



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:24 am GMT

PDB ID : 3N2K  
Title : TUBULIN-NSC 613862: RB3 Stathmin-like domain complex  
Authors : Barbier, P.; Dorleans, A.; Devred, F.; Sanz, L.; Allegro, D.; Alfonso, C.;  
Knossow, M.; Peyrot, V.; Andreu, J.M.  
Deposited on : 2010-05-18  
Resolution : 4.00 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

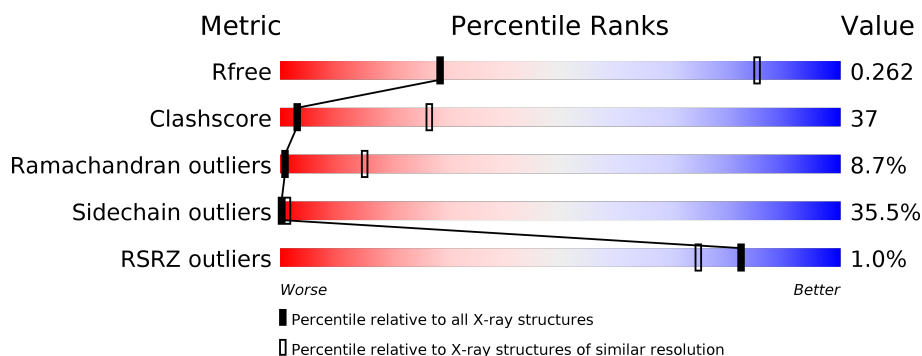
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
$R_{free}$	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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	451	<div> <div></div> <div> <div>41%</div> <div>37%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	C	451	<div> <div>%</div> <div> <div>44%</div> <div>33%</div> <div>15%</div> <div>• 5%</div> </div> </div>
2	B	445	<div> <div>%</div> <div> <div>27%</div> <div>46%</div> <div>19%</div> <div>• 6%</div> </div> </div>
2	D	445	<div> <div>%</div> <div> <div>24%</div> <div>45%</div> <div>22%</div> <div>5%</div> <div>•</div> </div> </div>
3	E	142	<div> <div>%</div> <div> <div>32%</div> <div>32%</div> <div>19%</div> <div>•</div> <div>13%</div> </div> </div>

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
6	GDP	D	600	-	-	X	-
7	K2N	D	700	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14225 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3300	2097	557	625	21			
1	C	429	Total	C	N	O	S	0	0	0
			3286	2084	554	627	21			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3251	2046	547	633	25			
2	D	427	Total	C	N	O	S	0	0	0
			3297	2071	559	643	24			

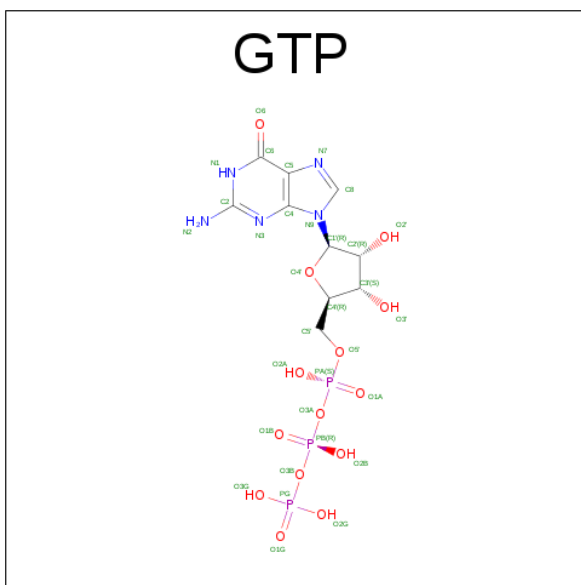
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			920	557	174	184	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	EXPRESSION TAG	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

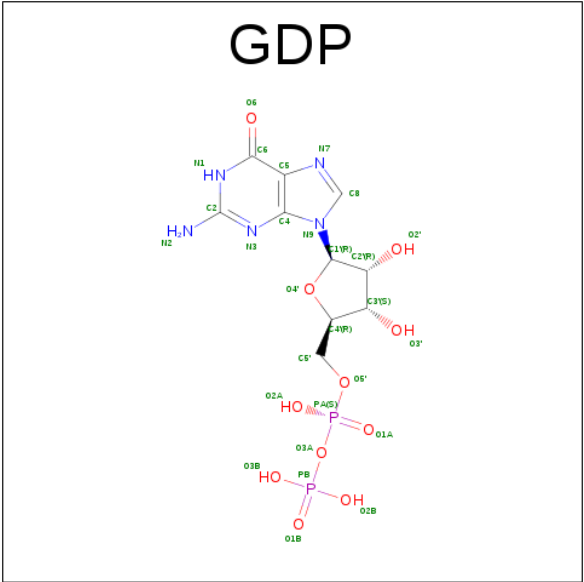


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

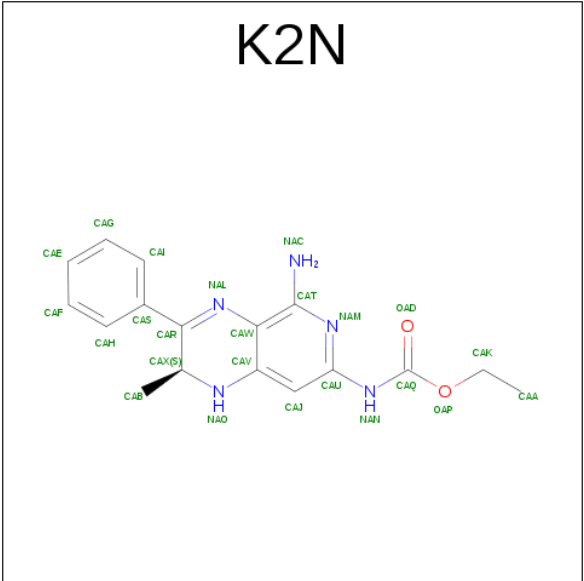
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
6	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 7 is ETHYL [(2S)-5-AMINO-2-METHYL-3-PHENYL-1,2-DIHYDROPYRIDO[3,4-B]PYRAZIN-7-YL]CARBAMATE (three-letter code: K2N) (formula: C<sub>17</sub>H<sub>19</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			24	17	5	2		

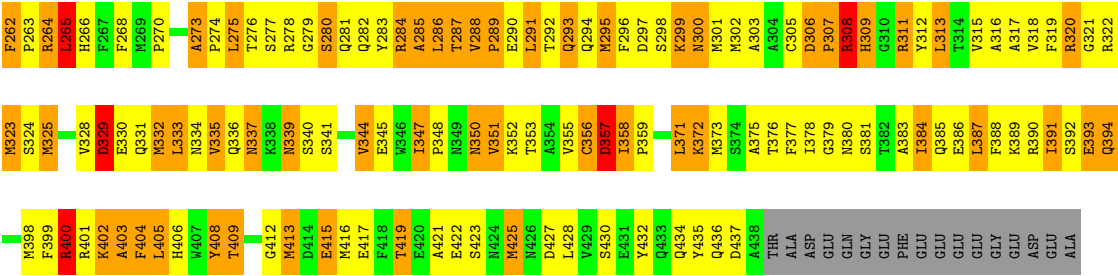
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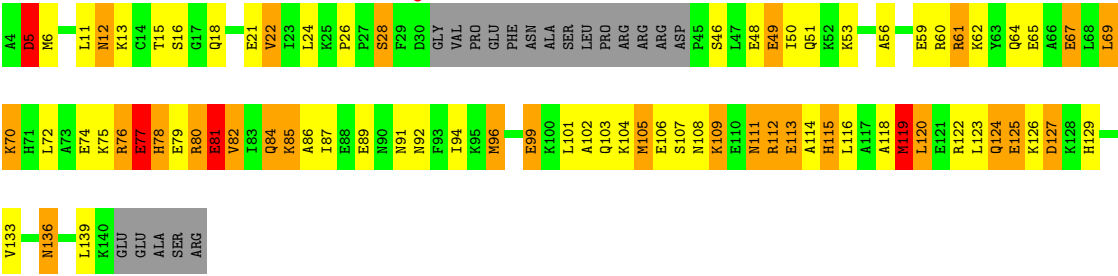
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			24	17	5	2		







● Molecule 3: Stathmin-4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	326.32Å 326.32Å 54.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.00 29.73 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-4.00) 99.6 (29.73-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 3.98Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.223 , 0.250 0.250 , 0.262	Depositor DCC
$R_{free}$ test set	1433 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	162.7	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 190.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	232.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, MG, K2N

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	0.79	0/3377	0.96	17/4593 (0.4%)
1	C	0.71	1/3360 (0.0%)	0.95	12/4572 (0.3%)
2	B	0.78	0/3323	0.97	11/4512 (0.2%)
2	D	0.85	2/3370 (0.1%)	1.01	14/4574 (0.3%)
3	E	0.82	2/928 (0.2%)	0.94	1/1243 (0.1%)
All	All	0.79	5/14358 (0.0%)	0.97	55/19494 (0.3%)

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	A	0	1
1	C	0	2
2	B	0	4
2	D	0	4
3	E	0	1
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	200	GLU	CD-OE1	7.30	1.33	1.25
1	C	168	GLU	CD-OE1	5.61	1.31	1.25
3	E	119	MET	SD-CE	5.50	2.08	1.77
3	E	105	MET	SD-CE	5.48	2.08	1.77
2	D	177	VAL	CB-CG2	5.39	1.64	1.52

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	ASP	CB-CG-OD2	7.46	125.01	118.30
1	C	120	ASP	CB-CG-OD2	7.32	124.88	118.30
1	A	248	LEU	CA-CB-CG	7.22	131.91	115.30
1	C	397	LEU	CA-CB-CG	7.10	131.63	115.30
2	D	297	ASP	CB-CG-OD2	7.06	124.65	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLY	Peptide
2	B	162	PRO	Peptide
2	B	248	LEU	Peptide
2	B	249	ASN	Peptide
2	B	262	PHE	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	A	3300	0	3162	186	0
1	C	3286	0	3133	186	0
2	B	3251	0	3074	276	0
2	D	3297	0	3116	358	0
3	E	920	0	816	61	0
4	A	32	0	12	5	0
4	C	32	0	12	7	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	7	0
6	D	28	0	12	12	0
7	B	24	0	19	8	0
7	D	24	0	19	23	0
All	All	14225	0	13387	1032	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 37.

The worst 5 of 1032 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)
3:E:96:MET:CE	3:E:96:MET:SD	2.01	1.47
3:E:105:MET:SD	3:E:105:MET:CE	2.08	1.42
3:E:119:MET:CE	3:E:119:MET:SD	2.08	1.41
2:D:387:LEU:O	2:D:390:ARG:HG2	1.41	1.18
2:D:287:THR:HG23	2:D:290:GLU:HB2	1.20	1.17

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	424/451 (94%)	327 (77%)	65 (15%)	32 (8%)	1	19
1	C	423/451 (94%)	331 (78%)	62 (15%)	30 (7%)	1	20
2	B	416/445 (94%)	306 (74%)	74 (18%)	36 (9%)	1	15
2	D	425/445 (96%)	295 (69%)	84 (20%)	46 (11%)	0	9
3	E	119/142 (84%)	80 (67%)	25 (21%)	14 (12%)	0	8
All	All	1807/1934 (93%)	1339 (74%)	310 (17%)	158 (9%)	1	15

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	PRO
1	A	73	THR
1	A	112	LYS
1	A	265	ILE
1	A	341	ILE

### 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	A	346/378 (92%)	243 (70%)	103 (30%)	0	3
1	C	344/378 (91%)	236 (69%)	108 (31%)	0	3
2	B	350/383 (91%)	217 (62%)	133 (38%)	0	0
2	D	353/383 (92%)	216 (61%)	137 (39%)	0	0
3	E	82/126 (65%)	40 (49%)	42 (51%)	0	0
All	All	1475/1648 (90%)	952 (64%)	523 (36%)	0	1

5 of 523 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	ARG
1	C	230	LEU
3	E	15	THR
1	C	31	GLN
1	C	119	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	380	ASN
1	C	128	GLN
2	D	380	ASN
2	B	385	GLN
1	C	85	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 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$
4	GTP	A	600	5	27,34,34	1.02	2 (7%)	27,54,54	1.81	5 (18%)
6	GDP	B	600	-	25,30,30	1.01	2 (8%)	26,47,47	1.93	5 (19%)
7	K2N	B	700	-	25,26,26	1.66	3 (12%)	26,36,36	3.20	13 (50%)
4	GTP	C	600	5	27,34,34	1.04	2 (7%)	27,54,54	2.08	7 (25%)
6	GDP	D	600	-	25,30,30	1.03	1 (4%)	26,47,47	2.06	5 (19%)
7	K2N	D	700	-	25,26,26	1.98	4 (16%)	26,36,36	2.86	11 (42%)

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	GTP	A	600	5	-	0/18/38/38	0/3/3/3
6	GDP	B	600	-	-	0/12/32/32	0/3/3/3
7	K2N	B	700	-	-	0/11/23/23	0/3/3/3
4	GTP	C	600	5	-	0/18/38/38	0/3/3/3
6	GDP	D	600	-	-	0/12/32/32	0/3/3/3
7	K2N	D	700	-	-	0/11/23/23	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	700	K2N	CAS-CAR	-6.62	1.38	1.48
7	B	700	K2N	CAS-CAR	-6.23	1.38	1.48
7	B	700	K2N	CAU-NAN	-2.52	1.35	1.40
4	A	600	GTP	O4'-C4'	-2.27	1.39	1.45
6	B	600	GDP	C2-N1	2.18	1.39	1.35

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	K2N	CAK-OAP-CAQ	-8.22	100.84	116.07
7	D	700	K2N	CAK-OAP-CAQ	-7.74	101.74	116.07
4	C	600	GTP	N3-C2-N1	-6.08	118.58	127.46
6	D	600	GDP	N3-C2-N1	-6.04	118.64	127.46
6	B	600	GDP	N3-C2-N1	-5.15	119.94	127.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GTP	5	0
6	B	600	GDP	7	0
7	B	700	K2N	8	0
4	C	600	GTP	7	0
6	D	600	GDP	12	0
7	D	700	K2N	23	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	428/451 (94%)	-0.21	2 (0%) 90 86	173, 213, 260, 322	0
1	C	429/451 (95%)	-0.16	6 (1%) 75 66	190, 236, 318, 350	0
2	B	420/445 (94%)	-0.21	5 (1%) 79 71	176, 220, 277, 315	0
2	D	427/445 (95%)	-0.16	5 (1%) 79 71	189, 246, 315, 389	0
3	E	123/142 (86%)	0.06	1 (0%) 86 79	216, 250, 323, 363	0
All	All	1827/1934 (94%)	-0.17	19 (1%) 82 74	173, 229, 306, 389	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	30	ASP	5.1
1	C	367	ASP	3.3
1	C	170	SER	3.1
1	C	143	GLY	2.9
1	A	438	ASP	2.8

### 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(Å <sup>2</sup> )	Q<0.9
7	K2N	B	700	24/24	0.92	0.33	0.32	61,64,68,71	0
7	K2N	D	700	24/24	0.86	0.32	0.15	71,74,80,81	0
6	GDP	D	600	28/28	0.91	0.30	-0.40	64,67,68,69	0
6	GDP	B	600	28/28	0.91	0.25	-0.70	64,67,68,68	0
4	GTP	A	600	32/32	0.94	0.17	-1.00	61,65,66,66	0
4	GTP	C	600	32/32	0.93	0.20	-1.02	55,64,66,66	0
5	MG	C	601	1/1	0.97	0.10	-1.36	43,43,43,43	0
5	MG	A	601	1/1	0.99	0.06	-2.68	40,40,40,40	0
5	MG	B	601	1/1	0.77	0.31	-	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.