



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 01:14 AM EST

PDB ID : 2QF2  
Title : Rat cytosolic PEPCCK in complex with oxaloacetic acid and GDP.  
Authors : Sullivan, S.M.; Holyoak, T.  
Deposited on : 2007-06-26  
Resolution : 1.65 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.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (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

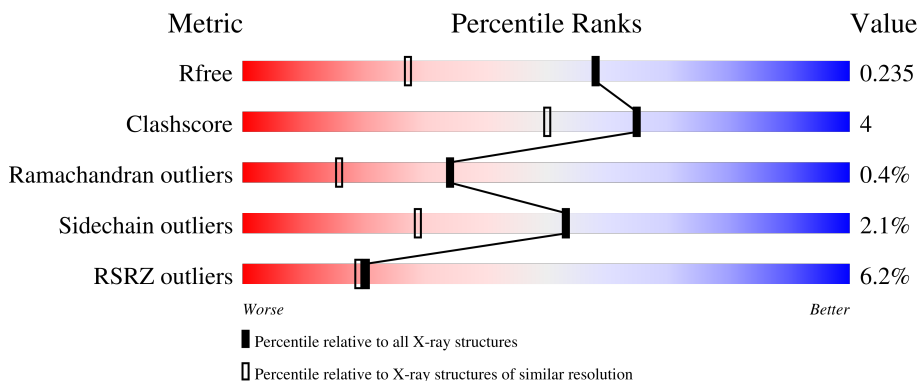
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	624	
1	B	624	

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 11386 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
			Total	C	N	O	S			
1	A	613	Total	C	N	O	S	0	45	0
			5075	3264	861	913	37			
1	B	606	Total	C	N	O	S	0	34	0
			4979	3209	841	896	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P07379
A	0	SER	-	expression tag	UNP P07379
B	-1	GLY	-	expression tag	UNP P07379
B	0	SER	-	expression tag	UNP P07379

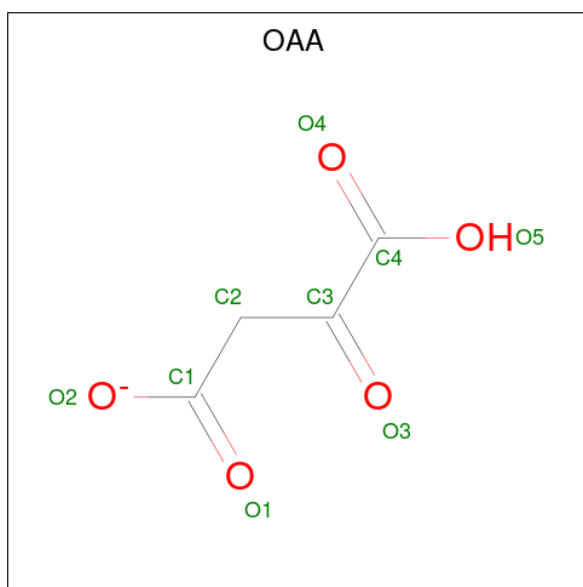
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Mn	0	2
			4	4		
2	B	3	Total	Mn	0	0
			3	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

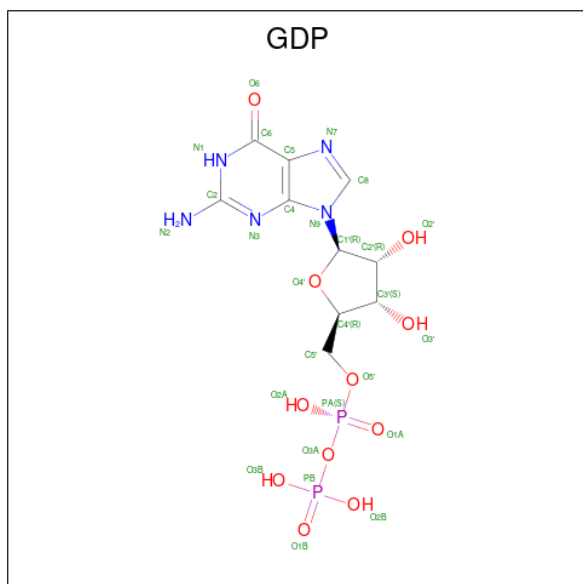
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is OXALOACETATE ION (three-letter code: OAA) (formula: C<sub>4</sub>H<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			9	4	5		
4	B	1	Total	C	O	0	1
			9	4	5		

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



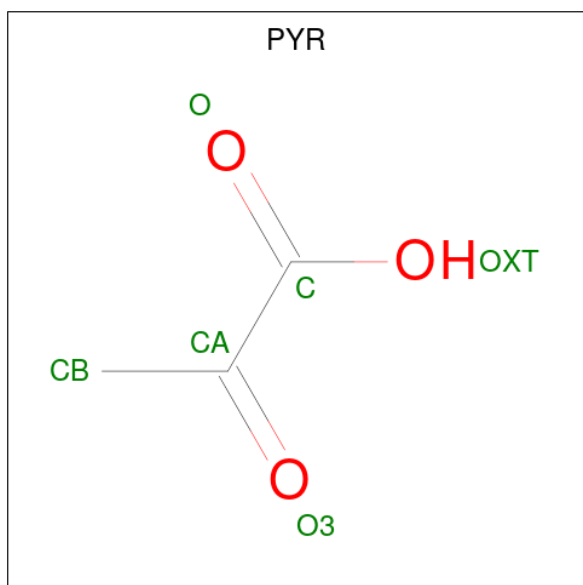
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			28	10	5	11	2		

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

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula:  $C_3H_4O_3$ ).



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

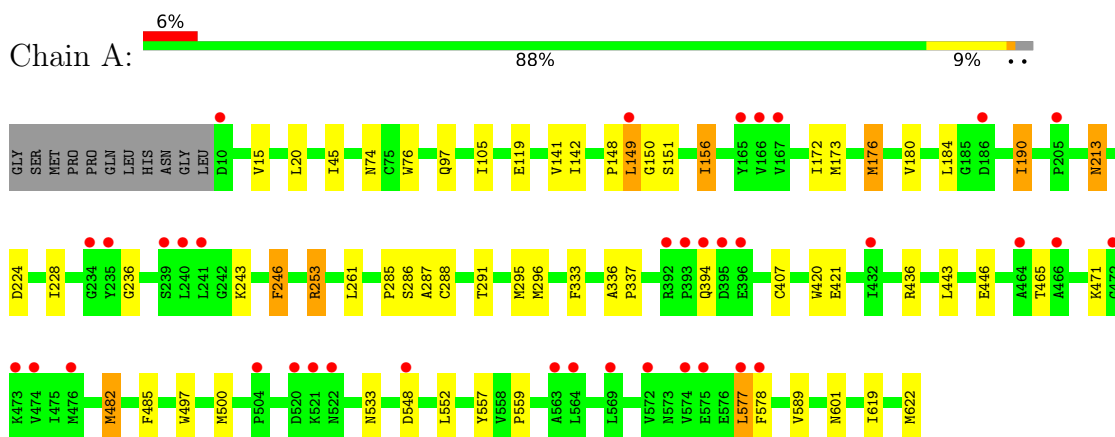
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	615	615	615	0	0
7	B	594	594	594	0	0

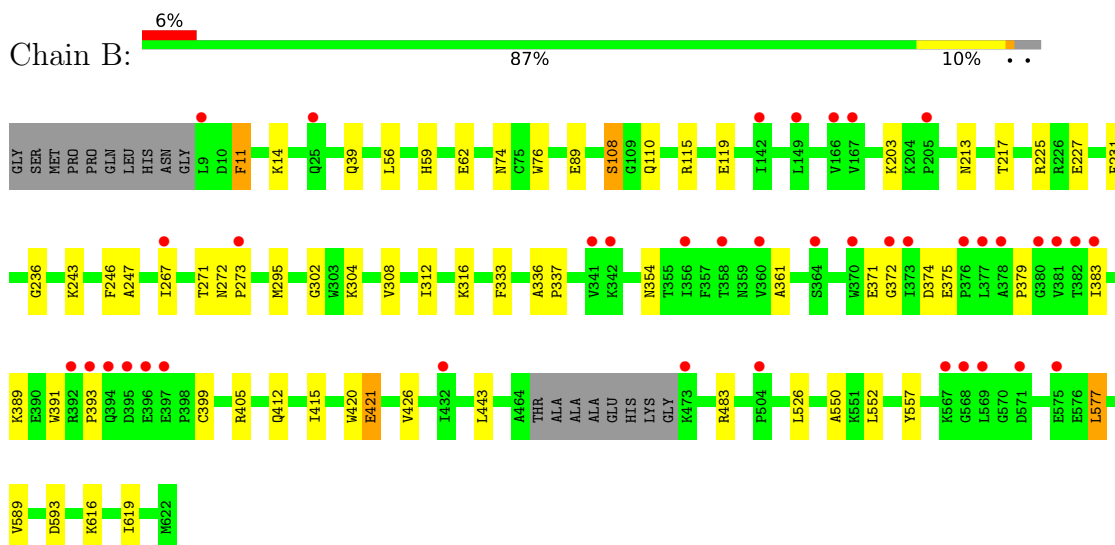
### 3 Residue-property plots [i](#)

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: Phosphoenolpyruvate carboxykinase, cytosolic [GTP]



- Molecule 1: Phosphoenolpyruvate carboxykinase, cytosolic [GTP]



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.51Å 119.11Å 86.71Å 90.00° 107.35° 90.00°	Depositor
Resolution (Å)	33.33 – 1.65 33.33 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.5 (33.33-1.65) 96.5 (33.33-1.65)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 1.65Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.204 , 0.238 0.203 , 0.235	Depositor DCC
$R_{free}$ test set	7148 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtrriage
Anisotropy	0.163	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	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 78.34 % 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 7.0665e-07. 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, NA, GDP, OAA, PYR

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	0.39	0/5313	0.55	0/7178
1	B	0.58	9/5206 (0.2%)	0.59	2/7031 (0.0%)
All	All	0.49	9/10519 (0.1%)	0.57	2/14209 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	PRO	C-N	9.96	1.50	1.33
1	B	375[A]	GLU	CG-CD	9.51	1.66	1.51
1	B	375[B]	GLU	CG-CD	9.51	1.66	1.51
1	B	379	PRO	C-O	8.14	1.39	1.23
1	B	375[A]	GLU	CD-OE1	7.46	1.33	1.25
1	B	375[B]	GLU	CD-OE1	7.46	1.33	1.25
1	B	374	ASP	C-N	6.56	1.49	1.34
1	B	371	GLU	C-O	5.35	1.33	1.23
1	B	372	GLY	C-O	5.24	1.32	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	379	PRO	O-C-N	6.55	134.34	123.20
1	B	108	SER	N-CA-C	5.91	126.95	111.00

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	5075	0	5146	43	0
1	B	4979	0	5052	40	0
2	A	4	0	0	1	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	9	0	2	1	0
4	B	9	0	2	3	0
5	A	56	0	24	3	0
5	B	28	0	12	0	0
6	A	6	0	0	0	0
6	B	6	0	0	0	0
7	A	615	0	0	1	0
7	B	594	0	0	5	0
All	All	11386	0	10238	84	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 4.

All (84) 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:B:267[A]:ILE:HD11	1:B:426:VAL:CG2	1.87	1.05
1:A:288[B]:CYS:SG	1:A:436[B]:ARG:HG3	2.02	0.99
1:B:267[A]:ILE:HD11	1:B:426:VAL:HG21	1.54	0.90
1:B:11[A]:PHE:CE1	1:B:14[A]:LYS:HD2	2.08	0.89
1:A:156[A]:ILE:HG12	1:A:184:LEU:HD13	1.58	0.86
2:A:624[A]:MN:MN	7:A:4142:HOH:O	1.35	0.82
1:B:108:SER:O	7:B:4456:HOH:O	2.02	0.77
1:A:287[B]:ALA:N	5:A:703[B]:GDP:O1B	2.17	0.77
1:B:225[A]:ARG:NE	1:B:227[A]:GLU:OE1	2.17	0.76
1:B:11[A]:PHE:HE1	1:B:14[A]:LYS:HD2	1.60	0.67
1:A:482[A]:MET:HG3	1:A:485:PHE:HB2	1.80	0.62
1:B:354:ASN:HB2	1:B:412:GLN:HE22	1.65	0.62
1:A:190:ILE:HD11	1:A:228:ILE:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267[A]:ILE:HG12	1:B:308:VAL:HB	1.84	0.59
1:A:497:TRP:HA	1:A:500[B]:MET:HE2	1.83	0.59
1:A:589[B]:VAL:HG11	1:A:619:ILE:HD12	1.85	0.59
1:B:11[A]:PHE:CD1	1:B:14[A]:LYS:HD2	2.38	0.59
1:B:593:ASP:OD2	1:B:616[B]:LYS:NZ	2.28	0.58
1:B:59:HIS:O	1:B:62[A]:GLU:HG2	2.03	0.58
1:A:288[B]:CYS:SG	1:A:436[B]:ARG:CG	2.88	0.57
1:B:203:LYS:HE2	7:B:4446:HOH:O	2.03	0.57
1:A:156[A]:ILE:HD11	1:A:184:LEU:HD22	1.87	0.57
1:A:286[B]:SER:O	1:A:465:THR:HG21	2.05	0.56
1:A:443:LEU:HB2	1:A:577:LEU:HD22	1.87	0.56
1:A:285[B]:PRO:O	1:A:288[B]:CYS:HB2	2.05	0.55
1:A:497:TRP:HA	1:A:500[B]:MET:CE	2.36	0.55
1:A:619:ILE:O	1:A:622:MET:HG2	2.06	0.55
1:A:482[A]:MET:CG	1:A:485:PHE:HB2	2.36	0.55
1:B:59:HIS:HD2	1:B:62[A]:GLU:OE2	1.90	0.54
1:A:105:ILE:O	1:A:601[B]:ASN:ND2	2.40	0.54
1:A:148[B]:PRO:O	1:A:150[B]:GLY:N	2.43	0.51
1:B:74:ASN:ND2	1:B:76:TRP:HE1	2.08	0.51
1:A:261:LEU:HD11	1:A:500[B]:MET:SD	2.51	0.50
1:A:420:TRP:CE2	1:A:421:GLU:HG3	2.46	0.49
1:A:296:MET:HE2	1:A:533:ASN:HB2	1.95	0.49
1:A:74:ASN:ND2	1:A:76:TRP:HE1	2.10	0.49
1:A:190:ILE:HD11	1:A:228:ILE:CD1	2.43	0.49
1:A:148[B]:PRO:HG2	1:A:151:SER:HB2	1.94	0.48
1:A:246:PHE:C	1:A:246:PHE:CD1	2.86	0.48
1:B:354:ASN:HD22	1:B:412:GLN:NE2	2.12	0.48
1:B:405:ARG:NH1	4:B:801[A]:OAA:H21	2.29	0.48
1:A:333:PHE:HD2	4:A:701[A]:OAA:H22	1.78	0.48
1:B:272:ASN:HB2	1:B:273:PRO:CD	2.44	0.48
1:A:246:PHE:C	1:A:246:PHE:HD1	2.16	0.47
1:B:89:GLU:OE2	1:B:483:ARG:NH1	2.37	0.47
1:B:272:ASN:HB2	1:B:273:PRO:HD2	1.95	0.47
1:B:295:MET:HA	1:B:415:ILE:HD11	1.97	0.47
1:A:172:ILE:HG22	1:A:173[A]:MET:HE2	1.98	0.46
1:B:247:ALA:HB1	1:B:312:ILE:HG21	1.97	0.46
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.98	0.46
1:A:173[A]:MET:HE2	1:A:407:CYS:SG	2.55	0.45
1:A:287[B]:ALA:HA	5:A:703[B]:GDP:H5'	1.99	0.45
1:A:436[B]:ARG:HH12	5:A:703[B]:GDP:C4'	2.29	0.44
1:A:287[B]:ALA:HB3	1:A:465:THR:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:THR:HB	1:B:304:LYS:HE3	1.99	0.43
1:A:224:ASP:OD2	1:A:253[A]:ARG:NH2	2.46	0.43
1:B:589:VAL:HG11	1:B:619:ILE:HD12	2.01	0.43
1:B:316[B]:LYS:HE3	7:B:4592:HOH:O	2.16	0.43
1:B:302:GLY:O	1:B:304:LYS:HE2	2.17	0.43
1:B:443:LEU:HB2	1:B:577[A]:LEU:HD22	2.01	0.43
1:B:405:ARG:HH12	4:B:801[A]:OAA:H21	1.84	0.43
1:A:149[B]:LEU:HD21	1:A:180:VAL:HG22	2.00	0.43
1:B:361:ALA:HB1	1:B:383:ILE:HG23	2.01	0.42
1:A:446:GLU:HB3	1:A:557:TYR:HB2	2.01	0.42
1:A:45:ILE:HA	1:A:141:VAL:HB	2.01	0.42
1:B:243:LYS:HE3	4:B:801[A]:OAA:H22	2.01	0.42
1:A:336:ALA:HB3	1:A:337:PRO:HD3	2.02	0.42
1:B:217:THR:HA	1:B:231:PHE:O	2.19	0.42
1:A:97[A]:GLN:HG2	1:A:119:GLU:OE1	2.20	0.42
1:A:15:VAL:HG21	1:A:20:LEU:HG	2.02	0.42
1:A:213:ASN:C	1:A:213:ASN:HD22	2.22	0.42
1:B:243:LYS:HE2	1:B:333:PHE:HB3	2.02	0.41
1:A:559:PRO:HD2	1:A:578[B]:PHE:CE1	2.55	0.41
1:B:115[B]:ARG:NH2	7:B:4594:HOH:O	2.53	0.41
1:B:550:ALA:HB1	1:B:557:TYR:HB3	2.01	0.41
1:B:526:LEU:HB3	1:B:577[A]:LEU:HG	2.02	0.41
1:B:420:TRP:CE2	1:B:421:GLU:HG2	2.56	0.41
1:A:173[A]:MET:CE	1:A:407:CYS:SG	3.09	0.40
1:A:291:THR:O	1:A:295:MET:HG2	2.20	0.40
1:B:391:TRP:CD2	1:B:399:CYS:HB3	2.56	0.40
1:A:142:ILE:HG23	1:A:176[B]:MET:CG	2.52	0.40
1:B:119[A]:GLU:HG3	7:B:4131:HOH:O	2.21	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	656/624 (105%)	626 (95%)	26 (4%)	4 (1%)	25	8
1	B	637/624 (102%)	620 (97%)	15 (2%)	2 (0%)	41	22
All	All	1293/1248 (104%)	1246 (96%)	41 (3%)	6 (0%)	34	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149[A]	LEU
1	A	149[B]	LEU
1	A	236	GLY
1	B	236	GLY
1	A	243	LYS
1	B	393	PRO

### 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	553/520 (106%)	536 (97%)	17 (3%)	40	14
1	B	543/520 (104%)	530 (98%)	13 (2%)	49	23
All	All	1096/1040 (105%)	1066 (97%)	30 (3%)	53	19

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156[A]	ILE
1	A	156[B]	ILE
1	A	176[A]	MET
1	A	176[B]	MET
1	A	190	ILE
1	A	213	ASN
1	A	246	PHE
1	A	253[A]	ARG
1	A	253[B]	ARG
1	A	394	GLN

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Mol	Chain	Res	Type
1	A	471	LYS
1	A	482[A]	MET
1	A	482[B]	MET
1	A	548[A]	ASP
1	A	548[B]	ASP
1	A	552	LEU
1	A	577	LEU
1	B	11[A]	PHE
1	B	11[B]	PHE
1	B	56[A]	LEU
1	B	56[B]	LEU
1	B	110[A]	GLN
1	B	110[B]	GLN
1	B	213	ASN
1	B	246	PHE
1	B	389	LYS
1	B	421	GLU
1	B	552	LEU
1	B	577[A]	LEU
1	B	577[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	208	ASN
1	A	213	ASN
1	A	238	ASN
1	A	297	ASN
1	A	515	ASN
1	B	34	ASN
1	B	36	GLN
1	B	59	HIS
1	B	74	ASN
1	B	99	GLN
1	B	208	ASN
1	B	213	ASN
1	B	292	ASN
1	B	297	ASN
1	B	388	ASN
1	B	412	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 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	OAA	A	701[A]	2	8,8,8	2.19	3 (37%)	9,10,10	1.17	0
5	GDP	A	702[A]	2	24,30,30	0.90	0	30,47,47	1.06	3 (10%)
6	PYR	A	4083[B]	2	5,5,5	2.93	3 (60%)	3,6,6	1.53	1 (33%)
4	OAA	B	801[A]	2	8,8,8	2.24	3 (37%)	9,10,10	1.14	0
6	PYR	B	4083[B]	2	5,5,5	2.93	3 (60%)	3,6,6	1.70	1 (33%)
5	GDP	B	802	2	24,30,30	0.84	0	30,47,47	1.18	4 (13%)
5	GDP	A	703[B]	-	24,30,30	0.96	1 (4%)	30,47,47	1.17	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	OAA	A	701[A]	2	-	2/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	A	702[A]	2	-	0/12/32/32	0/3/3/3
6	PYR	A	4083[B]	2	-	0/4/4/4	-
4	OAA	B	801[A]	2	-	4/8/8/8	-
6	PYR	B	4083[B]	2	-	1/4/4/4	-
5	GDP	B	802	2	-	0/12/32/32	0/3/3/3
5	GDP	A	703[B]	-	-	0/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801[A]	OAA	O3-C3	4.24	1.31	1.23
4	A	701[A]	OAA	O3-C3	4.21	1.31	1.23
6	B	4083[B]	PYR	CA-C	-3.98	1.40	1.54
6	A	4083[B]	PYR	CA-C	-3.97	1.40	1.54
6	B	4083[B]	PYR	O3-CA	3.75	1.31	1.23
6	A	4083[B]	PYR	O-C	3.73	1.32	1.22
6	A	4083[B]	PYR	O3-CA	3.60	1.31	1.23
6	B	4083[B]	PYR	O-C	3.59	1.32	1.22
4	B	801[A]	OAA	O4-C4	3.43	1.31	1.22
4	A	701[A]	OAA	O4-C4	3.32	1.31	1.22
4	A	701[A]	OAA	O1-C1	2.80	1.31	1.22
4	B	801[A]	OAA	O1-C1	2.68	1.31	1.22
5	A	703[B]	GDP	C6-N1	-2.49	1.34	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	703[B]	GDP	PA-O3A-PB	-3.46	120.97	132.83
5	B	802	GDP	PA-O3A-PB	-2.61	123.88	132.83
5	A	702[A]	GDP	C5-C6-N1	2.48	118.33	113.95
6	B	4083[B]	PYR	OXT-C-CA	2.45	120.67	113.97
5	B	802	GDP	O6-C6-C5	-2.41	119.67	124.37
6	A	4083[B]	PYR	OXT-C-CA	2.37	120.46	113.97
5	A	702[A]	GDP	PA-O3A-PB	-2.36	124.72	132.83
5	B	802	GDP	C5-C6-N1	2.34	118.09	113.95
5	A	703[B]	GDP	C8-N7-C5	2.32	107.42	102.99
5	B	802	GDP	C8-N7-C5	2.21	107.20	102.99
5	A	702[A]	GDP	C8-N7-C5	2.16	107.11	102.99
5	A	703[B]	GDP	C5-C6-N1	2.14	117.73	113.95
5	A	703[B]	GDP	C3'-C2'-C1'	2.03	104.03	100.98

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801[A]	OAA	C2-C3-C4-O5
4	A	701[A]	OAA	O2-C1-C2-C3
4	B	801[A]	OAA	C1-C2-C3-O3
4	B	801[A]	OAA	C1-C2-C3-C4
6	B	4083[B]	PYR	OXT-C-CA-O3
4	A	701[A]	OAA	O1-C1-C2-C3
4	B	801[A]	OAA	O1-C1-C2-C3

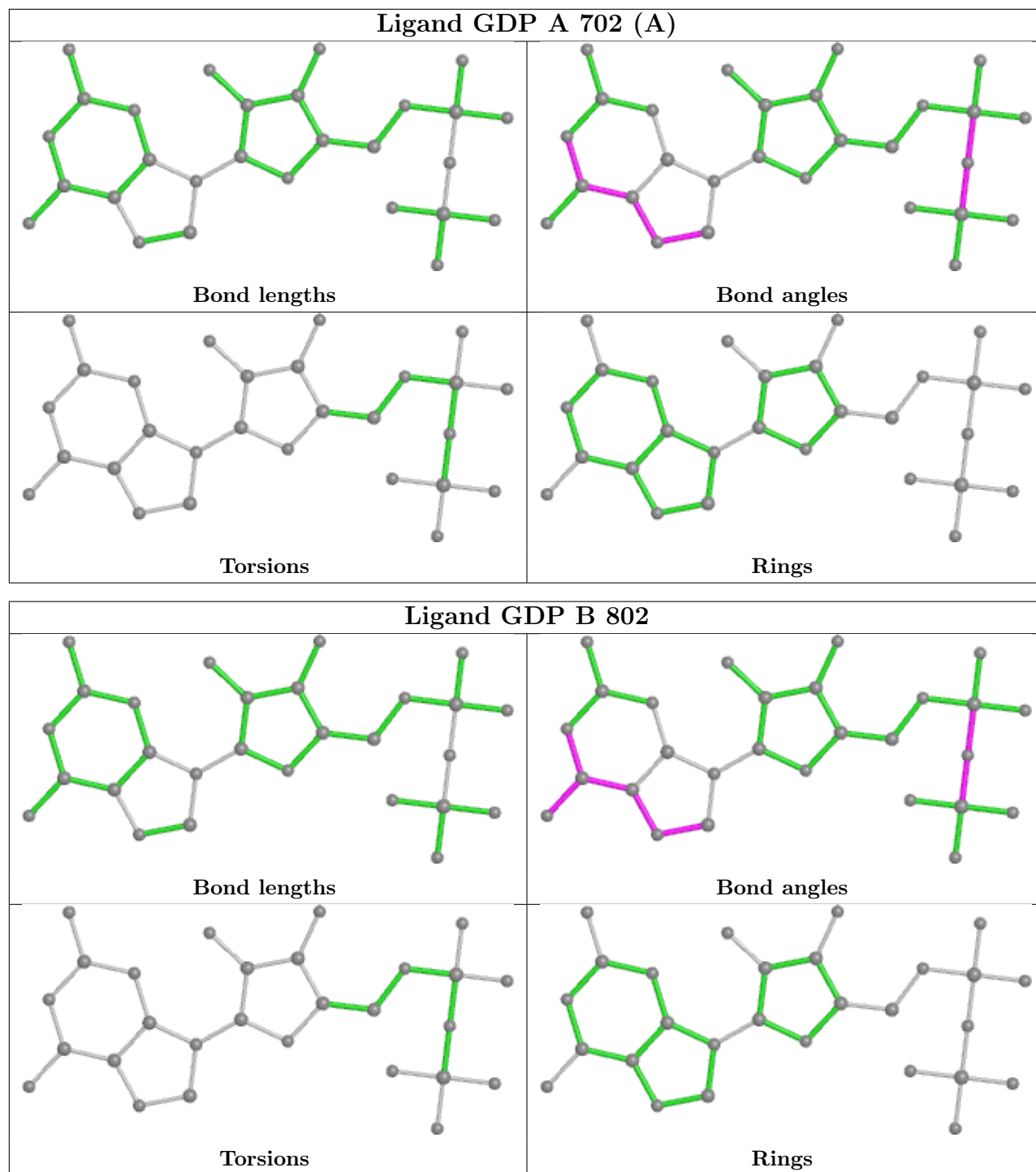
There are no ring outliers.

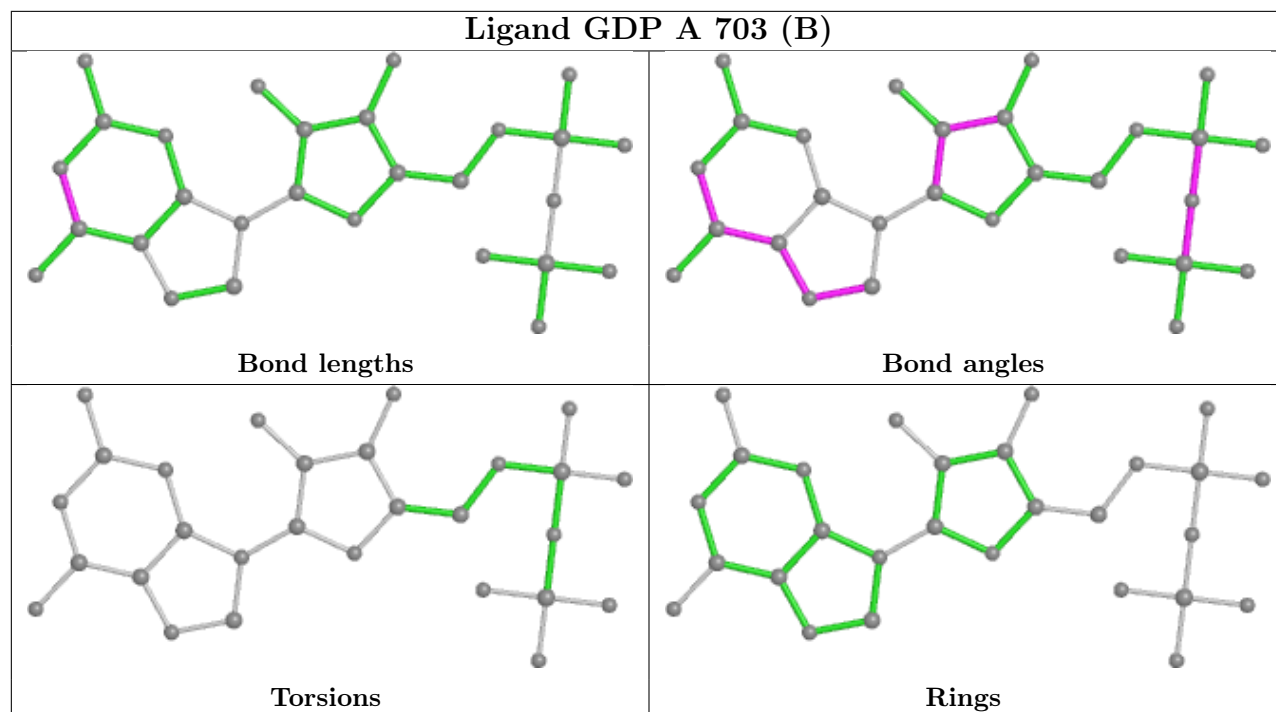
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701[A]	OAA	1	0
4	B	801[A]	OAA	3	0
5	A	703[B]	GDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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	613/624 (98%)	0.31	37 (6%) 21 20	11, 17, 25, 34	11 (1%)
1	B	606/624 (97%)	0.26	39 (6%) 19 18	8, 16, 26, 36	0
All	All	1219/1248 (97%)	0.28	76 (6%) 20 19	8, 17, 25, 36	11 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	393	PRO	7.0
1	B	9	LEU	6.5
1	A	393	PRO	5.6
1	A	504	PRO	5.4
1	A	575	GLU	5.2
1	B	394	GLN	5.1
1	A	394	GLN	5.0
1	B	395	ASP	4.7
1	A	149[A]	LEU	4.5
1	B	392	ARG	4.4
1	A	396	GLU	4.3
1	B	267[A]	ILE	4.0
1	A	392	ARG	4.0
1	A	578[A]	PHE	3.9
1	B	397	GLU	3.9
1	B	396	GLU	3.7
1	A	473	LYS	3.7
1	B	504	PRO	3.7
1	B	473	LYS	3.7
1	A	474	VAL	3.6
1	A	522	ASN	3.5
1	B	205	PRO	3.3
1	B	377	LEU	3.2
1	A	572	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	577	LEU	3.1
1	A	165	TYR	3.1
1	A	472	GLY	3.1
1	B	571	ASP	3.0
1	A	520	ASP	3.0
1	A	205	PRO	3.0
1	A	521	LYS	3.0
1	A	240	LEU	3.0
1	B	166	VAL	2.9
1	A	563	ALA	2.9
1	A	166	VAL	2.8
1	B	342	LYS	2.8
1	A	186	ASP	2.7
1	B	569	LEU	2.7
1	A	235	TYR	2.6
1	B	370	TRP	2.6
1	A	574	VAL	2.6
1	A	464	ALA	2.6
1	B	273	PRO	2.6
1	B	567	LYS	2.5
1	A	466	ALA	2.5
1	B	341	VAL	2.5
1	A	241	LEU	2.5
1	B	383	ILE	2.5
1	B	364[A]	SER	2.5
1	A	234	GLY	2.5
1	A	395	ASP	2.4
1	B	575	GLU	2.4
1	A	432	ILE	2.3
1	A	10	ASP	2.3
1	A	167	VAL	2.3
1	B	381	VAL	2.3
1	A	569	LEU	2.3
1	B	167	VAL	2.3
1	B	358	THR	2.3
1	B	382	THR	2.2
1	B	378	ALA	2.2
1	B	380	GLY	2.2
1	B	25	GLN	2.1
1	B	376	PRO	2.1
1	A	564	LEU	2.1
1	B	568	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	373	ILE	2.1
1	B	432	ILE	2.1
1	A	548[A]	ASP	2.1
1	B	149	LEU	2.1
1	B	142	ILE	2.1
1	B	360	VAL	2.1
1	A	239	SER	2.1
1	B	356	ILE	2.1
1	A	476	MET	2.0
1	B	372	GLY	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 monosaccharides 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, 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.

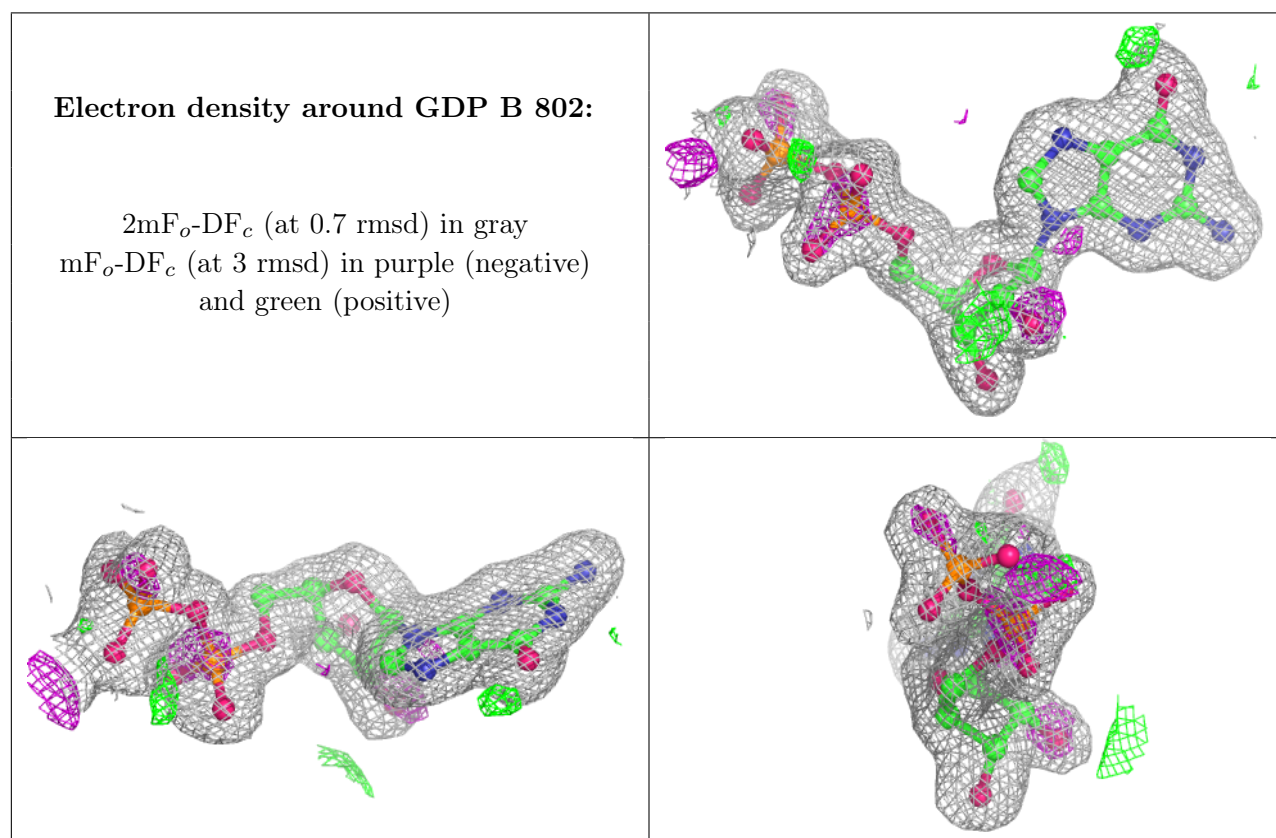
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	OAA	B	801[A]	9/9	0.79	0.27	23,25,26,27	9
6	PYR	B	4083[B]	6/6	0.81	0.20	24,27,27,28	6
6	PYR	A	4083[B]	6/6	0.84	0.17	14,17,17,18	6
4	OAA	A	701[A]	9/9	0.93	0.19	23,24,24,25	9
5	GDP	B	802	28/28	0.95	0.10	26,27,28,29	0
5	GDP	A	703[B]	28/28	0.97	0.10	16,18,19,20	28
2	MN	A	624[A]	1/1	0.97	0.06	20,20,20,20	1
3	NA	B	800	1/1	0.97	0.09	27,27,27,27	0
5	GDP	A	702[A]	28/28	0.97	0.08	16,21,21,22	28
3	NA	A	700	1/1	0.98	0.10	28,28,28,28	0
2	MN	A	625[B]	1/1	0.98	0.08	19,19,19,19	1
2	MN	A	626	1/1	0.98	0.06	32,32,32,32	0
2	MN	B	626	1/1	0.99	0.06	23,23,23,23	0

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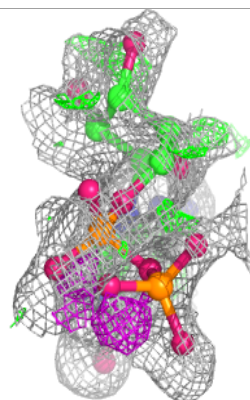
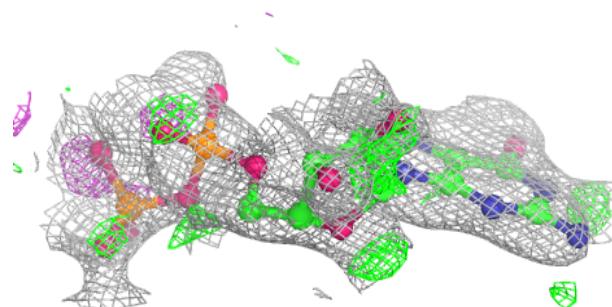
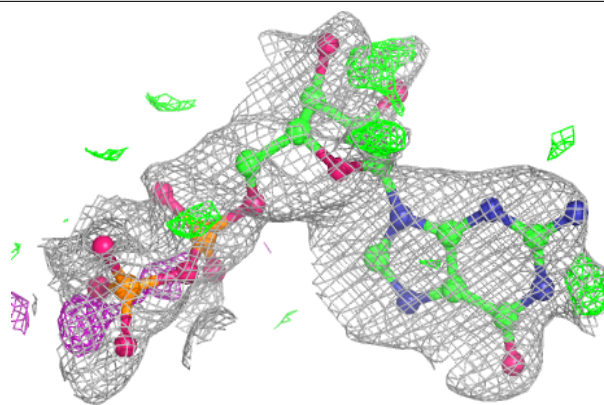
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	B	624	1/1	0.99	0.05	27,27,27,27	1
2	MN	B	623	1/1	1.00	0.04	18,18,18,18	0
2	MN	A	623	1/1	1.00	0.04	19,19,19,19	0

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.

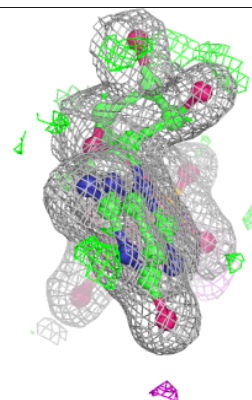
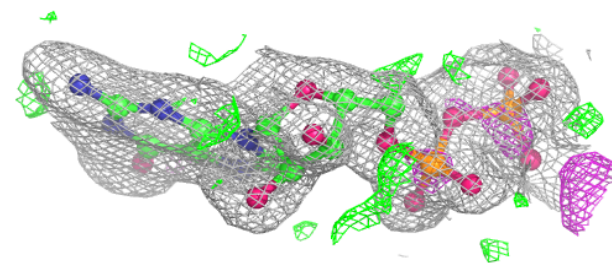
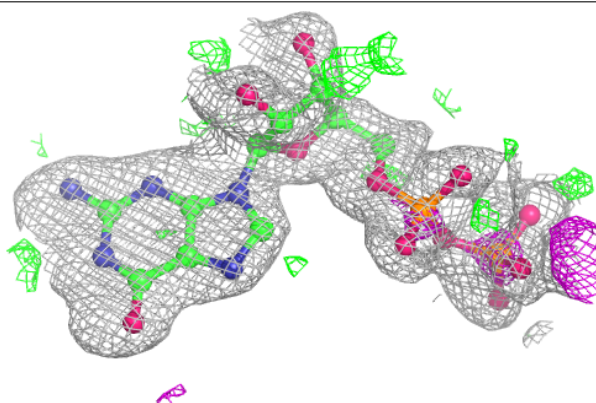


**Electron density around GDP A 703 (B):**

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

**Electron density around GDP A 702 (A):**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.