



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:48 PM BST

PDB ID : 3G37
EMDB ID: : EMD-1674
Title : Cryo-EM structure of actin filament in the presence of phosphate
Authors : Wakabayshi, T.; Murakami, K.; Yasunaga, T.; Noguchi, T.Q.; Uyeda, T.Q.
Deposited on : 2009-02-02
Resolution : 6.00 Å(reported)

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

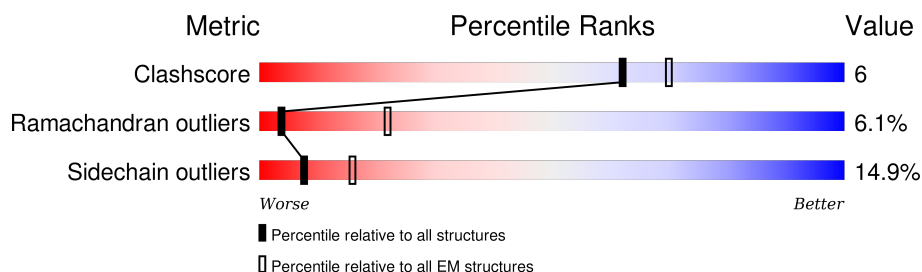
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.00 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	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	O	376	70% 25% . .
1	P	376	66% 27% 5% .
1	Q	376	65% 26% 8% .
1	R	376	69% 24% 6% .
1	S	376	65% 26% 7% .
1	T	376	67% 27% 6% .
1	U	376	66% 26% 7% .
1	V	376	65% 27% 7% .
1	W	376	66% 25% 8% .

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Mol	Chain	Length	Quality of chain
1	X	376	 68% 26% 6% •
1	Y	376	 70% 24% 5% •
1	Z	376	 68% 24% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	Y	801	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35808 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, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	P	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	Q	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	R	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	S	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	T	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	U	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	V	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	W	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	X	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	Y	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	Z	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		

There are 12 discrepancies between the modelled and reference sequences:

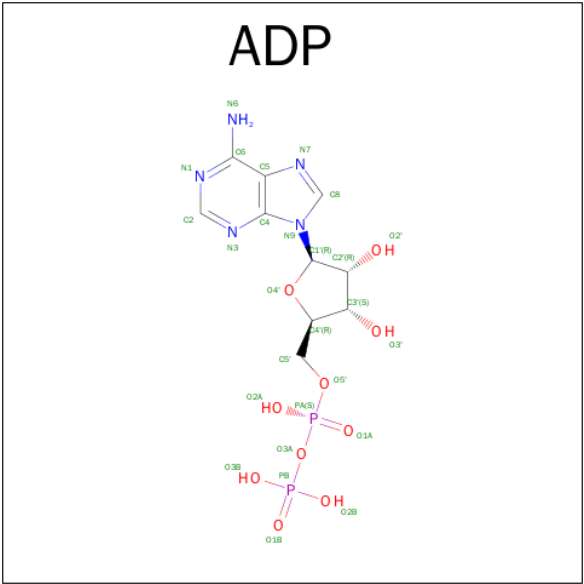
Chain	Residue	Modelled	Actual	Comment	Reference
O	0	ACE	-	ACETYLATION	UNP P68135
P	0	ACE	-	ACETYLATION	UNP P68135
Q	0	ACE	-	ACETYLATION	UNP P68135
R	0	ACE	-	ACETYLATION	UNP P68135
S	0	ACE	-	ACETYLATION	UNP P68135
T	0	ACE	-	ACETYLATION	UNP P68135

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Chain	Residue	Modelled	Actual	Comment	Reference
U	0	ACE	-	ACETYLATION	UNP P68135
V	0	ACE	-	ACETYLATION	UNP P68135
W	0	ACE	-	ACETYLATION	UNP P68135
X	0	ACE	-	ACETYLATION	UNP P68135
Y	0	ACE	-	ACETYLATION	UNP P68135
Z	0	ACE	-	ACETYLATION	UNP P68135

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



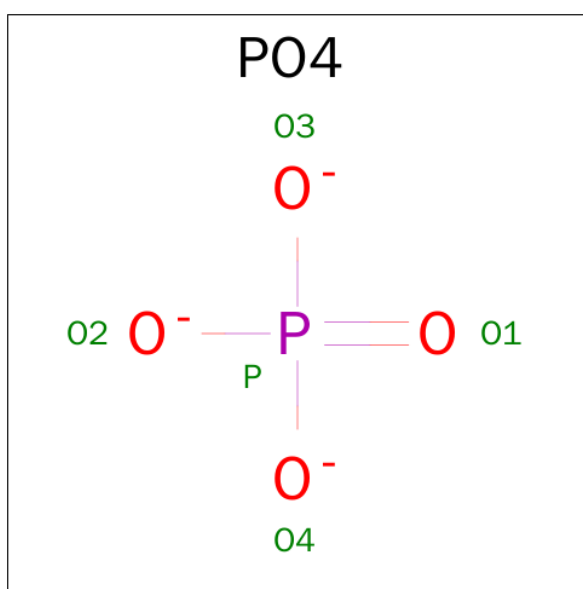
Mol	Chain	Residues	Atoms					AltConf
2	O	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	P	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	R	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	S	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	V	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
2	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
3	P	1	Total	O	P	0
			15	12	3	
3	O	1	Total	O	P	0
			15	12	3	
3	O	1	Total	O	P	0
			15	12	3	
3	O	1	Total	O	P	0
			15	12	3	
3	P	1	Total	O	P	0
			15	12	3	
3	P	1	Total	O	P	0
			15	12	3	
3	R	1	Total	O	P	0
			15	12	3	

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Mol	Chain	Residues	Atoms			AltConf
3	Q	1	Total 15	O 12	P 3	0
3	Q	1	Total 15	O 12	P 3	0
3	Q	1	Total 15	O 12	P 3	0
3	R	1	Total 15	O 12	P 3	0
3	R	1	Total 15	O 12	P 3	0
3	T	1	Total 20	O 16	P 4	0
3	T	1	Total 20	O 16	P 4	0
3	S	1	Total 15	O 12	P 3	0
3	S	1	Total 15	O 12	P 3	0
3	S	1	Total 15	O 12	P 3	0
3	T	1	Total 20	O 16	P 4	0
3	T	1	Total 20	O 16	P 4	0
3	U	1	Total 15	O 12	P 3	0
3	U	1	Total 15	O 12	P 3	0
3	U	1	Total 15	O 12	P 3	0
3	V	1	Total 10	O 8	P 2	0
3	V	1	Total 10	O 8	P 2	0
3	X	1	Total 15	O 12	P 3	0
3	W	1	Total 15	O 12	P 3	0
3	W	1	Total 15	O 12	P 3	0
3	W	1	Total 15	O 12	P 3	0

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Mol	Chain	Residues	Atoms			AltConf
3	X	1	Total	O	P	0
			15	12	3	
3	X	1	Total	O	P	0
			15	12	3	
3	Z	1	Total	O	P	0
			15	12	3	
3	Y	1	Total	O	P	0
			15	12	3	
3	Y	1	Total	O	P	0
			15	12	3	
3	Y	1	Total	O	P	0
			15	12	3	
3	Z	1	Total	O	P	0
			15	12	3	
3	Z	1	Total	O	P	0
			15	12	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	P	5	Total	Mg	0
			5	5	
4	Q	7	Total	Mg	0
			7	7	
4	V	6	Total	Mg	0
			6	6	
4	W	6	Total	Mg	0
			6	6	
4	Z	6	Total	Mg	0
			6	6	
4	T	6	Total	Mg	0
			6	6	
4	U	6	Total	Mg	0
			6	6	
4	X	6	Total	Mg	0
			6	6	
4	O	6	Total	Mg	0
			6	6	
4	R	6	Total	Mg	0
			6	6	
4	Y	6	Total	Mg	0
			6	6	

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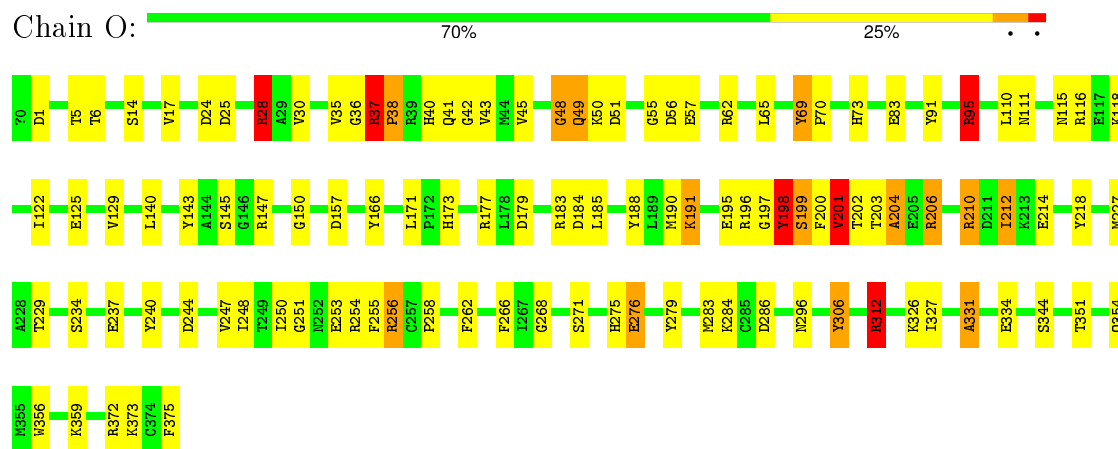
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	S	6	6	6	0

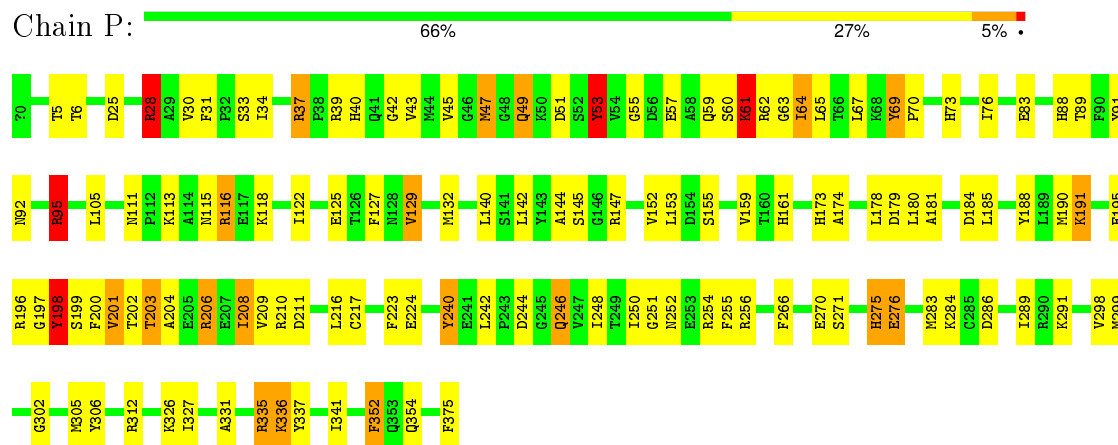
3 Residue-property plots

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.

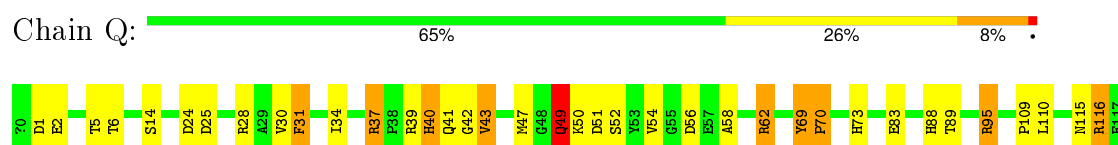
- Molecule 1: Actin, alpha skeletal muscle

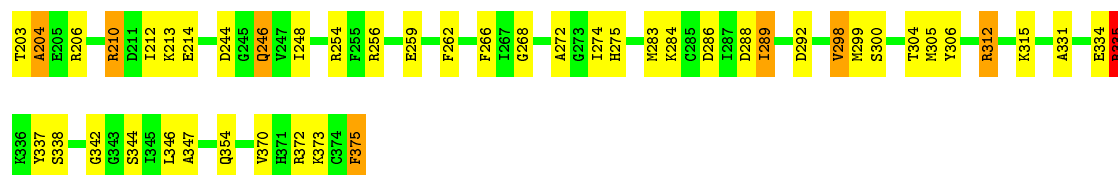


- Molecule 1: Actin, alpha skeletal muscle



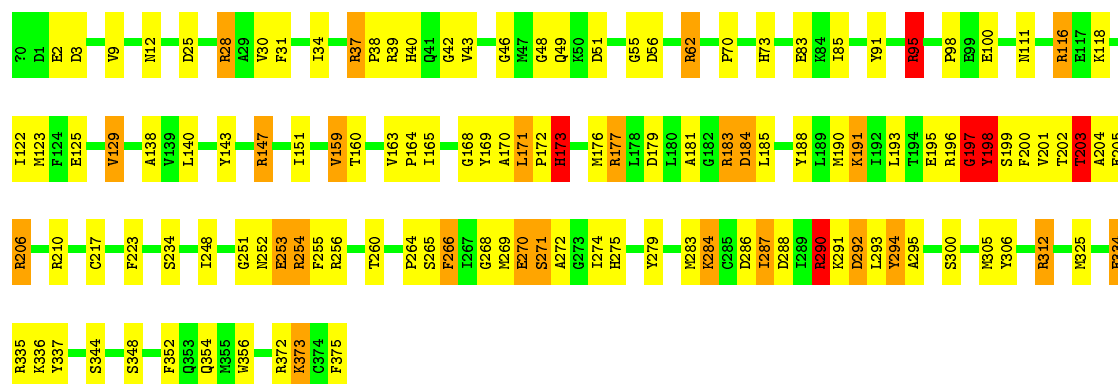
- Molecule 1: Actin, alpha skeletal muscle





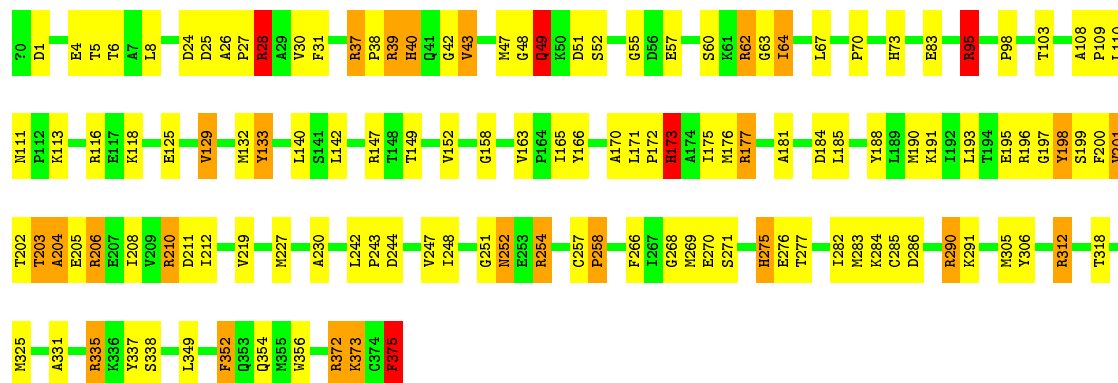
- Molecule 1: Actin, alpha skeletal muscle

Chain U: 66% 26% 7% •



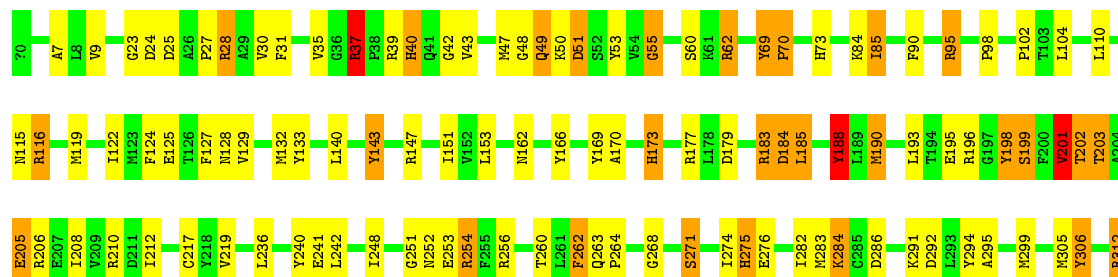
- Molecule 1: Actin, alpha skeletal muscle

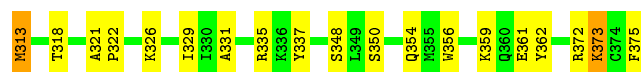
Chain V: 65% 27% 7% •



- Molecule 1: Actin, alpha skeletal muscle

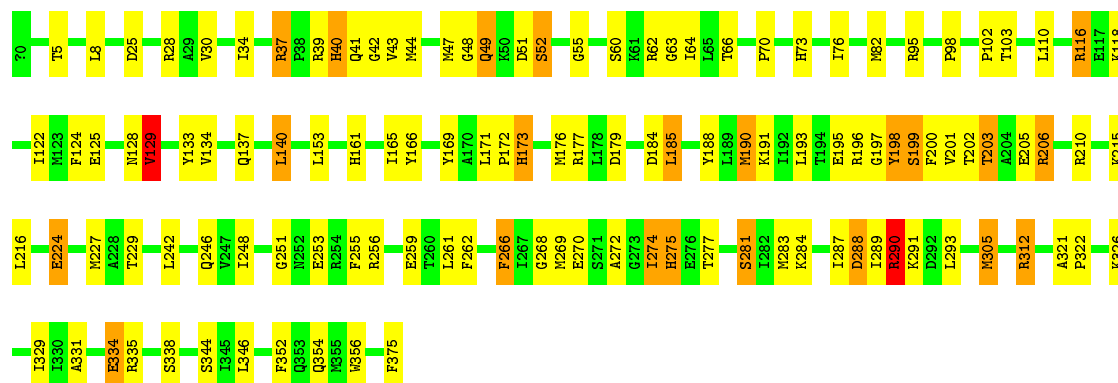
Chain W: 66% 25% 8% •





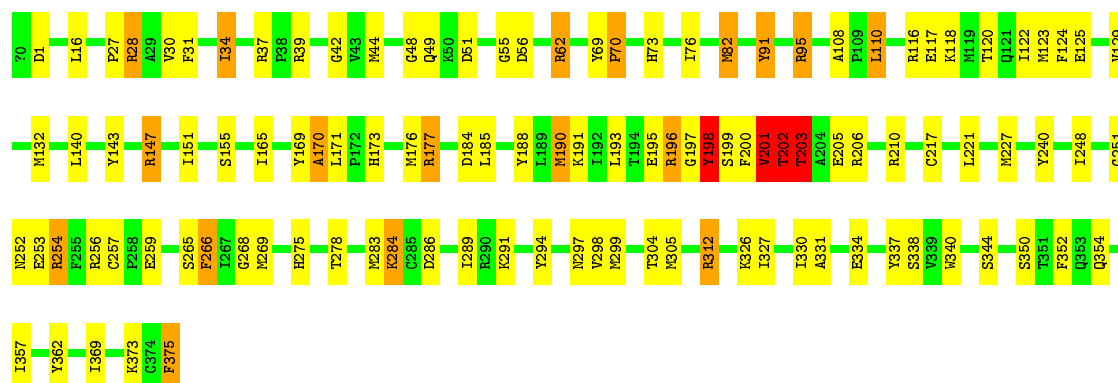
- Molecule 1: Actin, alpha skeletal muscle

Chain X: 68% 26% 6%



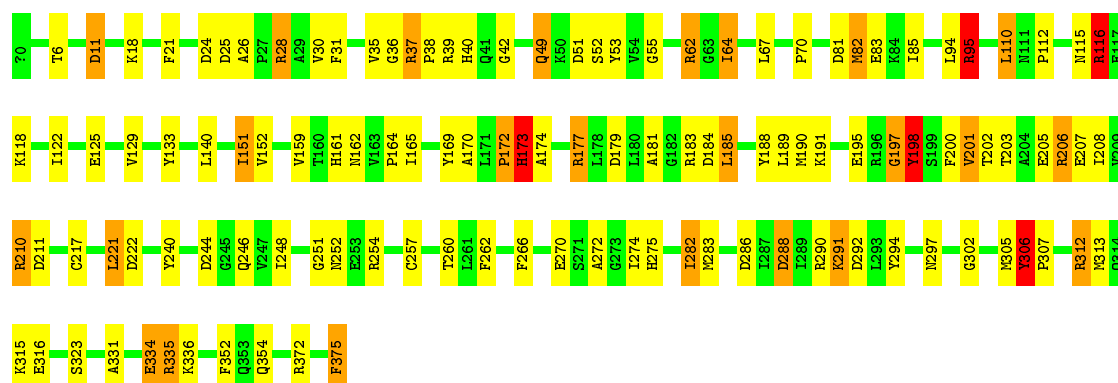
- Molecule 1: Actin, alpha skeletal muscle

Chain Y: 70% 24% 5%



- Molecule 1: Actin, alpha skeletal muscle

Chain Z: 68% 24% 6%



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FSC at 0.143 cut-off	Depositor
Microscope	HITACHI EF2000	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	100000	Depositor
Image detector	CCD	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, PO4, HIC, MG, 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	O	0.73	0/2984	1.47	30/4042 (0.7%)
1	P	0.91	9/2984 (0.3%)	1.48	36/4042 (0.9%)
1	Q	0.80	4/2984 (0.1%)	1.52	31/4042 (0.8%)
1	R	0.87	3/2984 (0.1%)	1.48	27/4042 (0.7%)
1	S	0.74	1/2984 (0.0%)	1.49	30/4042 (0.7%)
1	T	0.74	0/2984	1.46	23/4042 (0.6%)
1	U	0.73	0/2984	1.44	29/4042 (0.7%)
1	V	0.71	0/2984	1.45	34/4042 (0.8%)
1	W	0.73	0/2984	1.48	34/4042 (0.8%)
1	X	0.72	0/2984	1.45	29/4042 (0.7%)
1	Y	0.72	0/2984	1.40	27/4042 (0.7%)
1	Z	0.72	0/2984	1.44	27/4042 (0.7%)
All	All	0.76	17/35808 (0.0%)	1.46	357/48504 (0.7%)

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	O	0	18
1	P	0	17
1	Q	0	25
1	R	0	16
1	S	0	21
1	T	0	19
1	U	0	25
1	V	0	19
1	W	0	24
1	X	0	14
1	Y	0	22

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Z	0	23
All	All	0	243

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	167	GLU	CD-OE1	-17.54	1.06	1.25
1	R	167	GLU	CD-OE2	12.87	1.39	1.25
1	P	62	ARG	C-N	12.41	1.55	1.33
1	P	61	LYS	CG-CD	10.97	1.89	1.52
1	Q	187	ASP	CG-OD2	-9.47	1.03	1.25

The worst 5 of 357 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	269	MET	CG-SD-CE	-16.11	74.43	100.20
1	S	288	ASP	CB-CG-OD1	14.03	130.92	118.30
1	R	166	TYR	CB-CG-CD1	-13.80	112.72	121.00
1	Q	187	ASP	CB-CG-OD2	12.64	129.68	118.30
1	R	166	TYR	CB-CG-CD2	12.48	128.49	121.00

There are no chirality outliers.

5 of 243 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	28	ARG	Sidechain
1	O	38	PRO	Peptide
1	O	50	LYS	Peptide
1	O	69	TYR	Sidechain
1	O	91	TYR	Sidechain

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	O	2936	0	2896	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	2936	0	2895	38	0
1	Q	2936	0	2896	52	0
1	R	2936	0	2896	35	0
1	S	2936	0	2896	40	0
1	T	2936	0	2896	42	0
1	U	2936	0	2896	37	0
1	V	2936	0	2896	48	0
1	W	2936	0	2896	41	0
1	X	2936	0	2896	37	0
1	Y	2936	0	2896	33	0
1	Z	2936	0	2896	23	0
2	O	27	0	12	1	0
2	P	27	0	12	0	0
2	Q	27	0	12	0	0
2	R	27	0	12	0	0
2	S	27	0	12	0	0
2	T	27	0	12	0	0
2	U	27	0	12	1	0
2	V	27	0	12	0	0
2	W	27	0	12	0	0
2	X	27	0	12	0	0
2	Y	27	0	12	0	0
2	Z	27	0	12	0	0
3	O	15	0	0	0	0
3	P	15	0	0	1	0
3	Q	15	0	0	0	0
3	R	15	0	0	1	0
3	S	15	0	0	0	0
3	T	20	0	0	1	0
3	U	15	0	0	0	0
3	V	10	0	0	0	0
3	W	15	0	0	0	0
3	X	15	0	0	0	0
3	Y	15	0	0	2	0
3	Z	15	0	0	0	0
4	O	6	0	0	0	0
4	P	5	0	0	0	0
4	Q	7	0	0	0	0
4	R	6	0	0	0	0
4	S	6	0	0	0	0
4	T	6	0	0	0	0
4	U	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	6	0	0	0	0
4	W	6	0	0	0	0
4	X	6	0	0	0	0
4	Y	6	0	0	0	0
4	Z	6	0	0	0	0
All	All	35808	0	34895	391	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.

The worst 5 of 391 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:P:61:LYS:CD	1:P:61:LYS:CG	1.89	1.50
1:Q:202:THR:HG23	1:Q:203:THR:H	1.48	0.78
1:P:202:THR:HG23	1:P:203:THR:H	1.50	0.76
1:O:201:VAL:HG13	1:O:202:THR:HG22	1.68	0.74
1:V:275:HIS:CD2	1:V:276:GLU:H	2.05	0.74

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	O	373/376 (99%)	283 (76%)	66 (18%)	24 (6%)	2	25
1	P	373/376 (99%)	298 (80%)	54 (14%)	21 (6%)	2	28
1	Q	373/376 (99%)	281 (75%)	66 (18%)	26 (7%)	1	22
1	R	373/376 (99%)	295 (79%)	52 (14%)	26 (7%)	1	22
1	S	373/376 (99%)	286 (77%)	67 (18%)	20 (5%)	2	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	373/376 (99%)	275 (74%)	73 (20%)	25 (7%)	1	23
1	U	373/376 (99%)	284 (76%)	66 (18%)	23 (6%)	2	25
1	V	373/376 (99%)	293 (79%)	56 (15%)	24 (6%)	2	25
1	W	373/376 (99%)	288 (77%)	60 (16%)	25 (7%)	1	23
1	X	373/376 (99%)	292 (78%)	63 (17%)	18 (5%)	3	31
1	Y	373/376 (99%)	292 (78%)	64 (17%)	17 (5%)	3	32
1	Z	373/376 (99%)	289 (78%)	59 (16%)	25 (7%)	1	23
All	All	4476/4512 (99%)	3456 (77%)	746 (17%)	274 (6%)	4	25

5 of 274 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	42	GLY
1	O	51	ASP
1	O	129	VAL
1	O	254	ARG
1	P	42	GLY

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	O	317/317 (100%)	272 (86%)	45 (14%)	4	26
1	P	317/317 (100%)	269 (85%)	48 (15%)	3	23
1	Q	317/317 (100%)	269 (85%)	48 (15%)	3	23
1	R	317/317 (100%)	275 (87%)	42 (13%)	5	28
1	S	317/317 (100%)	265 (84%)	52 (16%)	3	20
1	T	317/317 (100%)	275 (87%)	42 (13%)	5	28
1	U	317/317 (100%)	265 (84%)	52 (16%)	3	20
1	V	317/317 (100%)	269 (85%)	48 (15%)	3	23
1	W	317/317 (100%)	279 (88%)	38 (12%)	6	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	317/317 (100%)	266 (84%)	51 (16%)	3	20
1	Y	317/317 (100%)	276 (87%)	41 (13%)	5	29
1	Z	317/317 (100%)	259 (82%)	58 (18%)	2	15
All	All	3804/3804 (100%)	3239 (85%)	565 (15%)	7	24

5 of 565 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	173	HIS
1	U	284	LYS
1	Z	115	ASN
1	T	244	ASP
1	U	49	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	V	173	HIS
1	W	111	ASN
1	Z	246	GLN
1	W	87	HIS
1	W	173	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	O	73	1	6,11,12	1.68	1 (16%)	6,14,16	0.59	0
1	HIC	P	73	1	6,11,12	2.86	1 (16%)	6,14,16	2.29	2 (33%)
1	HIC	Q	73	1	6,11,12	2.95	1 (16%)	6,14,16	2.32	3 (50%)
1	HIC	R	73	1	6,11,12	2.98	1 (16%)	6,14,16	2.51	3 (50%)
1	HIC	S	73	1	6,11,12	3.38	1 (16%)	6,14,16	2.77	2 (33%)
1	HIC	T	73	1	6,11,12	2.79	1 (16%)	6,14,16	1.98	2 (33%)
1	HIC	U	73	1	6,11,12	2.91	1 (16%)	6,14,16	1.45	1 (16%)
1	HIC	V	73	1	6,11,12	3.17	1 (16%)	6,14,16	2.29	2 (33%)
1	HIC	W	73	1	6,11,12	3.28	1 (16%)	6,14,16	3.44	2 (33%)
1	HIC	X	73	1	6,11,12	3.27	1 (16%)	6,14,16	1.74	2 (33%)
1	HIC	Y	73	1	6,11,12	3.10	1 (16%)	6,14,16	2.52	2 (33%)
1	HIC	Z	73	1	6,11,12	3.32	1 (16%)	6,14,16	3.18	2 (33%)

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	O	73	1	-	0/4/6/8	0/1/1/1
1	HIC	P	73	1	-	0/4/6/8	0/1/1/1
1	HIC	Q	73	1	-	0/4/6/8	0/1/1/1
1	HIC	R	73	1	-	0/4/6/8	0/1/1/1
1	HIC	S	73	1	-	0/4/6/8	0/1/1/1
1	HIC	T	73	1	-	0/4/6/8	0/1/1/1
1	HIC	U	73	1	-	0/4/6/8	0/1/1/1
1	HIC	V	73	1	-	0/4/6/8	0/1/1/1
1	HIC	W	73	1	-	0/4/6/8	0/1/1/1
1	HIC	X	73	1	-	0/4/6/8	0/1/1/1
1	HIC	Y	73	1	-	0/4/6/8	0/1/1/1
1	HIC	Z	73	1	-	0/4/6/8	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	73	HIC	CZ-NE2	-7.97	1.26	1.48
1	Z	73	HIC	CZ-NE2	-7.96	1.27	1.48
1	W	73	HIC	CZ-NE2	-7.89	1.27	1.48
1	X	73	HIC	CZ-NE2	-7.81	1.27	1.48
1	V	73	HIC	CZ-NE2	-7.65	1.27	1.48

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	73	HIC	CZ-NE2-CE1	-4.63	100.52	125.34
1	Z	73	HIC	CZ-NE2-CE1	-4.39	101.79	125.34
1	S	73	HIC	CZ-NE2-CE1	-3.81	104.92	125.34
1	Y	73	HIC	CZ-NE2-CE1	-3.40	107.13	125.34
1	R	73	HIC	CZ-NE2-CE1	-3.34	107.45	125.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	O	73	HIC	2	0
1	P	73	HIC	1	0
1	Q	73	HIC	3	0
1	R	73	HIC	3	0
1	S	73	HIC	3	0
1	T	73	HIC	2	0
1	U	73	HIC	2	0
1	V	73	HIC	3	0
1	W	73	HIC	3	0
1	X	73	HIC	3	0
1	Y	73	HIC	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 120 ligands modelled in this entry, 72 are monoatomic - leaving 48 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	O	800	4	24,29,29	0.99	2 (8%)	23,45,45	1.38	3 (13%)
3	PO4	O	801	-	4,4,4	1.68	1 (25%)	6,6,6	0.55	0
3	PO4	O	802	-	4,4,4	1.74	1 (25%)	6,6,6	0.42	0
3	PO4	O	803	-	4,4,4	1.99	1 (25%)	6,6,6	0.52	0
2	ADP	P	800	4	24,29,29	0.95	2 (8%)	23,45,45	1.31	3 (13%)
3	PO4	P	801	-	4,4,4	1.92	1 (25%)	6,6,6	0.54	0
3	PO4	P	802	-	4,4,4	1.49	1 (25%)	6,6,6	0.35	0
3	PO4	P	803	-	4,4,4	1.78	1 (25%)	6,6,6	1.21	1 (16%)
2	ADP	Q	800	4	24,29,29	0.95	1 (4%)	23,45,45	1.33	3 (13%)
3	PO4	Q	801	4	4,4,4	1.74	1 (25%)	6,6,6	0.72	0
3	PO4	Q	802	-	4,4,4	1.80	1 (25%)	6,6,6	0.38	0
3	PO4	Q	803	-	4,4,4	1.72	1 (25%)	6,6,6	0.51	0
2	ADP	R	800	4	24,29,29	0.99	2 (8%)	23,45,45	1.53	4 (17%)
3	PO4	R	801	-	4,4,4	1.82	1 (25%)	6,6,6	0.49	0
3	PO4	R	802	-	4,4,4	1.43	1 (25%)	6,6,6	0.41	0
3	PO4	R	803	-	4,4,4	1.94	1 (25%)	6,6,6	0.96	0
2	ADP	S	800	4	24,29,29	0.91	1 (4%)	23,45,45	1.29	3 (13%)
3	PO4	S	801	-	4,4,4	1.35	1 (25%)	6,6,6	0.42	0
3	PO4	S	802	-	4,4,4	1.82	1 (25%)	6,6,6	0.34	0
3	PO4	S	803	-	4,4,4	1.86	1 (25%)	6,6,6	0.54	0
3	PO4	T	376	-	4,4,4	1.65	1 (25%)	6,6,6	0.57	0
2	ADP	T	800	4	24,29,29	0.84	1 (4%)	23,45,45	1.46	4 (17%)
3	PO4	T	801	4	4,4,4	1.70	1 (25%)	6,6,6	0.56	0
3	PO4	T	802	-	4,4,4	1.83	1 (25%)	6,6,6	0.37	0
3	PO4	T	803	-	4,4,4	1.79	1 (25%)	6,6,6	0.67	0
2	ADP	U	800	4	24,29,29	0.83	1 (4%)	23,45,45	1.53	4 (17%)
3	PO4	U	801	-	4,4,4	1.82	1 (25%)	6,6,6	0.96	1 (16%)
3	PO4	U	802	-	4,4,4	1.39	1 (25%)	6,6,6	0.43	0
3	PO4	U	803	-	4,4,4	1.67	1 (25%)	6,6,6	0.40	0
2	ADP	V	800	4	24,29,29	0.92	2 (8%)	23,45,45	1.31	3 (13%)
3	PO4	V	802	-	4,4,4	1.80	1 (25%)	6,6,6	0.45	0
3	PO4	V	803	-	4,4,4	1.73	1 (25%)	6,6,6	0.55	0
2	ADP	W	800	4	24,29,29	0.91	2 (8%)	23,45,45	1.30	4 (17%)
3	PO4	W	801	-	4,4,4	1.69	1 (25%)	6,6,6	0.56	0
3	PO4	W	802	-	4,4,4	1.62	1 (25%)	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	W	803	-	4,4,4	1.71	1 (25%)	6,6,6	0.58	0
2	ADP	X	800	4	24,29,29	0.91	2 (8%)	23,45,45	1.46	5 (21%)
3	PO4	X	801	-	4,4,4	1.50	1 (25%)	6,6,6	0.39	0
3	PO4	X	802	-	4,4,4	1.71	1 (25%)	6,6,6	0.43	0
3	PO4	X	803	-	4,4,4	1.73	1 (25%)	6,6,6	0.73	0
2	ADP	Y	800	4	24,29,29	0.87	1 (4%)	23,45,45	1.29	3 (13%)
3	PO4	Y	801	4	4,4,4	2.01	1 (25%)	6,6,6	0.36	0
3	PO4	Y	802	-	4,4,4	1.87	1 (25%)	6,6,6	0.34	0
3	PO4	Y	803	-	4,4,4	1.82	1 (25%)	6,6,6	0.66	0
2	ADP	Z	800	4	24,29,29	0.88	1 (4%)	23,45,45	1.33	2 (8%)
3	PO4	Z	801	-	4,4,4	1.77	1 (25%)	6,6,6	0.59	0
3	PO4	Z	802	-	4,4,4	1.91	1 (25%)	6,6,6	0.54	0
3	PO4	Z	803	-	4,4,4	1.62	1 (25%)	6,6,6	0.48	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	ADP	O	800	4	-	0/12/32/32	0/3/3/3
3	PO4	O	801	-	-	0/0/0/0	0/0/0/0
3	PO4	O	802	-	-	0/0/0/0	0/0/0/0
3	PO4	O	803	-	-	0/0/0/0	0/0/0/0
2	ADP	P	800	4	-	0/12/32/32	0/3/3/3
3	PO4	P	801	-	-	0/0/0/0	0/0/0/0
3	PO4	P	802	-	-	0/0/0/0	0/0/0/0
3	PO4	P	803	-	-	0/0/0/0	0/0/0/0
2	ADP	Q	800	4	-	0/12/32/32	0/3/3/3
3	PO4	Q	801	4	-	0/0/0/0	0/0/0/0
3	PO4	Q	802	-	-	0/0/0/0	0/0/0/0
3	PO4	Q	803	-	-	0/0/0/0	0/0/0/0
2	ADP	R	800	4	-	0/12/32/32	0/3/3/3
3	PO4	R	801	-	-	0/0/0/0	0/0/0/0
3	PO4	R	802	-	-	0/0/0/0	0/0/0/0
3	PO4	R	803	-	-	0/0/0/0	0/0/0/0
2	ADP	S	800	4	-	0/12/32/32	0/3/3/3
3	PO4	S	801	-	-	0/0/0/0	0/0/0/0
3	PO4	S	802	-	-	0/0/0/0	0/0/0/0
3	PO4	S	803	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	T	376	-	-	0/0/0/0	0/0/0/0
2	ADP	T	800	4	-	0/12/32/32	0/3/3/3
3	PO4	T	801	4	-	0/0/0/0	0/0/0/0
3	PO4	T	802	-	-	0/0/0/0	0/0/0/0
3	PO4	T	803	-	-	0/0/0/0	0/0/0/0
2	ADP	U	800	4	-	0/12/32/32	0/3/3/3
3	PO4	U	801	-	-	0/0/0/0	0/0/0/0
3	PO4	U	802	-	-	0/0/0/0	0/0/0/0
3	PO4	U	803	-	-	0/0/0/0	0/0/0/0
2	ADP	V	800	4	-	0/12/32/32	0/3/3/3
3	PO4	V	802	-	-	0/0/0/0	0/0/0/0
3	PO4	V	803	-	-	0/0/0/0	0/0/0/0
2	ADP	W	800	4	-	0/12/32/32	0/3/3/3
3	PO4	W	801	-	-	0/0/0/0	0/0/0/0
3	PO4	W	802	-	-	0/0/0/0	0/0/0/0
3	PO4	W	803	-	-	0/0/0/0	0/0/0/0
2	ADP	X	800	4	-	0/12/32/32	0/3/3/3
3	PO4	X	801	-	-	0/0/0/0	0/0/0/0
3	PO4	X	802	-	-	0/0/0/0	0/0/0/0
3	PO4	X	803	-	-	0/0/0/0	0/0/0/0
2	ADP	Y	800	4	-	0/12/32/32	0/3/3/3
3	PO4	Y	801	4	-	0/0/0/0	0/0/0/0
3	PO4	Y	802	-	-	0/0/0/0	0/0/0/0
3	PO4	Y	803	-	-	0/0/0/0	0/0/0/0
2	ADP	Z	800	4	-	0/12/32/32	0/3/3/3
3	PO4	Z	801	-	-	0/0/0/0	0/0/0/0
3	PO4	Z	802	-	-	0/0/0/0	0/0/0/0
3	PO4	Z	803	-	-	0/0/0/0	0/0/0/0

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	800	ADP	C2'-C1'	-2.63	1.49	1.53
2	P	800	ADP	C2'-C1'	-2.39	1.49	1.53
2	W	800	ADP	C2'-C1'	-2.30	1.50	1.53
2	O	800	ADP	C2'-C1'	-2.22	1.50	1.53
2	W	800	ADP	PB-O2B	-2.20	1.47	1.54

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	800	ADP	O3B-PB-O1B	-3.26	99.99	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	800	ADP	O3B-PB-O1B	-3.26	100.00	110.63
2	R	800	ADP	O3B-PB-O1B	-3.25	100.01	110.63
2	W	800	ADP	O3B-PB-O1B	-3.25	100.02	110.63
2	Z	800	ADP	O3B-PB-O1B	-3.25	100.02	110.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	800	ADP	1	0
3	P	803	PO4	1	0
3	R	801	PO4	1	0
3	T	803	PO4	1	0
2	U	800	ADP	1	0
3	Y	801	PO4	2	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.