



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:42 PM UTC

PDB ID : 6Y09 / pdb_00006y09
Title : Crystal structure of Atg16L in complex with GTP-bound Rab33B (Q92L)
Authors : Pantoom, S.; Wu, Y.W.
Deposited on : 2020-02-07
Resolution : 2.40 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

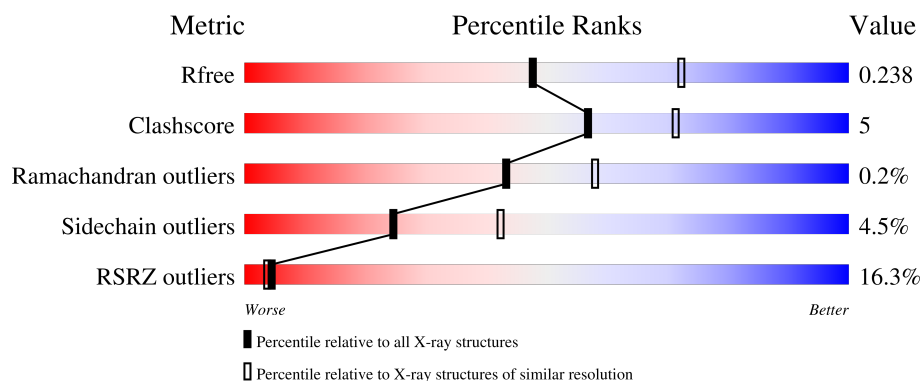
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 ≥ 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	192	3% 85% 7% 8%
1	B	192	3% 81% 9% 9%
2	C	126	27% 53% 12% 32%
2	D	126	31% 54% 13% 32%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PEG	B	305	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4629 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-33B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1422	901	257	255	9			
1	B	175	Total	C	N	O	S	0	0	0
			1414	895	256	254	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP Q9H082
A	28	PRO	-	expression tag	UNP Q9H082
A	29	MET	-	expression tag	UNP Q9H082
A	92	LEU	GLN	engineered mutation	UNP Q9H082
B	27	GLY	-	expression tag	UNP Q9H082
B	28	PRO	-	expression tag	UNP Q9H082
B	29	MET	-	expression tag	UNP Q9H082
B	92	LEU	GLN	engineered mutation	UNP Q9H082

- Molecule 2 is a protein called Autophagy-related protein 16-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	86	Total	C	N	O	S	0	0	0
			711	432	131	145	3			
2	D	86	Total	C	N	O	S	0	0	0
			711	432	131	145	3			

There are 2 discrepancies between the modelled and reference sequences:

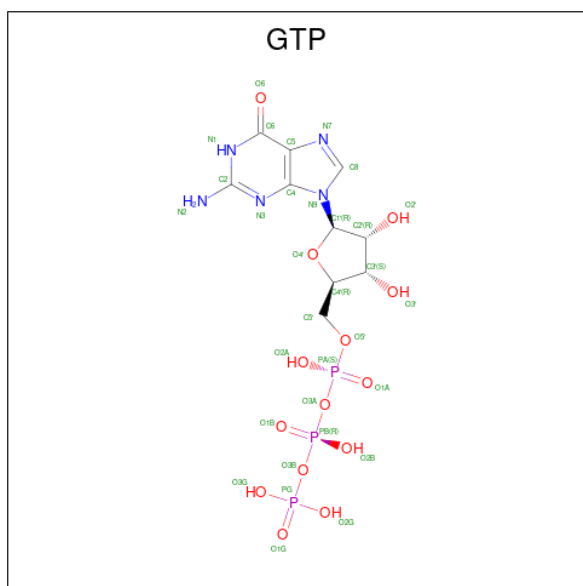
Chain	Residue	Modelled	Actual	Comment	Reference
C	140	MET	-	initiating methionine	UNP Q8C0J2
D	140	MET	-	initiating methionine	UNP Q8C0J2

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

Interest" by depositor).

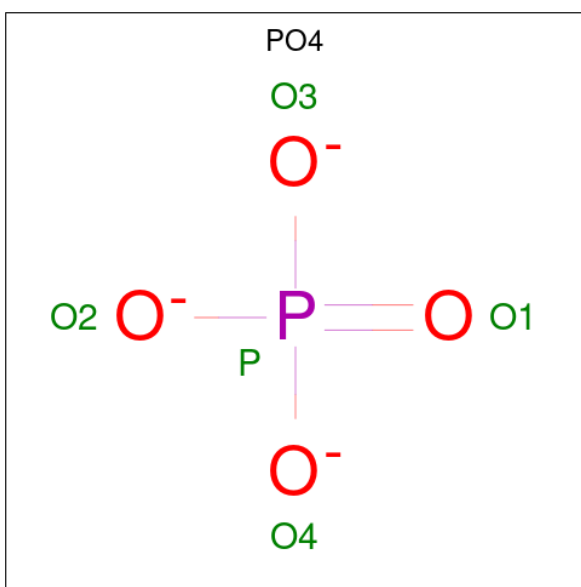
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



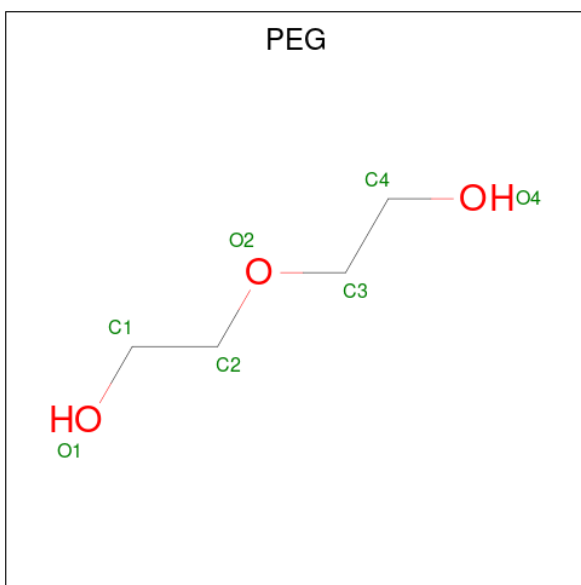
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	B	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



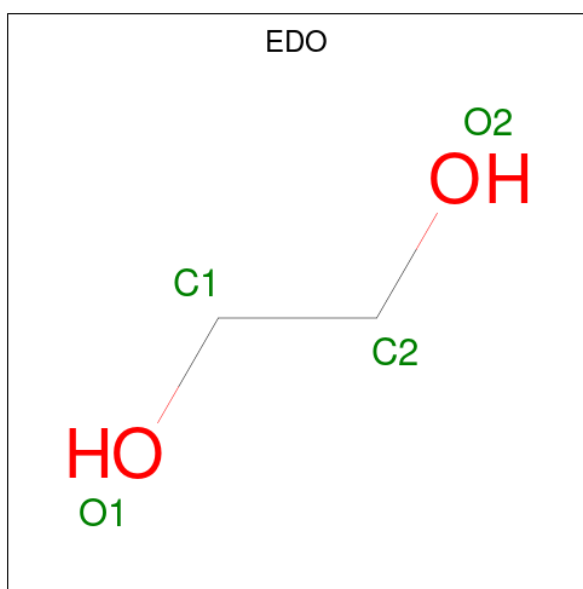
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

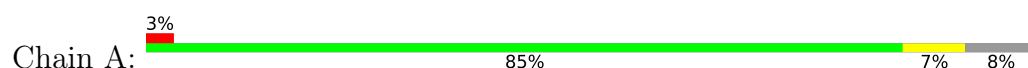
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	98	Total 98	O 98	0	0
8	C	9	Total 9	O 9	0	0
8	B	88	Total 88	O 88	0	0
8	D	19	Total 19	O 19	0	0

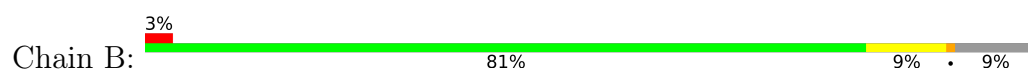
3 Residue-property plots [i](#)

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.

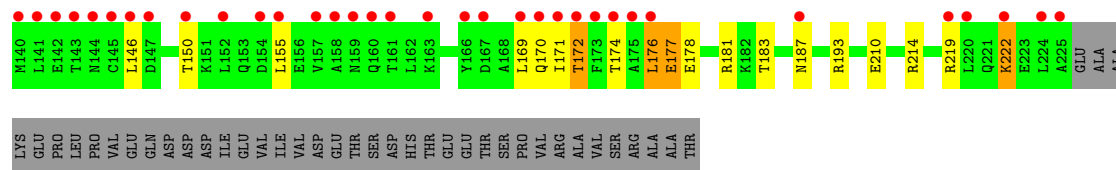
- Molecule 1: Ras-related protein Rab-33B



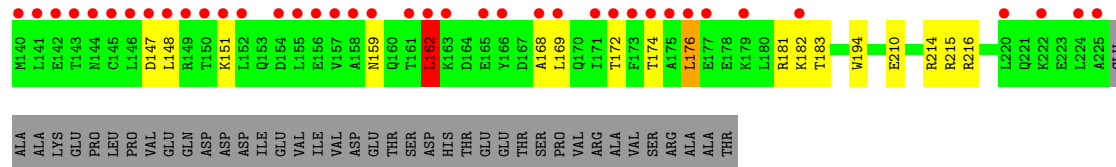
- Molecule 1: Ras-related protein Rab-33B



- Molecule 2: Autophagy-related protein 16-1



- Molecule 2: Autophagy-related protein 16-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.95Å 132.42Å 155.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.40 48.17 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.17-2.40) 99.9 (48.17-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 1.9_1692	Depositor
R, R_{free}	0.192 , 0.231 0.202 , 0.238	Depositor DCC
R_{free} test set	2337 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtrriage
Anisotropy	0.811	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4629	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1185e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, PEG, EDO, GTP, PO4

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	0.53	0/1454	0.79	0/1964
1	B	0.61	0/1446	0.84	0/1953
2	C	0.44	0/714	0.67	0/957
2	D	0.39	0/714	0.73	1/957 (0.1%)
All	All	0.52	0/4328	0.78	1/5831 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	174	THR	N-CA-C	-6.22	105.69	113.28

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	1422	0	1415	7	0
1	B	1414	0	1404	14	0
2	C	711	0	713	12	0
2	D	711	0	713	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	32	0	12	0	0
4	B	32	0	12	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	21	0	30	3	0
6	B	42	0	60	9	0
7	B	8	0	12	1	0
8	A	98	0	0	0	0
8	B	88	0	0	0	0
8	C	9	0	0	0	0
8	D	19	0	0	0	0
All	All	4629	0	4371	40	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 5.

All (40) 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:A:162:LEU:HD11	6:A:305:PEG:H31	1.67	0.76
2:D:159:ASN:HA	2:D:162:LEU:HB3	1.66	0.76
2:C:193:ARG:HG2	2:D:194:TRP:HH2	1.52	0.74
1:B:118:ASN:HD22	6:B:311:PEG:H12	1.54	0.73
2:D:162:LEU:C	2:D:162:LEU:HD12	2.14	0.72
2:C:170:GLN:HG3	2:C:171:ILE:HG12	1.72	0.70
1:A:90:ALA:O	1:A:96:ARG:NH1	2.33	0.60
1:A:51:TYR:OH	1:A:57:ARG:NH1	2.34	0.60
2:C:210:GLU:OE2	2:C:214:ARG:NH2	2.36	0.59
2:D:215:ARG:HH21	2:D:216:ARG:HB2	1.67	0.58
2:C:146:LEU:O	2:C:150:THR:HG22	2.06	0.55
2:D:210:GLU:HG2	2:D:214:ARG:NH1	2.22	0.53
2:C:193:ARG:HG2	2:D:194:TRP:CH2	2.39	0.53
2:D:168:ALA:O	2:D:172:THR:HG23	2.09	0.53
1:B:181:ASN:ND2	6:B:305:PEG:O1	2.41	0.51
2:C:183:THR:HG22	2:D:183:THR:HG22	1.93	0.51
1:B:170:HIS:CE1	7:B:307:EDO:H22	2.46	0.50
1:B:47:THR:HG23	1:B:71:ARG:NH1	2.26	0.50
1:B:181:ASN:HD22	6:B:305:PEG:HO1	1.60	0.50
1:B:137:LEU:HB2	6:B:309:PEG:H41	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:169:LEU:HA	2:C:172:THR:HG22	1.94	0.49
2:C:178:GLU:OE2	2:C:181:ARG:NH1	2.44	0.49
1:B:52:ARG:HH22	6:B:305:PEG:H22	1.77	0.49
1:A:125:LEU:O	1:A:129:ILE:HG12	2.14	0.47
1:B:131:GLU:OE2	6:B:310:PEG:H42	2.15	0.46
2:C:176:LEU:HD23	2:D:176:LEU:HD13	1.99	0.45
2:C:171:ILE:HA	2:C:174:THR:OG1	2.18	0.44
1:B:118:ASN:HD22	6:B:311:PEG:C1	2.28	0.44
1:B:143:ARG:NH2	1:B:170:HIS:O	2.39	0.43
1:B:198:LYS:HE3	1:B:204:PRO:O	2.19	0.43
2:C:219:ARG:HA	2:C:222:LYS:HE3	2.00	0.43
1:B:120:ALA:HB1	6:B:306:PEG:H11	2.01	0.43
6:A:306:PEG:H41	6:A:306:PEG:H21	1.62	0.43
1:A:162:LEU:CD1	6:A:305:PEG:H12	2.50	0.42
1:A:144:ILE:HG22	1:A:173:PRO:HG2	2.01	0.42
6:B:305:PEG:H11	6:B:305:PEG:H32	1.83	0.41
2:C:177:GLU:HG3	2:D:176:LEU:HD11	2.03	0.41
1:B:116:MET:HE2	1:B:156:ILE:HD13	2.03	0.41
1:B:35:LYS:HE3	1:B:87:TRP:CE2	2.55	0.41
1:A:72:GLU:HG2	1:A:85:GLN:HG3	2.04	0.40

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	174/192 (91%)	169 (97%)	5 (3%)	0	100	100
1	B	173/192 (90%)	170 (98%)	3 (2%)	0	100	100
2	C	84/126 (67%)	84 (100%)	0	0	100	100
2	D	84/126 (67%)	79 (94%)	4 (5%)	1 (1%)	10	16
All	All	515/636 (81%)	502 (98%)	12 (2%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	162	LEU

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	156/170 (92%)	154 (99%)	2 (1%)	61	80
1	B	155/170 (91%)	150 (97%)	5 (3%)	34	56
2	C	77/112 (69%)	71 (92%)	6 (8%)	11	20
2	D	77/112 (69%)	69 (90%)	8 (10%)	7	10
All	All	465/564 (82%)	444 (96%)	21 (4%)	24	42

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	GLU
1	A	197	HIS
2	C	155	LEU
2	C	172	THR
2	C	176	LEU
2	C	177	GLU
2	C	187	ASN
2	C	222	LYS
1	B	62	THR
1	B	68	VAL
1	B	143	ARG
1	B	198	LYS
1	B	202	HIS
2	D	147	ASP
2	D	148	LEU
2	D	151	LYS
2	D	162	LEU
2	D	169	LEU
2	D	176	LEU

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Mol	Chain	Res	Type
2	D	181	ARG
2	D	182	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
2	C	187	ASN
1	B	123	HIS
1	B	202	HIS
2	D	188	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	PEG	B	306	-	6,6,6	0.62	0	5,5,5	0.33	0
6	PEG	B	309	-	6,6,6	0.56	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	C	301	-	4,4,4	0.90	0	6,6,6	0.50	0
7	EDO	B	307	-	3,3,3	0.49	0	2,2,2	0.40	0
5	PO4	A	303	-	4,4,4	0.77	0	6,6,6	0.45	0
7	EDO	B	304	-	3,3,3	0.54	0	2,2,2	0.32	0
6	PEG	A	306	-	6,6,6	0.55	0	5,5,5	0.54	0
6	PEG	B	305	-	6,6,6	0.56	0	5,5,5	0.42	0
6	PEG	B	308	-	6,6,6	0.71	0	5,5,5	0.34	0
5	PO4	B	303	-	4,4,4	0.72	0	6,6,6	0.64	0
4	GTP	B	302	3	33,34,34	1.03	3 (9%)	50,54,54	1.52	8 (16%)
6	PEG	A	305	-	6,6,6	0.52	0	5,5,5	0.50	0
4	GTP	A	302	3	33,34,34	0.95	2 (6%)	50,54,54	1.49	10 (20%)
6	PEG	A	304	-	6,6,6	0.67	0	5,5,5	0.48	0
6	PEG	B	310	-	6,6,6	0.52	0	5,5,5	0.43	0
6	PEG	B	311	-	6,6,6	0.66	0	5,5,5	0.30	0
5	PO4	D	301	-	4,4,4	0.93	0	6,6,6	0.51	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	PEG	B	306	-	-	2/4/4/4	-
6	PEG	B	309	-	-	0/4/4/4	-
7	EDO	B	307	-	-	0/1/1/1	-
7	EDO	B	304	-	-	0/1/1/1	-
6	PEG	A	306	-	-	1/4/4/4	-
6	PEG	B	305	-	-	1/4/4/4	-
6	PEG	B	308	-	-	1/4/4/4	-
6	PEG	B	310	-	-	1/4/4/4	-
6	PEG	A	305	-	-	0/4/4/4	-
4	GTP	B	302	3	-	2/22/38/38	0/3/3/3
4	GTP	A	302	3	-	4/22/38/38	0/3/3/3
6	PEG	A	304	-	-	0/4/4/4	-
6	PEG	B	311	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	GTP	PB-O3A	2.38	1.62	1.59
4	B	302	GTP	PA-O3A	2.23	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	GTP	C2-N3	2.11	1.38	1.33
4	A	302	GTP	C2-N3	2.05	1.38	1.33
4	A	302	GTP	PA-O3A	2.02	1.61	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	GTP	C5-C4-N3	-4.67	120.96	128.39
4	B	302	GTP	C2-N3-C4	4.45	119.97	112.30
4	A	302	GTP	C5-C4-N3	-4.23	121.66	128.39
4	A	302	GTP	C2-N3-C4	3.97	119.13	112.30
4	B	302	GTP	N9-C8-N7	-2.85	108.12	113.40
4	A	302	GTP	N9-C8-N7	-2.80	108.20	113.40
4	B	302	GTP	N9-C4-N3	2.78	131.52	125.95
4	B	302	GTP	C8-N7-C5	2.60	108.89	104.26
4	B	302	GTP	C2-N1-C6	-2.57	120.44	125.11
4	A	302	GTP	C8-N7-C5	2.52	108.75	104.26
4	A	302	GTP	N9-C4-N3	2.51	130.98	125.95
4	A	302	GTP	C2-N1-C6	-2.49	120.60	125.11
4	A	302	GTP	O2B-PB-O3B	2.44	113.88	107.27
4	B	302	GTP	O6-C6-C5	-2.32	120.41	126.53
4	A	302	GTP	C5-C6-N1	2.21	118.89	113.25
4	A	302	GTP	O2A-PA-O3A	2.18	113.16	107.27
4	B	302	GTP	C5-C6-N1	2.15	118.73	113.25
4	A	302	GTP	O2G-PG-O3B	2.06	111.53	104.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	GTP	C5'-O5'-PA-O3A
4	A	302	GTP	C5'-O5'-PA-O2A
6	B	310	PEG	C1-C2-O2-C3
6	A	306	PEG	C4-C3-O2-C2
6	B	306	PEG	C1-C2-O2-C3
6	B	305	PEG	C1-C2-O2-C3
4	B	302	GTP	PA-O3A-PB-O1B
4	A	302	GTP	PA-O3A-PB-O2B
6	B	311	PEG	C1-C2-O2-C3
6	B	306	PEG	C4-C3-O2-C2
6	B	308	PEG	C1-C2-O2-C3
4	A	302	GTP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	B	302	GTP	PA-O3A-PB-O2B

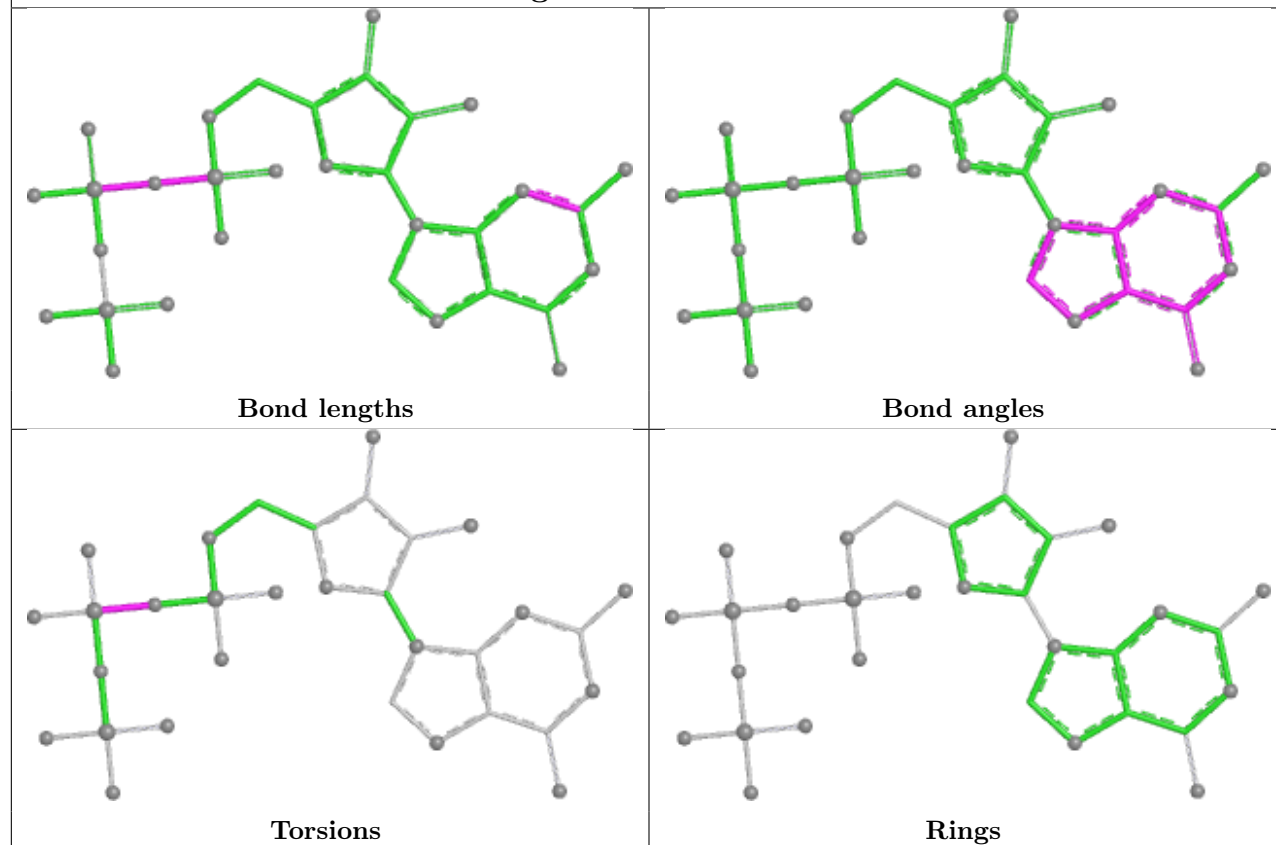
There are no ring outliers.

8 monomers are involved in 13 short contacts:

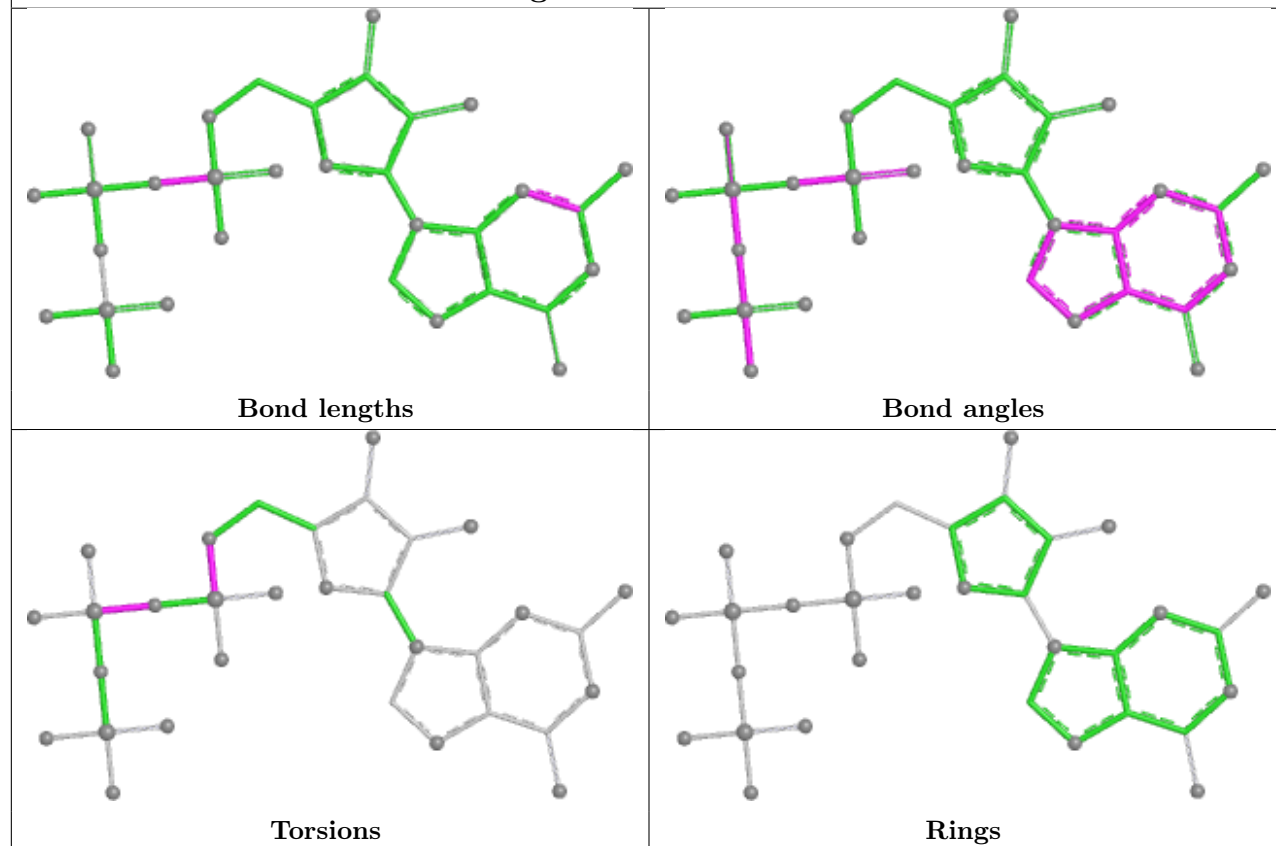
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	306	PEG	1	0
6	B	309	PEG	1	0
7	B	307	EDO	1	0
6	A	306	PEG	1	0
6	B	305	PEG	4	0
6	A	305	PEG	2	0
6	B	310	PEG	1	0
6	B	311	PEG	2	0

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 B 302



Ligand GTP A 302



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	176/192 (91%)	-0.09	6 (3%) 48 44	30, 41, 82, 117	0
1	B	175/192 (91%)	-0.05	6 (3%) 48 44	29, 41, 87, 129	0
2	C	86/126 (68%)	1.75	34 (39%) 1 0	42, 97, 139, 161	0
2	D	86/126 (68%)	1.95	39 (45%) 0 0	44, 102, 149, 157	0
All	All	523/636 (82%)	0.56	85 (16%) 4 4	29, 48, 134, 161	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	162	LEU	7.2
1	B	204	PRO	6.7
2	D	155	LEU	5.6
2	C	225	ALA	5.5
2	D	148	LEU	5.5
2	C	171	ILE	5.4
2	D	225	ALA	5.2
2	D	169	LEU	5.2
2	D	149	ARG	5.1
2	D	143	THR	4.7
1	A	204	PRO	4.5
2	C	173	PHE	4.2
2	C	160	GLN	4.2
1	A	205	LEU	4.2
1	B	30	ARG	4.2
2	D	152	LEU	4.2
2	C	174	THR	4.2
1	B	202	HIS	4.0
2	C	169	LEU	4.0
2	C	224	LEU	3.9
2	D	161	THR	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	157	VAL	3.9
2	D	158	ALA	3.8
2	D	168	ALA	3.8
2	D	173	PHE	3.7
2	C	140	MET	3.7
2	C	220	LEU	3.7
1	A	203	LYS	3.7
2	D	142	GLU	3.6
2	D	172	THR	3.6
2	D	179	LYS	3.6
2	D	140	MET	3.6
1	A	60	ASP	3.6
2	C	143	THR	3.5
2	C	146	LEU	3.5
2	D	154	ASP	3.5
2	C	141	LEU	3.5
1	A	30	ARG	3.5
2	C	157	VAL	3.5
2	C	142	GLU	3.4
2	C	155	LEU	3.4
2	D	159	ASN	3.4
2	D	171	ILE	3.3
1	B	31	SER	3.2
2	D	150	THR	3.0
2	C	161	THR	3.0
2	C	166	TYR	3.0
2	D	147	ASP	3.0
2	D	166	TYR	2.9
2	C	175	ALA	2.9
2	D	141	LEU	2.8
2	D	165	GLU	2.8
2	D	163	LYS	2.8
2	D	151	LYS	2.8
2	D	175	ALA	2.7
2	C	170	GLN	2.7
2	C	159	ASN	2.7
2	C	163	LYS	2.7
2	C	150	THR	2.7
1	A	202	HIS	2.7
2	D	176	LEU	2.6
2	C	145	CYS	2.6
2	D	182	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	146	LEU	2.5
2	C	222	LYS	2.5
1	B	60	ASP	2.5
1	B	203	LYS	2.5
2	C	176	LEU	2.5
2	C	219	ARG	2.5
2	C	152	LEU	2.5
2	C	158	ALA	2.4
2	D	220	LEU	2.3
2	C	154	ASP	2.3
2	C	167	ASP	2.3
2	D	224	LEU	2.3
2	D	145	CYS	2.2
2	D	222	LYS	2.2
2	C	144	ASN	2.2
2	D	177	GLU	2.2
2	C	187	ASN	2.1
2	D	156	GLU	2.0
2	D	144	ASN	2.0
2	C	172	THR	2.0
2	D	174	THR	2.0
2	C	147	ASP	2.0

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 oligosaccharides 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(Å ²)	Q<0.9
5	PO4	D	301	5/5	0.73	0.30	155,157,158,160	0

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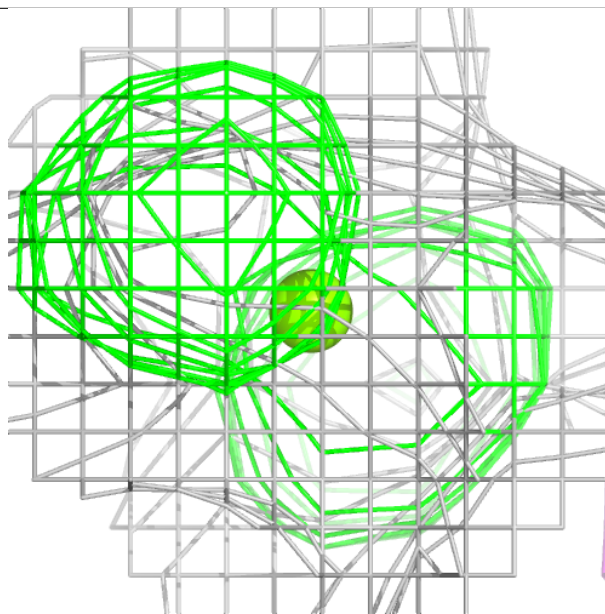
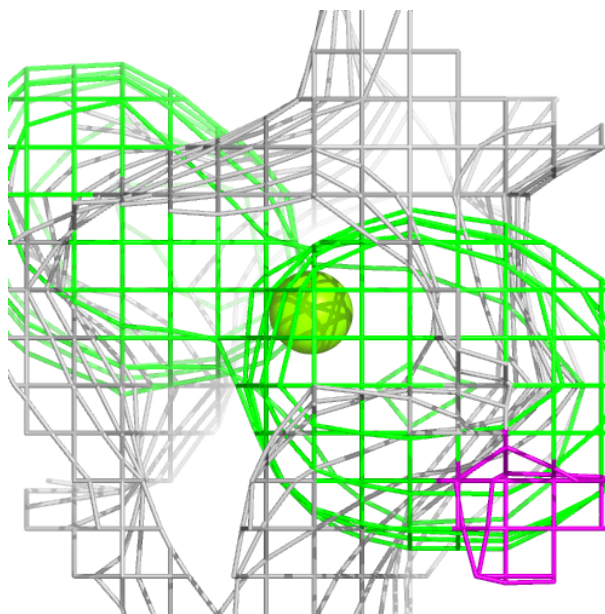
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	B	306	7/7	0.76	0.29	87,90,92,92	0
6	PEG	A	304	7/7	0.77	0.32	65,87,97,99	0
5	PO4	C	301	5/5	0.79	0.18	117,118,121,121	0
6	PEG	B	309	7/7	0.82	0.26	67,79,85,88	0
6	PEG	B	310	7/7	0.82	0.21	75,81,84,86	0
6	PEG	B	308	7/7	0.83	0.25	66,84,90,91	0
3	MG	B	301	1/1	0.85	0.20	53,53,53,53	0
6	PEG	B	311	7/7	0.85	0.27	62,78,92,95	0
7	EDO	B	307	4/4	0.85	0.21	48,54,64,74	0
5	PO4	A	303	5/5	0.86	0.18	69,74,80,81	0
5	PO4	B	303	5/5	0.86	0.17	61,70,73,77	0
6	PEG	B	305	7/7	0.86	0.24	71,82,99,102	0
6	PEG	A	305	7/7	0.87	0.25	85,90,93,94	0
6	PEG	A	306	7/7	0.89	0.22	52,55,77,77	0
7	EDO	B	304	4/4	0.94	0.12	36,41,41,49	0
4	GTP	B	302	32/32	0.98	0.05	30,41,45,46	0
4	GTP	A	302	32/32	0.98	0.06	27,40,46,58	0
3	MG	A	301	1/1	1.00	0.05	41,41,41,41	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.

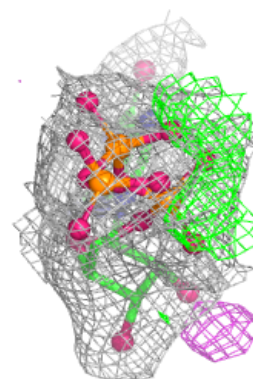
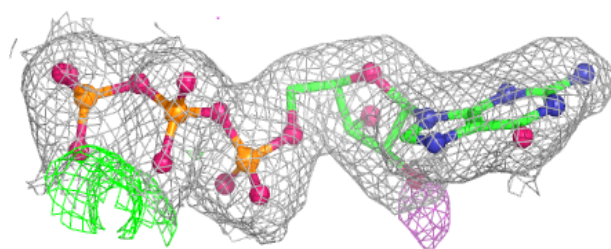
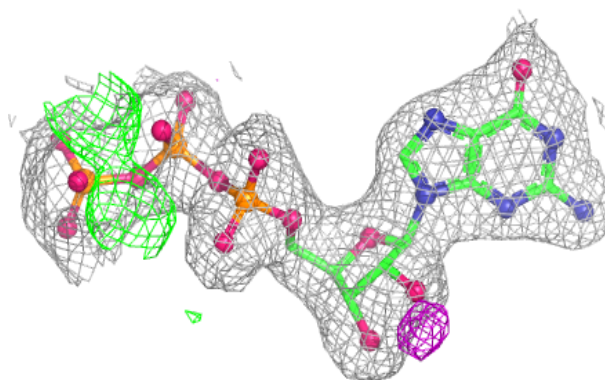
Electron density around MG B 301:

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

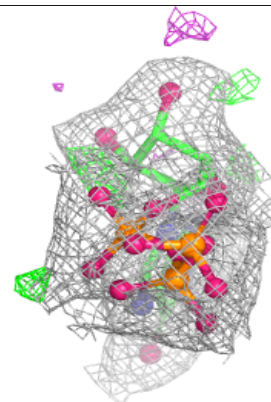
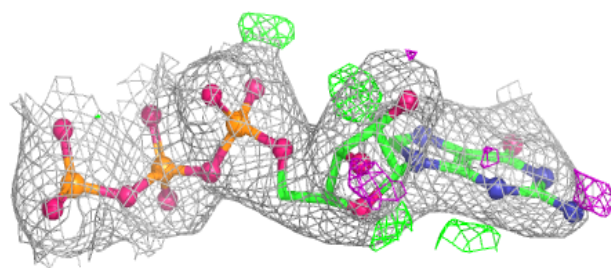
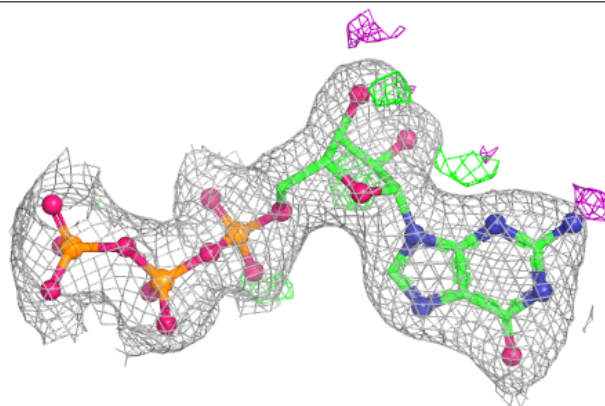


Electron density around GTP B 302:

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

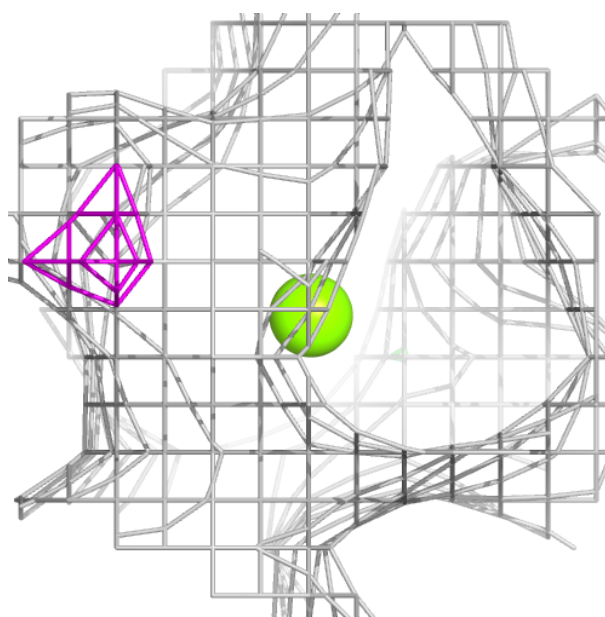
**Electron density around GTP A 302:**

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



Electron density around MG A 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.