



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 31, 2017 – 10:56 AM EST

PDB ID : 5MW1
EMDB ID: : EMD-4117
Title : cryoEM structure of crenactin double helical filament at 3.8Å resolution
Authors : Izore, T.; Lowe, J.
Deposited on : 2017-01-17
Resolution : 3.80 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 : 1.7.1 (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) : rb-20028442

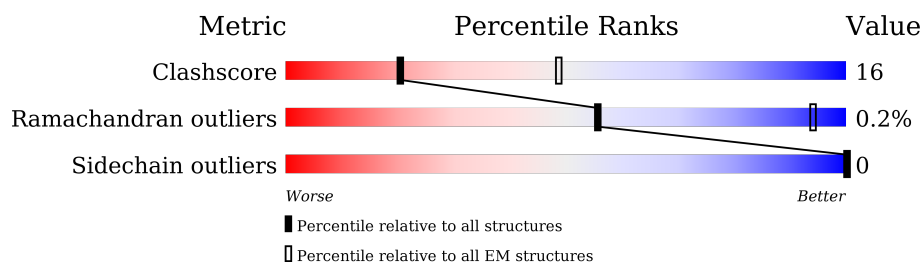
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	432	63% 35% .
1	B	432	62% 36% .
1	C	432	63% 35% .
1	D	432	62% 36% ..
1	E	432	64% 35% .
1	F	432	63% 35% .

2 Entry composition [i](#)

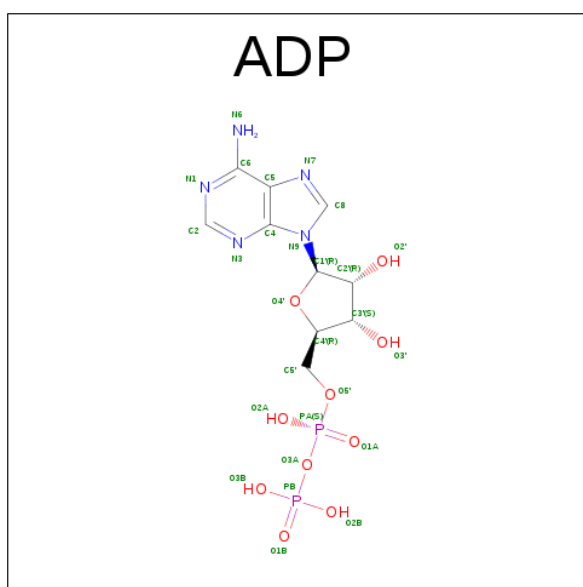
There are 2 unique types of molecules in this entry. The entry contains 20358 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Actin/actin family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	426	Total	C	N	O	S	0	0
			3366	2158	577	625	6		
1	A	426	Total	C	N	O	S	0	0
			3366	2158	577	625	6		
1	C	426	Total	C	N	O	S	0	0
			3366	2158	577	625	6		
1	D	426	Total	C	N	O	S	0	0
			3366	2158	577	625	6		
1	E	426	Total	C	N	O	S	0	0
			3366	2158	577	625	6		
1	F	426	Total	C	N	O	S	0	0
			3366	2158	577	625	6		

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

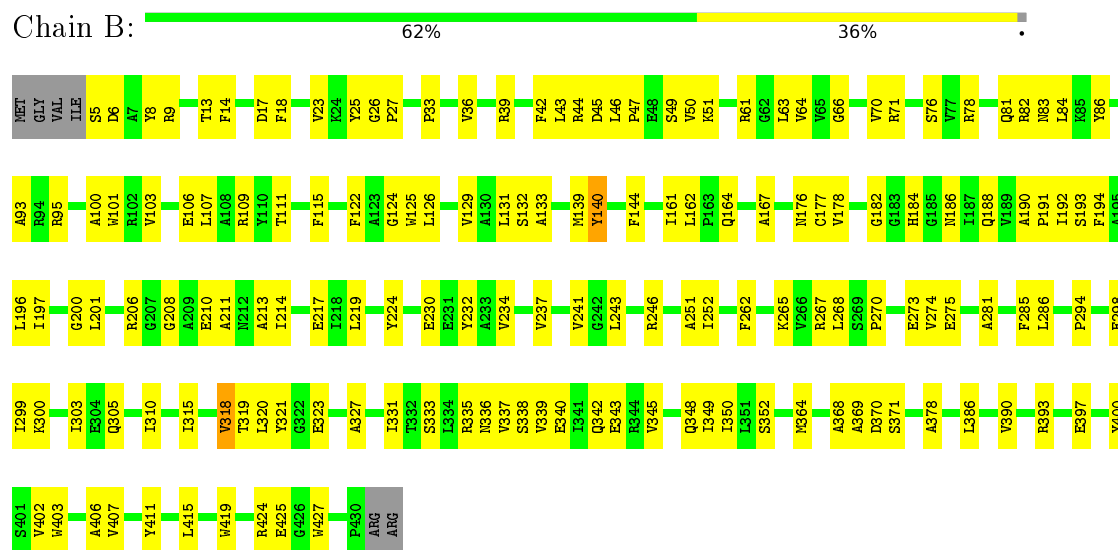


Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total 27	C 10	N 5	O 10	P 2	0
2	A	1	Total 27	C 10	N 5	O 10	P 2	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0

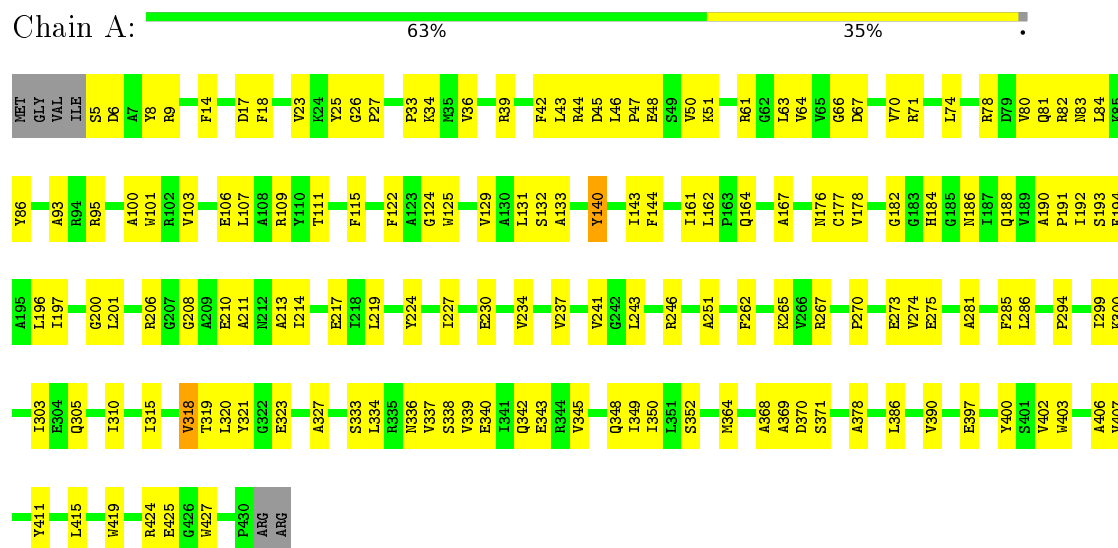
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Actin/actin family protein

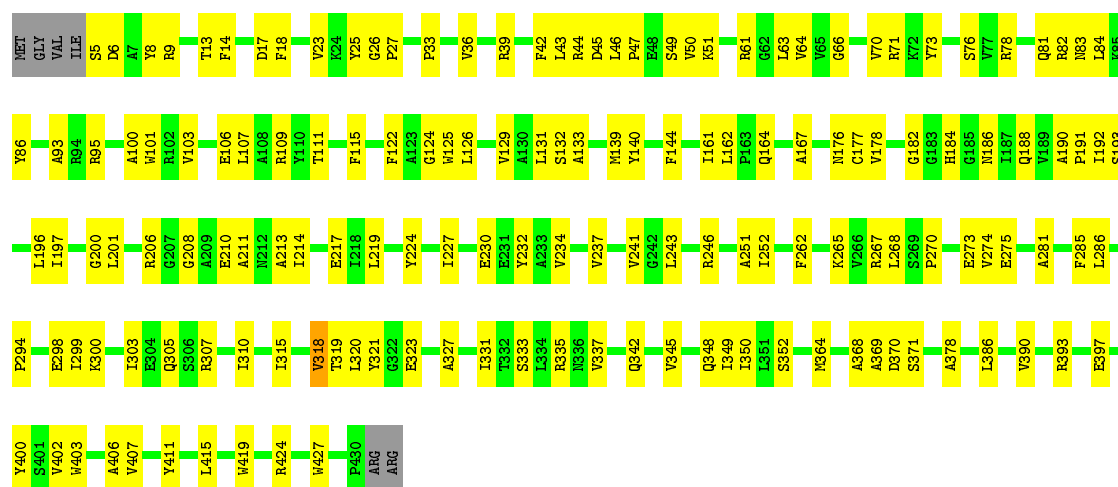


- Molecule 1: Actin/actin family protein



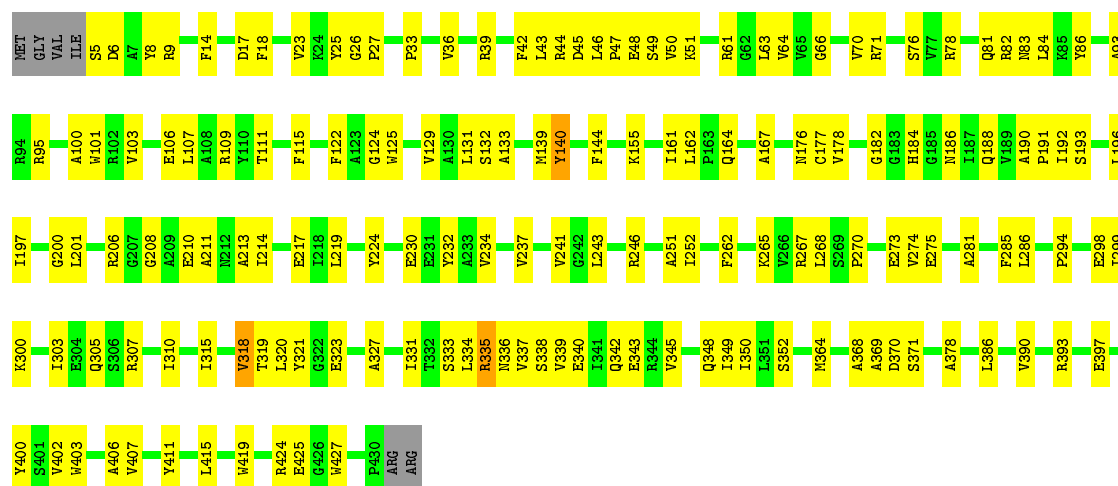
- Molecule 1: Actin/actin family protein

Chain C: 



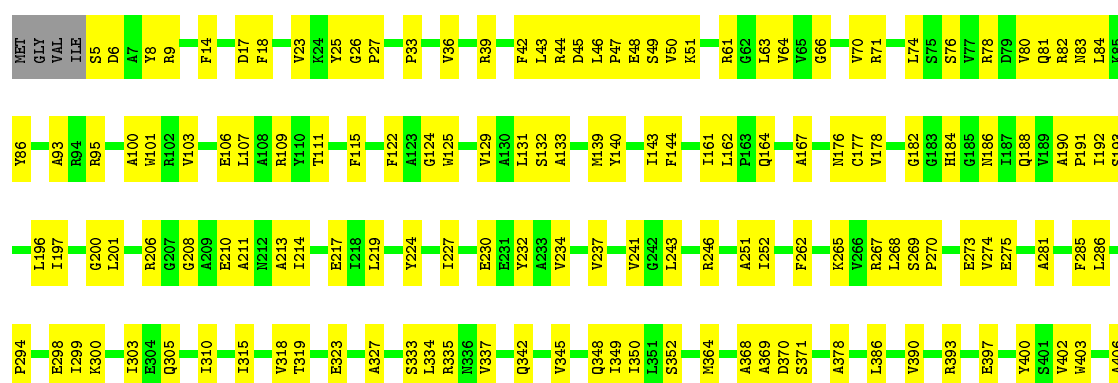
- Molecule 1: Actin/actin family protein

Chain D: 



- Molecule 1: Actin/actin family protein

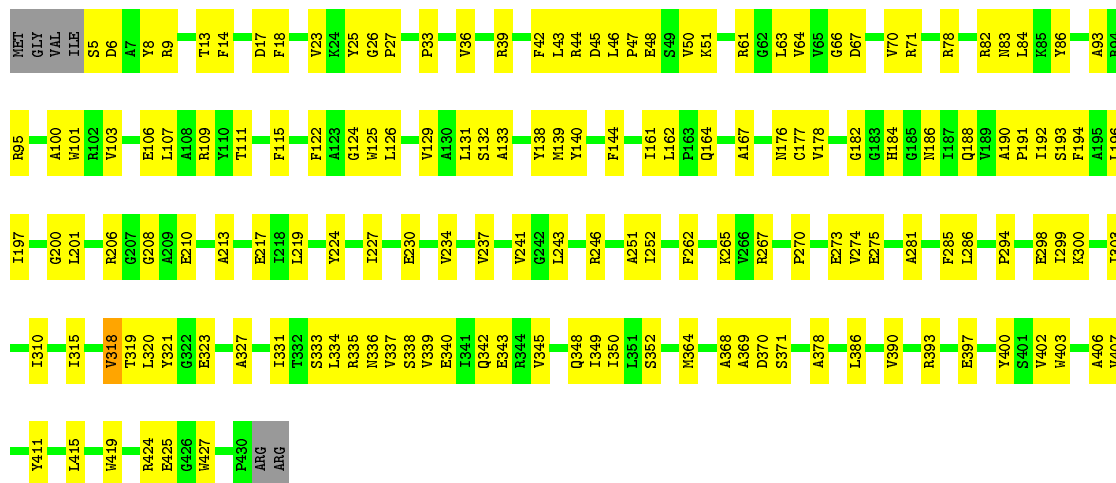
Chain E: 





- Molecule 1: Actin/actin family protein

Chain F: 63% 35% .



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	470396	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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: 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	0.80	2/3436 (0.1%)	0.74	2/4671 (0.0%)
1	B	0.82	2/3436 (0.1%)	0.72	1/4671 (0.0%)
1	C	0.83	2/3436 (0.1%)	0.76	3/4671 (0.1%)
1	D	0.80	2/3436 (0.1%)	0.73	3/4671 (0.1%)
1	E	0.82	0/3436	0.74	2/4671 (0.0%)
1	F	0.77	2/3436 (0.1%)	0.71	2/4671 (0.0%)
All	All	0.81	10/20616 (0.0%)	0.74	13/28026 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	GLU	CG-CD	8.38	1.64	1.51
1	C	140	TYR	CG-CD1	-8.11	1.28	1.39
1	D	140	TYR	CG-CD1	-6.17	1.31	1.39
1	A	140	TYR	CE1-CZ	-5.65	1.31	1.38
1	B	140	TYR	CE1-CZ	-5.57	1.31	1.38

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLU	OE1-CD-OE2	-14.18	106.28	123.30
1	F	230	GLU	OE1-CD-OE2	-8.23	113.42	123.30
1	C	393	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	A	230	GLU	CG-CD-OE1	7.03	132.35	118.30
1	D	393	ARG	NE-CZ-NH1	6.94	123.77	120.30

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	A	3366	0	3409	120	0
1	B	3366	0	3409	124	0
1	C	3366	0	3409	115	0
1	D	3366	0	3409	130	0
1	E	3366	0	3409	117	0
1	F	3366	0	3409	113	0
2	A	27	0	12	1	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	1	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
All	All	20358	0	20526	649	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 16.

The worst 5 of 649 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:197:ILE:HG22	1:B:200:GLY:H	1.40	0.85
1:C:197:ILE:HG22	1:C:200:GLY:H	1.41	0.85
1:A:197:ILE:HG22	1:A:200:GLY:H	1.40	0.85
1:F:197:ILE:HG22	1:F:200:GLY:H	1.41	0.85
1:E:197:ILE:HG22	1:E:200:GLY:H	1.42	0.84

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	424/432 (98%)	395 (93%)	28 (7%)	1 (0%)	52	86
1	B	424/432 (98%)	394 (93%)	29 (7%)	1 (0%)	52	86
1	C	424/432 (98%)	394 (93%)	29 (7%)	1 (0%)	52	86
1	D	424/432 (98%)	394 (93%)	29 (7%)	1 (0%)	52	86
1	E	424/432 (98%)	393 (93%)	30 (7%)	1 (0%)	52	86
1	F	424/432 (98%)	395 (93%)	28 (7%)	1 (0%)	52	86
All	All	2544/2592 (98%)	2365 (93%)	173 (7%)	6 (0%)	56	86

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	318	VAL
1	A	318	VAL
1	C	318	VAL
1	D	318	VAL
1	E	318	VAL

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	358/363 (99%)	358 (100%)	0	100	100
1	B	358/363 (99%)	358 (100%)	0	100	100
1	C	358/363 (99%)	358 (100%)	0	100	100
1	D	358/363 (99%)	358 (100%)	0	100	100
1	E	358/363 (99%)	358 (100%)	0	100	100
1	F	358/363 (99%)	358 (100%)	0	100	100
All	All	2148/2178 (99%)	2148 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	176	ASN
1	C	336	ASN
1	F	188	GLN
1	C	188	GLN
1	D	164	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 ⓘ

6 ligands 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	ADP	A	501	-	24,29,29	1.18	2 (8%)	23,45,45	1.80	2 (8%)
2	ADP	B	501	-	24,29,29	1.16	1 (4%)	23,45,45	1.80	2 (8%)
2	ADP	C	501	-	24,29,29	1.28	3 (12%)	23,45,45	1.78	4 (17%)
2	ADP	D	501	-	24,29,29	1.26	2 (8%)	23,45,45	1.71	4 (17%)
2	ADP	E	501	-	24,29,29	1.28	1 (4%)	23,45,45	1.91	4 (17%)
2	ADP	F	501	-	24,29,29	1.24	1 (4%)	23,45,45	1.72	3 (13%)

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	501	-	-	0/12/32/32	0/3/3/3
2	ADP	B	501	-	-	0/12/32/32	0/3/3/3
2	ADP	C	501	-	-	0/12/32/32	0/3/3/3
2	ADP	D	501	-	-	0/12/32/32	0/3/3/3
2	ADP	E	501	-	-	0/12/32/32	0/3/3/3
2	ADP	F	501	-	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	ADP	PB-O3B	-3.04	1.44	1.54
2	D	501	ADP	C4-N3	-2.49	1.31	1.35
2	A	501	ADP	PB-O3B	-2.38	1.46	1.54
2	C	501	ADP	PB-O3B	-2.11	1.47	1.54
2	C	501	ADP	O4'-C4'	-2.00	1.40	1.45

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	ADP	N3-C2-N1	-7.02	123.36	128.87
2	E	501	ADP	N3-C2-N1	-6.99	123.38	128.87
2	A	501	ADP	N3-C2-N1	-6.82	123.52	128.87
2	C	501	ADP	N3-C2-N1	-6.24	123.97	128.87
2	F	501	ADP	N3-C2-N1	-6.17	124.03	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ADP	1	0
2	B	501	ADP	1	0
2	C	501	ADP	1	0
2	D	501	ADP	1	0
2	E	501	ADP	1	0
2	F	501	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.