



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 01:54 PM EST

PDB ID : 4NXV
Title : Crystal structure of the cytosolic domain of human MiD51
Authors : Richter, V.; Kvansakul, M.; Ryan, M.T.
Deposited on : 2013-12-09
Resolution : 2.30 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 types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

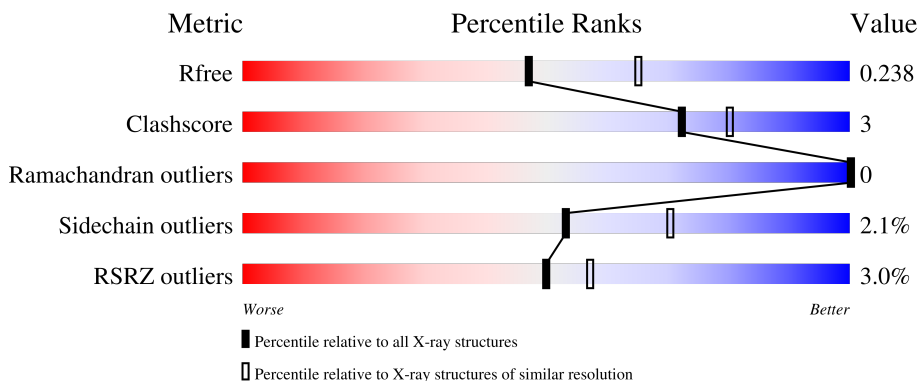
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	347	 2% 88% 6% • 5%
1	B	347	 % 88% 6% 5%
1	C	347	 3% 86% 11% • •
1	D	347	 5% 81% 14% 5%

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
4	GOL	C	502	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21344 atoms, of which 10472 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.

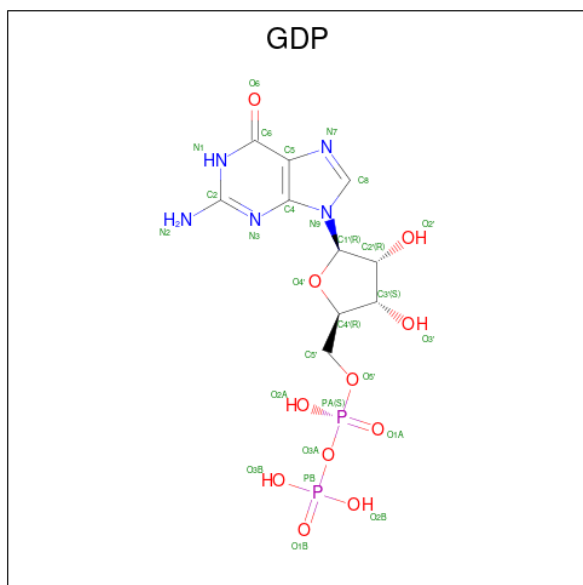
- Molecule 1 is a protein called Mitochondrial dynamic protein MID51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	330	5179	1657	2594	436	480	12	0	1	0
1	B	330	5204	1661	2613	438	480	12	0	0	0
1	C	337	5255	1682	2631	444	486	12	0	0	0
1	D	331	5156	1656	2578	432	478	12	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLY	-	expression tag	UNP Q9NQG6
A	118	SER	-	expression tag	UNP Q9NQG6
B	117	GLY	-	expression tag	UNP Q9NQG6
B	118	SER	-	expression tag	UNP Q9NQG6
C	117	GLY	-	expression tag	UNP Q9NQG6
C	118	SER	-	expression tag	UNP Q9NQG6
D	117	GLY	-	expression tag	UNP Q9NQG6
D	118	SER	-	expression tag	UNP Q9NQG6

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



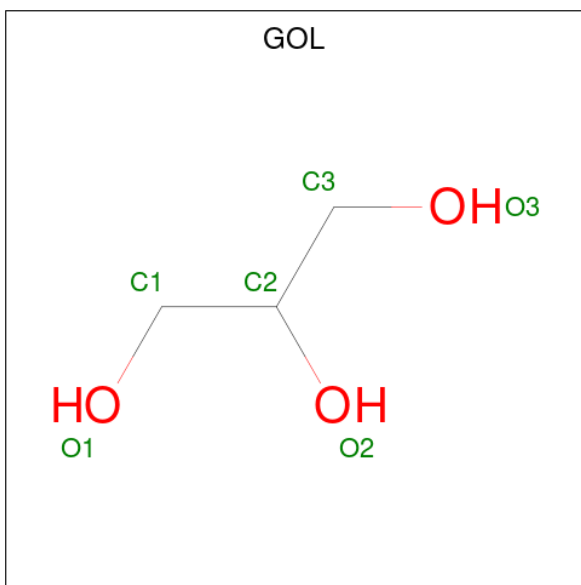
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		
2	B	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		
2	C	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		
2	D	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C H O 14 3 8 3	0	0

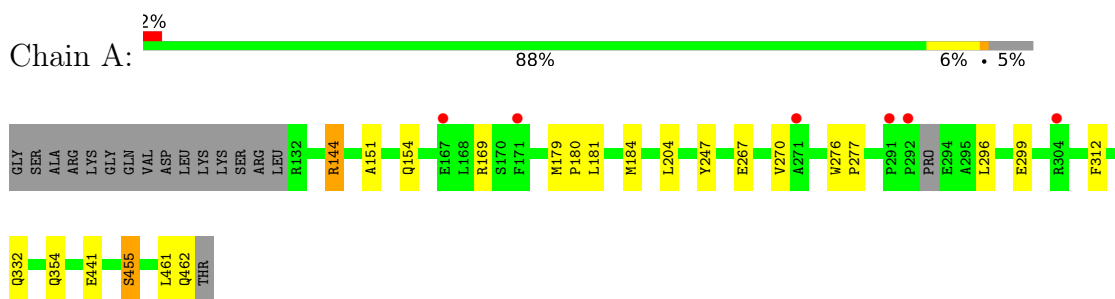
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	96	Total O 96 96	0	0
5	B	113	Total O 113 113	0	0
5	C	99	Total O 99 99	0	0
5	D	48	Total O 48 48	0	0

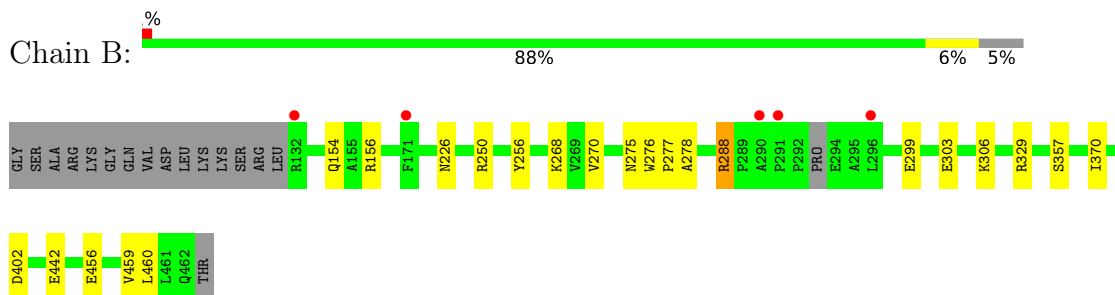
3 Residue-property plots [i](#)

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.

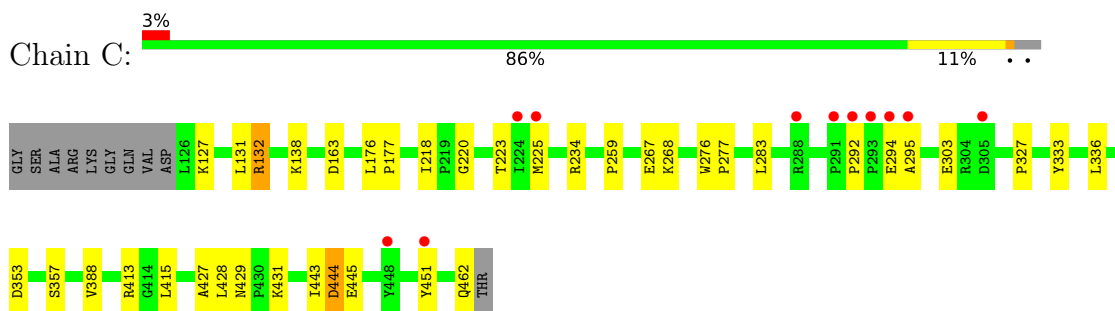
- Molecule 1: Mitochondrial dynamic protein MID51



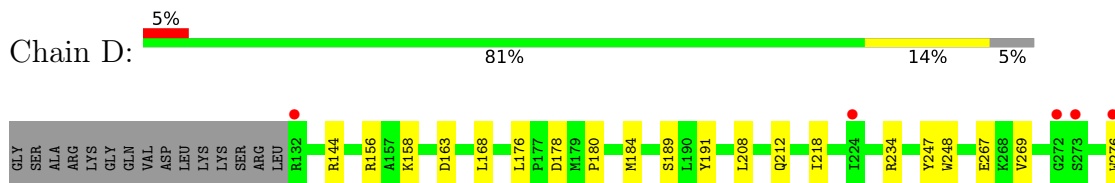
- Molecule 1: Mitochondrial dynamic protein MID51

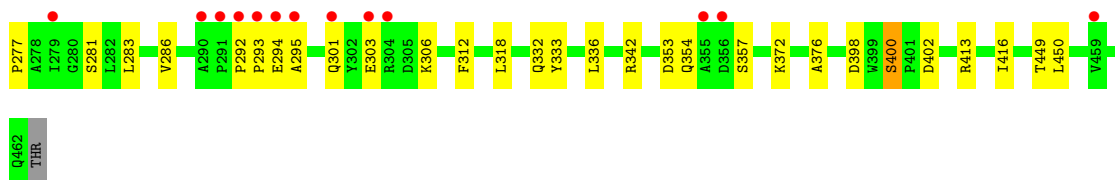


- Molecule 1: Mitochondrial dynamic protein MID51



- Molecule 1: Mitochondrial dynamic protein MID51





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.34Å 79.09Å 80.05Å 65.81° 84.36° 64.08°	Depositor
Resolution (Å)	39.05 – 2.30 39.05 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.05-2.30) 98.1 (39.05-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.191 , 0.237 0.193 , 0.238	Depositor DCC
R_{free} test set	3169 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtrriage
Anisotropy	0.508	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21344	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, GDP, GOL

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	0.26	0/2645	0.47	0/3608
1	B	0.26	0/2648	0.46	0/3609
1	C	0.26	0/2683	0.48	0/3662
1	D	0.25	0/2641	0.46	0/3608
All	All	0.26	0/10617	0.47	0/14487

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2585	2594	2589	17	1
1	B	2591	2613	2609	11	1
1	C	2624	2631	2626	23	0
1	D	2578	2578	2572	26	0
2	A	28	12	12	1	0
2	B	28	12	12	0	0
2	C	28	12	12	0	0
2	D	28	12	12	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	1	0
4	C	6	8	8	2	0
5	A	96	0	0	2	0
5	B	113	0	0	2	0
5	C	99	0	0	2	0
5	D	48	0	0	1	0
All	All	10872	10472	10452	72	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 3.

All (72) 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:250:ARG:NH1	3:B:504:SO4:O4	2.01	0.93
1:B:156:ARG:NH1	1:B:303:GLU:OE2	2.08	0.86
1:A:144:ARG:NH2	1:C:444:ASP:OD1	2.16	0.79
1:D:372:LYS:NZ	5:D:637:HOH:O	2.15	0.79
1:B:154:GLN:NE2	5:B:652:HOH:O	2.29	0.66
1:C:292:PRO:HA	1:C:294:GLU:H	1.62	0.63
1:A:144:ARG:NH2	1:C:444:ASP:O	2.32	0.62
1:D:376:ALA:HB1	1:D:449:THR:HG21	1.81	0.61
1:A:169:ARG:NH2	5:A:624:HOH:O	2.36	0.58
1:A:332:GLN:OE1	5:A:683:HOH:O	2.17	0.58
1:B:303:GLU:HG2	1:B:306:LYS:HB2	1.86	0.57
1:B:299:GLU:OE1	5:B:658:HOH:O	2.18	0.57
1:C:327:PRO:HA	4:C:502:GOL:H32	1.87	0.57
1:D:156:ARG:NE	1:D:303:GLU:OE2	2.36	0.57
1:D:353:ASP:O	1:D:357:SER:N	2.38	0.56
1:D:292:PRO:HB3	1:D:295:ALA:HB2	1.87	0.56
1:D:163:ASP:HB3	1:D:283:LEU:HD22	1.88	0.55
1:A:299:GLU:OE2	1:B:288:ARG:NH1	2.31	0.54
1:A:461:LEU:O	1:A:462:GLN:HB2	2.06	0.54
1:B:357:SER:O	1:D:413:ARG:NH1	2.40	0.54
1:C:138:LYS:NZ	5:C:684:HOH:O	2.41	0.53
1:A:441:GLU:N	1:A:441:GLU:OE1	2.41	0.53
1:D:402:ASP:OD1	1:D:402:ASP:N	2.42	0.52
1:D:184:MET:HE1	1:D:312:PHE:HE2	1.74	0.51
1:A:179:MET:HG2	1:A:181:LEU:HG	1.93	0.51
1:A:184:MET:HB3	1:A:204:LEU:HD22	1.94	0.48
1:D:180:PRO:HG2	1:D:247:TYR:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:VAL:HB	1:D:301:GLN:HB3	1.96	0.47
1:D:398:ASP:OD1	1:D:400:SER:OG	2.34	0.46
1:C:176:LEU:N	1:C:177:PRO:CD	2.79	0.46
1:D:333:TYR:HB3	1:D:336:LEU:HD12	1.98	0.45
1:C:428:LEU:HD12	1:C:428:LEU:N	2.32	0.45
1:A:180:PRO:HG2	1:A:247:TYR:HB3	1.98	0.45
1:A:354:GLN:HA	1:C:413:ARG:HH12	1.82	0.45
1:A:267:GLU:HB2	1:A:296:LEU:CD1	2.47	0.44
1:D:267:GLU:OE2	1:D:295:ALA:HB1	2.17	0.44
1:C:220:GLY:O	1:C:223:THR:OG1	2.30	0.44
1:C:259:PRO:HB2	4:C:502:GOL:H2	1.99	0.44
2:A:501:GDP:H2'	2:A:501:GDP:N3	2.33	0.44
1:D:212:GLN:HE22	1:D:318:LEU:HD23	1.83	0.44
1:B:275:ASN:ND2	1:B:278:ALA:HB2	2.34	0.43
1:C:333:TYR:HB3	1:C:336:LEU:HD12	1.99	0.43
1:C:163:ASP:HB3	1:C:283:LEU:HD22	2.00	0.43
1:C:218:ILE:HD11	1:C:234:ARG:CZ	2.48	0.43
1:C:388:VAL:HG21	1:C:415:LEU:HD13	1.99	0.43
1:A:276:TRP:N	1:A:277:PRO:CD	2.82	0.43
1:B:276:TRP:HB2	1:B:277:PRO:HD3	1.99	0.43
1:A:179:MET:SD	1:A:181:LEU:HD11	2.59	0.43
1:B:370:ILE:HG21	1:B:460:LEU:HG	2.01	0.43
1:C:132:ARG:HG2	1:C:132:ARG:HH11	1.83	0.42
1:D:189:SER:HA	1:D:342:ARG:NH2	2.34	0.42
1:C:225:MET:SD	1:C:336:LEU:HD11	2.60	0.42
1:A:151:ALA:CB	1:C:443:ILE:HG21	2.49	0.42
1:D:303:GLU:HB2	1:D:306:LYS:HB2	2.00	0.42
1:A:296:LEU:HG	1:A:312:PHE:HB2	2.00	0.41
1:B:329:ARG:NH2	1:B:442:GLU:OE1	2.38	0.41
1:D:176:LEU:C	1:D:178:ASP:H	2.24	0.41
1:C:276:TRP:N	1:C:277:PRO:CD	2.84	0.41
1:D:293:PRO:HA	1:D:294:GLU:HA	1.77	0.41
1:C:267:GLU:OE2	1:C:295:ALA:HB1	2.20	0.41
1:D:158:LYS:HE3	1:D:191:TYR:HA	2.03	0.41
1:D:416:ILE:HG13	1:D:450:LEU:HD13	2.02	0.41
1:C:303:GLU:OE1	5:C:692:HOH:O	2.22	0.41
1:D:168:LEU:HD13	1:D:184:MET:HE1	2.03	0.41
1:D:208:LEU:HG	1:D:248:TRP:CZ2	2.55	0.41
1:C:127:LYS:O	1:C:131:LEU:HG	2.20	0.40
1:D:218:ILE:HD11	1:D:234:ARG:CZ	2.51	0.40
1:C:427:ALA:HB3	1:C:428:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:TRP:N	1:D:277:PRO:CD	2.83	0.40
1:A:184:MET:HE1	1:A:312:PHE:HE2	1.86	0.40
1:C:353:ASP:O	1:C:357:SER:N	2.54	0.40
1:D:176:LEU:CD1	1:D:269:VAL:HG12	2.51	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:455:SER:OG	1:B:256:TYR:OH[1_655]	2.19	0.01

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	327/347 (94%)	320 (98%)	7 (2%)	0	100	100
1	B	326/347 (94%)	321 (98%)	5 (2%)	0	100	100
1	C	335/347 (96%)	324 (97%)	11 (3%)	0	100	100
1	D	330/347 (95%)	320 (97%)	10 (3%)	0	100	100
All	All	1318/1388 (95%)	1285 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	280/298 (94%)	276 (99%)	4 (1%)	67	81
1	B	282/298 (95%)	275 (98%)	7 (2%)	47	65
1	C	283/298 (95%)	275 (97%)	8 (3%)	43	60
1	D	278/298 (93%)	273 (98%)	5 (2%)	59	75
All	All	1123/1192 (94%)	1099 (98%)	24 (2%)	53	70

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ARG
1	A	154	GLN
1	A	270	VAL
1	A	455	SER
1	B	226	ASN
1	B	268	LYS
1	B	270	VAL
1	B	288	ARG
1	B	402	ASP
1	B	456	GLU
1	B	459	VAL
1	C	132	ARG
1	C	268	LYS
1	C	429	ASN
1	C	431	LYS
1	C	444	ASP
1	C	445	GLU
1	C	451	TYR
1	C	462	GLN
1	D	144	ARG
1	D	281	SER
1	D	332	GLN
1	D	354	GLN
1	D	400	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	301	GLN
1	C	307	HIS
1	C	429	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	C	501	-	24,30,30	1.90	3 (12%)	30,47,47	1.52	7 (23%)
2	GDP	D	501	-	24,30,30	1.89	3 (12%)	30,47,47	1.50	6 (20%)
2	GDP	B	501	-	24,30,30	1.87	3 (12%)	30,47,47	1.47	7 (23%)
2	GDP	A	501	-	24,30,30	1.89	4 (16%)	30,47,47	1.55	8 (26%)
3	SO4	B	504	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	502	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	B	503	-	4,4,4	0.16	0	6,6,6	0.09	0
3	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.05	0
4	GOL	C	502	-	5,5,5	0.33	0	5,5,5	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	C	501	-	-	4/12/32/32	0/3/3/3
2	GDP	D	501	-	-	6/12/32/32	0/3/3/3
2	GDP	B	501	-	-	3/12/32/32	0/3/3/3
2	GDP	A	501	-	-	6/12/32/32	0/3/3/3
4	GOL	C	502	-	-	4/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	GDP	C2-N2	5.51	1.47	1.34
2	D	501	GDP	C2-N2	5.49	1.47	1.34
2	B	501	GDP	C2-N2	5.43	1.47	1.34
2	A	501	GDP	C2-N2	5.40	1.47	1.34
2	A	501	GDP	C4-N3	4.62	1.48	1.37
2	D	501	GDP	C4-N3	4.61	1.48	1.37
2	C	501	GDP	C4-N3	4.59	1.48	1.37
2	B	501	GDP	C4-N3	4.52	1.48	1.37
2	C	501	GDP	C2-N1	2.94	1.44	1.37
2	B	501	GDP	C2-N1	2.91	1.44	1.37
2	A	501	GDP	C2-N1	2.86	1.44	1.37
2	D	501	GDP	C2-N1	2.84	1.44	1.37
2	A	501	GDP	C5-C6	-2.03	1.43	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	GDP	PA-O3A-PB	-3.58	120.55	132.83
2	A	501	GDP	PA-O3A-PB	-3.43	121.05	132.83
2	C	501	GDP	C8-N7-C5	3.31	109.29	102.99
2	A	501	GDP	C8-N7-C5	3.25	109.17	102.99
2	C	501	GDP	PA-O3A-PB	-3.21	121.81	132.83
2	D	501	GDP	C8-N7-C5	3.19	109.06	102.99
2	B	501	GDP	C8-N7-C5	3.18	109.04	102.99
2	B	501	GDP	PA-O3A-PB	-3.06	122.32	132.83
2	C	501	GDP	N1-C2-N3	-2.98	117.76	123.32
2	A	501	GDP	N1-C2-N3	-2.96	117.80	123.32
2	D	501	GDP	N1-C2-N3	-2.92	117.86	123.32
2	B	501	GDP	N1-C2-N3	-2.88	117.93	123.32
2	A	501	GDP	C5-C6-N1	2.73	118.77	113.95
2	D	501	GDP	C5-C6-N1	2.56	118.48	113.95
2	C	501	GDP	O4'-C4'-C3'	2.50	110.07	105.11
2	C	501	GDP	C5-C6-N1	2.48	118.33	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	GDP	C5-C6-N1	2.42	118.22	113.95
2	C	501	GDP	C3'-C2'-C1'	2.38	104.56	100.98
2	B	501	GDP	N2-C2-N1	2.37	121.75	116.71
2	A	501	GDP	N2-C2-N1	2.36	121.73	116.71
2	B	501	GDP	O4'-C4'-C3'	2.33	109.73	105.11
2	A	501	GDP	C3'-C2'-C1'	2.32	104.47	100.98
2	D	501	GDP	C3'-C2'-C1'	2.31	104.46	100.98
2	C	501	GDP	N2-C2-N1	2.31	121.64	116.71
2	D	501	GDP	N2-C2-N1	2.24	121.48	116.71
2	B	501	GDP	C3'-C2'-C1'	2.21	104.30	100.98
2	A	501	GDP	O4'-C4'-C3'	2.13	109.33	105.11
2	A	501	GDP	O6-C6-C5	-2.07	120.32	124.37

There are no chirality outliers.

All (23) torsion outliers are listed below:

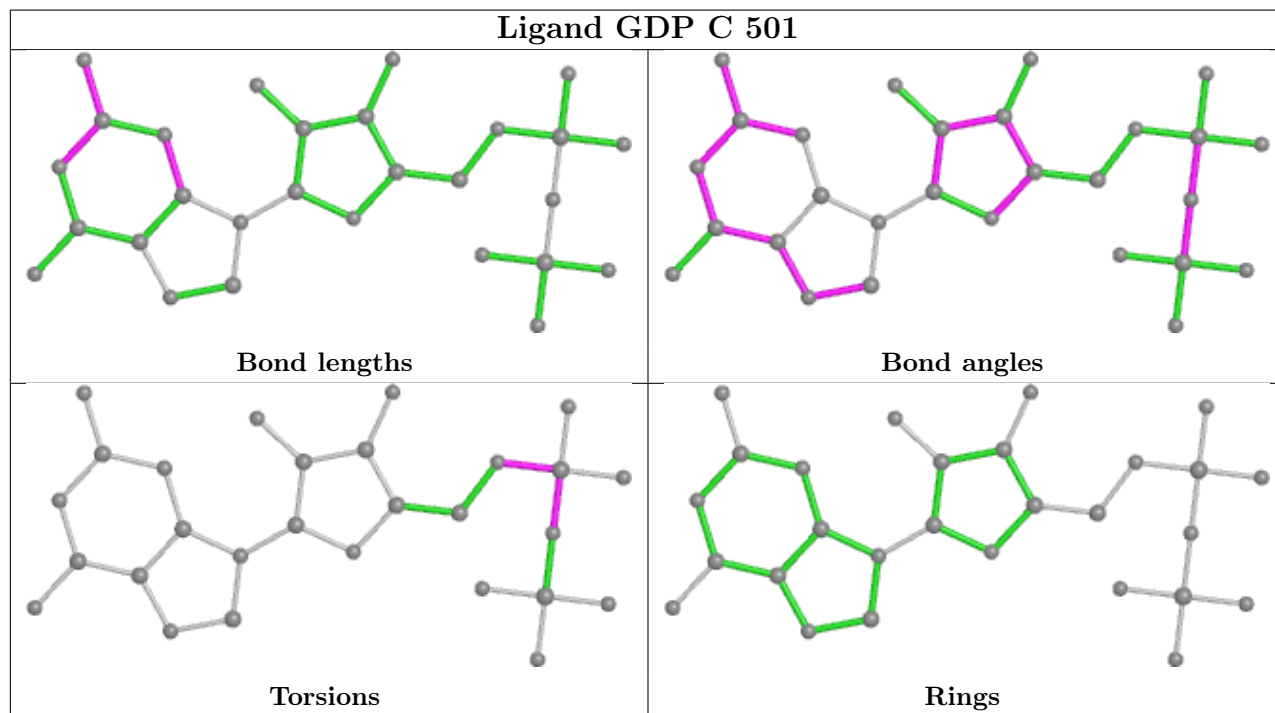
Mol	Chain	Res	Type	Atoms
2	A	501	GDP	PA-O3A-PB-O3B
2	A	501	GDP	PB-O3A-PA-O5'
2	A	501	GDP	C3'-C4'-C5'-O5'
2	C	501	GDP	C5'-O5'-PA-O1A
2	C	501	GDP	C5'-O5'-PA-O2A
2	D	501	GDP	PA-O3A-PB-O2B
2	D	501	GDP	O4'-C4'-C5'-O5'
2	D	501	GDP	C3'-C4'-C5'-O5'
4	C	502	GOL	C1-C2-C3-O3
4	C	502	GOL	O2-C2-C3-O3
2	A	501	GDP	O4'-C4'-C5'-O5'
2	B	501	GDP	PB-O3A-PA-O1A
2	C	501	GDP	PB-O3A-PA-O1A
4	C	502	GOL	O1-C1-C2-O2
2	D	501	GDP	PB-O3A-PA-O5'
2	D	501	GDP	PA-O3A-PB-O3B
2	B	501	GDP	C5'-O5'-PA-O3A
2	C	501	GDP	C5'-O5'-PA-O3A
2	B	501	GDP	C5'-O5'-PA-O1A
2	A	501	GDP	PA-O3A-PB-O2B
4	C	502	GOL	O1-C1-C2-C3
2	D	501	GDP	C5'-O5'-PA-O1A
2	A	501	GDP	PA-O3A-PB-O1B

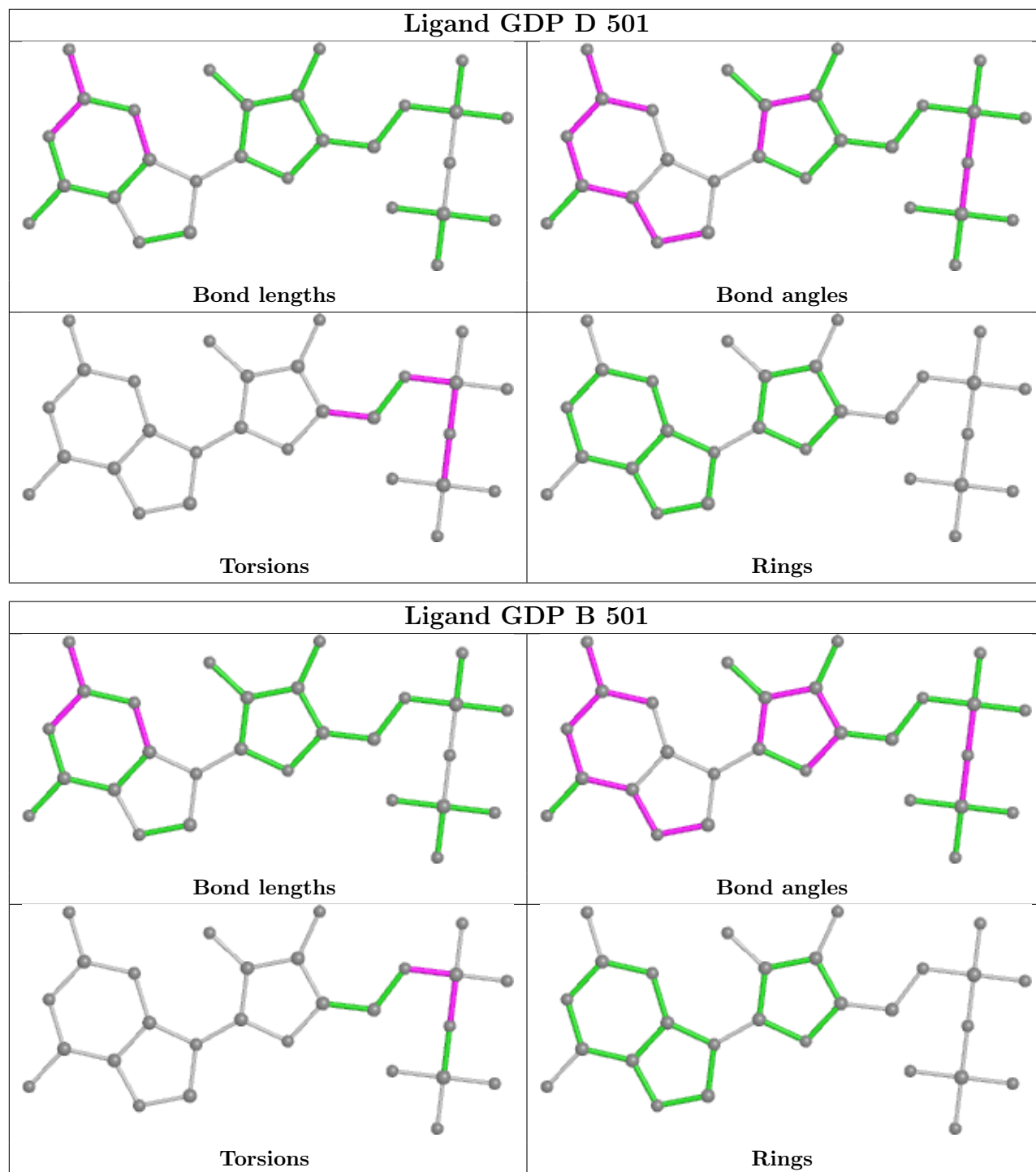
There are no ring outliers.

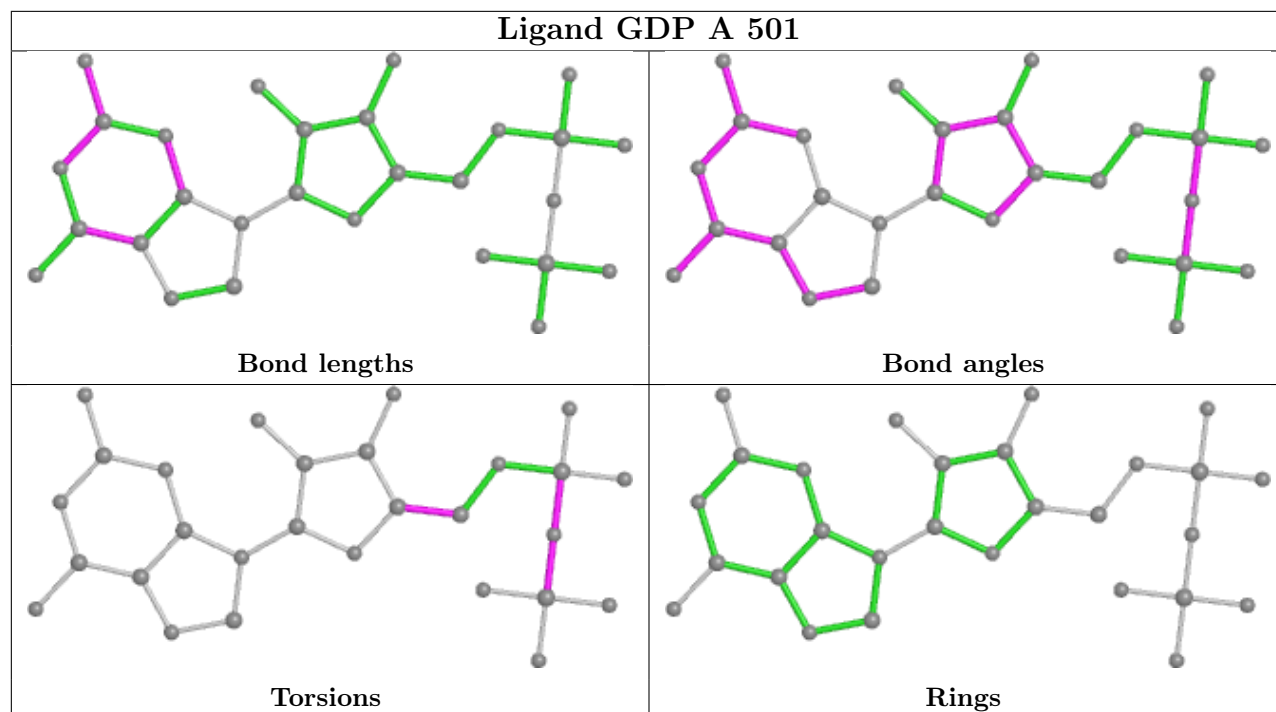
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GDP	1	0
3	B	504	SO4	1	0
4	C	502	GOL	2	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, 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	330/347 (95%)	-0.09	6 (1%) 68 74	27, 43, 71, 94	0
1	B	330/347 (95%)	-0.26	5 (1%) 73 79	23, 40, 70, 98	0
1	C	337/347 (97%)	-0.20	11 (3%) 46 53	25, 42, 73, 103	0
1	D	331/347 (95%)	0.06	18 (5%) 25 32	29, 52, 85, 125	0
All	All	1328/1388 (95%)	-0.12	40 (3%) 50 57	23, 45, 77, 125	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	295	ALA	6.3
1	D	293	PRO	5.3
1	D	291	PRO	4.9
1	D	295	ALA	4.7
1	B	291	PRO	4.4
1	C	451	TYR	4.4
1	D	294	GLU	3.9
1	C	293	PRO	3.7
1	A	304	ARG	3.7
1	C	225	MET	3.6
1	B	296	LEU	3.6
1	D	355	ALA	3.4
1	C	224	ILE	3.3
1	C	292	PRO	3.3
1	D	272	GLY	3.2
1	D	224	ILE	3.2
1	D	290	ALA	3.2
1	A	292	PRO	3.2
1	D	292	PRO	3.2
1	B	290	ALA	3.0
1	A	291	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	291	PRO	2.7
1	C	294	GLU	2.6
1	D	304	ARG	2.6
1	D	279	ILE	2.5
1	C	305	ASP	2.4
1	C	448	TYR	2.3
1	D	459	VAL	2.3
1	B	171	PHE	2.3
1	D	276	TRP	2.2
1	C	288	ARG	2.2
1	D	273	SER	2.1
1	D	132	ARG	2.1
1	D	356	ASP	2.1
1	D	303	GLU	2.1
1	B	132	ARG	2.1
1	D	301	GLN	2.0
1	A	171	PHE	2.0
1	A	167	GLU	2.0
1	A	271	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

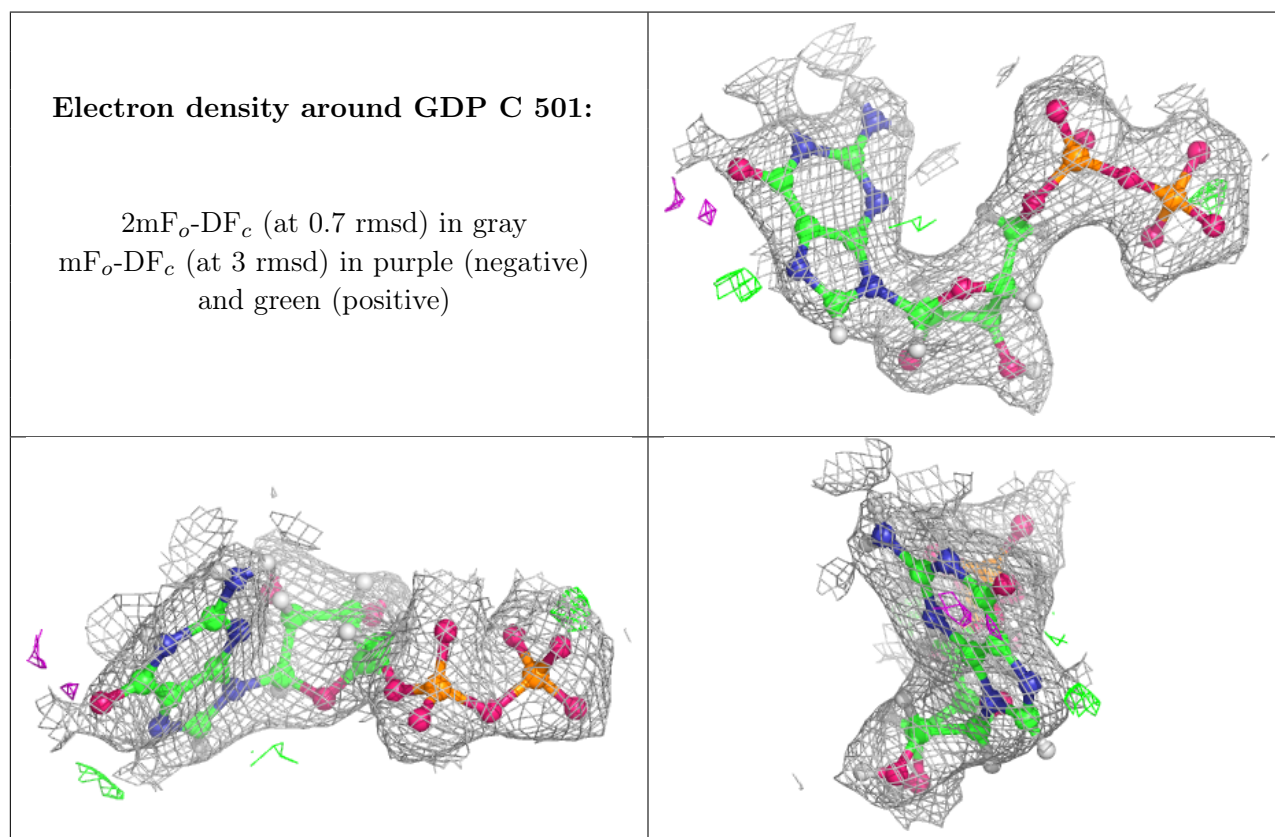
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	C	502	6/6	0.50	0.60	52,62,69,76	14
3	SO4	B	504	5/5	0.61	0.29	105,106,108,109	0
3	SO4	A	502	5/5	0.92	0.16	95,98,101,101	0
2	GDP	C	501	28/28	0.96	0.12	31,47,60,77	0

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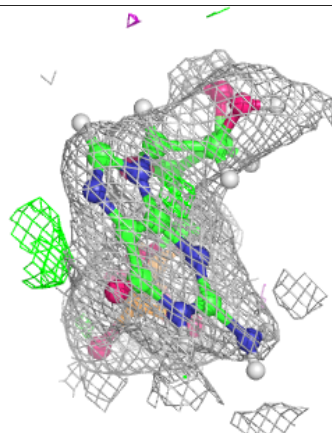
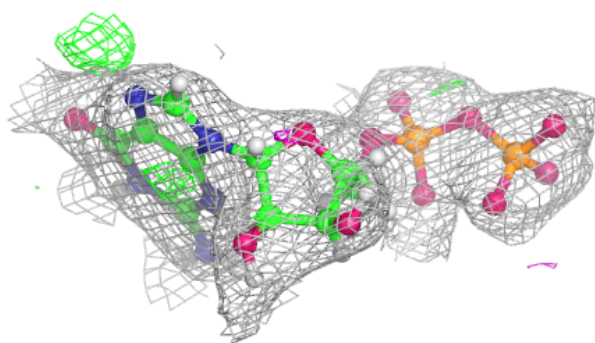
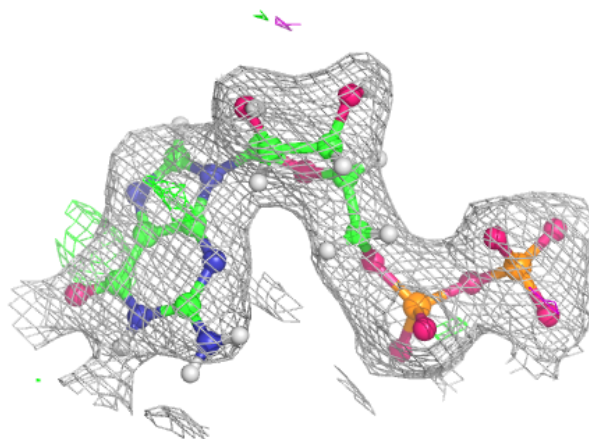
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GDP	B	501	28/28	0.96	0.14	34,44,53,55	0
2	GDP	D	501	28/28	0.97	0.14	38,44,53,90	0
2	GDP	A	501	28/28	0.97	0.20	35,45,55,56	0
3	SO4	B	502	5/5	0.98	0.07	37,46,47,51	0
3	SO4	B	503	5/5	0.98	0.12	40,40,46,53	0

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



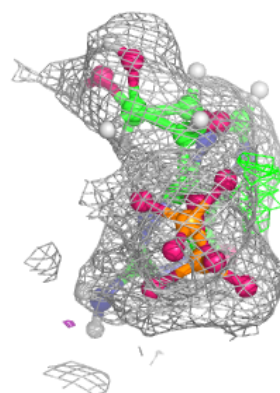
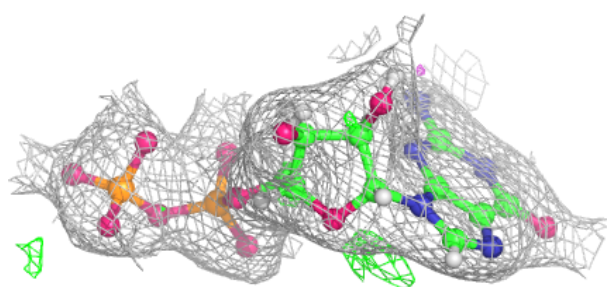
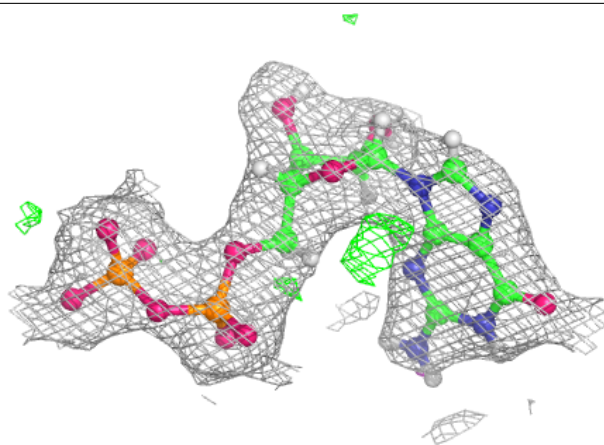
Electron density around GDP B 501:

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

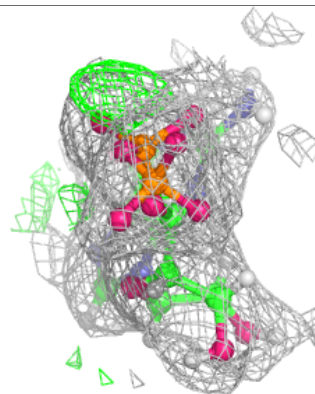
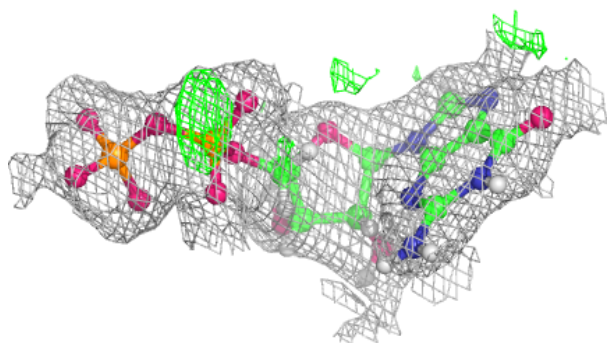
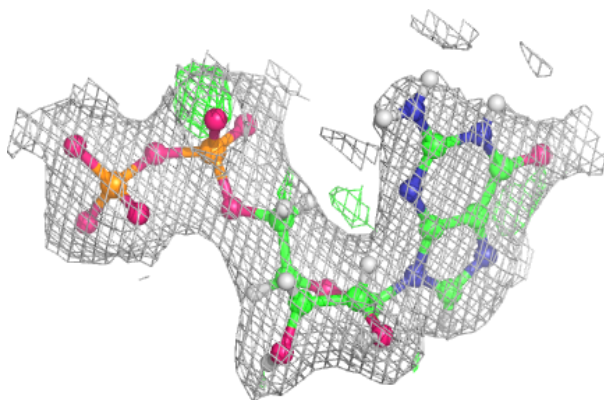


Electron density around GDP D 501:

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

**Electron density around GDP A 501:**

$2mF_o-DF_c$ (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.