



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:31 pm BST

PDB ID : 4ORO
Title : Structure of Influenza B PB2 cap-binding domain complex with GDP
Authors : Liu, Y.; Zheng, X.
Deposited on : 2014-02-11
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

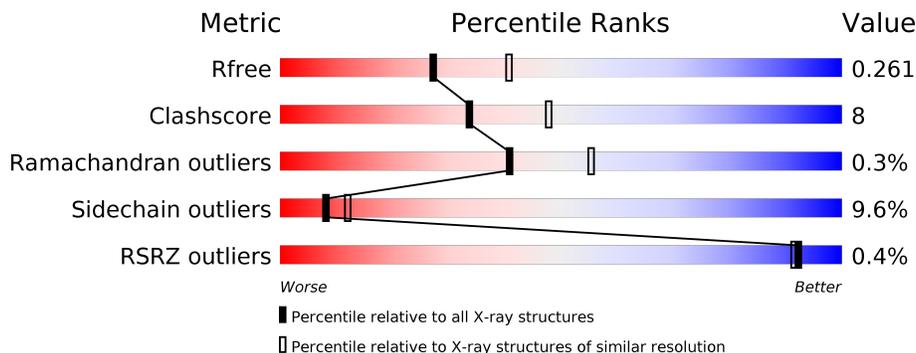
1 Overall quality at a glance i

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 ≥ 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	169	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 19%, green 78%);"></div> <div style="margin-left: 5px;">%</div> </div> <div style="display: flex; justify-content: space-between; width: 100%; margin-top: 5px;"> 78% 19% •• </div>
1	B	169	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 20%, green 78%);"></div> <div style="margin-left: 5px;">%</div> </div> <div style="display: flex; justify-content: space-between; width: 100%; margin-top: 5px;"> 78% 20% • </div>
1	C	169	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 15%, green 81%);"></div> <div style="margin-left: 5px;">%</div> </div> <div style="display: flex; justify-content: space-between; width: 100%; margin-top: 5px;"> 81% 15% • </div>
1	D	169	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, green 74%, yellow 22%, orange 5%, red 5%);"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%; margin-top: 5px;"> 74% 22% • </div>

2 Entry composition [i](#)

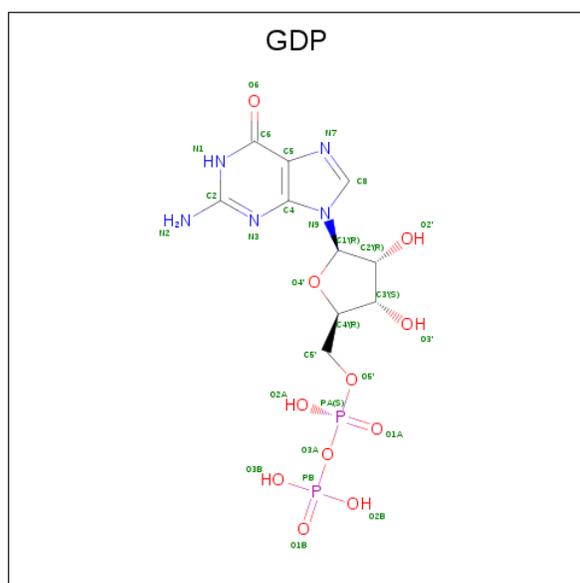
There are 3 unique types of molecules in this entry. The entry contains 5819 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polymerase PB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	169	Total 1371	C 859	N 251	O 251	S 10	0	0	0
1	B	169	Total 1371	C 859	N 251	O 251	S 10	0	0	0
1	C	169	Total 1371	C 859	N 251	O 251	S 10	0	0	0
1	D	169	Total 1371	C 859	N 251	O 251	S 10	0	0	0

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

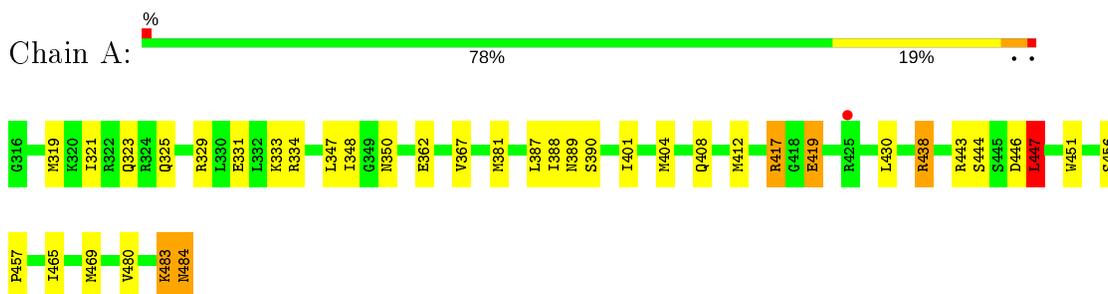
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total	O	0	0
			63	63		
3	B	51	Total	O	0	0
			51	51		
3	C	51	Total	O	0	0
			51	51		
3	D	58	Total	O	0	0
			58	58		

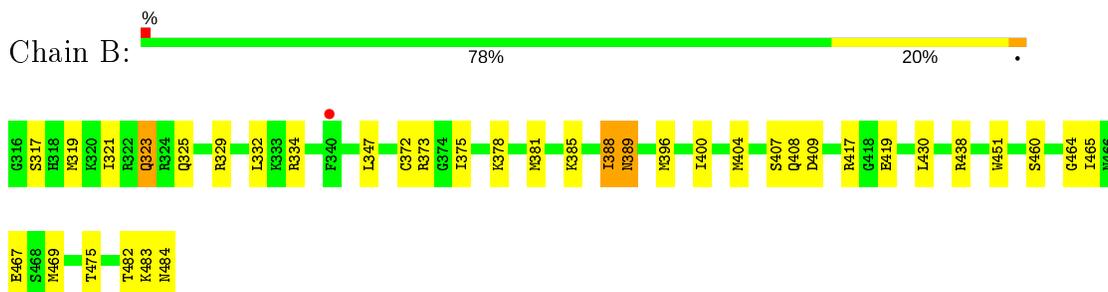
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

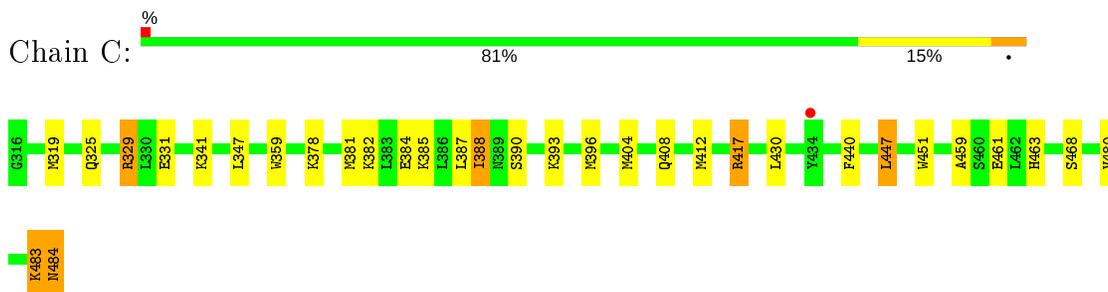
- Molecule 1: Polymerase PB2



- Molecule 1: Polymerase PB2



- Molecule 1: Polymerase PB2



- Molecule 1: Polymerase PB2



E461	L462	H463	G464	I465	M466	E467	S468	M469	L476	V480	V481	T482	K483	M484
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.42Å 42.77Å 118.41Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	39.47 – 2.40 39.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.9 (39.47-2.40) 95.9 (39.47-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.199 , 0.270 0.197 , 0.261	Depositor DCC
R_{free} test set	1625 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtrriage
Anisotropy	0.270	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 8.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.470 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5819	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4431e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	1.08	1/1391 (0.1%)	0.96	1/1853 (0.1%)
1	B	1.00	0/1391	0.88	1/1853 (0.1%)
1	C	1.04	0/1391	0.94	0/1853
1	D	1.05	0/1391	0.89	0/1853
All	All	1.04	1/5564 (0.0%)	0.92	2/7412 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	GLU	CG-CD	5.60	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	LEU	CA-CB-CG	5.46	127.85	115.30
1	B	388	ILE	CB-CA-C	-5.08	101.45	111.60

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	1371	0	1386	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1371	0	1386	22	0
1	C	1371	0	1386	23	0
1	D	1371	0	1386	28	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
2	C	28	0	12	0	0
2	D	28	0	12	0	0
3	A	63	0	0	1	0
3	B	51	0	0	0	0
3	C	51	0	0	1	0
3	D	58	0	0	0	0
All	All	5819	0	5592	95	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 8.

All (95) 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:465:ILE:HD11	1:B:469:MET:CE	1.90	1.02
1:B:465:ILE:HD11	1:B:469:MET:HE3	1.05	1.01
1:B:465:ILE:CD1	1:B:469:MET:HE3	1.90	1.01
1:D:329:ARG:H	1:D:437:GLN:HE22	1.29	0.81
1:B:465:ILE:CD1	1:B:469:MET:CE	2.56	0.74
1:A:319:MET:HG2	1:A:325:GLN:HG3	1.73	0.71
1:A:401:ILE:HD11	1:A:444:SER:HB2	1.74	0.69
1:D:424:ASN:C	1:D:424:ASN:HD22	1.97	0.68
1:A:348:ILE:HG13	1:A:350:ASN:HB2	1.76	0.68
1:D:417:ARG:HH21	1:D:450:GLN:NE2	1.93	0.66
1:C:388:ILE:HD11	1:C:396:MET:HG2	1.81	0.63
1:C:390:SER:HB3	1:C:484:ASN:HB2	1.81	0.63
1:B:319:MET:HG2	1:B:325:GLN:HG3	1.82	0.61
1:C:459:ALA:HB1	1:C:461:GLU:OE1	2.00	0.60
1:A:412:MET:HA	1:A:447:LEU:HD13	1.84	0.59
1:C:387:LEU:HD12	1:C:480:VAL:HG23	1.83	0.59
1:B:464:GLY:HA3	1:B:475:THR:HB	1.86	0.58
1:D:453:TYR:CE2	1:D:476:LEU:HD13	2.39	0.58
1:C:331:GLU:HG2	1:D:429:LEU:HD13	1.87	0.57
1:D:465:ILE:HD11	1:D:469:MET:SD	2.45	0.56
1:B:372:CYS:SG	1:B:388:ILE:CG2	2.93	0.56
1:D:466:ASN:HD22	1:D:466:ASN:C	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ALA:HB1	1:C:461:GLU:CD	2.27	0.55
1:D:385:LYS:NZ	1:D:480:VAL:HG12	2.21	0.54
1:B:396:MET:HB2	1:B:469:MET:HE2	1.89	0.54
1:B:378:LYS:HE2	1:B:407:SER:HA	1.90	0.53
1:B:483:LYS:HA	1:B:484:ASN:C	2.29	0.53
1:D:319:MET:HG2	1:D:325:GLN:HG3	1.91	0.52
1:D:424:ASN:ND2	1:D:428:GLN:H	2.09	0.51
1:C:329:ARG:HD3	3:C:651:HOH:O	2.09	0.51
1:C:484:ASN:HD22	1:C:484:ASN:C	2.14	0.51
1:D:385:LYS:HZ3	1:D:480:VAL:HG12	1.75	0.51
1:D:329:ARG:O	1:D:329:ARG:HG3	2.09	0.51
1:A:388:ILE:HG22	1:A:389:ASN:O	2.10	0.50
1:C:393:LYS:HA	1:C:396:MET:HE2	1.94	0.50
1:C:412:MET:HA	1:C:447:LEU:HD13	1.92	0.50
1:D:341:LYS:HG3	1:D:359:TRP:CE2	2.47	0.50
1:D:432:PRO:O	1:D:436:LEU:HD22	2.11	0.50
1:A:404:MET:HE2	1:A:451:TRP:CE2	2.47	0.49
1:A:333:LYS:HE3	3:A:658:HOH:O	2.12	0.48
1:D:461:GLU:HG2	1:D:462:LEU:HD13	1.95	0.48
1:C:381:MET:HA	1:C:408:GLN:O	2.12	0.48
1:B:372:CYS:SG	1:B:388:ILE:HG21	2.54	0.48
1:C:382:LYS:HD3	1:C:384:GLU:CD	2.35	0.48
1:D:417:ARG:HH21	1:D:450:GLN:HE22	1.58	0.48
1:A:348:ILE:HD11	1:A:350:ASN:HD22	1.79	0.47
1:A:388:ILE:HG21	1:A:388:ILE:HD13	1.69	0.47
1:A:465:ILE:HD11	1:A:469:MET:HA	1.97	0.47
1:D:397:ARG:NH1	1:D:467:GLU:O	2.48	0.46
1:B:381:MET:O	1:B:409:ASP:HA	2.15	0.46
1:A:404:MET:HE1	1:A:451:TRP:CG	2.50	0.46
1:D:462:LEU:HG	1:D:480:VAL:HG21	1.98	0.46
1:A:387:LEU:HD12	1:A:480:VAL:HG23	1.97	0.46
1:D:465:ILE:CD1	1:D:469:MET:SD	3.03	0.46
1:D:465:ILE:HD11	1:D:469:MET:HA	1.98	0.45
1:A:438:ARG:HH11	1:A:438:ARG:HB3	1.82	0.45
1:D:424:ASN:C	1:D:424:ASN:ND2	2.68	0.45
1:A:321:ILE:HA	1:A:334:ARG:HB3	1.99	0.45
1:A:381:MET:HA	1:A:408:GLN:O	2.17	0.44
1:C:319:MET:HG2	1:C:325:GLN:HG3	2.00	0.44
1:B:396:MET:CB	1:B:469:MET:HE2	2.48	0.44
1:B:323:GLN:O	1:B:323:GLN:HG3	2.16	0.44
1:B:388:ILE:HD13	1:B:388:ILE:HG21	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ILE:HG22	1:A:389:ASN:N	2.32	0.44
1:A:483:LYS:HA	1:A:484:ASN:HA	1.72	0.44
1:A:319:MET:HG2	1:A:325:GLN:CG	2.46	0.43
1:A:443:ARG:CZ	1:A:446:ASP:OD2	2.66	0.43
1:B:389:ASN:HD22	1:B:389:ASN:H	1.66	0.43
1:C:417:ARG:HA	1:C:417:ARG:HE	1.83	0.43
1:C:393:LYS:HA	1:C:396:MET:CE	2.49	0.43
1:C:463:HIS:HB3	1:C:483:LYS:NZ	2.32	0.43
1:D:456:SER:OG	1:D:464:GLY:HA3	2.18	0.43
1:B:400:ILE:O	1:B:404:MET:HG3	2.19	0.43
1:B:404:MET:HE1	1:B:451:TRP:CG	2.54	0.43
1:C:341:LYS:HD3	1:C:359:TRP:CZ2	2.53	0.43
1:D:413:PHE:O	1:D:416:VAL:HG12	2.19	0.43
1:C:440:PHE:CD1	1:C:447:LEU:HB2	2.54	0.42
1:C:387:LEU:CD1	1:C:480:VAL:HG23	2.46	0.42
1:C:388:ILE:HD13	1:C:388:ILE:HG21	1.61	0.42
1:D:463:HIS:O	1:D:480:VAL:HG23	2.19	0.42
1:B:404:MET:HE2	1:B:451:TRP:CE2	2.54	0.42
1:B:321:ILE:HA	1:B:334:ARG:HB3	2.02	0.42
1:C:404:MET:HE2	1:C:451:TRP:CE2	2.54	0.42
1:B:465:ILE:O	1:B:475:THR:HA	2.19	0.42
1:D:417:ARG:NH2	1:D:450:GLN:NE2	2.65	0.42
1:C:388:ILE:HG22	1:C:480:VAL:O	2.20	0.41
1:A:331:GLU:O	1:A:367:VAL:HA	2.20	0.41
1:A:456:SER:HB3	1:A:457:PRO:HD2	2.03	0.41
1:B:381:MET:HA	1:B:408:GLN:O	2.20	0.41
1:A:401:ILE:HD11	1:A:444:SER:CB	2.47	0.41
1:A:417:ARG:HE	1:A:417:ARG:HA	1.86	0.41
1:D:437:GLN:HG3	1:D:441:LEU:HD22	2.03	0.41
1:C:483:LYS:HA	1:C:484:ASN:HA	1.75	0.41
1:D:383:LEU:C	1:D:383:LEU:HD23	2.42	0.40
1:D:462:LEU:HG	1:D:480:VAL:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	167/169 (99%)	162 (97%)	5 (3%)	0	100	100
1	B	167/169 (99%)	161 (96%)	6 (4%)	0	100	100
1	C	167/169 (99%)	162 (97%)	5 (3%)	0	100	100
1	D	167/169 (99%)	159 (95%)	6 (4%)	2 (1%)	13	19
All	All	668/676 (99%)	644 (96%)	22 (3%)	2 (0%)	41	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	469	MET
1	D	370	GLY

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	149/149 (100%)	137 (92%)	12 (8%)	11	18
1	B	149/149 (100%)	133 (89%)	16 (11%)	6	9
1	C	149/149 (100%)	138 (93%)	11 (7%)	13	22
1	D	149/149 (100%)	131 (88%)	18 (12%)	5	6
All	All	596/596 (100%)	539 (90%)	57 (10%)	8	12

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
1	A	329	ARG
1	A	347	LEU
1	A	362	GLU

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Mol	Chain	Res	Type
1	A	390	SER
1	A	417	ARG
1	A	419	GLU
1	A	430	LEU
1	A	438	ARG
1	A	447	LEU
1	A	483	LYS
1	A	484	ASN
1	B	317	SER
1	B	323	GLN
1	B	329	ARG
1	B	332	LEU
1	B	347	LEU
1	B	373	ARG
1	B	375	ILE
1	B	385	LYS
1	B	389	ASN
1	B	417	ARG
1	B	419	GLU
1	B	430	LEU
1	B	438	ARG
1	B	460	SER
1	B	467	GLU
1	B	482	THR
1	C	329	ARG
1	C	347	LEU
1	C	378	LYS
1	C	385	LYS
1	C	388	ILE
1	C	417	ARG
1	C	430	LEU
1	C	447	LEU
1	C	468	SER
1	C	483	LYS
1	C	484	ASN
1	D	317	SER
1	D	332	LEU
1	D	338	ARG
1	D	373	ARG
1	D	381	MET
1	D	386	LEU
1	D	390	SER

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Mol	Chain	Res	Type
1	D	402	LEU
1	D	407	SER
1	D	424	ASN
1	D	436	LEU
1	D	441	LEU
1	D	443	ARG
1	D	465	ILE
1	D	466	ASN
1	D	468	SER
1	D	476	LEU
1	D	482	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	GLN
1	A	350	ASN
1	A	354	GLN
1	A	484	ASN
1	B	323	GLN
1	B	354	GLN
1	B	389	ASN
1	B	414	GLN
1	B	450	GLN
1	B	484	ASN
1	C	325	GLN
1	C	354	GLN
1	C	414	GLN
1	C	484	ASN
1	D	414	GLN
1	D	424	ASN
1	D	437	GLN
1	D	450	GLN
1	D	466	ASN
1	D	470	ASN

5.3.3 RNA

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](#)

4 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
2	GDP	D	501	-	24,30,30	1.69	5 (20%)	31,47,47	2.30	8 (25%)
2	GDP	A	501	-	24,30,30	1.29	2 (8%)	31,47,47	2.03	7 (22%)
2	GDP	C	501	-	24,30,30	1.56	4 (16%)	31,47,47	2.29	11 (35%)
2	GDP	B	501	-	24,30,30	1.61	4 (16%)	31,47,47	2.12	10 (32%)

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	D	501	-	-	2/12/32/32	0/3/3/3
2	GDP	A	501	-	-	2/12/32/32	0/3/3/3
2	GDP	C	501	-	-	2/12/32/32	0/3/3/3
2	GDP	B	501	-	-	2/12/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	GDP	C6-C5	5.37	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	GDP	C6-C5	5.00	1.50	1.41
2	B	501	GDP	C6-C5	4.84	1.49	1.41
2	B	501	GDP	O4'-C1'	4.47	1.47	1.41
2	A	501	GDP	C6-C5	4.17	1.48	1.41
2	D	501	GDP	O4'-C1'	2.90	1.45	1.41
2	C	501	GDP	C2-N1	-2.81	1.30	1.35
2	D	501	GDP	C2'-C1'	-2.79	1.49	1.53
2	D	501	GDP	C5-C4	2.59	1.47	1.40
2	C	501	GDP	C5-C4	2.45	1.47	1.40
2	A	501	GDP	C2'-C1'	-2.43	1.50	1.53
2	B	501	GDP	C5-C4	2.42	1.47	1.40
2	D	501	GDP	C8-N7	2.31	1.38	1.34
2	C	501	GDP	C2'-C1'	-2.30	1.50	1.53
2	B	501	GDP	C2'-C1'	-2.29	1.50	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	GDP	C6-C5-C4	-6.57	114.53	120.80
2	C	501	GDP	C6-C5-C4	-6.48	114.61	120.80
2	D	501	GDP	C1'-N9-C4	-5.22	117.47	126.64
2	A	501	GDP	C1'-N9-C4	-4.99	117.88	126.64
2	D	501	GDP	C5-C6-N1	-4.68	117.03	123.43
2	C	501	GDP	C6-N1-C2	4.62	123.27	115.93
2	D	501	GDP	C4-C5-N7	-4.52	104.69	109.40
2	B	501	GDP	C5-C6-N1	-4.43	117.37	123.43
2	B	501	GDP	C6-C5-C4	-4.39	116.60	120.80
2	D	501	GDP	C6-C5-C4	-4.34	116.65	120.80
2	D	501	GDP	C6-N1-C2	4.20	122.60	115.93
2	B	501	GDP	C1'-N9-C4	-4.19	119.27	126.64
2	B	501	GDP	C6-N1-C2	4.03	122.34	115.93
2	C	501	GDP	C2-N3-C4	3.91	119.83	115.36
2	A	501	GDP	C6-N1-C2	3.53	121.53	115.93
2	C	501	GDP	C1'-N9-C4	-3.36	120.74	126.64
2	C	501	GDP	N2-C2-N3	3.27	123.13	117.79
2	C	501	GDP	C5-C6-N1	-3.19	119.07	123.43
2	D	501	GDP	O3B-PB-O3A	-3.12	94.17	104.64
2	D	501	GDP	C2-N3-C4	3.11	118.91	115.36
2	C	501	GDP	N3-C2-N1	-3.11	123.07	127.22
2	B	501	GDP	PA-O3A-PB	-3.10	122.20	132.83
2	B	501	GDP	C4-C5-N7	-2.90	106.38	109.40
2	C	501	GDP	PA-O3A-PB	-2.86	123.02	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	GDP	C5'-C4'-C3'	-2.57	105.54	115.18
2	B	501	GDP	O2A-PA-O1A	2.57	124.95	112.24
2	C	501	GDP	C4-C5-N7	-2.43	106.87	109.40
2	B	501	GDP	O2B-PB-O3A	-2.35	96.74	104.64
2	B	501	GDP	O3B-PB-O3A	2.31	112.39	104.64
2	A	501	GDP	C5-C6-N1	-2.30	120.28	123.43
2	A	501	GDP	C2-N3-C4	2.27	117.95	115.36
2	C	501	GDP	N2-C2-N1	-2.26	113.74	117.25
2	C	501	GDP	O5'-C5'-C4'	-2.22	101.36	108.99
2	A	501	GDP	PA-O3A-PB	-2.16	125.43	132.83
2	A	501	GDP	N3-C2-N1	-2.08	124.44	127.22
2	D	501	GDP	N3-C2-N1	-2.08	124.45	127.22

There are no chirality outliers.

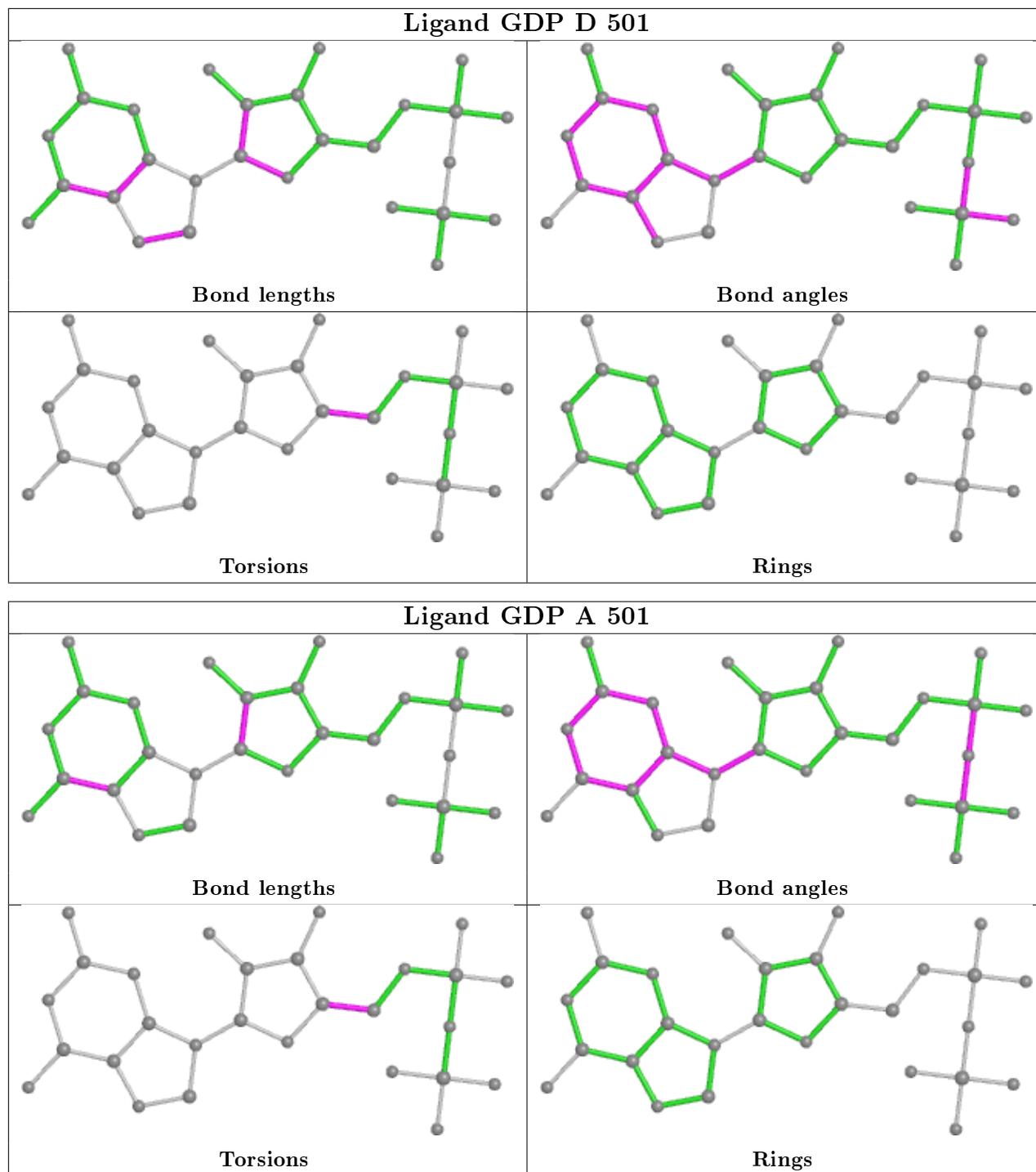
All (8) torsion outliers are listed below:

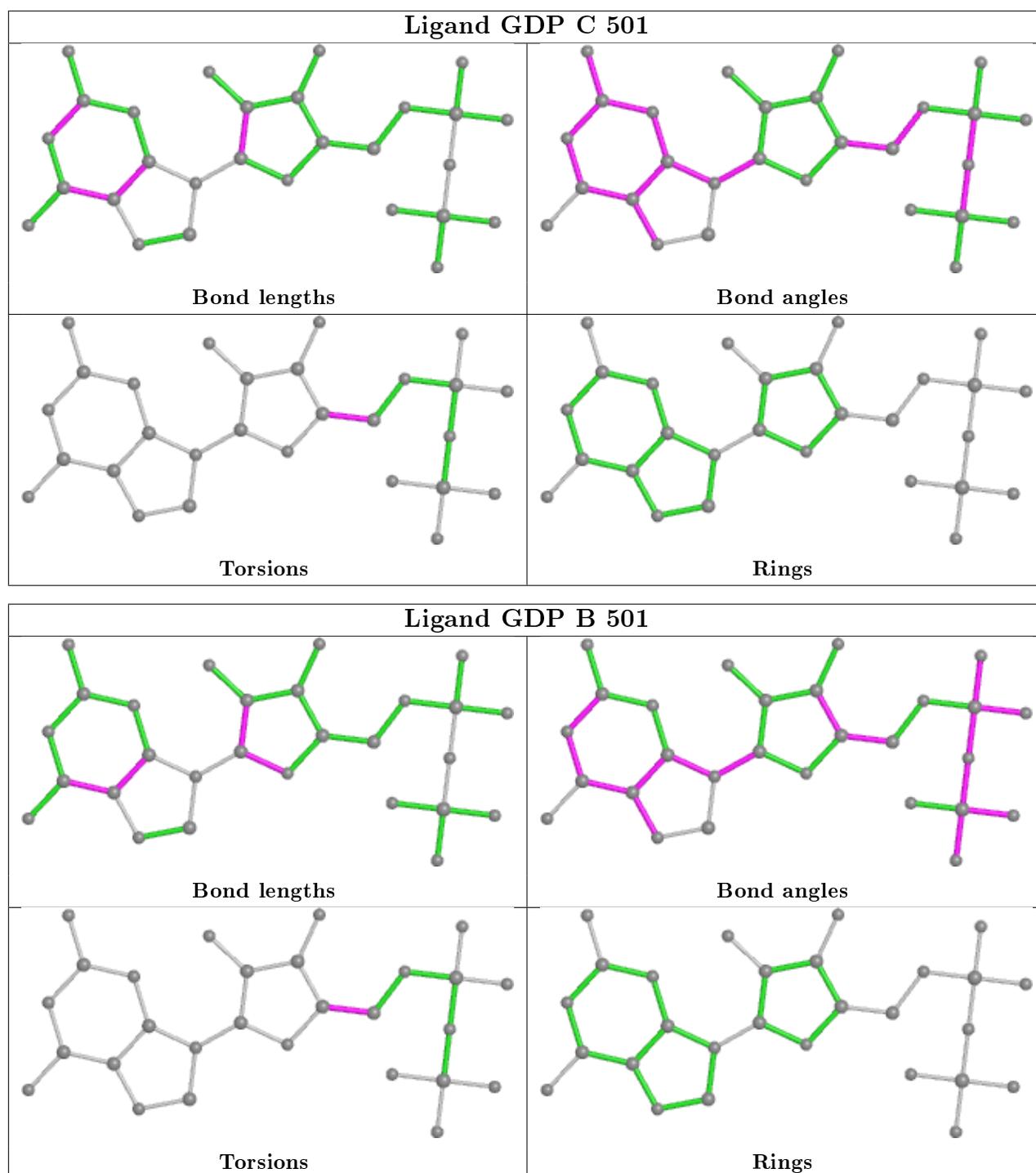
Mol	Chain	Res	Type	Atoms
2	A	501	GDP	O4'-C4'-C5'-O5'
2	C	501	GDP	O4'-C4'-C5'-O5'
2	D	501	GDP	O4'-C4'-C5'-O5'
2	D	501	GDP	C3'-C4'-C5'-O5'
2	B	501	GDP	O4'-C4'-C5'-O5'
2	B	501	GDP	C3'-C4'-C5'-O5'
2	A	501	GDP	C3'-C4'-C5'-O5'
2	C	501	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	169/169 (100%)	-0.42	1 (0%) 89 88	19, 29, 49, 58	0
1	B	169/169 (100%)	-0.40	1 (0%) 89 88	13, 30, 49, 58	1 (0%)
1	C	169/169 (100%)	-0.36	1 (0%) 89 88	13, 29, 46, 56	2 (1%)
1	D	169/169 (100%)	-0.43	0 100 100	18, 30, 47, 54	0
All	All	676/676 (100%)	-0.40	3 (0%) 92 91	13, 30, 48, 58	3 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	PHE	2.3
1	A	425	ARG	2.1
1	C	434	TYR	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](#)

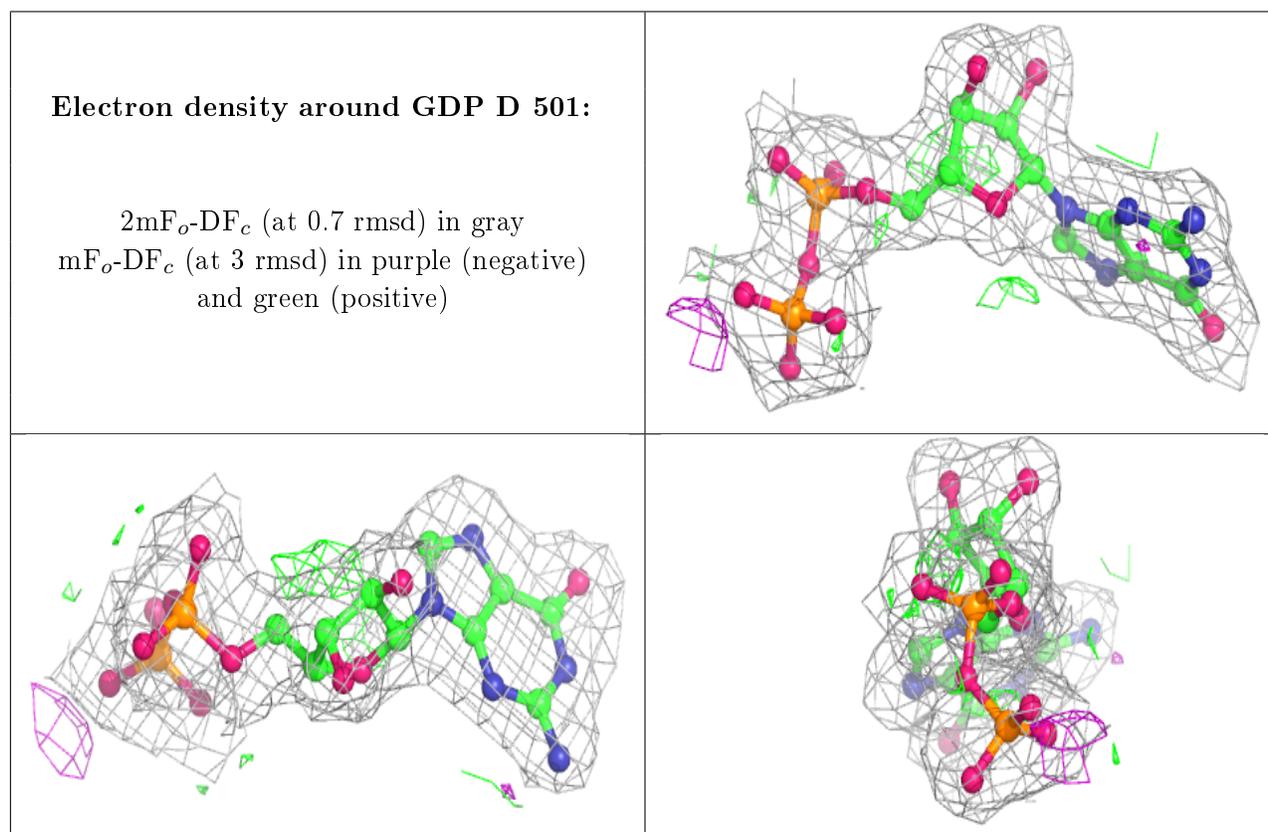
There are no carbohydrates in this entry.

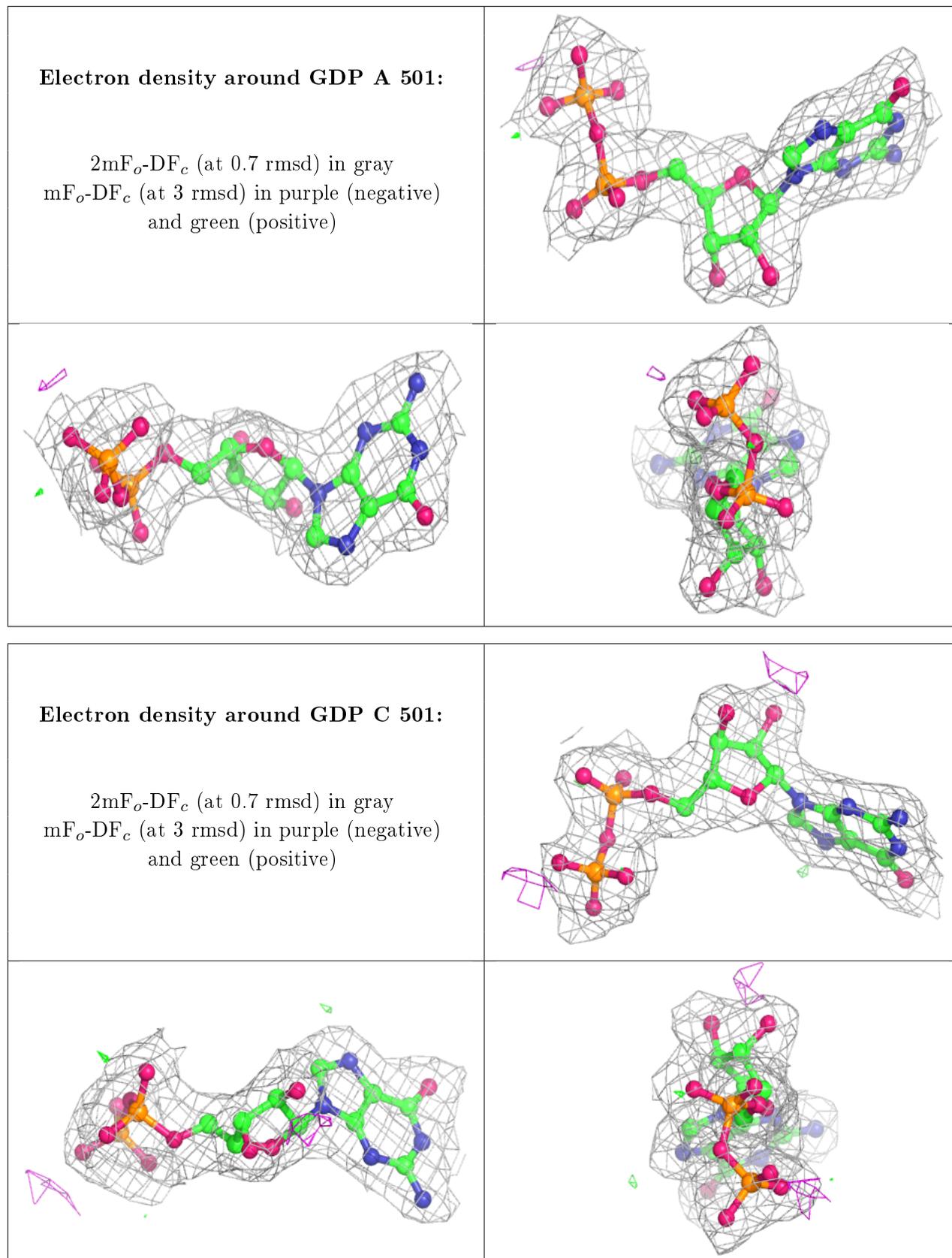
6.4 Ligands [i](#)

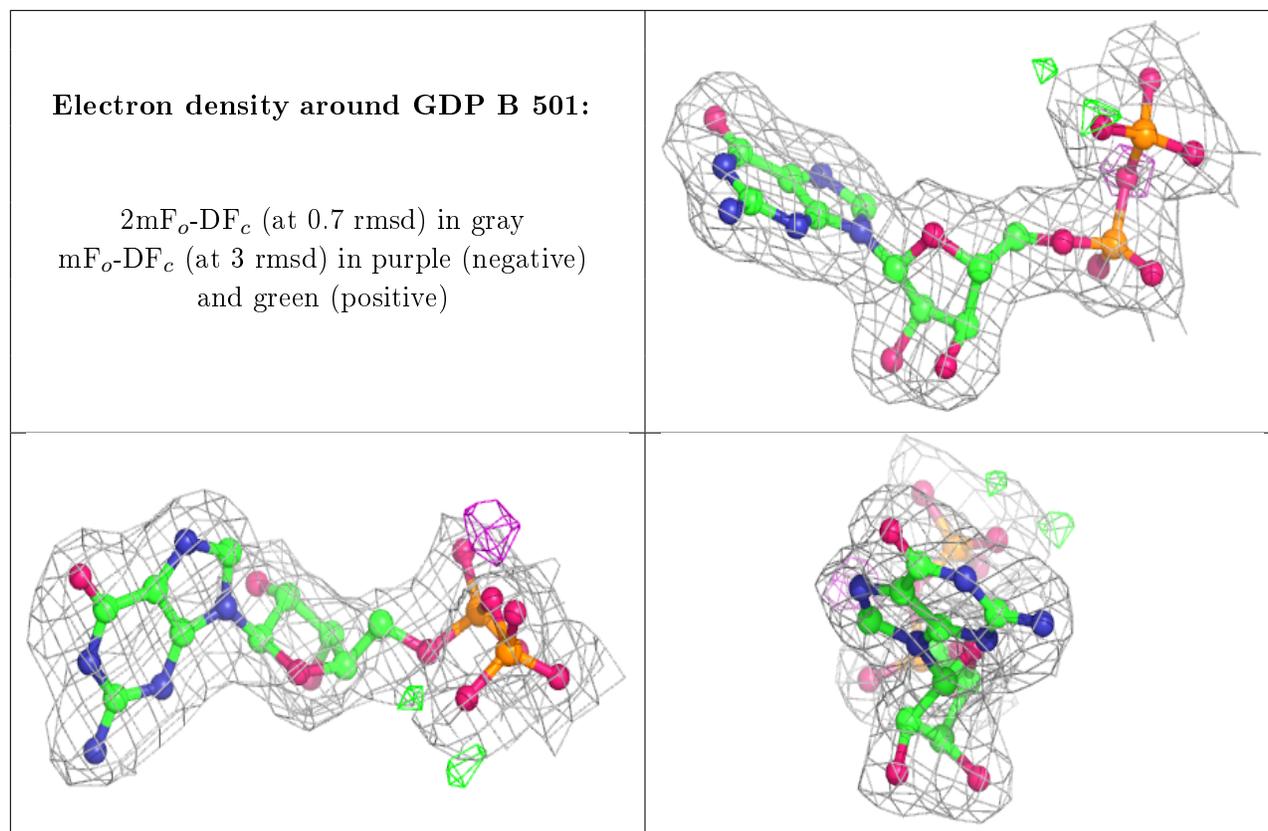
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GDP	D	501	28/28	0.98	0.10	14,19,22,24	0
2	GDP	A	501	28/28	0.98	0.11	8,19,23,24	0
2	GDP	C	501	28/28	0.98	0.10	10,19,24,25	0
2	GDP	B	501	28/28	0.98	0.10	8,15,21,22	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.







6.5 Other polymers [i](#)

There are no such residues in this entry.