



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 30, 2017 – 05:36 AM EDT

PDB ID : 5NOJ
EMDB ID: : EMD-3666
Title : Ca²⁺-induced Movement of Tropomyosin on Native Cardiac Thin Filaments
- "OPEN" state
Authors : Risi, C.; Eisner, J.; Belknap, B.; Heeley, D.H.; White, H.D.; Schroeder, G.F.;
Galkin, V.E.
Deposited on : unknown
Resolution : 11.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

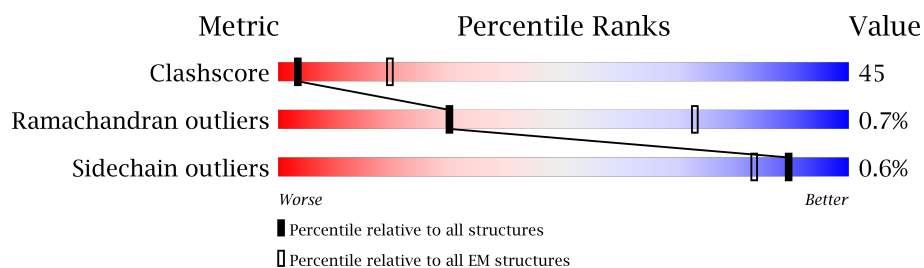
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.00 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	367	
1	B	367	
1	C	367	
1	D	367	
1	E	367	
2	F	136	
2	H	136	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16077 atoms, of which 270 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	367	Total	C	N	O	S	0	0
			2861	1813	481	548	19		
1	B	367	Total	C	N	O	S	0	0
			2861	1813	481	548	19		
1	C	367	Total	C	N	O	S	0	0
			2861	1813	481	548	19		
1	D	367	Total	C	N	O	S	0	0
			2861	1813	481	548	19		
1	E	367	Total	C	N	O	S	0	0
			2861	1813	481	548	19		

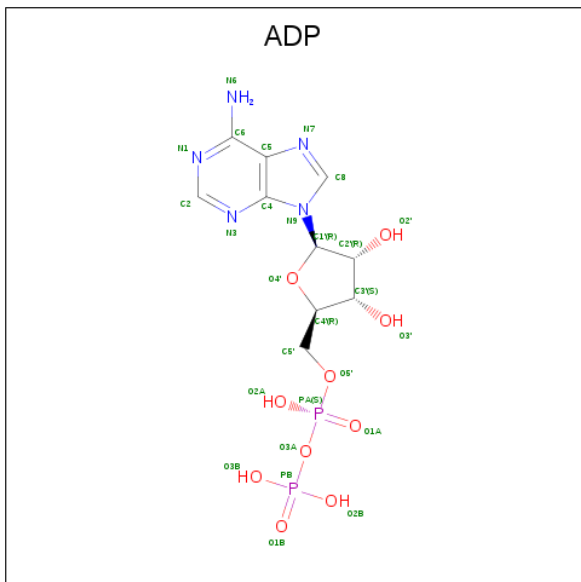
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299	LEU	MET	conflict	UNP P68137
A	358	SER	THR	conflict	UNP P68137
B	299	LEU	MET	conflict	UNP P68137
B	358	SER	THR	conflict	UNP P68137
C	299	LEU	MET	conflict	UNP P68137
C	358	SER	THR	conflict	UNP P68137
D	299	LEU	MET	conflict	UNP P68137
D	358	SER	THR	conflict	UNP P68137
E	299	LEU	MET	conflict	UNP P68137
E	358	SER	THR	conflict	UNP P68137

- Molecule 2 is a protein called cardiac alpha tropomyosin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	136	Total	C	H	N	O	0	0
			816	408	135	136	137		
2	H	136	Total	C	H	N	O	0	0
			816	408	135	136	137		

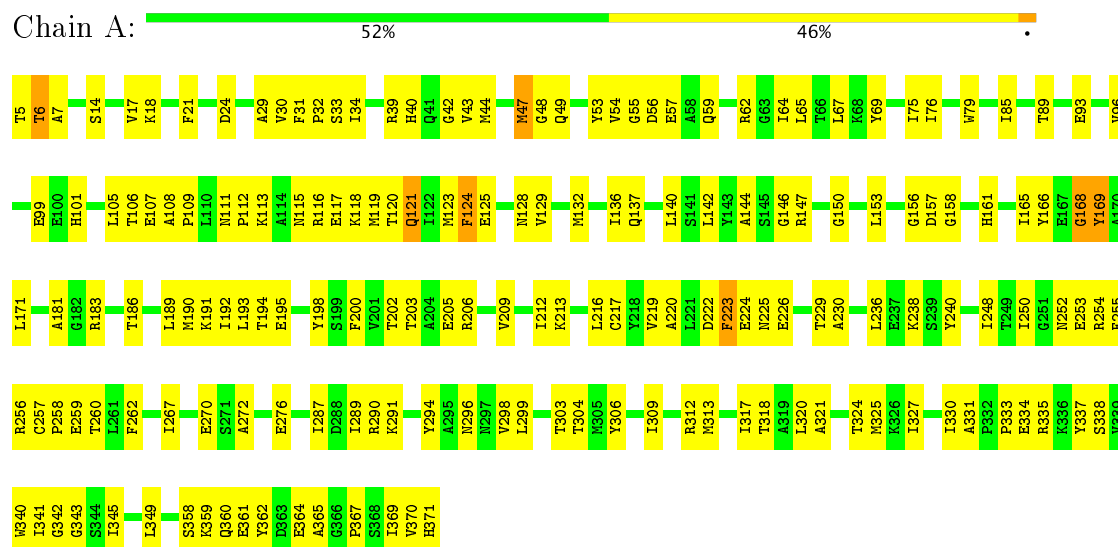
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



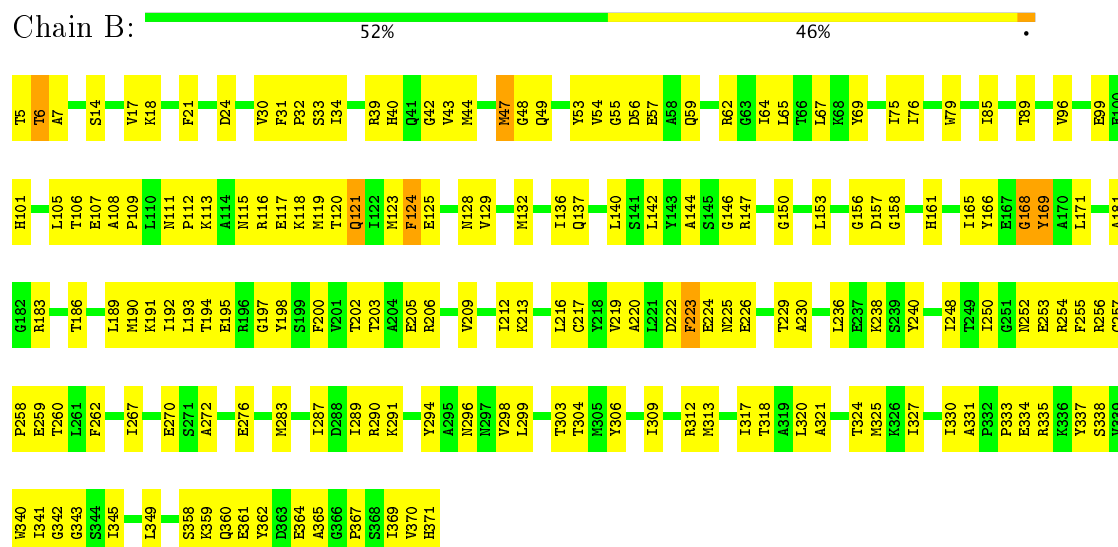
3 Residue-property plots

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.

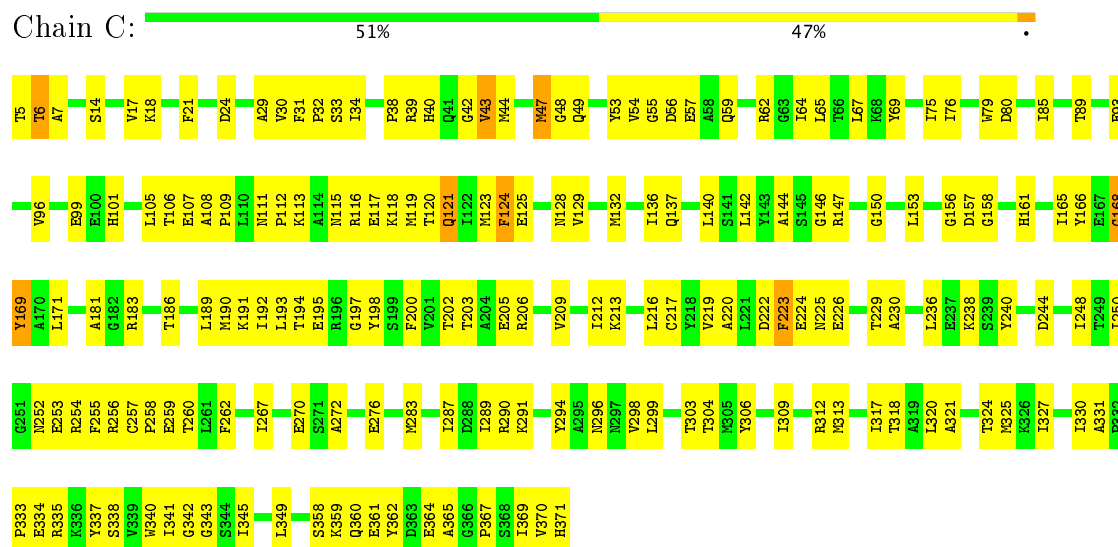
- Molecule 1: Actin, alpha skeletal muscle



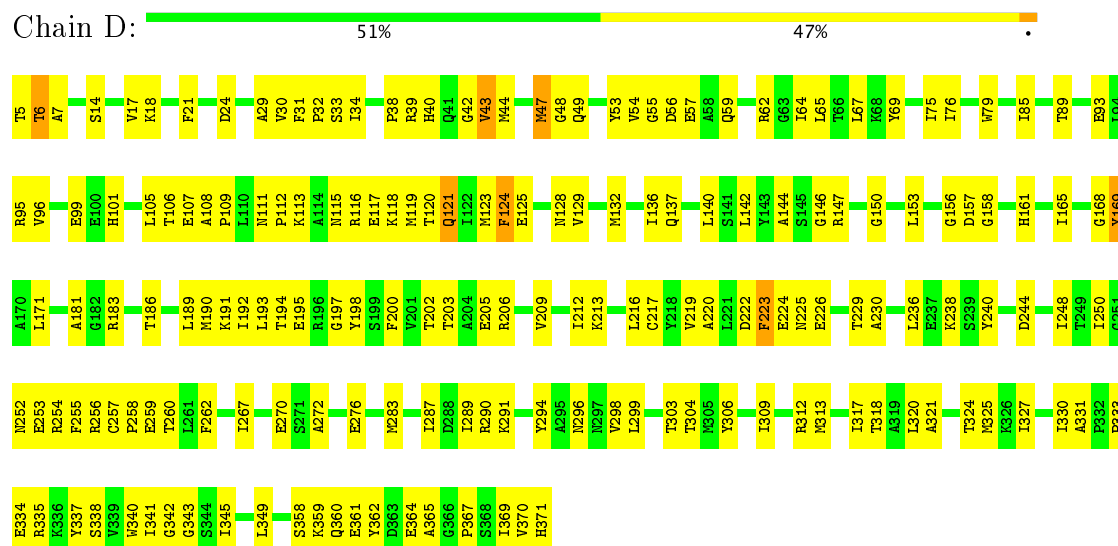
- Molecule 1: Actin, alpha skeletal muscle



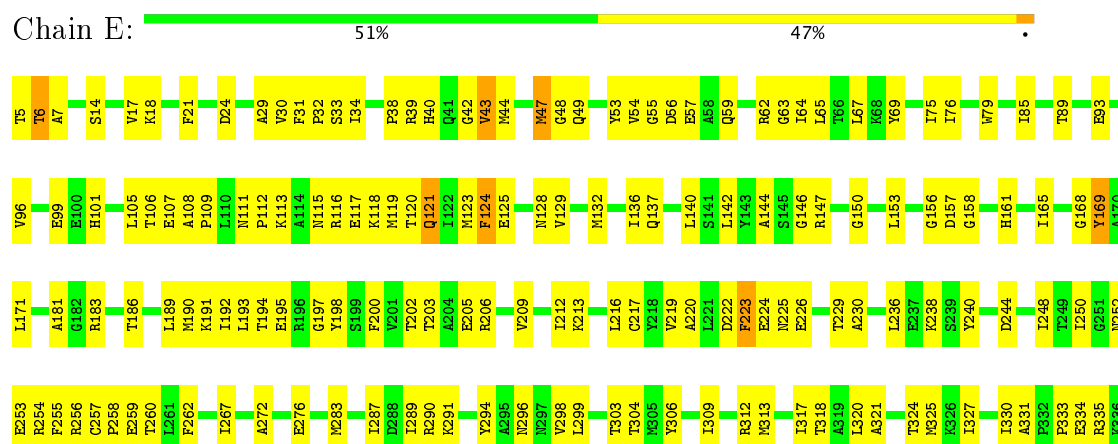
- Molecule 1: Actin, alpha skeletal muscle

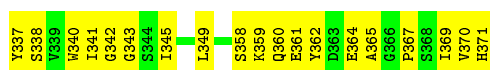


- Molecule 1: Actin, alpha skeletal muscle



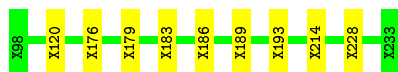
- Molecule 1: Actin, alpha skeletal muscle





- Molecule 2: cardiac alpha tropomyosin

Chain F: 93% 7%



- Molecule 2: cardiac alpha tropomyosin

Chain H: 93% 7%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.7°, rise=27.4 Å, axial sym=C1	Depositor
Number of segments used	3809	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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: MG, 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	0.37	2/2910 (0.1%)	0.52	0/3944
1	B	0.37	2/2910 (0.1%)	0.52	0/3944
1	C	0.37	2/2910 (0.1%)	0.52	0/3944
1	D	0.37	2/2910 (0.1%)	0.52	0/3944
1	E	0.37	2/2910 (0.1%)	0.52	0/3944
All	All	0.37	10/14550 (0.1%)	0.52	0/19720

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	1
1	E	0	1
All	All	0	8

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	PHE	CE2-CZ	6.66	1.50	1.37
1	C	124	PHE	CE2-CZ	6.64	1.50	1.37
1	B	124	PHE	CE2-CZ	6.63	1.50	1.37
1	D	124	PHE	CE2-CZ	6.61	1.50	1.37
1	E	124	PHE	CE2-CZ	6.59	1.49	1.37

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	GLY	Peptide
1	A	5	THR	Peptide
1	B	168	GLY	Peptide
1	B	5	THR	Peptide
1	C	5	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2861	0	2832	272	0
1	B	2861	0	2832	278	0
1	C	2861	0	2832	293	0
1	D	2861	0	2832	276	0
1	E	2861	0	2832	270	0
2	F	681	135	138	19	0
2	H	681	135	138	19	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	15807	270	14496	1355	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 45.

The worst 5 of 1355 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:124:PHE:HB3	1:B:359:LYS:NZ	1.58	1.19
1:D:124:PHE:HB3	1:D:359:LYS:NZ	1.58	1.19
1:E:124:PHE:HB3	1:E:359:LYS:NZ	1.58	1.18
1:A:124:PHE:HB3	1:A:359:LYS:NZ	1.58	1.18
1:D:365:ALA:HB1	1:D:369:ILE:HG12	1.18	1.18

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	364/367 (99%)	349 (96%)	13 (4%)	2 (0%)	32	74
1	B	364/367 (99%)	349 (96%)	13 (4%)	2 (0%)	32	74
1	C	364/367 (99%)	349 (96%)	12 (3%)	3 (1%)	22	67
1	D	364/367 (99%)	349 (96%)	12 (3%)	3 (1%)	22	67
1	E	364/367 (99%)	349 (96%)	12 (3%)	3 (1%)	22	67
All	All	1820/1835 (99%)	1745 (96%)	62 (3%)	13 (1%)	30	68

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	TYR
1	B	169	TYR
1	C	169	TYR
1	D	169	TYR
1	E	169	TYR

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	309/309 (100%)	307 (99%)	2 (1%)	89	94
1	B	309/309 (100%)	307 (99%)	2 (1%)	89	94
1	C	309/309 (100%)	307 (99%)	2 (1%)	89	94
1	D	309/309 (100%)	307 (99%)	2 (1%)	89	94
1	E	309/309 (100%)	307 (99%)	2 (1%)	89	94
All	All	1545/1545 (100%)	1535 (99%)	10 (1%)	89	94

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	47	MET
1	C	121	GLN
1	D	121	GLN
1	B	121	GLN
1	D	47	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	92	ASN
1	C	314	GLN
1	E	115	ASN
1	C	101	HIS
1	C	115	ASN

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	9,11,12	0.97	1 (11%)	7,14,16	1.04	0
1	HIC	B	73	1	9,11,12	0.96	1 (11%)	7,14,16	1.05	0
1	HIC	C	73	1	9,11,12	0.97	1 (11%)	7,14,16	1.05	0
1	HIC	D	73	1	9,11,12	0.95	1 (11%)	7,14,16	1.04	0
1	HIC	E	73	1	9,11,12	0.96	1 (11%)	7,14,16	1.04	0

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	73	HIC	CA-C	2.29	1.53	1.50
1	D	73	HIC	CA-C	2.31	1.53	1.50
1	C	73	HIC	CA-C	2.31	1.53	1.50
1	A	73	HIC	CA-C	2.33	1.53	1.50
1	B	73	HIC	CA-C	2.33	1.53	1.50

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.

5.5 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
3	ADP	A	401	4	25,29,29	0.97	1 (4%)	24,45,45	1.64	2 (8%)
3	ADP	B	401	4	25,29,29	0.97	1 (4%)	24,45,45	1.64	2 (8%)
3	ADP	C	401	4	25,29,29	0.97	1 (4%)	24,45,45	1.64	2 (8%)
3	ADP	D	401	4	25,29,29	0.97	1 (4%)	24,45,45	1.62	2 (8%)
3	ADP	E	401	4	25,29,29	0.97	1 (4%)	24,45,45	1.64	2 (8%)

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
3	ADP	A	401	4	-	0/12/32/32	0/3/3/3
3	ADP	B	401	4	-	0/12/32/32	0/3/3/3
3	ADP	C	401	4	-	0/12/32/32	0/3/3/3
3	ADP	D	401	4	-	0/12/32/32	0/3/3/3
3	ADP	E	401	4	-	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)
3	B	401	ADP	C5-C4	3.11	1.47	1.40
3	C	401	ADP	C5-C4	3.11	1.47	1.40
3	A	401	ADP	C5-C4	3.12	1.47	1.40
3	E	401	ADP	C5-C4	3.13	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	ADP	C5-C4	3.14	1.47	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	N3-C2-N1	-5.94	123.68	128.86
3	C	401	ADP	N3-C2-N1	-5.93	123.69	128.86
3	E	401	ADP	N3-C2-N1	-5.92	123.70	128.86
3	B	401	ADP	N3-C2-N1	-5.91	123.71	128.86
3	D	401	ADP	N3-C2-N1	-5.83	123.78	128.86

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.