



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2024 – 02:40 pm GMT

PDB ID : 4V0O  
Title : Crystal structure of BBS1N in complex with ARL6DN, soaked with lead  
Authors : Mourao, A.; Lorentzen, E.  
Deposited on : 2014-09-17  
Resolution : 3.35 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

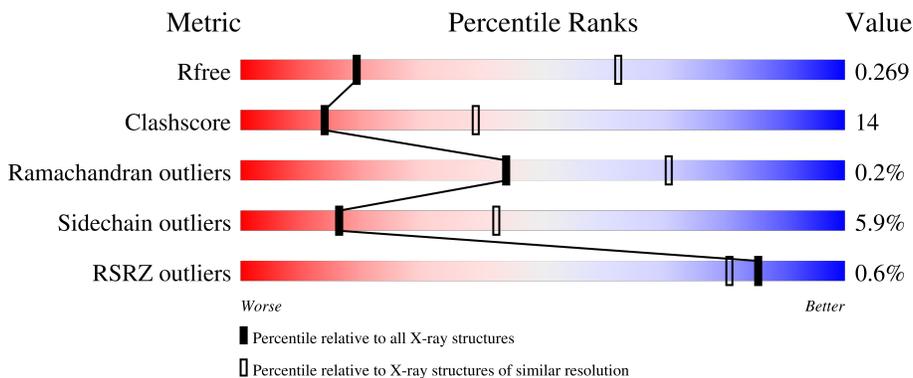
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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))
$R_{free}$	164625	1012 (3.40-3.32)
Clashscore	180529	1035 (3.40-3.32)
Ramachandran outliers	177936	1037 (3.40-3.32)
Sidechain outliers	177891	1037 (3.40-3.32)
RSRZ outliers	164620	1012 (3.40-3.32)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	169	 76% 21% ..
1	C	169	 75% 24% .
1	E	169	 71% 26% ..
1	G	169	 72% 25% ..
2	B	425	 50% 26% 22%

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Mol	Chain	Length	Quality of chain
2	D	425	
2	F	425	
2	H	425	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14519 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 ARF-LIKE SMALL GTPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	166	1265	809	215	235	6	0	0	0
1	C	166	1291	823	223	239	6	0	0	0
1	E	166	1278	816	219	237	6	0	0	0
1	G	166	1286	822	221	237	6	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP A8JF99
A	13	ALA	-	expression tag	UNP A8JF99
A	14	ALA	-	expression tag	UNP A8JF99
A	15	SER	-	expression tag	UNP A8JF99
C	12	GLY	-	expression tag	UNP A8JF99
C	13	ALA	-	expression tag	UNP A8JF99
C	14	ALA	-	expression tag	UNP A8JF99
C	15	SER	-	expression tag	UNP A8JF99
E	12	GLY	-	expression tag	UNP A8JF99
E	13	ALA	-	expression tag	UNP A8JF99
E	14	ALA	-	expression tag	UNP A8JF99
E	15	SER	-	expression tag	UNP A8JF99
G	12	GLY	-	expression tag	UNP A8JF99
G	13	ALA	-	expression tag	UNP A8JF99
G	14	ALA	-	expression tag	UNP A8JF99
G	15	SER	-	expression tag	UNP A8JF99

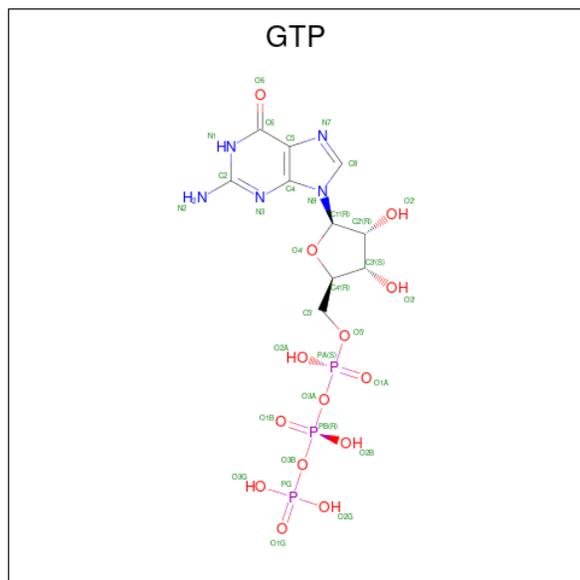
- Molecule 2 is a protein called BARDET-BIEDL SYNDROME 1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	333	Total 2428	C 1551	N 422	O 442	S 13	0	0	0
2	D	307	Total 2205	C 1401	N 387	O 405	S 12	0	0	0
2	F	309	Total 2230	C 1424	N 384	O 409	S 13	0	0	0
2	H	325	Total 2386	C 1525	N 411	O 437	S 13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	ARG	LYS	conflict	UNP A8JEA1
D	37	ARG	LYS	conflict	UNP A8JEA1
F	37	ARG	LYS	conflict	UNP A8JEA1
H	37	ARG	LYS	conflict	UNP A8JEA1

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

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

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

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

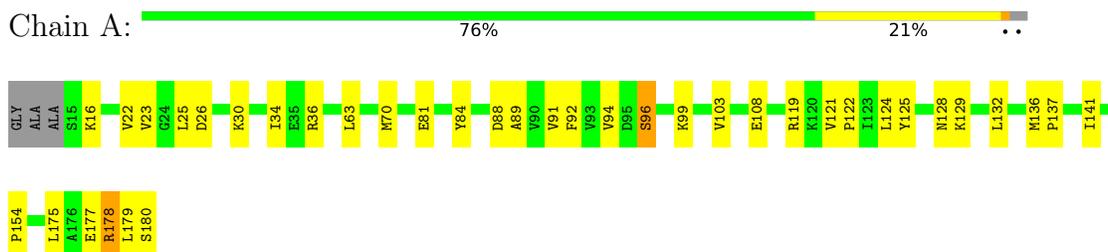
- Molecule 5 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Pb	0	0
			2	2		
5	B	4	Total	Pb	0	0
			4	4		
5	D	3	Total	Pb	0	0
			3	3		
5	E	1	Total	Pb	0	0
			1	1		
5	F	3	Total	Pb	0	0
			3	3		
5	G	1	Total	Pb	0	0
			1	1		
5	H	4	Total	Pb	0	0
			4	4		

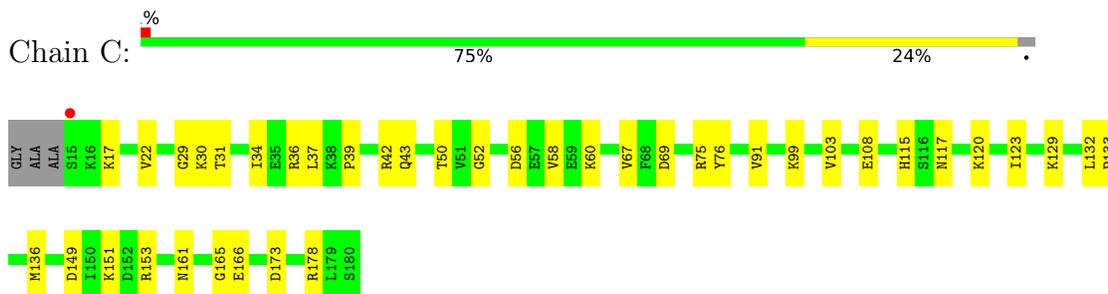
### 3 Residue-property plots [i](#)

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.

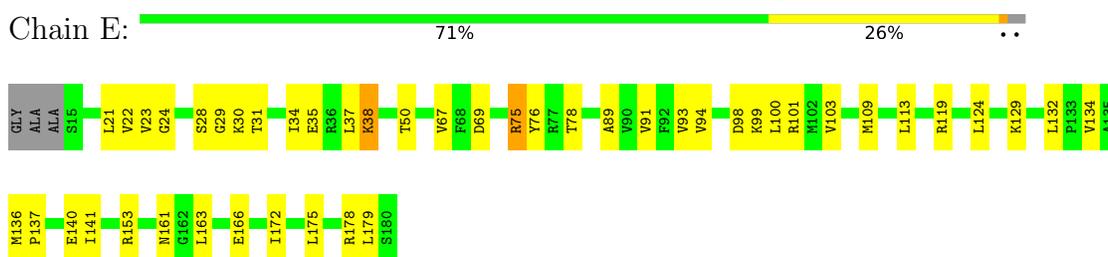
- Molecule 1: ARF-LIKE SMALL GTPASE



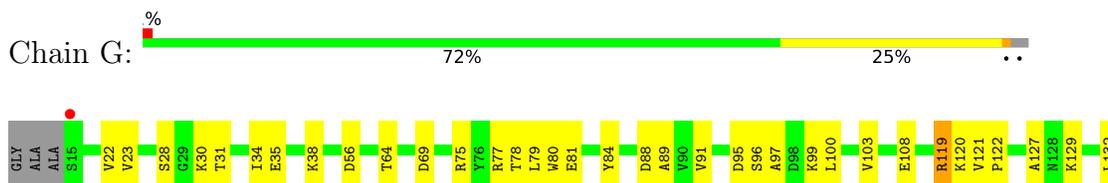
- Molecule 1: ARF-LIKE SMALL GTPASE



- Molecule 1: ARF-LIKE SMALL GTPASE



- Molecule 1: ARF-LIKE SMALL GTPASE







## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.70Å 123.70Å 439.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	96.27 – 3.35 96.27 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.2 (96.27-3.35) 99.3 (96.27-3.35)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 3.33Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.221 , 0.268 0.225 , 0.269	Depositor DCC
$R_{free}$ test set	2837 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	114.1	Xtrriage
Anisotropy	0.212	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: PB, MG, GTP

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	0.45	0/1291	0.65	0/1758
1	C	0.65	0/1317	0.77	0/1788
1	E	0.65	0/1304	0.78	0/1773
1	G	0.49	0/1312	0.67	0/1781
2	B	0.59	0/2480	0.79	2/3398 (0.1%)
2	D	0.47	0/2247	0.71	1/3077 (0.0%)
2	F	0.50	0/2276	0.73	0/3118
2	H	0.57	0/2437	0.78	1/3341 (0.0%)
All	All	0.55	0/14664	0.74	4/20034 (0.0%)

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
2	H	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	356	GLN	N-CA-C	-7.27	91.38	111.00
2	B	130	LEU	CA-CB-CG	5.37	127.66	115.30
2	D	80	LEU	CA-CB-CG	5.37	127.65	115.30
2	B	208	GLN	N-CA-C	5.17	124.95	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	355	GLY	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	1265	0	1248	25	0
1	C	1291	0	1297	34	0
1	E	1278	0	1272	36	0
1	G	1286	0	1294	30	0
2	B	2428	0	2359	74	0
2	D	2205	0	2101	72	0
2	F	2230	0	2145	70	0
2	H	2386	0	2329	79	0
3	A	32	0	12	4	0
3	C	32	0	12	3	0
3	E	32	0	12	5	0
3	G	32	0	12	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	2	0	0	0	0
5	B	4	0	0	0	0
5	D	3	0	0	0	0
5	E	1	0	0	0	0
5	F	3	0	0	1	0
5	G	1	0	0	0	0
5	H	4	0	0	0	0
All	All	14519	0	14093	405	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 14.

The worst 5 of 405 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:C:129:LYS:HB3	1:C:132:LEU:HD12	1.58	0.84
2:D:82:ILE:HG22	2:D:89:ALA:HB3	1.64	0.80
2:D:74:ALA:HB1	2:D:98:PRO:HG2	1.63	0.79
2:F:39:VAL:HG13	2:F:381:SER:HB2	1.64	0.79
2:F:91:GLU:O	2:F:92:HIS:ND1	2.17	0.78

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	164/169 (97%)	155 (94%)	9 (6%)	0	100	100
1	C	164/169 (97%)	152 (93%)	12 (7%)	0	100	100
1	E	164/169 (97%)	153 (93%)	11 (7%)	0	100	100
1	G	164/169 (97%)	154 (94%)	10 (6%)	0	100	100
2	B	329/425 (77%)	294 (89%)	34 (10%)	1 (0%)	37	65
2	D	299/425 (70%)	267 (89%)	31 (10%)	1 (0%)	37	65
2	F	303/425 (71%)	273 (90%)	29 (10%)	1 (0%)	37	65
2	H	321/425 (76%)	293 (91%)	28 (9%)	0	100	100
All	All	1908/2376 (80%)	1741 (91%)	164 (9%)	3 (0%)	44	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	209	PRO
2	F	65	GLY
2	D	65	GLY

### 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	132/142 (93%)	128 (97%)	4 (3%)	36 61
1	C	138/142 (97%)	136 (99%)	2 (1%)	62 78
1	E	135/142 (95%)	126 (93%)	9 (7%)	13 39
1	G	137/142 (96%)	132 (96%)	5 (4%)	30 56
2	B	243/352 (69%)	224 (92%)	19 (8%)	10 33
2	D	214/352 (61%)	196 (92%)	18 (8%)	9 30
2	F	221/352 (63%)	210 (95%)	11 (5%)	20 47
2	H	243/352 (69%)	225 (93%)	18 (7%)	11 36
All	All	1463/1976 (74%)	1377 (94%)	86 (6%)	16 42

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	296	LEU
2	H	70	ARG
2	F	317	VAL
1	G	78	THR
2	H	108	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	257	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 22 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
3	GTP	G	600	4	26,34,34	1.23	2 (7%)	32,54,54	1.64	7 (21%)
3	GTP	A	600	4	26,34,34	1.11	2 (7%)	32,54,54	1.47	5 (15%)
3	GTP	E	600	4	26,34,34	1.13	2 (7%)	32,54,54	1.72	10 (31%)
3	GTP	C	600	4	26,34,34	1.24	1 (3%)	32,54,54	1.74	9 (28%)

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
3	GTP	G	600	4	-	2/18/38/38	0/3/3/3
3	GTP	A	600	4	-	5/18/38/38	0/3/3/3
3	GTP	E	600	4	-	5/18/38/38	0/3/3/3
3	GTP	C	600	4	-	5/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	600	GTP	C5-C6	-4.57	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	600	GTP	C5-C6	-4.53	1.38	1.47
3	E	600	GTP	C5-C6	-4.12	1.39	1.47
3	A	600	GTP	C5-C6	-3.93	1.39	1.47
3	A	600	GTP	C2-N3	2.37	1.38	1.33

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	600	GTP	PA-O3A-PB	-3.95	119.27	132.83
3	A	600	GTP	PA-O3A-PB	-3.82	119.70	132.83
3	G	600	GTP	PB-O3B-PG	-3.80	119.80	132.83
3	C	600	GTP	PA-O3A-PB	-3.69	120.16	132.83
3	C	600	GTP	PB-O3B-PG	-3.43	121.07	132.83

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	600	GTP	O4'-C4'-C5'-O5'
3	G	600	GTP	PB-O3B-PG-O3G
3	A	600	GTP	O4'-C4'-C5'-O5'
3	E	600	GTP	O4'-C4'-C5'-O5'
3	A	600	GTP	PB-O3B-PG-O1G

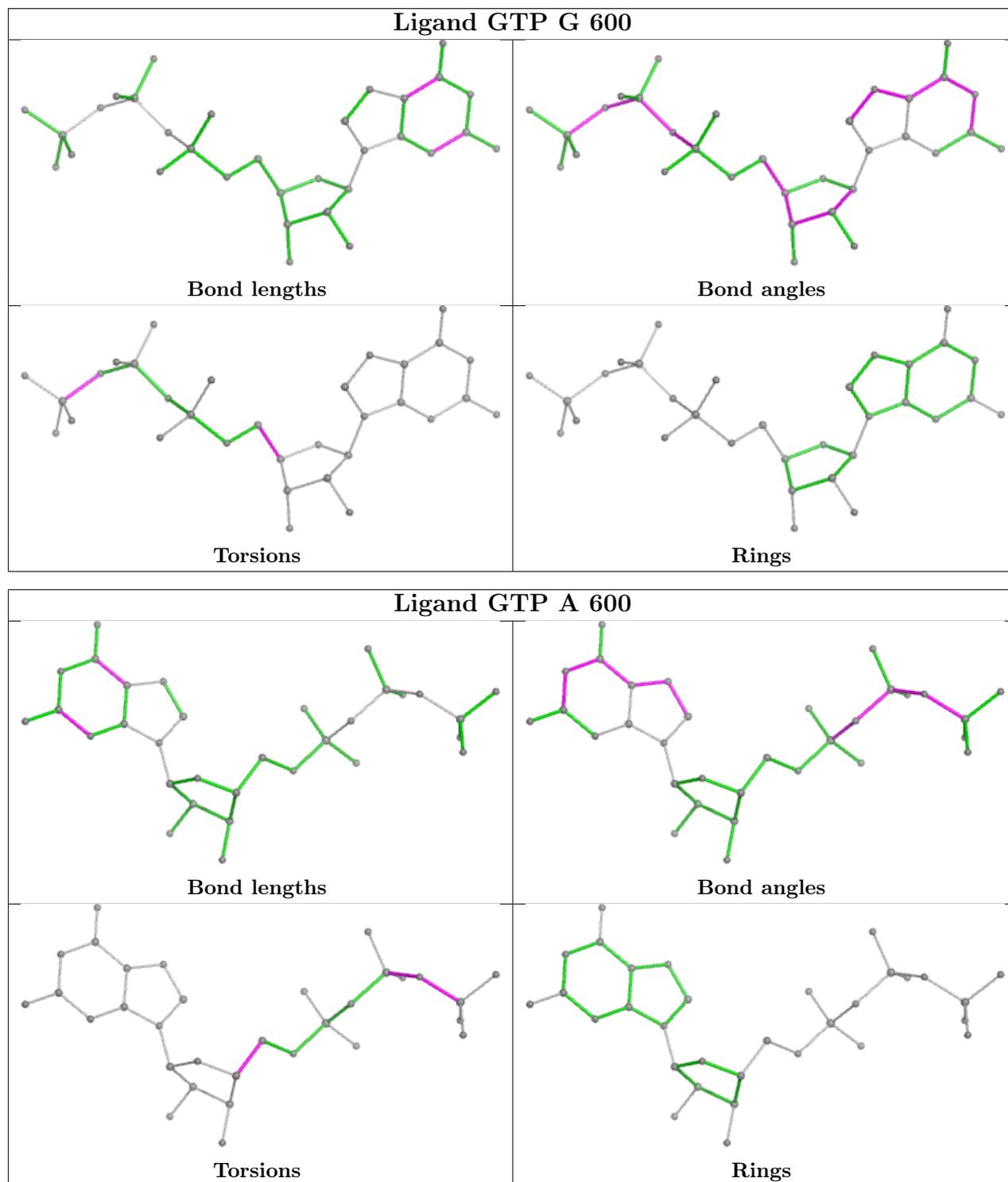
There are no ring outliers.

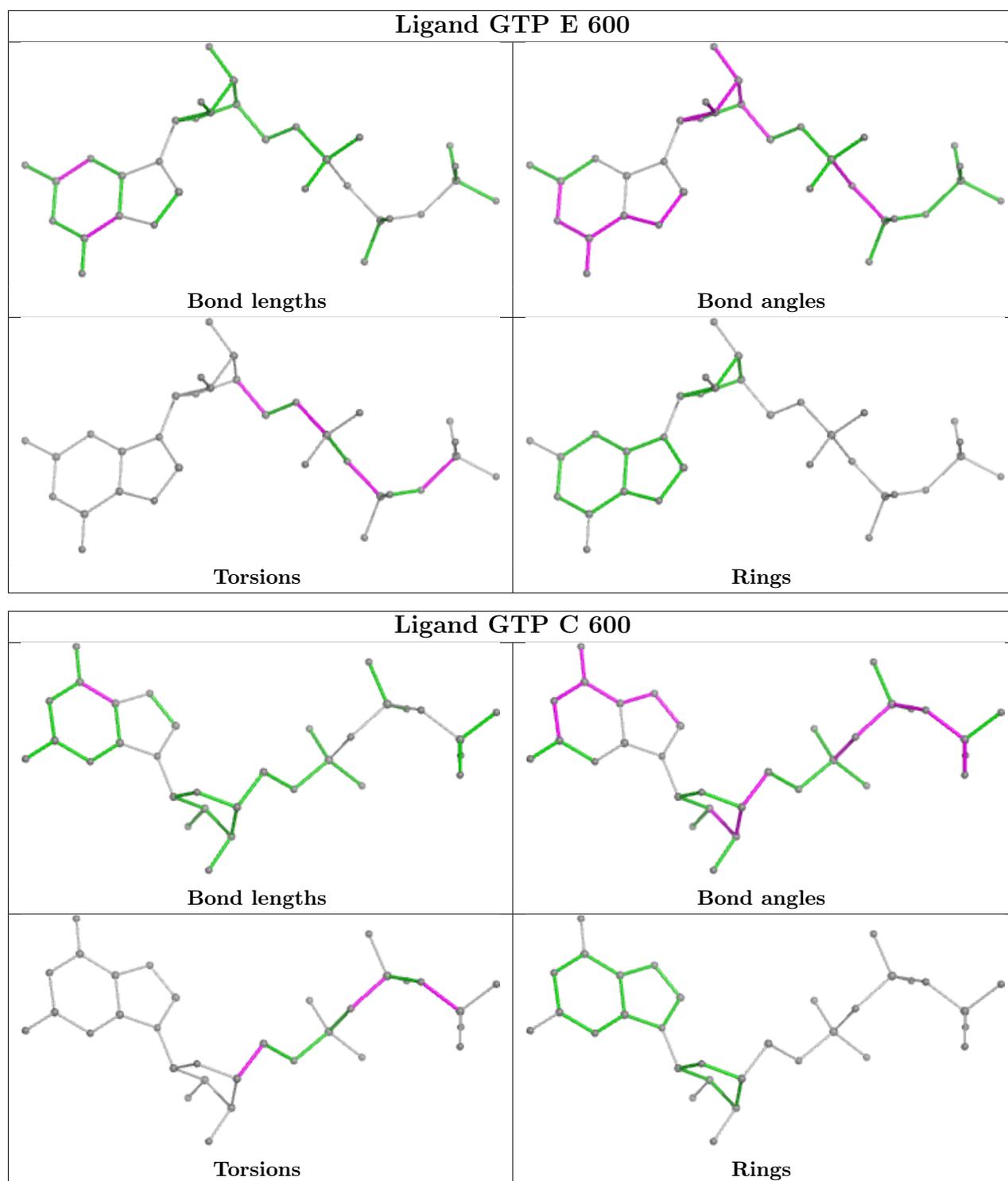
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	600	GTP	2	0
3	A	600	GTP	4	0
3	E	600	GTP	5	0
3	C	600	GTP	3	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.





## 5.7 Other polymers [\(i\)](#)

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 [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	166/169 (98%)	-0.74	0 <b>100</b> <b>100</b>	9, 35, 61, 85	0
1	C	166/169 (98%)	-0.87	1 (0%) <b>85</b> <b>81</b>	1, 4, 33, 48	0
1	E	166/169 (98%)	-0.85	0 <b>100</b> <b>100</b>	1, 8, 39, 66	0
1	G	166/169 (98%)	-0.80	1 (0%) <b>85</b> <b>81</b>	8, 24, 51, 60	0
2	B	333/425 (78%)	-0.76	1 (0%) <b>90</b> <b>89</b>	1, 16, 50, 81	0
2	D	307/425 (72%)	-0.46	3 (0%) <b>79</b> <b>72</b>	2, 44, 96, 105	0
2	F	309/425 (72%)	-0.46	3 (0%) <b>79</b> <b>72</b>	1, 37, 92, 120	0
2	H	325/425 (76%)	-0.78	2 (0%) <b>85</b> <b>81</b>	1, 16, 49, 77	0
All	All	1938/2376 (81%)	-0.69	11 (0%) <b>85</b> <b>81</b>	1, 21, 83, 120	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	147	GLU	3.6
2	B	144	ASN	3.4
2	F	104	TYR	3.1
2	F	254	ILE	2.9
2	F	140	PRO	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](#)

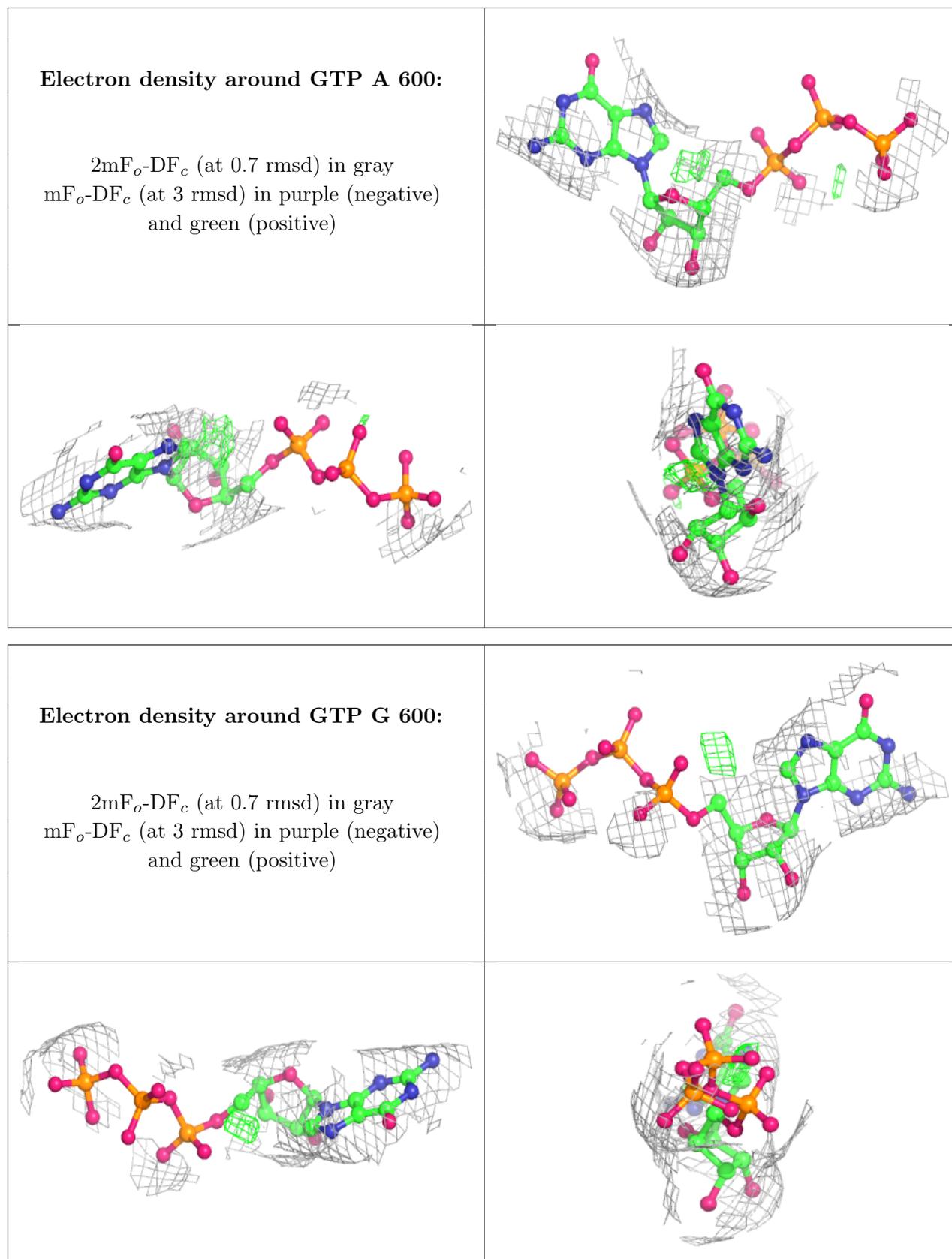
There are no monosaccharides in this entry.

## 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. 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.

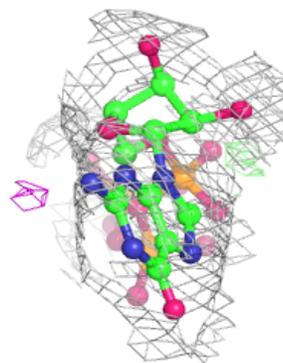
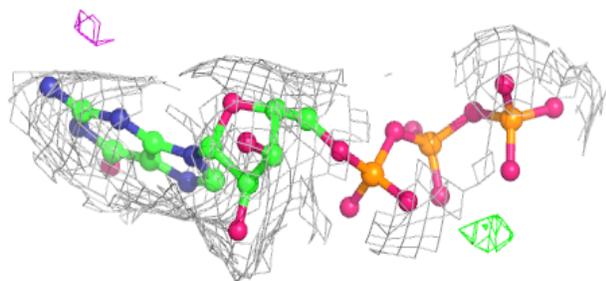
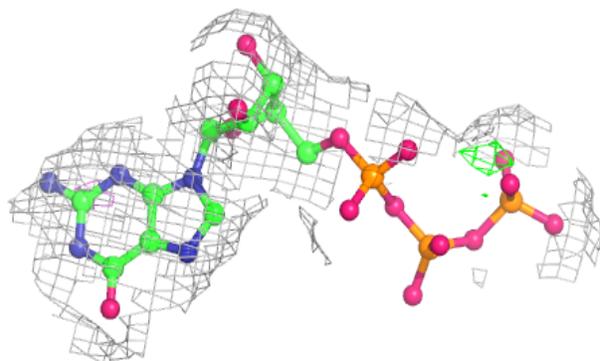
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PB	B	1429	1/1	0.74	0.08	66,66,66,66	1
5	PB	A	1181	1/1	0.83	0.05	170,170,170,170	1
5	PB	H	1429	1/1	0.85	0.05	84,84,84,84	1
5	PB	G	1181	1/1	0.86	0.05	106,106,106,106	1
5	PB	E	1181	1/1	0.86	0.08	120,120,120,120	1
5	PB	B	1427	1/1	0.87	0.06	85,85,85,85	1
5	PB	D	1428	1/1	0.88	0.05	140,140,140,140	1
5	PB	H	1427	1/1	0.90	0.11	16,16,16,16	1
5	PB	H	1428	1/1	0.90	0.06	89,89,89,89	1
5	PB	D	1427	1/1	0.90	0.10	79,79,79,79	1
5	PB	F	1426	1/1	0.92	0.10	83,83,83,83	1
5	PB	F	1428	1/1	0.93	0.07	83,83,83,83	1
5	PB	A	1182	1/1	0.95	0.04	112,112,112,112	1
3	GTP	A	600	32/32	0.96	0.05	29,35,46,48	0
3	GTP	G	600	32/32	0.97	0.05	15,19,25,26	0
5	PB	B	1428	1/1	0.97	0.06	12,12,12,12	1
5	PB	B	1426	1/1	0.97	0.10	33,33,33,33	1
5	PB	D	1426	1/1	0.97	0.07	35,35,35,35	1
5	PB	F	1427	1/1	0.97	0.05	23,23,23,23	1
5	PB	H	1426	1/1	0.98	0.09	35,35,35,35	1
4	MG	C	601	1/1	0.98	0.10	1,1,1,1	0
3	GTP	E	600	32/32	0.98	0.04	5,8,14,17	0
4	MG	A	601	1/1	0.98	0.08	29,29,29,29	0
3	GTP	C	600	32/32	0.99	0.04	1,3,4,4	0
4	MG	E	601	1/1	0.99	0.06	6,6,6,6	0
4	MG	G	601	1/1	0.99	0.07	15,15,15,15	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.

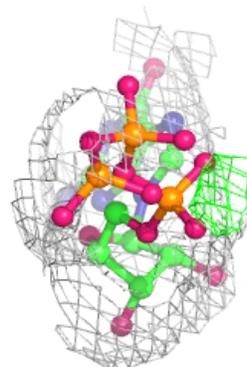
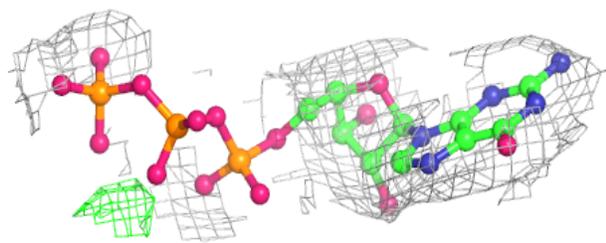
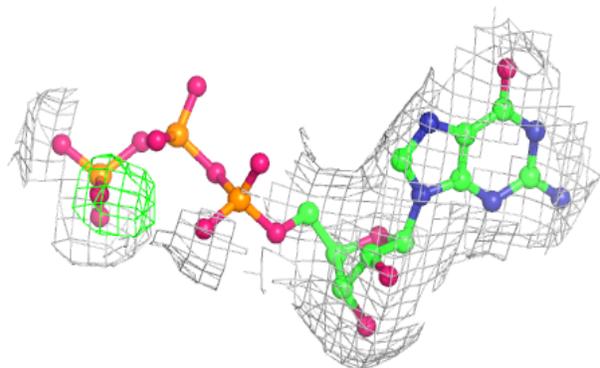


**Electron density around GTP E 600:**

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

**Electron density around GTP C 600:**

$2mF_o-DF_c$  (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.