



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:12 AM GMT

PDB ID : 3HKC  
Title : Tubulin-ABT751: RB3 stathmin-like domain complex  
Authors : Dorleans, A.; Gigant, B.; Ravelli, R.B.G.; Mailliet, P.; Mikol, V.; Knossow, M.  
Deposited on : 2009-05-23  
Resolution : 3.80 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

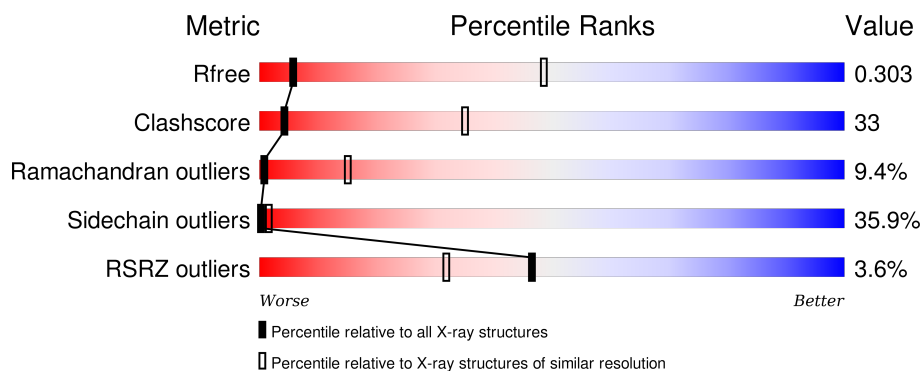
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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>4%</div> <div>39% 39% 14% • 5%</div> </div>
1	C	451	<div> <div>4%</div> <div>43% 35% 15% • 5%</div> </div>
2	B	445	<div> <div>3%</div> <div>29% 40% 23% • 6%</div> </div>
2	D	445	<div> <div>3%</div> <div>29% 42% 20% • 6%</div> </div>
3	E	142	<div> <div>0%</div> <div>35% 37% 13% • 13%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14145 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	427	Total	C	N	O	S	0	0	0
			3300	2097	558	624	21			
1	C	428	Total	C	N	O	S	0	0	0
			3270	2078	553	619	20			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3240	2038	546	632	24			
2	D	419	Total	C	N	O	S	0	0	0
			3239	2038	545	632	24			

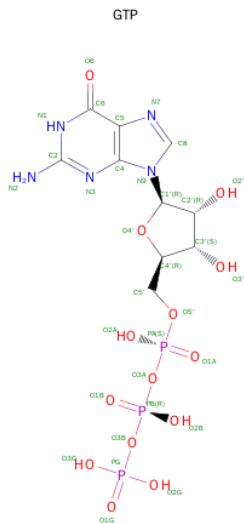
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			921	558	175	183	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>).

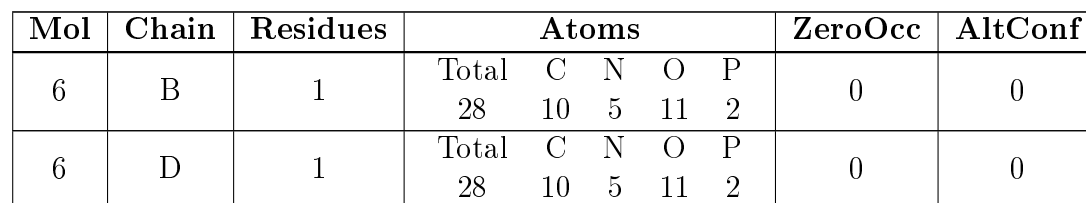


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

- 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:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



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- The chemical structure of E70 is a complex organic molecule. It features a central benzene ring substituted with a sulfonamide group (-SO<sub>2</sub>NH-) at the top position and a hydroxyl group (-OH) at the bottom position. The sulfonamide nitrogen is part of a five-membered ring system that includes a pyridine ring. The pyridine ring is substituted with a naphthalen-1-yl group (-NAP) at the 2-position and a 4-hydroxyphenyl group (-CAK) at the 4-position. The 4-hydroxyphenyl group is further substituted with a 4-hydroxyphenyl group (-CAI) at the 4-position. The central benzene ring is also substituted with a 4-hydroxyphenyl group (-CAH) at the 4-position and a 4-hydroxyphenyl group (-CAJ) at the 4-position. The molecule is highly symmetrical and contains several functional groups, including amine, sulfonamide, and hydroxyl groups.

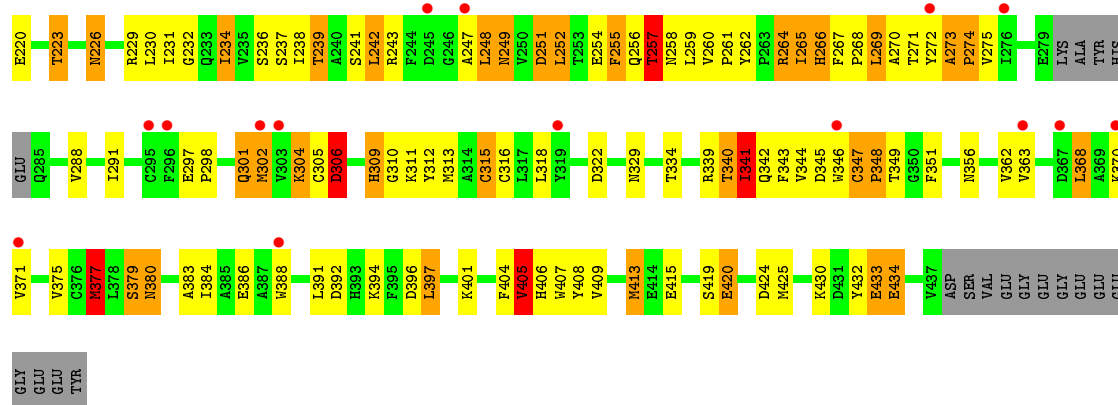
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			26	18	3	4	1		



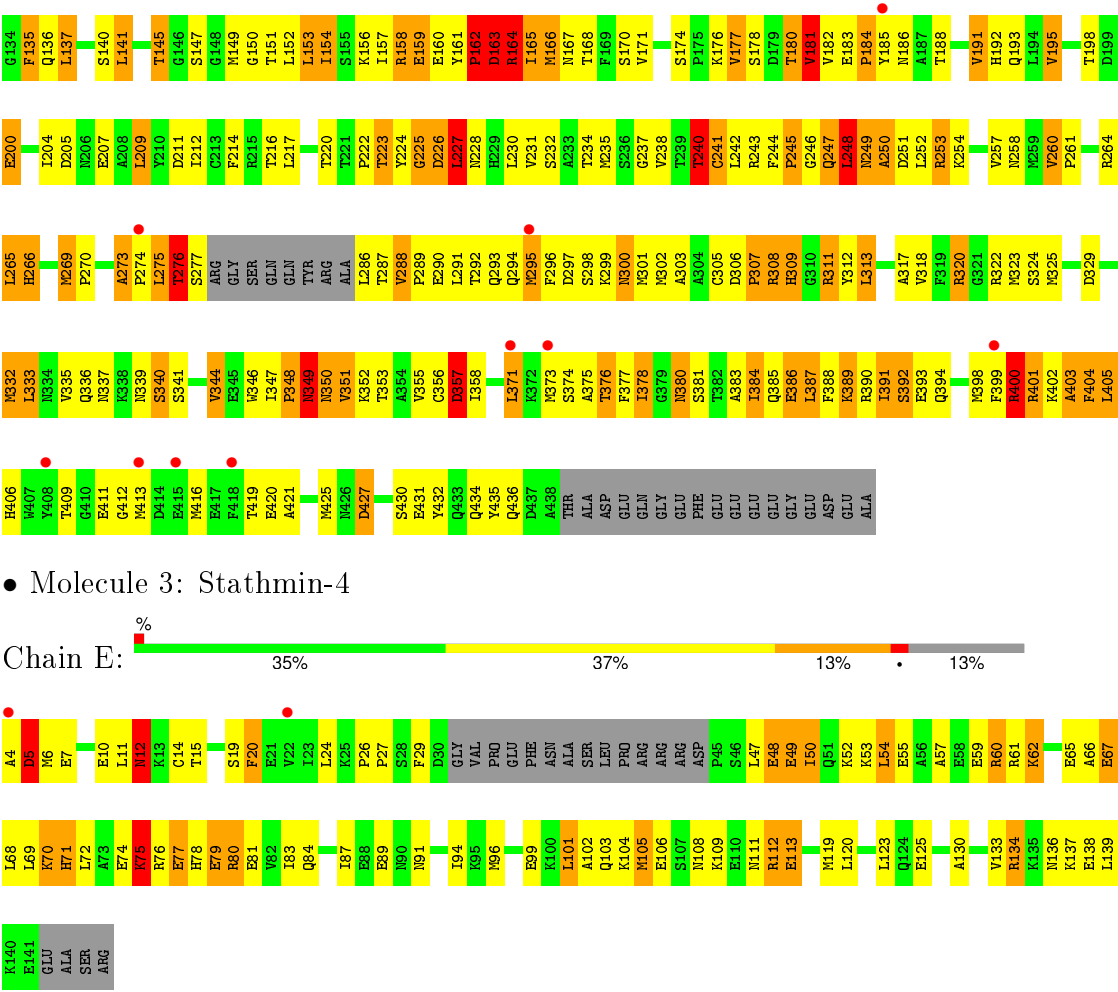
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			26	18	3	4	1		









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	329.24Å 329.24Å 53.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.80 48.19 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-3.80) 97.6 (48.19-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.203 , 0.252 0.273 , 0.303	Depositor DCC
$R_{free}$ test set	1664 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	172.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 245.7	EDS
Estimated twinning fraction	0.068 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 33054 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14145	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: GDP, GTP, MG, E70

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	0/3376	0.99	17/4588 (0.4%)
1	C	0.67	0/3344	0.91	11/4552 (0.2%)
2	B	0.68	0/3312	0.94	11/4498 (0.2%)
2	D	0.71	0/3311	0.95	10/4495 (0.2%)
3	E	0.75	0/929	0.92	2/1245 (0.2%)
All	All	0.72	0/14272	0.95	51/19378 (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	2
2	B	0	2
2	D	0	2
3	E	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	CB-CG-OD2	8.56	126.00	118.30
1	C	211	ASP	CB-CG-OD2	8.46	125.91	118.30
1	A	76	ASP	CB-CG-OD2	8.07	125.56	118.30
1	A	120	ASP	CB-CG-OD2	7.62	125.16	118.30
1	C	120	ASP	CB-CG-OD2	7.48	125.03	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	HIS	Peptide
1	A	82	THR	Peptide
2	B	162	PRO	Peptide
2	B	248	LEU	Peptide
2	D	162	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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	3169	185	0
1	C	3270	0	3122	180	0
2	B	3240	0	3056	269	0
2	D	3239	0	3058	269	0
3	E	921	0	814	41	0
4	A	32	0	12	4	0
4	C	32	0	12	4	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	3	0
6	D	28	0	12	4	0
7	B	26	0	17	5	0
7	D	26	0	17	5	0
All	All	14145	0	13301	912	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 33.

The worst 5 of 912 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:105:MET:SD	3:E:105:MET:CE	2.03	1.44
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.74	1.16
2:B:165:ILE:HD11	2:B:252:LEU:HG	1.25	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.22	1.15
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.17	1.15

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	422/451 (94%)	319 (76%)	70 (17%)	33 (8%)	1	20
1	C	422/451 (94%)	316 (75%)	70 (17%)	36 (8%)	1	17
2	B	415/445 (93%)	315 (76%)	58 (14%)	42 (10%)	1	13
2	D	415/445 (93%)	308 (74%)	64 (15%)	43 (10%)	1	12
3	E	120/142 (84%)	82 (68%)	24 (20%)	14 (12%)	0	9
All	All	1794/1934 (93%)	1340 (75%)	286 (16%)	168 (9%)	1	15

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	73	THR
1	A	164	LYS
1	A	191	THR
1	A	247	ALA

### 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	347/378 (92%)	229 (66%)	118 (34%)	0	2
1	C	340/378 (90%)	228 (67%)	112 (33%)	0	3
2	B	348/383 (91%)	221 (64%)	127 (36%)	0	1
2	D	348/383 (91%)	220 (63%)	128 (37%)	0	1
3	E	81/126 (64%)	41 (51%)	40 (49%)	0	0
All	All	1464/1648 (89%)	939 (64%)	525 (36%)	0	1

5 of 525 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	401	ARG
1	C	187	SER
3	E	5	ASP
2	B	434	GLN
1	C	84	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	380	ASN
1	C	133	GLN
2	D	339	ASN
2	B	385	GLN
1	C	85	GLN

### 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 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	-	25,34,34	0.95	2 (8%)	34,54,54	1.44	6 (17%)
6	GDP	B	600	-	23,30,30	1.13	2 (8%)	30,47,47	1.88	7 (23%)
7	E70	B	700	-	27,28,28	2.71	5 (18%)	37,39,39	1.90	6 (16%)
4	GTP	C	600	-	25,34,34	1.00	2 (8%)	34,54,54	1.93	9 (26%)
6	GDP	D	600	-	23,30,30	0.97	1 (4%)	30,47,47	1.97	6 (20%)
7	E70	D	700	-	27,28,28	3.54	7 (25%)	37,39,39	2.05	6 (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	GTP	A	600	-	-	0/18/38/38	0/3/3/3
6	GDP	B	600	-	-	0/12/32/32	0/3/3/3
7	E70	B	700	-	-	0/17/17/17	0/3/3/3
4	GTP	C	600	-	-	0/18/38/38	0/3/3/3
6	GDP	D	600	-	-	0/12/32/32	0/3/3/3
7	E70	D	700	-	-	0/17/17/17	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	700	E70	CAX-NAR	-4.69	1.34	1.42
7	B	700	E70	CAX-NAR	-3.08	1.37	1.42
7	B	700	E70	CAU-NAQ	-3.00	1.34	1.40
7	D	700	E70	CAU-NAQ	-2.47	1.35	1.40
4	C	600	GTP	O4'-C4'	-2.31	1.39	1.45

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	E70	OAC-SAZ-OAB	-7.76	109.25	119.54
7	D	700	E70	OAC-SAZ-OAB	-7.15	110.06	119.54
6	D	600	GDP	N3-C2-N1	-5.50	119.06	127.44
6	B	600	GDP	N3-C2-N1	-5.47	119.11	127.44
4	C	600	GTP	N3-C2-N1	-5.36	119.28	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GTP	4	0
6	B	600	GDP	3	0
7	B	700	E70	5	0
4	C	600	GTP	4	0
6	D	600	GDP	4	0
7	D	700	E70	5	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	427/451 (94%)	0.10	17 (3%) 42 28	46, 51, 52, 57	0
1	C	428/451 (94%)	0.17	18 (4%) 40 26	44, 51, 52, 62	0
2	B	419/445 (94%)	0.18	14 (3%) 50 34	49, 51, 52, 54	0
2	D	419/445 (94%)	0.12	15 (3%) 46 32	48, 51, 52, 54	0
3	E	124/142 (87%)	-0.34	2 (1%) 74 60	41, 50, 56, 59	0
All	All	1817/1934 (93%)	0.11	66 (3%) 46 32	41, 51, 52, 62	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	VAL	4.7
2	D	418	PHE	4.2
2	D	399	PHE	3.8
1	A	315	CYS	3.7
1	C	30	ILE	3.6

### 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	E70	D	700	26/26	0.92	0.36	1.48	52,53,57,59	0
7	E70	B	700	26/26	0.93	0.40	0.95	52,52,57,59	0
6	GDP	D	600	28/28	0.95	0.19	-0.78	48,51,52,52	0
6	GDP	B	600	28/28	0.86	0.22	-0.78	48,51,52,52	0
4	GTP	C	600	32/32	0.92	0.20	-1.07	48,49,50,51	0
4	GTP	A	600	32/32	0.95	0.13	-1.92	47,49,51,51	0
5	MG	C	601	1/1	0.97	0.06	-4.82	41,41,41,41	0
5	MG	A	601	1/1	0.98	0.10	-5.48	40,40,40,40	0
5	MG	B	601	1/1	0.82	0.90	-	47,47,47,47	0

## 6.5 Other polymers

There are no such residues in this entry.