



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:59 AM UTC

PDB ID : 4NCN / pdb_00004ncn
Title : Crystal structure of eukaryotic translation initiation factor eIF5B (517-858) from *Chaetomium thermophilum* in complex with GTP
Authors : Kuhle, B.; Ficner, R.
Deposited on : 2013-10-24
Resolution : 1.87 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

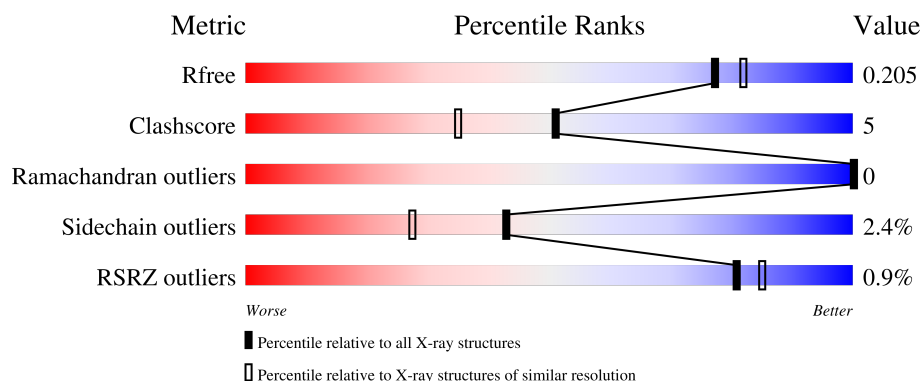
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	457	66% 8% 25%
1	B	457	65% 9% 25%

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
5	GOL	B	1006	-	-	X	-
6	ACY	B	1004	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6087 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 Eukaryotic translation initiation factor 5B-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	4	0
			2724	1720	481	513	10			
1	B	345	Total	C	N	O	S	0	4	0
			2725	1721	479	514	11			

There are 54 discrepancies between the modelled and reference sequences:

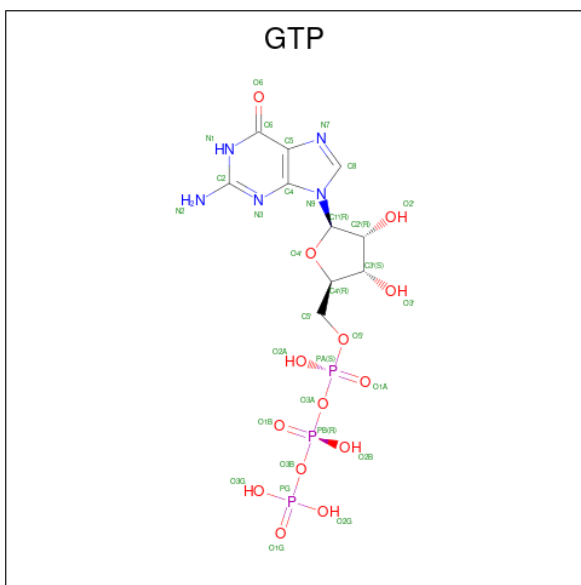
Chain	Residue	Modelled	Actual	Comment	Reference
A	514	SER	-	expression tag	UNP G0S8G9
A	515	HIS	-	expression tag	UNP G0S8G9
A	516	MET	-	expression tag	UNP G0S8G9
A	576	VAL	-	SEE REMARK 999	UNP G0S8G9
A	577	VAL	-	SEE REMARK 999	UNP G0S8G9
A	578	ASN	-	SEE REMARK 999	UNP G0S8G9
A	579	LYS	-	SEE REMARK 999	UNP G0S8G9
A	580	ASP	-	SEE REMARK 999	UNP G0S8G9
A	581	GLY	-	SEE REMARK 999	UNP G0S8G9
A	582	LYS	-	SEE REMARK 999	UNP G0S8G9
A	583	PHE	-	SEE REMARK 999	UNP G0S8G9
A	584	GLU	-	SEE REMARK 999	UNP G0S8G9
A	585	PHE	-	SEE REMARK 999	UNP G0S8G9
A	586	LYS	-	SEE REMARK 999	UNP G0S8G9
A	587	VAL	-	SEE REMARK 999	UNP G0S8G9
A	588	PRO	-	SEE REMARK 999	UNP G0S8G9
A	589	GLY	-	SEE REMARK 999	UNP G0S8G9
A	590	LEU	-	SEE REMARK 999	UNP G0S8G9
A	591	LEU	-	SEE REMARK 999	UNP G0S8G9
A	592	ILE	-	SEE REMARK 999	UNP G0S8G9
A	593	ILE	-	SEE REMARK 999	UNP G0S8G9
A	594	ASP	-	SEE REMARK 999	UNP G0S8G9
A	595	THR	-	SEE REMARK 999	UNP G0S8G9
A	596	PRO	-	SEE REMARK 999	UNP G0S8G9
A	597	GLY	-	SEE REMARK 999	UNP G0S8G9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	598	HIS	-	SEE REMARK 999	UNP G0S8G9
A	599	GLU	-	SEE REMARK 999	UNP G0S8G9
B	514	SER	-	expression tag	UNP G0S8G9
B	515	HIS	-	expression tag	UNP G0S8G9
B	516	MET	-	expression tag	UNP G0S8G9
B	576	VAL	-	SEE REMARK 999	UNP G0S8G9
B	577	VAL	-	SEE REMARK 999	UNP G0S8G9
B	578	ASN	-	SEE REMARK 999	UNP G0S8G9
B	579	LYS	-	SEE REMARK 999	UNP G0S8G9
B	580	ASP	-	SEE REMARK 999	UNP G0S8G9
B	581	GLY	-	SEE REMARK 999	UNP G0S8G9
B	582	LYS	-	SEE REMARK 999	UNP G0S8G9
B	583	PHE	-	SEE REMARK 999	UNP G0S8G9
B	584	GLU	-	SEE REMARK 999	UNP G0S8G9
B	585	PHE	-	SEE REMARK 999	UNP G0S8G9
B	586	LYS	-	SEE REMARK 999	UNP G0S8G9
B	587	VAL	-	SEE REMARK 999	UNP G0S8G9
B	588	PRO	-	SEE REMARK 999	UNP G0S8G9
B	589	GLY	-	SEE REMARK 999	UNP G0S8G9
B	590	LEU	-	SEE REMARK 999	UNP G0S8G9
B	591	LEU	-	SEE REMARK 999	UNP G0S8G9
B	592	ILE	-	SEE REMARK 999	UNP G0S8G9
B	593	ILE	-	SEE REMARK 999	UNP G0S8G9
B	594	ASP	-	SEE REMARK 999	UNP G0S8G9
B	595	THR	-	SEE REMARK 999	UNP G0S8G9
B	596	PRO	-	SEE REMARK 999	UNP G0S8G9
B	597	GLY	-	SEE REMARK 999	UNP G0S8G9
B	598	HIS	-	SEE REMARK 999	UNP G0S8G9
B	599	GLU	-	SEE REMARK 999	UNP G0S8G9

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

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

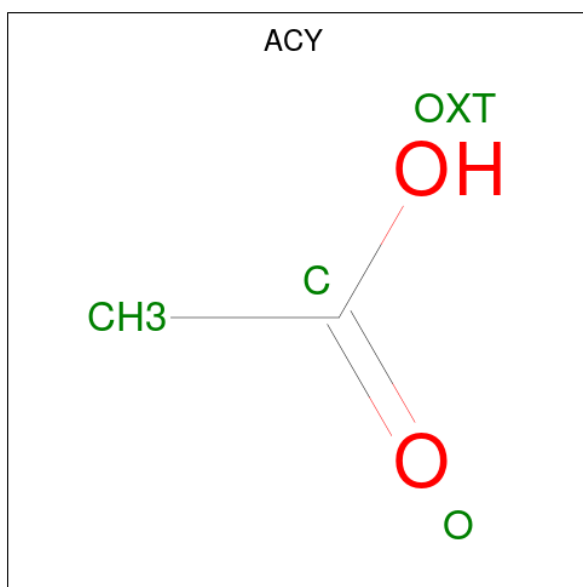
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		

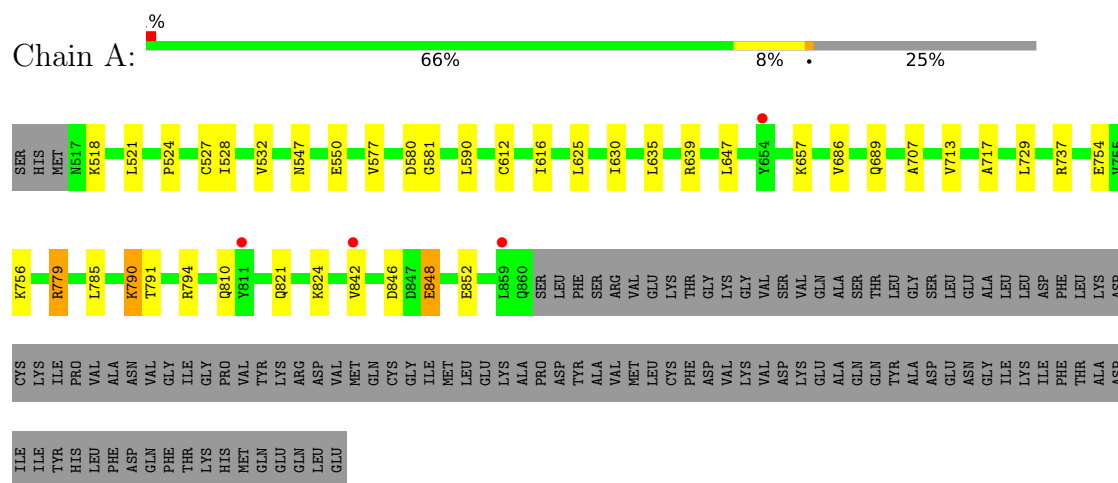
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	236	Total	O	0	5
			241	241		
7	B	272	Total	O	0	11
			283	283		

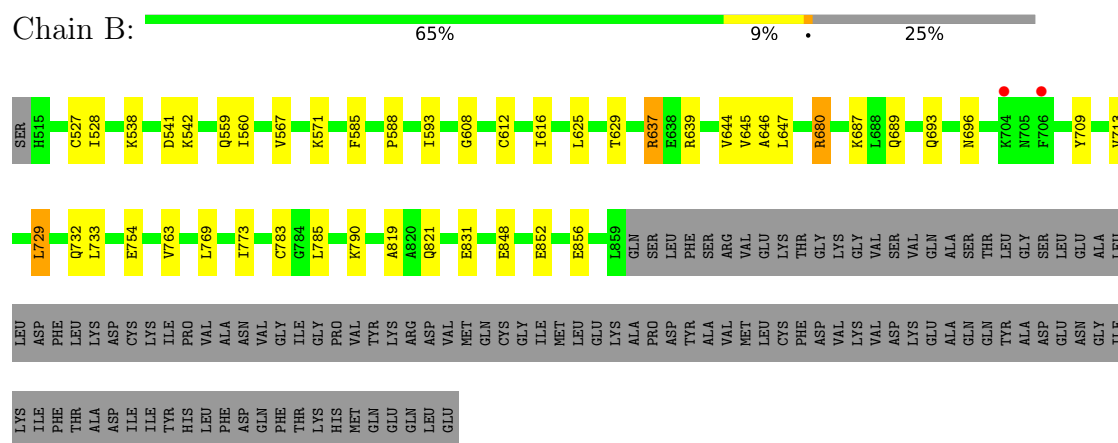
3 Residue-property plots

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 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: Eukaryotic translation initiation factor 5B-like protein



- Molecule 1: Eukaryotic translation initiation factor 5B-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.41Å 114.84Å 65.88Å 90.00° 102.41° 90.00°	Depositor
Resolution (Å)	46.65 – 1.87 46.65 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.65-1.87) 99.8 (46.65-1.87)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.164 , 0.204 0.166 , 0.205	Depositor DCC
R_{free} test set	3316 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6087	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: MG, NA, ACY, GTP, 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	1.01	2/2763 (0.1%)	1.09	3/3726 (0.1%)
1	B	1.01	1/2764 (0.0%)	1.04	1/3727 (0.0%)
All	All	1.01	3/5527 (0.1%)	1.06	4/7453 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	646	ALA	CA-CB	8.17	1.63	1.53
1	A	717	ALA	CA-CB	5.03	1.62	1.53
1	A	577	VAL	CA-CB	5.02	1.59	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	846	ASP	N-CA-C	8.74	122.83	110.50
1	A	848	GLU	N-CA-C	8.03	119.81	111.14
1	A	810	GLN	N-CA-C	-7.72	99.06	110.48
1	B	608	GLY	N-CA-C	-5.87	105.25	112.77

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	2724	0	2789	25	0
1	B	2725	0	2784	30	0
2	A	32	0	12	0	0
2	B	32	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	18	0	24	3	0
5	B	24	0	32	8	0
6	B	4	0	3	2	0
7	A	241	0	0	5	0
7	B	283	0	0	3	0
All	All	6087	0	5656	58	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 5.

All (58) 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:559:GLN:NE2	1:B:754:GLU:OE2	2.21	0.73
1:A:707:ALA:HA	1:A:737:ARG:HD3	1.69	0.72
1:A:794:ARG:NH1	7:A:1308:HOH:O	2.20	0.72
1:B:637:ARG:NH1	1:B:693:GLN:O	2.29	0.65
1:B:732:GLN:NE2	7:B:1290:HOH:O	2.25	0.65
1:A:532:VAL:O	5:A:1005:GOL:H11	1.97	0.64
1:B:541:ASP:HB3	5:B:1006:GOL:H12	1.79	0.63
1:B:538:LYS:HE3	5:B:1006:GOL:H11	1.81	0.62
1:B:639[B]:ARG:NH1	7:B:1365:HOH:O	2.21	0.62
1:B:625:LEU:HD22	1:B:689:GLN:HB3	1.83	0.61
1:A:639[A]:ARG:NH2	7:A:1240:HOH:O	2.33	0.61
5:A:1004:GOL:H2	7:A:1126:HOH:O	2.02	0.60
1:A:790:LYS:HE3	1:A:852:GLU:OE2	2.03	0.59
1:A:625:LEU:HD22	1:A:689:GLN:HB3	1.86	0.58
1:B:588:PRO:HA	5:B:1005:GOL:H12	1.85	0.57
1:B:773:ILE:H	6:B:1004:ACY:H2	1.70	0.57
1:A:639[A]:ARG:NH1	7:A:1271:HOH:O	2.39	0.56
1:B:527:CYS:HB2	1:B:612:CYS:HB3	1.87	0.55
1:B:848:GLU:O	1:B:852:GLU:HG3	2.06	0.55
1:A:635:LEU:CD2	1:A:639[B]:ARG:HH12	2.20	0.54
1:B:763:VAL:HG11	1:B:831:GLU:HA	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:LYS:HA	5:B:1006:GOL:H32	1.91	0.53
1:B:644:VAL:HG13	1:B:733:LEU:HD11	1.91	0.53
1:A:779:ARG:CZ	1:A:790:LYS:HB3	2.42	0.50
1:B:541:ASP:CB	5:B:1006:GOL:H12	2.41	0.50
1:A:527:CYS:HB2	1:A:612:CYS:HB3	1.94	0.50
1:A:518:LYS:HA	1:A:521:LEU:HG	1.93	0.50
1:A:790:LYS:HE2	1:A:848:GLU:OE2	2.12	0.49
1:B:528[B]:ILE:HD12	1:B:616:ILE:HB	1.94	0.49
1:B:567:VAL:HG11	5:B:1005:GOL:H32	1.94	0.48
1:B:713:VAL:HG21	1:B:729:LEU:HD13	1.95	0.47
1:A:754:GLU:HG2	1:A:756:LYS:HG2	1.96	0.47
1:A:528[B]:ILE:CD1	1:A:616:ILE:HD12	2.45	0.46
1:A:647:LEU:HD21	1:A:686:VAL:HG11	1.97	0.46
1:B:773:ILE:N	6:B:1004:ACY:H2	2.32	0.45
5:A:1006:GOL:H32	7:A:1203:HOH:O	2.15	0.45
1:A:779:ARG:HB3	1:A:842:VAL:CG2	2.46	0.45
1:B:713:VAL:CG2	1:B:729:LEU:HD13	2.46	0.45
1:B:538:LYS:CE	5:B:1006:GOL:H11	2.45	0.44
1:B:680:ARG:HH12	1:B:687:LYS:NZ	2.16	0.44
1:B:560:ILE:HG23	1:B:593:ILE:HG23	1.99	0.44
1:A:580:ASP:OD2	1:A:581:GLY:N	2.51	0.43
1:B:785:LEU:HD23	1:B:785:LEU:HA	1.77	0.43
1:A:779:ARG:O	1:A:842:VAL:HG22	2.18	0.43
1:A:635:LEU:HD23	1:A:639[B]:ARG:HH12	1.82	0.43
1:B:696:ASN:HB3	1:B:709:TYR:CD2	2.54	0.43
1:A:713[A]:VAL:CG2	1:A:729:LEU:HD13	2.49	0.42
1:A:524:PRO:O	1:A:590:LEU:HD12	2.18	0.42
1:B:571:LYS:HG2	1:B:585:PHE:CD2	2.54	0.42
1:B:645:VAL:HG12	1:B:647:LEU:HD12	2.02	0.42
1:A:635:LEU:HD22	1:A:639[B]:ARG:HH12	1.84	0.42
1:A:779:ARG:HA	1:A:791:THR:O	2.21	0.41
1:B:769:LEU:HG	1:B:819:ALA:HB2	2.02	0.41
1:B:680:ARG:O	1:B:680:ARG:HD2	2.21	0.41
1:B:783:CYS:SG	1:B:856:GLU:HA	2.61	0.41
1:A:779:ARG:NH2	1:A:790:LYS:HB3	2.36	0.40
1:A:756:LYS:HE2	1:A:824:LYS:NZ	2.36	0.40
5:B:1008:GOL:H12	7:B:1344[A]:HOH:O	2.21	0.40

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	A	346/457 (76%)	340 (98%)	6 (2%)	0	100	100
1	B	347/457 (76%)	341 (98%)	6 (2%)	0	100	100
All	All	693/914 (76%)	681 (98%)	12 (2%)	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	A	299/393 (76%)	291 (97%)	8 (3%)	39	23
1	B	299/393 (76%)	293 (98%)	6 (2%)	48	33
All	All	598/786 (76%)	584 (98%)	14 (2%)	43	29

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

Mol	Chain	Res	Type
1	A	547	ASN
1	A	550	GLU
1	A	630	ILE
1	A	657	LYS
1	A	779	ARG
1	A	785	LEU
1	A	790	LYS
1	A	821	GLN

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Mol	Chain	Res	Type
1	B	629	THR
1	B	637	ARG
1	B	680	ARG
1	B	729	LEU
1	B	790	LYS
1	B	821	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	628	GLN
1	A	705	ASN
1	A	792	ASN
1	A	810	GLN
1	B	623	HIS
1	B	677	ASN
1	B	685	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\# Z > 2$
5	GOL	A	1006	-	5,5,5	0.61	0	5,5,5	0.36	0
5	GOL	B	1007	-	5,5,5	0.72	0	5,5,5	0.89	0
5	GOL	A	1005	-	5,5,5	0.28	0	5,5,5	0.48	0
6	ACY	B	1004	-	3,3,3	0.83	0	3,3,3	0.73	0
2	GTP	A	1001	3,4	33,34,34	1.12	3 (9%)	50,54,54	1.78	13 (26%)
5	GOL	B	1006	-	5,5,5	0.30	0	5,5,5	0.98	0
5	GOL	B	1008	-	5,5,5	1.08	0	5,5,5	1.65	1 (20%)
5	GOL	A	1004	-	5,5,5	1.15	0	5,5,5	1.90	1 (20%)
5	GOL	B	1005	-	5,5,5	0.41	0	5,5,5	0.70	0
2	GTP	B	1001	3,4	33,34,34	1.14	2 (6%)	50,54,54	1.49	6 (12%)

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
5	GOL	A	1006	-	-	3/4/4/4	-
5	GOL	B	1007	-	-	2/4/4/4	-
5	GOL	A	1005	-	-	2/4/4/4	-
2	GTP	A	1001	3,4	-	0/22/38/38	0/3/3/3
5	GOL	B	1006	-	-	0/4/4/4	-
5	GOL	B	1008	-	-	2/4/4/4	-
5	GOL	A	1004	-	-	4/4/4/4	-
5	GOL	B	1005	-	-	4/4/4/4	-
2	GTP	B	1001	3,4	-	0/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GTP	PA-O3A	3.70	1.63	1.59
2	B	1001	GTP	C8-N7	2.94	1.40	1.32
2	B	1001	GTP	PA-O3A	2.62	1.62	1.59
2	A	1001	GTP	PB-O3B	2.60	1.62	1.59
2	A	1001	GTP	C8-N7	2.10	1.38	1.32

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	GTP	C2-N3-C4	5.09	121.07	112.30
2	B	1001	GTP	C5-C4-N3	-4.10	121.86	128.39
2	A	1001	GTP	C5-C4-N3	-3.99	122.04	128.39
5	A	1004	GOL	C3-C2-C1	3.69	125.31	111.80
2	A	1001	GTP	N9-C8-N7	-3.66	106.61	113.40
2	B	1001	GTP	O2B-PB-O3A	-3.23	98.55	107.27
2	B	1001	GTP	C2-N3-C4	3.20	117.81	112.30
2	A	1001	GTP	N2-C2-N1	3.17	123.46	116.76
2	B	1001	GTP	N9-C8-N7	-3.09	107.67	113.40
2	A	1001	GTP	N1-C2-N3	-2.66	118.46	123.32
2	A	1001	GTP	C5-C6-N1	2.65	120.00	113.25
2	A	1001	GTP	O3G-PG-O2G	2.61	117.58	107.80
2	B	1001	GTP	C2'-C1'-N9	-2.51	106.25	113.25
2	A	1001	GTP	O6-C6-C5	-2.39	120.22	126.53
2	A	1001	GTP	C8-N7-C5	2.32	108.40	104.26
5	B	1008	GOL	O1-C1-C2	2.29	120.67	110.38
2	A	1001	GTP	C2-N1-C6	-2.26	121.01	125.11
2	A	1001	GTP	O3A-PB-O1B	-2.23	103.98	110.70
2	A	1001	GTP	N9-C4-N3	2.21	130.38	125.95
2	B	1001	GTP	O4'-C1'-C2'	-2.18	101.96	106.62
2	A	1001	GTP	O3G-PG-O3B	-2.05	97.77	104.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1004	GOL	C1-C2-C3-O3
5	A	1005	GOL	O1-C1-C2-C3
5	A	1006	GOL	O1-C1-C2-C3
5	B	1005	GOL	O1-C1-C2-C3
5	B	1005	GOL	C1-C2-C3-O3
5	B	1008	GOL	O1-C1-C2-O2
5	B	1008	GOL	O1-C1-C2-C3
5	A	1004	GOL	O1-C1-C2-C3
5	B	1007	GOL	O1-C1-C2-C3
5	A	1005	GOL	O1-C1-C2-O2
5	B	1005	GOL	O1-C1-C2-O2
5	B	1005	GOL	O2-C2-C3-O3
5	A	1004	GOL	O2-C2-C3-O3
5	A	1004	GOL	O1-C1-C2-O2
5	A	1006	GOL	O1-C1-C2-O2
5	B	1007	GOL	O1-C1-C2-O2
5	A	1006	GOL	O2-C2-C3-O3

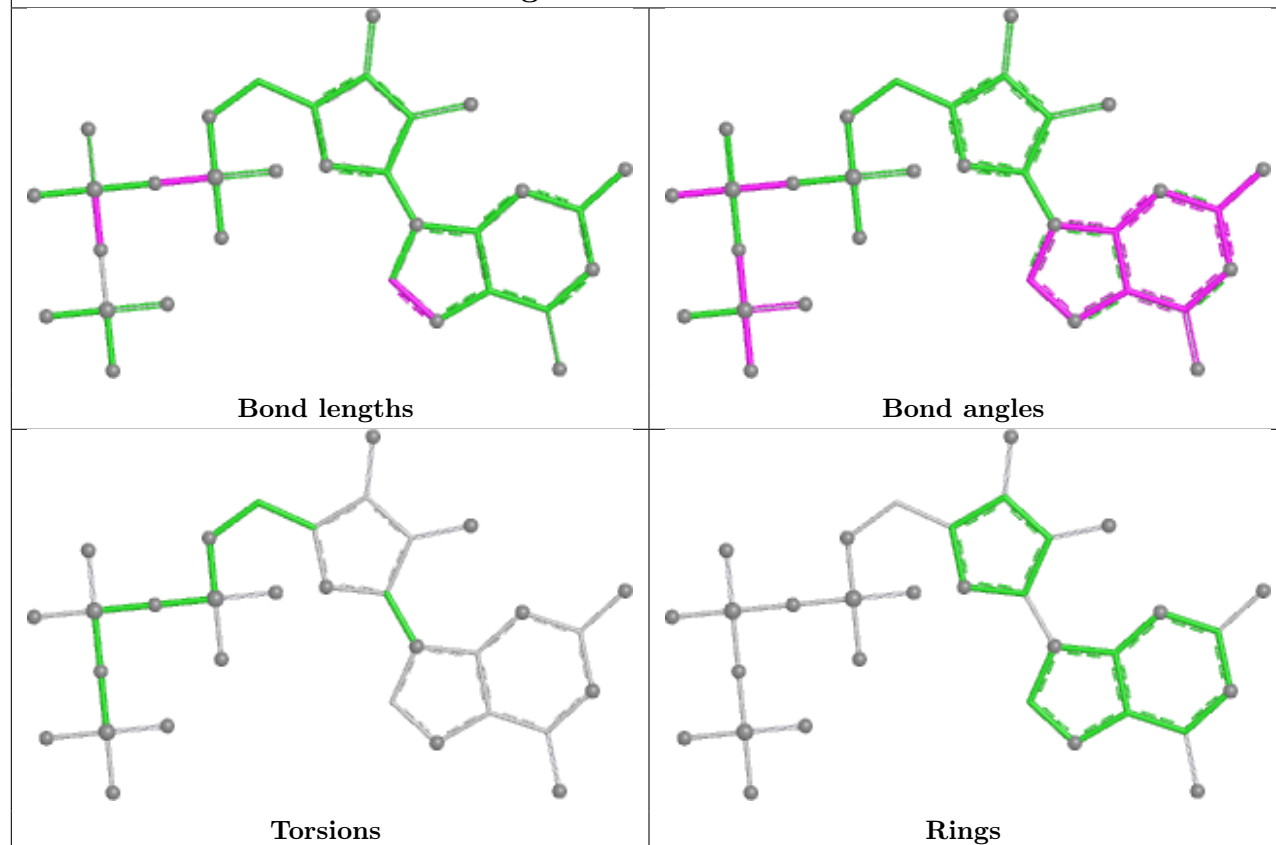
There are no ring outliers.

7 monomers are involved in 13 short contacts:

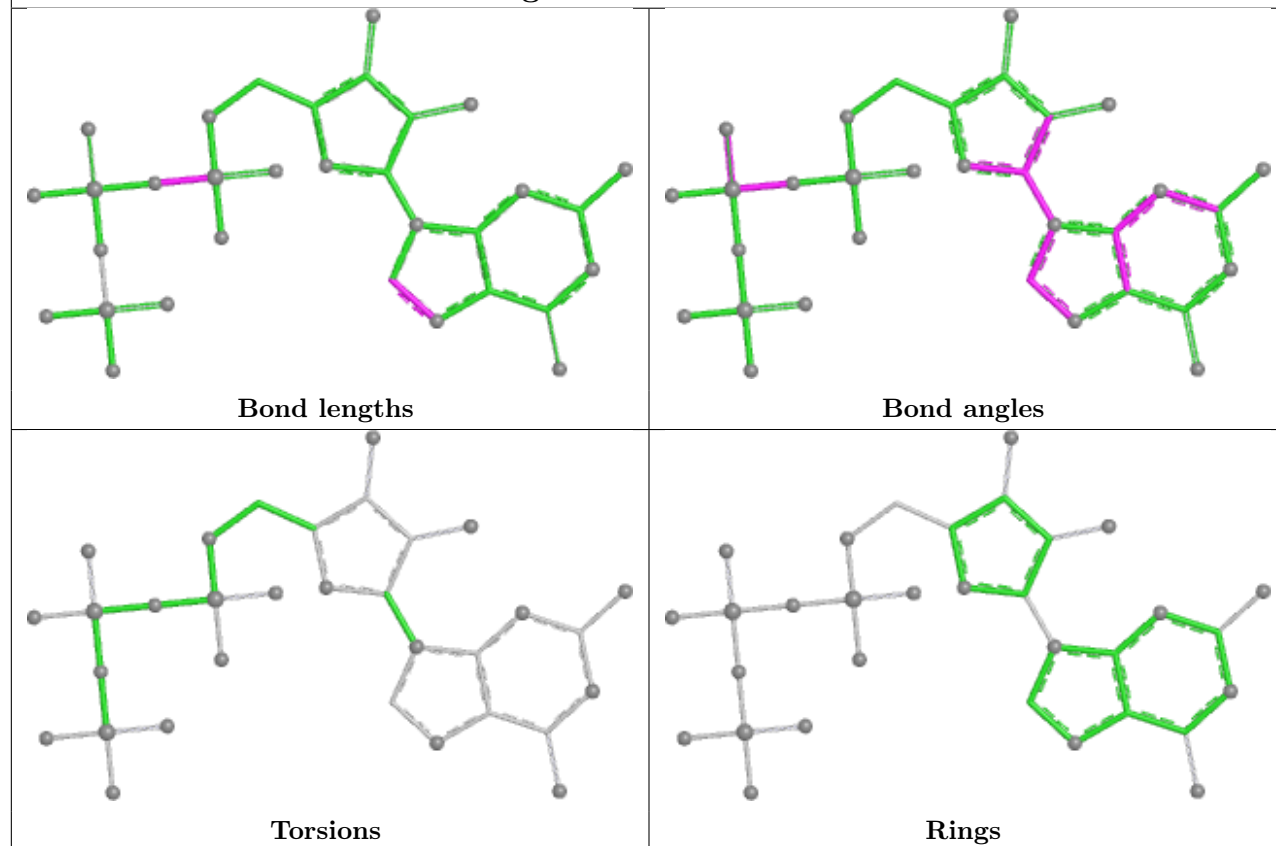
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1006	GOL	1	0
5	A	1005	GOL	1	0
6	B	1004	ACY	2	0
5	B	1006	GOL	5	0
5	B	1008	GOL	1	0
5	A	1004	GOL	1	0
5	B	1005	GOL	2	0

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.

Ligand GTP A 1001



Ligand GTP B 1001



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 [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	344/457 (75%)	-0.24	4 (1%) 76 81	9, 31, 79, 122	4 (1%)
1	B	345/457 (75%)	-0.37	2 (0%) 85 89	9, 29, 63, 95	4 (1%)
All	All	689/914 (75%)	-0.31	6 (0%) 81 85	9, 30, 72, 122	8 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	654	TYR	4.7
1	B	706	PHE	2.8
1	A	842	VAL	2.4
1	A	859	LEU	2.3
1	B	704	LYS	2.1
1	A	811	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](#)

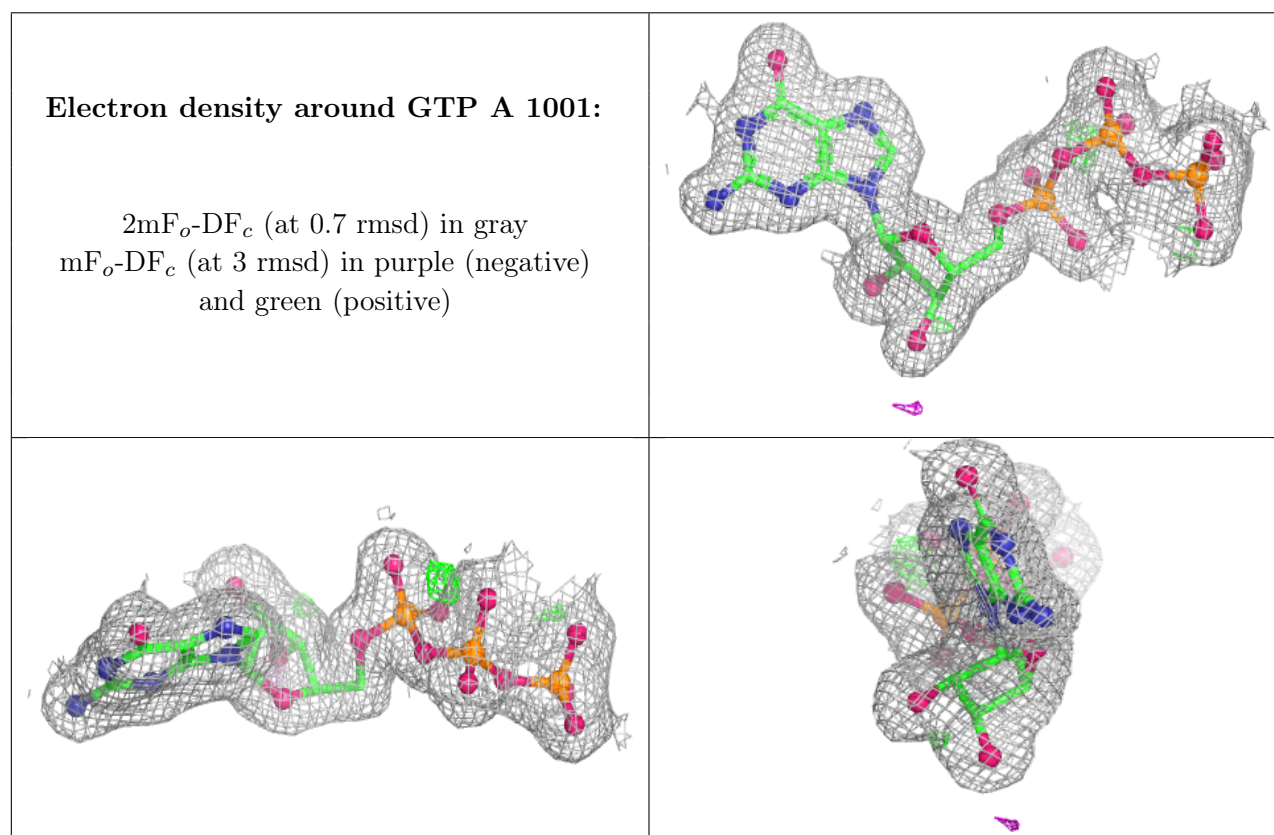
There are no oligosaccharides in this entry.

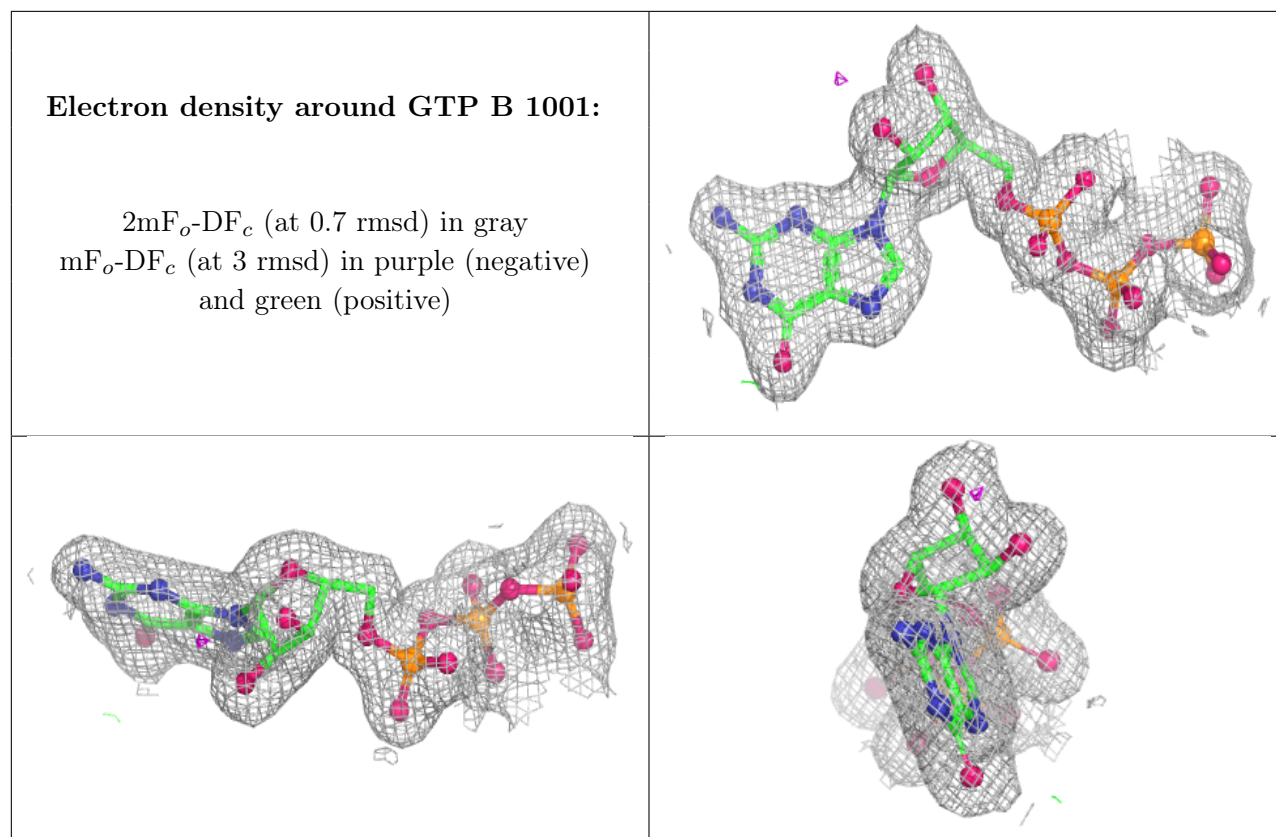
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
6	ACY	B	1004	4/4	0.65	0.15	39,52,58,60	0
5	GOL	A	1006	6/6	0.87	0.12	47,51,60,63	0
5	GOL	A	1004	6/6	0.88	0.15	27,28,40,55	0
5	GOL	B	1005	6/6	0.88	0.12	48,55,57,57	6
5	GOL	B	1007	6/6	0.88	0.13	38,47,55,57	0
5	GOL	B	1008	6/6	0.88	0.13	26,45,48,52	0
5	GOL	A	1005	6/6	0.88	0.13	37,51,54,56	0
5	GOL	B	1006	6/6	0.89	0.11	37,52,57,65	0
3	MG	A	1002	1/1	0.99	0.02	18,18,18,18	0
3	MG	B	1002	1/1	0.99	0.02	18,18,18,18	0
4	NA	A	1003	1/1	0.99	0.03	21,21,21,21	0
4	NA	B	1003	1/1	0.99	0.02	20,20,20,20	0
2	GTP	A	1001	32/32	0.99	0.03	12,18,22,24	0
2	GTP	B	1001	32/32	0.99	0.03	15,19,24,27	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.