



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 08:38 PM EDT

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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

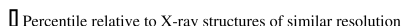
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

i

X-RAY DIFFRACTION

A.



Similar resolution
(#Entries, resolution range(Å))

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Mol	Chain	Length	Quality of chain
2	F	64	<p>11% 62% 36%</p>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6119 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 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 mutation	UNP P62491
B	4	GLY	-	cloning artifact	UNP P62491
B	5	SER	-	cloning artifact	UNP P62491
B	70	LEU	GLN	engineered mutation	UNP P62491
C	4	GLY	-	cloning artifact	UNP P62491
C	5	SER	-	cloning artifact	UNP P62491
C	70	LEU	GLN	engineered mutation	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			

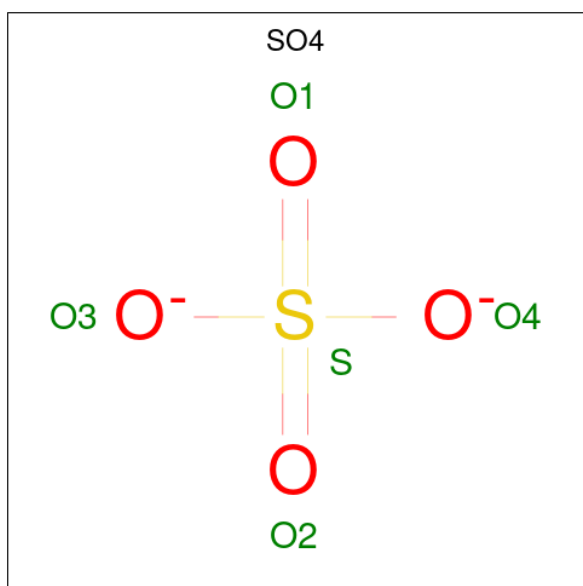
There are 6 discrepancies between the modelled and reference sequences:

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



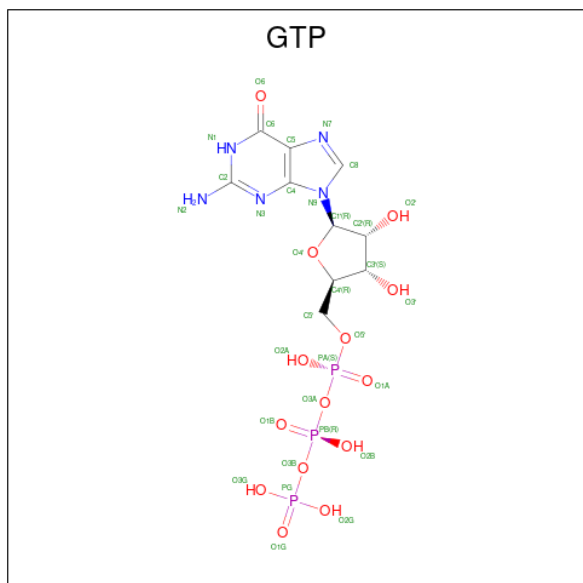
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

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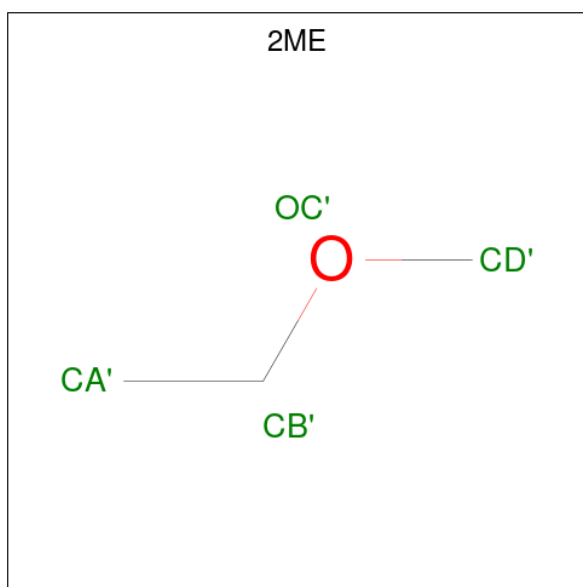
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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



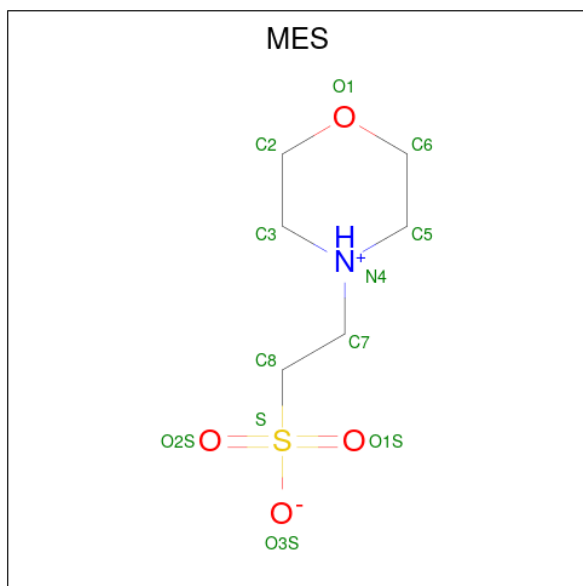
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is METHOXYETHANE (three-letter code: 2ME) (formula: C_3H_8O).



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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

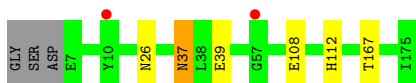
- Molecule 8 is water.

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

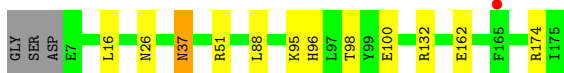
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

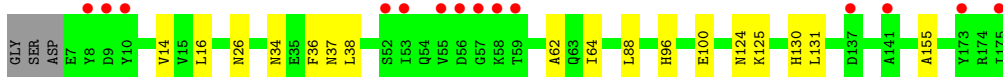
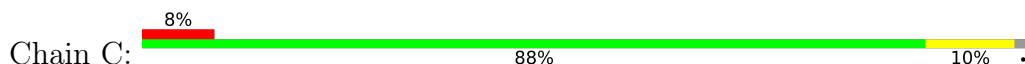
- Molecule 1: Ras-related protein Rab-11A



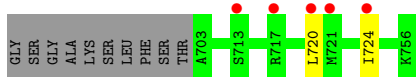
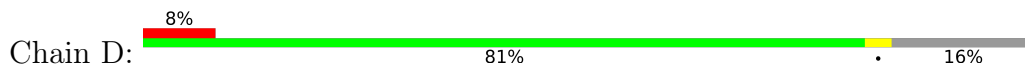
- Molecule 1: Ras-related protein Rab-11A



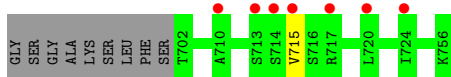
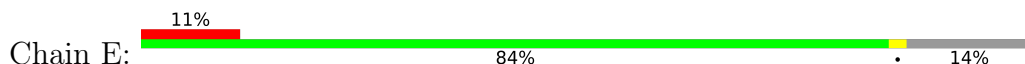
- Molecule 1: Ras-related protein Rab-11A



- Molecule 2: Rab11 family-interacting protein 3



- Molecule 2: Rab11 family-interacting protein 3



- Molecule 2: Rab11 family-interacting protein 3



GLY	SER	GLY	ALA	LYS	SER	LEU	PHE	SER	THR	ALA	PHE	SER	GLU	SER	LEU	ALA	GLU	ILE	SER	SER	VAL	S716	S717	D718	E719	L720	M721	E728	K756
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.237 0.205 , 0.239	Depositor DCC
R_{free} test set	3271 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6119	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, GTP, 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 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	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
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
5	A	32	0	12	0	0
5	B	32	0	12	0	0
5	C	32	0	12	1	0
6	B	4	0	8	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

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 3.

All (26) 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: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	6: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLU:HG3	1:A:112:HIS:CD2	2.51	0.46
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	5: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	Interatomic distance (Å)	Clash overlap (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%)	84	79
1	B	140/145 (97%)	139 (99%)	1 (1%)	84	79
1	C	131/145 (90%)	130 (99%)	1 (1%)	81	76
2	D	37/56 (66%)	37 (100%)	0	100	100
2	E	39/56 (70%)	38 (97%)	1 (3%)	46	30
2	F	32/56 (57%)	31 (97%)	1 (3%)	40	23
All	All	516/603 (86%)	511 (99%)	5 (1%)	76	69

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

Sometimes 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

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Mol	Chain	Res	Type
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 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 monosaccharides 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	$\# Z > 2$
4	SO4	C	2005	-	4,4,4	0.13	0	6,6,6	0.06	0
7	MES	B	1	-	12,12,12	2.13	1 (8%)	14,16,16	2.41	4 (28%)
6	2ME	B	2	-	3,3,3	0.47	0	2,2,2	0.27	0
4	SO4	A	2001	-	4,4,4	0.14	0	6,6,6	0.14	0
4	SO4	B	2004	-	4,4,4	0.14	0	6,6,6	0.07	0
5	GTP	B	200	3	26,34,34	1.02	2 (7%)	33,54,54	1.81	8 (24%)
4	SO4	C	2002	-	4,4,4	0.18	0	6,6,6	0.07	0
5	GTP	A	200	3	26,34,34	1.03	2 (7%)	33,54,54	1.72	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	2003	-	4,4,4	0.13	0	6,6,6	0.09	0
5	GTP	C	200	3	26,34,34	1.02	1 (3%)	33,54,54	1.87	8 (24%)

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
7	MES	B	1	-	-	1/6/14/14	0/1/1/1
6	2ME	B	2	-	-	0/0/1/1	-
5	GTP	B	200	3	-	2/18/38/38	0/3/3/3
5	GTP	A	200	3	-	2/18/38/38	0/3/3/3
5	GTP	C	200	3	-	2/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1	MES	C8-S	-7.07	1.67	1.77
5	C	200	GTP	C6-N1	3.47	1.39	1.33
5	B	200	GTP	C6-N1	3.32	1.38	1.33
5	A	200	GTP	C6-N1	3.32	1.38	1.33
5	A	200	GTP	C2-N1	2.07	1.39	1.35
5	B	200	GTP	C2-N1	2.02	1.39	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1	MES	C5-N4-C3	6.16	122.70	108.83
5	C	200	GTP	N3-C2-N1	-5.74	119.56	127.22
5	B	200	GTP	N3-C2-N1	-5.73	119.57	127.22
5	A	200	GTP	N3-C2-N1	-5.43	119.98	127.22
5	B	200	GTP	C2-N3-C4	4.18	120.13	115.36
5	C	200	GTP	C2-N3-C4	4.16	120.10	115.36
5	A	200	GTP	C2-N3-C4	4.09	120.02	115.36
7	B	1	MES	O2S-S-C8	3.62	111.28	106.92
5	C	200	GTP	C5-C6-N1	-3.12	119.17	123.43
5	B	200	GTP	C6-N1-C2	3.10	120.85	115.93
5	C	200	GTP	C6-N1-C2	3.08	120.82	115.93
7	B	1	MES	C7-N4-C3	3.03	118.98	111.23
5	B	200	GTP	C5-C6-N1	-3.03	119.29	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1	MES	C7-N4-C5	2.77	118.32	111.23
5	A	200	GTP	C5-C6-N1	-2.75	119.67	123.43
5	A	200	GTP	C6-N1-C2	2.65	120.14	115.93
5	C	200	GTP	PA-O3A-PB	-2.60	123.90	132.83
5	C	200	GTP	N2-C2-N1	2.49	121.13	117.25
5	A	200	GTP	N2-C2-N1	2.32	120.86	117.25
5	B	200	GTP	N2-C2-N1	2.26	120.77	117.25
5	B	200	GTP	PA-O3A-PB	-2.25	125.12	132.83
5	B	200	GTP	C6-C5-C4	-2.15	118.74	120.80
5	A	200	GTP	C6-C5-C4	-2.13	118.76	120.80
5	C	200	GTP	C6-C5-C4	-2.12	118.78	120.80
5	C	200	GTP	PB-O3B-PG	-2.11	125.58	132.83
5	B	200	GTP	PB-O3B-PG	-2.01	125.91	132.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	200	GTP	PA-O3A-PB-O1B
5	B	200	GTP	PA-O3A-PB-O1B
5	C	200	GTP	PA-O3A-PB-O1B
7	B	1	MES	C8-C7-N4-C5
5	A	200	GTP	PA-O3A-PB-O2B
5	B	200	GTP	PA-O3A-PB-O2B
5	C	200	GTP	PA-O3A-PB-O2B

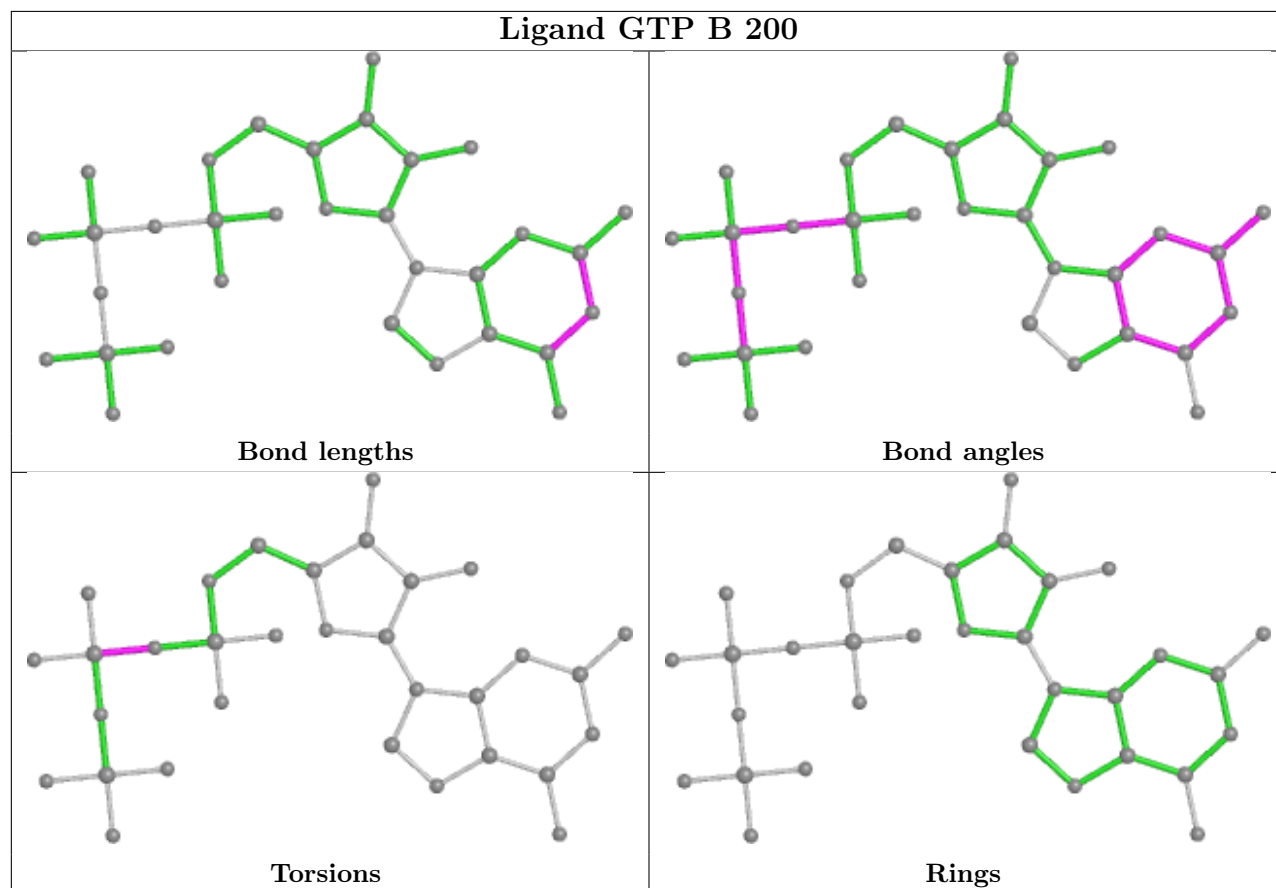
There are no ring outliers.

2 monomers are involved in 2 short contacts:

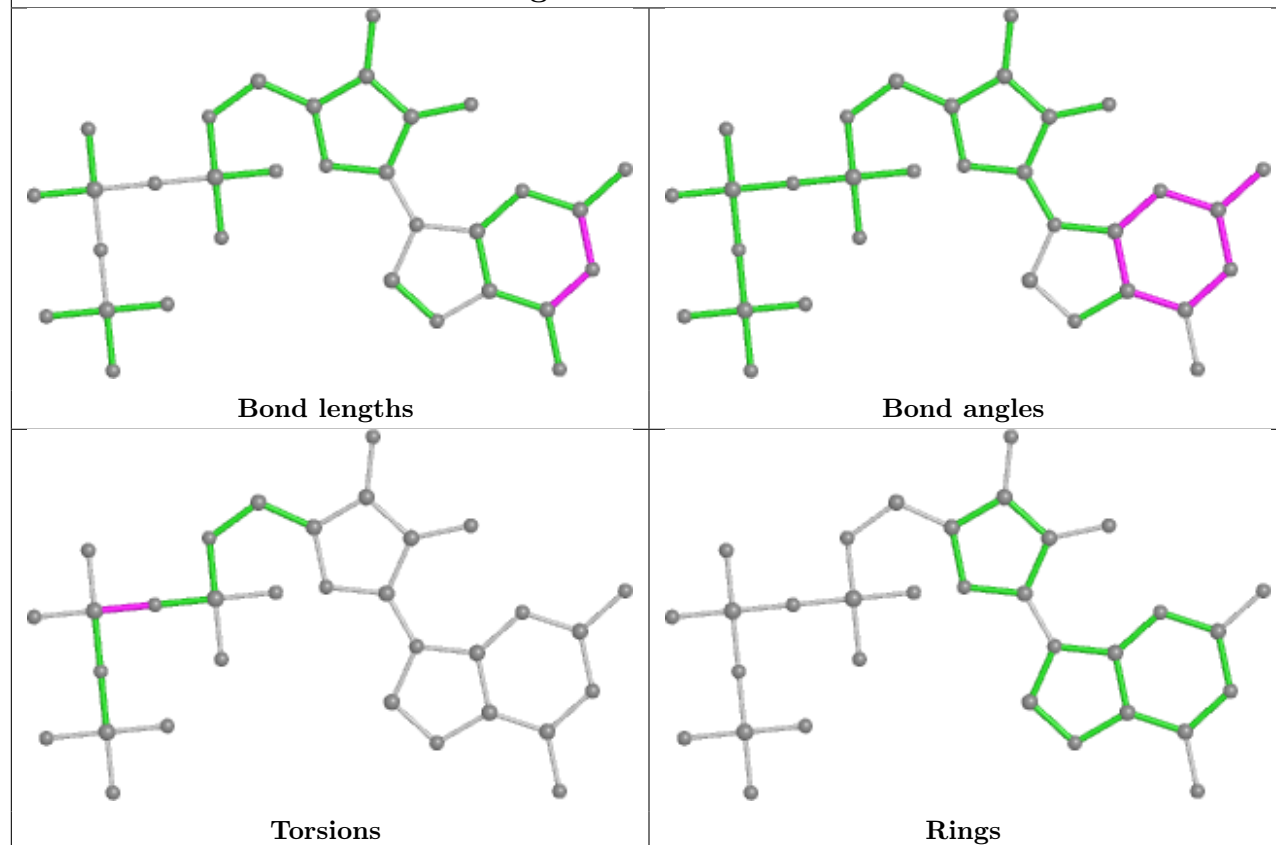
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2	2ME	1	0
5	C	200	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

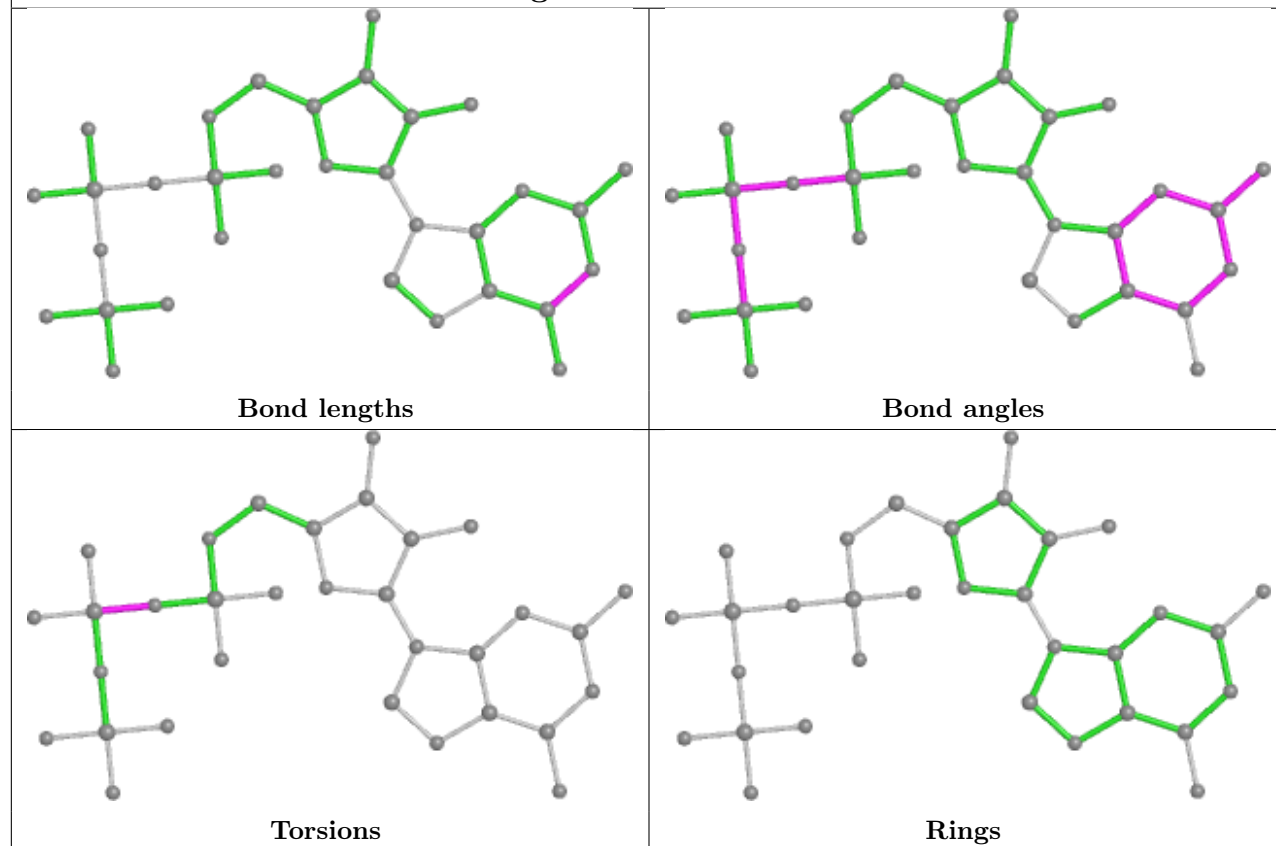
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand GTP A 200



Ligand GTP C 200



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

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, 95th 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 ²)	Q<0.9
1	A	169/172 (98%)	0.14	2 (1%) 79 79	18, 25, 33, 35	0
1	B	169/172 (98%)	0.08	1 (0%) 89 89	18, 23, 30, 33	0
1	C	169/172 (98%)	0.29	14 (8%) 11 11	21, 28, 42, 44	0
2	D	54/64 (84%)	0.56	5 (9%) 8 8	17, 31, 40, 42	0
2	E	55/64 (85%)	0.62	7 (12%) 3 3	24, 31, 42, 44	0
2	F	41/64 (64%)	0.77	7 (17%) 1 1	23, 34, 44, 47	0
All	All	657/708 (92%)	0.28	36 (5%) 25 24	17, 26, 40, 47	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	10	TYR	5.5
2	F	718	ASP	4.3
1	C	57	GLY	4.1
2	E	714	SER	4.1
1	C	173	TYR	3.9
1	A	57	GLY	3.9
2	D	717	ARG	3.7
1	C	59	THR	3.6
2	D	724	ILE	3.6
2	E	720	LEU	3.5
2	E	715	VAL	3.3
2	E	717	ARG	3.3
2	D	720	LEU	3.3
1	C	175	ILE	3.2
2	F	716	SER	3.2
2	F	721	MET	3.2
2	E	724	ILE	3.1
2	F	717	ARG	3.1
2	E	713	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	137	ASP	3.0
1	C	8	TYR	2.9
1	C	56	ASP	2.9
2	F	720	LEU	2.9
1	C	141	ALA	2.8
1	C	9	ASP	2.7
1	C	58	LYS	2.7
2	F	728	GLU	2.5
1	A	10	TYR	2.4
1	C	55	VAL	2.4
2	D	713	SER	2.3
2	F	719	GLU	2.2
1	B	165	PHE	2.2
1	C	53	ILE	2.2
1	C	52	SER	2.2
2	D	721	MET	2.2
2	E	710	ALA	2.2

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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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.

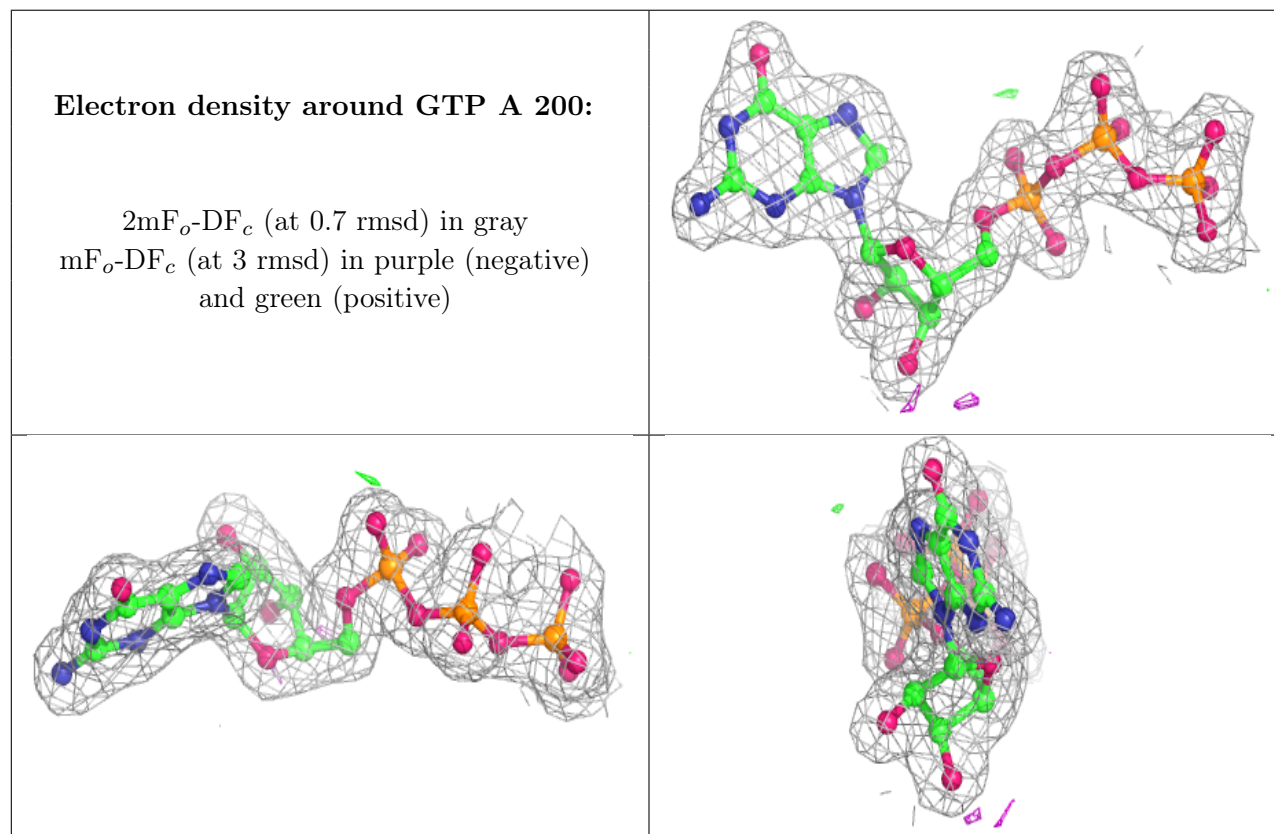
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MES	B	1	12/12	0.83	0.23	45,48,49,50	0
6	2ME	B	2	4/4	0.89	0.16	46,46,46,46	0
4	SO4	B	2004	5/5	0.95	0.11	60,60,60,60	0
5	GTP	A	200	32/32	0.98	0.08	17,23,24,25	0
5	GTP	B	200	32/32	0.98	0.08	18,19,20,21	0
5	GTP	C	200	32/32	0.98	0.08	20,25,26,29	0

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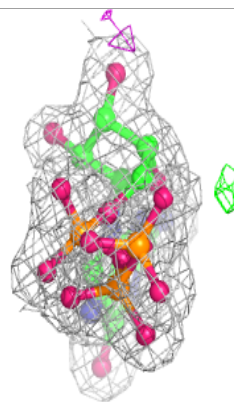
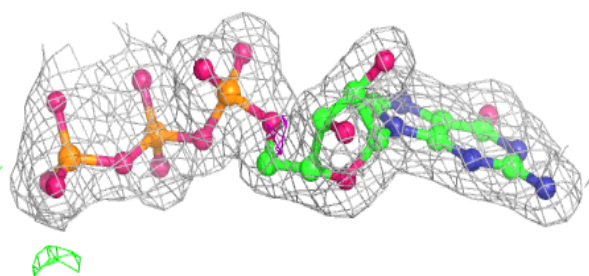
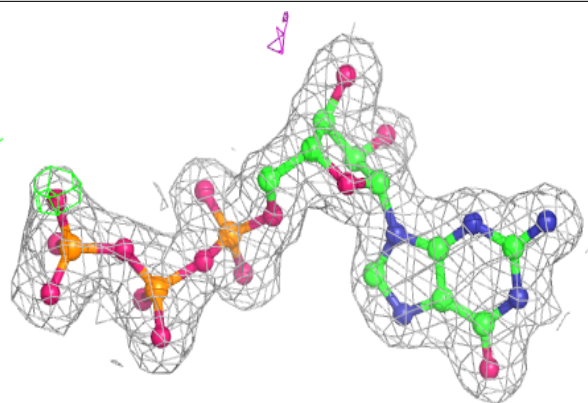
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	201	1/1	0.98	0.04	20,20,20,20	0
4	SO4	C	2005	5/5	0.98	0.14	51,51,51,51	0
4	SO4	A	2001	5/5	0.99	0.07	23,24,25,25	0
4	SO4	B	2003	5/5	0.99	0.07	31,32,33,33	0
3	MG	B	201	1/1	0.99	0.08	20,20,20,20	0
4	SO4	C	2002	5/5	0.99	0.06	27,28,29,29	0
3	MG	C	201	1/1	0.99	0.04	23,23,23,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

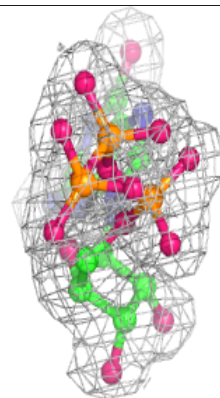
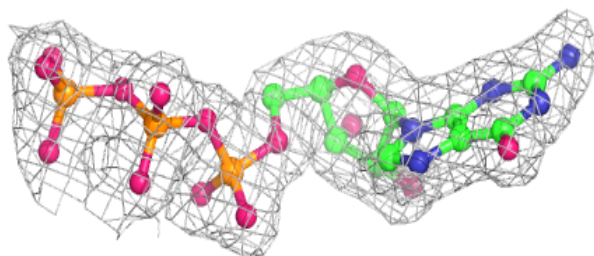
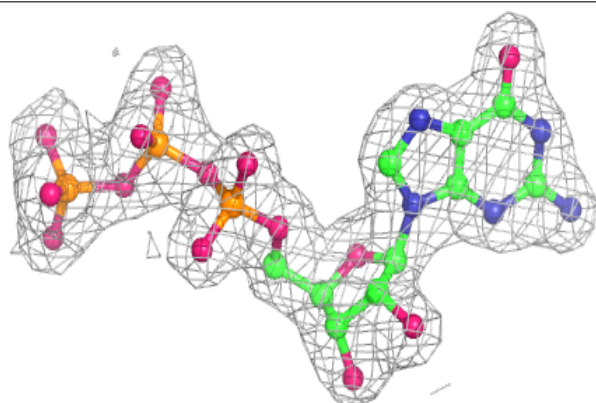


Electron density around GTP B 200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GTP C 200:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.