



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 03:59 PM EDT

PDB ID : 1DEJ  
Title : CRYSTAL STRUCTURE OF A DICTYOSTELIUM/TETRAHYMENA CHIMERA ACTIN (MUTANT 646: Q228K/T229A/A230Y/A231K/S232E/E360H) IN COMPLEX WITH HUMAN GELSOLIN SEGMENT 1  
Authors : Matsuura, Y.; Stewart, M.; Kawamoto, M.; Kamiya, N.; Saeki, K.; Yasunaga, T.; Wakabayashi, T.  
Deposited on : 1999-11-15  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

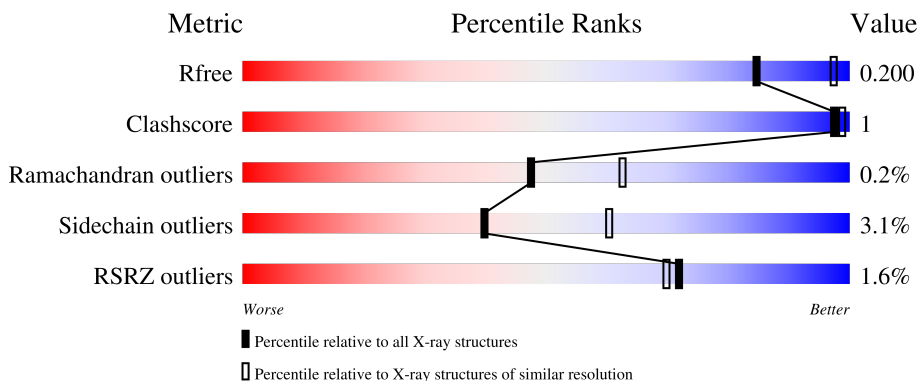
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


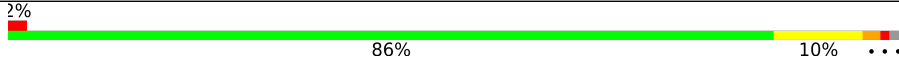
The reported resolution of this entry is 2.40 Å.

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S	127	 89% 9% .
2	A	375	 2% 86% 10% ...

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4329 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 GELSOLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	S	127	1005	649	166	187	3	8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	35	CYS	ASN	engineered mutation	UNP P06396
S	1	MET	-	expression tag	UNP P06396
S	2	GLY	-	expression tag	UNP P06396
S	3	SER	-	expression tag	UNP P06396

- Molecule 2 is a protein called CHIMERIC ACTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	368	2885	1830	485	551	19	27	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	HIS	GLU	SEE REMARK 999	UNP P07830
A	73	HIC	HIS	modified residue	UNP P07830

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	2	Total	Ca	0	0
			2	2		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
4	A	1	31	10	5	13	3	0	0


- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	150	Total O 150 150	0	0
5	A	255	Total O 255 255	0	0

### 3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

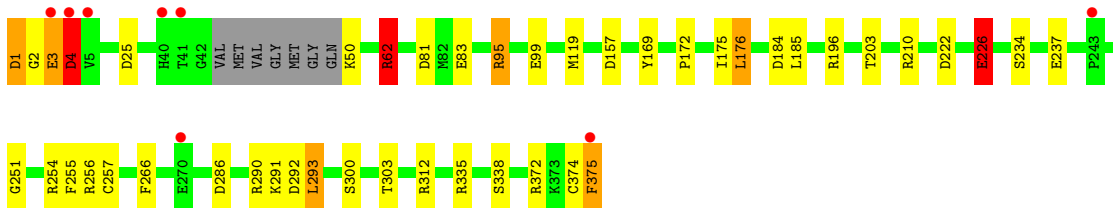
- Molecule 1: GELSOLIN

Chain S:  89% 9%



- Molecule 2: CHIMERIC ACTIN

Chain A:  2% 86% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.89Å 69.39Å 183.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 29.62 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.40) 93.6 (29.62-2.40)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	16.65 (at 2.39Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.171 , 0.214 0.163 , 0.200	Depositor DCC
$R_{free}$ test set	1396 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.4	Xtrriage
Anisotropy	0.248	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 63.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4329	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: CA, HIC, ATP

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  >5	RMSZ	# Z  >5
1	S	0.73	1/1031 (0.1%)	1.50	20/1392 (1.4%)
2	A	1.07	8/2935 (0.3%)	1.85	53/3967 (1.3%)
All	All	0.99	9/3966 (0.2%)	1.76	73/5359 (1.4%)

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
2	A	1	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4	ASP	CG-OD2	30.55	1.95	1.25
2	A	50	LYS	CB-CG	26.37	2.23	1.52
1	S	1	MET	C-N	10.33	1.51	1.33
2	A	3	GLU	CB-CG	9.95	1.71	1.52
2	A	2	GLY	N-CA	9.59	1.60	1.46
2	A	2	GLY	CA-C	8.47	1.65	1.51
2	A	1	ASP	C-N	7.53	1.46	1.33
2	A	291	LYS	CG-CD	6.95	1.76	1.52
2	A	1	ASP	CA-C	5.86	1.68	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	256	ARG	CD-NE-CZ	32.35	168.90	123.60
2	A	3	GLU	CA-CB-CG	-28.84	49.95	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4	ASP	CB-CG-OD1	22.78	138.80	118.30
2	A	62	ARG	CD-NE-CZ	22.56	155.19	123.60
2	A	375	PHE	N-CA-CB	19.53	145.75	110.60
2	A	4	ASP	OD1-CG-OD2	-19.14	86.93	123.30
2	A	50	LYS	CA-CB-CG	-18.41	72.90	113.40
2	A	95	ARG	CD-NE-CZ	17.74	148.44	123.60
2	A	256	ARG	NE-CZ-NH1	17.51	129.06	120.30
2	A	3	GLU	CB-CG-CD	-16.91	68.53	114.20
2	A	372	ARG	CD-NE-CZ	16.23	146.32	123.60
2	A	372	ARG	NE-CZ-NH2	-15.32	112.64	120.30
1	S	1	MET	C-N-CA	12.35	148.23	122.30
2	A	286	ASP	CB-CG-OD2	11.73	128.86	118.30
2	A	372	ARG	NE-CZ-NH1	11.09	125.84	120.30
2	A	95	ARG	NE-CZ-NH1	10.11	125.36	120.30
1	S	1	MET	O-C-N	-9.91	106.35	123.20
2	A	312	ARG	NE-CZ-NH1	9.81	125.20	120.30
2	A	375	PHE	CB-CG-CD1	-9.76	113.97	120.80
1	S	111	TYR	CB-CG-CD2	-9.74	115.16	121.00
2	A	256	ARG	NE-CZ-NH2	-9.26	115.67	120.30
2	A	95	ARG	NE-CZ-NH2	-9.04	115.78	120.30
2	A	290	ARG	NE-CZ-NH2	-8.91	115.84	120.30
2	A	50	LYS	CB-CG-CD	-8.75	88.85	111.60
2	A	1	ASP	O-C-N	-8.70	108.42	123.20
1	S	39	ASP	CB-CG-OD1	8.65	126.08	118.30
2	A	25	ASP	CB-CG-OD1	8.36	125.82	118.30
2	A	266	PHE	CB-CG-CD2	8.22	126.55	120.80
1	S	93	ARG	NE-CZ-NH2	8.17	124.39	120.30
2	A	290	ARG	NE-CZ-NH1	8.14	124.37	120.30
2	A	81	ASP	CB-CG-OD1	7.80	125.32	118.30
2	A	1	ASP	CB-CA-C	-7.77	94.86	110.40
1	S	93	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	S	87	ASP	CB-CG-OD2	-7.64	111.42	118.30
2	A	292	ASP	CB-CG-OD2	7.63	125.17	118.30
1	S	111	TYR	CB-CG-CD1	7.53	125.52	121.00
2	A	169	TYR	CB-CG-CD2	-7.39	116.56	121.00
1	S	1	MET	CA-C-N	7.32	130.85	116.20
2	A	256	ARG	CG-CD-NE	7.16	126.83	111.80
2	A	83	GLU	OE1-CD-OE2	7.04	131.75	123.30
1	S	42	THR	CA-CB-CG2	-6.95	102.67	112.40
2	A	196	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	S	88	ASP	CB-CG-OD1	6.32	123.99	118.30
2	A	1	ASP	CA-C-N	6.28	128.76	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	1	MET	CG-SD-CE	6.12	110.00	100.20
2	A	303	THR	CA-CB-CG2	6.07	120.90	112.40
2	A	184	ASP	CB-CG-OD2	5.98	123.68	118.30
1	S	112	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	S	12	LYS	CB-CG-CD	5.73	126.49	111.60
2	A	300	SER	N-CA-CB	-5.72	101.92	110.50
2	A	176	LEU	CA-CB-CG	5.68	128.36	115.30
2	A	210	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	S	1	MET	CB-CA-C	5.64	121.68	110.40
2	A	254	ARG	NE-CZ-NH1	5.61	123.10	120.30
2	A	222	ASP	CB-CG-OD1	5.59	123.33	118.30
2	A	119	MET	CA-CB-CG	5.58	122.79	113.30
2	A	374	CYS	CA-CB-SG	-5.56	103.99	114.00
2	A	312	ARG	NE-CZ-NH2	-5.49	117.56	120.30
2	A	99	GLU	OE1-CD-OE2	-5.46	116.74	123.30
2	A	286	ASP	OD1-CG-OD2	-5.36	113.12	123.30
1	S	55	ARG	CB-CG-CD	5.33	125.45	111.60
1	S	118	TYR	CA-CB-CG	5.29	123.46	113.40
2	A	374	CYS	CA-C-N	-5.25	105.66	117.20
2	A	266	PHE	CB-CG-CD1	-5.24	117.13	120.80
2	A	293	LEU	CB-CG-CD1	5.22	119.88	111.00
1	S	87	ASP	CB-CG-OD1	5.16	122.95	118.30
2	A	196	ARG	CD-NE-CZ	5.15	130.81	123.60
2	A	157	ASP	CB-CG-OD1	5.15	122.93	118.30
2	A	226	GLU	CB-CG-CD	5.11	127.99	114.20
2	A	62	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	A	210	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	S	39	ASP	OD1-CG-OD2	-5.02	113.76	123.30
1	S	25	GLU	OE1-CD-OE2	-5.01	117.29	123.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	375	PHE	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	4	ASP	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	S	1005	0	971	0	12
2	A	2885	0	2847	6	0
3	A	1	0	0	0	0
3	S	2	0	0	0	0
4	A	31	0	12	0	0
5	A	255	0	0	1	0
5	S	150	0	0	0	12
All	All	4329	0	3830	6	12

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 (6) 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:A:62:ARG:HH21	2:A:203:THR:HG22	1.80	0.47
2:A:237:GLU:HG2	2:A:251:GLY:HA2	1.99	0.45
2:A:335:ARG:HA	2:A:338:SER:OG	2.17	0.45
2:A:95:ARG:HD2	5:A:1460:HOH:O	2.19	0.42
2:A:172:PRO:HA	2:A:175:ILE:HD12	2.03	0.40
2:A:226:GLU:HB3	2:A:255:PHE:CZ	2.57	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1:MET:CA	5:S:216:HOH:O[3_645]	1.03	1.17
1:S:1:MET:CG	5:S:254:HOH:O[3_645]	1.08	1.12
1:S:1:MET:SD	5:S:238:HOH:O[3_645]	1.23	0.97
1:S:1:MET:CB	5:S:254:HOH:O[3_645]	1.35	0.85
1:S:1:MET:CE	5:S:165:HOH:O[3_645]	1.38	0.82
1:S:1:MET:N	5:S:216:HOH:O[3_645]	1.47	0.73
1:S:1:MET:CE	5:S:238:HOH:O[3_645]	1.75	0.45
1:S:1:MET:C	5:S:216:HOH:O[3_645]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1:MET:CA	5:S:254:HOH:O[3_645]	2.01	0.19
1:S:1:MET:SD	5:S:265:HOH:O[3_645]	2.10	0.10
1:S:1:MET:N	5:S:254:HOH:O[3_645]	2.12	0.08
1:S:1:MET:CG	5:S:238:HOH:O[3_645]	2.19	0.01

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	S	125/127 (98%)	121 (97%)	4 (3%)	0	100	100
2	A	361/375 (96%)	352 (98%)	8 (2%)	1 (0%)	41	55
All	All	486/502 (97%)	473 (97%)	12 (2%)	1 (0%)	47	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	4	ASP

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	S	104/104 (100%)	101 (97%)	3 (3%)	42	62
2	A	310/315 (98%)	300 (97%)	10 (3%)	39	59
All	All	414/419 (99%)	401 (97%)	13 (3%)	40	60

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	16	GLU
1	S	36	LEU
1	S	55	ARG
2	A	1	ASP
2	A	3	GLU
2	A	62	ARG
2	A	176	LEU
2	A	185	LEU
2	A	226	GLU
2	A	234	SER
2	A	257	CYS
2	A	293	LEU
2	A	375	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	161	HIS
2	A	280	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](#)

1 non-standard protein/DNA/RNA residue is 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	8,11,12	0.68	0	6,14,16	1.24	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	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	ATP	A	1376	3	26,33,33	1.35	3 (11%)	31,52,52	1.39	5 (16%)

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	ATP	A	1376	3	-	1/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1376	ATP	C8-N7	-3.16	1.29	1.34
4	A	1376	ATP	C2-N1	2.43	1.38	1.33
4	A	1376	ATP	PG-O3G	-2.05	1.47	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1376	ATP	C1'-N9-C4	3.88	133.45	126.64
4	A	1376	ATP	C5-C6-N6	3.10	125.06	120.35
4	A	1376	ATP	O4'-C4'-C3'	2.52	110.10	105.11
4	A	1376	ATP	C4-C5-N7	2.31	111.80	109.40
4	A	1376	ATP	O4'-C1'-C2'	-2.09	103.88	106.93

There are no chirality outliers.

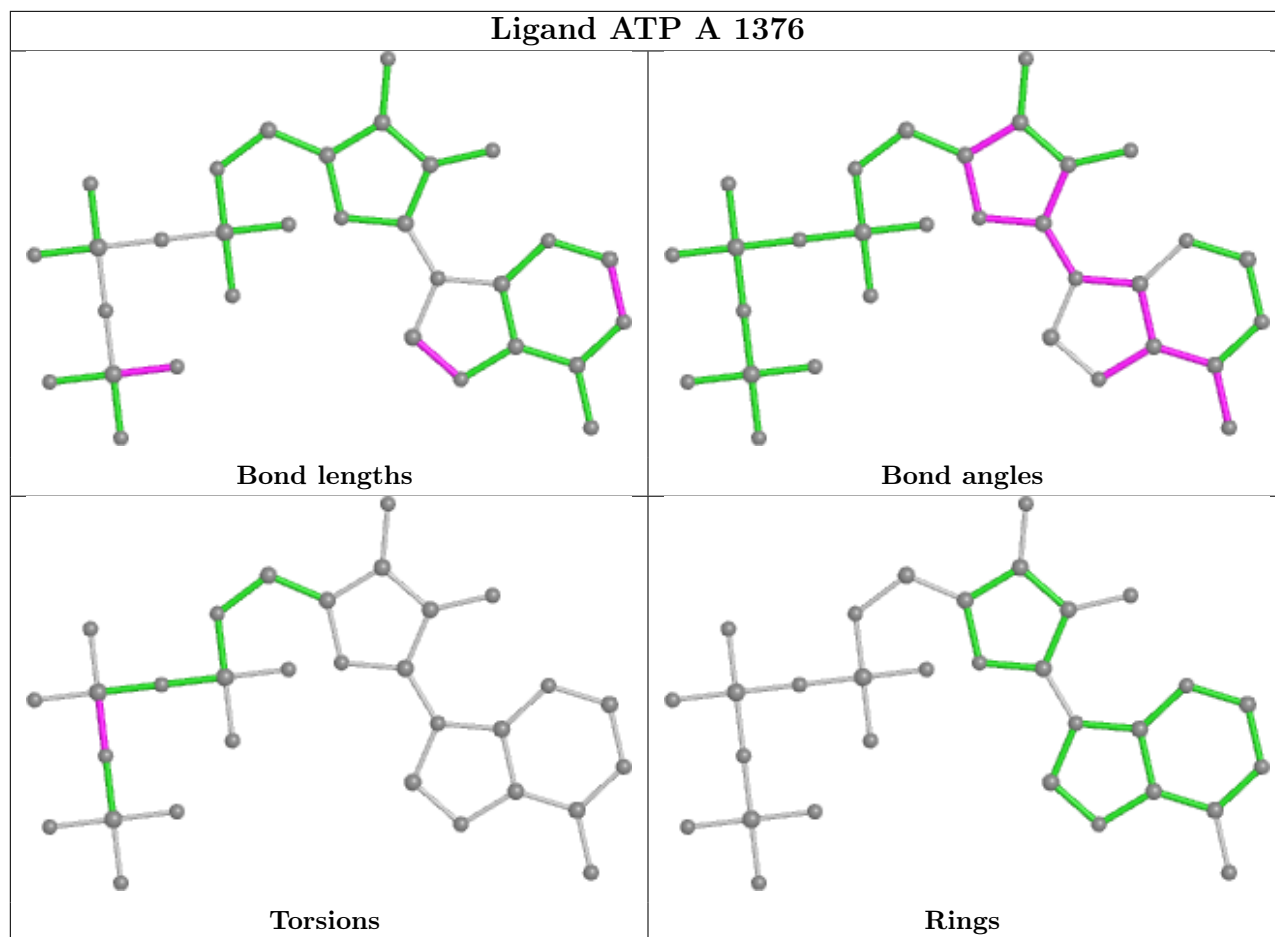
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1376	ATP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2:GLY	C	3:GLU	N	2.43

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	S	126/127 (99%)	-0.77	0 <b>100</b> <b>100</b>	13, 22, 34, 60	0
2	A	365/375 (97%)	-0.48	8 (2%) 62 60	14, 23, 52, 94	5 (1%)
All	All	491/502 (97%)	-0.55	8 (1%) 72 70	13, 23, 47, 94	5 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	3	GLU	6.6
2	A	41	THR	5.6
2	A	5	VAL	4.2
2	A	4	ASP	4.2
2	A	270	GLU	2.4
2	A	243	PRO	2.4
2	A	375	PHE	2.2
2	A	40	HIS	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	HIC	A	73	11/12	0.97	0.12	20,25,38,41	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

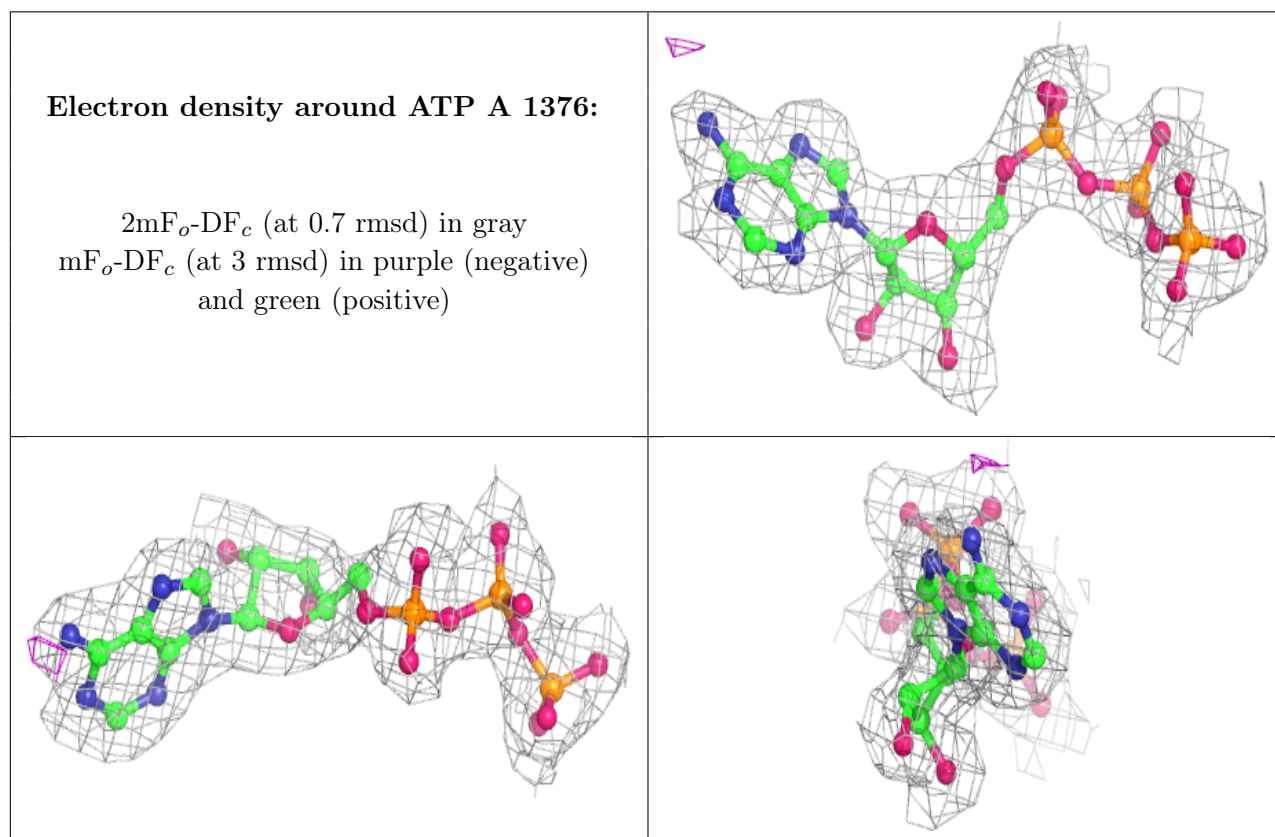


## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	S	128	1/1	0.99	0.04	20,20,20,20	0
3	CA	S	129	1/1	0.99	0.05	21,21,21,21	0
3	CA	A	377	1/1	0.99	0.07	21,21,21,21	0
4	ATP	A	1376	31/31	0.99	0.08	15,19,24,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.