wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:51 PM BST

PDB ID	:	3J8A
EMDB ID:	:	EMD-6124
Title	:	Structure of the F-actin-tropomyosin complex
Authors	:	von der Ecken, J.; Mueller, M.; Lehman, W.; Manstein, J.M.; Penczek, A.P.; Raunser, S.
Deposited on	:	2014-10-08
Resolution	:	3.70 Å(reported)
Based on PDB ID	:	4A7N

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

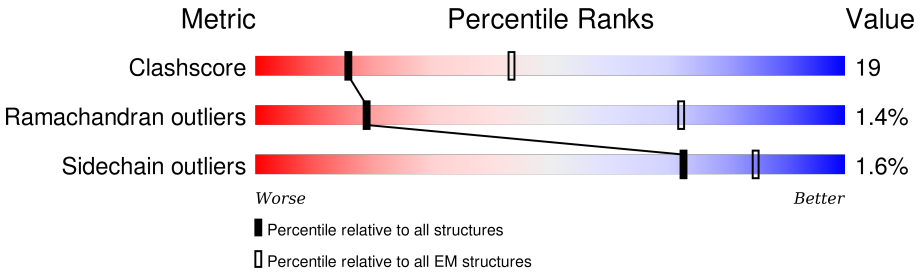
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 3.70 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	F	135	99% ·
1	G	135	99% ·
2	A	375	59% 38% · ·
2	B	375	57% 40% · ·
2	C	375	57% 40% · ·
2	D	375	57% 39% · ·
2	E	375	55% 42% · ·

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15800 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 tropomyosin alpha-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	F	135	Total 675	C 405	N 135	O 135	0	0
1	G	135	Total 675	C 405	N 135	O 135	0	0

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

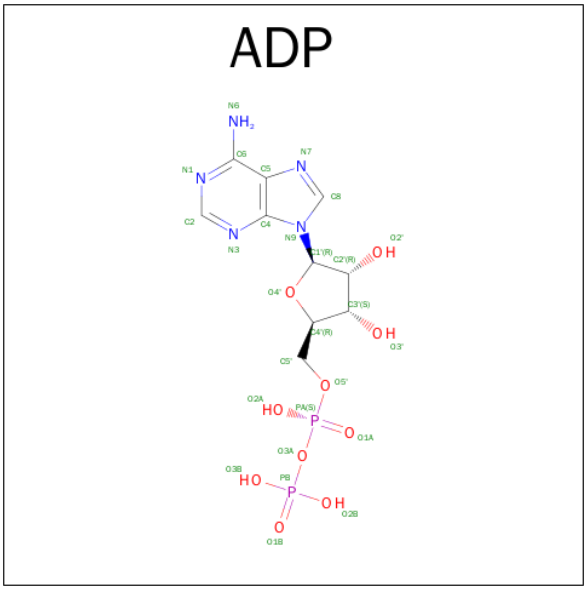
Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	367	Total 2862	C 1813	N 481	O 548	S 20	0	0
2	B	367	Total 2862	C 1813	N 481	O 548	S 20	0	0
2	C	367	Total 2862	C 1813	N 481	O 548	S 20	0	0
2	D	367	Total 2862	C 1813	N 481	O 548	S 20	0	0
2	E	367	Total 2862	C 1813	N 481	O 548	S 20	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).



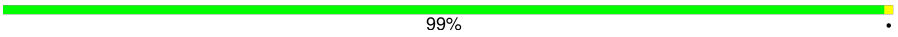
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

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 errors 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.

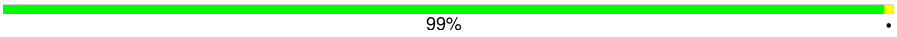
- Molecule 1: tropomyosin alpha-1

Chain F:



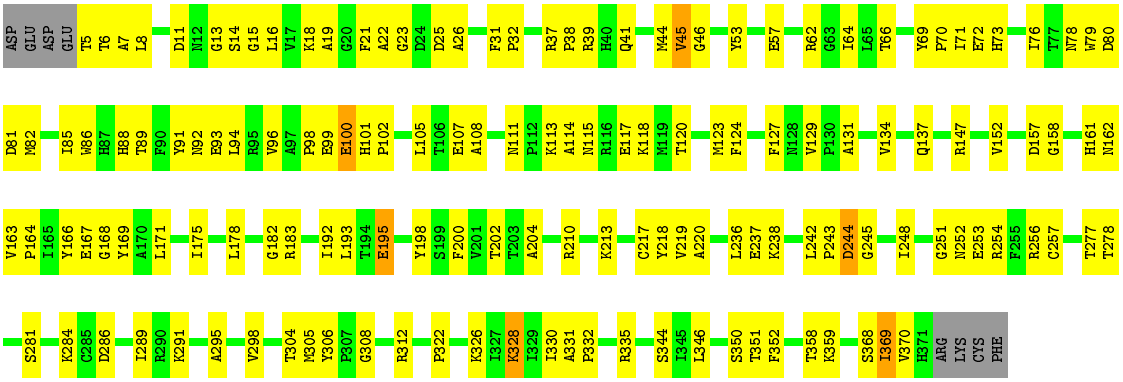
- Molecule 1: tropomyosin alpha-1

Chain G:



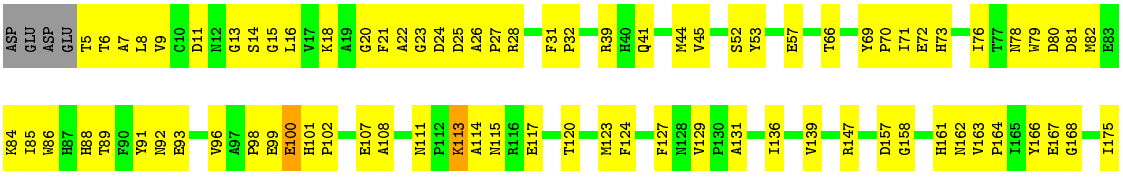
- Molecule 2: Actin, alpha skeletal muscle

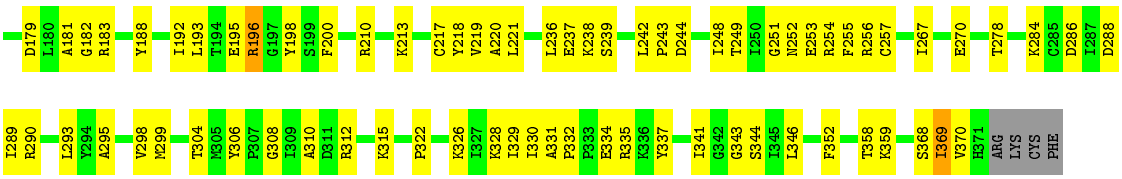
Chain A:



- Molecule 2: Actin, alpha skeletal muscle

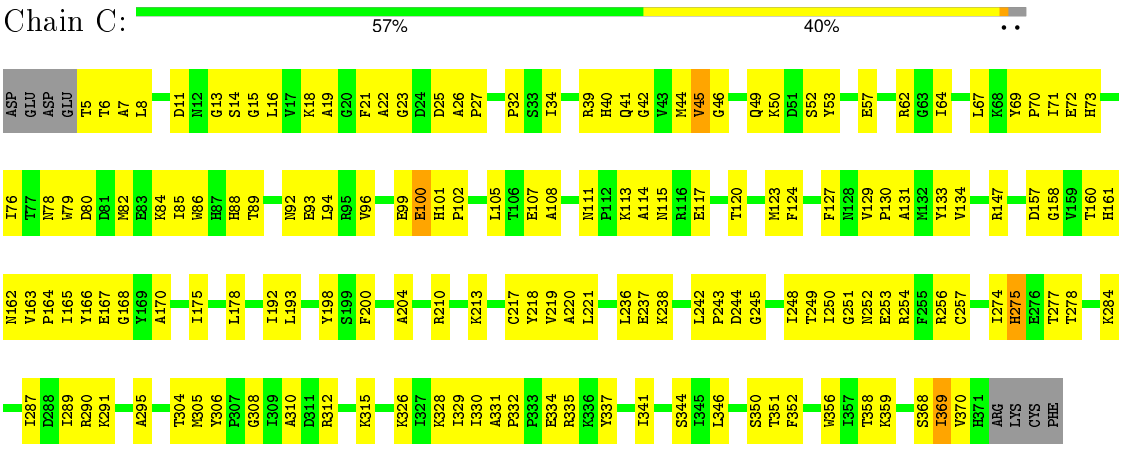
Chain B:





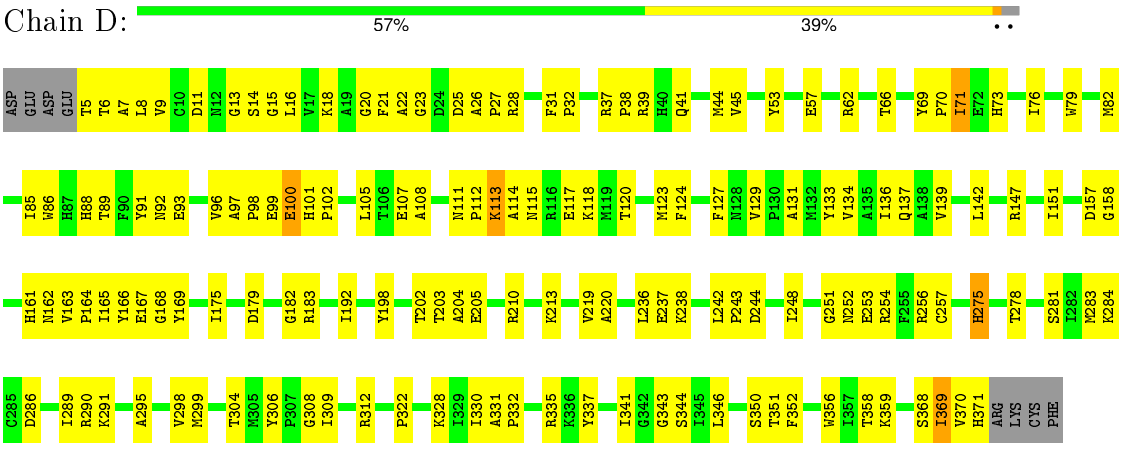
• Molecule 2: Actin, alpha skeletal muscle

Chain C:



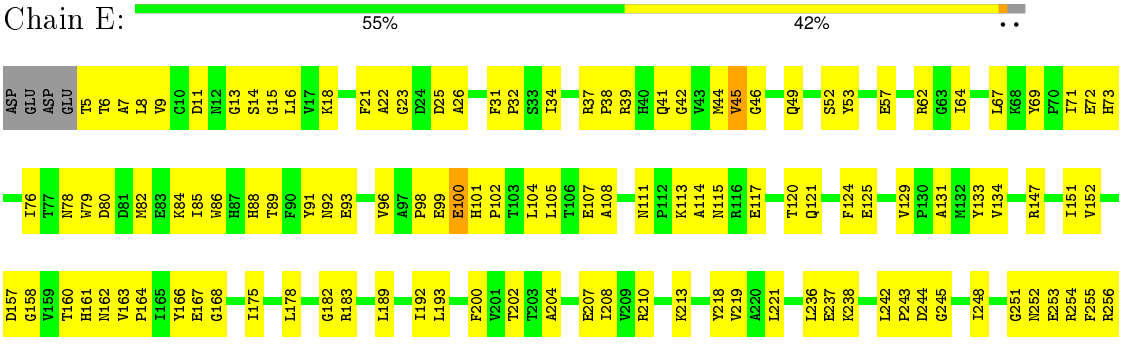
• Molecule 2: Actin, alpha skeletal muscle

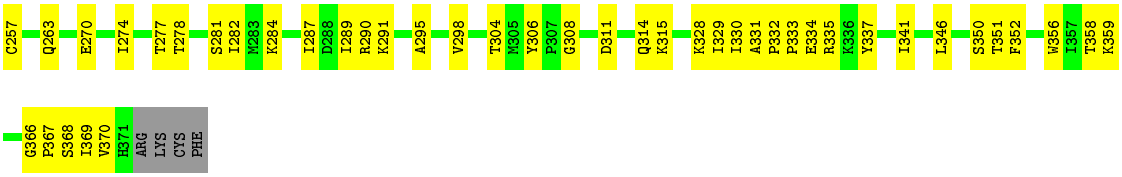
Chain D:



• Molecule 2: Actin, alpha skeletal muscle

Chain E:




C257
Q263
E270
I274
T277
T278
S281
I282
M283
K284
I287
D288
I289
R290
K291
A295
V298
T304
M305
Y306
P307
G308
D311
Q314
K315
K328
I329
I330
A331
P332
P333
E334
R335
K336
Y337
I341
L346
S350
T351
F352
W356
I357
T358
K359
G366
P367
S368
I369
V370
H371
ARG
LYS
CYS
PHE

4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC 0.5	Depositor
CTF correction method	each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1460	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	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	$\#\|Z\| > 2$
2	A	0.28	0/2911	0.54	0/3945
2	B	0.27	0/2911	0.52	0/3945
2	C	0.27	0/2911	0.54	0/3945
2	D	0.27	0/2911	0.53	0/3945
2	E	0.27	0/2911	0.54	0/3945
All	All	0.27	0/14555	0.53	0/19725

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

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	F	675	0	137	1	0
1	G	675	0	137	1	0
2	A	2862	0	2832	121	0
2	B	2862	0	2832	122	0
2	C	2862	0	2832	121	0
2	D	2862	0	2832	119	0
2	E	2862	0	2832	117	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
4	A	27	0	12	1	0
4	B	27	0	12	2	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
All	All	15800	0	14494	576	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 19.

The worst 5 of 576 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:B:102:PRO:HB3	2:B:131:ALA:HB3	1.57	0.87
2:A:114:ALA:HB1	2:A:117:GLU:HB2	1.55	0.86
2:E:114:ALA:HB1	2:E:117:GLU:HB2	1.56	0.85
2:B:124:PHE:HE1	2:B:359:LYS:HG3	1.41	0.84
2:E:102:PRO:HB3	2:E:131:ALA:HB3	1.59	0.84

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	
2	A	364/375 (97%)	318 (87%)	41 (11%)	5 (1%)	14	60
2	B	364/375 (97%)	317 (87%)	42 (12%)	5 (1%)	14	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	364/375 (97%)	318 (87%)	41 (11%)	5 (1%)	14	60
2	D	364/375 (97%)	316 (87%)	43 (12%)	5 (1%)	14	60
2	E	364/375 (97%)	318 (87%)	41 (11%)	5 (1%)	14	60
All	All	1820/1875 (97%)	1587 (87%)	208 (11%)	25 (1%)	19	60

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	22	ALA
2	A	45	VAL
2	A	252	ASN
2	A	369	ILE
2	B	22	ALA

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	
2	A	309/317 (98%)	304 (98%)	5 (2%)	70	90
2	B	309/317 (98%)	304 (98%)	5 (2%)	70	90
2	C	309/317 (98%)	305 (99%)	4 (1%)	76	91
2	D	309/317 (98%)	304 (98%)	5 (2%)	70	90
2	E	309/317 (98%)	304 (98%)	5 (2%)	70	90
All	All	1545/1585 (98%)	1521 (98%)	24 (2%)	72	90

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	100	GLU
2	C	334	GLU
2	E	263	GLN
2	C	161	HIS
2	C	275	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	111	ASN
2	C	275	HIS
2	E	88	HIS
2	C	88	HIS
2	E	111	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
2	HIC	A	73	2	6,11,12	3.20	1 (16%)	6,14,16	0.76	0
2	HIC	B	73	2	6,11,12	3.19	1 (16%)	6,14,16	0.79	0
2	HIC	C	73	2	6,11,12	3.19	1 (16%)	6,14,16	0.78	0
2	HIC	D	73	2	6,11,12	3.19	1 (16%)	6,14,16	0.77	0
2	HIC	E	73	2	6,11,12	3.18	1 (16%)	6,14,16	0.77	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
2	HIC	A	73	2	-	0/4/6/8	0/1/1/1
2	HIC	B	73	2	-	0/4/6/8	0/1/1/1
2	HIC	C	73	2	-	0/4/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIC	D	73	2	-	0/4/6/8	0/1/1/1
2	HIC	E	73	2	-	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)
2	A	73	HIC	CZ-NE2	-7.66	1.27	1.48
2	B	73	HIC	CZ-NE2	-7.64	1.27	1.48
2	D	73	HIC	CZ-NE2	-7.63	1.27	1.48
2	C	73	HIC	CZ-NE2	-7.63	1.27	1.48
2	E	73	HIC	CZ-NE2	-7.62	1.27	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	73	HIC	1	0
2	B	73	HIC	2	0
2	C	73	HIC	1	0
2	D	73	HIC	1	0
2	E	73	HIC	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\|>2$
4	ADP	A	402	3	24,29,29	0.95	1 (4%)	23,45,45	1.64	2 (8%)
4	ADP	B	402	3	24,29,29	0.96	1 (4%)	23,45,45	1.67	1 (4%)
4	ADP	C	402	3	24,29,29	0.99	1 (4%)	23,45,45	1.68	1 (4%)
4	ADP	D	402	3	24,29,29	0.97	1 (4%)	23,45,45	1.69	1 (4%)
4	ADP	E	402	3	24,29,29	0.96	1 (4%)	23,45,45	1.72	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
4	ADP	A	402	3	-	0/12/32/32	0/3/3/3
4	ADP	B	402	3	-	0/12/32/32	0/3/3/3
4	ADP	C	402	3	-	0/12/32/32	0/3/3/3
4	ADP	D	402	3	-	0/12/32/32	0/3/3/3
4	ADP	E	402	3	-	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)
4	E	402	ADP	C5-C4	2.97	1.47	1.40
4	B	402	ADP	C5-C4	3.02	1.47	1.40
4	A	402	ADP	C5-C4	3.07	1.47	1.40
4	D	402	ADP	C5-C4	3.11	1.47	1.40
4	C	402	ADP	C5-C4	3.13	1.47	1.40

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	402	ADP	N3-C2-N1	-6.57	123.71	128.87
4	C	402	ADP	N3-C2-N1	-6.29	123.93	128.87
4	B	402	ADP	N3-C2-N1	-6.23	123.98	128.87
4	A	402	ADP	N3-C2-N1	-6.13	124.06	128.87
4	D	402	ADP	N3-C2-N1	-6.13	124.06	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	ADP	1	0
4	B	402	ADP	2	0
4	C	402	ADP	1	0
4	D	402	ADP	1	0
4	E	402	ADP	1	0

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.