



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 09:49 PM EDT

PDB ID : 1C0G
Title : CRYSTAL STRUCTURE OF 1:1 COMPLEX BETWEEN GELSOLIN SEGMENT 1 AND A DICTYOSTELIUM/TETRAHYMENA CHIMERA ACTIN (MUTANT 228: Q228K/T229A/A230Y/E360H)
Authors : Matsuura, Y.; Stewart, M.; Kawamoto, M.; Kamiya, N.; Saeki, K.; Yasunaga, T.; Wakabayashi, T.
Deposited on : unknown
Resolution : 2.00 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

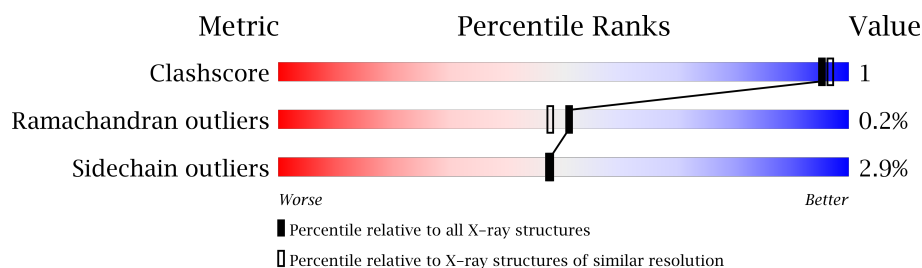
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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 on the lower 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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	S	127	 92% 7% .
2	A	375	 87% 9% ...

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4386 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 PROTEIN (GELSOLIN SEGMENT 1).

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1	MET	-	EXPRESSION ARTIFACT	UNP P06396
S	2	GLY	-	EXPRESSION ARTIFACT	UNP P06396
S	3	SER	-	EXPRESSION ARTIFACT	UNP P06396

- Molecule 2 is a protein called PROTEIN (CHIMERIC ACTIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	368	Total	C	N	O	S	27	0	0
			2878	1825	484	550	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIC	HIS	MODIFIED RESIDUE	UNP P07830
A	225	ALA	GLN	CONFLICT	UNP P07830
A	228	LYS	ALA	SEE REMARK 999	UNP P07830
A	229	ALA	THR	SEE REMARK 999	UNP P07830
A	230	TYR	ALA	SEE REMARK 999	UNP P07830
A	360	HIS	GLU	SEE REMARK 999	UNP P07830

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

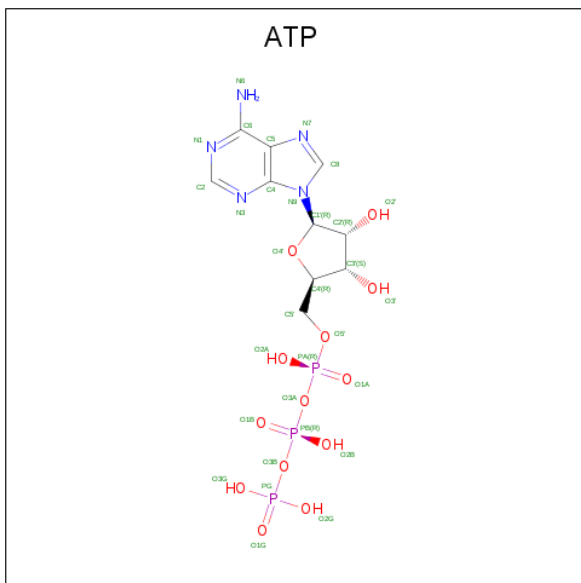
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	170	Total O 170 170	0	0
5	A	299	Total O 299 299	0	0

3 Residue-property plots [i](#)

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


Note EDS was not executed.

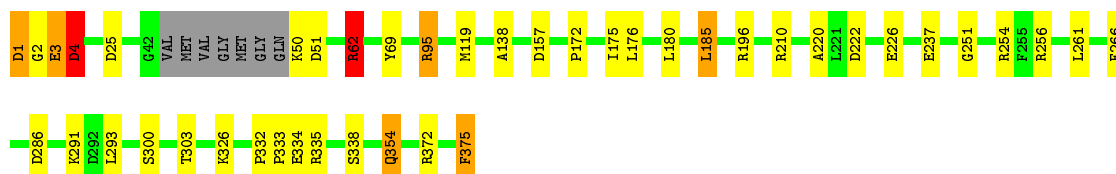
- Molecule 1: PROTEIN (GELSOLIN SEGMENT 1)

Chain S:  92% 7% .



- Molecule 2: PROTEIN (CHIMERIC ACTIN)

Chain A:  87% 9% ...



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.86Å 69.03Å 181.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4386	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.75	1/1031 (0.1%)	1.43	12/1392 (0.9%)
2	A	1.19	8/2928 (0.3%)	1.66	42/3959 (1.1%)
All	All	1.09	9/3959 (0.2%)	1.60	54/5351 (1.0%)

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	S	0	1
2	A	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	GLU	CB-CG	52.06	2.51	1.52
1	S	1	MET	C-N	15.82	1.61	1.33
2	A	50	LYS	CB-CG	11.94	1.84	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	4	ASP	CG-OD2	7.17	1.41	1.25
2	A	4	ASP	CG-OD1	-7.02	1.09	1.25
2	A	1	ASP	CA-C	5.86	1.68	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3	GLU	CA-CB-CG	-27.52	52.85	113.40
2	A	256	ARG	CD-NE-CZ	25.54	159.36	123.60
2	A	372	ARG	NE-CZ-NH2	-22.32	109.14	120.30
2	A	256	ARG	NE-CZ-NH1	19.24	129.92	120.30
1	S	1	MET	O-C-N	-17.57	93.34	123.20
2	A	4	ASP	CB-CG-OD2	-15.47	104.38	118.30
2	A	62	ARG	CD-NE-CZ	14.82	144.35	123.60
1	S	1	MET	CA-C-N	14.12	144.44	116.20
2	A	95	ARG	NE-CZ-NH1	13.80	127.20	120.30
2	A	3	GLU	CB-CG-CD	-13.65	77.34	114.20
2	A	95	ARG	NE-CZ-NH2	-13.09	113.76	120.30
2	A	256	ARG	NE-CZ-NH2	-12.35	114.13	120.30
2	A	50	LYS	CA-CB-CG	-12.27	86.40	113.40
2	A	372	ARG	CD-NE-CZ	11.26	139.36	123.60
2	A	95	ARG	CD-NE-CZ	9.62	137.08	123.60
2	A	372	ARG	NE-CZ-NH1	9.60	125.10	120.30
2	A	326	LYS	CD-CE-NZ	9.55	133.67	111.70
2	A	1	ASP	O-C-N	-8.70	108.42	123.20
2	A	25	ASP	CB-CG-OD1	8.63	126.06	118.30
2	A	62	ARG	NE-CZ-NH1	8.61	124.61	120.30
2	A	62	ARG	NE-CZ-NH2	-8.58	116.01	120.30
2	A	210	ARG	NE-CZ-NH1	8.49	124.54	120.30
2	A	375	PHE	N-CA-CB	8.16	125.28	110.60
2	A	286	ASP	CB-CG-OD2	8.00	125.50	118.30
2	A	1	ASP	CB-CA-C	-7.77	94.86	110.40
1	S	1	MET	C-N-CA	7.60	138.26	122.30
2	A	210	ARG	NE-CZ-NH2	-7.51	116.54	120.30
2	A	210	ARG	CD-NE-CZ	7.35	133.89	123.60
2	A	157	ASP	CB-CG-OD1	7.27	124.84	118.30
2	A	375	PHE	CB-CG-CD1	-7.08	115.85	120.80
1	S	99	GLU	OE1-CD-OE2	-6.77	115.18	123.30
2	A	266	PHE	CB-CG-CD2	6.77	125.54	120.80
2	A	334	GLU	OE1-CD-OE2	-6.66	115.30	123.30
2	A	254	ARG	CD-NE-CZ	6.43	132.61	123.60
2	A	185	LEU	CB-CG-CD1	6.43	121.93	111.00
2	A	1	ASP	CA-C-N	6.28	128.76	116.20
2	A	222	ASP	CB-CG-OD1	6.26	123.93	118.30
1	S	1	MET	CG-SD-CE	6.12	110.00	100.20
1	S	23	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	A	372	ARG	NH1-CZ-NH2	5.78	125.76	119.40
2	A	50	LYS	CB-CG-CD	-5.78	96.58	111.60
1	S	82	PHE	CB-CG-CD2	5.75	124.82	120.80
2	A	303	THR	CA-CB-CG2	5.72	120.41	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	69	TYR	CB-CG-CD1	5.70	124.42	121.00
1	S	1	MET	CB-CA-C	5.64	121.68	110.40
1	S	118	TYR	CA-CB-CG	5.61	124.06	113.40
1	S	82	PHE	CB-CG-CD1	-5.60	116.88	120.80
1	S	98	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	A	375	PHE	CB-CG-CD2	5.55	124.69	120.80
2	A	300	SER	N-CA-CB	-5.41	102.38	110.50
2	A	196	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	A	119	MET	CA-CB-CG	5.26	122.25	113.30
2	A	291	LYS	CG-CD-CE	-5.07	96.70	111.90
1	S	116	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	4	ASP	Sidechain
1	S	1	MET	Peptide

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	10
2	A	2878	0	2838	11	0
3	A	1	0	0	0	0
3	S	2	0	0	0	0
4	A	31	0	12	0	0
5	A	299	0	0	2	0
5	S	170	0	0	0	10
All	All	4386	0	3821	11	10

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 (11) 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:220:ALA:HB1	2:A:226:GLU:HG3	1.88	0.56
2:A:237:GLU:HG2	2:A:251:GLY:HA2	1.91	0.53
2:A:95:ARG:HD2	5:A:470:HOH:O	2.15	0.46
2:A:180:LEU:HD22	2:A:261:LEU:HD23	1.98	0.45
2:A:172:PRO:HA	2:A:175:ILE:HD12	1.98	0.45
2:A:354:GLN:H	2:A:354:GLN:HG2	1.57	0.43
2:A:335:ARG:HA	2:A:338:SER:OG	2.19	0.42
2:A:332:PRO:HA	2:A:333:PRO:HD3	1.92	0.41
2:A:62:ARG:HH11	2:A:62:ARG:HG2	1.85	0.41
2:A:220:ALA:CB	2:A:226:GLU:HG3	2.50	0.41
2:A:138:ALA:HA	5:A:668:HOH:O	2.20	0.41

All (10) 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:223:HOH:O[3_645]	0.32	1.88
1:S:1:MET:CG	5:S:269:HOH:O[3_645]	0.70	1.50
1:S:1:MET:SD	5:S:247:HOH:O[3_645]	0.82	1.38
1:S:1:MET:CE	5:S:247:HOH:O[3_645]	1.20	1.00
1:S:1:MET:N	5:S:223:HOH:O[3_645]	1.47	0.73
1:S:1:MET:C	5:S:223:HOH:O[3_645]	1.48	0.72
1:S:1:MET:CB	5:S:269:HOH:O[3_645]	1.57	0.63
1:S:1:MET:CE	5:S:167:HOH:O[3_645]	1.71	0.49
1:S:1:MET:CB	5:S:223:HOH:O[3_645]	1.80	0.40
1:S:1:MET:CG	5:S:247:HOH:O[3_645]	2.17	0.03

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	361/375 (96%)	355 (98%)	5 (1%)	1 (0%)	44	40
All	All	486/502 (97%)	476 (98%)	9 (2%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	4	ASP

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 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%)	48	47
2	A	309/314 (98%)	300 (97%)	9 (3%)	48	47
All	All	413/418 (99%)	401 (97%)	12 (3%)	48	47

All (12) 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	51	ASP
2	A	62	ARG
2	A	176	LEU
2	A	185	LEU
2	A	293	LEU
2	A	354	GLN
2	A	375	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	59	GLN
2	A	128	ASN
2	A	280	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	9,11,12	1.09	1 (11%)	7,14,16	1.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIC	A	73	2	-	0/4/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	73	HIC	CA-C	2.23	1.53	1.50

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 carbohydrates 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	376	3	27,33,33	1.33	4 (14%)	25,52,52	1.09	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	376	3	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	376	ATP	C8-N7	-2.99	1.29	1.34
4	A	376	ATP	PG-O2G	-2.16	1.45	1.54
4	A	376	ATP	C5-N7	-2.06	1.32	1.39
4	A	376	ATP	PG-O3B	2.74	1.64	1.60

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	376	ATP	C1'-N9-C4	2.09	130.25	126.64
4	A	376	ATP	C4-C5-N7	2.50	111.83	109.41

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	1
1	S	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	2.90
1	S	1:MET	C	2:GLY	N	1.61

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.