291 (92%)	26 (8%)	12	41
All	All	1585/1585 (100%)	1455 (92%)	130 (8%)	17	41

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	39	ARG
1	A	40	HIS
1	A	43	VAL
1	A	47	MET
1	A	49	GLN
1	A	66	THR
1	A	69	TYR
1	A	87	HIS
1	A	113	LYS
1	A	128	ASN
1	A	159	VAL
1	A	171	LEU
1	A	183	ARG
1	A	192	ILE
1	A	196	ARG
1	A	202	THR
1	A	209	VAL
1	A	211	ASP
1	A	241	GLU
1	A	246	GLN
1	A	291	LYS
1	A	315	LYS
1	A	326	LYS
1	A	328	LYS
1	A	356	TRP
1	B	5	THR
1	B	39	ARG
1	B	40	HIS
1	B	43	VAL
1	B	47	MET

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Mol	Chain	Res	Type
1	B	49	GLN
1	B	66	THR
1	B	69	TYR
1	B	87	HIS
1	B	113	LYS
1	B	128	ASN
1	B	159	VAL
1	B	171	LEU
1	B	183	ARG
1	B	192	ILE
1	B	196	ARG
1	B	202	THR
1	B	209	VAL
1	B	211	ASP
1	B	241	GLU
1	B	246	GLN
1	B	291	LYS
1	B	315	LYS
1	B	326	LYS
1	B	328	LYS
1	B	356	TRP
1	C	5	THR
1	C	39	ARG
1	C	40	HIS
1	C	43	VAL
1	C	47	MET
1	C	49	GLN
1	C	66	THR
1	C	69	TYR
1	C	87	HIS
1	C	113	LYS
1	C	128	ASN
1	C	159	VAL
1	C	171	LEU
1	C	183	ARG
1	C	192	ILE
1	C	196	ARG
1	C	202	THR
1	C	209	VAL
1	C	211	ASP
1	C	241	GLU
1	C	246	GLN

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Mol	Chain	Res	Type
1	C	291	LYS
1	C	315	LYS
1	C	326	LYS
1	C	328	LYS
1	C	356	TRP
1	D	5	THR
1	D	39	ARG
1	D	40	HIS
1	D	43	VAL
1	D	47	MET
1	D	49	GLN
1	D	66	THR
1	D	69	TYR
1	D	87	HIS
1	D	113	LYS
1	D	128	ASN
1	D	159	VAL
1	D	171	LEU
1	D	183	ARG
1	D	192	ILE
1	D	196	ARG
1	D	202	THR
1	D	209	VAL
1	D	211	ASP
1	D	241	GLU
1	D	246	GLN
1	D	291	LYS
1	D	315	LYS
1	D	326	LYS
1	D	328	LYS
1	D	356	TRP
1	E	5	THR
1	E	39	ARG
1	E	40	HIS
1	E	43	VAL
1	E	47	MET
1	E	49	GLN
1	E	66	THR
1	E	69	TYR
1	E	87	HIS
1	E	113	LYS
1	E	128	ASN

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Mol	Chain	Res	Type
1	E	159	VAL
1	E	171	LEU
1	E	183	ARG
1	E	192	ILE
1	E	196	ARG
1	E	202	THR
1	E	209	VAL
1	E	211	ASP
1	E	241	GLU
1	E	246	GLN
1	E	291	LYS
1	E	315	LYS
1	E	326	LYS
1	E	328	LYS
1	E	356	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	225	ASN
1	A	314	GLN
1	A	353	GLN
1	B	137	GLN
1	B	225	ASN
1	B	314	GLN
1	B	353	GLN
1	C	40	HIS
1	C	137	GLN
1	C	225	ASN
1	C	314	GLN
1	C	353	GLN
1	D	40	HIS
1	D	137	GLN
1	D	225	ASN
1	D	314	GLN
1	D	353	GLN
1	E	137	GLN
1	E	225	ASN
1	E	314	GLN
1	E	353	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HIC	A	73	1	10,11,12	2.64	3 (30%)	7,14,16	1.90	3 (42%)
1	HIC	B	73	1	10,11,12	2.64	3 (30%)	7,14,16	1.90	3 (42%)
1	HIC	C	73	1	10,11,12	2.64	3 (30%)	7,14,16	1.89	3 (42%)
1	HIC	D	73	1	10,11,12	2.63	3 (30%)	7,14,16	1.89	3 (42%)
1	HIC	E	73	1	10,11,12	2.65	3 (30%)	7,14,16	1.89	3 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HIC	A	73	1	-	0/4/6/8	0/1/1/1
1	HIC	B	73	1	-	0/4/6/8	0/1/1/1
1	HIC	C	73	1	-	0/4/6/8	0/1/1/1
1	HIC	D	73	1	-	0/4/6/8	0/1/1/1
1	HIC	E	73	1	-	0/4/6/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	HIC	CD2-CG	2.30	1.39	1.36
1	A	73	HIC	CD2-CG	2.33	1.39	1.36
1	C	73	HIC	CD2-CG	2.35	1.39	1.36
1	E	73	HIC	CD2-CG	2.35	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	HIC	CD2-CG	2.37	1.39	1.36
1	A	73	HIC	CE1-NE2	3.40	1.40	1.36
1	D	73	HIC	CE1-NE2	3.40	1.40	1.36
1	C	73	HIC	CE1-NE2	3.41	1.41	1.36
1	E	73	HIC	CE1-NE2	3.42	1.41	1.36
1	B	73	HIC	CE1-NE2	3.46	1.41	1.36
1	B	73	HIC	CA-C	6.70	1.59	1.50
1	C	73	HIC	CA-C	6.71	1.59	1.50
1	D	73	HIC	CA-C	6.72	1.59	1.50
1	A	73	HIC	CA-C	6.72	1.59	1.50
1	E	73	HIC	CA-C	6.75	1.59	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	73	HIC	CB-CA-C	-3.60	104.47	111.41
1	B	73	HIC	CB-CA-C	-3.60	104.48	111.41
1	A	73	HIC	CB-CA-C	-3.60	104.48	111.41
1	D	73	HIC	CB-CA-C	-3.58	104.51	111.41
1	C	73	HIC	CB-CA-C	-3.58	104.51	111.41
1	B	73	HIC	O-C-CA	-2.58	117.88	124.96
1	A	73	HIC	O-C-CA	-2.58	117.88	124.96
1	E	73	HIC	O-C-CA	-2.58	117.88	124.96
1	D	73	HIC	O-C-CA	-2.57	117.89	124.96
1	C	73	HIC	O-C-CA	-2.57	117.90	124.96
1	C	73	HIC	CG-CD2-NE2	-2.36	105.22	107.78
1	A	73	HIC	CG-CD2-NE2	-2.36	105.22	107.78
1	B	73	HIC	CG-CD2-NE2	-2.36	105.22	107.78
1	D	73	HIC	CG-CD2-NE2	-2.33	105.25	107.78
1	E	73	HIC	CG-CD2-NE2	-2.32	105.26	107.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	A	376	-	25,29,29	1.09	1 (4%)	25,45,45	1.61	4 (16%)
2	ADP	B	376	-	25,29,29	1.09	1 (4%)	25,45,45	1.62	4 (16%)
2	ADP	C	376	-	25,29,29	1.09	1 (4%)	25,45,45	1.62	4 (16%)
2	ADP	D	376	-	25,29,29	1.08	1 (4%)	25,45,45	1.62	4 (16%)
2	ADP	E	376	-	25,29,29	1.08	1 (4%)	25,45,45	1.61	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	376	-	-	0/12/32/32	0/3/3/3
2	ADP	B	376	-	-	0/12/32/32	0/3/3/3
2	ADP	C	376	-	-	0/12/32/32	0/3/3/3
2	ADP	D	376	-	-	0/12/32/32	0/3/3/3
2	ADP	E	376	-	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	376	ADP	C2-N1	2.94	1.39	1.33
2	E	376	ADP	C2-N1	2.94	1.39	1.33
2	B	376	ADP	C2-N1	2.95	1.39	1.33
2	A	376	ADP	C2-N1	2.96	1.39	1.33
2	C	376	ADP	C2-N1	2.97	1.39	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	376	ADP	N3-C2-N1	-4.28	125.20	128.86
2	C	376	ADP	N3-C2-N1	-4.25	125.22	128.86
2	D	376	ADP	N3-C2-N1	-4.24	125.23	128.86
2	A	376	ADP	N3-C2-N1	-4.23	125.24	128.86
2	E	376	ADP	N3-C2-N1	-4.17	125.30	128.86
2	A	376	ADP	O3B-PB-O2B	2.03	115.60	107.59
2	C	376	ADP	O3B-PB-O2B	2.04	115.65	107.59
2	D	376	ADP	O3B-PB-O2B	2.04	115.66	107.59
2	E	376	ADP	O3B-PB-O2B	2.04	115.66	107.59
2	B	376	ADP	O3B-PB-O2B	2.05	115.69	107.59
2	D	376	ADP	C2-N1-C6	2.19	122.47	118.75
2	E	376	ADP	C2-N1-C6	2.20	122.50	118.75
2	A	376	ADP	C2-N1-C6	2.22	122.52	118.75
2	B	376	ADP	C2-N1-C6	2.22	122.52	118.75
2	C	376	ADP	C2-N1-C6	2.22	122.53	118.75
2	A	376	ADP	C4-C5-N7	4.17	113.44	109.41
2	D	376	ADP	C4-C5-N7	4.19	113.45	109.41
2	B	376	ADP	C4-C5-N7	4.20	113.47	109.41
2	C	376	ADP	C4-C5-N7	4.21	113.47	109.41
2	E	376	ADP	C4-C5-N7	4.22	113.49	109.41

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1
1	D	1
1	C	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	72:GLU	C	73:HIC	N	3.48
1	B	72:GLU	C	73:HIC	N	3.48
1	C	72:GLU	C	73:HIC	N	3.48
1	D	72:GLU	C	73:HIC	N	3.48
1	E	72:GLU	C	73:HIC	N	3.48