



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 12:09 AM EDT

PDB ID : 5O74  
Title : Crystal structure of human Rab1b covalently bound to the GEF domain of DrrA/SidM from Legionella pneumophila in the presence of GDP  
Authors : Cigler, M.; Mueller, T.; Horn-Ghetko, D.; von Wrisberg, M.K.; Fottner, M.; Goody, R.S.; Itzen, A.; Mueller, M.P.; Lang, K.  
Deposited on : 2017-06-08  
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](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:

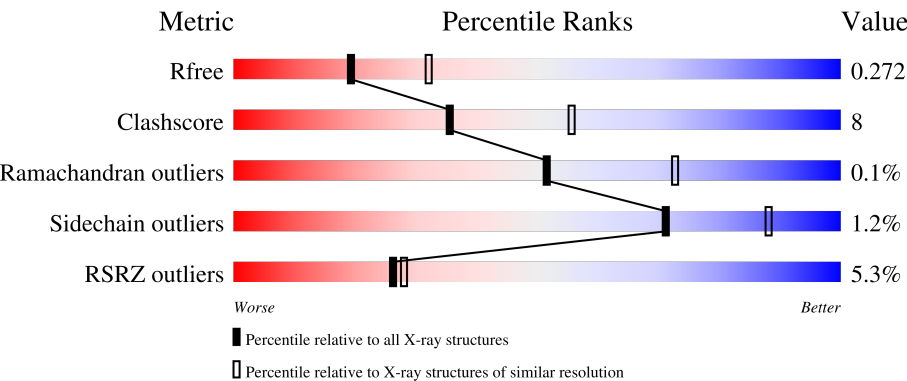
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

# 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 <sub>free</sub>	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  $\geq 3$ , 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	197	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>82%14%..</div></div>
1	C	197	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>81%17%. </div></div>
1	E	197	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>77%19%.. </div></div>
1	G	197	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>81%16%.. </div></div>

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Mol	Chain	Length	Quality of chain
1	I	197	
1	K	197	
2	B	180	
2	D	180	
2	F	180	
2	H	180	
2	J	180	
2	L	180	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	9MN	B	79	-	-	-	X
2	9MN	D	79	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33987 atoms, of which 16983 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 Multifunctional virulence effector protein DrrA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	191	Total	C	H	N	O	S	0	0	0
			2998	939	1505	254	291	9			
1	C	192	Total	C	H	N	O	S	0	0	0
			3012	943	1512	255	293	9			
1	E	191	Total	C	H	N	O	S	0	0	0
			2998	939	1505	254	291	9			
1	G	192	Total	C	H	N	O	S	0	0	0
			3012	943	1512	255	293	9			
1	I	193	Total	C	H	N	O	S	0	0	0
			3024	944	1521	256	293	10			
1	K	191	Total	C	H	N	O	S	0	0	0
			2987	934	1499	254	291	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	GLY	-	expression tag	UNP Q29ST3
A	338	HIS	-	expression tag	UNP Q29ST3
A	339	MET	-	expression tag	UNP Q29ST3
A	512	CYS	ASP	engineered mutation	UNP Q29ST3
C	337	GLY	-	expression tag	UNP Q29ST3
C	338	HIS	-	expression tag	UNP Q29ST3
C	339	MET	-	expression tag	UNP Q29ST3
C	512	CYS	ASP	engineered mutation	UNP Q29ST3
E	337	GLY	-	expression tag	UNP Q29ST3
E	338	HIS	-	expression tag	UNP Q29ST3
E	339	MET	-	expression tag	UNP Q29ST3
E	512	CYS	ASP	engineered mutation	UNP Q29ST3
G	337	GLY	-	expression tag	UNP Q29ST3
G	338	HIS	-	expression tag	UNP Q29ST3
G	339	MET	-	expression tag	UNP Q29ST3
G	512	CYS	ASP	engineered mutation	UNP Q29ST3
I	337	GLY	-	expression tag	UNP Q29ST3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	338	HIS	-	expression tag	UNP Q29ST3
I	339	MET	-	expression tag	UNP Q29ST3
I	512	CYS	ASP	engineered mutation	UNP Q29ST3
K	337	GLY	-	expression tag	UNP Q29ST3
K	338	HIS	-	expression tag	UNP Q29ST3
K	339	MET	-	expression tag	UNP Q29ST3
K	512	CYS	ASP	engineered mutation	UNP Q29ST3

- Molecule 2 is a protein called Ras-related protein Rab-1B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	170	Total	C	H	N	O	S	0	0	0
			2716	868	1356	220	268	4			
2	D	161	Total	C	H	N	O	S	0	0	0
			2593	828	1300	210	251	4			
2	F	165	Total	C	H	N	O	S	0	0	0
			2641	843	1323	215	256	4			
2	H	170	Total	C	H	N	O	S	0	0	0
			2721	868	1361	220	268	4			
2	J	164	Total	C	H	N	O	S	0	0	0
			2628	841	1313	213	257	4			
2	L	152	Total	C	H	N	O	S	0	0	0
			2429	775	1216	201	233	4			

There are 54 discrepancies between the modelled and reference sequences:

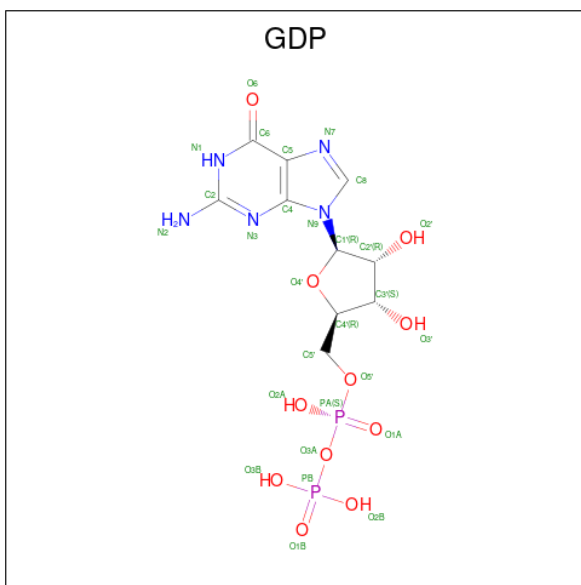
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q9H0U4
B	2	ALA	-	expression tag	UNP Q9H0U4
B	79	9MN	ARG	engineered mutation	UNP Q9H0U4
B	175	HIS	-	expression tag	UNP Q9H0U4
B	176	HIS	-	expression tag	UNP Q9H0U4
B	177	HIS	-	expression tag	UNP Q9H0U4
B	178	HIS	-	expression tag	UNP Q9H0U4
B	179	HIS	-	expression tag	UNP Q9H0U4
B	180	HIS	-	expression tag	UNP Q9H0U4
D	1	MET	-	initiating methionine	UNP Q9H0U4
D	2	ALA	-	expression tag	UNP Q9H0U4
D	79	9MN	ARG	engineered mutation	UNP Q9H0U4
D	175	HIS	-	expression tag	UNP Q9H0U4
D	176	HIS	-	expression tag	UNP Q9H0U4
D	177	HIS	-	expression tag	UNP Q9H0U4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	178	HIS	-	expression tag	UNP Q9H0U4
D	179	HIS	-	expression tag	UNP Q9H0U4
D	180	HIS	-	expression tag	UNP Q9H0U4
F	1	MET	-	initiating methionine	UNP Q9H0U4
F	2	ALA	-	expression tag	UNP Q9H0U4
F	79	9MN	ARG	engineered mutation	UNP Q9H0U4
F	175	HIS	-	expression tag	UNP Q9H0U4
F	176	HIS	-	expression tag	UNP Q9H0U4
F	177	HIS	-	expression tag	UNP Q9H0U4
F	178	HIS	-	expression tag	UNP Q9H0U4
F	179	HIS	-	expression tag	UNP Q9H0U4
F	180	HIS	-	expression tag	UNP Q9H0U4
H	1	MET	-	initiating methionine	UNP Q9H0U4
H	2	ALA	-	expression tag	UNP Q9H0U4
H	79	9MN	ARG	engineered mutation	UNP Q9H0U4
H	175	HIS	-	expression tag	UNP Q9H0U4
H	176	HIS	-	expression tag	UNP Q9H0U4
H	177	HIS	-	expression tag	UNP Q9H0U4
H	178	HIS	-	expression tag	UNP Q9H0U4
H	179	HIS	-	expression tag	UNP Q9H0U4
H	180	HIS	-	expression tag	UNP Q9H0U4
J	1	MET	-	initiating methionine	UNP Q9H0U4
J	2	ALA	-	expression tag	UNP Q9H0U4
J	79	9MN	ARG	engineered mutation	UNP Q9H0U4
J	175	HIS	-	expression tag	UNP Q9H0U4
J	176	HIS	-	expression tag	UNP Q9H0U4
J	177	HIS	-	expression tag	UNP Q9H0U4
J	178	HIS	-	expression tag	UNP Q9H0U4
J	179	HIS	-	expression tag	UNP Q9H0U4
J	180	HIS	-	expression tag	UNP Q9H0U4
L	1	MET	-	initiating methionine	UNP Q9H0U4
L	2	ALA	-	expression tag	UNP Q9H0U4
L	79	9MN	ARG	engineered mutation	UNP Q9H0U4
L	175	HIS	-	expression tag	UNP Q9H0U4
L	176	HIS	-	expression tag	UNP Q9H0U4
L	177	HIS	-	expression tag	UNP Q9H0U4
L	178	HIS	-	expression tag	UNP Q9H0U4
L	179	HIS	-	expression tag	UNP Q9H0U4
L	180	HIS	-	expression tag	UNP Q9H0U4

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).

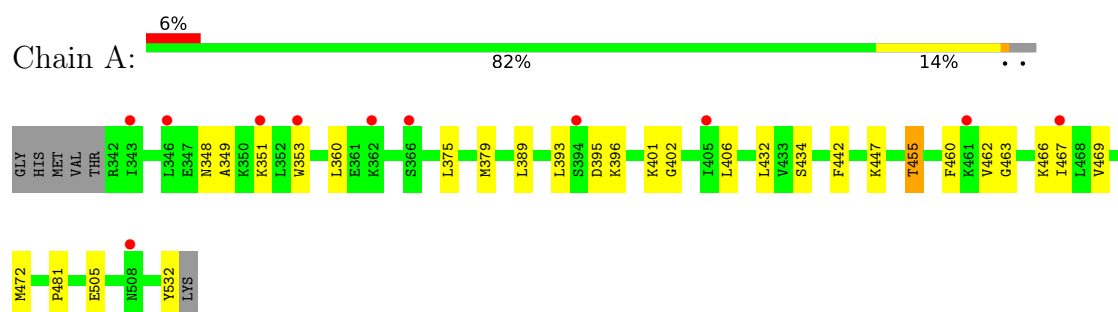


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0
3	D	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0
3	F	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0
3	H	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0
3	J	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0
3	L	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0

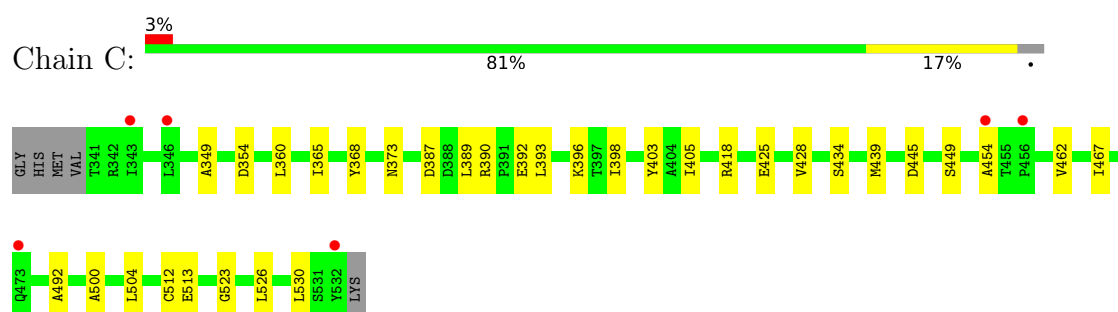
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

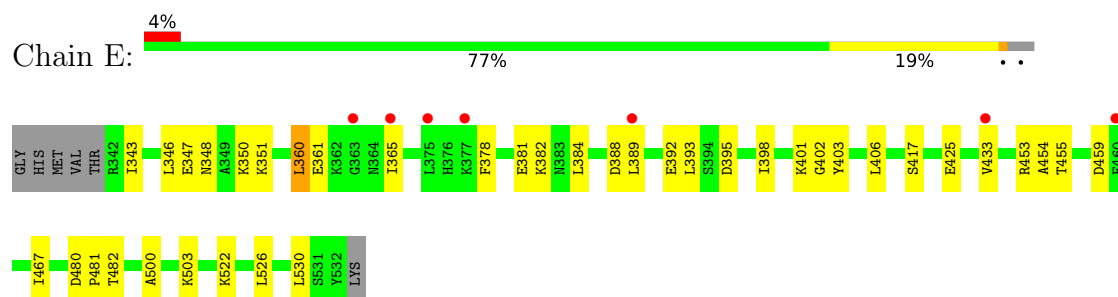
- Molecule 1: Multifunctional virulence effector protein DrrA



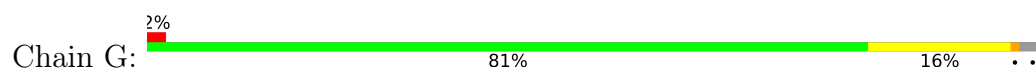
- Molecule 1: Multifunctional virulence effector protein DrrA

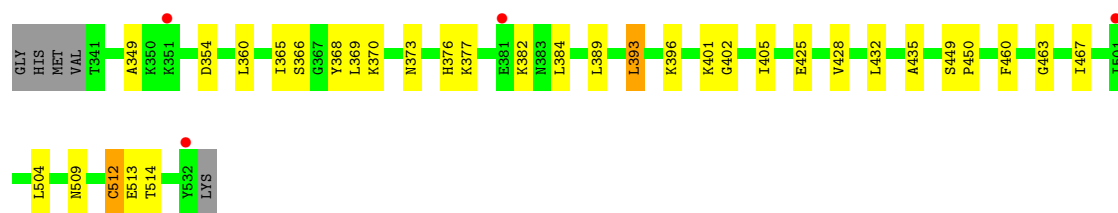


- Molecule 1: Multifunctional virulence effector protein DrrA

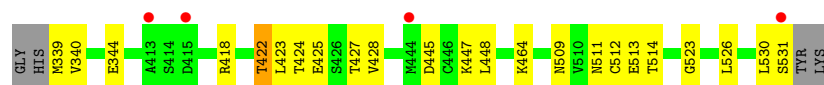
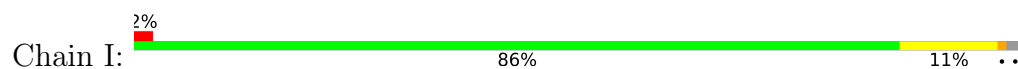


- Molecule 1: Multifunctional virulence effector protein DrrA

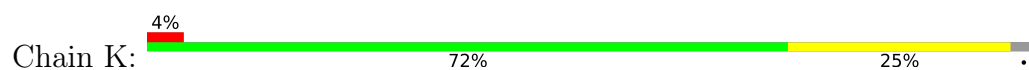




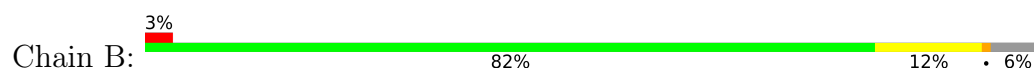
• Molecule 1: Multifunctional virulence effector protein DrrA



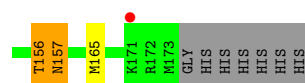
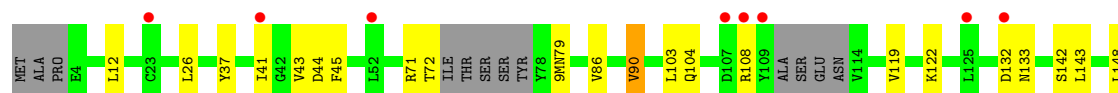
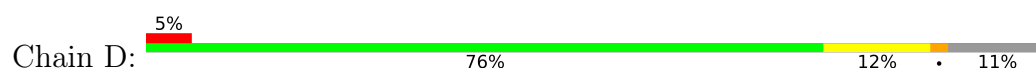
• Molecule 1: Multifunctional virulence effector protein DrrA



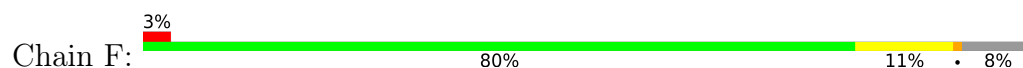
• Molecule 2: Ras-related protein Rab-1B



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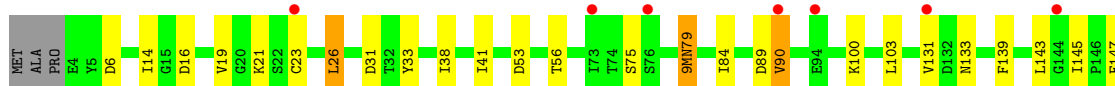
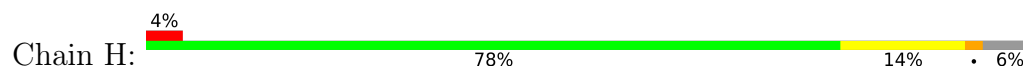


• Molecule 2: Ras-related protein Rab-1B

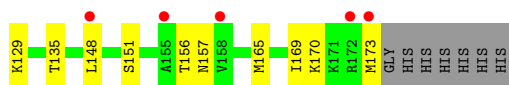
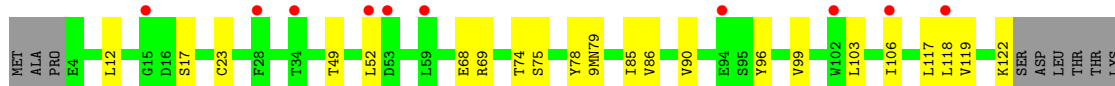




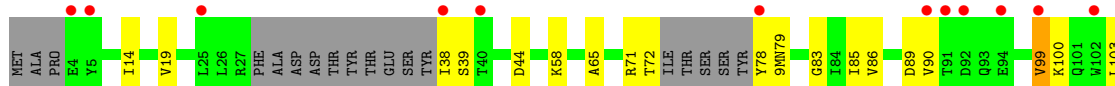
• Molecule 2: Ras-related protein Rab-1B



• Molecule 2: Ras-related protein Rab-1B



• Molecule 2: Ras-related protein Rab-1B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.91Å 87.45Å 93.17Å 114.61° 97.69° 100.74°	Depositor
Resolution (Å)	46.52 – 2.50 46.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.52-2.50) 98.0 (46.52-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.229 , 0.266 0.234 , 0.272	Depositor DCC
$R_{free}$ test set	3618 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	33987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 9MN

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	0.30	0/1518	0.54	0/2044
1	C	0.30	0/1525	0.51	0/2054
1	E	0.35	0/1518	0.57	1/2044 (0.0%)
1	G	0.31	0/1525	0.53	1/2054 (0.0%)
1	I	0.29	0/1527	0.51	0/2056
1	K	0.31	0/1512	0.55	0/2036
2	B	0.31	0/1364	0.58	1/1841 (0.1%)
2	D	0.31	0/1294	0.53	1/1742 (0.1%)
2	F	0.29	0/1320	0.57	1/1778 (0.1%)
2	H	0.32	0/1364	0.59	1/1841 (0.1%)
2	J	0.32	0/1318	0.54	0/1777
2	L	0.34	0/1210	0.62	1/1625 (0.1%)
All	All	0.31	0/16995	0.55	7/22892 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	99	VAL	CG1-CB-CG2	8.36	124.28	110.90
2	F	90	VAL	CG1-CB-CG2	8.06	123.79	110.90
2	B	90	VAL	CG1-CB-CG2	8.05	123.78	110.90
2	H	90	VAL	CG1-CB-CG2	7.81	123.40	110.90
2	D	90	VAL	CA-CB-CG1	7.55	122.22	110.90

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	1493	1505	1505	21	0
1	C	1500	1512	1512	32	0
1	E	1493	1505	1505	36	2
1	G	1500	1512	1512	23	0
1	I	1503	1521	1521	17	2
1	K	1488	1499	1503	39	0
2	B	1360	1356	1341	15	1
2	D	1293	1300	1280	20	0
2	F	1318	1323	1309	10	1
2	H	1360	1361	1341	22	0
2	J	1315	1313	1293	18	0
2	L	1213	1216	1209	42	0
3	B	28	10	12	0	0
3	D	28	10	12	0	0
3	F	28	10	12	0	0
3	H	28	10	12	1	0
3	J	28	10	12	1	0
3	L	28	10	12	0	0
All	All	17004	16983	16903	275	3

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 8.

The worst 5 of 275 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:I:425:GLU:OE2	1:I:428:VAL:N	2.13	0.81
2:L:129:LYS:NZ	2:L:149:GLU:OE2	2.13	0.80
1:G:512:CYS:SG	1:G:513:GLU:N	2.54	0.80
1:C:390:ARG:NH1	1:C:445:ASP:O	2.16	0.77
2:B:132:ASP:OD2	2:B:134:THR:OG1	2.02	0.77

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:ASN:H	2:F:159:GLU:OE2[1_455]	1.53	0.07
1:E:459:ASP:OD2	1:I:464:LYS:H[1_565]	1.56	0.04
1:E:459:ASP:OD2	1:I:464:LYS:N[1_565]	2.17	0.03

## 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	189/197 (96%)	187 (99%)	2 (1%)	0	100	100
1	C	190/197 (96%)	188 (99%)	2 (1%)	0	100	100
1	E	189/197 (96%)	188 (100%)	1 (0%)	0	100	100
1	G	190/197 (96%)	188 (99%)	2 (1%)	0	100	100
1	I	191/197 (97%)	189 (99%)	2 (1%)	0	100	100
1	K	189/197 (96%)	187 (99%)	2 (1%)	0	100	100
2	B	167/180 (93%)	164 (98%)	3 (2%)	0	100	100
2	D	154/180 (86%)	150 (97%)	2 (1%)	2 (1%)	12	21
2	F	160/180 (89%)	154 (96%)	6 (4%)	0	100	100
2	H	167/180 (93%)	163 (98%)	4 (2%)	0	100	100
2	J	159/180 (88%)	156 (98%)	3 (2%)	0	100	100
2	L	143/180 (79%)	139 (97%)	3 (2%)	1 (1%)	22	39
All	All	2088/2262 (92%)	2053 (98%)	32 (2%)	3 (0%)	51	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	157	ASN
2	D	122	LYS
2	L	122	LYS

### 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	166/171 (97%)	164 (99%)	2 (1%)	71	88
1	C	167/171 (98%)	166 (99%)	1 (1%)	86	95
1	E	166/171 (97%)	165 (99%)	1 (1%)	86	95
1	G	167/171 (98%)	166 (99%)	1 (1%)	86	95
1	I	168/171 (98%)	167 (99%)	1 (1%)	86	95
1	K	166/171 (97%)	165 (99%)	1 (1%)	86	95
2	B	147/155 (95%)	144 (98%)	3 (2%)	55	79
2	D	139/155 (90%)	136 (98%)	3 (2%)	52	77
2	F	142/155 (92%)	139 (98%)	3 (2%)	53	78
2	H	147/155 (95%)	145 (99%)	2 (1%)	67	86
2	J	141/155 (91%)	139 (99%)	2 (1%)	67	86
2	L	130/155 (84%)	128 (98%)	2 (2%)	65	85
All	All	1846/1956 (94%)	1824 (99%)	22 (1%)	71	88

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	26	LEU
2	J	49	THR
1	I	422	THR
2	J	135	THR
2	D	133	ASN

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

Mol	Chain	Res	Type
1	A	496	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are 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
2	9MN	H	79	1,2	14,15,17	1.57	2 (14%)	11,16,19	1.30	2 (18%)
2	9MN	L	79	1,2	14,15,17	1.59	2 (14%)	11,16,19	0.99	0
2	9MN	D	79	1,2	14,15,17	1.78	2 (14%)	11,16,19	3.46	5 (45%)
2	9MN	B	79	1,2	14,15,17	1.61	2 (14%)	11,16,19	1.26	1 (9%)
2	9MN	F	79	1,2	14,15,17	1.66	2 (14%)	11,16,19	1.48	2 (18%)
2	9MN	J	79	1,2	14,15,17	1.74	2 (14%)	11,16,19	2.96	5 (45%)

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	9MN	H	79	1,2	-	5/14/15/18	-
2	9MN	L	79	1,2	-	5/14/15/18	-
2	9MN	D	79	1,2	-	9/14/15/18	-
2	9MN	B	79	1,2	-	10/14/15/18	-
2	9MN	F	79	1,2	-	7/14/15/18	-
2	9MN	J	79	1,2	-	8/14/15/18	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	79	9MN	C10-NZ	5.82	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	79	9MN	C10-NZ	5.79	1.46	1.33
2	F	79	9MN	C10-NZ	5.52	1.45	1.33
2	L	79	9MN	C10-NZ	5.35	1.45	1.33
2	B	79	9MN	C10-NZ	5.33	1.45	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	79	9MN	C12-C10-NZ	8.38	130.52	116.42
2	J	79	9MN	C12-C10-NZ	6.95	128.12	116.42
2	D	79	9MN	O11-C10-NZ	-4.71	114.13	123.01
2	J	79	9MN	O11-C10-C12	-3.78	115.11	122.02
2	D	79	9MN	O11-C10-C12	-3.65	115.34	122.02

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	79	9MN	N-CA-CB-C6
2	B	79	9MN	C-CA-CB-C6
2	F	79	9MN	C-CA-CB-C6
2	J	79	9MN	N-CA-CB-C6
2	J	79	9MN	C-CA-CB-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	79	9MN	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are 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	GDP	D	500	-	24,30,30	0.94	1 (4%)	30,47,47	1.21	4 (13%)
3	GDP	F	500	-	24,30,30	1.02	2 (8%)	30,47,47	1.37	4 (13%)
3	GDP	J	500	-	24,30,30	0.98	1 (4%)	30,47,47	1.37	4 (13%)
3	GDP	L	500	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	3 (10%)
3	GDP	H	500	-	24,30,30	0.98	1 (4%)	30,47,47	1.28	3 (10%)
3	GDP	B	500	-	24,30,30	0.93	1 (4%)	30,47,47	1.36	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
3	GDP	D	500	-	-	4/12/32/32	0/3/3/3
3	GDP	F	500	-	-	4/12/32/32	0/3/3/3
3	GDP	J	500	-	-	5/12/32/32	0/3/3/3
3	GDP	L	500	-	-	8/12/32/32	0/3/3/3
3	GDP	H	500	-	-	4/12/32/32	0/3/3/3
3	GDP	B	500	-	-	3/12/32/32	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)
3	F	500	GDP	C6-N1	-2.80	1.33	1.37
3	J	500	GDP	C6-N1	-2.69	1.33	1.37
3	L	500	GDP	C6-N1	-2.55	1.34	1.37
3	D	500	GDP	C6-N1	-2.41	1.34	1.37
3	H	500	GDP	C6-N1	-2.40	1.34	1.37

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	500	GDP	PA-O3A-PB	-4.51	117.35	132.83
3	J	500	GDP	PA-O3A-PB	-4.33	117.97	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	500	GDP	PA-O3A-PB	-4.00	119.11	132.83
3	L	500	GDP	PA-O3A-PB	-3.93	119.34	132.83
3	D	500	GDP	PA-O3A-PB	-3.72	120.05	132.83

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

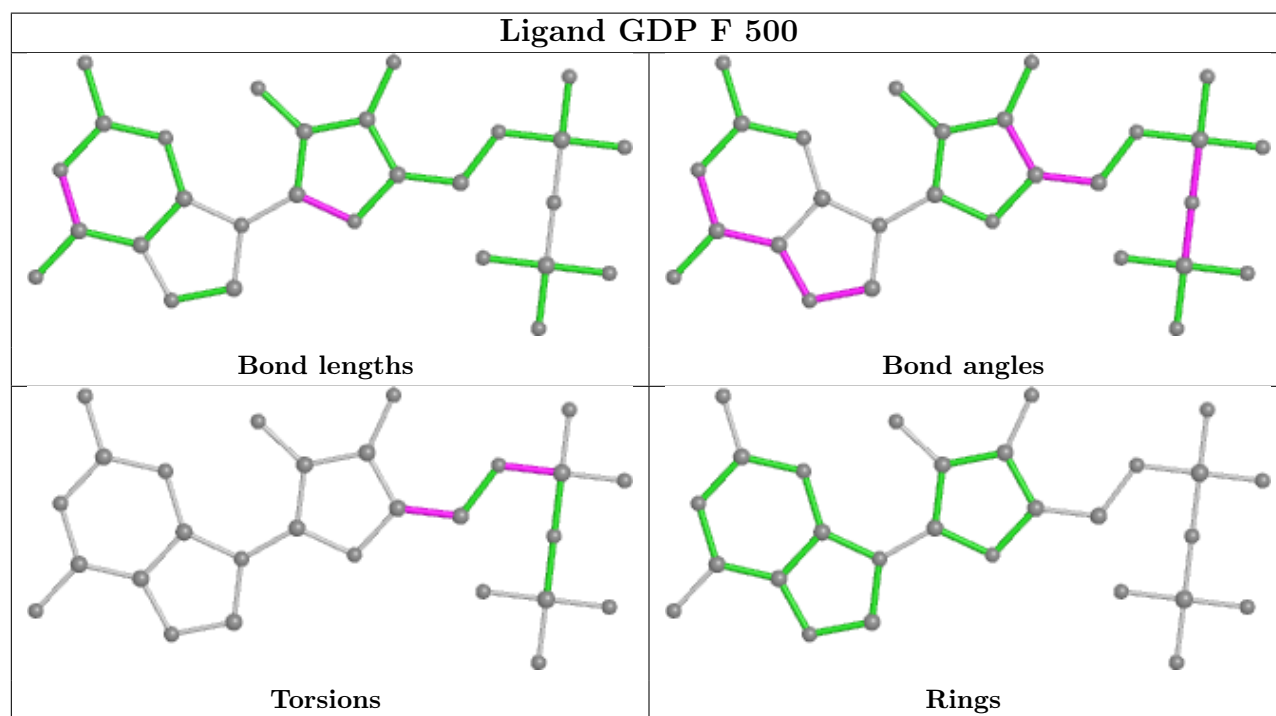
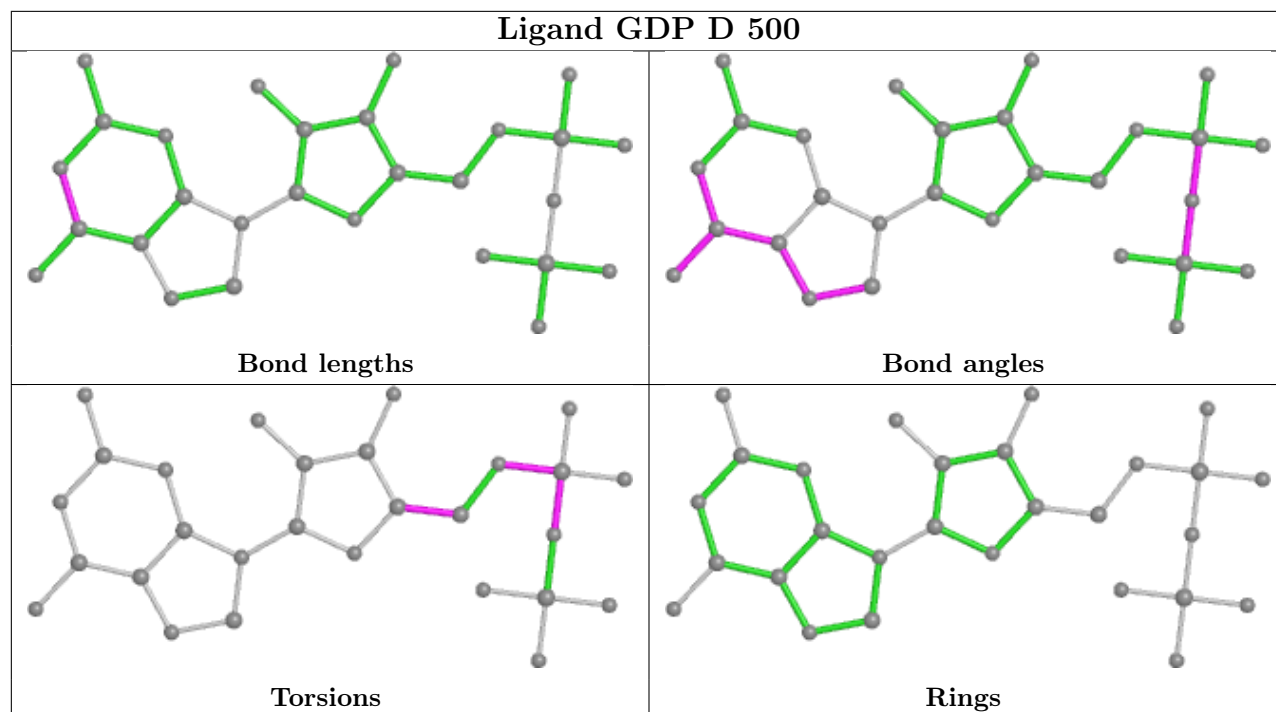
Mol	Chain	Res	Type	Atoms
3	D	500	GDP	C5'-O5'-PA-O1A
3	J	500	GDP	PA-O3A-PB-O3B
3	L	500	GDP	PA-O3A-PB-O2B
3	L	500	GDP	PA-O3A-PB-O3B
3	L	500	GDP	C5'-O5'-PA-O3A

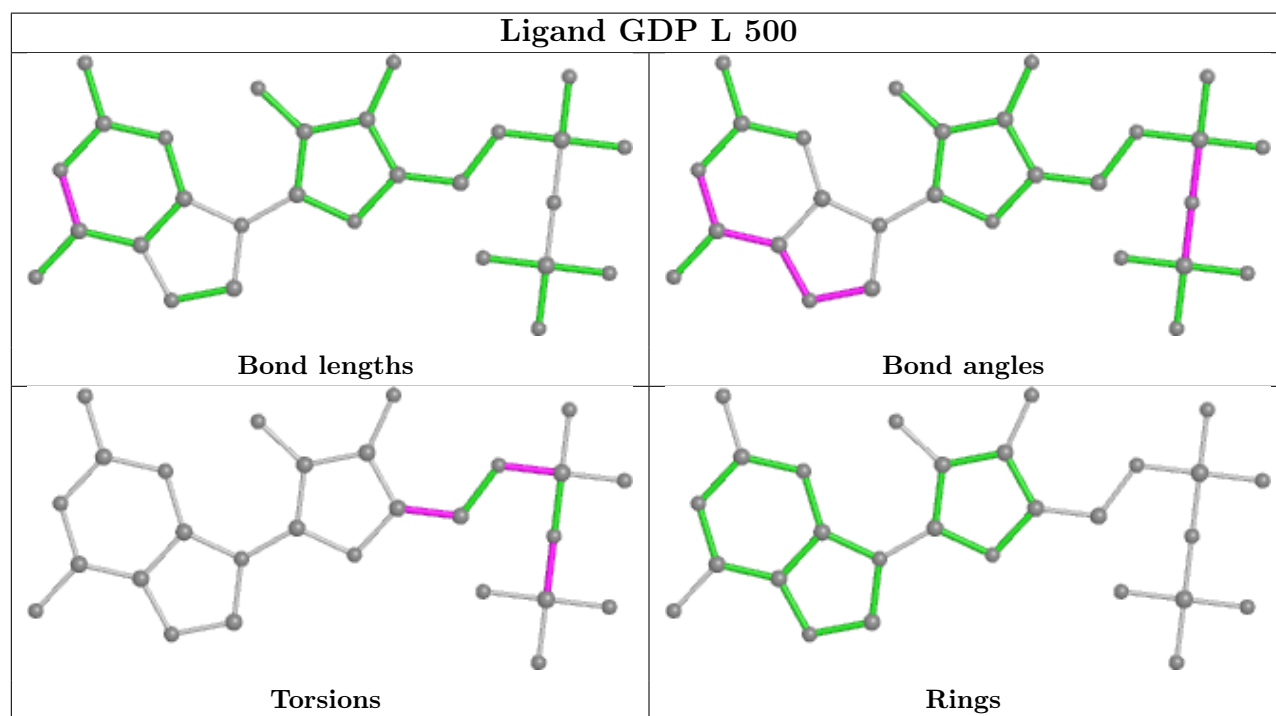
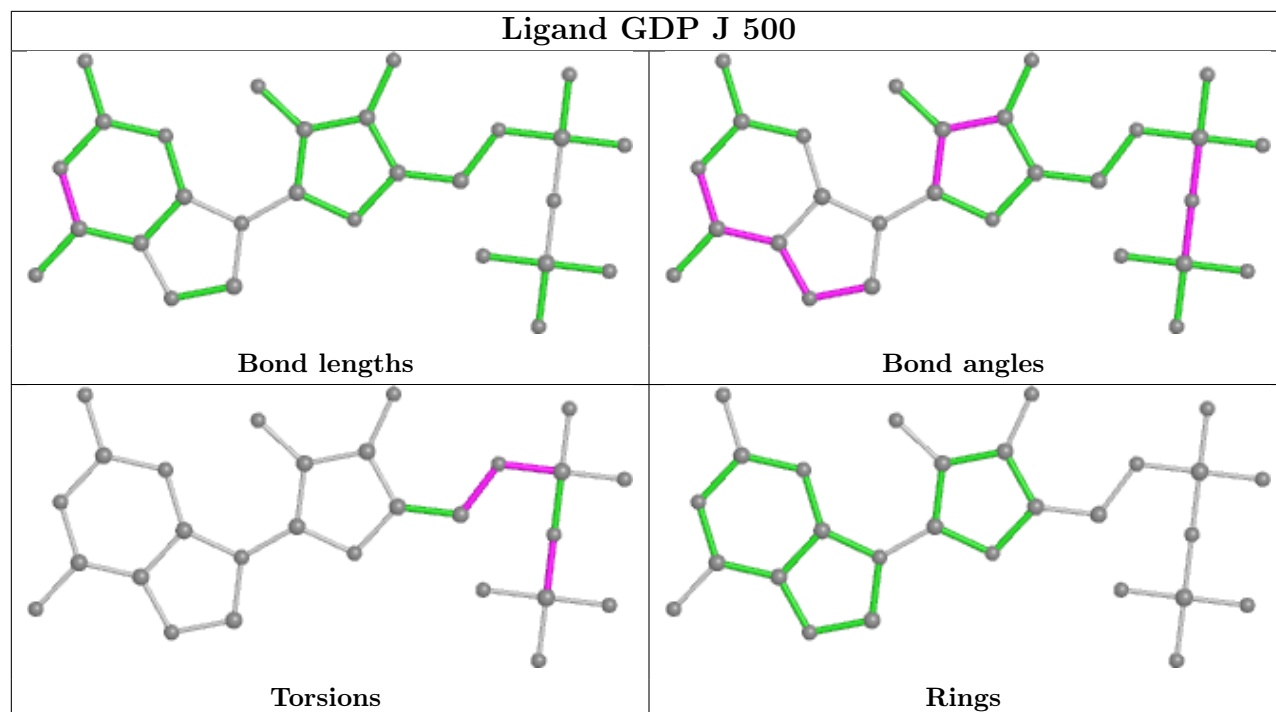
There are no ring outliers.

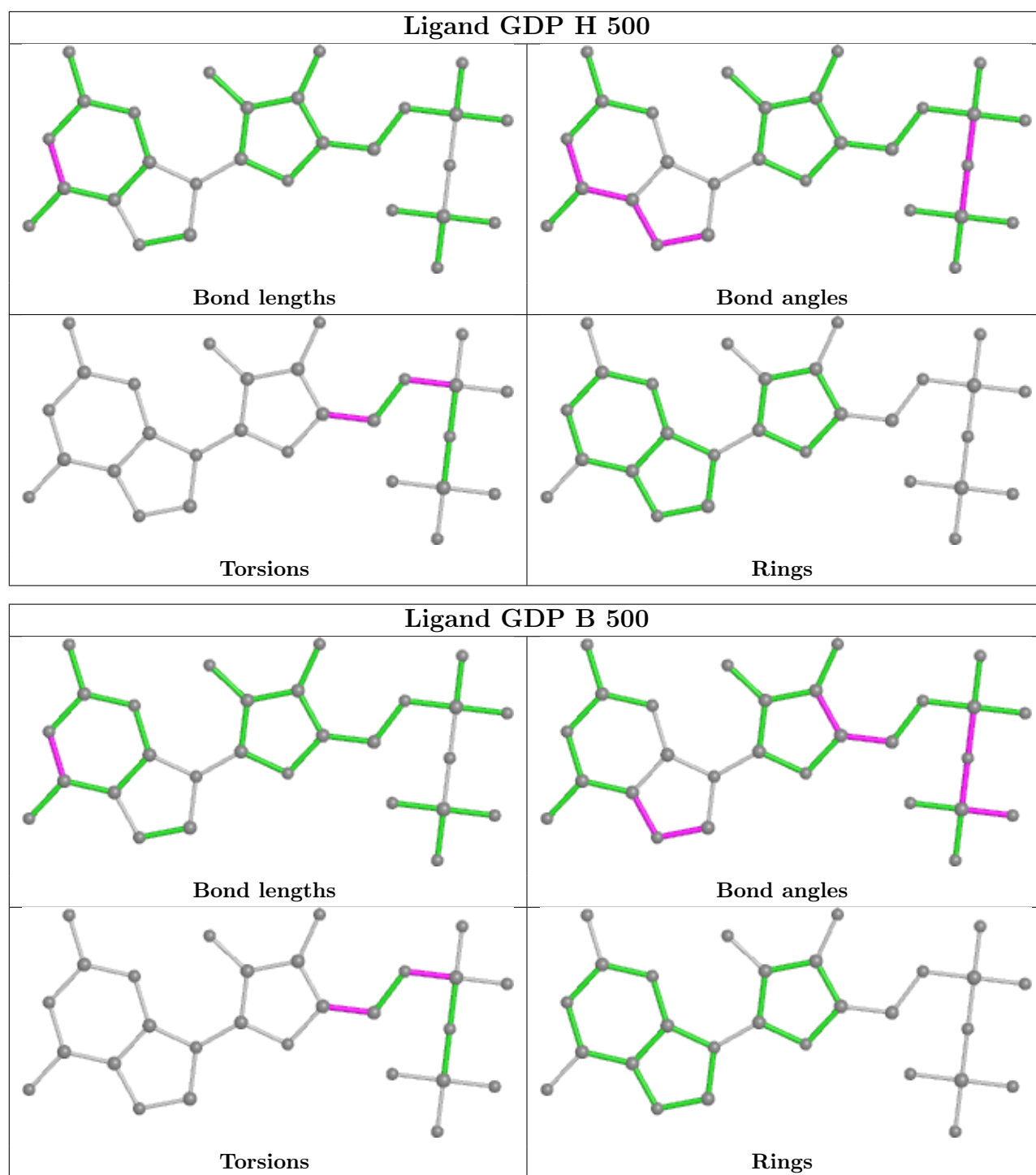
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	500	GDP	1	0
3	H	500	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 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 [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, 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	191/197 (96%)	0.54	11 (5%) 23 24	38, 64, 102, 131	0
1	C	192/197 (97%)	0.44	6 (3%) 49 52	39, 61, 96, 113	0
1	E	191/197 (96%)	0.52	7 (3%) 41 45	37, 67, 113, 138	0
1	G	192/197 (97%)	0.41	4 (2%) 63 66	36, 63, 103, 138	0
1	I	193/197 (97%)	0.53	4 (2%) 63 66	45, 61, 87, 101	0
1	K	191/197 (96%)	0.51	8 (4%) 36 39	43, 68, 106, 151	0
2	B	169/180 (93%)	0.50	5 (2%) 50 53	44, 65, 96, 135	0
2	D	160/180 (88%)	0.44	9 (5%) 24 25	45, 71, 107, 144	0
2	F	164/180 (91%)	0.45	6 (3%) 41 45	37, 60, 89, 106	0
2	H	169/180 (93%)	0.47	7 (4%) 37 40	35, 63, 106, 132	0
2	J	163/180 (90%)	0.81	15 (9%) 9 9	52, 79, 114, 134	0
2	L	151/180 (83%)	1.17	30 (19%) 1 1	46, 82, 125, 158	0
All	All	2126/2262 (93%)	0.56	112 (5%) 26 28	35, 67, 108, 158	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	52	LEU	6.9
2	L	129	LYS	5.8
2	J	158	VAL	5.1
2	L	148	LEU	4.9
2	L	94	GLU	4.7

### 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, 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
2	9MN	D	79	16/18	0.72	0.42	93,140,168,169	0
2	9MN	J	79	16/18	0.75	0.30	76,137,185,188	0
2	9MN	F	79	16/18	0.79	0.31	73,133,159,160	0
2	9MN	B	79	16/18	0.79	0.43	82,146,181,186	0
2	9MN	H	79	16/18	0.82	0.38	68,157,192,195	0
2	9MN	L	79	16/18	0.84	0.50	95,182,236,241	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

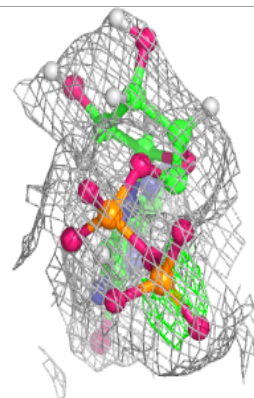
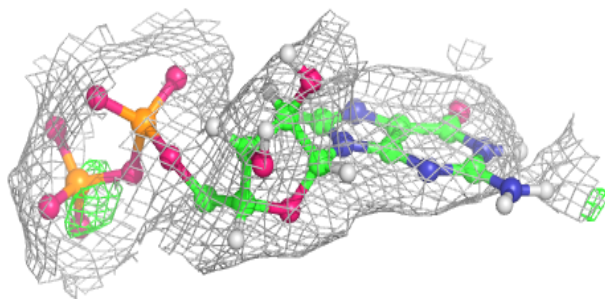
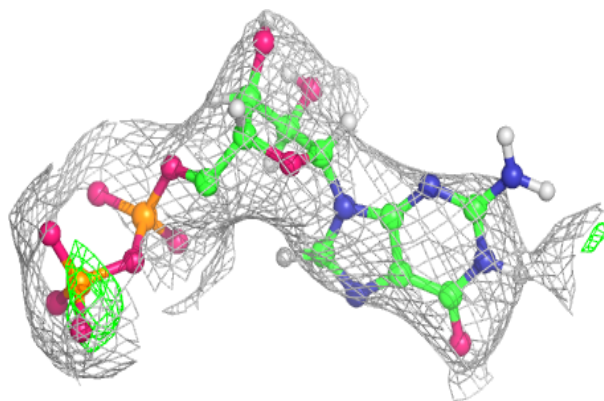
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	GDP	D	500	28/28	0.79	0.18	79,97,153,176	0
3	GDP	J	500	28/28	0.79	0.23	82,124,178,189	0
3	GDP	F	500	28/28	0.81	0.23	44,82,117,131	0
3	GDP	L	500	28/28	0.89	0.18	67,91,140,141	0
3	GDP	H	500	28/28	0.93	0.19	40,84,127,131	0
3	GDP	B	500	28/28	0.94	0.19	54,80,124,148	0

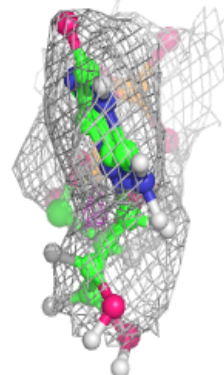
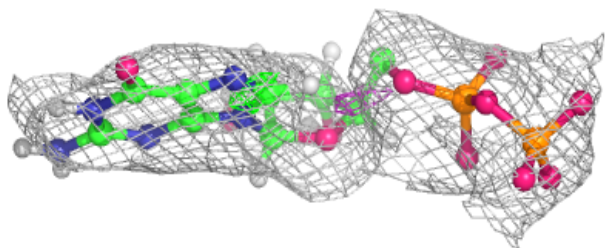
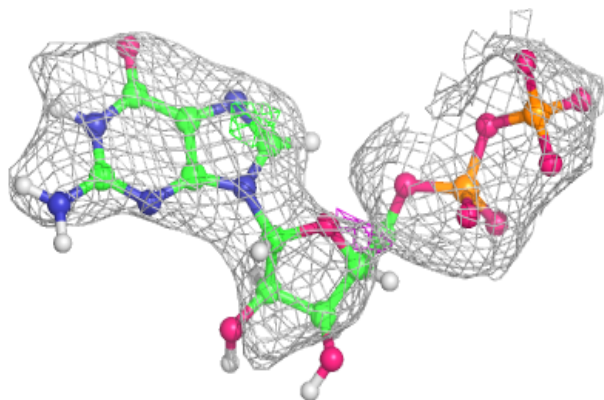
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GDP D 500:**

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

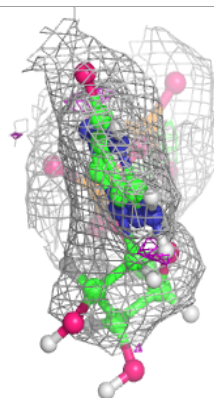
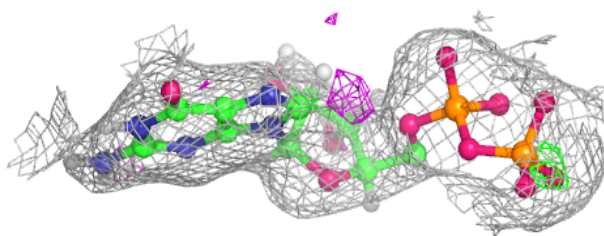
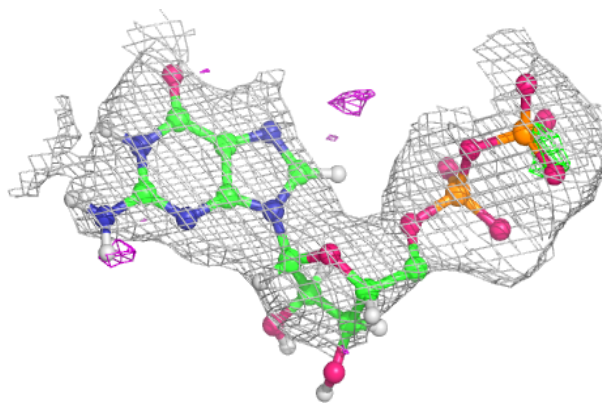
**Electron density around GDP J 500:**

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

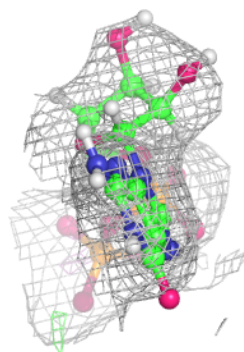
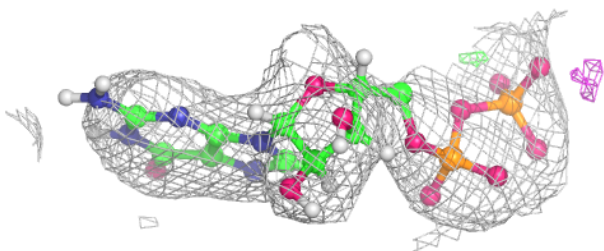
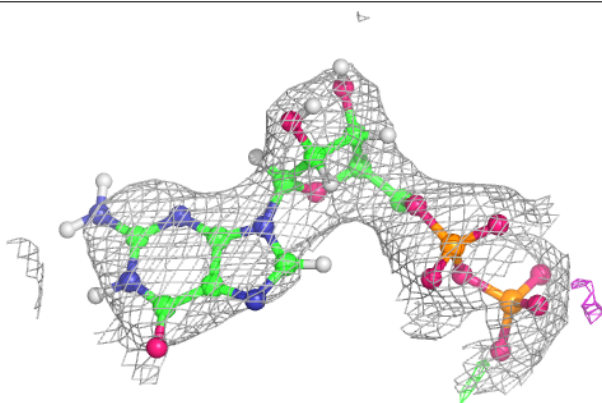


**Electron density around GDP F 500:**

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

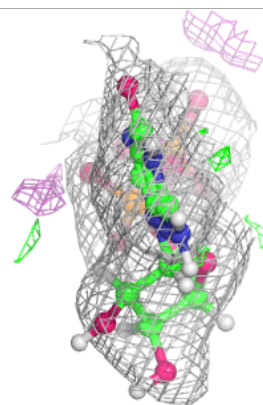
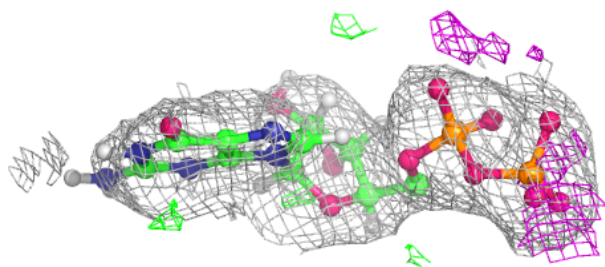
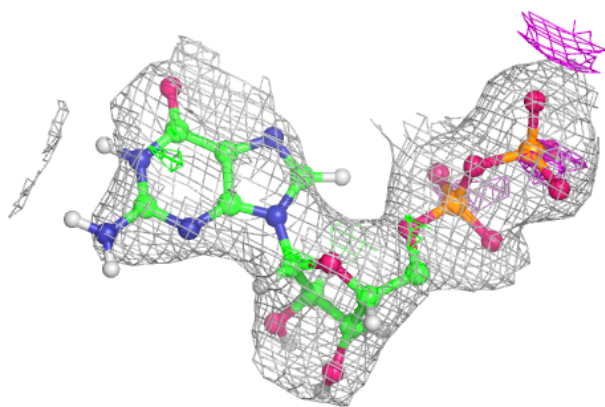
**Electron density around GDP L 500:**

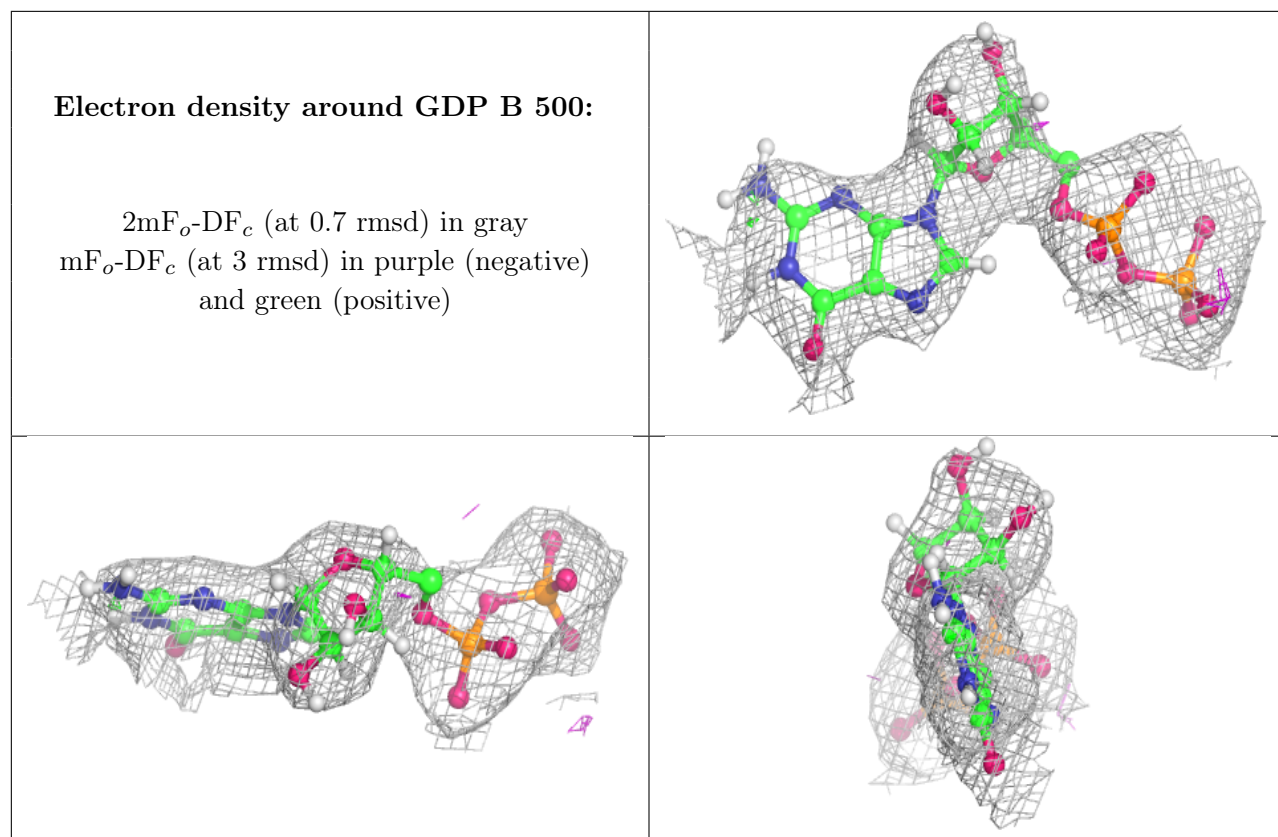
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GDP H 500:**

$2mF_o-DF_c$  (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.