Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 05:56 PM EST

PDB ID	:	3D6T
Title	:	Structure of the ROC domain from the Parkinson's disease-associated leucine-rich repeat kinase 2 reveals a dimeric GTPase
Authors	:	Deng, J.
Deposited on	:	2008-05-20
Resolution	:	2.43 Å(reported)

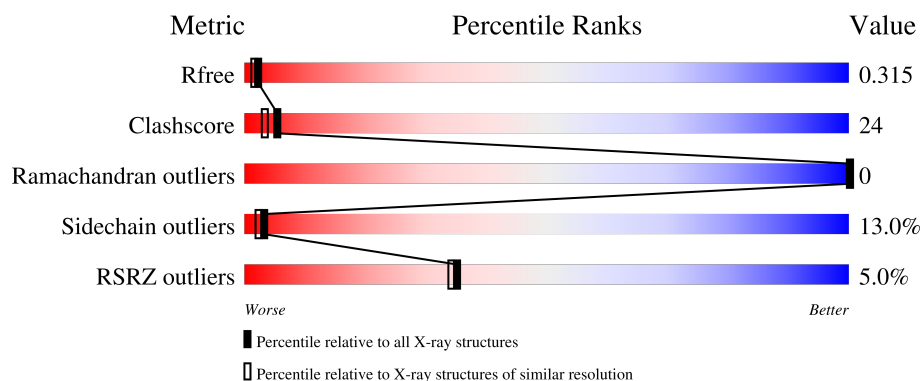# 1   Overall quality at a glance   ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	Percentile Ranks	Value
Rfree		0.315
Clashscore		24
Ramachandran outliers		0
Sidechain outliers		13.0%
RSRZ outliers		5.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	B	171	4% ▮ 49% 19% 6% 27%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 1029 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 Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	B	125	994	646	165	178	5	36	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1335	MSE	-	initiating methionine	UNP Q5S007

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
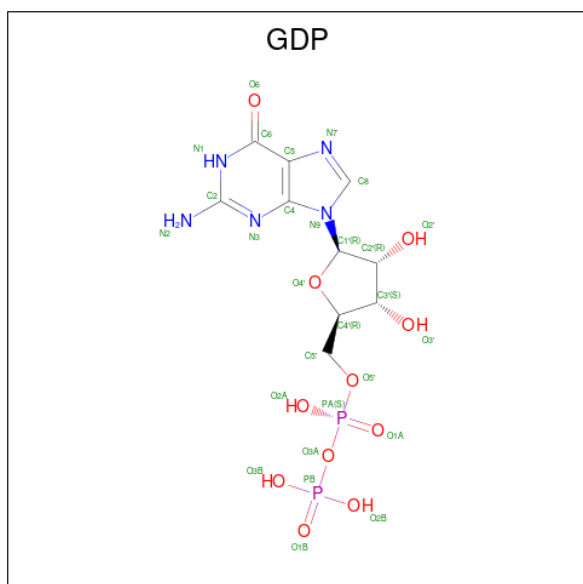
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total	O	0	0
			6	6		

3 Residue-property plots ⓘ

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. 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. 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: Leucine-rich repeat serine/threonine-protein kinase 2
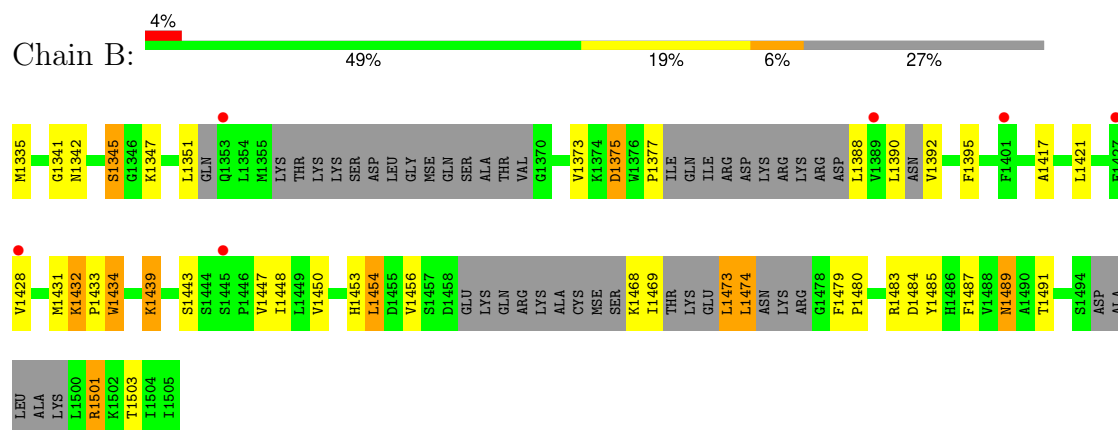
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	69.92Å 53.17Å 42.74Å 90.00° 112.76° 90.00°	Depositor
Resolution (Å)	21.09 – 2.43 21.09 – 2.43	Depositor EDS
% Data completeness (in resolution range)	93.0 (21.09-2.43) 92.9 (21.09-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.74 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.307 0.250 , 0.315	Depositor DCC
R_{free} test set	230 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å^2)	51.6	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 65.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.031 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	1029	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.68% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	B	1.03	0/1006	1.00	2/1343 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1454	LEU	CA-CB-CG	5.41	127.74	115.30
1	B	1434	TRP	CB-CA-C	-5.01	100.38	110.40

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	B	994	0	1000	46	0
2	B	1	0	0	0	0
3	B	28	0	12	0	0
4	B	6	0	0	0	0
All	All	1029	0	1012	46	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 24.

All (46) 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:1335:MSE:HE2	1:B:1390:LEU:CD2	2.05	0.87
1:B:1501:ARG:CG	1:B:1501:ARG:HH21	1.94	0.80
1:B:1474:LEU:HD22	1:B:1474:LEU:H	1.51	0.75
1:B:1501:ARG:HH21	1:B:1501:ARG:CB	2.01	0.72
1:B:1335:MSE:HE2	1:B:1390:LEU:HD22	1.72	0.72
1:B:1432:LYS:HG2	1:B:1479:PHE:CZ	2.25	0.71
1:B:1501:ARG:HH21	1:B:1501:ARG:HG2	1.56	0.69
1:B:1417:ALA:HB1	1:B:1431:MSE:SE	2.46	0.65
1:B:1432:LYS:HD3	1:B:1479:PHE:HZ	1.63	0.64
1:B:1432:LYS:HG2	1:B:1479:PHE:HZ	1.66	0.60
1:B:1474:LEU:H	1:B:1474:LEU:CD2	2.14	0.60
1:B:1421:LEU:O	1:B:1421:LEU:HG	2.01	0.60
1:B:1342:ASN:O	1:B:1345:SER:OG	2.20	0.59
1:B:1485:TYR:HE2	1:B:1487:PHE:HE2	1.50	0.59
1:B:1484:ASP:CG	1:B:1485:TYR:H	2.05	0.59
1:B:1432:LYS:CG	1:B:1479:PHE:HZ	2.19	0.55
1:B:1432:LYS:HD3	1:B:1479:PHE:CZ	2.40	0.55
1:B:1432:LYS:HG2	1:B:1479:PHE:CE1	2.43	0.54
1:B:1468:LYS:HG2	1:B:1469:ILE:H	1.74	0.53
1:B:1501:ARG:HH21	1:B:1501:ARG:HB3	1.71	0.52
1:B:1432:LYS:CD	1:B:1479:PHE:HZ	2.23	0.52
1:B:1501:ARG:HG2	1:B:1501:ARG:NH2	2.26	0.51
1:B:1489:ASN:HD22	1:B:1489:ASN:C	2.15	0.50
1:B:1341:GLY:O	1:B:1347:LYS:HE3	2.13	0.49
1:B:1485:TYR:HE2	1:B:1487:PHE:CE2	2.29	0.49
1:B:1351:LEU:CD2	1:B:1392:VAL:HG11	2.44	0.48
1:B:1484:ASP:CG	1:B:1485:TYR:N	2.66	0.48
1:B:1375:ASP:O	1:B:1377:PRO:HD3	2.12	0.48
1:B:1431:MSE:O	1:B:1431:MSE:HG3	2.13	0.48
1:B:1485:TYR:CE2	1:B:1487:PHE:HE2	2.31	0.48
1:B:1447:VAL:HG21	1:B:1480:PRO:HG2	1.95	0.47
1:B:1474:LEU:CD2	1:B:1474:LEU:N	2.77	0.47
1:B:1473:LEU:HB3	1:B:1479:PHE:CE2	2.51	0.46
1:B:1431:MSE:O	1:B:1434:TRP:HB2	2.16	0.46
1:B:1432:LYS:N	1:B:1433:PRO:CD	2.79	0.45
1:B:1501:ARG:CB	1:B:1501:ARG:NH2	2.74	0.45
1:B:1439:LYS:HE3	1:B:1443:SER:HB3	1.98	0.44
1:B:1351:LEU:HD22	1:B:1392:VAL:HG11	2.00	0.44
1:B:1503:THR:O	1:B:1503:THR:HG22	2.18	0.43
1:B:1453:HIS:HB3	1:B:1456:VAL:CG2	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1485:TYR:CE2	1:B:1487:PHE:CE2	3.06	0.43
1:B:1448:ILE:HD13	1:B:1503:THR:HG22	2.01	0.43
1:B:1474:LEU:HD22	1:B:1474:LEU:N	2.28	0.42
1:B:1373:VAL:HA	1:B:1392:VAL:O	2.20	0.41
1:B:1347:LYS:HE2	1:B:1395:PHE:O	2.20	0.41
1:B:1501:ARG:O	1:B:1501:ARG:HG3	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	B	107/171 (63%)	102 (95%)	5 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	B	108/142 (76%)	94 (87%)	14 (13%)	3	2

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1345	SER
1	B	1375	ASP
1	B	1388	LEU
1	B	1428	VAL
1	B	1432	LYS
1	B	1439	LYS
1	B	1450	VAL
1	B	1454	LEU
1	B	1473	LEU
1	B	1474	LEU
1	B	1483	ARG
1	B	1489	ASN
1	B	1491	THR
1	B	1501	ARG

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

Mol	Chain	Res	Type
1	B	1489	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	GDP	B	1	2	25,30,30	1.07	1 (4%)	30,47,47	1.95	8 (26%)

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	B	1	2	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	GDP	C1'-N9	-2.13	1.44	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1	GDP	O4'-C1'-N9	-5.51	101.44	108.75
3	B	1	GDP	O3A-PA-O1A	3.92	122.50	110.70
3	B	1	GDP	N1-C2-N3	-2.68	118.42	123.32
3	B	1	GDP	O3'-C3'-C2'	-2.60	103.48	111.82
3	B	1	GDP	C8-N7-C5	2.59	106.96	102.55
3	B	1	GDP	O6-C6-C5	-2.47	119.43	124.32
3	B	1	GDP	C2'-C3'-C4'	2.28	107.01	102.61
3	B	1	GDP	O6-C6-N1	2.10	123.12	120.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	GDP	PA-O3A-PB-O2B
3	B	1	GDP	O4'-C4'-C5'-O5'
3	B	1	GDP	PA-O3A-PB-O3B
3	B	1	GDP	C5'-O5'-PA-O1A

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP B 1

Bond lengths   Bond angles

Torsions   Rings
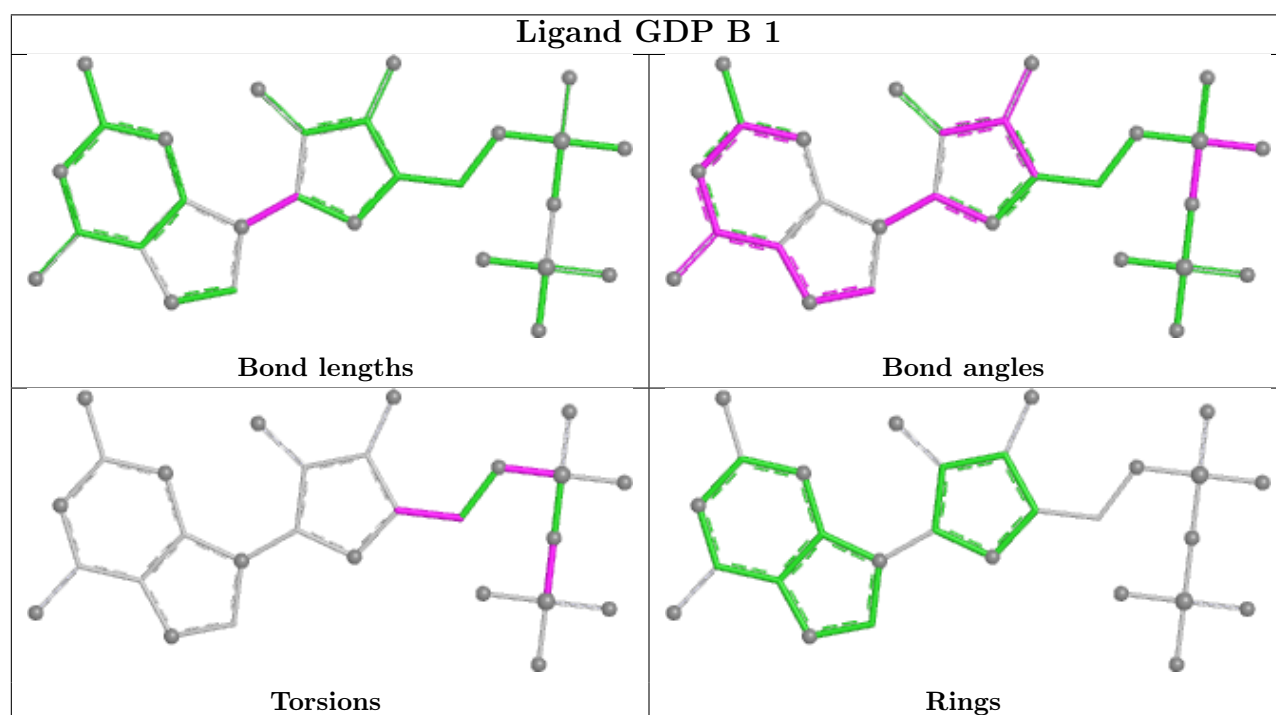
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

Warning: The R factor obtained from EDS is 0.2652, which does not match the depositor's R factor of 0.211. Please interpret the results in this section carefully.

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(Å²)	Q<0.9
1	B	120/171 (70%)	0.36	6 (5%)	35	34	11, 29, 48, 54	12 (10%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1428	VAL	3.8
1	B	1427	GLU	2.6
1	B	1445	SER	2.6
1	B	1353	GLN	2.4
1	B	1389	VAL	2.3
1	B	1401	PHE	2.2

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

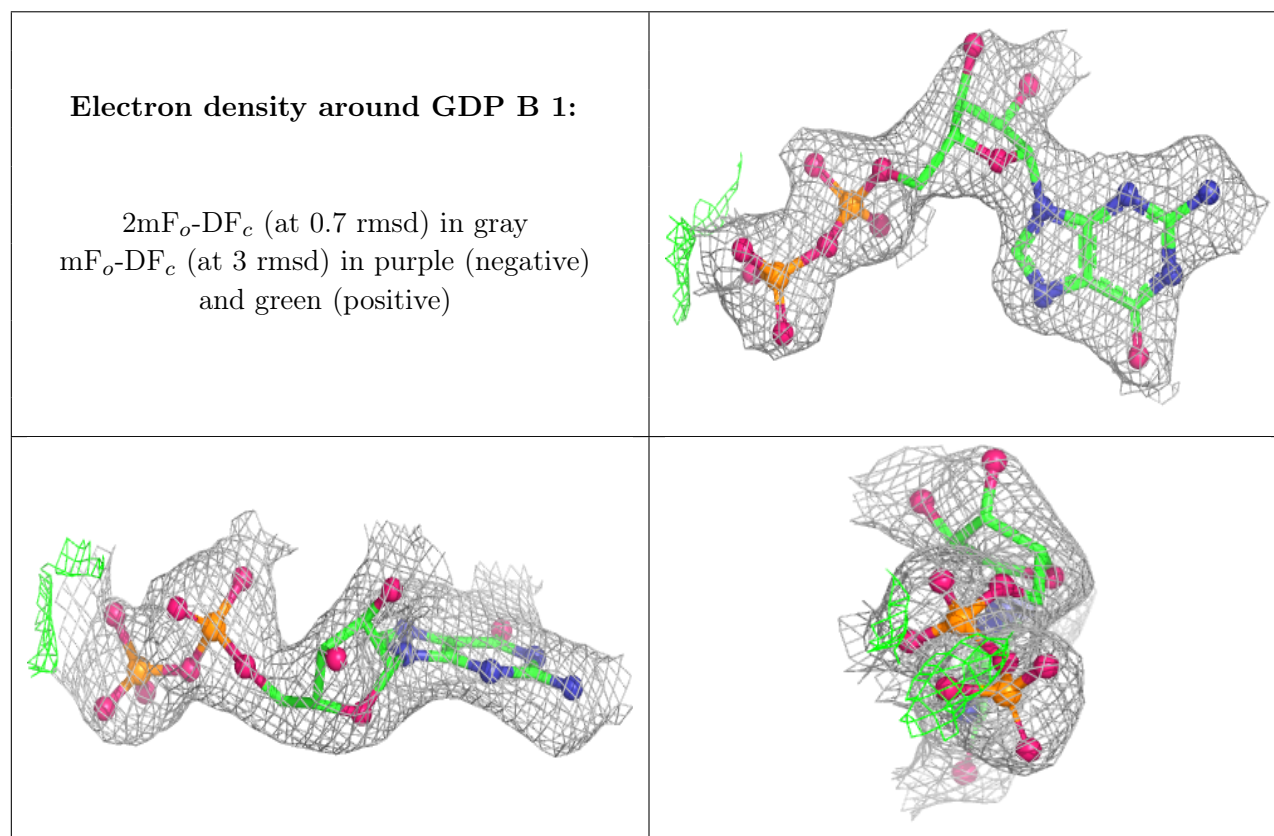There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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.

Full wwPDB X-ray Structure Validation Report

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
2	MG	B	2	1/1	0.89	0.23	41,41,41,41	0
3	GDP	B	1	28/28	0.97	0.06	28,37,41,46	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 1:

$2mF_o$-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 ⓘ

There are no such residues in this entry.