wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 02:37 PM EST

PDB ID	:	1CC0
Title	:	CRYSTAL STRUCTURE OF THE RHOA.GDP-RHOGDI COMPLEX
Authors	:	Longenecker, K.L.; Read, P.; Derewenda, U.; Dauter, Z.; Garrard, S.; Walker, L.; Somlyo, A.V.; Somlyo, A.P.; Nakamoto, R.K.; Derewenda, Z.S.
Deposited on	:	1999-03-03
Resolution	:	5.00 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

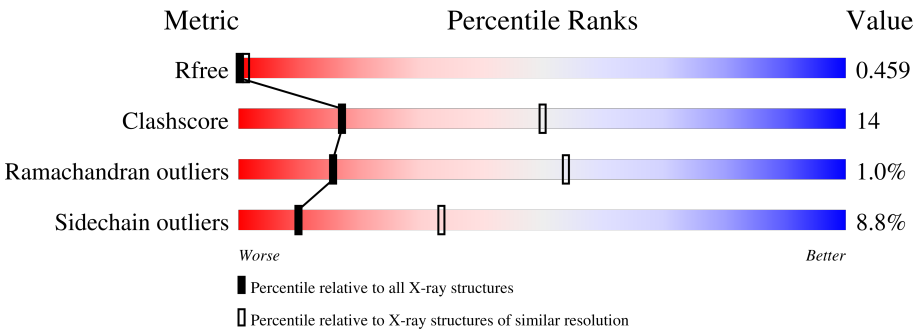
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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}	130704	1140 (6.20-3.80)
Clashscore	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	190	63% 24% 9% • •
1	C	190	60% 27% 8% • •
2	E	204	69% 19% • 12%
2	F	204	69% 19% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5174 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 transforming protein rhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	187	1415	896	239	270	10	0	0	10
1	C	187	1415	896	239	270	10	0	0	10

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASN	PHE	conflict	UNP P61586
C	25	ASN	PHE	conflict	UNP P61586

- Molecule 2 is a protein called rho GDP dissociation inhibitor alpha.

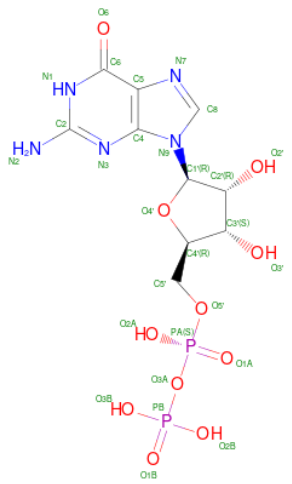
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	180	1143	748	183	208	4	0	0	44
2	F	180	1143	748	183	208	4	0	0	44

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

GDP



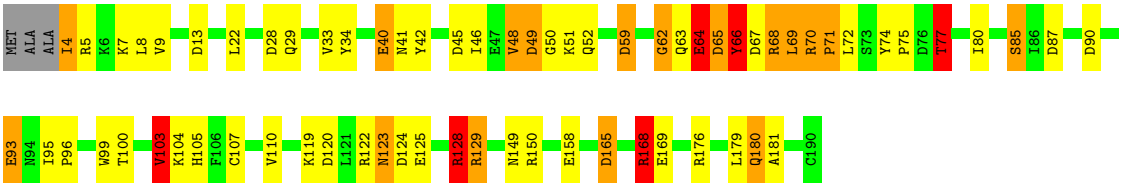
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
4	C	1	28	10	5	11	2	0	0

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. 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. 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.

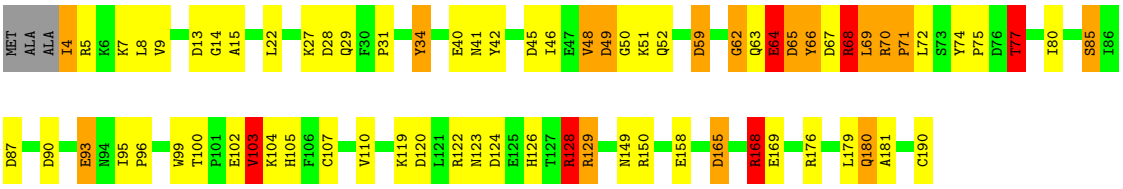
- Molecule 1: transforming protein rhoA

Chain A:



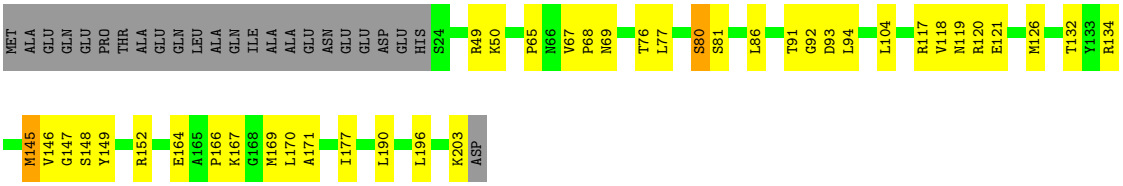
- Molecule 1: transforming protein rhoA

Chain C:



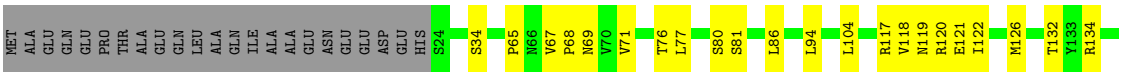
- Molecule 2: rho GDP dissociation inhibitor alpha

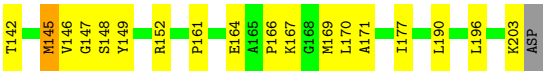
Chain E:



- Molecule 2: rho GDP dissociation inhibitor alpha

Chain F:




T142
M145
V146
G147
S148
Y149
R152
P161
E164
A165
P166
K167
G168
M169
L170
A171
I177
L190
L196
K203
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	139.30Å 139.30Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 5.00 19.97 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-5.00) 99.2 (19.97-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.94Å)	Xtriage
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available) 0.481 , 0.459	Depositor DCC
R_{free} test set	642 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	138.6	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.67	EDS
Total number of atoms	5174	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, GDP

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	1.00	2/1432 (0.1%)	2.12	48/1937 (2.5%)
1	C	1.00	2/1432 (0.1%)	2.12	49/1937 (2.5%)
2	E	0.58	0/1124	0.93	1/1515 (0.1%)
2	F	0.59	0/1124	0.92	1/1515 (0.1%)
All	All	0.84	4/5112 (0.1%)	1.70	99/6904 (1.4%)

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
1	A	0	5
1	C	0	5
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	GLU	CD-OE2	5.85	1.32	1.25
1	C	93	GLU	CD-OE2	5.76	1.31	1.25
1	C	93	GLU	CG-CD	5.35	1.59	1.51
1	A	93	GLU	CG-CD	5.35	1.59	1.51

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	122	ARG	NE-CZ-NH2	-16.36	112.12	120.30
1	A	122	ARG	NE-CZ-NH2	-16.21	112.20	120.30
1	A	176	ARG	NE-CZ-NH2	-15.41	112.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	176	ARG	NE-CZ-NH2	-15.39	112.61	120.30
1	C	150	ARG	NE-CZ-NH2	-15.31	112.64	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	VAL	Peptide
1	A	49	ASP	Peptide
1	A	50	GLY	Peptide
1	A	62	GLY	Mainchain
1	A	64	GLU	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	1415	0	1392	56	7
1	C	1415	0	1394	61	16
2	E	1143	0	1100	34	20
2	F	1143	0	1100	39	6
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	28	0	12	0	0
4	C	28	0	12	0	0
All	All	5174	0	5010	143	26

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 143 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:F:67:VAL:CA	2:F:68:PRO:N	1.83	1.41
1:C:71:PRO:HB3	2:F:148:SER:OG	1.28	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PRO:HB3	2:E:148:SER:OG	1.45	1.14
1:A:71:PRO:HB3	2:E:148:SER:CB	1.83	1.08
1:C:105:HIS:CD2	2:F:145:MET:CE	2.37	1.06

The worst 5 of 26 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)
2:E:91:THR:O	1:C:34:TYR:CE2[6_554]	0.52	1.68
2:E:91:THR:O	1:C:34:TYR:CZ[6_554]	1.09	1.11
1:A:123:ASN:OD1	1:C:129:ARG:NH1[7_555]	1.17	1.03
2:E:80:SER:OG	2:E:80:SER:OG[10_665]	1.20	1.00
2:E:91:THR:O	1:C:34:TYR:CD2[6_554]	1.33	0.87

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	175/190 (92%)	164 (94%)	8 (5%)	3 (2%)	9 43
1	C	175/190 (92%)	164 (94%)	8 (5%)	3 (2%)	9 43
2	E	134/204 (66%)	132 (98%)	2 (2%)	0	100 100
2	F	134/204 (66%)	132 (98%)	2 (2%)	0	100 100
All	All	618/788 (78%)	592 (96%)	20 (3%)	6 (1%)	15 54

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	C	41	ASN
1	A	64	GLU

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Mol	Chain	Res	Type
1	A	66	TYR
1	C	64	GLU

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	156/164 (95%)	143 (92%)	13 (8%)	11	36
1	C	156/164 (95%)	143 (92%)	13 (8%)	11	36
2	E	122/180 (68%)	111 (91%)	11 (9%)	9	32
2	F	122/180 (68%)	110 (90%)	12 (10%)	8	28
All	All	556/688 (81%)	507 (91%)	49 (9%)	10	33

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	69	LEU
1	C	168	ARG
1	C	71	PRO
1	C	103	VAL
2	F	76	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	119	ASN
2	F	130	GLN
2	E	130	GLN
1	C	180	GLN
2	F	69	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	GDP	A	201	3	24,30,30	1.59	3 (12%)	30,47,47	1.55	4 (13%)
4	GDP	C	202	3	24,30,30	1.59	3 (12%)	30,47,47	1.54	4 (13%)

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
4	GDP	A	201	3	-	1/12/32/32	0/3/3/3
4	GDP	C	202	3	-	1/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	202	GDP	C5-C4	-5.10	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	GDP	C5-C4	-5.07	1.30	1.43
4	C	202	GDP	C5-C6	-2.59	1.42	1.47
4	A	201	GDP	C4-N3	-2.59	1.31	1.37
4	A	201	GDP	C5-C6	-2.58	1.42	1.47

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	201	GDP	O3B-PB-O2B	3.75	121.96	107.64
4	C	202	GDP	O3B-PB-O2B	3.74	121.92	107.64
4	A	201	GDP	O2'-C2'-C1'	-3.25	98.85	110.85
4	A	201	GDP	O4'-C1'-C2'	-3.24	102.19	106.93
4	C	202	GDP	O2'-C2'-C1'	-3.24	98.89	110.85

There are no chirality outliers.

All (2) torsion outliers are listed below:

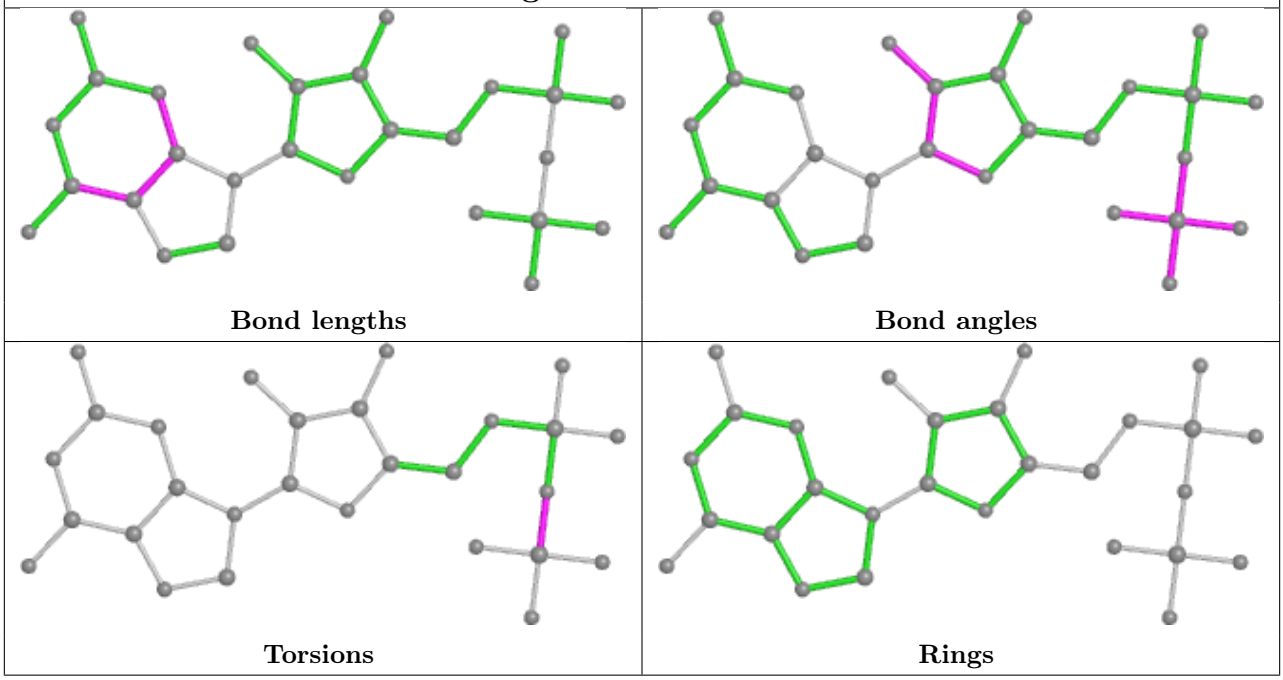
Mol	Chain	Res	Type	Atoms
4	A	201	GDP	PA-O3A-PB-O1B
4	C	202	GDP	PA-O3A-PB-O1B

There are no ring outliers.

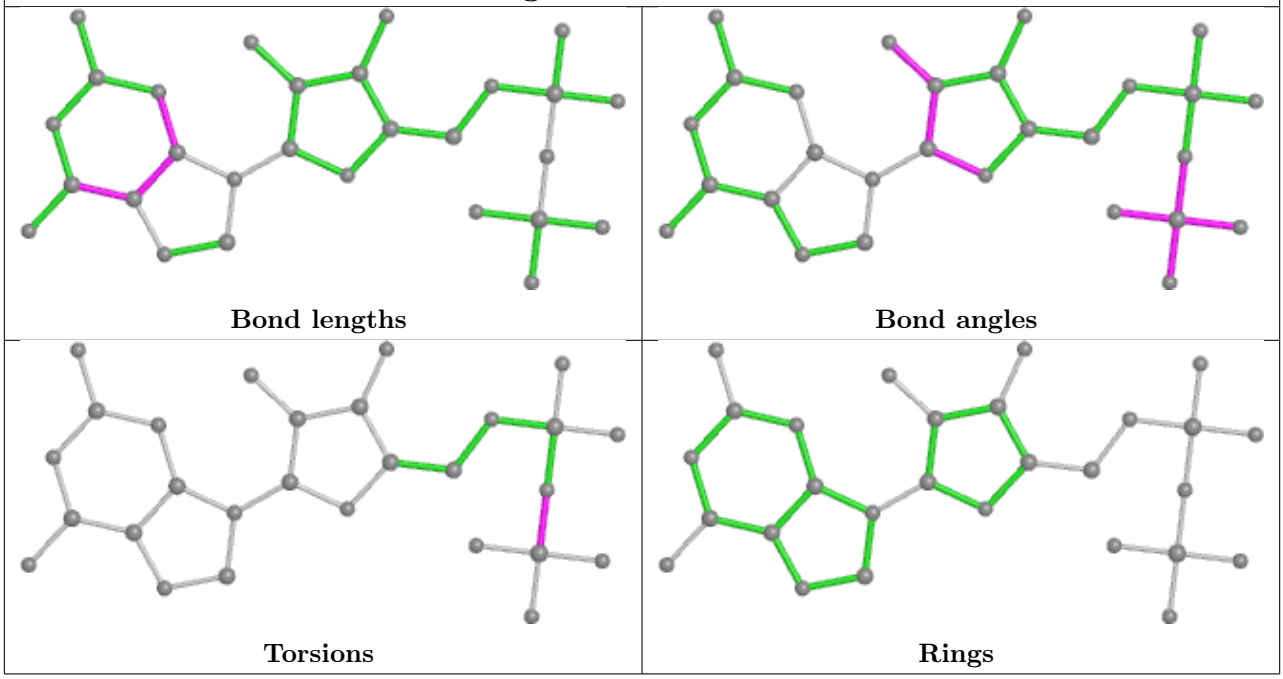
No monomer is involved in short contacts.

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 then 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 GDP A 201



Ligand GDP C 202



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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

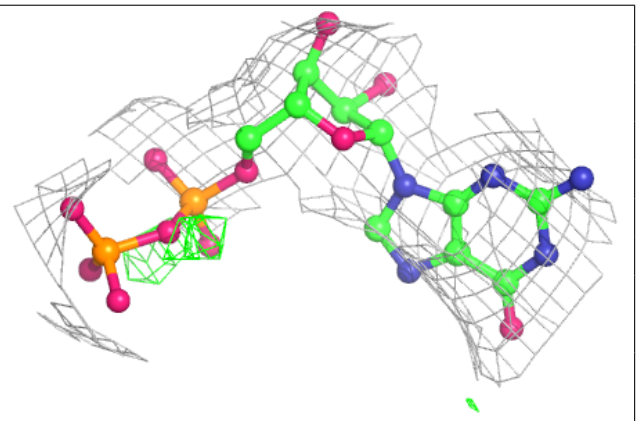
6.4 Ligands (i)

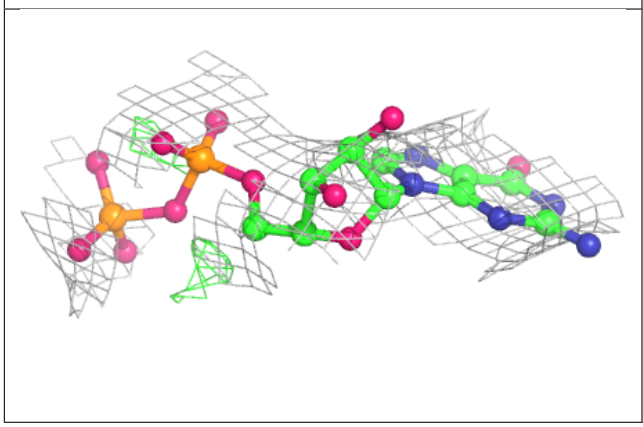
Unable to reproduce the depositors R factor - this section is therefore empty.

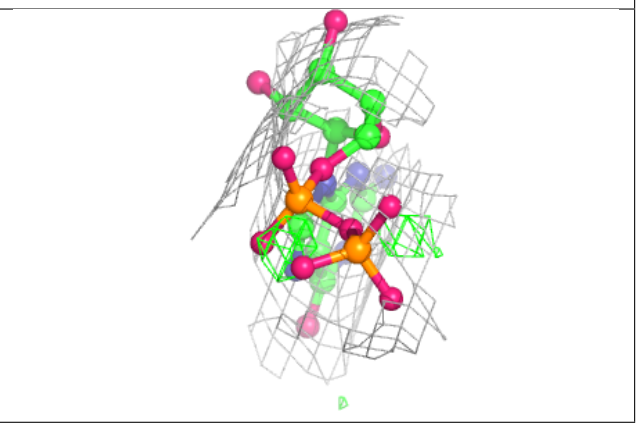
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP A 201:

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

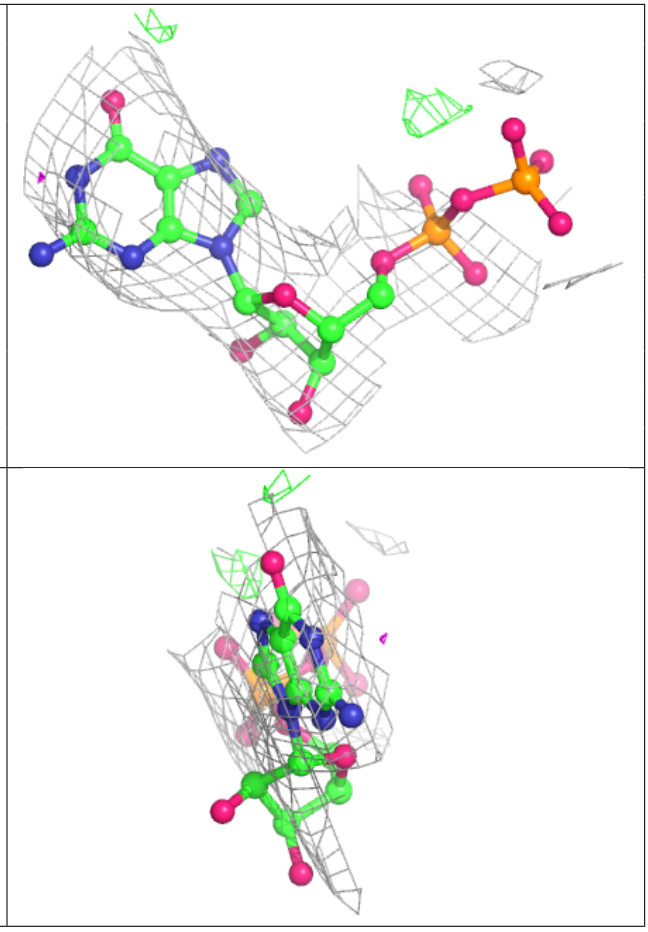






Electron density around GDP C 202:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.