wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 03:56 AM EDT

PDB ID	:	7JMK
Title	:	GTP-specific succinyl-CoA synthetase complexed with Mg-GDP in space group P32
Authors	:	Huang, J.; Fraser, M.E.
Deposited on	:	2020-08-01
Resolution	:	2.50 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:

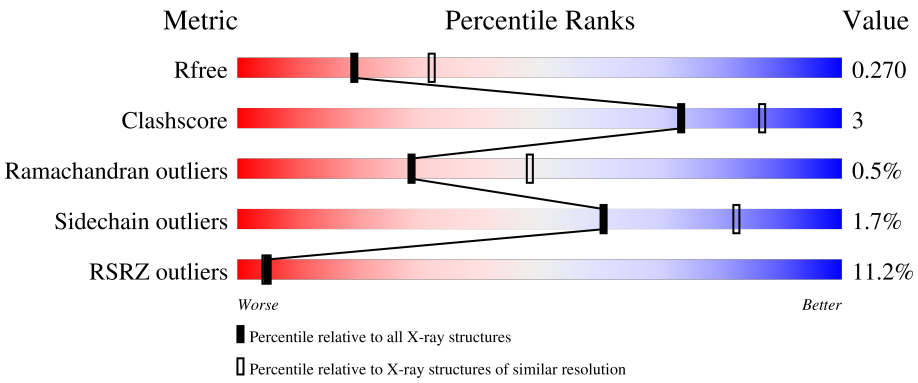
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 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	305	2%, 90%, 8%
1	C	305	3%, 92%, 5%
2	B	395	18%, 84%, 11%
3	D	395	15%, 81%, 9%, 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20236 atoms, of which 10155 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 Succinate–CoA ligase [ADP/GDP-forming] subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	297	4446	1391	2244	385	414	12	0	1	0
1	C	297	4433	1386	2239	384	414	10	0	0	0

- Molecule 2 is a protein called Succinate–CoA ligase [GDP-forming] subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	379	5787	1814	2916	483	560	14	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P53590

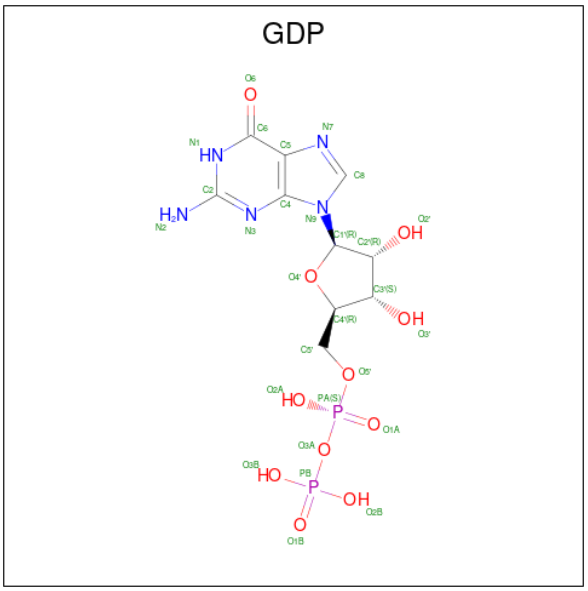
- Molecule 3 is a protein called Succinyl-CoA ligase [GDP-forming] subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	D	354	5417	1703	2726	449	525	14	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP P53590

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
4	B	1	86	20	30	10	22	4	0	1

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	B	1	1	1	0	0

- Molecule 6 is water.

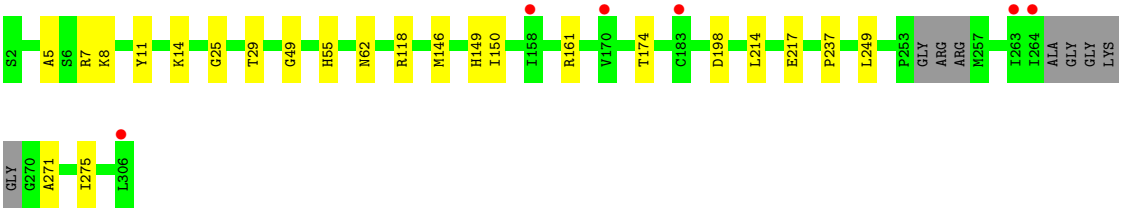
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	28	28	28	0	0
6	B	8	8	8	0	0
6	C	25	25	25	0	0
6	D	5	5	5	0	0

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.

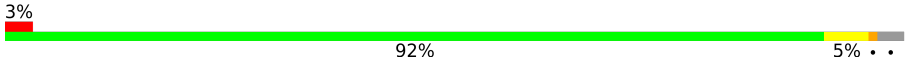
• Molecule 1: Succinate–CoA ligase [ADP/GDP-forming] subunit alpha, mitochondrial

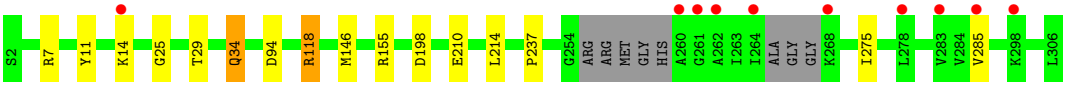
Chain A:



• Molecule 1: Succinate–CoA ligase [ADP/GDP-forming] subunit alpha, mitochondrial

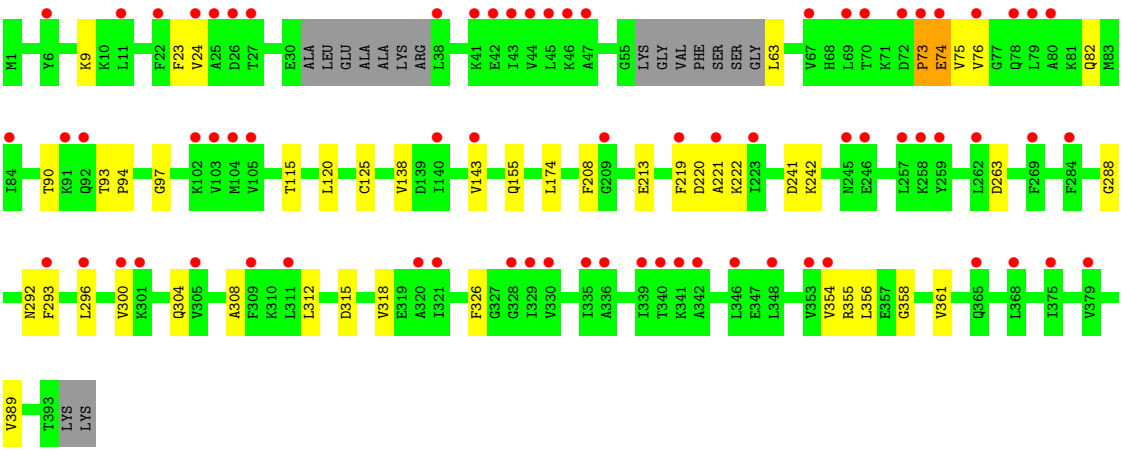
Chain C:





• Molecule 2: Succinate–CoA ligase [GDP-forming] subunit beta, mitochondrial

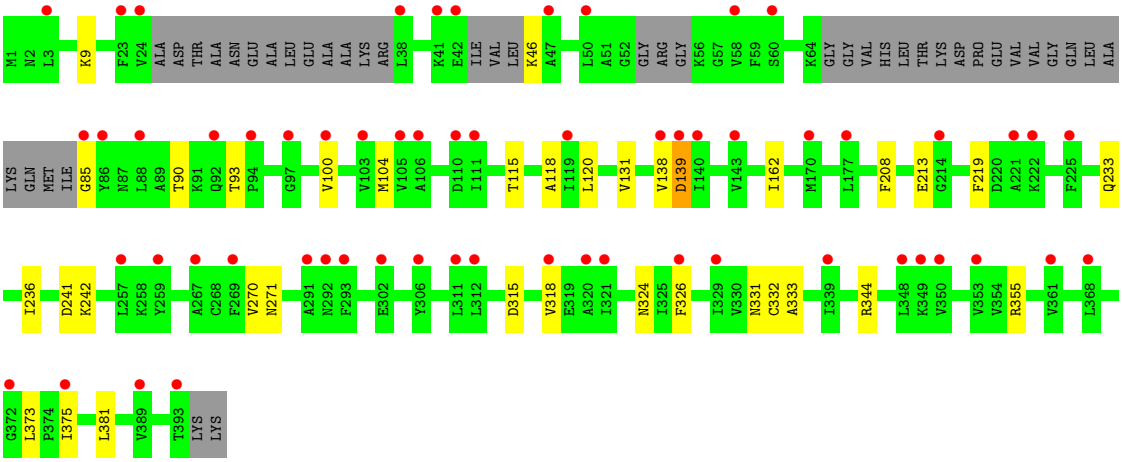
Chain B:



• Molecule 3: Succinyl-CoA ligase [GDP-forming] subunit beta, mitochondrial

Chain D:

15%
81%
9%
10%


M1 N2 L3 K9 F23 V24 ALA ASP THR ALA ASN GLU ALA LEU GLU ALA ALA LYS ARG L38 K41 E42 ILE VAL LEU K46 A47 L50 A51 G52 GLY ARG GLY K56 G57 V58 F59 S60 K64 GLY GLY VAL HIS LEU THR LYS ASP PRO GLU VAL VAL GLY GLN LEU ALA
LYS GLN MET ILE G85 Y86 N87 L88 A89 T90 K91 Q92 T93 P94 G97 V100 V103 M104 V105 A106 D110 I111 T115 A118 I119 L120 V131 V138 D139 I140 V143 I162 M170 L177 F208 E213 G214 F219 D220 A221 K222 F225 Q233
I236 D241 K242 L257 K258 Y259 A267 C268 F269 V270 N271 A291 N292 F293 E302 Y306 L311 L312 D315 V318 E319 A320 I321 N324 I325 F326 I329 V330 N331 C332 A333 I339 R344 L348 K349 V350 V353 V354 R355 V361 L368
G372 L373 P374 I375 L381 V389 T393 LYS LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	99.76Å 99.76Å 134.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.00 – 2.50 53.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (53.00-2.50) 99.8 (53.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev_3885	Depositor
R, R_{free}	0.240 , 0.269 0.241 , 0.270	Depositor DCC
R_{free} test set	2676 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l 0.156 for h,-h-k,-l 0.044 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20236	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: GDP, MG, CME

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	0.24	0/2245	0.42	0/3035
1	C	0.24	0/2233	0.42	0/3018
2	B	0.25	0/2905	0.41	0/3921
3	D	0.25	0/2711	0.41	0/3652
All	All	0.25	0/10094	0.41	0/13626

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 (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	2202	2244	2244	10	0
1	C	2194	2239	2239	7	0
2	B	2871	2916	2916	29	0
3	D	2691	2726	2726	22	0
4	B	56	30	24	1	0
5	B	1	0	0	0	0
6	A	28	0	0	0	0
6	B	8	0	0	0	0
6	C	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	5	0	0	0	0
All	All	10081	10155	10149	67	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 3.

The worst 5 of 67 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:C:34:GLN:N	1:C:34:GLN:OE1	2.06	0.89
3:D:46:LYS:N	3:D:104:MET:O	2.15	0.80
1:C:94:ASP:OD1	1:C:118:ARG:NH1	2.16	0.79
1:C:25:GLY:O	1:C:29:THR:HG23	1.84	0.77
1:C:7:ARG:NH2	1:C:198:ASP:OD1	2.19	0.75

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	292/305 (96%)	286 (98%)	4 (1%)	2 (1%)	22	39
1	C	291/305 (95%)	285 (98%)	5 (2%)	1 (0%)	41	61
2	B	373/395 (94%)	356 (95%)	14 (4%)	3 (1%)	19	35
3	D	343/395 (87%)	325 (95%)	17 (5%)	1 (0%)	41	61
All	All	1299/1400 (93%)	1252 (96%)	40 (3%)	7 (0%)	29	48

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	PRO

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Mol	Chain	Res	Type
2	B	74	GLU
2	B	138	VAL
1	C	237	PRO
1	A	271	ALA

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	236/238 (99%)	232 (98%)	4 (2%)	60	82
1	C	234/238 (98%)	229 (98%)	5 (2%)	53	78
2	B	308/319 (97%)	301 (98%)	7 (2%)	50	76
3	D	288/318 (91%)	286 (99%)	2 (1%)	84	94
All	All	1066/1113 (96%)	1048 (98%)	18 (2%)	60	82

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	118	ARG
3	D	344	ARG
3	D	326	PHE
2	B	293	PHE
1	C	34	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
3	CME	D	332	3	8,9,10	0.99	0	5,9,11	0.82	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
3	CME	D	332	3	-	3/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	332	CME	N-CA-CB-SG
3	D	332	CME	CZ-CE-SD-SG
3	D	332	CME	CE-SD-SG-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	332	CME	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is 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	B	401[B]	5	24,30,30	1.24	4 (16%)	30,47,47	1.11	2 (6%)
4	GDP	B	401[A]	-	24,30,30	1.23	3 (12%)	30,47,47	1.12	2 (6%)

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	B	401[B]	5	-	4/12/32/32	0/3/3/3
4	GDP	B	401[A]	-	-	2/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401[B]	GDP	C5-C6	-3.81	1.39	1.47
4	B	401[A]	GDP	C5-C6	-3.75	1.39	1.47
4	B	401[A]	GDP	C5-C4	-2.76	1.36	1.43
4	B	401[B]	GDP	C5-C4	-2.73	1.36	1.43
4	B	401[B]	GDP	C6-N1	-2.26	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	401[B]	GDP	C2-N1-C6	-4.12	117.52	125.10
4	B	401[A]	GDP	C2-N1-C6	-4.11	117.53	125.10
4	B	401[B]	GDP	C5-C6-N1	3.06	119.35	113.95
4	B	401[A]	GDP	C5-C6-N1	3.05	119.33	113.95

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401[A]	GDP	PA-O3A-PB-O3B
4	B	401[B]	GDP	PA-O3A-PB-O3B
4	B	401[B]	GDP	C5'-O5'-PA-O3A
4	B	401[A]	GDP	PA-O3A-PB-O2B
4	B	401[B]	GDP	PA-O3A-PB-O2B

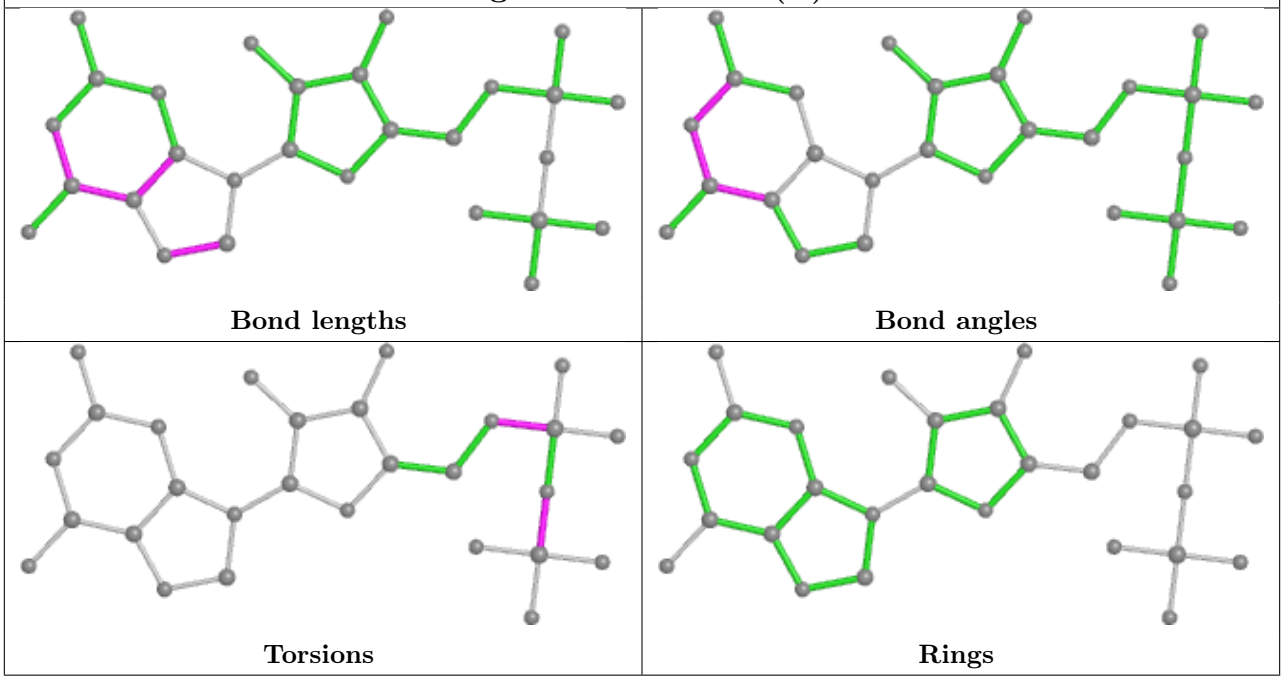
There are no ring outliers.

1 monomer is involved in 1 short contact:

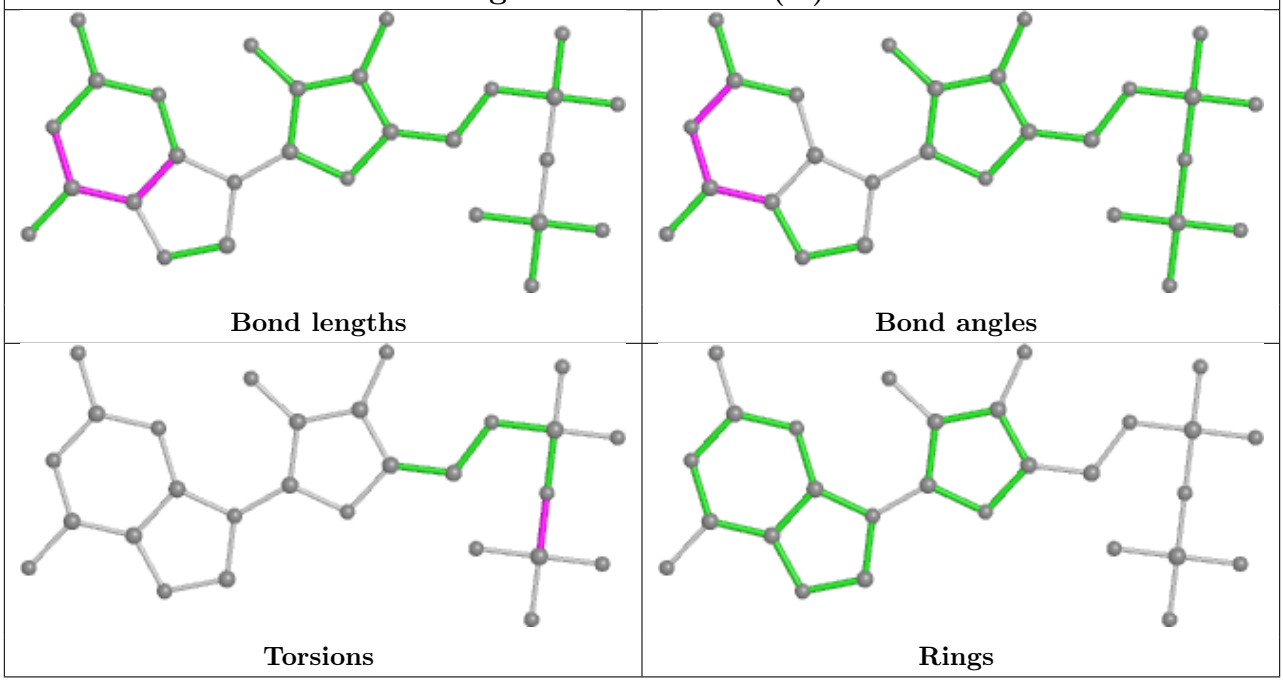
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401[B]	GDP	1	0

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 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 B 401 (B)



Ligand GDP B 401 (A)



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)

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	297/305 (97%)	0.48	6 (2%) 65 68	42, 69, 108, 146	0
1	C	297/305 (97%)	0.50	10 (3%) 45 48	46, 71, 113, 142	0
2	B	379/395 (95%)	1.11	72 (18%) 1 1	51, 104, 149, 225	0
3	D	353/395 (89%)	0.98	60 (16%) 1 1	54, 104, 142, 176	0
All	All	1326/1400 (94%)	0.80	148 (11%) 5 4	42, 87, 140, 225	0

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	329	ILE	7.8
3	D	140	ILE	7.2
3	D	41	LYS	6.2
2	B	76	VAL	6.1
2	B	43	ILE	6.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CME	D	332	10/11	0.87	0.14	99,119,144,144	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

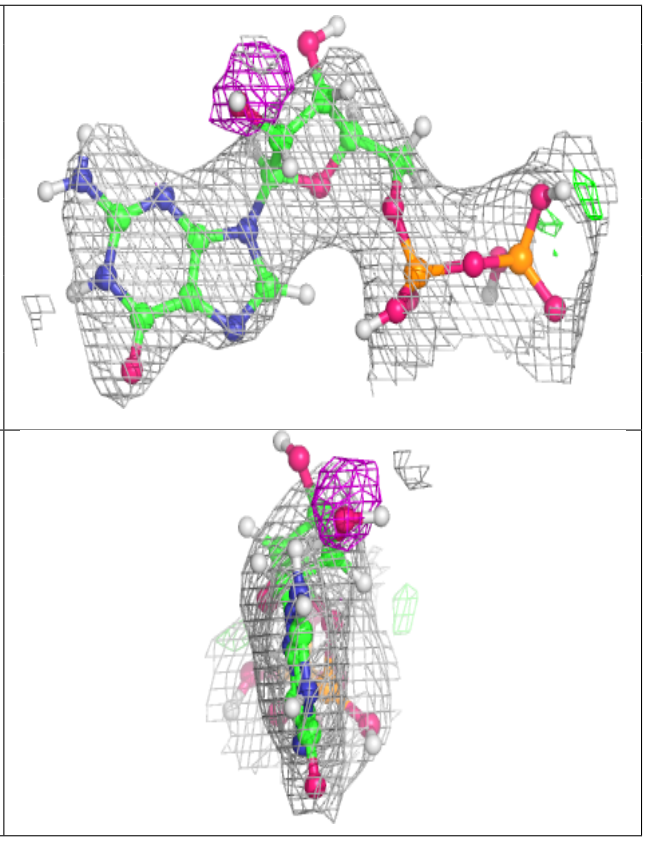
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GDP	B	401[A]	28/28	0.86	0.25	103,108,132,137	43
4	GDP	B	401[B]	28/28	0.86	0.25	104,108,132,134	43
5	MG	B	402	1/1	0.92	0.26	104,104,104,104	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.

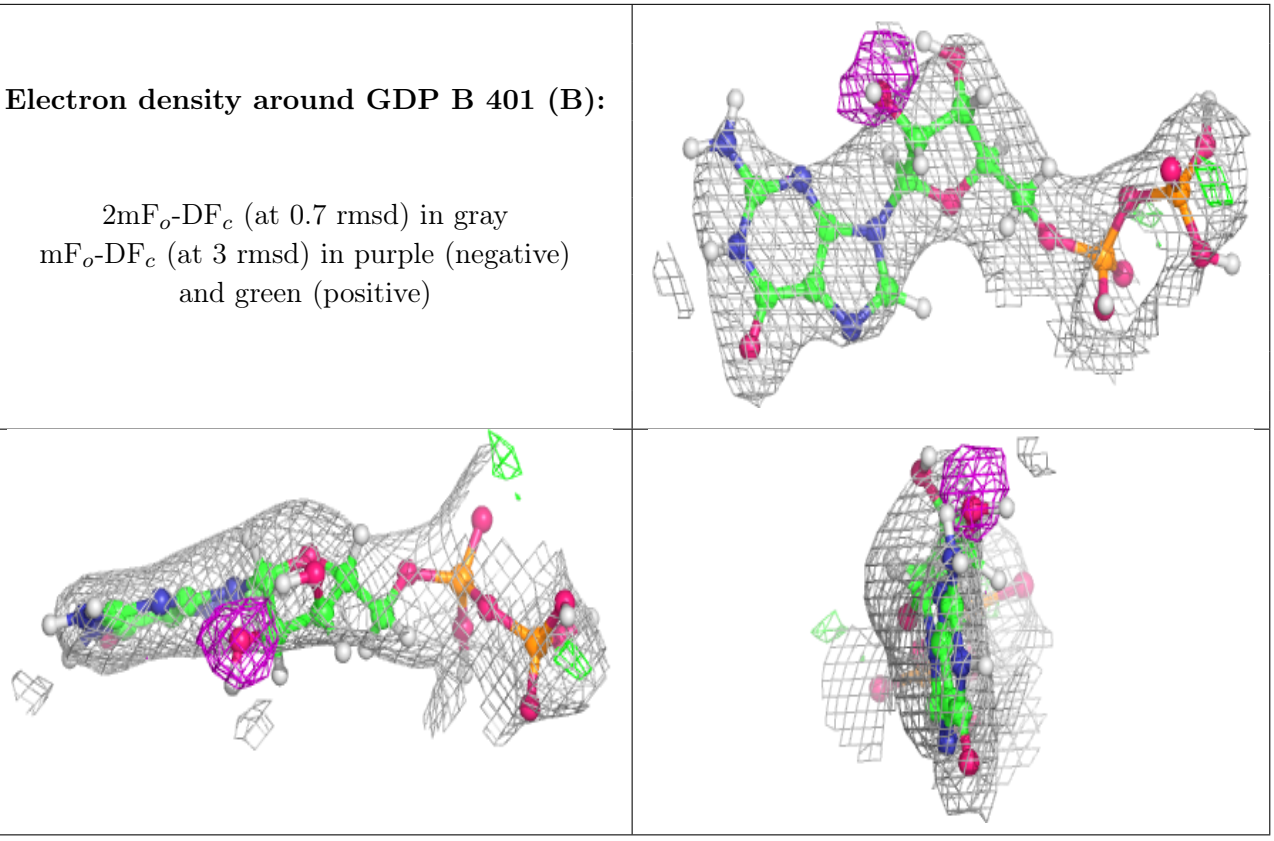
Electron density around GDP B 401 (A):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



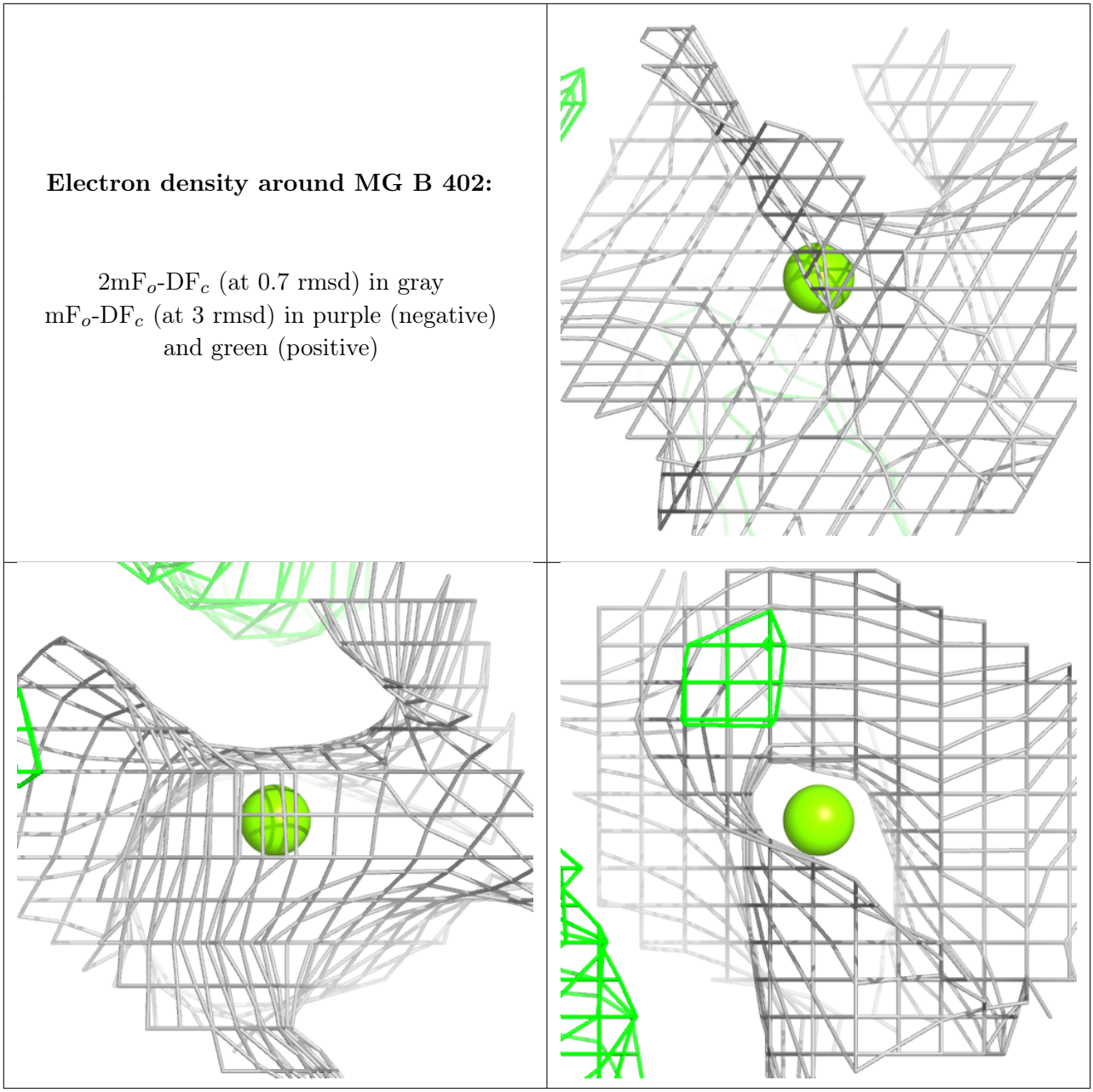
Electron density around GDP B 401 (B):

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



Electron density around MG B 402:

$2mF_o$-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.