



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:40 PM BST

PDB ID : 2Y83  
EMDB ID: : EMD-1872  
Title : Actin filament pointed end  
Authors : Narita, A.; Oda, T.; Maeda, Y.  
Deposited on : 2011-02-02  
Resolution : 22.90 Å(reported)  
Based on PDB ID : 2ZWH

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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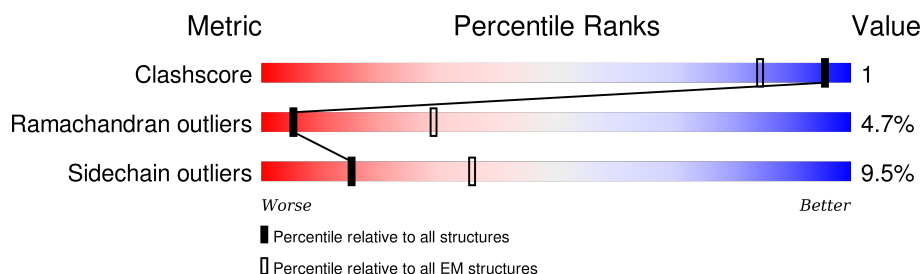
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 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 22.90 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	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  $\geq 3$ , 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	O	375	79% 18% ..
1	P	375	79% 18% ..
1	Q	375	79% 16% .
1	R	375	82% 15% ..
1	S	375	79% 17% ..
1	T	375	82% 14% ..

## 2 Entry composition [i](#)

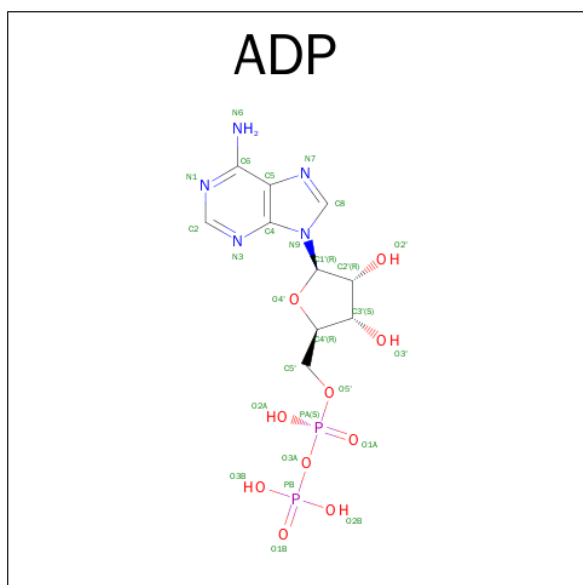
There are 3 unique types of molecules in this entry. The entry contains 33546 atoms, of which 15780 are hydrogens and 0 are deuteriums.

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	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	493	565	21		
1	P	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	493	565	21		
1	Q	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	493	565	21		
1	R	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	493	565	21		
1	S	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	493	565	21		
1	T	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	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	O	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	P	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	Q	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	R	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	S	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	T	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

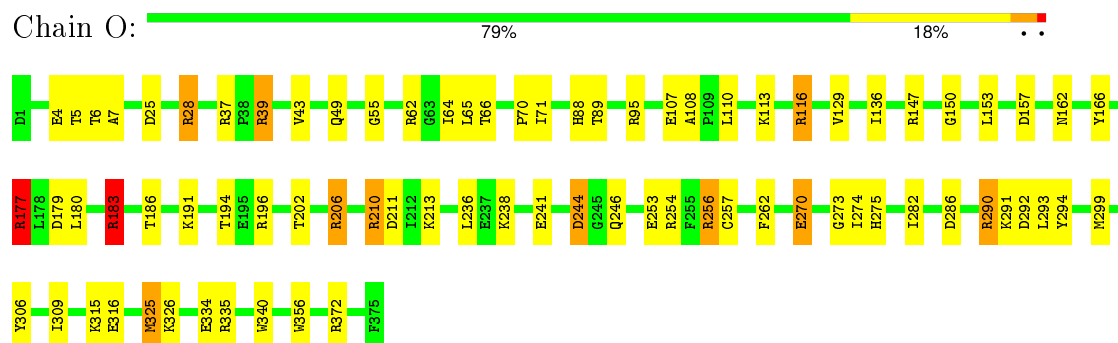
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	P	1	Total	Ca	0
			1	1	
3	Q	1	Total	Ca	0
			1	1	
3	T	1	Total	Ca	0
			1	1	
3	O	1	Total	Ca	0
			1	1	
3	R	1	Total	Ca	0
			1	1	
3	S	1	Total	Ca	0
			1	1	

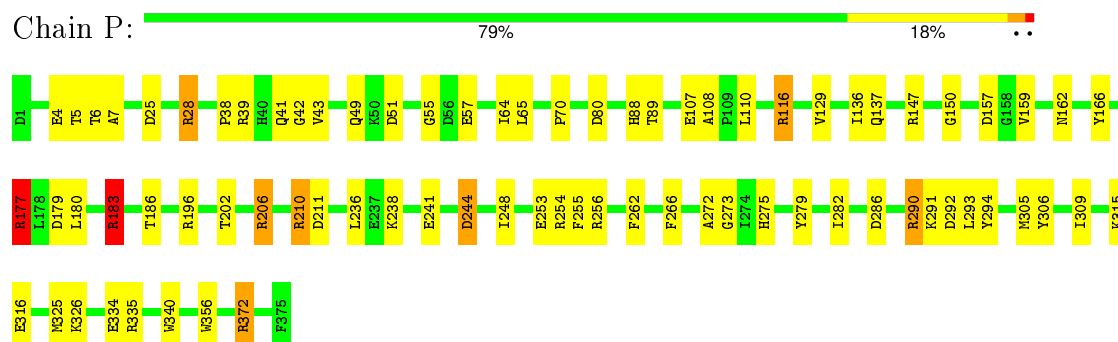
### 3 Residue-property plots

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

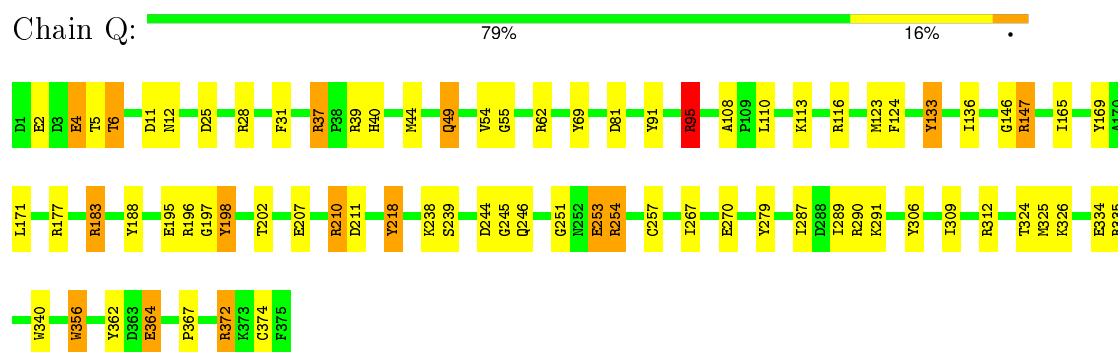
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



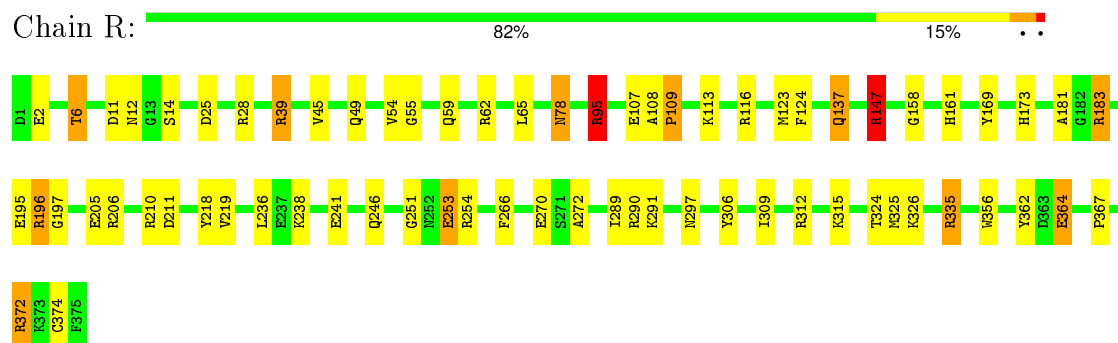
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



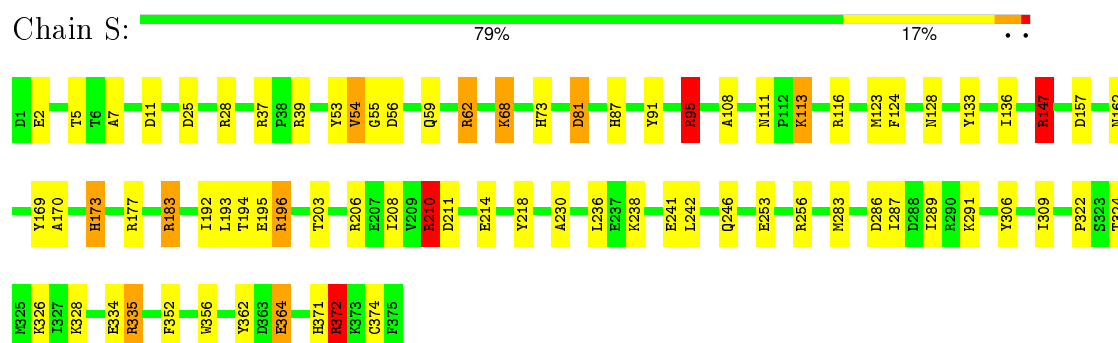
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



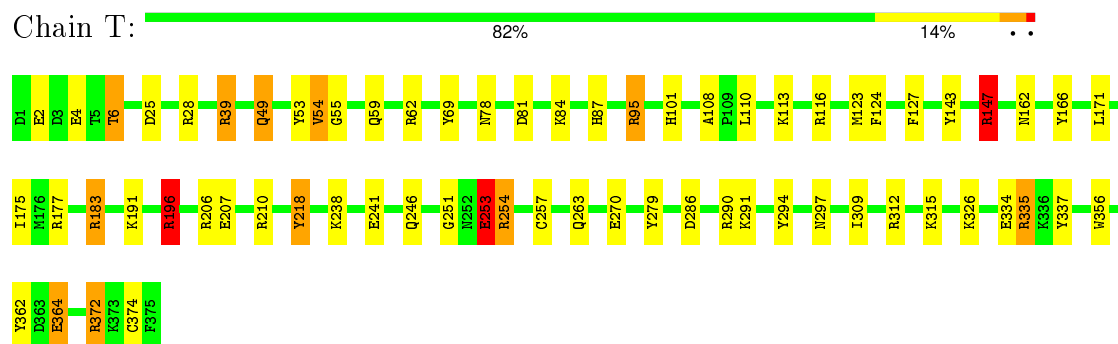
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE AND AMPLITUDE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	34	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	8000	Depositor
Magnification	40000	Depositor
Image detector	KODAK SO163 FILM	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.79	0/2996	1.26	17/4058 (0.4%)
1	P	0.79	0/2996	1.27	19/4058 (0.5%)
1	Q	0.69	0/2996	1.24	24/4058 (0.6%)
1	R	0.69	0/2996	1.18	17/4058 (0.4%)
1	S	0.68	0/2996	1.20	17/4058 (0.4%)
1	T	0.70	0/2996	1.23	28/4058 (0.7%)
All	All	0.72	0/17976	1.23	122/24348 (0.5%)

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	14
1	P	0	13
1	Q	0	13
1	R	0	12
1	S	0	16
1	T	0	12
All	All	0	80

There are no bond length outliers.

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	183	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	S	183	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	Q	183	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	Q	91	TYR	CB-CG-CD2	-9.42	115.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	218	TYR	CB-CG-CD2	-9.40	115.36	121.00
1	Q	210	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	R	183	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	Q	218	TYR	CB-CG-CD1	9.12	126.47	121.00
1	O	290	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	P	290	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	Q	62	ARG	NE-CZ-NH2	-8.47	116.07	120.30
1	S	169	TYR	CB-CG-CD2	-8.46	115.92	121.00
1	O	206	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	Q	91	TYR	CB-CG-CD1	8.38	126.03	121.00
1	P	206	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	O	210	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	S	169	TYR	CB-CG-CD1	8.30	125.98	121.00
1	T	254	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	Q	254	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	P	39	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	T	116	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	T	206	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	P	166	TYR	CB-CG-CD1	-7.60	116.44	121.00
1	O	62	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	O	166	TYR	CB-CG-CD1	-7.58	116.45	121.00
1	R	62	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	P	210	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	R	210	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	S	372	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	Q	124	PHE	CB-CG-CD2	-7.42	115.61	120.80
1	Q	124	PHE	CB-CG-CD1	7.29	125.90	120.80
1	T	143	TYR	CB-CG-CD2	-7.28	116.63	121.00
1	R	124	PHE	CB-CG-CD1	7.23	125.86	120.80
1	R	124	PHE	CB-CG-CD2	-7.12	115.82	120.80
1	T	124	PHE	CB-CG-CD2	-7.10	115.83	120.80
1	S	124	PHE	CB-CG-CD2	-7.05	115.87	120.80
1	T	143	TYR	CB-CG-CD1	7.03	125.22	121.00
1	S	62	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	T	290	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	R	372	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	Q	372	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	T	124	PHE	CB-CG-CD1	6.86	125.60	120.80
1	S	147	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	S	124	PHE	CB-CG-CD1	6.85	125.59	120.80
1	S	37	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	T	147	ARG	NE-CZ-NH1	6.74	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	11	ASP	CB-CG-OD1	6.74	124.36	118.30
1	O	177	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	T	210	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	R	147	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	T	279	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	S	95	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	T	372	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	S	210	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	T	337	TYR	CB-CG-CD2	-6.56	117.06	121.00
1	O	116	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	O	62	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	Q	62	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	R	62	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	T	218	TYR	CB-CG-CD2	-6.41	117.16	121.00
1	T	39	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	P	177	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	T	337	TYR	CB-CG-CD1	6.33	124.80	121.00
1	T	196	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	T	147	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	S	256	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	O	291	LYS	C-N-CA	6.09	136.93	121.70
1	P	166	TYR	CB-CG-CD2	6.06	124.64	121.00
1	P	266	PHE	CB-CG-CD1	6.05	125.04	120.80
1	T	294	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	S	335	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	T	218	TYR	CB-CG-CD1	6.04	124.62	121.00
1	Q	95	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	O	326	LYS	N-CA-CB	6.01	121.41	110.60
1	P	291	LYS	C-N-CA	5.99	136.67	121.70
1	O	166	TYR	CB-CG-CD2	5.96	124.58	121.00
1	Q	133	TYR	CB-CG-CD1	5.94	124.56	121.00
1	R	95	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	S	206	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	R	290	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	T	95	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	R	335	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	R	39	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	T	279	TYR	CB-CG-CD1	5.87	124.52	121.00
1	Q	183	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	T	335	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	Q	37	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	R	28	ARG	NE-CZ-NH2	-5.80	117.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	356	TRP	CA-CB-CG	5.80	124.72	113.70
1	P	254	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	T	6	THR	N-CA-CB	5.71	121.16	110.30
1	Q	147	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	P	196	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	Q	11	ASP	CB-CG-OD1	5.68	123.41	118.30
1	O	196	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	P	266	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	T	294	TYR	CB-CG-CD1	5.55	124.33	121.00
1	O	39	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	O	28	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	T	196	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	O	183	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	P	177	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	P	272	ALA	CB-CA-C	5.51	118.37	110.10
1	O	254	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	P	183	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	Q	279	TYR	CB-CG-CD2	-5.34	117.79	121.00
1	R	11	ASP	CB-CG-OD1	5.31	123.08	118.30
1	R	6	THR	N-CA-CB	5.31	120.38	110.30
1	P	57	GLU	N-CA-CB	5.30	120.15	110.60
1	P	28	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	Q	28	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	S	147	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	S	28	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	Q	6	THR	N-CA-CB	5.19	120.17	110.30
1	R	254	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	P	326	LYS	N-CA-CB	5.11	119.80	110.60
1	R	78	ASN	N-CA-CB	5.08	119.75	110.60
1	Q	69	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	T	290	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	P	279	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	O	325	MET	N-CA-C	5.02	124.55	111.00
1	Q	133	TYR	CB-CG-CD2	-5.01	117.99	121.00

There are no chirality outliers.

All (80) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	108	ALA	Peptide
1	O	116	ARG	Sidechain
1	O	177	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	O	179	ASP	Peptide
1	O	183	ARG	Sidechain
1	O	206	ARG	Sidechain
1	O	256	ARG	Sidechain
1	O	28	ARG	Sidechain
1	O	306	TYR	Sidechain
1	O	335	ARG	Sidechain
1	O	37	ARG	Sidechain
1	O	372	ARG	Sidechain
1	O	65	LEU	Peptide
1	O	95	ARG	Sidechain
1	P	108	ALA	Peptide
1	P	116	ARG	Sidechain
1	P	177	ARG	Sidechain
1	P	179	ASP	Peptide
1	P	183	ARG	Sidechain
1	P	206	ARG	Sidechain
1	P	255	PHE	Sidechain
1	P	256	ARG	Sidechain
1	P	28	ARG	Sidechain
1	P	306	TYR	Sidechain
1	P	335	ARG	Sidechain
1	P	372	ARG	Sidechain
1	P	65	LEU	Peptide
1	Q	108	ALA	Peptide
1	Q	116	ARG	Sidechain
1	Q	177	ARG	Sidechain
1	Q	188	TYR	Sidechain
1	Q	196	ARG	Sidechain
1	Q	198	TYR	Sidechain
1	Q	239	SER	Peptide
1	Q	254	ARG	Sidechain
1	Q	306	TYR	Peptide
1	Q	312	ARG	Sidechain
1	Q	335	ARG	Sidechain
1	Q	39	ARG	Sidechain
1	Q	95	ARG	Sidechain
1	R	108	ALA	Peptide
1	R	116	ARG	Sidechain
1	R	147	ARG	Sidechain
1	R	196	ARG	Sidechain
1	R	206	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	R	266	PHE	Sidechain
1	R	306	TYR	Peptide
1	R	312	ARG	Sidechain
1	R	335	ARG	Sidechain
1	R	45	VAL	Peptide
1	R	65	LEU	Peptide
1	R	95	ARG	Sidechain
1	S	108	ALA	Peptide
1	S	116	ARG	Sidechain
1	S	133	TYR	Sidechain
1	S	147	ARG	Sidechain
1	S	173	HIS	Sidechain
1	S	177	ARG	Sidechain
1	S	193	LEU	Peptide
1	S	196	ARG	Sidechain
1	S	210	ARG	Sidechain
1	S	306	TYR	Peptide
1	S	335	ARG	Sidechain
1	S	372	ARG	Sidechain
1	S	39	ARG	Sidechain
1	S	53	TYR	Sidechain
1	S	7	ALA	Peptide
1	S	95	ARG	Sidechain
1	T	108	ALA	Peptide
1	T	147	ARG	Sidechain
1	T	177	ARG	Sidechain
1	T	196	ARG	Sidechain
1	T	254	ARG	Sidechain
1	T	28	ARG	Sidechain
1	T	312	ARG	Sidechain
1	T	335	ARG	Sidechain
1	T	39	ARG	Sidechain
1	T	53	TYR	Sidechain
1	T	69	TYR	Peptide
1	T	95	ARG	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	2933	2618	2894	10	0
1	P	2933	2618	2894	9	0
1	Q	2933	2618	2894	8	0
1	R	2933	2618	2894	3	0
1	S	2933	2618	2894	13	0
1	T	2933	2618	2894	6	0
2	O	27	12	12	0	0
2	P	27	12	12	0	0
2	Q	27	12	12	0	0
2	R	27	12	12	0	0
2	S	27	12	12	0	0
2	T	27	12	12	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
All	All	17766	15780	17436	47	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 1.

All (47) 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:Q:253:GLU:H	1:Q:253:GLU:CD	2.02	0.64
1:S:208:ILE:HD12	1:S:242:LEU:HD22	1.83	0.61
1:T:54:VAL:HG22	1:T:55:GLY:H	1.70	0.57
1:R:253:GLU:CD	1:R:253:GLU:H	2.08	0.56
1:T:253:GLU:H	1:T:253:GLU:CD	2.09	0.56
1:P:262:PHE:HA	1:P:273:GLY:HA3	1.88	0.56
1:O:262:PHE:HA	1:O:273:GLY:HA3	1.86	0.56
1:S:113:LYS:HZ2	1:S:371:HIS:CE1	2.24	0.54
1:P:150:GLY:HA2	1:P:293:LEU:HA	1.90	0.54
1:O:150:GLY:HA2	1:O:293:LEU:HA	1.90	0.54
1:Q:54:VAL:HG22	1:Q:55:GLY:H	1.75	0.51
1:S:54:VAL:HG22	1:S:55:GLY:H	1.76	0.51
1:O:186:THR:HG23	1:O:210:ARG:HA	1.92	0.50
1:S:136:ILE:H	1:S:136:ILE:HD12	1.77	0.50
1:O:153:LEU:HD11	1:O:274:ILE:HB	1.93	0.49
1:R:364:GLU:H	1:R:364:GLU:CD	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:364:GLU:H	1:Q:364:GLU:CD	2.15	0.49
1:S:286:ASP:CG	1:S:287:ILE:H	2.17	0.48
1:S:364:GLU:CD	1:S:364:GLU:H	2.17	0.48
1:P:4:GLU:CD	1:P:5:THR:H	2.18	0.47
1:Q:287:ILE:HA	1:Q:290:ARG:HH12	1.79	0.47
1:O:270:GLU:H	1:O:270:GLU:CD	2.17	0.47
1:O:4:GLU:CD	1:O:5:THR:H	2.18	0.46
1:Q:136:ILE:H	1:Q:136:ILE:HD12	1.80	0.46
1:S:195:GLU:CD	1:T:113:LYS:HZ3	2.19	0.46
1:S:253:GLU:CD	1:S:253:GLU:H	2.19	0.46
1:S:87:HIS:CE1	1:S:91:TYR:CE1	3.06	0.44
1:Q:40:HIS:CE1	1:S:170:ALA:HA	2.52	0.44
1:T:364:GLU:CD	1:T:364:GLU:H	2.20	0.44
1:P:186:THR:HG23	1:P:210:ARG:HA	1.99	0.44
1:O:282:ILE:HD13	1:O:294:TYR:CE2	2.53	0.44
1:O:253:GLU:H	1:O:253:GLU:CD	2.21	0.43
1:P:253:GLU:H	1:P:253:GLU:CD	2.22	0.43
1:S:68:LYS:HZ1	1:S:81:ASP:CG	2.22	0.43
1:P:136:ILE:HD12	1:P:136:ILE:H	1.84	0.43
1:Q:4:GLU:CD	1:Q:5:THR:H	2.22	0.42
1:P:282:ILE:HD13	1:P:294:TYR:CE2	2.54	0.42
1:Q:165:ILE:HD12	1:Q:169:TYR:CE1	2.55	0.41
1:S:210:ARG:HH21	1:S:214:GLU:CD	2.24	0.41
1:R:109:PRO:HB2	1:R:161:HIS:CG	2.56	0.41
1:O:64:ILE:H	1:O:64:ILE:HD12	1.85	0.41
1:T:84:LYS:HA	1:T:87:HIS:CD2	2.55	0.41
1:T:87:HIS:CD2	1:T:127:PHE:CZ	3.09	0.41
1:P:248:ILE:H	1:P:248:ILE:HD12	1.85	0.41
1:S:62:ARG:HH22	1:S:211:ASP:CG	2.24	0.41
1:O:136:ILE:H	1:O:136:ILE:HD12	1.87	0.40
1:P:107:GLU:CD	1:P:116:ARG:HH12	2.25	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	O	373/375 (100%)	301 (81%)	57 (15%)	15 (4%)	4	35
1	P	373/375 (100%)	306 (82%)	50 (13%)	17 (5%)	3	33
1	Q	373/375 (100%)	299 (80%)	55 (15%)	19 (5%)	2	30
1	R	373/375 (100%)	298 (80%)	53 (14%)	22 (6%)	2	27
1	S	373/375 (100%)	301 (81%)	54 (14%)	18 (5%)	3	32
1	T	373/375 (100%)	301 (81%)	57 (15%)	15 (4%)	4	35
All	All	2238/2250 (100%)	1806 (81%)	326 (15%)	106 (5%)	5	32

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	70	PRO
1	O	180	LEU
1	P	70	PRO
1	P	180	LEU
1	Q	6	THR
1	Q	49	GLN
1	Q	81	ASP
1	Q	324	THR
1	R	6	THR
1	R	78	ASN
1	R	137	GLN
1	R	173	HIS
1	S	2	GLU
1	S	81	ASP
1	S	95	ARG
1	S	236	LEU
1	T	49	GLN
1	O	129	VAL
1	O	246	GLN
1	O	290	ARG
1	O	309	ILE
1	P	43	VAL
1	P	129	VAL
1	P	236	LEU
1	P	290	ARG
1	P	309	ILE
1	Q	95	ARG

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Mol	Chain	Res	Type
1	Q	146	GLY
1	Q	244	ASP
1	Q	267	ILE
1	R	2	GLU
1	R	55	GLY
1	R	236	LEU
1	R	272	ALA
1	R	324	THR
1	S	194	THR
1	S	289	ILE
1	T	6	THR
1	O	43	VAL
1	O	236	LEU
1	O	244	ASP
1	P	110	LEU
1	Q	2	GLU
1	Q	251	GLY
1	R	95	ARG
1	R	253	GLU
1	R	315	LYS
1	R	374	CYS
1	S	25	ASP
1	S	203	THR
1	S	324	THR
1	T	2	GLU
1	T	110	LEU
1	O	25	ASP
1	O	89	THR
1	O	110	LEU
1	P	25	ASP
1	P	51	ASP
1	Q	25	ASP
1	Q	110	LEU
1	Q	309	ILE
1	Q	362	TYR
1	Q	374	CYS
1	R	25	ASP
1	R	362	TYR
1	S	5	THR
1	S	128	ASN
1	S	309	ILE
1	S	362	TYR

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Mol	Chain	Res	Type
1	T	25	ASP
1	T	62	ARG
1	T	253	GLU
1	T	315	LYS
1	O	7	ALA
1	P	7	ALA
1	P	244	ASP
1	Q	245	GLY
1	Q	257	CYS
1	R	181	ALA
1	R	197	GLY
1	R	251	GLY
1	R	309	ILE
1	T	257	CYS
1	T	309	ILE
1	T	374	CYS
1	P	89	THR
1	P	137	GLN
1	S	73	HIS
1	S	230	ALA
1	S	322	PRO
1	S	374	CYS
1	T	54	VAL
1	T	362	TYR
1	P	42	GLY
1	Q	197	GLY
1	Q	289	ILE
1	S	54	VAL
1	O	55	GLY
1	P	55	GLY
1	R	289	ILE
1	O	71	ILE
1	P	38	PRO
1	R	158	GLY
1	T	251	GLY
1	T	175	ILE
1	R	54	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	O	318/318 (100%)	285 (90%)	33 (10%)	9	36
1	P	318/318 (100%)	290 (91%)	28 (9%)	12	45
1	Q	318/318 (100%)	286 (90%)	32 (10%)	9	38
1	R	318/318 (100%)	287 (90%)	31 (10%)	10	40
1	S	318/318 (100%)	291 (92%)	27 (8%)	13	48
1	T	318/318 (100%)	288 (91%)	30 (9%)	11	42
All	All	1908/1908 (100%)	1727 (90%)	181 (10%)	15	41

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	6	THR
1	O	39	ARG
1	O	49	GLN
1	O	66	THR
1	O	88	HIS
1	O	107	GLU
1	O	113	LYS
1	O	147	ARG
1	O	157	ASP
1	O	162	ASN
1	O	177	ARG
1	O	183	ARG
1	O	191	LYS
1	O	194	THR
1	O	202	THR
1	O	211	ASP
1	O	213	LYS
1	O	238	LYS
1	O	241	GLU
1	O	244	ASP
1	O	256	ARG
1	O	257	CYS
1	O	270	GLU
1	O	275	HIS
1	O	286	ASP
1	O	292	ASP

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Mol	Chain	Res	Type
1	O	299	MET
1	O	315	LYS
1	O	316	GLU
1	O	325	MET
1	O	334	GLU
1	O	340	TRP
1	O	356	TRP
1	P	6	THR
1	P	41	GLN
1	P	49	GLN
1	P	64	ILE
1	P	80	ASP
1	P	88	HIS
1	P	147	ARG
1	P	157	ASP
1	P	159	VAL
1	P	162	ASN
1	P	177	ARG
1	P	183	ARG
1	P	202	THR
1	P	211	ASP
1	P	238	LYS
1	P	241	GLU
1	P	244	ASP
1	P	275	HIS
1	P	286	ASP
1	P	292	ASP
1	P	305	MET
1	P	315	LYS
1	P	316	GLU
1	P	325	MET
1	P	334	GLU
1	P	340	TRP
1	P	356	TRP
1	P	372	ARG
1	Q	4	GLU
1	Q	12	ASN
1	Q	31	PHE
1	Q	37	ARG
1	Q	44	MET
1	Q	49	GLN
1	Q	113	LYS

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Mol	Chain	Res	Type
1	Q	123	MET
1	Q	133	TYR
1	Q	147	ARG
1	Q	171	LEU
1	Q	183	ARG
1	Q	195	GLU
1	Q	198	TYR
1	Q	202	THR
1	Q	207	GLU
1	Q	210	ARG
1	Q	211	ASP
1	Q	218	TYR
1	Q	238	LYS
1	Q	246	GLN
1	Q	253	GLU
1	Q	270	GLU
1	Q	291	LYS
1	Q	325	MET
1	Q	326	LYS
1	Q	334	GLU
1	Q	340	TRP
1	Q	356	TRP
1	Q	364	GLU
1	Q	367	PRO
1	Q	372	ARG
1	R	12	ASN
1	R	14	SER
1	R	39	ARG
1	R	49	GLN
1	R	59	GLN
1	R	107	GLU
1	R	109	PRO
1	R	113	LYS
1	R	123	MET
1	R	137	GLN
1	R	147	ARG
1	R	169	TYR
1	R	183	ARG
1	R	195	GLU
1	R	196	ARG
1	R	205	GLU
1	R	211	ASP

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Mol	Chain	Res	Type
1	R	218	TYR
1	R	219	VAL
1	R	238	LYS
1	R	241	GLU
1	R	246	GLN
1	R	270	GLU
1	R	291	LYS
1	R	297	ASN
1	R	325	MET
1	R	326	LYS
1	R	356	TRP
1	R	364	GLU
1	R	367	PRO
1	R	372	ARG
1	S	56	ASP
1	S	59	GLN
1	S	68	LYS
1	S	111	ASN
1	S	113	LYS
1	S	123	MET
1	S	147	ARG
1	S	157	ASP
1	S	162	ASN
1	S	173	HIS
1	S	183	ARG
1	S	192	ILE
1	S	196	ARG
1	S	210	ARG
1	S	218	TYR
1	S	238	LYS
1	S	241	GLU
1	S	246	GLN
1	S	283	MET
1	S	291	LYS
1	S	326	LYS
1	S	328	LYS
1	S	334	GLU
1	S	352	PHE
1	S	356	TRP
1	S	364	GLU
1	S	372	ARG
1	T	4	GLU

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Mol	Chain	Res	Type
1	T	49	GLN
1	T	59	GLN
1	T	78	ASN
1	T	81	ASP
1	T	101	HIS
1	T	123	MET
1	T	147	ARG
1	T	162	ASN
1	T	166	TYR
1	T	171	LEU
1	T	183	ARG
1	T	191	LYS
1	T	196	ARG
1	T	207	GLU
1	T	218	TYR
1	T	238	LYS
1	T	241	GLU
1	T	246	GLN
1	T	253	GLU
1	T	263	GLN
1	T	270	GLU
1	T	286	ASP
1	T	291	LYS
1	T	297	ASN
1	T	326	LYS
1	T	334	GLU
1	T	356	TRP
1	T	364	GLU
1	T	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	88	HIS
1	O	173	HIS
1	O	246	GLN
1	P	88	HIS
1	Q	40	HIS
1	R	73	HIS
1	R	87	HIS
1	R	92	ASN
1	S	246	GLN

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Mol	Chain	Res	Type
1	T	87	HIS
1	T	297	ASN

### 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 ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	400	3	24,29,29	0.89	0	23,45,45	1.59	4 (17%)
2	ADP	P	400	3	24,29,29	0.89	0	23,45,45	1.61	4 (17%)
2	ADP	Q	400	3	24,29,29	0.81	0	23,45,45	1.30	5 (21%)
2	ADP	R	400	3	24,29,29	0.78	0	23,45,45	1.43	3 (13%)
2	ADP	S	400	3	24,29,29	0.72	0	23,45,45	1.20	3 (13%)
2	ADP	T	400	3	24,29,29	0.74	0	23,45,45	0.98	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
2	ADP	O	400	3	-	0/12/32/32	0/3/3/3
2	ADP	P	400	3	-	0/12/32/32	0/3/3/3
2	ADP	Q	400	3	-	0/12/32/32	0/3/3/3
2	ADP	R	400	3	-	0/12/32/32	0/3/3/3
2	ADP	S	400	3	-	0/12/32/32	0/3/3/3
2	ADP	T	400	3	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	400	ADP	O3B-PB-O1B	-4.66	95.43	110.63
2	P	400	ADP	O3B-PB-O1B	-4.61	95.57	110.63
2	R	400	ADP	O3B-PB-O1B	-4.47	96.04	110.63
2	S	400	ADP	O3B-PB-O1B	-3.42	99.47	110.63
2	Q	400	ADP	O3B-PB-O1B	-3.17	100.30	110.63
2	T	400	ADP	O3B-PB-O1B	-2.90	101.17	110.63
2	P	400	ADP	C4'-O4'-C1'	-2.79	106.68	109.64
2	Q	400	ADP	C1'-N9-C4	-2.55	123.96	126.81
2	O	400	ADP	C4'-O4'-C1'	-2.54	106.95	109.64
2	O	400	ADP	O5'-PA-O1A	-2.13	100.50	109.21
2	P	400	ADP	O5'-PA-O1A	-2.12	100.54	109.21
2	Q	400	ADP	C4'-O4'-C1'	-2.02	107.50	109.64
2	S	400	ADP	O2B-PB-O1B	2.11	117.51	110.63
2	Q	400	ADP	O3B-PB-O2B	2.35	116.07	107.44
2	R	400	ADP	O2B-PB-O1B	2.40	118.47	110.63
2	Q	400	ADP	O2B-PB-O1B	2.41	118.49	110.63
2	T	400	ADP	O3B-PB-O2B	2.53	116.74	107.44
2	S	400	ADP	O3B-PB-O2B	2.77	117.61	107.44
2	R	400	ADP	O2A-PA-O3A	3.25	119.19	105.27
2	P	400	ADP	O2A-PA-O3A	3.26	119.23	105.27
2	O	400	ADP	O2A-PA-O3A	3.33	119.56	105.27

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.