



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:30 AM GMT

PDB ID : 2HV8  
Title : Crystal structure of GTP-bound Rab11 in complex with FIP3  
Authors : Eathiraj, S.; Mishra, A.; Prekeris, R.; Lambright, D.G.  
Deposited on : 2006-07-27  
Resolution : 1.86 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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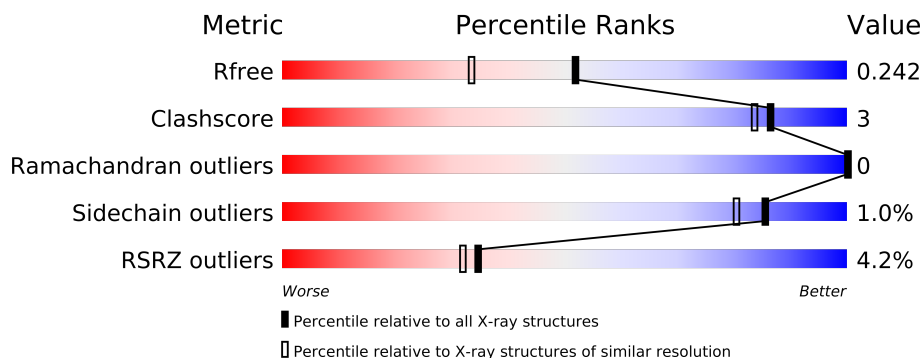
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.86 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))
$R_{free}$	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	172	
1	B	172	
1	C	172	
2	D	64	
2	E	64	
2	F	64	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	C	2005	-	X
7	MES	B	1	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6119 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ras-related protein Rab-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1324	840	231	252	1			
1	B	169	Total	C	N	O	S	0	0	0
			1332	845	233	253	1			
1	C	169	Total	C	N	O	S	0	0	0
			1302	831	227	243	1			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLY	-	CLONING ARTIFACT	UNP P62491
A	5	SER	-	CLONING ARTIFACT	UNP P62491
A	70	LEU	GLN	ENGINEERED	UNP P62491
B	4	GLY	-	CLONING ARTIFACT	UNP P62491
B	5	SER	-	CLONING ARTIFACT	UNP P62491
B	70	LEU	GLN	ENGINEERED	UNP P62491
C	4	GLY	-	CLONING ARTIFACT	UNP P62491
C	5	SER	-	CLONING ARTIFACT	UNP P62491
C	70	LEU	GLN	ENGINEERED	UNP P62491

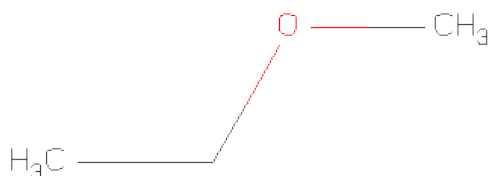
- Molecule 2 is a protein called Rab11 family-interacting protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	54	Total	C	N	O	S	0	0	0
			398	254	67	76	1			
2	E	55	Total	C	N	O	S	0	0	0
			400	254	65	80	1			
2	F	41	Total	C	N	O	S	0	0	0
			317	199	54	62	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	693	GLY	-	CLONING ARTIFACT	UNP O75154
D	694	SER	-	CLONING ARTIFACT	UNP O75154
E	693	GLY	-	CLONING ARTIFACT	UNP O75154
E	694	SER	-	CLONING ARTIFACT	UNP O75154
F	693	GLY	-	CLONING ARTIFACT	UNP O75154
F	694	SER	-	CLONING ARTIFACT	UNP O75154

- Molecule 3 is METHOXYETHANE (three-letter code: 2ME) (formula: C<sub>3</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

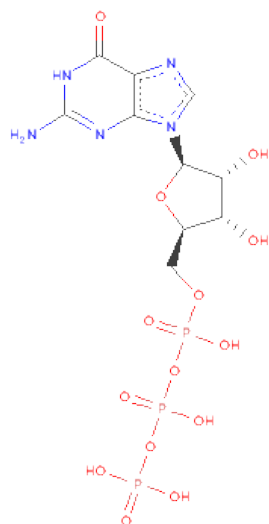
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



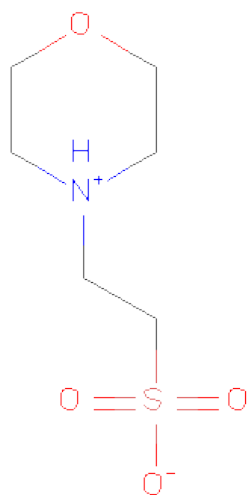
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	257	Total	O	0	0
			257	257		
8	B	297	Total	O	0	0
			297	297		
8	C	199	Total	O	0	0
			199	199		
8	D	62	Total	O	0	0
			62	62		
8	E	49	Total	O	0	0
			49	49		
8	F	42	Total	O	0	0
			42	42		

### 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: Ras-related protein Rab-11A

Chain A: 



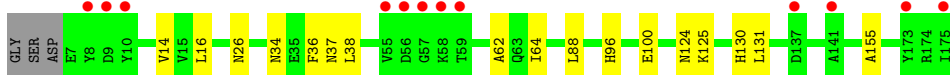
- Molecule 1: Ras-related protein Rab-11A

Chain B: 



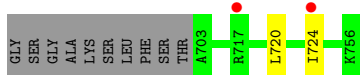
- Molecule 1: Ras-related protein Rab-11A

Chain C: 



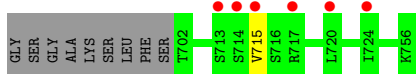
- Molecule 2: Rab11 family-interacting protein 3

Chain D: 



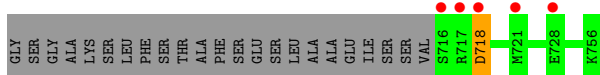
- Molecule 2: Rab11 family-interacting protein 3

Chain E: 



- Molecule 2: Rab11 family-interacting protein 3

Chain F: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.29Å 52.60Å 70.68Å 90.00° 105.56° 90.00°	Depositor
Resolution (Å)	8.00 – 1.86 33.46 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.2 (8.00-1.86) 98.2 (33.46-1.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.203 , 0.237 0.206 , 0.242	Depositor DCC
$R_{free}$ test set	3271 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 64411 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6119	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 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, SO4, MES, 2ME

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	0.36	0/1346	0.49	0/1824
1	B	0.36	0/1353	0.52	0/1830
1	C	0.35	0/1324	0.51	0/1797
2	D	0.35	0/401	0.43	0/546
2	E	0.34	0/403	0.44	0/549
2	F	0.34	0/319	0.44	0/432
All	All	0.36	0/5146	0.49	0/6978

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1324	0	1301	5	1
1	B	1332	0	1329	8	0
1	C	1302	0	1275	11	0
2	D	398	0	372	1	0
2	E	400	0	372	0	0
2	F	317	0	298	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	8	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0
6	A	32	0	12	0	0
6	B	32	0	12	0	0
6	C	32	0	12	1	0
7	B	12	0	12	0	0
8	A	257	0	0	0	0
8	B	297	0	0	1	1
8	C	199	0	0	0	0
8	D	62	0	0	0	0
8	E	49	0	0	0	0
8	F	42	0	0	1	0
All	All	6119	0	5003	26	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (26) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:26:ASN:HD21	1:B:37:ASN:H	1.37	0.72
1:A:26:ASN:HD21	1:A:37:ASN:H	1.41	0.66
1:B:51:ARG:NH2	1:B:162:GLU:OE1	2.31	0.64
1:C:26:ASN:HD21	1:C:37:ASN:H	1.45	0.63
1:B:26:ASN:ND2	1:B:37:ASN:H	1.99	0.60
1:C:26:ASN:ND2	1:C:37:ASN:H	2.01	0.57
1:B:174:ARG:NE	8:B:2287:HOH:O	2.37	0.57
1:A:26:ASN:ND2	1:A:37:ASN:H	2.03	0.56
1:B:132:ARG:HE	3:B:2:2ME:HD'2	1.72	0.54
1:A:108:GLU:HG3	1:A:112:HIS:HD2	1.73	0.54
1:A:37:ASN:ND2	1:A:39:GLU:H	2.06	0.54
1:C:130:HIS:CD2	1:C:131:LEU:HG	2.45	0.52
2:F:718:ASP:HB2	8:F:766:HOH:O	2.10	0.51
1:C:62:ALA:HB1	1:C:64:ILE:HD11	1.94	0.49
1:C:96:HIS:HD2	1:C:100:GLU:OE2	1.95	0.48
1:B:16:LEU:HD23	1:B:88:LEU:HB2	1.96	0.47
1:B:96:HIS:HD2	1:B:100:GLU:OE2	1.97	0.47
1:A:108:GLU:HG3	1:A:112:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:16:LEU:HD23	1:C:88:LEU:HB2	1.98	0.46
1:C:124:ASN:HD21	1:C:155:ALA:H	1.65	0.43
1:C:14:VAL:HB	1:C:64:ILE:HD13	2.01	0.43
1:C:125:LYS:HG2	6:C:200:GTP:C6	2.55	0.42
1:C:36:PHE:HE2	1:C:38:LEU:HD12	1.84	0.41
2:D:720:LEU:O	2:D:724:ILE:HG12	2.20	0.41
1:C:36:PHE:CE2	1:C:38:LEU:HD12	2.56	0.41
1:B:95:LYS:HD3	1:B:98:THR:HG23	2.03	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:A:167:THR:OG1	8:B:2287:HOH:O[4_455]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	B	167/172 (97%)	165 (99%)	2 (1%)	0	100	100
1	C	167/172 (97%)	164 (98%)	3 (2%)	0	100	100
2	D	52/64 (81%)	51 (98%)	1 (2%)	0	100	100
2	E	53/64 (83%)	53 (100%)	0	0	100	100
2	F	39/64 (61%)	38 (97%)	1 (3%)	0	100	100
All	All	645/708 (91%)	636 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	137/145 (94%)	136 (99%)	1 (1%)	91	87
1	B	140/145 (97%)	139 (99%)	1 (1%)	91	87
1	C	131/145 (90%)	130 (99%)	1 (1%)	89	85
2	D	37/56 (66%)	37 (100%)	0	100	100
2	E	39/56 (70%)	38 (97%)	1 (3%)	59	41
2	F	32/56 (57%)	31 (97%)	1 (3%)	52	32
All	All	516/603 (86%)	511 (99%)	5 (1%)	85	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	B	37	ASN
2	E	715	VAL
1	C	34	ASN
2	F	718	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	34	ASN
1	A	37	ASN
1	A	96	HIS
1	A	112	HIS
1	A	124	ASN
2	D	735	GLN
1	B	26	ASN
1	B	34	ASN
1	B	37	ASN
1	B	96	HIS
1	B	124	ASN
2	E	735	GLN
1	C	26	ASN
1	C	34	ASN
1	C	96	HIS
1	C	124	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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$
6	GTP	A	200	4	34,34,34	0.98	1 (2%)	51,54,54	1.39	7 (13%)
5	SO4	A	2001	-	4,4,4	0.27	0	6,6,6	0.18	0
7	MES	B	1	-	12,12,12	2.00	1 (8%)	16,16,16	2.31	4 (25%)
3	2ME	B	2	-	3,3,3	0.52	0	2,2,2	0.67	0
6	GTP	B	200	4	34,34,34	0.97	1 (2%)	51,54,54	1.44	9 (17%)
5	SO4	B	2003	-	4,4,4	0.28	0	6,6,6	0.10	0
5	SO4	B	2004	-	4,4,4	0.23	0	6,6,6	0.07	0
6	GTP	C	200	4	34,34,34	0.98	1 (2%)	51,54,54	1.50	10 (19%)
5	SO4	C	2002	-	4,4,4	0.29	0	6,6,6	0.10	0
5	SO4	C	2005	-	4,4,4	0.22	0	6,6,6	0.08	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
6	GTP	A	200	4	-	0/22/38/38	0/1/3/3
5	SO4	A	2001	-	-	0/0/0/0	0/0/0/0
7	MES	B	1	-	-	0/6/14/14	0/1/1/1
3	2ME	B	2	-	-	0/0/1/1	0/0/0/0
6	GTP	B	200	4	-	0/22/38/38	0/1/3/3
5	SO4	B	2003	-	-	0/0/0/0	0/0/0/0
5	SO4	B	2004	-	-	0/0/0/0	0/0/0/0
6	GTP	C	200	4	-	0/22/38/38	0/1/3/3
5	SO4	C	2002	-	-	0/0/0/0	0/0/0/0
5	SO4	C	2005	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1	MES	C8-S	-6.08	1.67	1.78
6	A	200	GTP	C2-N3	3.70	1.38	1.33
6	B	200	GTP	C2-N3	3.66	1.38	1.33
6	C	200	GTP	C2-N3	3.62	1.38	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1	MES	C5-N4-C3	6.53	122.70	109.75
6	C	200	GTP	C6-C5-N7	-3.68	133.64	134.14
6	B	200	GTP	C2-N3-C4	3.58	120.13	115.09
6	C	200	GTP	C2-N3-C4	3.57	120.10	115.09
6	A	200	GTP	C6-C5-N7	-3.54	133.66	134.14
6	A	200	GTP	C2-N3-C4	3.51	120.02	115.09
7	B	1	MES	C8-C7-N4	-3.25	106.87	112.44
6	A	200	GTP	C5-C4-N3	-3.12	121.41	125.94
6	B	200	GTP	C5-C4-N3	-3.12	121.42	125.94
6	C	200	GTP	C5-C4-N3	-3.01	121.58	125.94
6	C	200	GTP	N2-C2-N1	2.97	121.13	117.86
6	B	200	GTP	O4'-C1'-N9	2.96	111.19	108.44
6	A	200	GTP	N3-C4-N9	2.86	131.10	126.91
6	B	200	GTP	N3-C4-N9	2.86	131.10	126.91
7	B	1	MES	C7-N4-C3	2.80	118.98	111.66
6	C	200	GTP	N3-C4-N9	2.75	130.94	126.91
6	A	200	GTP	N2-C2-N1	2.73	120.86	117.86
6	B	200	GTP	C6-C5-N7	-2.72	133.77	134.14
6	C	200	GTP	PA-O3A-PB	-2.66	123.90	131.68
6	B	200	GTP	N2-C2-N1	2.64	120.77	117.86
7	B	1	MES	C7-N4-C5	2.55	118.32	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	200	GTP	O4'-C1'-N9	2.42	110.69	108.44
6	B	200	GTP	C4-C5-N7	-2.38	107.48	109.52
6	A	200	GTP	C4-C5-N7	-2.27	107.58	109.52
6	C	200	GTP	C4-C5-N7	-2.27	107.58	109.52
6	B	200	GTP	PA-O3A-PB	-2.24	125.12	131.68
6	C	200	GTP	N7-C8-N9	-2.21	108.09	114.36
6	A	200	GTP	N7-C8-N9	-2.21	108.11	114.36
6	B	200	GTP	N7-C8-N9	-2.19	108.17	114.36
6	C	200	GTP	PB-O3B-PG	-2.08	125.58	131.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	169/172 (98%)	0.12	2 (1%) 75 73	18, 25, 33, 35	0
1	B	169/172 (98%)	0.07	1 (0%) 86 87	18, 23, 30, 33	0
1	C	169/172 (98%)	0.26	12 (7%) 16 14	21, 28, 42, 44	0
2	D	54/64 (84%)	0.45	2 (3%) 39 36	17, 31, 40, 42	0
2	E	55/64 (85%)	0.50	6 (10%) 6 6	24, 31, 42, 44	0
2	F	41/64 (64%)	0.61	5 (12%) 5 5	23, 34, 44, 47	0
All	All	657/708 (92%)	0.23	28 (4%) 35 31	17, 26, 40, 47	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	10	TYR	4.8
2	F	718	ASP	4.1
1	C	173	TYR	4.0
1	C	57	GLY	3.9
1	A	57	GLY	3.7
1	C	175	ILE	3.4
2	E	724	ILE	3.3
1	C	56	ASP	3.2
2	D	717	ARG	3.1
2	E	717	ARG	3.1
2	F	716	SER	3.0
2	E	714	SER	2.9
1	C	59	THR	2.7
2	E	715	VAL	2.6
1	C	137	ASP	2.5
2	D	724	ILE	2.5
1	C	58	LYS	2.5
2	F	717	ARG	2.5
2	E	720	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	141	ALA	2.5
1	C	8	TYR	2.4
2	F	721	MET	2.3
1	C	55	VAL	2.3
2	F	728	GLU	2.2
1	B	165	PHE	2.2
1	C	9	ASP	2.1
1	A	10	TYR	2.1
2	E	713	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
7	MES	B	1	12/12	0.22	3.70	45,48,49,50	0
5	SO4	C	2005	5/5	0.13	2.12	51,51,51,51	0
3	2ME	B	2	4/4	0.12	0.22	46,46,46,46	0
5	SO4	B	2004	5/5	0.12	-0.11	60,60,60,60	0
6	GTP	C	200	32/32	0.09	-0.77	20,25,26,29	0
6	GTP	A	200	32/32	0.08	-0.81	17,23,24,25	0
6	GTP	B	200	32/32	0.09	-0.83	18,19,20,21	0
5	SO4	B	2003	5/5	0.07	-1.39	31,32,33,33	0
5	SO4	A	2001	5/5	0.06	-1.48	23,24,25,25	0
5	SO4	C	2002	5/5	0.06	-2.19	27,28,29,29	0
4	MG	B	201	1/1	0.08	-2.65	20,20,20,20	0
4	MG	A	201	1/1	0.05	-2.72	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	C	201	1/1	0.06	-2.80	23,23,23,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.