



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:39 pm BST

PDB ID : 5V9H  
Title : Structure of the H477R variant of rat cytosolic PEPCK in complex with phosphoglycolate and GDP.  
Authors : Holyoak, T.; Cui, D.S.  
Deposited on : 2017-03-23  
Resolution : 2.15 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](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

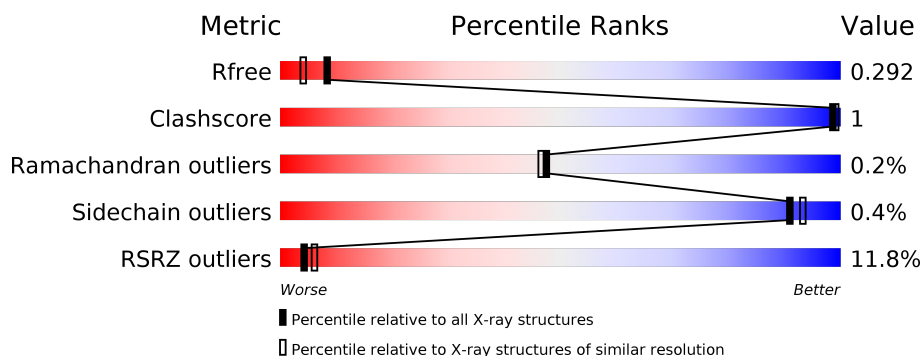
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	622	
1	B	622	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9988 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.

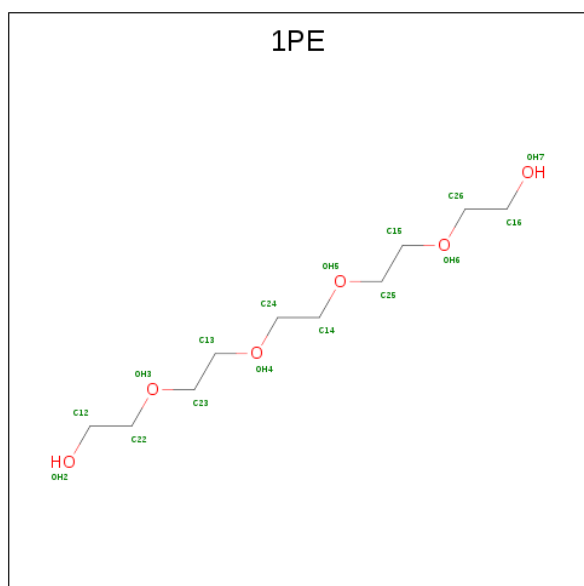
- Molecule 1 is a protein called Phosphoenolpyruvate carboxykinase, cytosolic [GTP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	2	0
			4809	3075	822	880	32			
1	B	609	Total	C	N	O	S	0	2	0
			4797	3069	820	876	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	477	ARG	HIS	engineered mutation	UNP P07379
B	477	ARG	HIS	engineered mutation	UNP P07379

- Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		

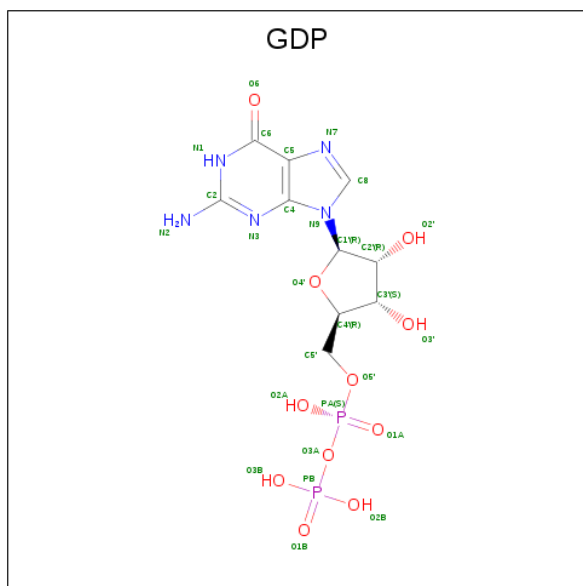
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

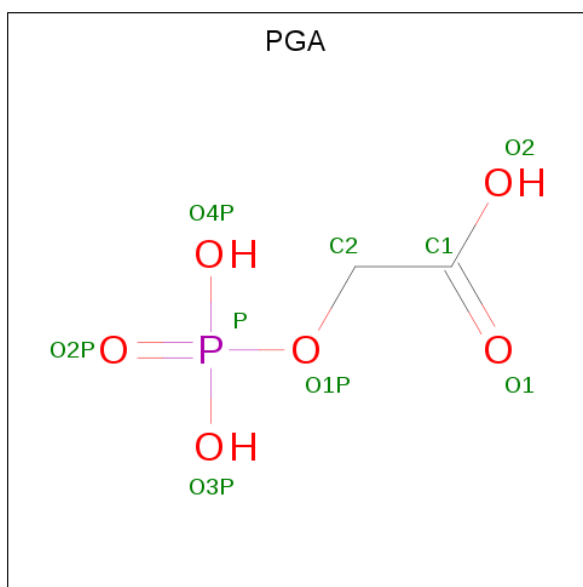
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mn	0	0
			3	3		
3	A	3	Total	Mn	0	0
			3	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).





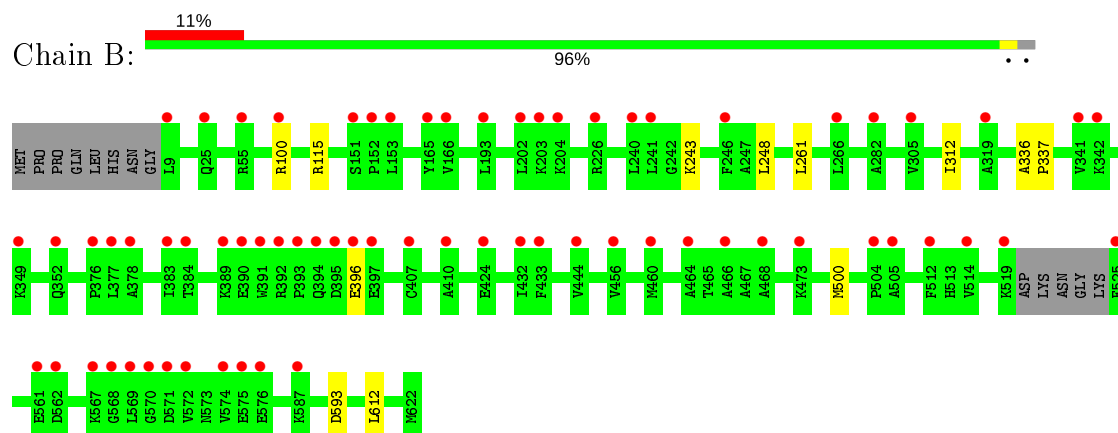
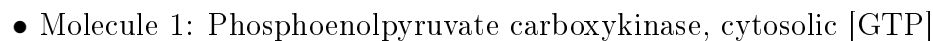
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			9	2	6	1		
6	B	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	154	Total	O	0	0
			154	154		
7	B	136	Total	O	0	0
			136	136		



- Molecule 1: Phosphoenolpyruvate carboxykinase, cytosolic [GTP]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.48 Å 119.43 Å 88.17 Å 90.00° 105.30° 90.00°	Depositor
Resolution (Å)	85.04 – 2.15 29.75 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.5 (85.04-2.15) 98.6 (29.75-2.14)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.14 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.241 , 0.285 0.247 , 0.292	Depositor DCC
$R_{free}$ test set	3345 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.09 % 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 4.6235e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GDP, NA, MN, 1PE, PGA

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	0.37	0/4940	0.57	0/6687
1	B	0.36	0/4928	0.56	0/6672
All	All	0.37	0/9868	0.57	0/13359

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	4809	0	4761	6	0
1	B	4797	0	4754	4	0
2	A	10	0	13	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	12	0	0
5	B	28	0	12	0	0
6	A	9	0	2	0	0
6	B	9	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	154	0	0	0	0
7	B	136	0	0	0	0
All	All	9988	0	9556	10	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 1.

All (10) 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:336:ALA:HB3	1:A:337:PRO:HD3	1.86	0.57
1:A:261:LEU:HD11	1:A:500[B]:MET:SD	2.45	0.56
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.92	0.51
1:B:593:ASP:HA	1:B:612:LEU:HD21	1.98	0.45
1:B:261:LEU:HD11	1:B:500[B]:MET:SD	2.59	0.43
1:A:266:LEU:HD21	1:A:282:ALA:HB3	2.01	0.42
1:A:221:HIS:CE1	1:A:249:ARG:HD2	2.54	0.42
1:A:95:ILE:N	1:A:95:ILE:HD12	2.34	0.42
1:B:248:LEU:HG	1:B:312:ILE:HD12	2.02	0.42
1:A:550:ALA:HB1	1:A:557:TYR:HB3	2.03	0.41

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	609/622 (98%)	592 (97%)	16 (3%)	1 (0%)	47	46
1	B	607/622 (98%)	590 (97%)	16 (3%)	1 (0%)	47	46
All	All	1216/1244 (98%)	1182 (97%)	32 (3%)	2 (0%)	47	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	LYS
1	A	243	LYS

### 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	511/519 (98%)	510 (100%)	1 (0%)	93	96
1	B	510/519 (98%)	507 (99%)	3 (1%)	86	90
All	All	1021/1038 (98%)	1017 (100%)	4 (0%)	91	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	MET
1	B	100	ARG
1	B	115	ARG
1	B	396	GLU

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

Mol	Chain	Res	Type
1	A	7	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	$\# Z  > 2$
5	GDP	A	706	3	24,30,30	1.24	2 (8%)	31,47,47	1.96	8 (25%)
5	GDP	B	705	3	24,30,30	1.22	2 (8%)	31,47,47	1.91	7 (22%)
6	PGA	B	706	3	5,8,8	0.67	0	6,11,11	1.12	0
6	PGA	A	707	3	5,8,8	0.67	0	6,11,11	1.20	0
2	1PE	A	701	-	9,9,15	0.42	0	8,8,14	0.39	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
5	GDP	A	706	3	-	1/12/32/32	0/3/3/3
5	GDP	B	705	3	-	3/12/32/32	0/3/3/3
6	PGA	B	706	3	-	4/4/6/6	-
6	PGA	A	707	3	-	4/4/6/6	-
2	1PE	A	701	-	-	4/7/7/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	706	GDP	C6-C5	4.35	1.48	1.41
5	B	705	GDP	C6-C5	4.31	1.48	1.41
5	B	705	GDP	C5-C4	2.57	1.47	1.40
5	A	706	GDP	C5-C4	2.55	1.47	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	706	GDP	C2-N3-C4	5.15	121.23	115.36
5	B	705	GDP	C2-N3-C4	5.12	121.20	115.36
5	A	706	GDP	C6-C5-C4	-4.01	116.97	120.80
5	B	705	GDP	C6-N1-C2	3.98	122.26	115.93
5	B	705	GDP	C6-C5-C4	-3.96	117.02	120.80
5	A	706	GDP	C6-N1-C2	3.81	121.99	115.93
5	B	705	GDP	C5-C6-N1	-3.77	118.28	123.43
5	A	706	GDP	C5-C6-N1	-3.68	118.39	123.43
5	B	705	GDP	N3-C2-N1	-3.58	122.45	127.22
5	A	706	GDP	N3-C2-N1	-3.43	122.65	127.22
5	B	705	GDP	PA-O3A-PB	-2.79	123.26	132.83
5	A	706	GDP	C4-C5-N7	-2.69	106.60	109.40
5	A	706	GDP	PA-O3A-PB	-2.41	124.56	132.83
5	B	705	GDP	C4-C5-N7	-2.37	106.93	109.40
5	A	706	GDP	C3'-C2'-C1'	2.32	104.47	100.98

There are no chirality outliers.

All (16) torsion outliers are listed below:

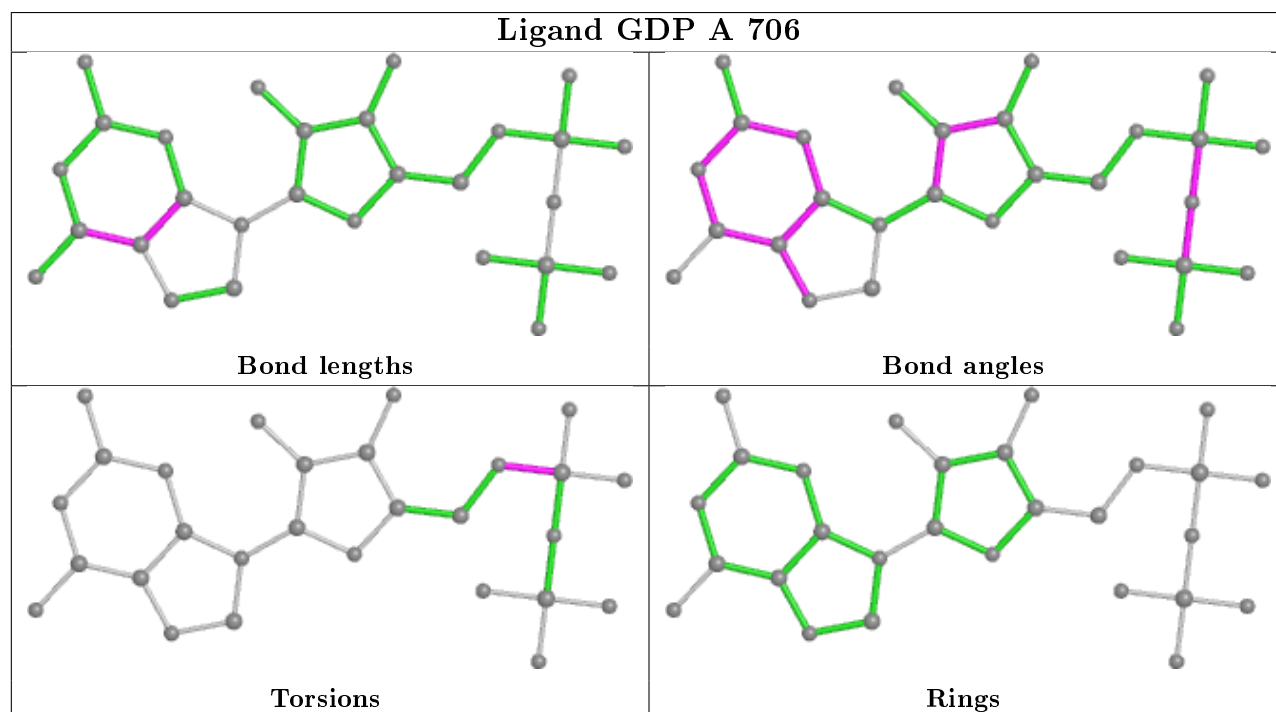
Mol	Chain	Res	Type	Atoms
5	B	705	GDP	C5'-O5'-PA-O3A
5	B	705	GDP	C5'-O5'-PA-O1A
6	B	706	PGA	C2-O1P-P-O2P
6	B	706	PGA	C2-O1P-P-O3P
6	B	706	PGA	C2-O1P-P-O4P
6	A	707	PGA	C2-O1P-P-O2P
6	A	707	PGA	C2-O1P-P-O3P
6	A	707	PGA	C2-O1P-P-O4P
6	A	707	PGA	C1-C2-O1P-P
2	A	701	1PE	OH2-C12-C22-OH3
6	B	706	PGA	C1-C2-O1P-P
2	A	701	1PE	C14-C24-OH4-C13
2	A	701	1PE	C13-C23-OH3-C22
2	A	701	1PE	C23-C13-OH4-C24
5	A	706	GDP	C5'-O5'-PA-O1A
5	B	705	GDP	C5'-O5'-PA-O2A

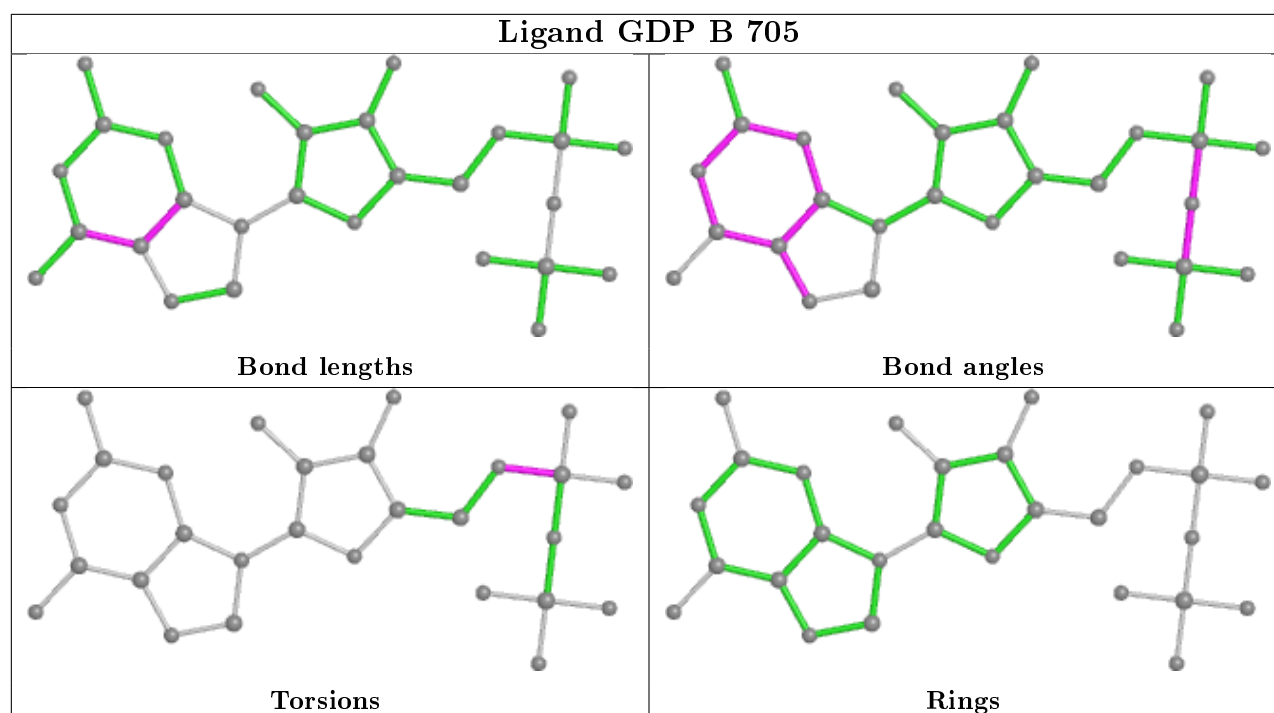
There are no ring outliers.

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 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, 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	611/622 (98%)	0.79	75 (12%) 4 5	25, 43, 69, 106	0
1	B	609/622 (97%)	0.77	69 (11%) 5 7	29, 46, 72, 100	0
All	All	1220/1244 (98%)	0.78	144 (11%) 4 6	25, 45, 71, 106	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	GLN	11.0
1	B	568	GLY	8.5
1	A	7	ASN	6.4
1	B	394	GLN	5.9
1	B	152	PRO	5.6
1	A	472	GLY	5.5
1	A	9	LEU	5.5
1	A	574	VAL	5.3
1	A	569	LEU	5.2
1	A	392	ARG	5.1
1	B	473	LYS	5.0
1	A	504	PRO	4.8
1	A	474	VAL	4.8
1	B	505	ALA	4.7
1	B	9	LEU	4.6
1	A	166	VAL	4.5
1	B	392	ARG	4.5
1	B	432	ILE	4.3
1	A	466	ALA	4.1
1	A	396	GLU	4.0
1	B	570	GLY	4.0
1	B	561	GLU	4.0
1	A	395	ASP	3.9
1	A	70	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	378	ALA	3.7
1	A	432	ILE	3.7
1	A	153	LEU	3.7
1	B	153	LEU	3.7
1	B	567	LYS	3.6
1	A	525	PHE	3.6
1	A	390	GLU	3.6
1	B	504	PRO	3.6
1	A	204	LYS	3.5
1	B	456	VAL	3.5
1	B	575	GLU	3.5
1	A	152	PRO	3.5
1	A	572	VAL	3.4
1	B	166	VAL	3.4
1	B	525	PHE	3.3
1	B	569	LEU	3.3
1	A	165	TYR	3.3
1	A	575	GLU	3.3
1	A	473	LYS	3.3
1	A	391	TRP	3.3
1	B	574	VAL	3.3
1	A	55	ARG	3.3
1	A	471	LYS	3.2
1	B	562	ASP	3.2
1	B	396	GLU	3.2
1	A	562	ASP	3.2
1	B	266	LEU	3.2
1	B	25	GLN	3.2
1	A	431	ILE	3.2
1	A	576	GLU	3.1
1	A	341	VAL	3.1
1	B	204	LYS	3.1
1	A	149	LEU	3.1
1	A	377	LEU	3.1
1	B	377	LEU	3.0
1	B	466	ALA	3.0
1	A	202	LEU	3.0
1	B	391	TRP	2.9
1	A	424	GLU	2.9
1	B	571	ASP	2.9
1	A	205	PRO	2.9
1	B	514	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	240	LEU	2.8
1	A	282	ALA	2.8
1	A	567	LYS	2.8
1	B	587	LYS	2.8
1	B	572	VAL	2.8
1	B	576	GLU	2.8
1	A	511	ILE	2.7
1	B	393	PRO	2.7
1	B	319	ALA	2.7
1	A	283	ALA	2.7
1	A	407	CYS	2.6
1	B	389	LYS	2.6
1	A	319	ALA	2.6
1	A	241	LEU	2.5
1	B	341	VAL	2.5
1	A	512	PHE	2.5
1	A	456	VAL	2.5
1	A	25	GLN	2.5
1	B	203	LYS	2.5
1	A	378	ALA	2.4
1	B	390	GLU	2.4
1	B	464	ALA	2.4
1	B	342	LYS	2.4
1	B	383	ILE	2.4
1	B	305	VAL	2.3
1	A	561	GLU	2.3
1	B	151	SER	2.3
1	B	349	LYS	2.3
1	B	352	GLN	2.3
1	B	165	TYR	2.3
1	B	407	CYS	2.3
1	B	460	MET	2.3
1	B	55	ARG	2.3
1	A	470	HIS	2.3
1	B	100	ARG	2.3
1	B	444	VAL	2.3
1	A	349	LYS	2.3
1	B	282	ALA	2.3
1	B	433	PHE	2.3
1	B	376	PRO	2.3
1	A	8	GLY	2.3
1	A	240	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	169	SER	2.2
1	A	467	ALA	2.2
1	B	193	LEU	2.2
1	A	376	PRO	2.2
1	A	393	PRO	2.2
1	A	505	ALA	2.2
1	B	410	ALA	2.2
1	A	236	GLY	2.2
1	A	266	LEU	2.2
1	B	468	ALA	2.2
1	A	267	ILE	2.1
1	A	185	GLY	2.1
1	A	161	THR	2.1
1	A	358	THR	2.1
1	A	464	ALA	2.1
1	A	433	PHE	2.1
1	B	246	PHE	2.1
1	B	397	GLU	2.1
1	A	577	LEU	2.1
1	A	584	PHE	2.1
1	B	384	THR	2.1
1	B	395	ASP	2.1
1	A	348	ILE	2.1
1	A	381	VAL	2.1
1	A	246	PHE	2.1
1	B	512	PHE	2.1
1	A	66	ILE	2.0
1	A	160	LEU	2.0
1	A	613	ARG	2.0
1	B	226	ARG	2.0
1	B	424	GLU	2.0
1	B	202	LEU	2.0
1	B	241	LEU	2.0
1	A	568	GLY	2.0
1	A	570	GLY	2.0
1	B	519	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

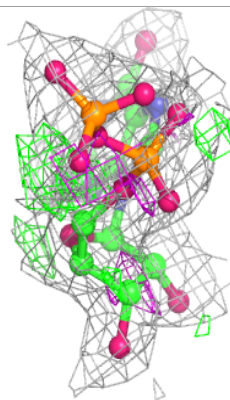
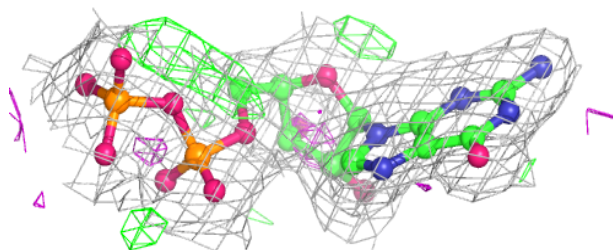
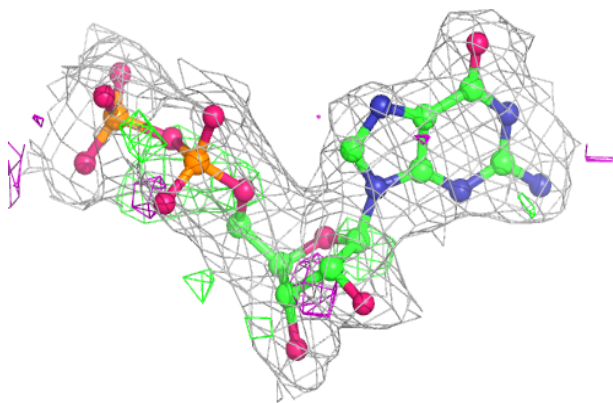
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	NA	B	704	1/1	0.68	0.19	67,67,67,67	0
4	NA	A	705	1/1	0.85	0.15	58,58,58,58	0
2	1PE	A	701	10/16	0.87	0.23	33,34,35,35	10
6	PGA	A	707	9/9	0.92	0.12	36,37,39,40	0
5	GDP	A	706	28/28	0.92	0.14	40,44,47,47	0
5	GDP	B	705	28/28	0.92	0.14	48,51,52,54	0
3	MN	A	703	1/1	0.94	0.03	60,60,60,60	0
6	PGA	B	706	9/9	0.96	0.12	47,48,51,51	0
3	MN	A	702	1/1	0.97	0.06	43,43,43,43	0
3	MN	B	702	1/1	0.98	0.07	44,44,44,44	0
3	MN	B	701	1/1	0.98	0.03	56,56,56,56	0
3	MN	B	703	1/1	0.98	0.11	38,38,38,38	0
3	MN	A	704	1/1	0.98	0.10	31,31,31,31	0

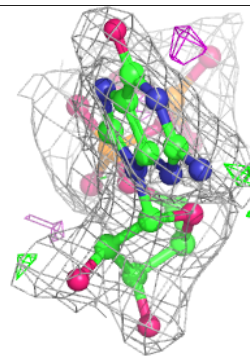
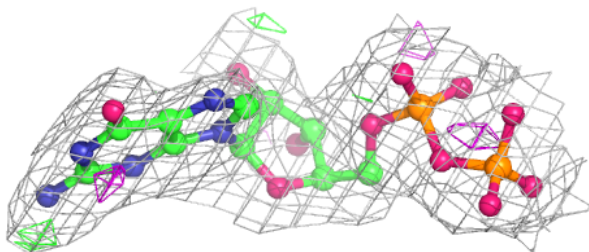
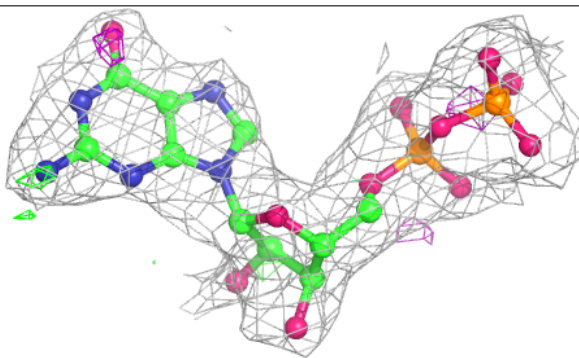
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GDP A 706:**

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

**Electron density around GDP B 705:**

$2mF_o-DF_c$  (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.