



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:05 AM UTC

PDB ID : 3DZI / pdb_00003dzi
Title : Crystal structure of human CD38 extracellular domain, ribose-5'-phosphate intermediate/GTP complex
Authors : Liu, Q.; Kriksunov, I.A.; Jiang, H.; Graeff, R.; Lin, H.; Lee, H.C.; Hao, Q.
Deposited on : 2008-07-29
Resolution : 1.73 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

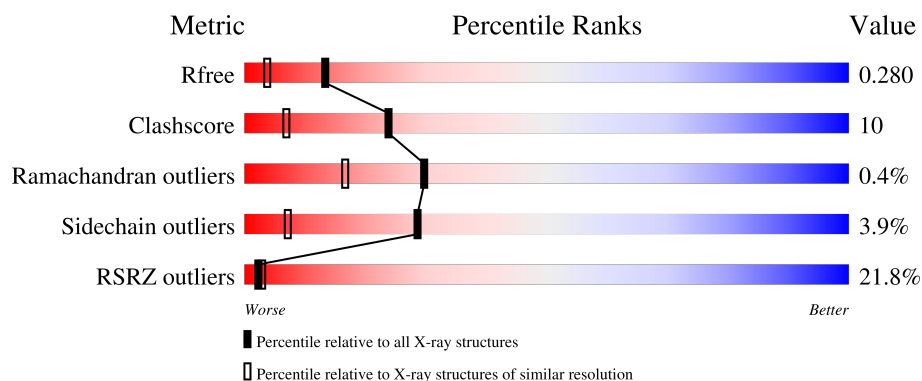
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	262	21% 76% 19% • •
1	B	262	21% 75% 18% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4534 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 ADP-ribosyl cyclase 1.

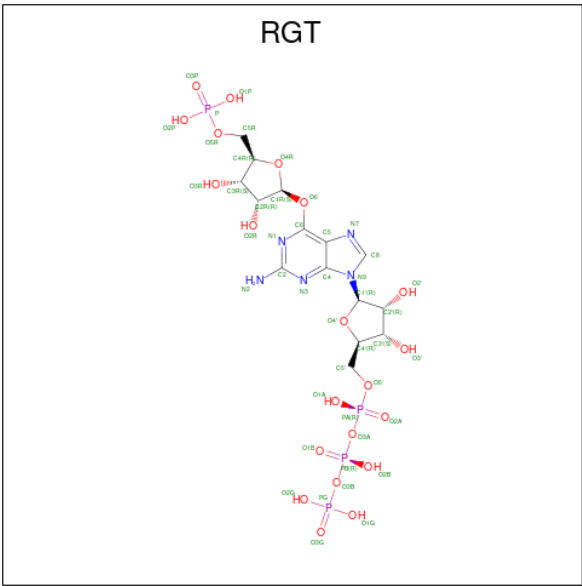
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	B	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	expression tag	UNP P28907
A	40	ARG	-	expression tag	UNP P28907
A	41	GLU	-	expression tag	UNP P28907
A	42	ALA	-	expression tag	UNP P28907
A	43	GLU	-	expression tag	UNP P28907
A	44	ALA	-	expression tag	UNP P28907
A	49	THR	GLN	engineered mutation	UNP P28907
A	100	ASP	ASN	engineered mutation	UNP P28907
A	164	ASP	ASN	engineered mutation	UNP P28907
A	209	ASP	ASN	engineered mutation	UNP P28907
A	219	ASP	ASN	engineered mutation	UNP P28907
B	39	LYS	-	expression tag	UNP P28907
B	40	ARG	-	expression tag	UNP P28907
B	41	GLU	-	expression tag	UNP P28907
B	42	ALA	-	expression tag	UNP P28907
B	43	GLU	-	expression tag	UNP P28907
B	44	ALA	-	expression tag	UNP P28907
B	49	THR	GLN	engineered mutation	UNP P28907
B	100	ASP	ASN	engineered mutation	UNP P28907
B	164	ASP	ASN	engineered mutation	UNP P28907
B	209	ASP	ASN	engineered mutation	UNP P28907
B	219	ASP	ASN	engineered mutation	UNP P28907

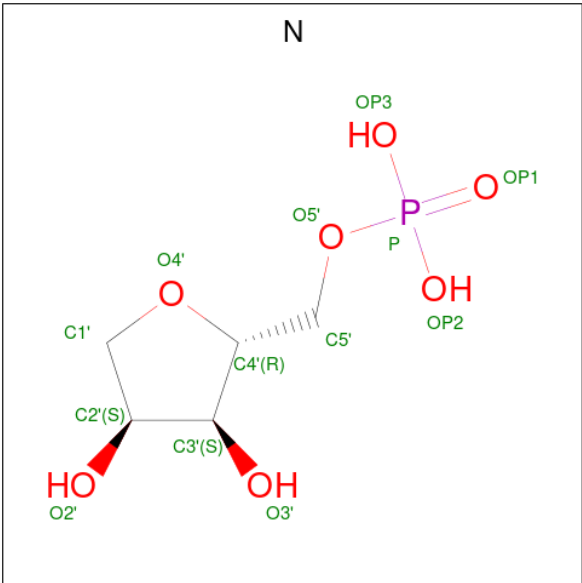
- Molecule 2 is 2-amino-9-{5-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-D-ribofuranosyl}-9H-purin-6-yl 5-O-phosphono-beta-D-ribofuranoside

(CCD ID: RGT) (formula: $C_{15}H_{25}N_5O_{21}P_4$).



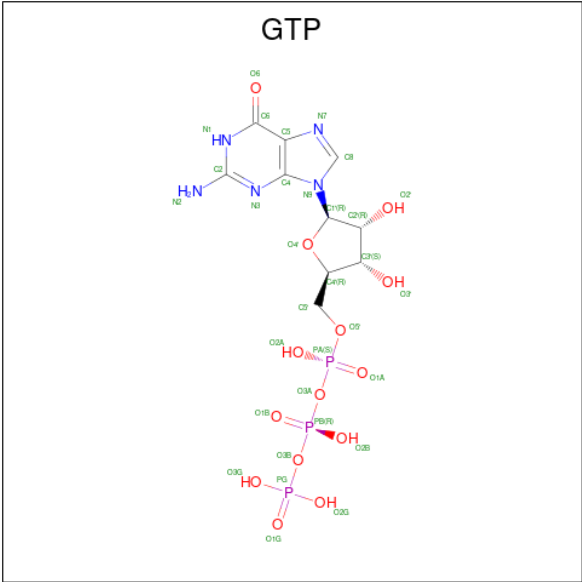
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			45	15	5	21	4		

- Molecule 3 is ANY 5'-MONOPHOSPHATE NUCLEOTIDE (CCD ID: N) (formula: $C_5H_{11}O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			13	5	7	1		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

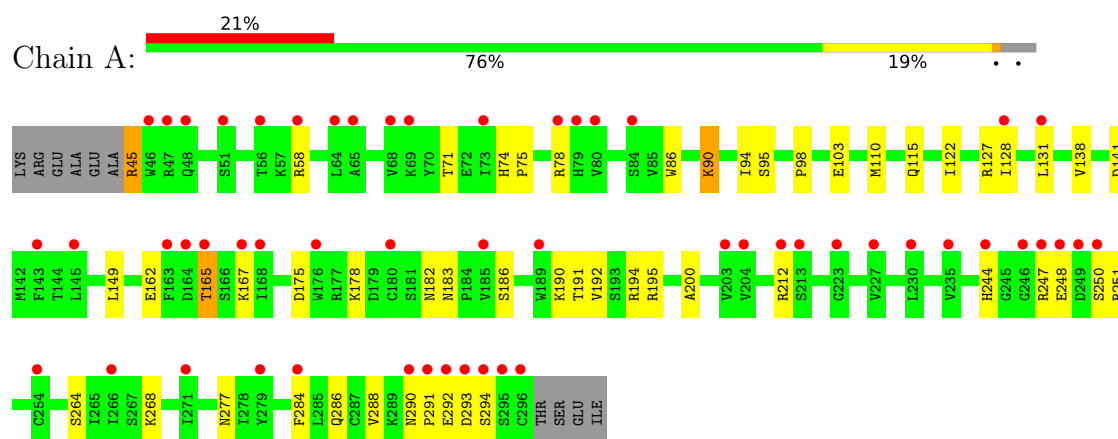
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	180	Total	O	0	0
			180	180		
5	B	164	Total	O	0	0
			164	164		

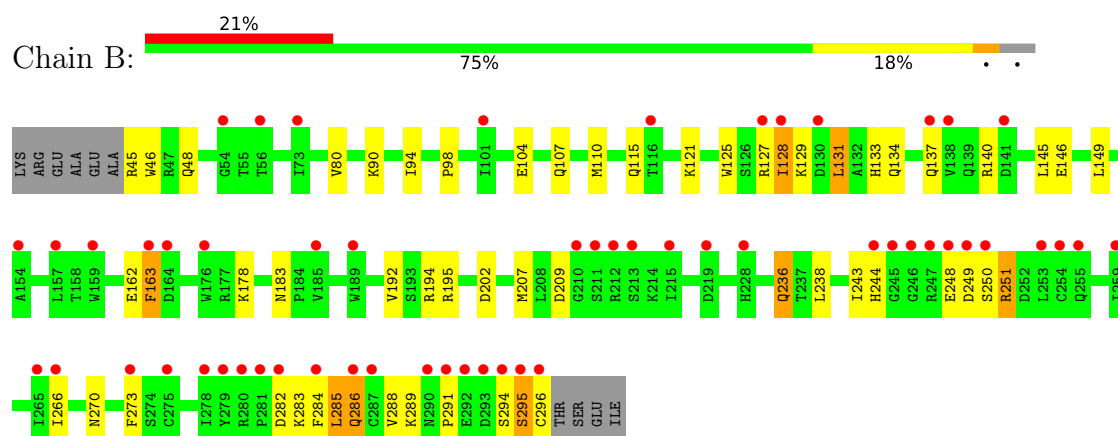
3 Residue-property plots [i](#)

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: ADP-ribosyl cyclase 1



• Molecule 1: ADP-ribosyl cyclase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.67Å 52.75Å 65.13Å 106.09° 91.92° 95.27°	Depositor
Resolution (Å)	20.00 – 1.73 20.00 – 1.73	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-1.73) 95.7 (20.00-1.73)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.3.0021	Depositor
R, R_{free}	0.177 , 0.211 0.256 , 0.280	Depositor DCC
R_{free} test set	2721 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4534	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% 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: GTP, RGT

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	0.89	2/2101 (0.1%)	0.96	0/2846
1	B	0.86	2/2101 (0.1%)	0.93	0/2846
All	All	0.88	4/4202 (0.1%)	0.95	0/5692

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	PHE	N-CA	-7.47	1.36	1.46
1	A	71	THR	C-O	5.29	1.30	1.24
1	B	162	GLU	CA-C	-5.08	1.46	1.52
1	A	138	VAL	C-O	5.03	1.29	1.24

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	2050	0	1976	36	0
1	B	2050	0	1976	45	0
2	A	45	0	19	2	0
3	B	13	0	9	5	0
4	B	32	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	180	0	0	6	0
5	B	164	0	0	7	0
All	All	4534	0	3992	83	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 10.

All (83) 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)
2:A:301:RGT:O6	2:A:301:RGT:C1R	1.93	1.17
1:B:202:ASP:HB3	5:B:488:HOH:O	1.64	0.95
3:B:301:N:C1'	4:B:302:GTP:O6	2.16	0.93
1:A:165:THR:HG23	1:A:167:LYS:H	1.31	0.92
3:B:301:N:H1'	4:B:302:GTP:O6	1.76	0.86
1:A:115:GLN:HE22	1:A:149:LEU:H	1.24	0.84
1:A:127:ARG:HG2	1:A:212:ARG:NE	1.93	0.82
1:B:115:GLN:HE22	1:B:149:LEU:H	1.22	0.81
1:A:195:ARG:HD3	5:A:425:HOH:O	1.83	0.78
1:B:244:HIS:CD2	1:B:250:SER:HB3	2.25	0.71
1:A:175:ASP:OD1	1:A:178:LYS:HG3	1.92	0.69
1:A:268:LYS:HD3	1:B:163:PHE:CE1	2.26	0.69
1:A:183:ASN:ND2	1:A:186:SER:H	1.93	0.66
2:A:301:RGT:O6	2:A:301:RGT:O4R	2.13	0.66
3:B:301:N:O4'	4:B:302:GTP:O6	2.14	0.66
1:B:244:HIS:HD2	1:B:250:SER:HB3	1.61	0.66
1:A:75:PRO:O	1:A:78:ARG:HB2	1.96	0.64
1:A:268:LYS:HD3	1:B:163:PHE:HE1	1.59	0.64
1:A:127:ARG:HG2	1:A:212:ARG:HE	1.63	0.63
1:B:286:GLN:HE21	1:B:286:GLN:HA	1.62	0.63
1:B:238:LEU:HB3	1:B:266:ILE:HD13	1.81	0.62
1:B:115:GLN:NE2	1:B:149:LEU:H	1.95	0.62
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.83	0.60
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.82	0.60
1:A:183:ASN:HD21	1:A:186:SER:H	1.49	0.59
1:B:282:ASP:O	1:B:286:GLN:HG2	2.03	0.59
1:B:125:TRP:O	3:B:301:N:H5'	2.03	0.59
1:B:45:ARG:HG3	1:B:46:TRP:H	1.69	0.58
1:B:104:GLU:HA	1:B:107:GLN:HG2	1.85	0.58
1:B:195:ARG:HD3	5:B:541:HOH:O	2.04	0.57
3:B:301:N:H1'	4:B:302:GTP:C6	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TRP:CZ2	1:A:90:LYS:HG3	2.39	0.57
1:B:45:ARG:HG3	1:B:46:TRP:N	2.19	0.56
1:B:283:LYS:HZ1	1:B:296:CYS:HA	1.70	0.56
1:B:244:HIS:HD2	1:B:250:SER:CB	2.19	0.55
1:A:110:MET:HE1	1:A:192:VAL:CG1	2.36	0.55
1:B:194:ARG:HD2	5:B:588:HOH:O	2.09	0.53
1:B:266:ILE:HD11	1:B:273:PHE:CB	2.38	0.53
1:A:103:GLU:OE1	1:A:194:ARG:NH1	2.31	0.52
1:A:247:ARG:HG2	1:A:248:GLU:HG3	1.93	0.51
1:A:45:ARG:HA	5:A:475:HOH:O	2.11	0.51
1:A:244:HIS:HD2	1:A:250:SER:HB3	1.76	0.50
1:B:202:ASP:CB	5:B:488:HOH:O	2.41	0.50
1:A:122:ILE:HD12	1:A:200:ALA:HA	1.94	0.49
1:B:98:PRO:O	1:B:183:ASN:HA	2.11	0.49
1:B:283:LYS:NZ	1:B:296:CYS:HA	2.27	0.49
1:A:74:HIS:HE1	5:A:477:HOH:O	1.95	0.49
1:B:289:LYS:O	1:B:291:PRO:HD3	2.13	0.48
1:B:284:PHE:O	1:B:288:VAL:HG23	2.12	0.48
1:A:286:GLN:NE2	1:A:290:ASN:HD22	2.10	0.48
1:B:266:ILE:HD11	1:B:273:PHE:CA	2.44	0.47
1:A:251:ARG:H	1:A:251:ARG:HD3	1.79	0.46
1:A:127:ARG:CG	1:A:212:ARG:HE	2.28	0.46
1:A:291:PRO:C	1:A:293:ASP:H	2.23	0.46
1:B:90:LYS:CG	1:B:94:ILE:HG13	2.46	0.46
1:B:128:ILE:HB	1:B:209:ASP:HB2	1.97	0.46
1:A:244:HIS:HE1	1:A:277:ASN:OD1	1.98	0.45
1:A:286:GLN:HE22	1:A:290:ASN:HD22	1.64	0.45
1:B:134:GLN:HB3	1:B:285:LEU:HD11	1.99	0.45
1:A:264:SER:HG	1:B:163:PHE:HZ	1.61	0.45
1:B:45:ARG:HB2	5:B:508:HOH:O	2.16	0.45
1:B:145:LEU:HD21	1:B:192:VAL:HG23	1.99	0.45
1:A:291:PRO:C	1:A:293:ASP:N	2.75	0.45
1:A:94:ILE:O	1:A:95:SER:HB2	2.18	0.44
1:B:121:LYS:NZ	5:B:601:HOH:O	2.50	0.44
1:A:127:ARG:N	1:A:127:ARG:HD2	2.33	0.43
1:A:98:PRO:O	1:A:183:ASN:HA	2.18	0.43
1:B:110:MET:SD	1:B:192:VAL:HG12	2.59	0.43
1:B:125:TRP:CZ3	1:B:129:LYS:HB3	2.54	0.42
1:A:141:ASP:HA	5:A:476:HOH:O	2.18	0.42
1:B:251:ARG:HD3	1:B:251:ARG:H	1.83	0.42
1:B:207:MET:HG2	1:B:243:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LEU:HD12	1:B:243:ILE:HG21	2.01	0.42
1:B:294:SER:O	1:B:295:SER:C	2.62	0.42
1:A:284:PHE:O	1:A:288:VAL:HG23	2.20	0.41
1:B:133:HIS:NE2	1:B:146:GLU:HB2	2.36	0.41
1:A:182:ASN:HD21	1:B:178:LYS:HE2	1.86	0.41
1:B:248:GLU:HG3	1:B:249:ASP:H	1.84	0.41
1:A:190:LYS:NZ	5:A:478:HOH:O	2.54	0.41
1:A:103:GLU:HG2	1:A:191:THR:OG1	2.21	0.40
5:A:421:HOH:O	1:B:163:PHE:HD2	2.05	0.40
1:B:48:GLN:HG3	5:B:559:HOH:O	2.20	0.40
1:B:236:GLN:H	1:B:236:GLN:HG2	1.72	0.40

There are no symmetry-related clashes.

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	250/262 (95%)	237 (95%)	13 (5%)	0	100	100
1	B	250/262 (95%)	234 (94%)	14 (6%)	2 (1%)	16	4
All	All	500/524 (95%)	471 (94%)	27 (5%)	2 (0%)	30	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	295	SER
1	B	128	ILE

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	233/241 (97%)	225 (97%)	8 (3%)	32	10
1	B	233/241 (97%)	223 (96%)	10 (4%)	26	6
All	All	466/482 (97%)	448 (96%)	18 (4%)	28	7

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	58	ARG
1	A	90	LYS
1	A	128	ILE
1	A	131	LEU
1	A	165	THR
1	A	292	GLU
1	A	294	SER
1	B	80	VAL
1	B	127	ARG
1	B	131	LEU
1	B	137	GLN
1	B	140	ARG
1	B	236	GLN
1	B	251	ARG
1	B	270	ASN
1	B	285	LEU
1	B	286	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	74	HIS
1	A	83	GLN
1	A	115	GLN

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Mol	Chain	Res	Type
1	A	137	GLN
1	A	139	GLN
1	A	171	GLN
1	A	182	ASN
1	A	183	ASN
1	A	244	HIS
1	A	290	ASN
1	B	48	GLN
1	B	83	GLN
1	B	115	GLN
1	B	134	GLN
1	B	137	GLN
1	B	171	GLN
1	B	229	ASN
1	B	236	GLN
1	B	244	HIS
1	B	255	GLN
1	B	270	ASN
1	B	286	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](#)

3 ligands are modelled in this entry.

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	$\# Z > 2$
2	RGT	A	301	-	47,48,48	5.34	10 (21%)	71,76,76	3.86	23 (32%)
3	N	B	301	-	13,13,13	0.66	0	16,19,19	1.34	3 (18%)
4	GTP	B	302	-	33,34,34	1.25	5 (15%)	50,54,54	1.63	10 (20%)

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
2	RGT	A	301	-	-	11/31/64/64	0/4/4/4
3	N	B	301	-	-	0/6/19/19	0/1/1/1
4	GTP	B	302	-	-	2/22/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RGT	O6-C1R	34.83	1.93	1.41
2	A	301	RGT	O6-C6	-5.53	1.24	1.36
2	A	301	RGT	C6-N1	4.78	1.39	1.32
4	B	302	GTP	PB-O3A	3.38	1.63	1.59
2	A	301	RGT	PB-O3B	3.32	1.63	1.59
2	A	301	RGT	C4-N3	3.17	1.38	1.34
4	B	302	GTP	PA-O3A	3.09	1.62	1.59
2	A	301	RGT	C8-N7	3.03	1.37	1.31
4	B	302	GTP	PB-O3B	2.98	1.62	1.59
2	A	301	RGT	C5-C6	-2.96	1.36	1.41
4	B	302	GTP	C2-N3	2.43	1.39	1.33
2	A	301	RGT	C5-N7	-2.34	1.34	1.39
2	A	301	RGT	C2-N1	2.18	1.39	1.35
2	A	301	RGT	PB-O3A	2.14	1.61	1.59
4	B	302	GTP	C5-N7	-2.00	1.35	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RGT	C6-O6-C1R	21.74	149.79	117.05
2	A	301	RGT	O4R-C1R-O6	-16.03	77.07	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RGT	O6-C1R-C2R	9.51	122.13	106.69
2	A	301	RGT	N1-C2-N3	-5.14	117.60	125.48
2	A	301	RGT	C2-N1-C6	4.77	122.59	115.96
2	A	301	RGT	N9-C8-N7	-4.25	107.90	113.94
2	A	301	RGT	C5-C4-N3	-4.22	122.74	127.18
4	B	302	GTP	C2-N3-C4	4.19	119.52	112.30
4	B	302	GTP	C5-C4-N3	-4.07	121.91	128.39
2	A	301	RGT	N3-C4-N9	3.81	131.82	126.99
4	B	302	GTP	O4'-C1'-N9	3.58	116.48	108.36
4	B	302	GTP	O6-C6-C5	-3.37	117.65	126.53
2	A	301	RGT	O4'-C1'-N9	3.16	114.17	108.09
4	B	302	GTP	N9-C4-N3	3.07	132.09	125.95
2	A	301	RGT	C5-C6-N1	-2.82	119.72	123.49
2	A	301	RGT	N2-C2-N3	2.78	121.39	117.22
2	A	301	RGT	C4-N9-C8	2.73	108.61	105.74
4	B	302	GTP	C5-C6-N1	2.73	120.20	113.25
4	B	302	GTP	N9-C8-N7	-2.67	108.46	113.40
2	A	301	RGT	C4-C5-C6	2.64	117.81	115.22
4	B	302	GTP	C2-N1-C6	-2.61	120.38	125.11
2	A	301	RGT	N2-C2-N1	2.52	121.00	117.22
2	A	301	RGT	C4-N9-C1'	-2.48	120.84	126.63
2	A	301	RGT	C5-N7-C8	2.46	107.31	103.45
2	A	301	RGT	C2R-C3R-C4R	2.39	107.22	102.61
2	A	301	RGT	C1R-C2R-C3R	2.35	105.22	102.29
2	A	301	RGT	O2R-C2R-C1R	-2.33	105.25	111.82
4	B	302	GTP	N1-C2-N3	-2.27	119.17	123.32
2	A	301	RGT	C2-N3-C4	2.25	119.53	113.51
4	B	302	GTP	C3'-C2'-C1'	-2.23	97.24	101.46
2	A	301	RGT	C3'-C2'-C1'	-2.19	97.33	101.46
3	B	301	N	O5'-C5'-C4'	2.14	116.30	108.99
3	B	301	N	OP2-P-OP3	2.05	115.49	107.80
3	B	301	N	O4'-C1'-C2'	2.04	109.29	105.76
2	A	301	RGT	C6-C5-N7	-2.03	131.44	133.82
2	A	301	RGT	O4R-C1R-C2R	2.01	107.53	104.98

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	RGT	C5-C6-O6-C1R
2	A	301	RGT	N1-C6-O6-C1R
2	A	301	RGT	C5'-O5'-PA-O1A

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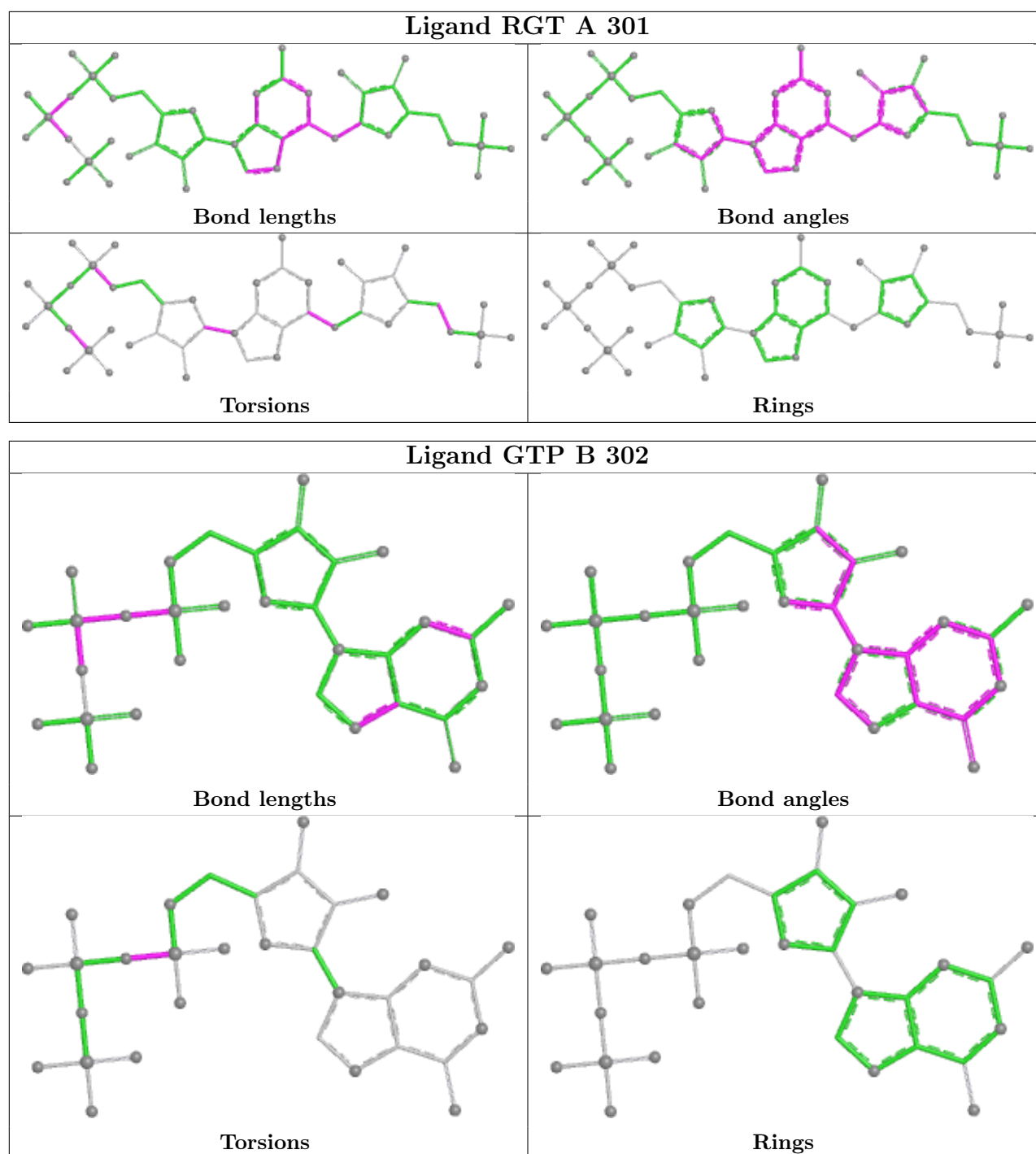
Mol	Chain	Res	Type	Atoms
2	A	301	RGT	C2'-C1'-N9-C8
4	B	302	GTP	PB-O3A-PA-O1A
2	A	301	RGT	C2'-C1'-N9-C4
2	A	301	RGT	C5'-O5'-PA-O2A
2	A	301	RGT	C5'-O5'-PA-O3A
2	A	301	RGT	PB-O3B-PG-O3G
2	A	301	RGT	C4R-C5R-O5R-P
2	A	301	RGT	PB-O3B-PG-O1G
2	A	301	RGT	PB-O3B-PG-O2G
4	B	302	GTP	PB-O3A-PA-O2A

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RGT	2	0
3	B	301	N	5	0
4	B	302	GTP	4	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 [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	252/262 (96%)	1.44	54 (21%) 2 3	31, 37, 51, 73	0
1	B	252/262 (96%)	1.43	56 (22%) 2 3	33, 38, 46, 51	0
All	All	504/524 (96%)	1.43	110 (21%) 2 3	31, 38, 47, 73	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	GLY	5.7
1	B	249	ASP	5.6
1	B	295	SER	5.6
1	A	292	GLU	5.3
1	B	293	ASP	5.1
1	A	249	ASP	4.8
1	A	293	ASP	4.8
1	A	248	GLU	4.7
1	B	290	ASN	4.7
1	B	292	GLU	4.5
1	B	250	SER	4.5
1	B	291	PRO	4.4
1	A	143	PHE	4.2
1	A	246	GLY	4.2
1	B	294	SER	4.1
1	A	80	VAL	4.1
1	B	245	GLY	3.9
1	B	254	CYS	3.7
1	A	73	ILE	3.6
1	A	46	TRP	3.5
1	B	176	TRP	3.5
1	A	164	ASP	3.5
1	B	296	CYS	3.5
1	B	141	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	165	THR	3.4
1	B	287	CYS	3.4
1	A	247	ARG	3.4
1	B	266	ILE	3.4
1	A	294	SER	3.4
1	A	296	CYS	3.2
1	B	259	ILE	3.1
1	B	128	ILE	3.0
1	B	127	ARG	3.0
1	A	65	ALA	3.0
1	A	51	SER	3.0
1	A	78	ARG	3.0
1	B	248	GLU	2.9
1	A	58	ARG	2.9
1	B	286	GLN	2.9
1	B	244	HIS	2.8
1	A	279	TYR	2.8
1	B	247	ARG	2.8
1	B	215	ILE	2.8
1	A	47	ARG	2.7
1	A	79	HIS	2.7
1	A	185	VAL	2.6
1	A	212	ARG	2.6
1	A	213	SER	2.6
1	B	213	SER	2.6
1	A	291	PRO	2.6
1	B	54	GLY	2.6
1	B	116	THR	2.6
1	A	295	SER	2.6
1	B	212	ARG	2.6
1	B	284	PHE	2.5
1	A	290	ASN	2.5
1	A	266	ILE	2.5
1	B	228	HIS	2.5
1	B	189	TRP	2.5
1	B	279	TYR	2.5
1	B	282	ASP	2.4
1	A	163	PHE	2.4
1	A	230	LEU	2.4
1	A	128	ILE	2.4
1	A	227	VAL	2.4
1	A	235	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	167	LYS	2.4
1	B	281	PRO	2.4
1	A	250	SER	2.3
1	B	157	LEU	2.3
1	A	271	ILE	2.3
1	B	273	PHE	2.3
1	A	176	TRP	2.3
1	B	275	CYS	2.3
1	B	265	ILE	2.3
1	B	278	ILE	2.3
1	B	138	VAL	2.3
1	A	244	HIS	2.2
1	A	64	LEU	2.2
1	B	130	ASP	2.2
1	A	48	GLN	2.2
1	B	73	ILE	2.2
1	B	280	ARG	2.2
1	A	84	SER	2.2
1	B	253	LEU	2.2
1	B	255	GLN	2.2
1	B	211	SER	2.2
1	B	219	ASP	2.2
1	A	189	TRP	2.2
1	B	159	TRP	2.2
1	A	131	LEU	2.2
1	B	163	PHE	2.2
1	A	180	CYS	2.1
1	A	254	CYS	2.1
1	A	145	LEU	2.1
1	B	101	ILE	2.1
1	A	68	VAL	2.1
1	A	203	VAL	2.1
1	A	204	VAL	2.1
1	B	164	ASP	2.1
1	A	168	ILE	2.1
1	B	210	GLY	2.0
1	B	154	ALA	2.0
1	B	137	GLN	2.0
1	B	185	VAL	2.0
1	A	56	THR	2.0
1	B	56	THR	2.0
1	A	223	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	284	PHE	2.0
1	A	69	LYS	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](#)

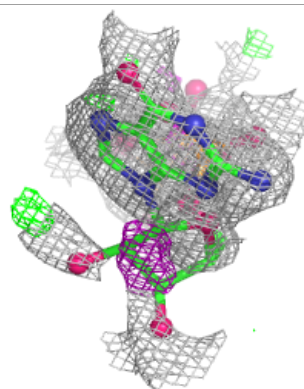
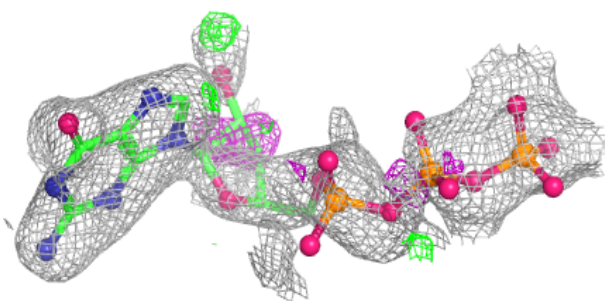
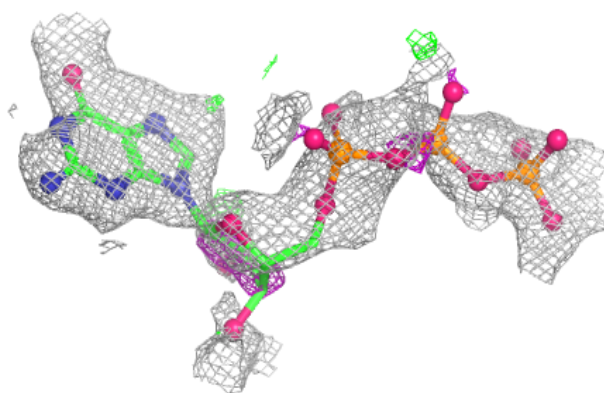
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GTP	B	302	32/32	0.65	0.14	52,69,106,106	0
2	RGT	A	301	45/45	0.67	0.16	38,50,106,107	0
3	N	B	301	13/13	0.68	0.18	57,64,70,71	0

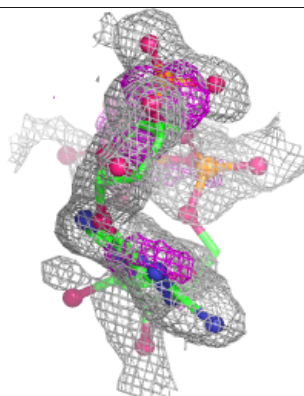
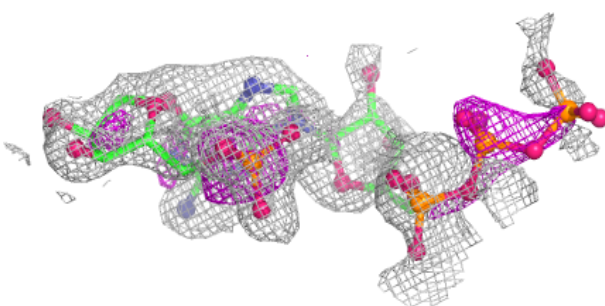
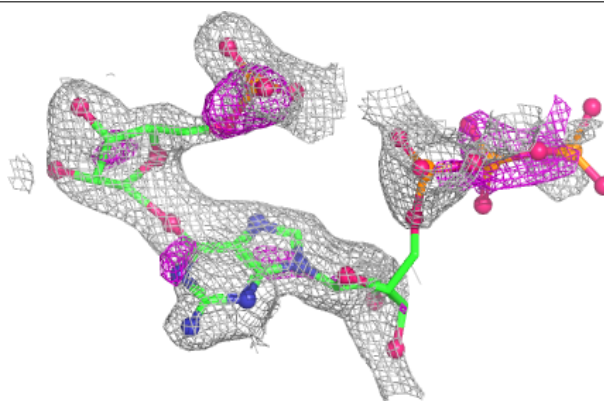
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP B 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 RGT 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.