



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:50 am BST

PDB ID : 5CK5  
Title : Signal recognition particle receptor SRb-GDP-Mg from *Chaetomium thermophilum*  
Authors : Jadhav, B.R.; Wild, K.; Sinning, I.  
Deposited on : 2015-07-15  
Resolution : 2.40 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

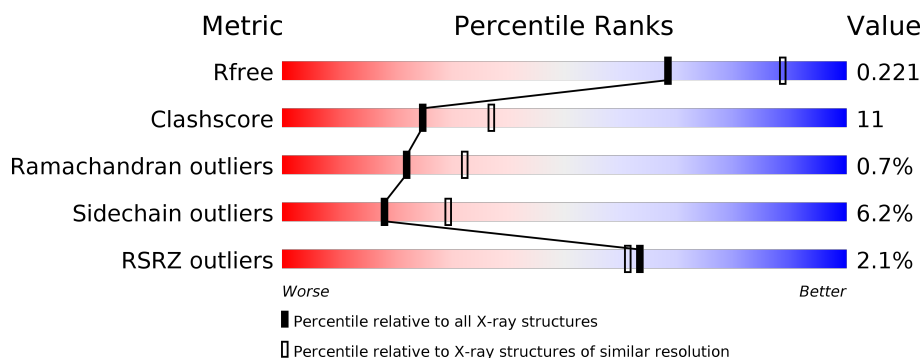
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	316	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>18%</div> <div>•</div> <div>30%</div> </div> </div>
1	B	316	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>19%</div> <div></div> <div>30%</div> </div> </div>
1	C	316	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>21%</div> <div>•</div> <div>32%</div> </div> </div>
1	D	316	<div> <div>3%</div> <div> <div></div> <div>45%</div> <div>17%</div> <div>•</div> <div>35%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6887 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 Putative signal recognition particle protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1713	1097	296	316	4			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1095	292	315	4			
1	C	215	Total	C	N	O	S	0	0	0
			1666	1066	290	306	4			
1	D	206	Total	C	N	O	S	0	0	0
			1594	1025	275	290	4			

There are 44 discrepancies between the modelled and reference sequences:

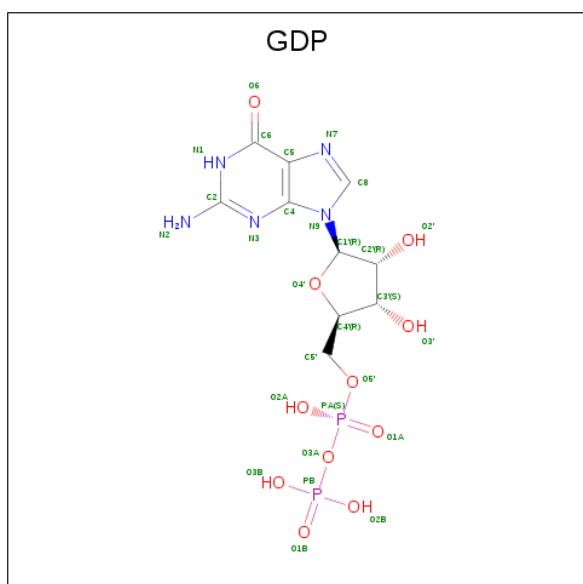
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	initiating methionine	UNP G0S401
A	33	LYS	-	expression tag	UNP G0S401
A	34	HIS	-	expression tag	UNP G0S401
A	35	HIS	-	expression tag	UNP G0S401
A	36	HIS	-	expression tag	UNP G0S401
A	37	HIS	-	expression tag	UNP G0S401
A	38	HIS	-	expression tag	UNP G0S401
A	39	HIS	-	expression tag	UNP G0S401
A	40	PRO	-	expression tag	UNP G0S401
A	41	MET	-	expression tag	UNP G0S401
A	42	GLY	-	expression tag	UNP G0S401
B	32	MET	-	initiating methionine	UNP G0S401
B	33	LYS	-	expression tag	UNP G0S401
B	34	HIS	-	expression tag	UNP G0S401
B	35	HIS	-	expression tag	UNP G0S401
B	36	HIS	-	expression tag	UNP G0S401
B	37	HIS	-	expression tag	UNP G0S401
B	38	HIS	-	expression tag	UNP G0S401
B	39	HIS	-	expression tag	UNP G0S401
B	40	PRO	-	expression tag	UNP G0S401
B	41	MET	-	expression tag	UNP G0S401

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Chain	Residue	Modelled	Actual	Comment	Reference
B	42	GLY	-	expression tag	UNP G0S401
C	32	MET	-	initiating methionine	UNP G0S401
C	33	LYS	-	expression tag	UNP G0S401
C	34	HIS	-	expression tag	UNP G0S401
C	35	HIS	-	expression tag	UNP G0S401
C	36	HIS	-	expression tag	UNP G0S401
C	37	HIS	-	expression tag	UNP G0S401
C	38	HIS	-	expression tag	UNP G0S401
C	39	HIS	-	expression tag	UNP G0S401
C	40	PRO	-	expression tag	UNP G0S401
C	41	MET	-	expression tag	UNP G0S401
C	42	GLY	-	expression tag	UNP G0S401
D	32	MET	-	initiating methionine	UNP G0S401
D	33	LYS	-	expression tag	UNP G0S401
D	34	HIS	-	expression tag	UNP G0S401
D	35	HIS	-	expression tag	UNP G0S401
D	36	HIS	-	expression tag	UNP G0S401
D	37	HIS	-	expression tag	UNP G0S401
D	38	HIS	-	expression tag	UNP G0S401
D	39	HIS	-	expression tag	UNP G0S401
D	40	PRO	-	expression tag	UNP G0S401
D	41	MET	-	expression tag	UNP G0S401
D	42	GLY	-	expression tag	UNP G0S401

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	26	Total	O	0	0
			26	26		
4	C	23	Total	O	0	0
			23	23		
4	D	15	Total	O	0	0
			15	15		

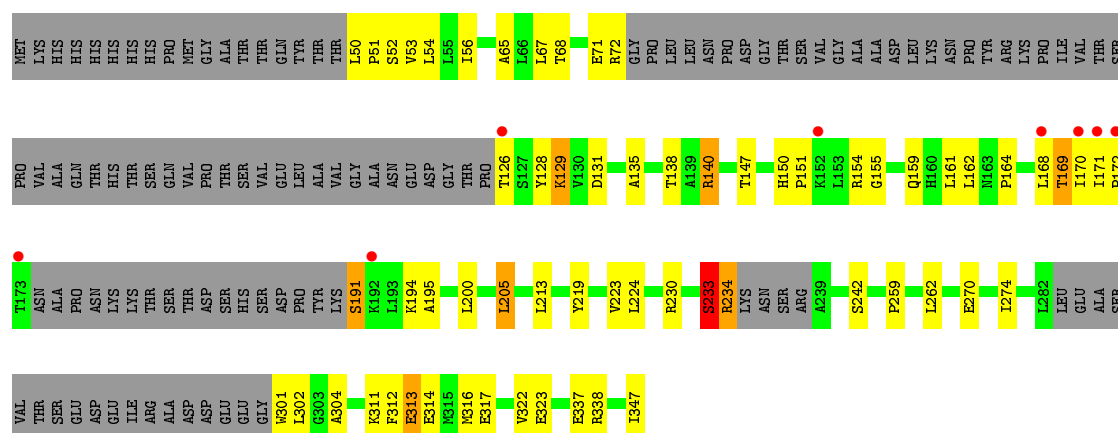
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $\text{RSRZ} > 2$ ). 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.

- [illegible]

- Chain B:
- 
- 51% 19% 30%
- 1%
- AMINO ACID
- ASP  
SER  
GLU  
E299  
G300  
A304  
S307  
K311  
F312  
E313  
E314  
G327  
W328  
V329  
D332  
G333  
P334  
E337  
R338  
W339  
W340  
R341  
E345  
R346  
I347
- HIS  
THR  
SER  
GLN  
VAL  
PRO  
THR  
SER  
VAL  
GLU  
LEU  
ALA  
VAL  
GLY  
ALA  
ASN  
GLU  
ASP  
GLY  
THR  
PRO  
T126  
S127  
Y128  
G136  
R140  
D146  
T147  
H150  
P151  
K152  
L153  
R154  
G155  
T156  
T157  
L158  
L161  
L162  
N163  
P164  
L168  
T169  
I170  
H174  
ALA  
PRO  
ASN  
LYS  
THR  
LYS  
THR  
ILE  
VAL  
SER  
THR
- ASP  
SER  
GLU  
E299  
G300  
A304  
S307  
K311  
F312  
E313  
E314  
G327  
W328  
V329  
D332  
G333  
P334  
E337  
R338  
W339  
W340  
R341  
E345  
R346  
I347
- HIS  
THR  
SER  
GLN  
VAL  
PRO  
THR  
SER  
VAL  
GLU  
LEU  
ALA  
VAL  
GLY  
ALA  
ASN  
GLU  
ASP  
GLY  
THR  
PRO  
T126  
S127  
Y128  
G136  
R140  
D146  
T147  
H150  
P151  
K152  
L153  
R154  
G155  
T156  
T157  
L158  
L161  
L162  
N163  
P164  
L168  
T169  
I170  
H174  
ALA  
PRO  
ASN  
LYS  
THR  
LYS  
THR  
ILE  
VAL  
SER  
THR

- Chain C:  46% 21% 32%

- Molecule 1: Putative signal recognition particle protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.10Å 137.97Å 64.31Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	64.20 – 2.40 64.21 – 2.38	Depositor EDS
% Data completeness (in resolution range)	95.2 (64.20-2.40) 92.2 (64.21-2.38)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, $R_{free}$	0.186 , 0.223 0.184 , 0.221	Depositor DCC
$R_{free}$ test set	2139 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.387 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: GDP, MG

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	0.48	0/1747	0.68	1/2360 (0.0%)
1	B	0.54	0/1739	0.64	0/2350
1	C	0.46	0/1698	0.69	0/2292
1	D	0.45	0/1624	0.67	0/2193
All	All	0.49	0/6808	0.67	1/9195 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	LEU	CA-CB-CG	6.25	129.69	115.30

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	1713	0	1747	39	1
1	B	1706	0	1732	35	0
1	C	1666	0	1704	41	0
1	D	1594	0	1637	35	0
2	A	28	0	12	3	0
2	B	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	12	1	0
2	D	28	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	28	0	0	1	0
4	B	26	0	0	0	0
4	C	23	0	0	3	1
4	D	15	0	0	3	0
All	All	6887	0	6868	147	1

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 11.

All (147) 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:50:LEU:O	1:B:191:SER:OG	1.91	0.87
1:C:140:ARG:NH2	4:C:501:HOH:O	2.10	0.83
1:B:200:LEU:HD13	1:B:205:LEU:HD13	1.62	0.80
1:C:71:GLU:HA	1:C:136:GLY:HA3	1.67	0.76
1:C:259:PRO:HG2	1:C:262:LEU:HD13	1.72	0.72
1:A:243:ILE:O	4:A:501:HOH:O	2.09	0.71
1:C:49:THR:HG22	1:C:50:LEU:H	1.55	0.70
1:A:49:THR:HG22	1:A:50:LEU:H	1.58	0.68
1:A:170:ILE:HG12	1:A:171:ILE:N	2.08	0.68
1:C:317:GLU:OE1	4:C:502:HOH:O	2.12	0.67
1:A:130:VAL:HG22	1:A:170:ILE:HG13	1.77	0.67
1:A:224:LEU:HB2	1:A:302:LEU:HD11	1.77	0.66
1:B:228:GLN:O	1:B:232:HIS:ND1	2.29	0.64
1:B:54:LEU:HB2	1:B:193:LEU:HD11	1.80	0.64
1:A:327:GLY:HA2	1:A:334:PRO:HG2	1.80	0.63
1:B:304:ALA:HB3	1:B:307:SER:HB2	1.81	0.62
1:A:213:LEU:HG	1:A:270:GLU:HG3	1.81	0.62
1:B:70:PHE:O	1:B:136:GLY:HA3	2.00	0.62
1:D:301:TRP:NE1	1:D:304:ALA:O	2.26	0.62
1:D:301:TRP:N	4:D:502:HOH:O	2.33	0.61
1:D:140:ARG:NH2	1:D:337:GLU:OE1	2.31	0.60
1:C:259:PRO:HD2	1:C:262:LEU:HD22	1.82	0.60
1:A:132:LEU:HD23	1:A:132:LEU:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:PRO:HG2	1:D:262:LEU:HD13	1.84	0.60
1:C:54:LEU:HD21	1:C:168:LEU:HD11	1.83	0.60
1:A:170:ILE:HG23	1:A:189:TYR:HB2	1.85	0.59
1:B:67:LEU:HD22	1:B:146:ASP:HB2	1.83	0.58
1:B:341:ARG:O	1:B:345:GLU:HG3	2.02	0.58
1:B:273:ARG:O	1:B:277:THR:HG22	2.04	0.57
1:C:171:ILE:HG23	1:C:186:SER:OG	2.04	0.57
1:D:205:LEU:HD11	1:D:213:LEU:HD13	1.86	0.57
1:A:196:VAL:HB	1:A:245:VAL:HG22	1.87	0.57
1:D:230:ARG:O	1:D:233:SER:HB2	2.05	0.57
1:D:128:TYR:N	1:D:169:THR:O	2.37	0.56
1:A:50:LEU:O	1:A:191:SER:OG	2.24	0.55
1:B:151:PRO:HA	1:B:154:ARG:HD2	1.88	0.55
1:D:54:LEU:HD13	1:D:168:LEU:HD21	1.88	0.55
1:B:327:GLY:HA2	1:B:334:PRO:HG2	1.88	0.55
1:A:166:PRO:HB2	1:A:193:LEU:HB3	1.89	0.55
1:D:71:GLU:O	1:D:135:ALA:HB3	2.07	0.54
1:A:150:HIS:HE1	1:A:152:LYS:HG3	1.72	0.54
1:C:246:LEU:HB2	1:C:342:TRP:CZ3	2.42	0.54
1:D:311:LYS:HB3	1:D:313:GLU:HG2	1.89	0.54
1:D:150:HIS:CG	1:D:151:PRO:HD2	2.43	0.53
1:C:270:GLU:O	1:C:274:ILE:HG13	2.09	0.53
1:B:56:ILE:HG22	1:B:147:THR:HG21	1.91	0.53
1:B:70:PHE:CE1	1:B:140:ARG:HD2	2.43	0.53
1:C:233:SER:O	1:C:237:SER:OG	2.12	0.53
1:A:259:PRO:HG2	1:A:262:LEU:HD13	1.92	0.52
1:A:274:ILE:O	1:A:278:ARG:HG3	2.08	0.52
1:C:272:GLY:HA2	1:C:275:ARG:HG2	1.92	0.52
1:D:270:GLU:O	1:D:274:ILE:HG13	2.10	0.52
1:A:323:GLU:OE1	1:A:342:TRP:NE1	2.29	0.52
1:B:270:GLU:O	1:B:274:ILE:HG13	2.10	0.52
1:B:68:THR:O	1:B:72:ARG:HG3	2.10	0.52
1:C:211:ASP:O	1:C:215:GLN:HG3	2.10	0.52
1:C:215:GLN:O	1:C:218:SER:OG	2.29	0.51
1:A:130:VAL:O	1:A:172:PRO:HA	2.11	0.50
1:B:126:THR:HG21	1:B:156:THR:HB	1.93	0.50
1:D:164:PRO:HG3	1:D:233:SER:OG	2.11	0.50
1:D:200:LEU:HD13	1:D:205:LEU:HD23	1.94	0.50
1:A:150:HIS:CE1	1:A:152:LYS:HG3	2.46	0.50
1:A:273:ARG:HG3	1:B:333:GLY:C	2.32	0.50
1:A:311:LYS:O	1:A:314:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLY:O	1:D:159:GLN:N	2.43	0.49
1:C:129:LYS:HG2	1:C:171:ILE:HD11	1.95	0.49
1:C:232:HIS:O	1:C:234:ARG:HG3	2.12	0.49
1:C:342:TRP:O	1:C:346:ARG:HD2	2.13	0.48
1:D:322:VAL:O	4:D:501:HOH:O	2.20	0.48
1:B:158:LEU:HD23	1:B:161:LEU:HD12	1.96	0.48
1:B:163:ASN:HA	1:B:164:PRO:HD3	1.73	0.48
1:B:225:LEU:HD21	1:B:300:GLY:HA2	1.95	0.47
1:D:65:ALA:O	1:D:68:THR:HG22	2.13	0.47
1:C:154:ARG:O	1:C:157:THR:HB	2.14	0.47
1:C:270:GLU:CD	1:C:273:ARG:HE	2.17	0.47
1:C:315:MET:HB3	1:C:320:MET:HG3	1.95	0.47
1:C:337:GLU:HB2	4:C:513:HOH:O	2.14	0.47
1:A:54:LEU:HA	1:A:54:LEU:HD12	1.72	0.47
1:D:233:SER:C	1:D:234:ARG:HD2	2.35	0.47
1:A:273:ARG:O	1:A:277:THR:OG1	2.32	0.47
1:D:219:TYR:O	1:D:223:VAL:HG23	2.14	0.47
1:D:312:PHE:HB3	1:D:322:VAL:HG13	1.97	0.47
1:D:52:SER:HB2	4:D:506:HOH:O	2.16	0.46
1:C:70:PHE:CE1	1:C:140:ARG:HD2	2.50	0.46
1:D:224:LEU:HB2	1:D:302:LEU:HD11	1.98	0.46
1:D:53:VAL:HG22	1:D:195:ALA:HB3	1.97	0.46
1:C:278:ARG:C	1:C:280:LYS:H	2.19	0.46
1:D:191:SER:OG	1:D:191:SER:O	2.33	0.46
1:C:64:THR:OG1	2:C:401:GDP:O1B	2.34	0.45
1:B:311:LYS:O	1:B:314:GLU:HG2	2.16	0.45
1:C:54:LEU:HD23	1:C:193:LEU:HD13	1.97	0.45
1:D:161:LEU:O	1:D:230:ARG:HB2	2.16	0.45
1:B:232:HIS:O	1:B:233:SER:OG	2.28	0.45
1:D:129:LYS:HA	1:D:171:ILE:HG13	1.99	0.45
1:A:56:ILE:HG13	1:A:198:PHE:HD1	1.82	0.45
1:B:150:HIS:ND1	1:B:152:LYS:HB2	2.31	0.45
1:A:327:GLY:HA2	1:A:334:PRO:CG	2.46	0.45
1:A:63:LYS:HG3	2:A:401:GDP:O3B	2.17	0.45
1:A:276:LYS:HE3	1:B:332:ASP:O	2.17	0.44
1:A:49:THR:HG22	1:A:50:LEU:N	2.30	0.44
1:B:158:LEU:HD23	1:B:158:LEU:HA	1.82	0.44
1:C:247:ILE:HB	1:C:324:VAL:HG22	1.98	0.44
1:C:341:ARG:O	1:C:345:GLU:HG3	2.17	0.44
1:A:159:GLN:HA	1:A:162:LEU:HD22	2.00	0.44
1:A:270:GLU:O	1:A:274:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ARG:O	1:A:345:GLU:HB2	2.18	0.44
1:B:311:LYS:HB3	1:B:313:GLU:OE1	2.18	0.44
1:D:311:LYS:O	1:D:314:GLU:HG2	2.17	0.44
1:A:301:TRP:NE1	1:A:304:ALA:O	2.45	0.43
1:D:128:TYR:HB2	1:D:170:ILE:HD13	2.01	0.43
1:C:163:ASN:O	1:C:166:PRO:HG3	2.18	0.43
1:A:312:PHE:HB3	1:A:322:VAL:HG13	2.00	0.43
1:C:221:TYR:HE2	1:C:275:ARG:HB3	1.83	0.43
1:D:56:ILE:HG22	1:D:147:THR:HG21	2.01	0.42
1:D:233:SER:HB3	1:D:234:ARG:H	1.58	0.42
1:A:301:TRP:HE1	1:A:304:ALA:C	2.22	0.42
1:C:170:ILE:HB	1:C:171:ILE:H	1.62	0.42
1:C:220:LEU:O	1:C:224:LEU:HG	2.19	0.42
1:A:330:ILE:HG12	2:A:401:GDP:C6	2.55	0.42
1:A:209:ASP:O	1:B:341:ARG:NH2	2.51	0.41
1:A:336:ALA:O	1:A:339:TRP:HB2	2.19	0.41
1:B:333:GLY:HA3	1:B:334:PRO:HD2	1.87	0.41
1:C:52:SER:HB2	1:C:145:ILE:CD1	2.49	0.41
1:D:194:LYS:HB3	1:D:347:ILE:HG22	2.01	0.41
1:B:128:TYR:CE1	1:B:168:LEU:HD22	2.55	0.41
1:B:66:LEU:HD11	1:B:340:TRP:CH2	2.55	0.41
1:C:274:ILE:O	1:C:278:ARG:HG3	2.20	0.41
1:C:245:VAL:HB	1:C:322:VAL:HG13	2.02	0.41
1:C:63:LYS:HA	1:C:199:LEU:HD23	2.02	0.41
1:B:248:ALA:HB1	1:B:339:TRP:CZ2	2.55	0.41
1:C:130:VAL:HG21	1:C:143:LEU:HD22	2.02	0.41
1:C:279:GLN:O	1:C:281:GLY:N	2.54	0.41
1:C:71:GLU:O	1:C:135:ALA:HB3	2.21	0.41
1:C:209:ASP:OD1	1:C:210:GLY:N	2.54	0.41
1:D:50:LEU:HB2	1:D:51:PRO:HD2	2.03	0.41
1:B:151:PRO:HA	1:B:154:ARG:CD	2.49	0.41
1:A:251:LYS:NZ	2:A:401:GDP:O4'	2.47	0.40
1:B:168:LEU:HA	1:B:168:LEU:HD23	1.92	0.40
1:D:67:LEU:O	1:D:71:GLU:HG3	2.21	0.40
1:B:205:LEU:HD22	1:B:263:VAL:HG22	2.03	0.40
1:A:201:ASP:CG	1:A:251:LYS:HD2	2.42	0.40
1:B:170:ILE:HG23	1:B:189:TYR:HB2	2.03	0.40
1:C:219:TYR:O	1:C:223:VAL:HG23	2.22	0.40
1:D:151:PRO:HA	1:D:154:ARG:HD2	2.03	0.40
1:C:140:ARG:HB3	1:C:142:PHE:CE1	2.56	0.40
1:D:154:ARG:HG2	1:D:219:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:THR:O	1:A:72:ARG:N	2.41	0.40

All (1) 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)
1:A:64:THR:OG1	4:C:502:HOH:O[2_544]	2.14	0.06

## 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	213/316 (67%)	206 (97%)	5 (2%)	2 (1%)	17	25
1	B	211/316 (67%)	207 (98%)	4 (2%)	0	100	100
1	C	207/316 (66%)	197 (95%)	8 (4%)	2 (1%)	15	23
1	D	196/316 (62%)	192 (98%)	2 (1%)	2 (1%)	15	23
All	All	827/1264 (65%)	802 (97%)	19 (2%)	6 (1%)	22	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ALA
1	D	233	SER
1	C	279	GLN
1	A	233	SER
1	D	172	PRO
1	C	170	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/264 (69%)	175 (96%)	8 (4%)	28	45
1	B	181/264 (69%)	173 (96%)	8 (4%)	28	45
1	C	178/264 (67%)	168 (94%)	10 (6%)	21	34
1	D	170/264 (64%)	152 (89%)	18 (11%)	6	9
All	All	712/1056 (67%)	668 (94%)	44 (6%)	18	29

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	A	156	THR
1	A	162	LEU
1	A	170	ILE
1	A	205	LEU
1	A	236	ASN
1	A	242	SER
1	A	277	THR
1	B	162	LEU
1	B	207	ASP
1	B	209	ASP
1	B	219	TYR
1	B	256	THR
1	B	277	THR
1	B	329	VAL
1	B	337	GLU
1	C	150	HIS
1	C	170	ILE
1	C	193	LEU
1	C	235	LYS
1	C	236	ASN
1	C	256	THR
1	C	316	MET
1	C	317	GLU

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Mol	Chain	Res	Type
1	C	322	VAL
1	C	323	GLU
1	D	72	ARG
1	D	126	THR
1	D	129	LYS
1	D	131	ASP
1	D	138	THR
1	D	140	ARG
1	D	162	LEU
1	D	169	THR
1	D	191	SER
1	D	205	LEU
1	D	233	SER
1	D	234	ARG
1	D	242	SER
1	D	313	GLU
1	D	316	MET
1	D	317	GLU
1	D	323	GLU
1	D	338	ARG

Some 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](#)

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
2	GDP	C	401	3	24,30,30	1.11	2 (8%)	31,47,47	1.94	8 (25%)
2	GDP	A	401	3	24,30,30	1.16	1 (4%)	31,47,47	2.05	7 (22%)
2	GDP	D	401	3	24,30,30	1.14	2 (8%)	31,47,47	1.92	8 (25%)
2	GDP	B	401	3	24,30,30	1.22	2 (8%)	31,47,47	1.91	9 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	C	401	3	-	2/12/32/32	0/3/3/3
2	GDP	A	401	3	-	1/12/32/32	0/3/3/3
2	GDP	D	401	3	-	3/12/32/32	0/3/3/3
2	GDP	B	401	3	-	5/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GDP	C6-C5	4.24	1.48	1.41
2	D	401	GDP	C6-C5	3.83	1.48	1.41
2	C	401	GDP	C6-C5	3.75	1.47	1.41
2	A	401	GDP	C6-C5	3.68	1.47	1.41
2	B	401	GDP	C5-C4	2.65	1.47	1.40
2	C	401	GDP	C5-C4	2.50	1.47	1.40
2	D	401	GDP	C5-C4	2.26	1.46	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	GDP	C2-N3-C4	5.50	121.63	115.36
2	D	401	GDP	C2-N3-C4	5.36	121.48	115.36
2	A	401	GDP	C6-C5-C4	-4.97	116.06	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GDP	C2-N3-C4	4.40	120.39	115.36
2	A	401	GDP	C6-N1-C2	4.33	122.81	115.93
2	A	401	GDP	C2-N3-C4	4.18	120.13	115.36
2	B	401	GDP	C5-C6-N1	-4.18	117.72	123.43
2	A	401	GDP	C5-C6-N1	-4.06	117.88	123.43
2	B	401	GDP	C6-N1-C2	3.84	122.04	115.93
2	D	401	GDP	PA-O3A-PB	-3.77	119.90	132.83
2	C	401	GDP	PA-O3A-PB	-3.71	120.11	132.83
2	C	401	GDP	C6-C5-C4	-3.45	117.51	120.80
2	D	401	GDP	C6-N1-C2	3.36	121.27	115.93
2	B	401	GDP	PA-O3A-PB	-3.33	121.39	132.83
2	D	401	GDP	C6-C5-C4	-3.33	117.62	120.80
2	A	401	GDP	C4-C5-N7	-3.29	105.97	109.40
2	C	401	GDP	C6-N1-C2	3.28	121.13	115.93
2	B	401	GDP	C6-C5-C4	-3.24	117.70	120.80
2	A	401	GDP	N3-C2-N1	-3.17	123.00	127.22
2	C	401	GDP	C3'-C2'-C1'	3.16	105.74	100.98
2	C	401	GDP	N3-C2-N1	-3.09	123.11	127.22
2	C	401	GDP	C5-C6-N1	-3.04	119.28	123.43
2	D	401	GDP	C5-C6-N1	-2.99	119.34	123.43
2	D	401	GDP	C4-C5-N7	-2.97	106.30	109.40
2	D	401	GDP	N3-C2-N1	-2.89	123.36	127.22
2	B	401	GDP	O4'-C1'-C2'	-2.67	103.03	106.93
2	B	401	GDP	C4-C5-N7	-2.66	106.62	109.40
2	B	401	GDP	N3-C2-N1	-2.62	123.73	127.22
2	A	401	GDP	C1'-N9-C4	-2.36	122.50	126.64
2	B	401	GDP	O2B-PB-O3A	2.30	112.35	104.64
2	C	401	GDP	C4-C5-N7	-2.26	107.04	109.40
2	D	401	GDP	C3'-C2'-C1'	2.20	104.30	100.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GDP	O4'-C4'-C5'-O5'
2	D	401	GDP	C5'-O5'-PA-O1A
2	B	401	GDP	C5'-O5'-PA-O3A
2	D	401	GDP	C5'-O5'-PA-O3A
2	B	401	GDP	C5'-O5'-PA-O1A
2	B	401	GDP	C5'-O5'-PA-O2A
2	D	401	GDP	C5'-O5'-PA-O2A
2	C	401	GDP	O4'-C4'-C5'-O5'

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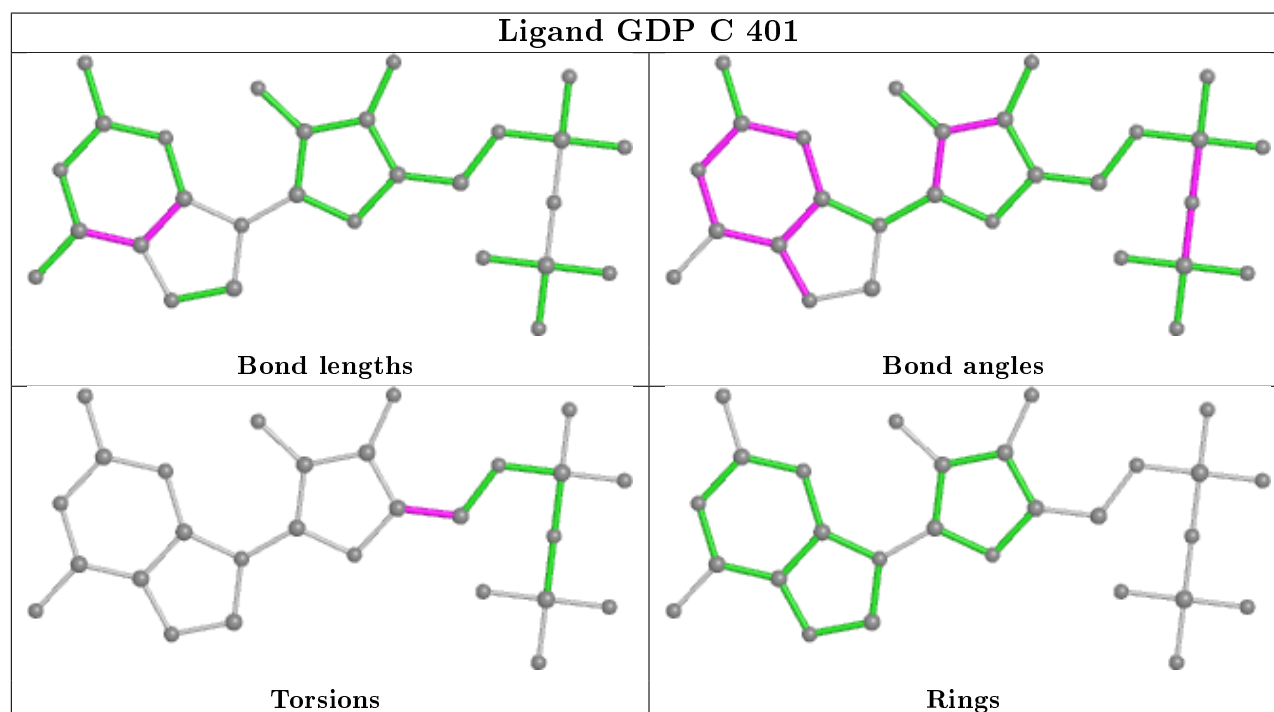
Mol	Chain	Res	Type	Atoms
2	C	401	GDP	C3'-C4'-C5'-O5'
2	B	401	GDP	PB-O3A-PA-O1A
2	B	401	GDP	PB-O3A-PA-O2A

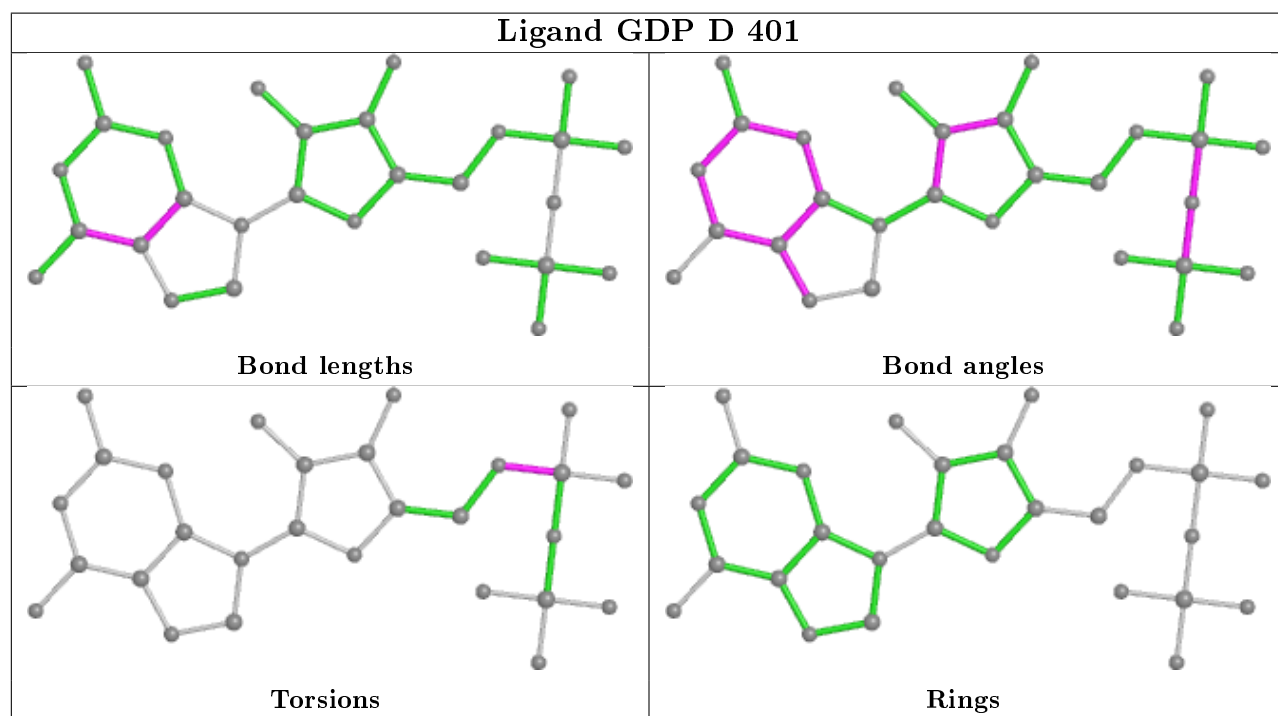
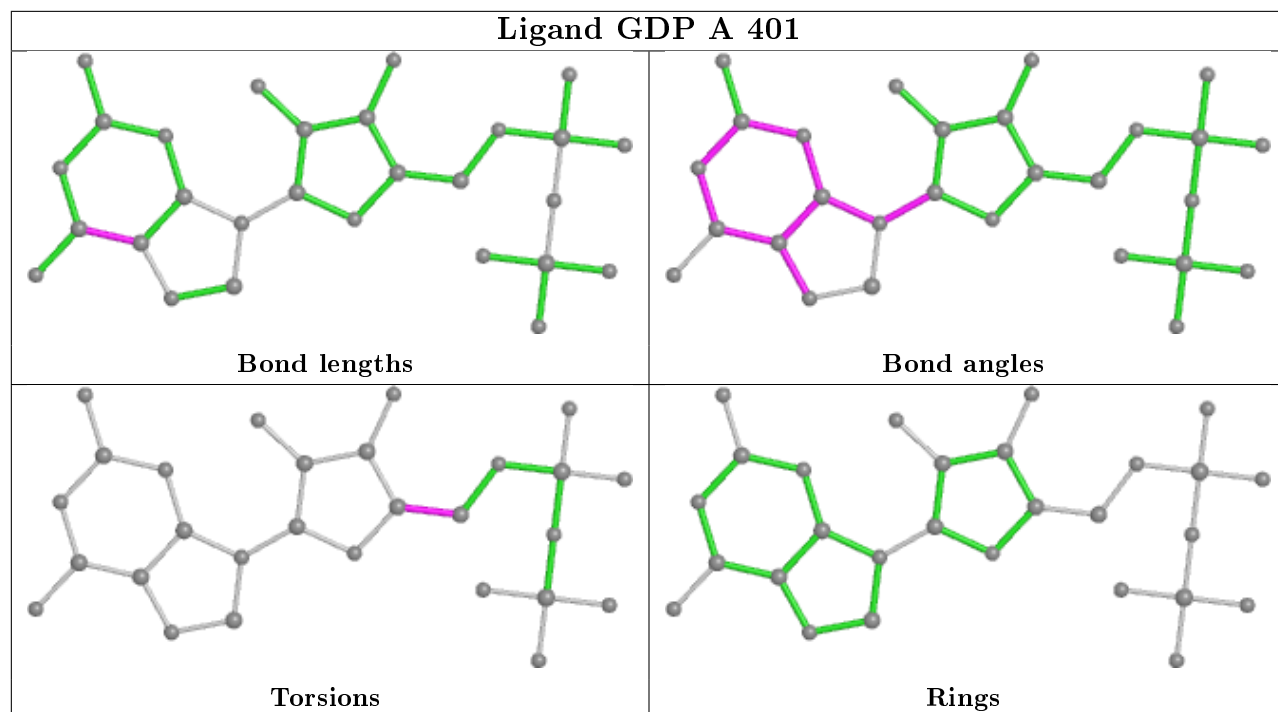
There are no ring outliers.

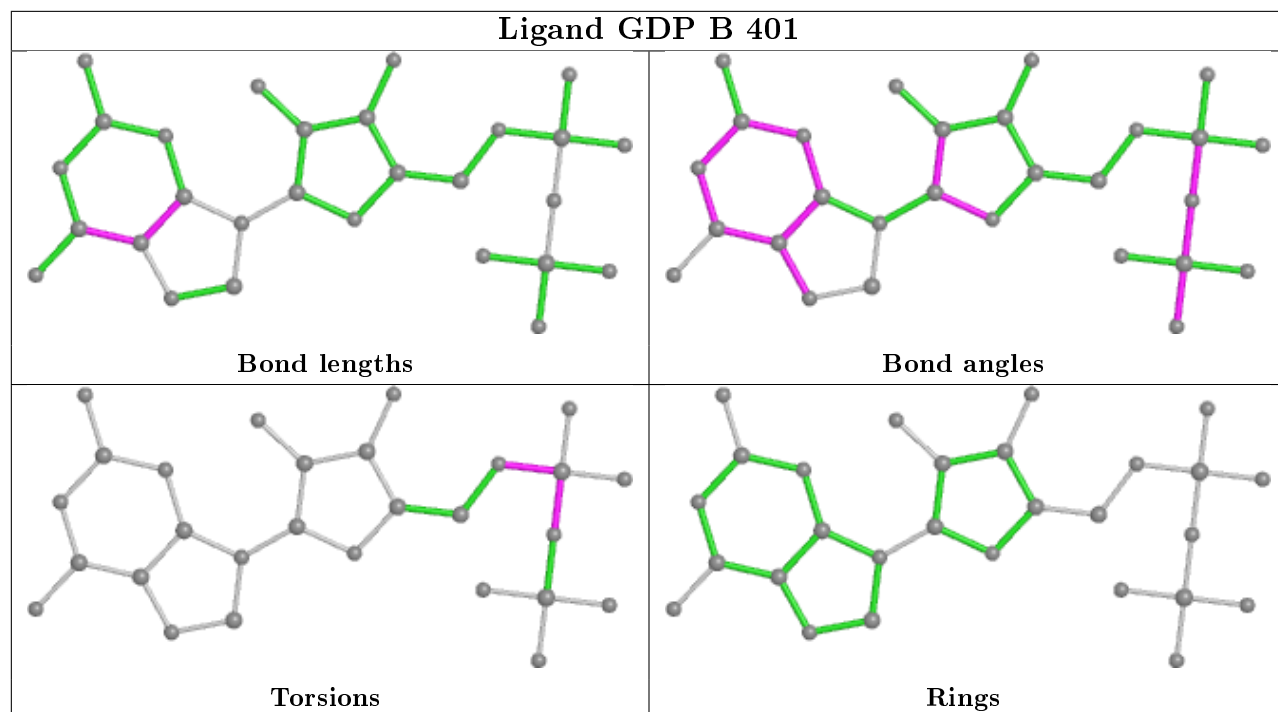
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	GDP	1	0
2	A	401	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	221/316 (69%)	-0.12	5 (2%) 60 58	26, 48, 90, 125	0
1	B	221/316 (69%)	-0.22	2 (0%) 84 82	25, 45, 79, 127	0
1	C	215/316 (68%)	-0.06	3 (1%) 75 73	31, 57, 98, 143	0
1	D	206/316 (65%)	0.07	8 (3%) 39 38	33, 57, 106, 137	0
All	All	863/1264 (68%)	-0.08	18 (2%) 63 61	25, 51, 98, 143	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	ALA	6.8
1	A	47	TYR	6.0
1	B	174	ASN	4.0
1	B	186	SER	3.6
1	D	192	LYS	3.2
1	D	172	PRO	3.2
1	D	170	ILE	2.9
1	D	173	THR	2.9
1	A	189	TYR	2.8
1	D	171	ILE	2.8
1	D	152	LYS	2.7
1	D	168	LEU	2.5
1	D	126	THR	2.4
1	C	127	SER	2.2
1	C	135	ALA	2.1
1	A	186	SER	2.1
1	A	134	ALA	2.0
1	A	132	LEU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

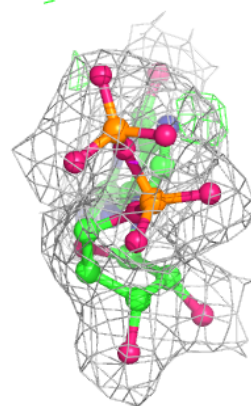
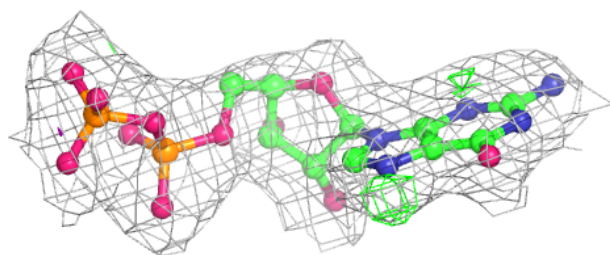
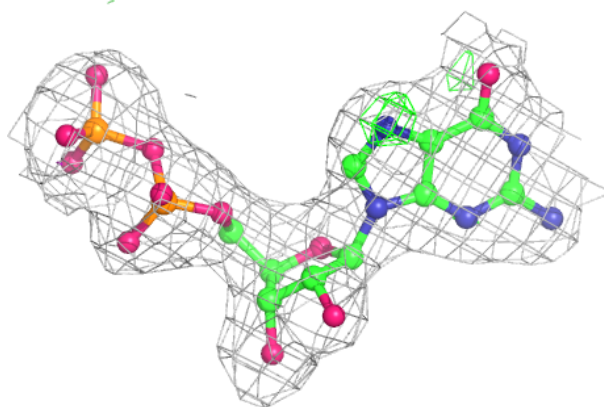
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	402	1/1	0.95	0.12	25,25,25,25	0
3	MG	D	402	1/1	0.95	0.06	69,69,69,69	0
3	MG	C	402	1/1	0.96	0.12	40,40,40,40	0
2	GDP	C	401	28/28	0.97	0.12	33,48,58,65	0
2	GDP	D	401	28/28	0.97	0.11	32,46,56,58	0
2	GDP	B	401	28/28	0.98	0.13	18,30,37,47	0
2	GDP	A	401	28/28	0.98	0.14	26,37,45,50	0
3	MG	B	402	1/1	0.99	0.10	22,22,22,22	0

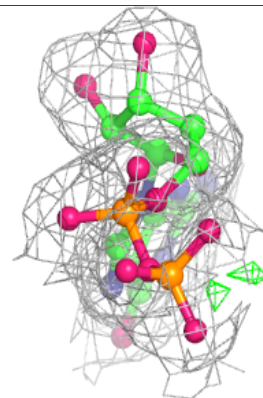
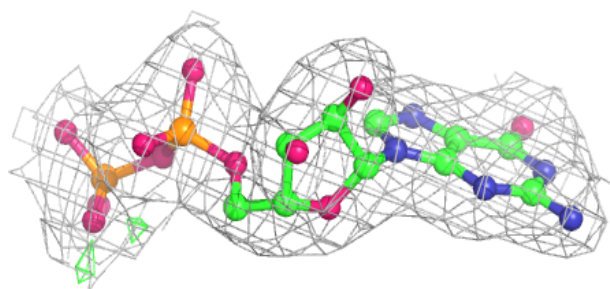
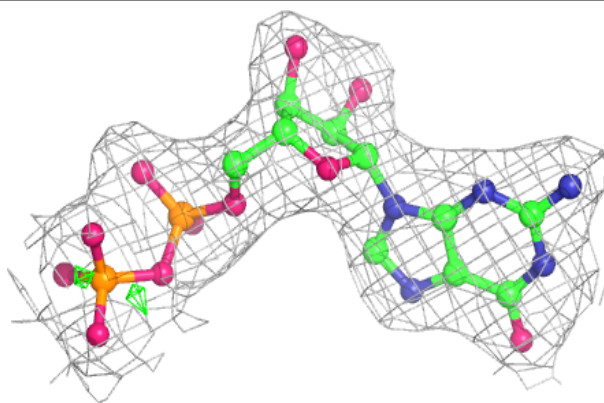
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GDP C 401:**

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

**Electron density around GDP D 401:**

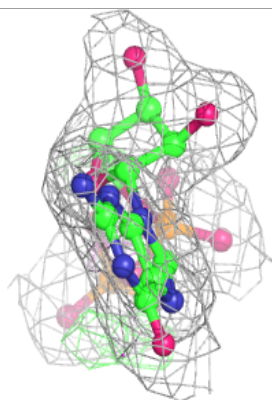
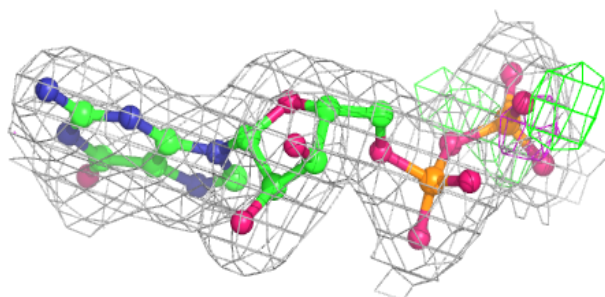
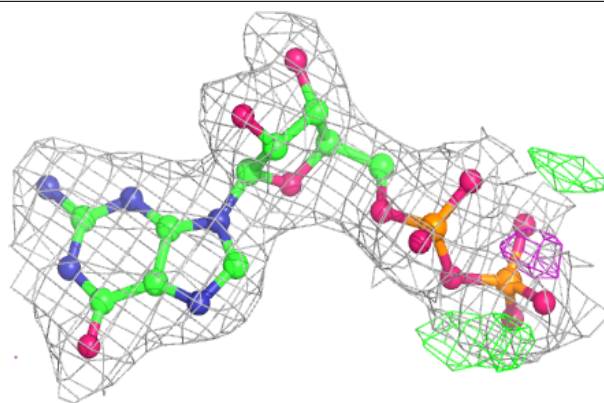
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



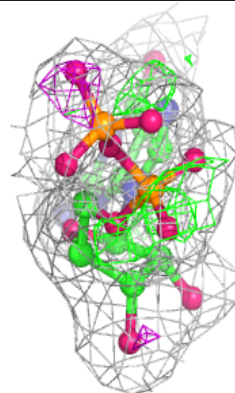
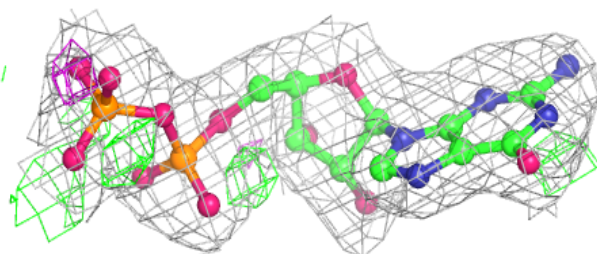
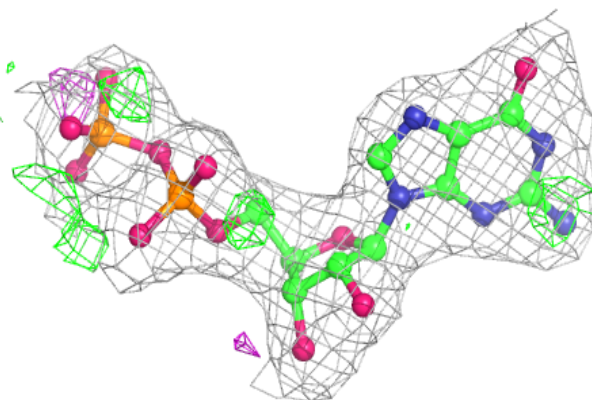


**Electron density around GDP B 401:**

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

**Electron density around GDP A 401:**

$2mF_o-DF_c$  (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.