



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID : 5OPD / pdb_00005opd
Title : Structure of phosphorylated EF-Tu in complex with GTP
Authors : Garcia-Pino, A.
Deposited on : 2017-08-09
Resolution : 2.75 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

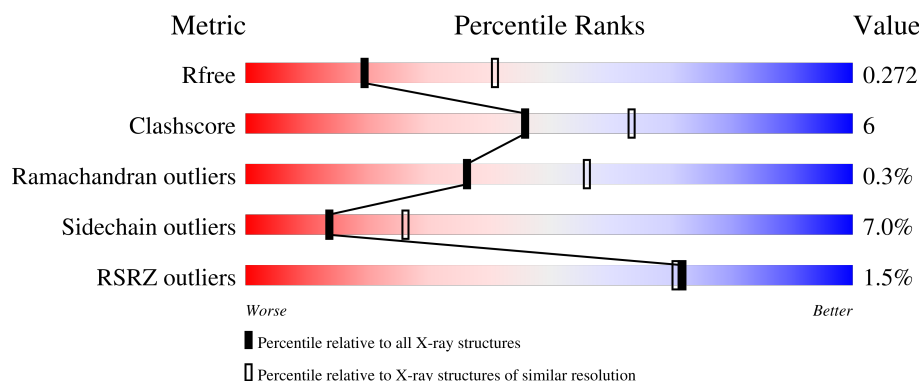
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

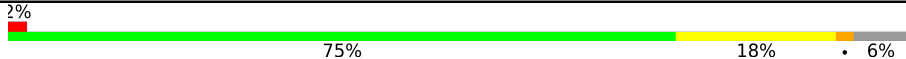
The reported resolution of this entry is 2.75 Å.

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	400	
1	B	400	

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	IOD	B	513	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6070 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 Elongation factor Tu 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	P	S	0	0	0
			2837	1800	482	541	1	13			
1	B	379	Total	C	N	O	P	S	0	0	0
			2816	1784	480	539	1	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	395	HIS	-	expression tag	UNP A8A5E6
A	396	HIS	-	expression tag	UNP A8A5E6
A	397	HIS	-	expression tag	UNP A8A5E6
A	398	HIS	-	expression tag	UNP A8A5E6
A	399	HIS	-	expression tag	UNP A8A5E6
A	400	HIS	-	expression tag	UNP A8A5E6
B	395	HIS	-	expression tag	UNP A8A5E6
B	396	HIS	-	expression tag	UNP A8A5E6
B	397	HIS	-	expression tag	UNP A8A5E6
B	398	HIS	-	expression tag	UNP A8A5E6
B	399	HIS	-	expression tag	UNP A8A5E6
B	400	HIS	-	expression tag	UNP A8A5E6

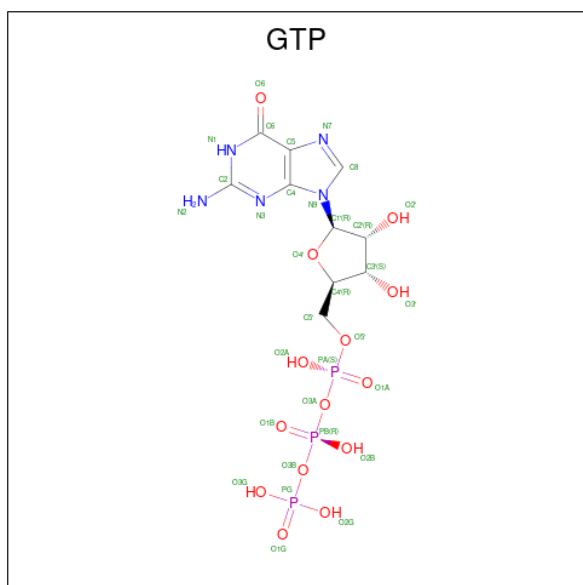
- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	I	0	0
			14	14		
2	B	14	Total	I	0	0
			14	14		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 32 10 5 14 3	0	0
4	B	1	Total C N O P 32 10 5 14 3	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Na 2 2	0	0
5	B	3	Total Na 3 3	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

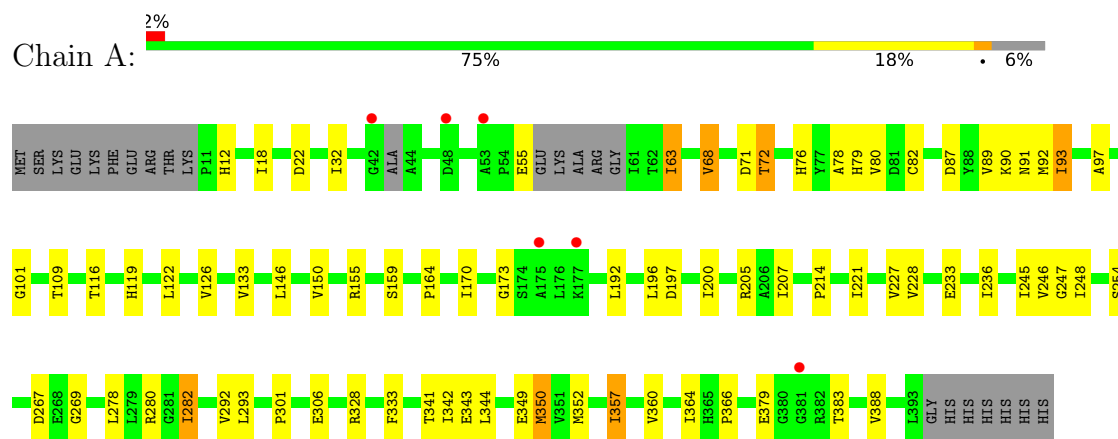
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	155	Total	O	0	0
			155	155		
7	B	157	Total	O	0	0
			157	157		

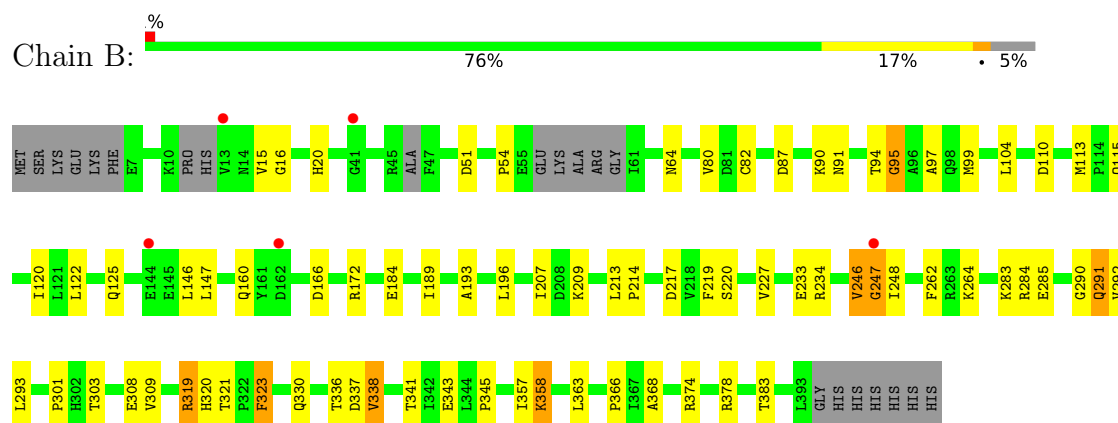
3 Residue-property plots [i](#)

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: Elongation factor Tu 1



• Molecule 1: Elongation factor Tu 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.84Å 61.88Å 65.48Å 70.37° 75.83° 89.41°	Depositor
Resolution (Å)	51.37 – 2.75 51.37 – 2.75	Depositor EDS
% Data completeness (in resolution range)	93.4 (51.37-2.75) 93.3 (51.37-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.181 , 0.258 0.186 , 0.272	Depositor DCC
R_{free} test set	978 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6070	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA, TPO, IOD, MG, GTP

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	0.84	0/2878	1.35	13/3905 (0.3%)
1	B	0.83	0/2853	1.37	13/3873 (0.3%)
All	All	0.84	0/5731	1.36	26/7778 (0.3%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	PHE	CA-CB-CG	-7.23	106.57	113.80
1	B	323	PHE	CA-CB-CG	7.01	120.81	113.80
1	A	247	GLY	CA-C-N	5.81	132.42	121.97
1	A	247	GLY	C-N-CA	5.81	132.42	121.97
1	A	349	GLU	CB-CG-CD	5.76	122.40	112.60
1	B	189	ILE	N-CA-C	-5.49	105.76	111.58
1	B	320	HIS	N-CA-C	-5.35	107.41	114.31
1	A	72	THR	N-CA-C	-5.28	102.85	110.40
1	B	247	GLY	CA-C-N	5.25	131.42	121.97
1	B	247	GLY	C-N-CA	5.25	131.42	121.97
1	B	358	LYS	N-CA-C	-5.23	102.00	110.32
1	A	164	PRO	CA-C-N	5.18	125.83	120.03
1	A	164	PRO	C-N-CA	5.18	125.83	120.03
1	B	95	GLY	CA-C-N	5.14	128.54	120.82
1	B	95	GLY	C-N-CA	5.14	128.54	120.82
1	A	173	GLY	N-CA-C	5.11	118.01	110.80
1	B	284	ARG	CA-C-N	5.08	127.59	120.28
1	B	284	ARG	C-N-CA	5.08	127.59	120.28
1	A	267	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	155	ARG	CA-C-N	5.04	126.99	120.44
1	A	155	ARG	C-N-CA	5.04	126.99	120.44
1	B	291	GLN	N-CA-C	-5.04	103.01	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	LYS	CA-C-N	5.01	127.25	120.38
1	B	283	LYS	C-N-CA	5.01	127.25	120.38
1	A	116	THR	CA-C-N	5.00	127.39	120.29
1	A	116	THR	C-N-CA	5.00	127.39	120.29

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	2837	0	2780	32	0
1	B	2816	0	2732	33	0
2	A	14	0	0	5	0
2	B	14	0	0	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	12	0	0
4	B	32	0	12	0	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
6	A	6	0	8	0	0
7	A	155	0	0	0	0
7	B	157	0	0	1	0
All	All	6070	0	5544	66	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 6.

All (66) 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)
2:B:513:IOD:I	7:B:654:HOH:O	2.71	0.78
1:B:193:ALA:HA	1:B:196:LEU:HD12	1.67	0.77
1:A:280:ARG:HD3	2:A:514:IOD:I	2.56	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HB	1:A:170:ILE:HG12	1.74	0.69
1:B:262:PHE:O	2:B:508:IOD:I	2.83	0.67
1:A:227:VAL:HG22	1:A:278:LEU:HG	1.76	0.67
1:B:246:VAL:HG22	1:B:368:ALA:HB2	1.77	0.65
1:A:32:ILE:HD11	1:A:192:LEU:HD23	1.77	0.64
1:A:97:ALA:HB3	2:A:508:IOD:I	2.68	0.64
1:B:319:ARG:NH1	1:B:323:PHE:HB3	2.12	0.64
1:B:357:ILE:HG22	1:B:358:LYS:O	1.98	0.63
1:A:214:PRO:HA	1:A:292:VAL:HG12	1.82	0.60
1:A:18:ILE:HG23	1:A:119:HIS:HB3	1.84	0.59
1:A:72:THR:HG21	1:A:197:ASP:OD2	2.02	0.59
1:A:221:ILE:HG12	1:A:227:VAL:HG23	1.86	0.57
1:A:82:CYS:HB3	1:A:87:ASP:HB2	1.84	0.57
1:A:101:GLY:HA3	1:A:200:ILE:HD12	1.86	0.57
1:B:104:LEU:HD22	1:B:120:ILE:HD11	1.87	0.57
1:B:110:ASP:HB3	1:B:113:MET:HE3	1.87	0.56
1:B:319:ARG:HH11	1:B:323:PHE:HB3	1.69	0.56
1:A:89:VAL:O	1:A:93:ILE:HG12	2.06	0.56
1:B:90:LYS:O	1:B:94:THR:HG22	2.06	0.54
1:A:350:MET:HE2	1:A:352:MET:HG2	1.91	0.53
1:B:219:PHE:HB2	1:B:227:VAL:HG12	1.91	0.53
1:A:63:ILE:HG12	1:A:90:LYS:HB3	1.90	0.53
1:A:343:GLU:HB2	1:A:360:VAL:HB	1.90	0.52
1:B:330:GLN:HB3	1:B:337:ASP:HB3	1.91	0.51
1:B:247:GLY:HA3	1:B:291:GLN:HG2	1.93	0.51
1:A:236:ILE:HA	1:A:269:GLY:O	2.12	0.50
1:B:16:GLY:HA3	1:B:99:MET:HE2	1.93	0.50
1:B:209:LYS:HB2	1:B:234:ARG:HB2	1.93	0.50
1:A:68:VAL:HG12	1:A:79:HIS:HB3	1.95	0.48
1:A:205:ARG:NH1	1:A:207:ILE:H	2.11	0.48
1:B:91:ASN:HB3	1:B:97:ALA:HB2	1.94	0.48
1:A:306:GLU:HG2	2:A:509:IOD:I	2.83	0.48
1:B:82:CYS:HB3	1:B:87:ASP:HB2	1.95	0.48
1:A:91:ASN:HB3	1:A:97:ALA:HB2	1.95	0.48
1:A:233:GLU:HG3	2:A:512:IOD:I	2.84	0.47
1:A:92:MET:HE3	1:A:122:LEU:HD23	1.96	0.47
1:B:233:GLU:HG3	2:B:513:IOD:I	2.85	0.47
1:B:15:VAL:HG12	1:B:16:GLY:N	2.30	0.47
1:B:54:PRO:O	1:B:64:ASN:HA	2.14	0.47
1:B:125:GLN:HB3	1:B:308:GLU:HG2	1.97	0.47
1:B:97:ALA:HB3	2:B:509:IOD:I	2.85	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLU:H	1:B:285:GLU:CD	2.23	0.45
1:B:338:VAL:HB	1:B:363:LEU:HD22	1.98	0.45
1:B:15:VAL:HG12	1:B:16:GLY:H	1.82	0.45
1:B:319:ARG:HD2	2:B:506:IOD:I	2.87	0.45
1:A:92:MET:HB3	1:A:126:VAL:HG21	1.99	0.45
1:A:254:SER:HB2	1:A:282:ILE:HD13	1.99	0.44
1:B:95:GLY:HA2	1:B:374:ARG:NH1	2.32	0.44
1:B:337:ASP:OD1	1:B:378:ARG:HD3	2.18	0.44
1:A:12:HIS:HE1	1:A:78:ALA:HB2	1.83	0.44
1:B:345:PRO:HG2	2:B:502:IOD:I	2.88	0.43
1:B:214:PRO:HA	1:B:292:VAL:HG12	2.00	0.43
1:A:301:PRO:HB2	1:A:366:PRO:HB2	2.00	0.43
1:A:71:ASP:OD1	1:A:76:HIS:HA	2.19	0.43
1:B:290:GLY:HA3	1:B:336:THR:HG22	2.00	0.43
1:A:357:ILE:HG22	2:A:510:IOD:I	2.89	0.42
1:A:55:GLU:HG2	1:A:63:ILE:O	2.19	0.42
1:A:342:ILE:HD12	1:A:344:LEU:HD21	2.01	0.42
1:A:146:LEU:O	1:A:150:VAL:HG23	2.20	0.41
1:B:301:PRO:HB2	1:B:366:PRO:HB2	2.02	0.41
1:B:147:LEU:HD13	1:B:172:ARG:HD3	2.03	0.41
1:A:126:VAL:HG12	1:A:388:VAL:HG21	2.03	0.40
1:B:20:HIS:ND1	1:B:115:GLN:HB2	2.36	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	370/400 (92%)	347 (94%)	22 (6%)	1 (0%)	36	56
1	B	370/400 (92%)	344 (93%)	25 (7%)	1 (0%)	36	56
All	All	740/800 (92%)	691 (93%)	47 (6%)	2 (0%)	36	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	ILE
1	B	248	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/331 (88%)	273 (94%)	19 (6%)	15	29
1	B	283/331 (86%)	262 (93%)	21 (7%)	13	24
All	All	575/662 (87%)	535 (93%)	40 (7%)	14	26

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	63	ILE
1	A	68	VAL
1	A	80	VAL
1	A	93	ILE
1	A	109	THR
1	A	159	SER
1	A	196	LEU
1	A	228	VAL
1	A	245	ILE
1	A	246	VAL
1	A	282	ILE
1	A	293	LEU
1	A	328	ARG
1	A	341	THR
1	A	350	MET
1	A	357	ILE
1	A	364	ILE
1	A	379	GLU
1	B	51	ASP
1	B	80	VAL

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Mol	Chain	Res	Type
1	B	122	LEU
1	B	146	LEU
1	B	160	GLN
1	B	166	ASP
1	B	184	GLU
1	B	207	ILE
1	B	213	LEU
1	B	217	ASP
1	B	220	SER
1	B	246	VAL
1	B	264	LYS
1	B	293	LEU
1	B	303	THR
1	B	309	VAL
1	B	319	ARG
1	B	321	THR
1	B	338	VAL
1	B	341	THR
1	B	343	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	85	HIS
1	A	91	ASN
1	A	356	ASN
1	A	365	HIS
1	B	64	ASN
1	B	125	GLN
1	B	320	HIS
1	B	356	ASN
1	B	365	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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$
1	TPO	B	383	1	8,10,11	0.88	0	10,14,16	1.13	1 (10%)
1	TPO	A	383	1	8,10,11	0.87	0	10,14,16	1.16	1 (10%)

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
1	TPO	B	383	1	-	0/9/11/13	-
1	TPO	A	383	1	-	1/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	383	TPO	P-OG1-CB	-2.45	116.68	123.33
1	A	383	TPO	P-OG1-CB	-2.02	117.84	123.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	383	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 35 are monoatomic - leaving 3 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	$\# Z > 2$
4	GTP	A	516	3	33,34,34	0.37	0	50,54,54	0.49	1 (2%)
6	GOL	A	519	-	5,5,5	0.17	0	5,5,5	0.38	0
4	GTP	B	516	3	33,34,34	0.42	0	50,54,54	0.60	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
4	GTP	A	516	3	-	4/22/38/38	0/3/3/3
6	GOL	A	519	-	-	0/4/4/4	-
4	GTP	B	516	3	-	3/22/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	516	GTP	O5'-PA-O1A	2.01	116.91	108.94

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	516	GTP	C5'-O5'-PA-O2A

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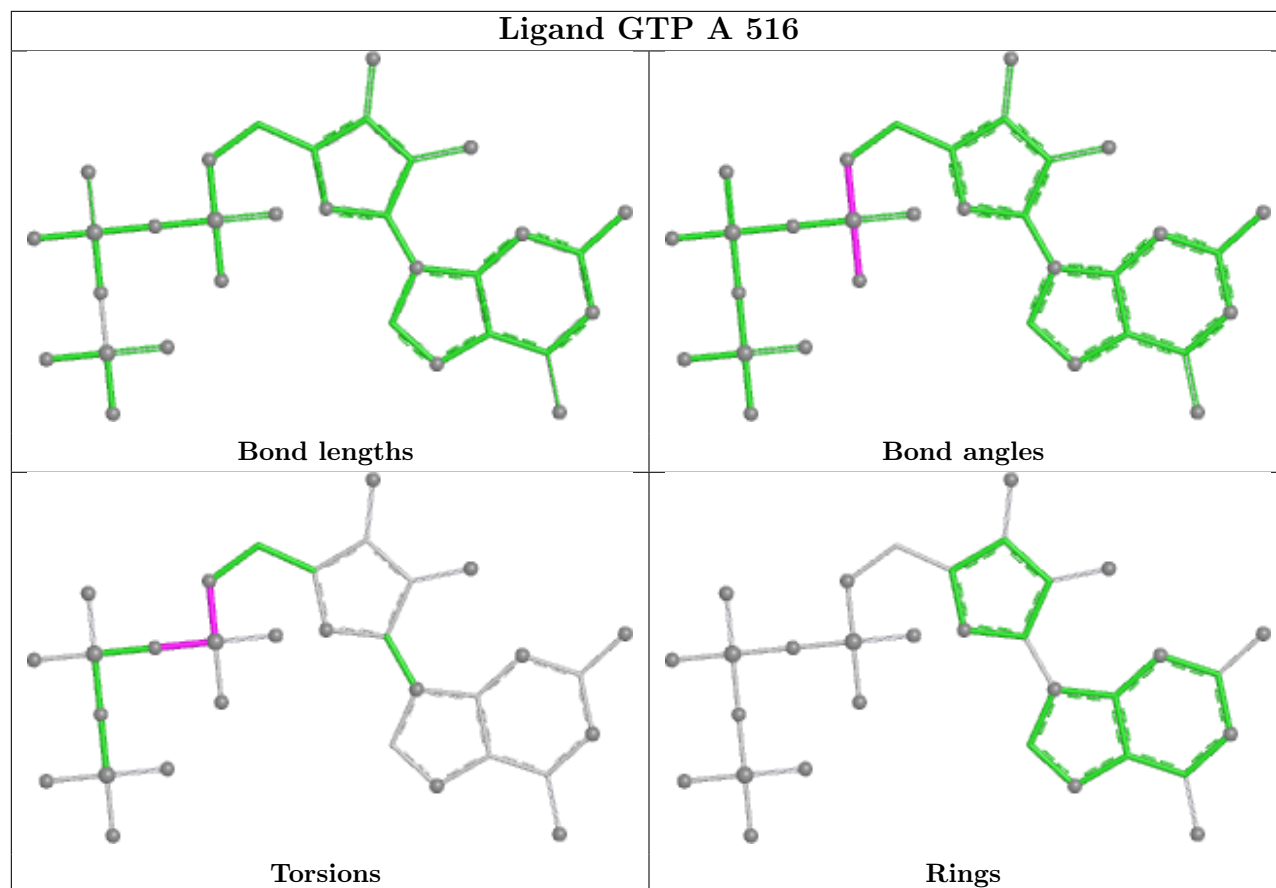
Mol	Chain	Res	Type	Atoms
4	B	516	GTP	PA-O3A-PB-O2B
4	A	516	GTP	C5'-O5'-PA-O3A
4	A	516	GTP	C5'-O5'-PA-O1A
4	A	516	GTP	PB-O3A-PA-O2A
4	B	516	GTP	PG-O3B-PB-O1B
4	B	516	GTP	PA-O3A-PB-O1B

There are no ring outliers.

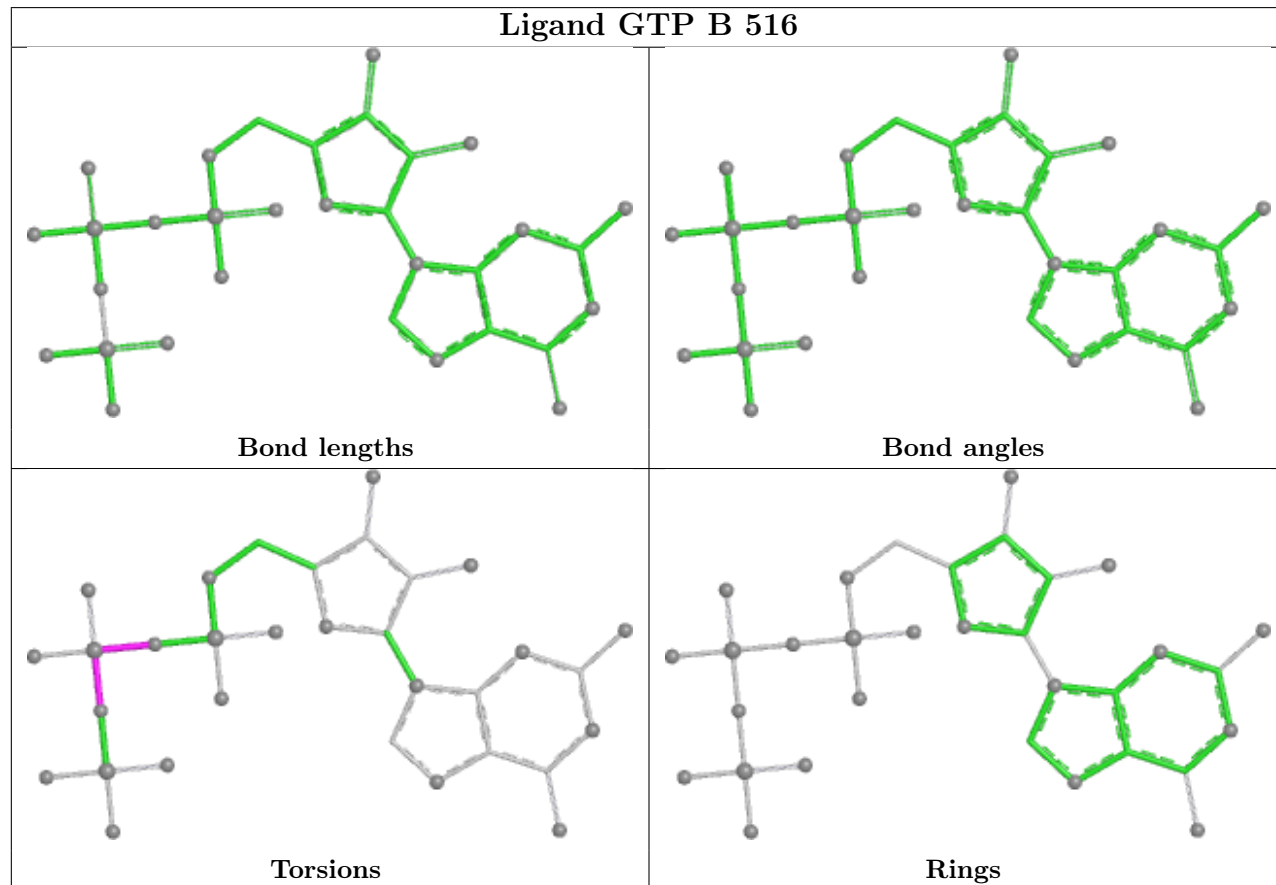
No monomer is involved in short contacts.

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.

Ligand GTP A 516



Ligand GTP B 516



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	376/400 (94%)	0.18	6 (1%) 70 69	5, 17, 35, 56	0
1	B	378/400 (94%)	0.20	5 (1%) 75 75	5, 18, 36, 54	0
All	All	754/800 (94%)	0.19	11 (1%) 72 71	5, 17, 36, 56	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	GLY	3.4
1	B	144	GLU	2.6
1	A	53	ALA	2.5
1	A	175	ALA	2.5
1	B	13	VAL	2.5
1	A	381	GLY	2.3
1	B	162	ASP	2.3
1	A	48	ASP	2.2
1	B	41	GLY	2.2
1	A	177	LYS	2.0
1	B	247	GLY	2.0

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, 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
1	TPO	A	383	11/12	0.96	0.07	15,17,19,19	0
1	TPO	B	383	11/12	0.97	0.07	15,18,20,21	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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.

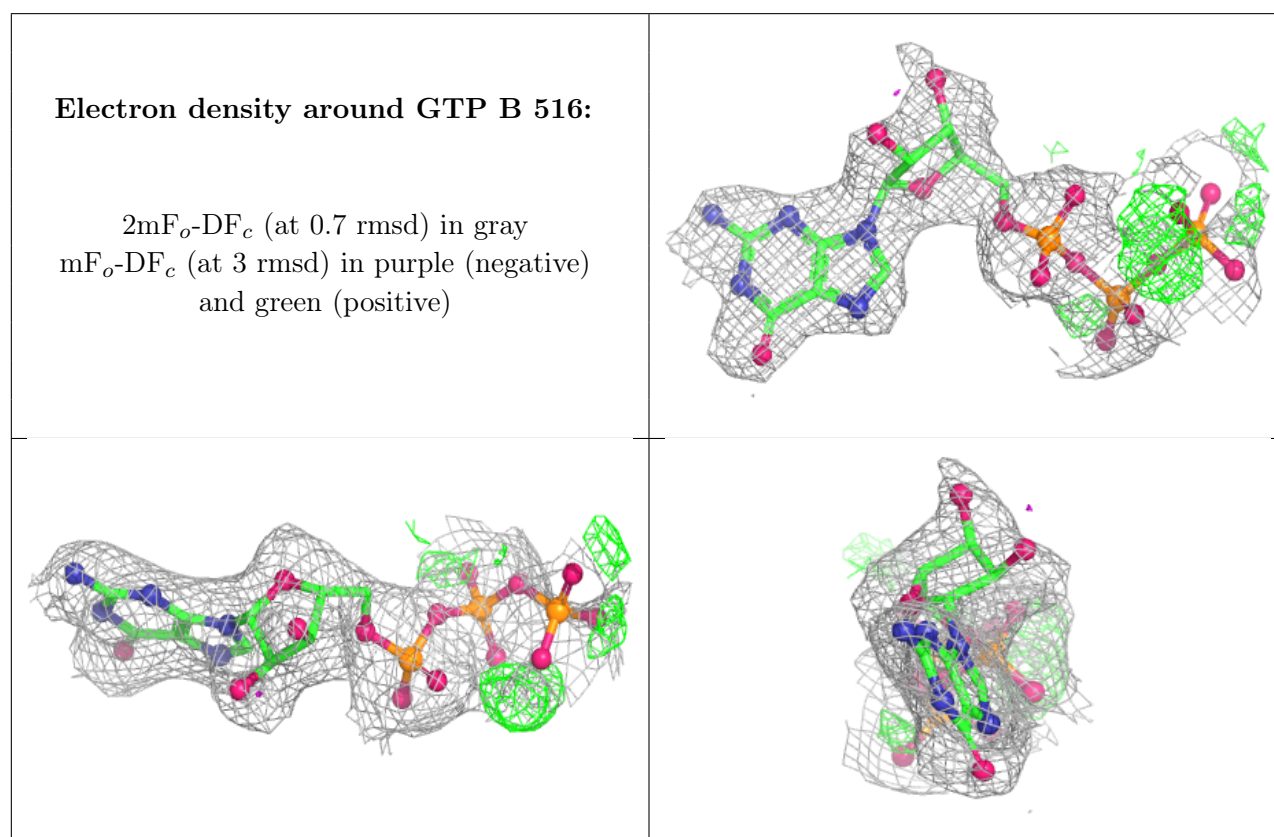
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	519	6/6	0.92	0.11	17,19,22,22	0
4	GTP	B	516	32/32	0.94	0.11	12,19,21,23	4
4	GTP	A	516	32/32	0.94	0.10	15,23,25,27	4
5	NA	B	518	1/1	0.95	0.20	3,3,3,3	0
5	NA	A	517	1/1	0.95	0.17	5,5,5,5	0
2	IOD	A	513	1/1	0.96	0.05	34,34,34,34	1
2	IOD	A	509	1/1	0.96	0.05	37,37,37,37	1
3	MG	A	515	1/1	0.97	0.13	9,9,9,9	0
5	NA	B	517	1/1	0.97	0.20	3,3,3,3	0
2	IOD	A	505	1/1	0.97	0.07	54,54,54,54	0
2	IOD	B	512	1/1	0.97	0.04	31,31,31,31	1
2	IOD	A	510	1/1	0.98	0.05	50,50,50,50	0
2	IOD	B	513	1/1	0.98	0.05	19,19,19,19	1
2	IOD	A	512	1/1	0.98	0.04	33,33,33,33	1
3	MG	B	515	1/1	0.98	0.14	3,3,3,3	0
2	IOD	A	504	1/1	0.98	0.03	28,28,28,28	0
2	IOD	A	514	1/1	0.98	0.04	65,65,65,65	0
2	IOD	B	506	1/1	0.98	0.05	13,13,13,13	1
5	NA	A	518	1/1	0.98	0.11	3,3,3,3	0
2	IOD	B	507	1/1	0.98	0.03	30,30,30,30	0
2	IOD	B	510	1/1	0.98	0.06	40,40,40,40	1
5	NA	B	519	1/1	0.98	0.16	3,3,3,3	0
2	IOD	B	511	1/1	0.98	0.05	14,14,14,14	1
2	IOD	A	507	1/1	0.99	0.03	27,27,27,27	1
2	IOD	A	508	1/1	0.99	0.03	24,24,24,24	1
2	IOD	B	514	1/1	0.99	0.03	46,46,46,46	0
2	IOD	B	502	1/1	0.99	0.02	27,27,27,27	1
2	IOD	B	503	1/1	0.99	0.01	23,23,23,23	0
2	IOD	B	504	1/1	0.99	0.02	41,41,41,41	0
2	IOD	B	505	1/1	0.99	0.02	6,6,6,6	1
2	IOD	A	503	1/1	0.99	0.04	5,5,5,5	1
2	IOD	A	501	1/1	0.99	0.02	47,47,47,47	0

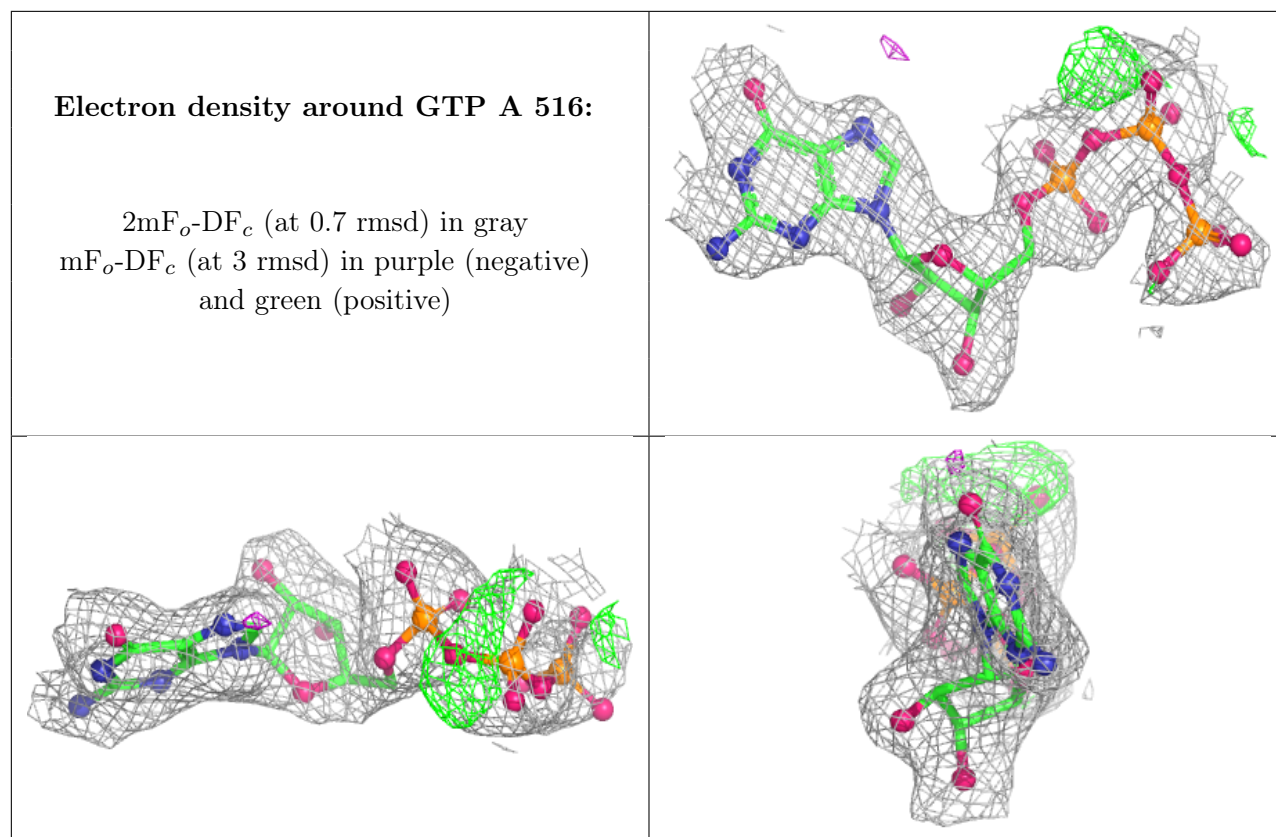
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IOD	B	508	1/1	0.99	0.04	16,16,16,16	1
2	IOD	B	509	1/1	0.99	0.02	24,24,24,24	1
2	IOD	A	511	1/1	0.99	0.05	65,65,65,65	0
2	IOD	A	502	1/1	0.99	0.05	47,47,47,47	0
2	IOD	B	501	1/1	1.00	0.02	24,24,24,24	1
2	IOD	A	506	1/1	1.00	0.03	17,17,17,17	1

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.