



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:47 AM GMT

PDB ID : 2IOA  
Title : E. coli Bifunctional glutathionylspermidine synthetase/amidase Incomplex with Mg<sup>2+</sup> and ADP and phosphinate inhibitor  
Authors : Pai, C.H.; Chiang, B.Y.; Ko, T.P.; Chou, C.C.; Chong, C.M.; Yen, F.J.; Coward, J.K.; Wang, A.H.-J.; Lin, C.H.  
Deposited on : 2006-10-10  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

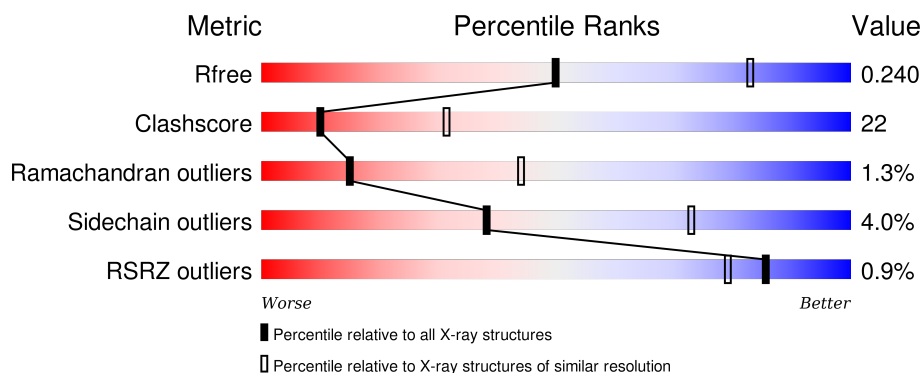
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	619	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 56%, green 37%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>56%</span> <span>37%</span> <span>• 5%</span> </div> </div>
1	B	619	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 58%, green 34%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>58%</span> <span>34%</span> <span>• 5%</span> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10089 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.

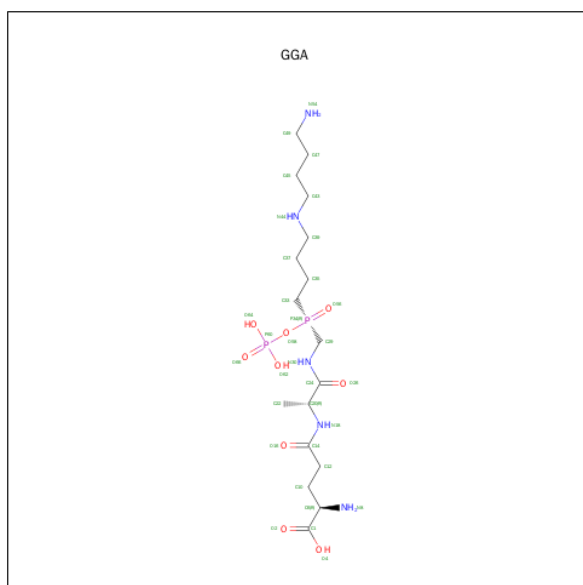
- Molecule 1 is a protein called Bifunctional glutathionylspermidine synthetase/amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4755	3051	813	872	19			
1	B	589	Total	C	N	O	S	0	0	0
			4753	3048	813	873	19			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

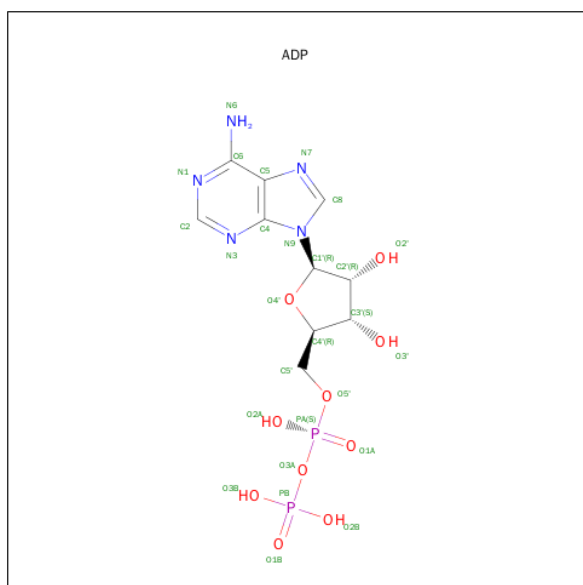
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is D-GAMMA-GLUTAMYL-N-{|(R)-{4-[(4-AMINO BUTYL)AMINO]BUTYL } (PHOSPHONOOXY)PHOSPHORYL] METHYL}-D-ALANINAMIDE (three-letter code: GGA) (formula: C<sub>17</sub>H<sub>37</sub>N<sub>5</sub>O<sub>9</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			33	17	5	9	2		
3	B	1	Total	C	N	O	P	0	0
			33	17	5	9	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

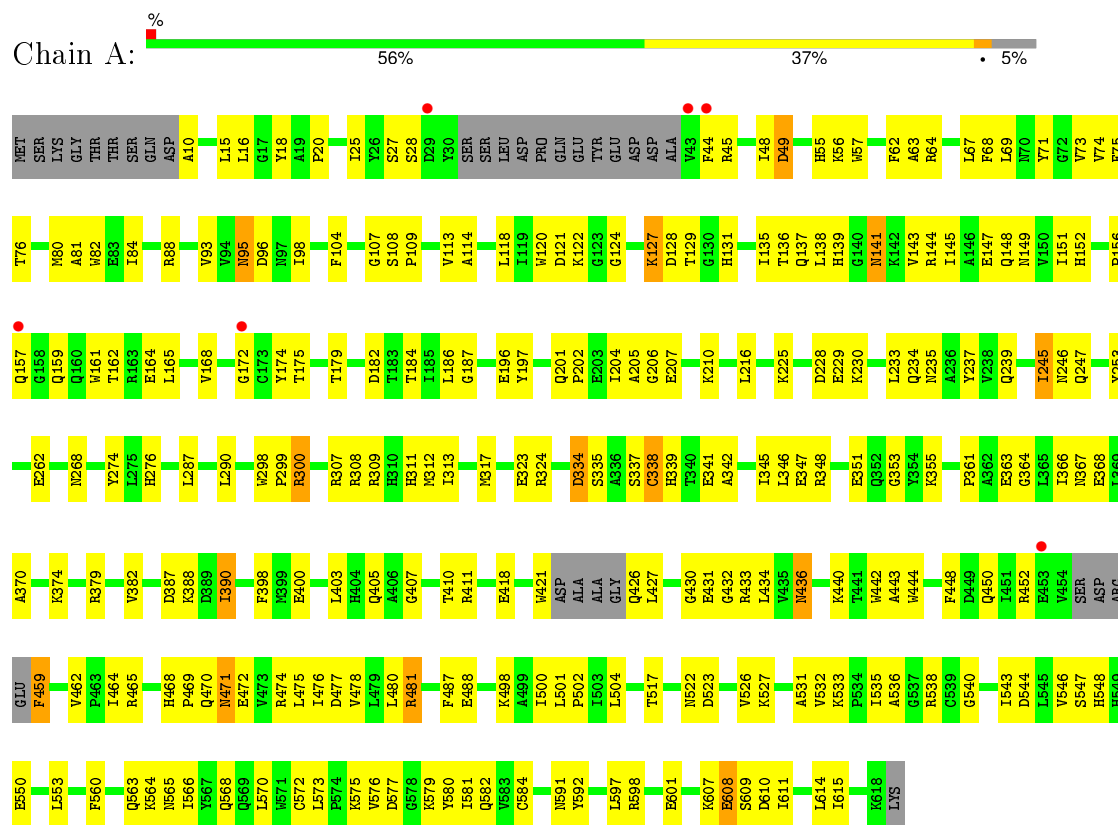
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	236	Total	O	0	0
			236	236		
5	B	221	Total	O	0	0
			221	221		

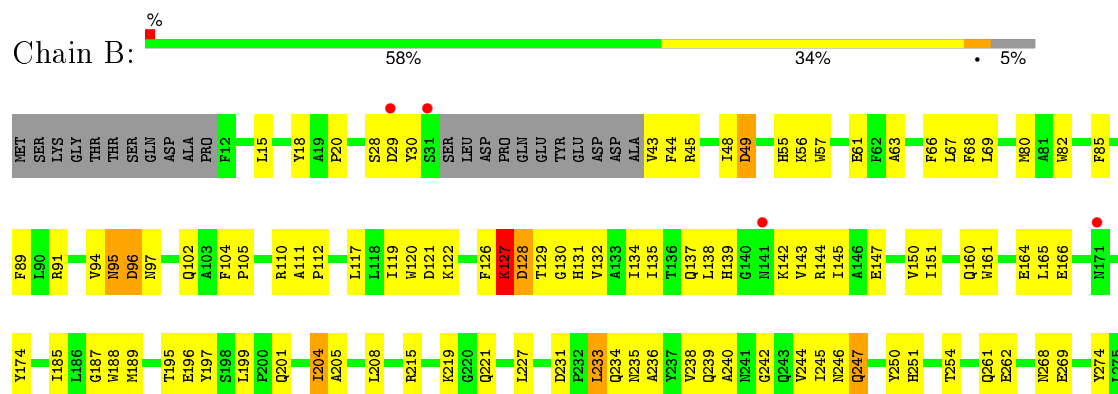
### 3 Residue-property plots

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 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: Bifunctional glutathionylspermidine synthetase/amidase



- Molecule 1: Bifunctional glutathionylspermidine synthetase/amidase



H276	R383	R481	Q568
R280	I384	P482	O572
V281	Q385	E483	D577
L282	Q386	V484	I581
D288	D387	L485	O584
F299	K388	V486	T587
R300	D389	F487	Y592
L301	I390	E488	O596
R302	Q397	P489	L597
L303	F398	L490	R598
R307	K399	V493	E601
R308	E400	I494	S602
R309	Q401	K498	L603
H310	E409		K607
H311	T410		E608
H312	L413	I503	S609
L313		L504	D610
T314	E418	H505	I611
R315			L614
R316	W421	R512	I615
D322	ASP	Y513	K618
E323	ALA	L514	LYS
R324	ALA	L515	
K327	G425	V521	
V328	Q426	R522	
D334	L427	E524	
S337	G430	L525	
C338	E431	V526	
H339	W439	K527	
T340	W444	T528	
E341	D449	V532	
A342		K533	
L344	R452	P534	
L345	E453	I535	
L346	V454	R538	
F347	SER	D544	
R348	ASP	S547	
E351	ARG	E551	
Q352	GLU	V552	
I360	A460	K555	
F361	R465	F560	
L365	T466	A561	
R377	G467	E562	
A378	H468	O563	
R379	P469	K564	
F380	Q470	N565	
F381	W471	I566	
V382	R474	V567	
	V478		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.03Å 75.29Å 84.66Å 70.09° 74.06° 77.55°	Depositor
Resolution (Å)	30.00 – 2.80 29.49 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 84.8 (29.49-2.69)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.23 (at 2.68Å)	Xtriage
Refinement program	XTALVIEW	Depositor
R, $R_{free}$	0.173 , 0.243 0.176 , 0.240	Depositor DCC
$R_{free}$ test set	3149 reflections (11.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 63.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 35215 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10089	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GGA, 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  >5	RMSZ	# Z  >5
1	A	0.43	0/4877	0.67	0/6621
1	B	0.43	0/4874	0.68	0/6615
All	All	0.43	0/9751	0.68	0/13236

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4755	0	4641	217	0
1	B	4753	0	4637	202	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	33	0	35	8	0
3	B	33	0	34	2	0
4	A	27	0	11	2	0
4	B	27	0	11	0	0
5	A	236	0	0	18	0
5	B	221	0	0	8	0
All	All	10089	0	9369	417	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 22.

The worst 5 of 417 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:A:245:ILE:O	5:A:4192:HOH:O	1.73	1.03
1:A:210:LYS:HD3	1:A:323:GLU:HB3	1.40	1.02
1:A:64:ARG:HG3	1:A:74:VAL:HG23	1.43	0.96
1:A:311:HIS:ND1	5:A:4195:HOH:O	1.97	0.96
1:A:341:GLU:HG2	1:A:611:ILE:HG13	1.48	0.93

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 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	A	581/619 (94%)	534 (92%)	40 (7%)	7 (1%)	16	47
1	B	581/619 (94%)	526 (90%)	47 (8%)	8 (1%)	14	42
All	All	1162/1238 (94%)	1060 (91%)	87 (8%)	15 (1%)	15	44

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	127	LYS
1	A	334	ASP
1	B	96	ASP
1	B	127	LYS

### 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	A	505/530 (95%)	489 (97%)	16 (3%)	46	80
1	B	505/530 (95%)	481 (95%)	24 (5%)	31	66
All	All	1010/1060 (95%)	970 (96%)	40 (4%)	38	73

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	128	ASP
1	B	247	GLN
1	B	524	GLU
1	B	204	ILE
1	B	261	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	568	GLN
1	B	201	GLN
1	B	522	ASN
1	B	55	HIS
1	B	131	HIS

### 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ADP	A	3001	2	22,29,29	1.90	3 (13%)	27,45,45	1.74	3 (11%)
3	GGA	A	6001	2	25,32,32	2.25	5 (20%)	26,42,42	1.57	5 (19%)
4	ADP	B	3002	2	22,29,29	2.00	3 (13%)	27,45,45	1.83	4 (14%)
3	GGA	B	6002	2	25,32,32	2.30	4 (16%)	26,42,42	1.70	5 (19%)

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	ADP	A	3001	2	-	0/12/32/32	0/3/3/3
3	GGA	A	6001	2	-	0/32/40/40	0/0/0/0
4	ADP	B	3002	2	-	0/12/32/32	0/3/3/3
3	GGA	B	6002	2	-	0/32/40/40	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	6002	GGA	P34-O56	-8.70	1.32	1.49
3	A	6001	GGA	P34-O56	-8.23	1.33	1.49
4	B	3002	ADP	O3'-C3'	-7.77	1.24	1.43
4	A	3001	ADP	O3'-C3'	-7.60	1.24	1.43
3	B	6002	GGA	P60-O64	-5.52	1.34	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	B	3002	ADP	N3-C2-N1	-7.12	123.44	128.89
4	A	3001	ADP	N3-C2-N1	-6.78	123.71	128.89
3	B	6002	GGA	O26-C24-C20	-3.19	112.81	120.45
3	A	6001	GGA	O26-C24-C20	-2.83	113.67	120.45
3	A	6001	GGA	C37-C39-N44	-2.71	105.18	111.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	ADP	2	0
3	A	6001	GGA	8	0
3	B	6002	GGA	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.

## 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	A	589/619 (95%)	-0.41	6 (1%) 84 77	7, 27, 48, 63	0
1	B	589/619 (95%)	-0.36	5 (0%) 87 81	8, 29, 48, 67	0
All	All	1178/1238 (95%)	-0.39	11 (0%) 85 79	7, 28, 48, 67	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	VAL	3.6
1	A	172	GLY	3.3
1	A	44	PHE	3.0
1	B	562	GLU	2.9
1	B	31	SER	2.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GGA	B	6002	33/33	0.94	0.20	1.23	22,37,54,56	0
3	GGA	A	6001	33/33	0.94	0.21	1.03	22,31,45,49	0
2	MG	A	5001	1/1	0.93	0.18	0.21	8,8,8,8	0
4	ADP	B	3002	27/27	0.99	0.14	-0.18	6,18,20,21	0
4	ADP	A	3001	27/27	0.98	0.12	-0.48	1,18,21,23	0
2	MG	B	5003	1/1	0.99	0.12	-0.67	10,10,10,10	0
2	MG	A	5002	1/1	0.95	0.14	-	8,8,8,8	0
2	MG	B	5004	1/1	0.97	0.12	-	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.