



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:22 PM UTC

PDB ID : 4RXO / pdb_00004rxo
Title : The structure of GTP-bound SAMHD1
Authors : Zhu, C.F.; Wei, W.; Peng, X.; Dong, Y.H.; Gong, Y.; Yu, X.F.
Deposited on : 2014-12-11
Resolution : 2.60 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

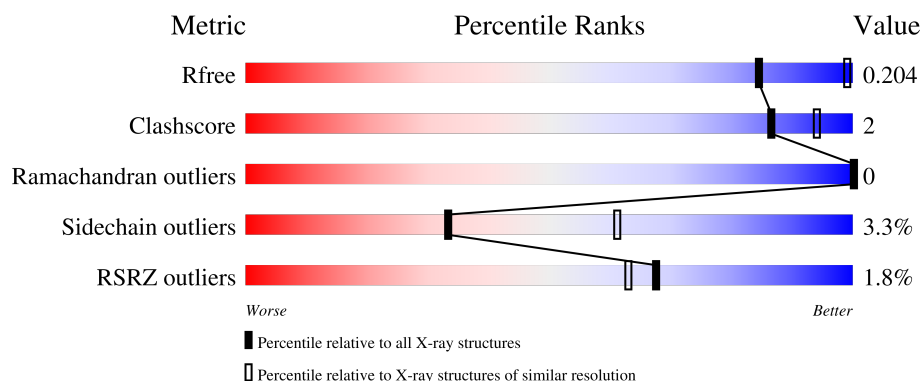
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	539	 2% 76% 8% 15%
1	B	539	 % 76% . 20%
1	C	539	 % 77% . 19%
1	D	539	 % 76% 6% . 18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14977 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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3737	2395	649	674	19			
1	B	433	Total	C	N	O	S	0	0	0
			3555	2282	615	641	17			
1	C	434	Total	C	N	O	S	0	0	0
			3559	2282	616	643	18			
1	D	444	Total	C	N	O	S	0	0	0
			3642	2335	633	656	18			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	expression tag	UNP Q9Y3Z3
A	89	GLY	-	expression tag	UNP Q9Y3Z3
A	90	SER	-	expression tag	UNP Q9Y3Z3
A	91	SER	-	expression tag	UNP Q9Y3Z3
A	92	HIS	-	expression tag	UNP Q9Y3Z3
A	93	HIS	-	expression tag	UNP Q9Y3Z3
A	94	HIS	-	expression tag	UNP Q9Y3Z3
A	95	HIS	-	expression tag	UNP Q9Y3Z3
A	96	HIS	-	expression tag	UNP Q9Y3Z3
A	97	HIS	-	expression tag	UNP Q9Y3Z3
A	98	SER	-	expression tag	UNP Q9Y3Z3
A	99	SER	-	expression tag	UNP Q9Y3Z3
A	100	GLY	-	expression tag	UNP Q9Y3Z3
A	101	GLU	-	expression tag	UNP Q9Y3Z3
A	102	ASN	-	expression tag	UNP Q9Y3Z3
A	103	LEU	-	expression tag	UNP Q9Y3Z3
A	104	TYR	-	expression tag	UNP Q9Y3Z3
A	105	PHE	-	expression tag	UNP Q9Y3Z3
A	106	GLN	-	expression tag	UNP Q9Y3Z3
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	SER	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	266	TYR	CYS	conflict	UNP Q9Y3Z3
B	88	MET	-	expression tag	UNP Q9Y3Z3
B	89	GLY	-	expression tag	UNP Q9Y3Z3
B	90	SER	-	expression tag	UNP Q9Y3Z3
B	91	SER	-	expression tag	UNP Q9Y3Z3
B	92	HIS	-	expression tag	UNP Q9Y3Z3
B	93	HIS	-	expression tag	UNP Q9Y3Z3
B	94	HIS	-	expression tag	UNP Q9Y3Z3
B	95	HIS	-	expression tag	UNP Q9Y3Z3
B	96	HIS	-	expression tag	UNP Q9Y3Z3
B	97	HIS	-	expression tag	UNP Q9Y3Z3
B	98	SER	-	expression tag	UNP Q9Y3Z3
B	99	SER	-	expression tag	UNP Q9Y3Z3
B	100	GLY	-	expression tag	UNP Q9Y3Z3
B	101	GLU	-	expression tag	UNP Q9Y3Z3
B	102	ASN	-	expression tag	UNP Q9Y3Z3
B	103	LEU	-	expression tag	UNP Q9Y3Z3
B	104	TYR	-	expression tag	UNP Q9Y3Z3
B	105	PHE	-	expression tag	UNP Q9Y3Z3
B	106	GLN	-	expression tag	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	SER	-	expression tag	UNP Q9Y3Z3
B	266	TYR	CYS	conflict	UNP Q9Y3Z3
C	88	MET	-	expression tag	UNP Q9Y3Z3
C	89	GLY	-	expression tag	UNP Q9Y3Z3
C	90	SER	-	expression tag	UNP Q9Y3Z3
C	91	SER	-	expression tag	UNP Q9Y3Z3
C	92	HIS	-	expression tag	UNP Q9Y3Z3
C	93	HIS	-	expression tag	UNP Q9Y3Z3
C	94	HIS	-	expression tag	UNP Q9Y3Z3
C	95	HIS	-	expression tag	UNP Q9Y3Z3
C	96	HIS	-	expression tag	UNP Q9Y3Z3
C	97	HIS	-	expression tag	UNP Q9Y3Z3
C	98	SER	-	expression tag	UNP Q9Y3Z3
C	99	SER	-	expression tag	UNP Q9Y3Z3
C	100	GLY	-	expression tag	UNP Q9Y3Z3
C	101	GLU	-	expression tag	UNP Q9Y3Z3
C	102	ASN	-	expression tag	UNP Q9Y3Z3
C	103	LEU	-	expression tag	UNP Q9Y3Z3
C	104	TYR	-	expression tag	UNP Q9Y3Z3
C	105	PHE	-	expression tag	UNP Q9Y3Z3
C	106	GLN	-	expression tag	UNP Q9Y3Z3

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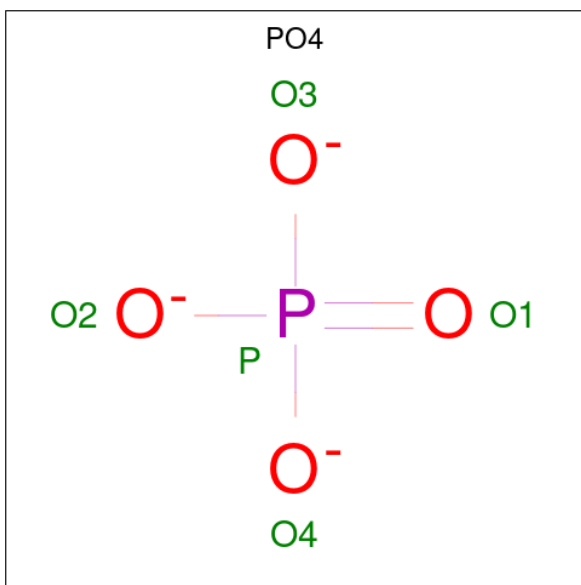
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Chain	Residue	Modelled	Actual	Comment	Reference
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	SER	-	expression tag	UNP Q9Y3Z3
C	266	TYR	CYS	conflict	UNP Q9Y3Z3
D	88	MET	-	expression tag	UNP Q9Y3Z3
D	89	GLY	-	expression tag	UNP Q9Y3Z3
D	90	SER	-	expression tag	UNP Q9Y3Z3
D	91	SER	-	expression tag	UNP Q9Y3Z3
D	92	HIS	-	expression tag	UNP Q9Y3Z3
D	93	HIS	-	expression tag	UNP Q9Y3Z3
D	94	HIS	-	expression tag	UNP Q9Y3Z3
D	95	HIS	-	expression tag	UNP Q9Y3Z3
D	96	HIS	-	expression tag	UNP Q9Y3Z3
D	97	HIS	-	expression tag	UNP Q9Y3Z3
D	98	SER	-	expression tag	UNP Q9Y3Z3
D	99	SER	-	expression tag	UNP Q9Y3Z3
D	100	GLY	-	expression tag	UNP Q9Y3Z3
D	101	GLU	-	expression tag	UNP Q9Y3Z3
D	102	ASN	-	expression tag	UNP Q9Y3Z3
D	103	LEU	-	expression tag	UNP Q9Y3Z3
D	104	TYR	-	expression tag	UNP Q9Y3Z3
D	105	PHE	-	expression tag	UNP Q9Y3Z3
D	106	GLN	-	expression tag	UNP Q9Y3Z3
D	107	GLY	-	expression tag	UNP Q9Y3Z3
D	108	SER	-	expression tag	UNP Q9Y3Z3
D	266	TYR	CYS	conflict	UNP Q9Y3Z3

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

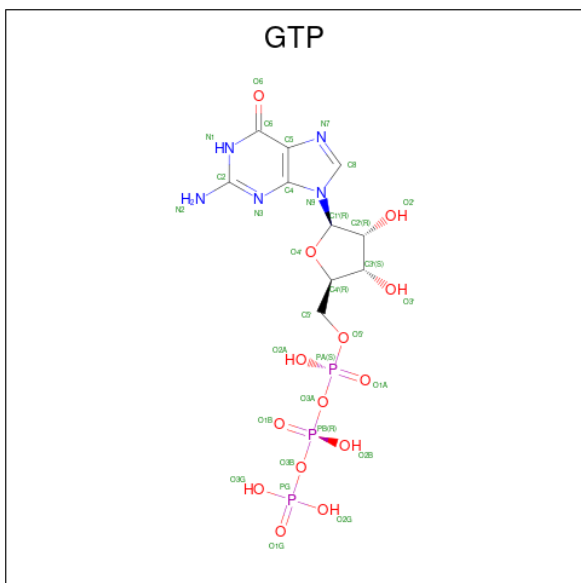
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0
3	C	1	Total 5	O 4	P 1	0	0
3	D	1	Total 5	O 4	P 1	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



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

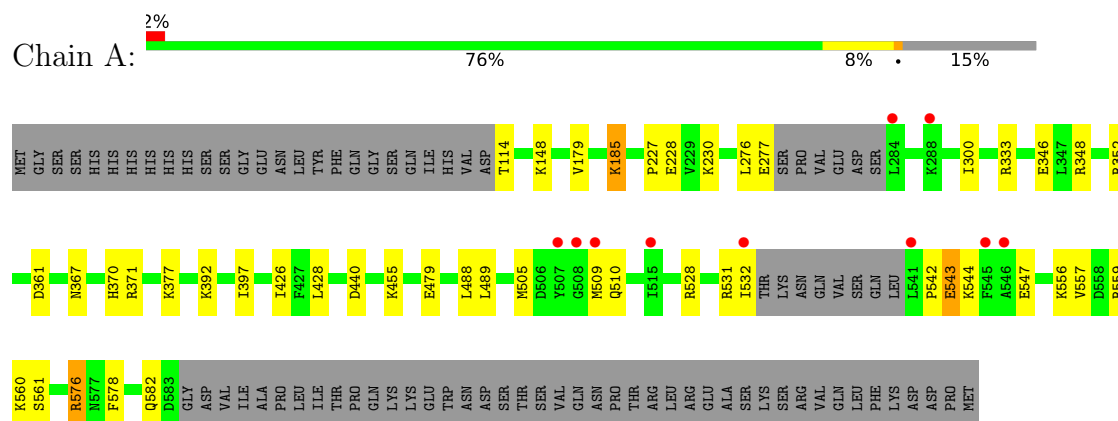
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	89	Total	O	0	0
			89	89		
5	C	76	Total	O	0	0
			76	76		
5	D	59	Total	O	0	0
			59	59		

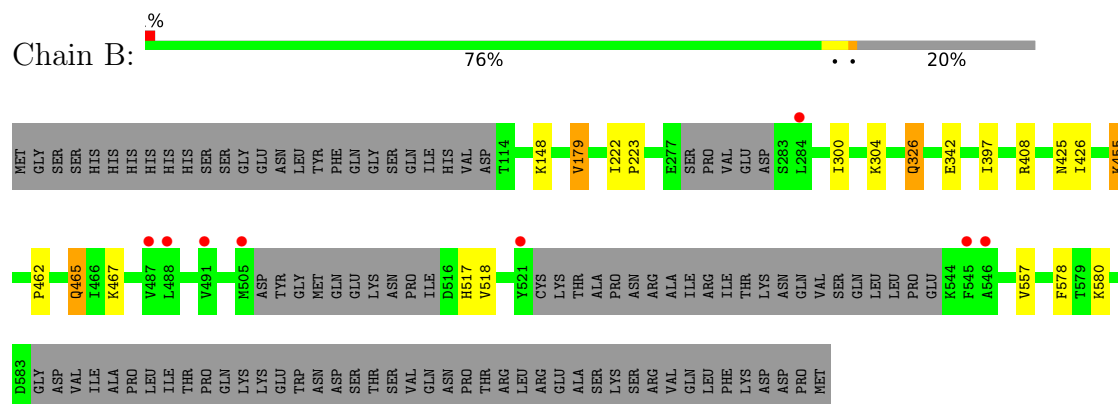
3 Residue-property plots [i](#)

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.

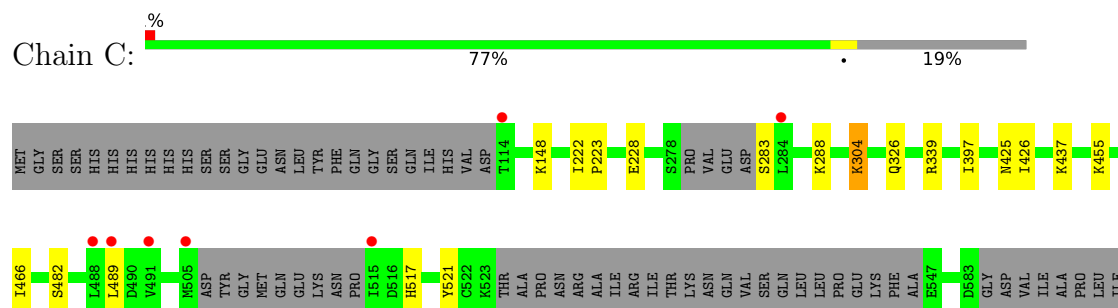
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



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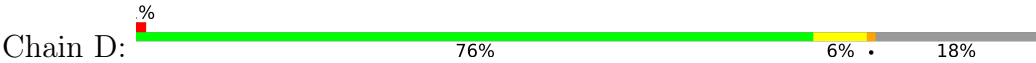


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



THR	PRO	GLN	LYS	LYS	GLU	TRP	ASN	ASP	THR	THR	VAL	GLN	PRO	THR	ARG	LEU	ARG	GLU	ALA	SER	LYS	SER	ARG	VAL	GLN	LEU	PHE	LYS	ASP	PRO	PRO	MET
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● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	SER	GLY	GLU	ASN	ASN	LEU	TYR	PHE	GLN	GLY	SER	GLN	ILE	HIS	VAL	ASP	T114	M115	R143	K148	L204	K230	P261	E277	SER	PRO	VAL	GLU	ASP	SER	L284	N306	R333	K336	E342	N345	R352	D353							
K354	D361	R371	K377	I397	N426	I426	K439	R442	I466	S482	K486	K494	A495	E496	M505	D506	GLY	MET	GLN	GLU	LYS	ASN	ASN	PRO	I515	D516	H517	K523	R531	I532	THR	LYS	ASN	GLN	VAL	SER	GLN	LEU	LEU	PRO	GLU	LYS	PHE	A546	E547										
Q548	L549	K560	R576	N577	K580	P581	Q582	D583	GLY	ASP	VAL	ILE	ALA	ALA	PRO	LEU	PRO	LEU	ILE	THR	PRO	GLN	LYS	LYS	GLU	TRP	ASN	ASP	SER	THR	SER	VAL	GLN	ASN	PRO	PRO	THR	ARG	LEU	ARG	GLU	ALA	ALA	SER	LYS	SER	ARG	VAL	GLN	PHE	LYS	ASP	ASP	PRO	MET

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.22Å 183.19Å 81.28Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.60) 96.6 (50.00-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.183 , 0.222 (Not available) , 0.204	Depositor DCC
R_{free} test set	3257 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14977	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: GTP, ZN, PO4

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	0.63	0/3826	0.86	5/5161 (0.1%)
1	B	0.62	0/3639	0.85	1/4906 (0.0%)
1	C	0.62	0/3642	0.84	0/4910
1	D	0.61	0/3727	0.84	2/5027 (0.0%)
All	All	0.62	0/14834	0.85	8/20004 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	LEU	N-CA-C	6.28	119.17	109.07
1	A	509	MET	N-CA-C	5.75	118.31	110.55
1	D	531	ARG	N-CA-C	5.63	118.35	111.82
1	D	547	GLU	N-CA-C	5.30	117.37	110.53
1	A	576	ARG	CG-CD-NE	-5.24	100.48	112.00
1	A	227	PRO	CA-C-N	5.19	127.55	120.54
1	A	227	PRO	C-N-CA	5.19	127.55	120.54
1	B	179	VAL	CB-CA-C	-5.06	105.31	112.14

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	3737	0	3703	23	0
1	B	3555	0	3520	15	0
1	C	3559	0	3527	8	0
1	D	3642	0	3613	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	B	64	0	24	0	0
4	C	32	0	12	0	0
4	D	32	0	12	0	0
5	A	108	0	0	2	0
5	B	89	0	0	2	0
5	C	76	0	0	0	0
5	D	59	0	0	2	0
All	All	14977	0	14411	62	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 2.

All (62) 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:D:371:ARG:NH1	1:D:505:MET:HE1	1.91	0.85
1:D:371:ARG:HH12	1:D:505:MET:HE1	1.54	0.70
1:A:179:VAL:HG22	1:A:300:ILE:HD13	1.76	0.67
1:D:439:LYS:HE3	1:D:442:ARG:HH21	1.61	0.66
1:B:179:VAL:HG22	1:B:300:ILE:HD13	1.77	0.64
1:A:576:ARG:HG2	1:A:578:PHE:CE2	2.34	0.62
1:D:371:ARG:NH1	1:D:505:MET:CE	2.63	0.61
1:D:306:ASN:HB3	1:D:517:HIS:HB3	1.83	0.60
1:A:576:ARG:HG2	1:A:578:PHE:CZ	2.37	0.60
1:D:560:LYS:HD2	1:D:560:LYS:N	2.19	0.57
1:B:179:VAL:CG2	1:B:300:ILE:HD13	2.34	0.57
1:A:179:VAL:CG2	1:A:300:ILE:HD13	2.34	0.57
1:A:505:MET:HB2	1:A:547:GLU:OE1	2.05	0.56
1:C:304:LYS:HA	1:C:304:LYS:HE2	1.87	0.55
1:A:346:GLU:OE1	1:A:348:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:PRO:HB3	1:A:543:GLU:OE1	2.08	0.54
1:D:371:ARG:HH11	1:D:505:MET:CE	2.23	0.52
1:A:556:LYS:NZ	5:A:850:HOH:O	2.43	0.52
1:B:326:GLN:HB2	5:B:973:HOH:O	2.09	0.51
1:A:333:ARG:NH2	1:D:361:ASP:OD1	2.43	0.51
1:D:560:LYS:HD2	1:D:560:LYS:H	1.76	0.50
1:A:543:GLU:N	1:A:543:GLU:CD	2.70	0.49
1:A:370:HIS:CG	1:A:505:MET:HE3	2.48	0.48
1:C:228:GLU:H	1:C:228:GLU:CD	2.22	0.48
1:A:582:GLN:NE2	5:A:851:HOH:O	2.35	0.47
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.95	0.47
1:D:560:LYS:H	1:D:560:LYS:CD	2.28	0.47
1:D:352:ARG:HG2	1:D:354:LYS:HG2	1.96	0.47
1:B:465:GLN:HA	1:B:465:GLN:OE1	2.15	0.46
1:C:339:ARG:HD3	1:C:521:TYR:CZ	2.50	0.45
1:B:397:ILE:HG21	1:B:426:ILE:HD11	1.99	0.45
1:B:455:LYS:HD3	1:B:557:VAL:HG13	1.99	0.44
1:D:143:ARG:HD3	5:D:803:HOH:O	2.17	0.44
1:C:397:ILE:HG21	1:C:426:ILE:HD11	2.00	0.43
1:B:557:VAL:HG12	1:B:557:VAL:O	2.18	0.43
1:A:543:GLU:CD	1:A:543:GLU:H	2.26	0.43
1:C:455:LYS:HD3	1:C:455:LYS:HA	1.72	0.43
1:D:560:LYS:N	1:D:560:LYS:CD	2.82	0.43
1:D:580:LYS:HE2	1:D:580:LYS:HB2	1.88	0.42
1:B:179:VAL:HG22	1:B:300:ILE:CD1	2.48	0.42
1:B:326:GLN:NE2	1:C:326:GLN:HG2	2.35	0.42
1:C:425:ASN:OD1	1:D:425:ASN:OD1	2.38	0.42
1:B:342:GLU:H	1:B:342:GLU:CD	2.27	0.42
1:D:115:MET:HA	5:D:833:HOH:O	2.20	0.42
1:D:397:ILE:HG21	1:D:426:ILE:HD11	2.01	0.42
1:A:185:LYS:HA	1:A:185:LYS:HD2	1.86	0.42
1:A:560:LYS:HG3	1:A:561:SER:N	2.35	0.41
1:B:462:PRO:HA	1:B:578:PHE:CD1	2.55	0.41
1:A:367:ASN:CG	1:A:543:GLU:HG2	2.45	0.41
1:B:222:ILE:HB	1:B:223:PRO:HD3	2.02	0.41
1:D:576:ARG:O	1:D:577:ASN:OD1	2.38	0.41
1:A:361:ASP:OD1	1:D:333:ARG:NH2	2.52	0.41
1:A:479:GLU:OE1	1:A:576:ARG:NH1	2.53	0.41
1:B:467:LYS:O	1:B:467:LYS:HG3	2.20	0.41
1:A:428:LEU:HD13	1:B:425:ASN:HB2	2.02	0.41
1:C:222:ILE:HB	1:C:223:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LYS:HE3	1:A:377:LYS:HB2	1.81	0.41
1:D:352:ARG:CZ	1:D:523:LYS:HD3	2.51	0.41
1:D:439:LYS:HE3	1:D:442:ARG:NH2	2.31	0.41
1:A:392:LYS:HD3	1:A:440:ASP:HB3	2.03	0.40
1:B:408:ARG:NH1	5:B:967:HOH:O	2.54	0.40
1:A:397:ILE:HG21	1:A:426:ILE:HD11	2.02	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	450/539 (84%)	445 (99%)	5 (1%)	0	100	100
1	B	425/539 (79%)	417 (98%)	8 (2%)	0	100	100
1	C	426/539 (79%)	419 (98%)	7 (2%)	0	100	100
1	D	436/539 (81%)	429 (98%)	7 (2%)	0	100	100
All	All	1737/2156 (81%)	1710 (98%)	27 (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	403/481 (84%)	386 (96%)	17 (4%)	26	52
1	B	384/481 (80%)	376 (98%)	8 (2%)	47	73
1	C	386/481 (80%)	377 (98%)	9 (2%)	44	71
1	D	393/481 (82%)	376 (96%)	17 (4%)	26	51
All	All	1566/1924 (81%)	1515 (97%)	51 (3%)	33	61

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	148	LYS
1	A	185	LYS
1	A	228	GLU
1	A	230	LYS
1	A	277	GLU
1	A	352	ARG
1	A	371	ARG
1	A	488	LEU
1	A	489	LEU
1	A	510	GLN
1	A	528	ARG
1	A	531	ARG
1	A	532	ILE
1	A	543	GLU
1	A	544	LYS
1	A	559	ARG
1	B	148	LYS
1	B	304	LYS
1	B	326	GLN
1	B	455	LYS
1	B	465	GLN
1	B	517	HIS
1	B	518	VAL
1	B	580	LYS
1	C	148	LYS
1	C	283	SER
1	C	288	LYS
1	C	304	LYS
1	C	437	LYS
1	C	466	ILE
1	C	482	SER
1	C	489	LEU

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Mol	Chain	Res	Type
1	C	517	HIS
1	D	148	LYS
1	D	204	LEU
1	D	230	LYS
1	D	261	PRO
1	D	336	LYS
1	D	342	GLU
1	D	345	ASN
1	D	352	ARG
1	D	371	ARG
1	D	377	LYS
1	D	482	SER
1	D	486	LYS
1	D	494	LYS
1	D	496	GLU
1	D	506	ASP
1	D	577	ASN
1	D	582	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	200	GLN
1	A	243	HIS
1	A	326	GLN
1	A	328	ASN
1	A	367	ASN
1	A	447	GLN
1	A	571	GLN
1	A	577	ASN
1	B	163	ASN
1	B	200	GLN
1	B	243	HIS
1	B	248	ASN
1	B	326	GLN
1	B	327	ASN
1	B	345	ASN
1	B	571	GLN
1	C	200	GLN
1	C	243	HIS
1	C	248	ASN

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Mol	Chain	Res	Type
1	C	303	ASN
1	C	447	GLN
1	C	571	GLN
1	D	163	ASN
1	D	200	GLN
1	D	243	HIS
1	D	567	GLN
1	D	571	GLN
1	D	577	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	B	803	-	33,34,34	1.22	5 (15%)	50,54,54	1.83	8 (16%)
3	PO4	A	702	2	4,4,4	1.31	0	6,6,6	0.87	0
3	PO4	C	703	2	4,4,4	1.27	0	6,6,6	0.34	0
4	GTP	D	702	-	33,34,34	1.39	6 (18%)	50,54,54	1.68	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GTP	C	702	-	33,34,34	1.14	4 (12%)	50,54,54	1.75	9 (18%)
3	PO4	D	703	2	4,4,4	1.21	0	6,6,6	0.62	0
3	PO4	B	804	2	4,4,4	1.09	0	6,6,6	0.20	0
4	GTP	B	801	-	33,34,34	1.22	4 (12%)	50,54,54	1.77	9 (18%)

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	D	702	-	-	7/22/38/38	0/3/3/3
4	GTP	B	803	-	-	5/22/38/38	0/3/3/3
4	GTP	C	702	-	-	7/22/38/38	0/3/3/3
4	GTP	B	801	-	-	7/22/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	GTP	C5-C4	3.31	1.47	1.38
4	D	702	GTP	PA-O3A	3.25	1.63	1.59
4	D	702	GTP	C5-C4	3.15	1.47	1.38
4	D	702	GTP	PB-O3A	3.05	1.62	1.59
4	B	803	GTP	C5-C4	2.91	1.46	1.38
4	B	801	GTP	C5-C4	2.87	1.46	1.38
4	B	803	GTP	PB-O3B	2.80	1.62	1.59
4	B	801	GTP	C5-N7	-2.65	1.33	1.39
4	D	702	GTP	C5-N7	-2.61	1.33	1.39
4	C	702	GTP	C5-N7	-2.49	1.34	1.39
4	B	801	GTP	C6-N1	-2.44	1.34	1.38
4	D	702	GTP	C6-N1	-2.44	1.34	1.38
4	B	801	GTP	PB-O3B	2.31	1.62	1.59
4	C	702	GTP	C6-N1	-2.27	1.34	1.38
4	B	803	GTP	C5-N7	-2.27	1.34	1.39
4	B	803	GTP	PB-O3A	2.18	1.61	1.59
4	C	702	GTP	PB-O3B	2.17	1.61	1.59
4	B	803	GTP	C6-N1	-2.16	1.34	1.38
4	D	702	GTP	PB-O3B	2.06	1.61	1.59

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	GTP	C5-C4-N3	-6.05	118.77	128.39
4	D	702	GTP	C5-C4-N3	-6.03	118.80	128.39
4	C	702	GTP	C5-C4-N3	-6.02	118.81	128.39
4	B	801	GTP	C5-C4-N3	-5.87	119.04	128.39
4	B	803	GTP	C2-N3-C4	5.27	121.38	112.30
4	D	702	GTP	N9-C4-N3	4.99	135.93	125.95
4	B	801	GTP	N9-C4-N3	4.91	135.77	125.95
4	C	702	GTP	N9-C4-N3	4.85	135.66	125.95
4	B	801	GTP	C2-N3-C4	4.72	120.42	112.30
4	C	702	GTP	C2-N3-C4	4.53	120.10	112.30
4	B	803	GTP	N9-C4-N3	4.50	134.95	125.95
4	D	702	GTP	C2-N3-C4	4.48	120.02	112.30
4	C	702	GTP	O3A-PB-O1B	-3.48	100.23	110.70
4	B	803	GTP	C6-C5-N7	3.45	136.56	130.29
4	B	801	GTP	C6-C5-N7	2.97	135.70	130.29
4	D	702	GTP	O2A-PA-O3A	2.81	114.88	107.27
4	B	803	GTP	C4-C5-N7	-2.77	106.28	110.67
4	C	702	GTP	C6-C5-N7	2.69	135.19	130.29
4	B	803	GTP	O3A-PA-O1A	-2.57	102.97	110.70
4	B	801	GTP	C4-C5-N7	-2.38	106.90	110.67
4	B	801	GTP	O3A-PB-O1B	-2.35	103.62	110.70
4	C	702	GTP	O6-C6-C5	-2.26	120.57	126.53
4	D	702	GTP	C6-C5-N7	2.24	134.36	130.29
4	B	801	GTP	C3'-C2'-C1'	2.23	105.68	101.46
4	B	803	GTP	O2B-PB-O3A	-2.18	101.38	107.27
4	C	702	GTP	O2A-PA-O1A	2.13	122.37	112.44
4	D	702	GTP	O6-C6-C5	-2.11	120.96	126.53
4	B	803	GTP	C8-N7-C5	2.10	108.00	104.26
4	B	801	GTP	C8-N7-C5	2.09	107.98	104.26
4	B	801	GTP	O2A-PA-O1A	2.08	122.10	112.44
4	C	702	GTP	C4-C5-N7	-2.05	107.42	110.67
4	C	702	GTP	O3G-PG-O2G	2.01	115.33	107.80

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	GTP	C5'-O5'-PA-O3A
4	B	801	GTP	C5'-O5'-PA-O1A
4	B	801	GTP	C5'-O5'-PA-O2A
4	B	803	GTP	C5'-O5'-PA-O1A
4	B	803	GTP	C5'-O5'-PA-O2A
4	D	702	GTP	C5'-O5'-PA-O1A

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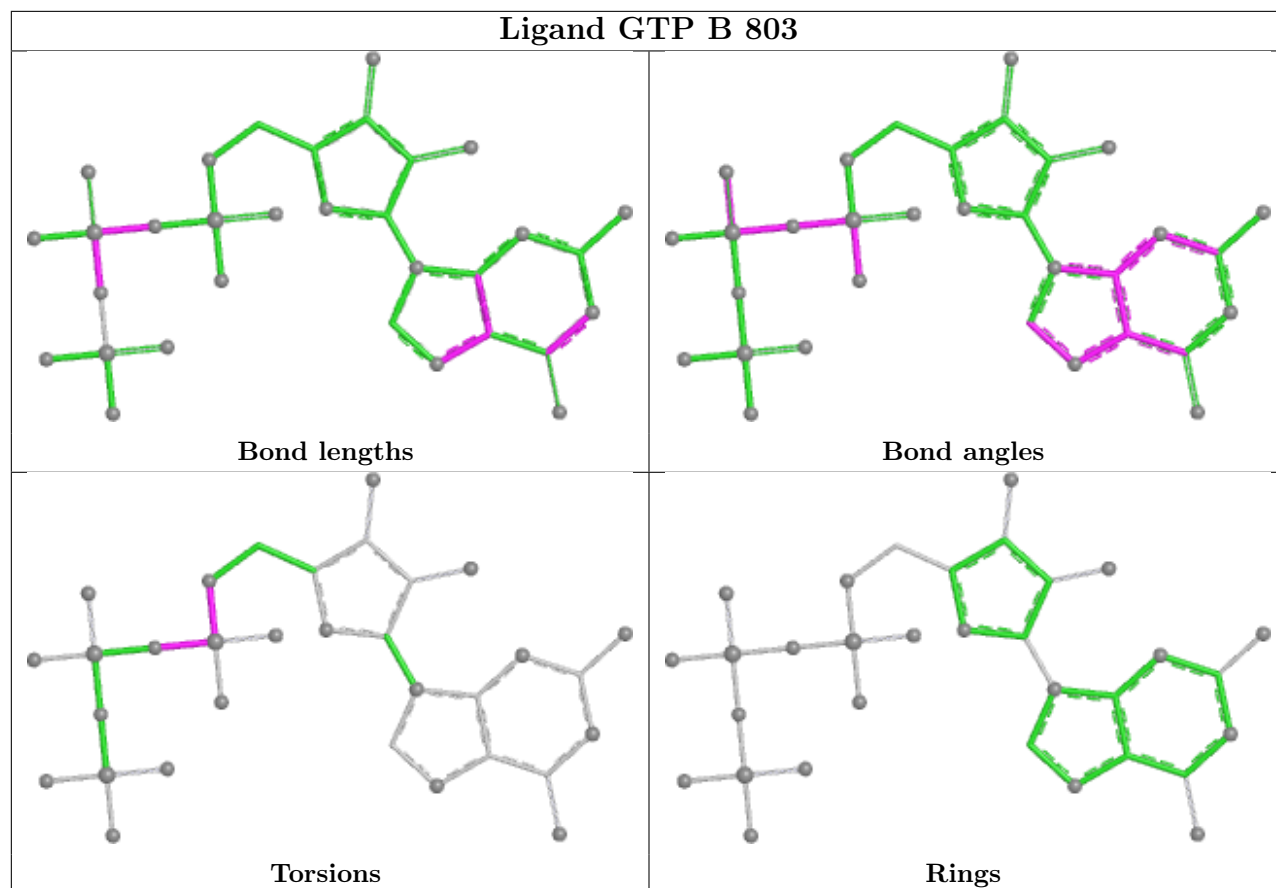
Mol	Chain	Res	Type	Atoms
4	D	702	GTP	C5'-O5'-PA-O2A
4	B	801	GTP	PG-O3B-PB-O1B
4	C	702	GTP	PG-O3B-PB-O1B
4	B	803	GTP	C5'-O5'-PA-O3A
4	C	702	GTP	C5'-O5'-PA-O3A
4	C	702	GTP	C5'-O5'-PA-O1A
4	C	702	GTP	C5'-O5'-PA-O2A
4	D	702	GTP	C5'-O5'-PA-O3A
4	B	801	GTP	PG-O3B-PB-O2B
4	B	803	GTP	PB-O3A-PA-O2A
4	C	702	GTP	PG-O3B-PB-O2B
4	B	801	GTP	C4'-C5'-O5'-PA
4	D	702	GTP	PG-O3B-PB-O1B
4	D	702	GTP	C4'-C5'-O5'-PA
4	C	702	GTP	C4'-C5'-O5'-PA
4	B	803	GTP	PB-O3A-PA-O1A
4	C	702	GTP	PB-O3A-PA-O2A
4	D	702	GTP	PG-O3B-PB-O2B
4	B	801	GTP	PA-O3A-PB-O1B
4	D	702	GTP	PA-O3A-PB-O2B

There are no ring outliers.

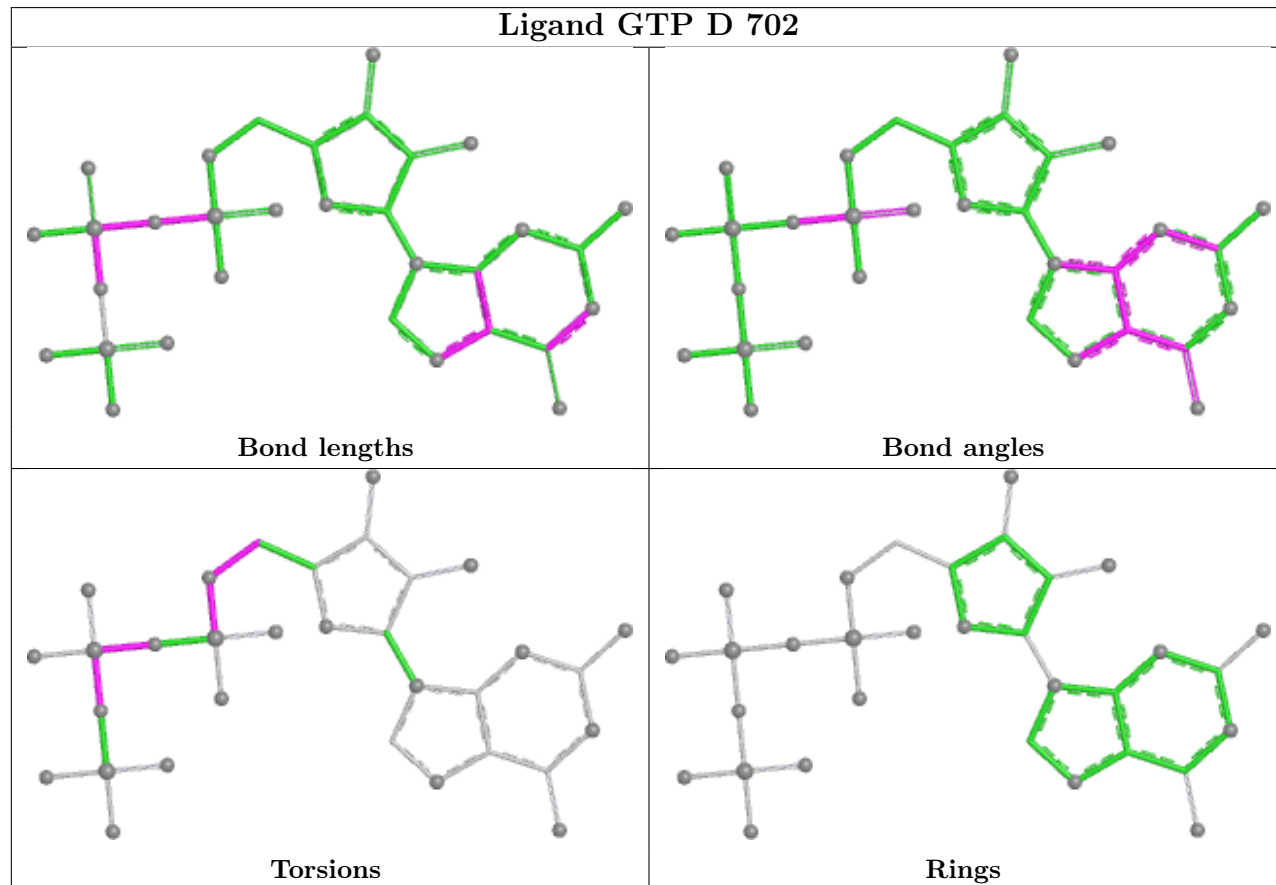
No monomer is involved in short contacts.

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.

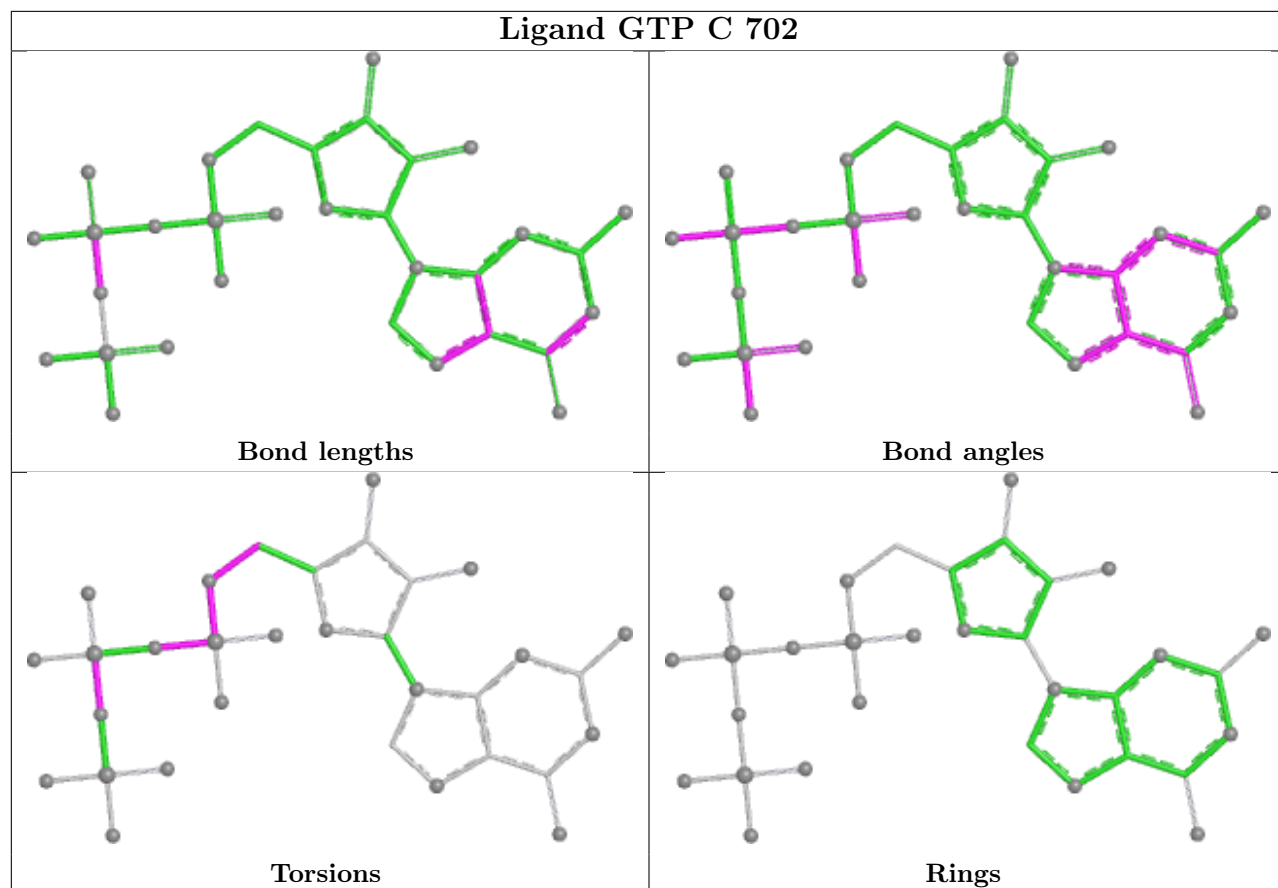
Ligand GTP B 803



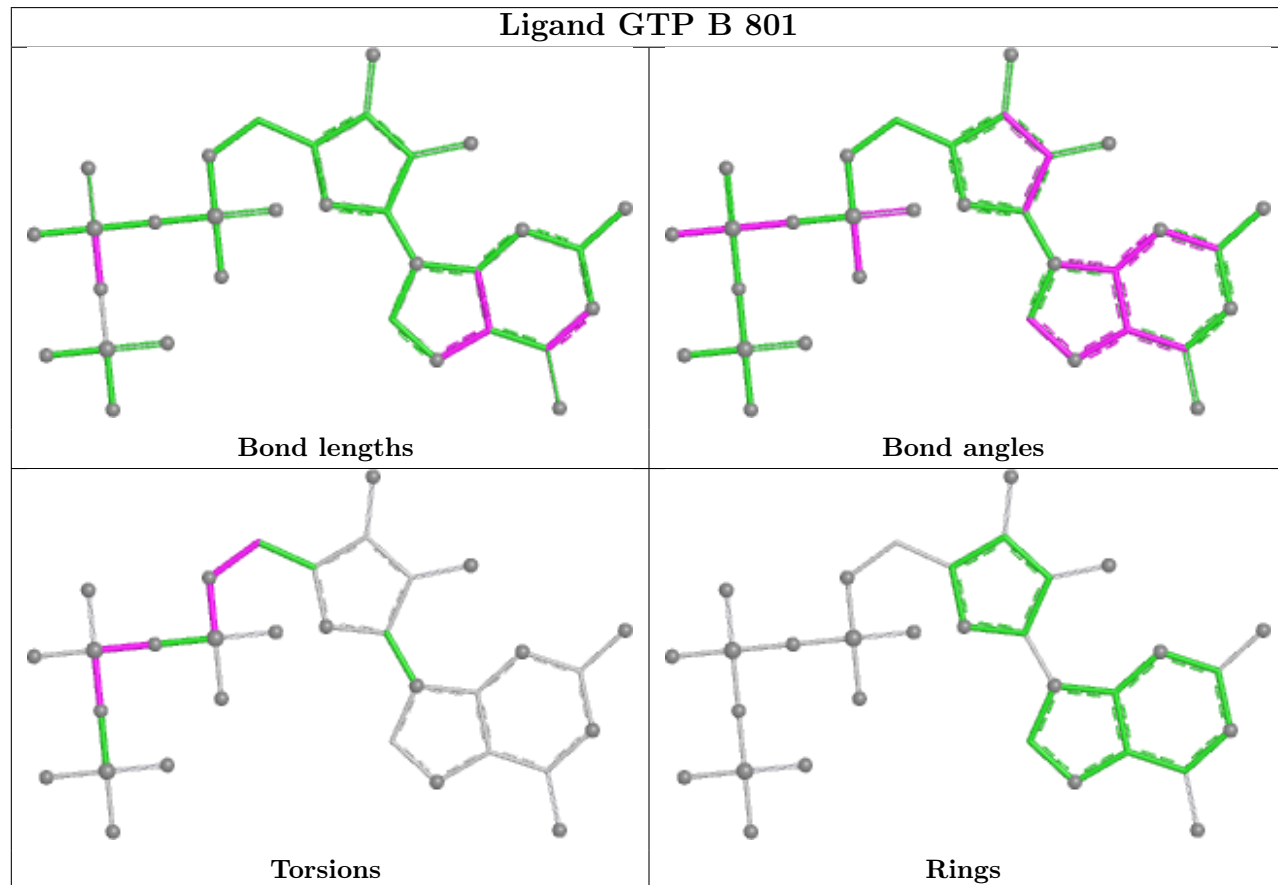
Ligand GTP D 702



Ligand GTP C 702



Ligand GTP B 801



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	456/539 (84%)	-0.02	10 (2%) 62 57	33, 59, 115, 143	0
1	B	433/539 (80%)	-0.08	8 (1%) 67 63	30, 55, 112, 150	0
1	C	434/539 (80%)	0.01	7 (1%) 70 66	33, 60, 117, 143	0
1	D	444/539 (82%)	0.03	6 (1%) 73 69	36, 63, 119, 145	0
All	All	1767/2156 (81%)	-0.01	31 (1%) 67 63	30, 59, 117, 150	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	532	ILE	3.6
1	D	546	ALA	3.3
1	A	546	ALA	3.2
1	C	515	ILE	3.0
1	A	284	LEU	3.0
1	A	507	TYR	2.9
1	B	491	VAL	2.9
1	A	532	ILE	2.9
1	B	546	ALA	2.8
1	B	521	TYR	2.7
1	C	284	LEU	2.7
1	C	488	LEU	2.7
1	D	515	ILE	2.6
1	B	545	PHE	2.5
1	D	466	ILE	2.5
1	B	488	LEU	2.5
1	C	489	LEU	2.5
1	D	284	LEU	2.5
1	A	541	LEU	2.5
1	A	508	GLY	2.4
1	C	491	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	509	MET	2.3
1	A	515	ILE	2.2
1	B	505	MET	2.2
1	C	505	MET	2.2
1	A	545	PHE	2.2
1	D	549	LEU	2.1
1	B	487	VAL	2.1
1	C	114	THR	2.1
1	A	288	LYS	2.0
1	B	284	LEU	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](#)

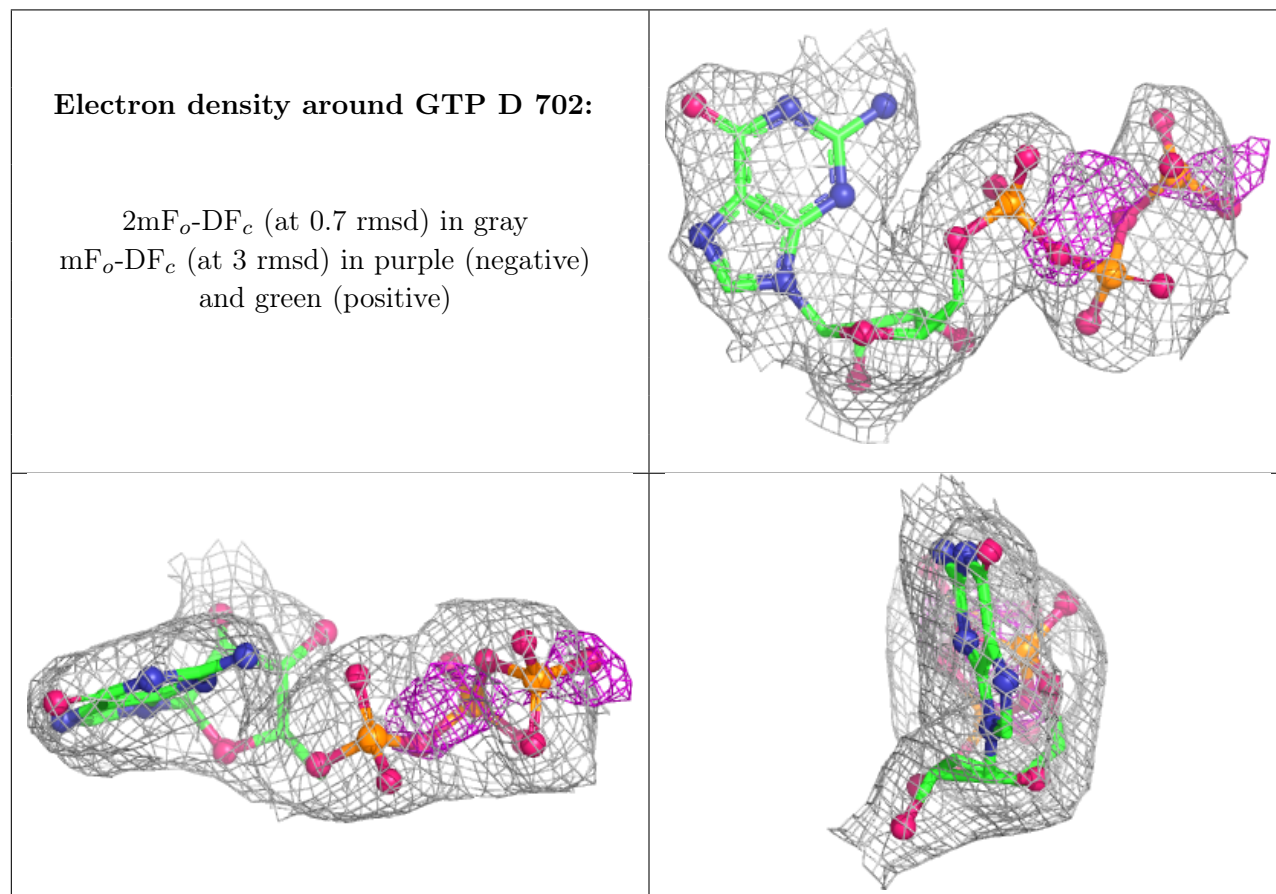
There are no oligosaccharides in this entry.

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.

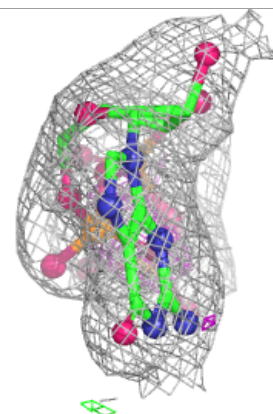
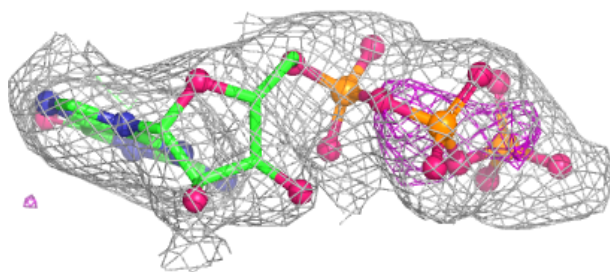
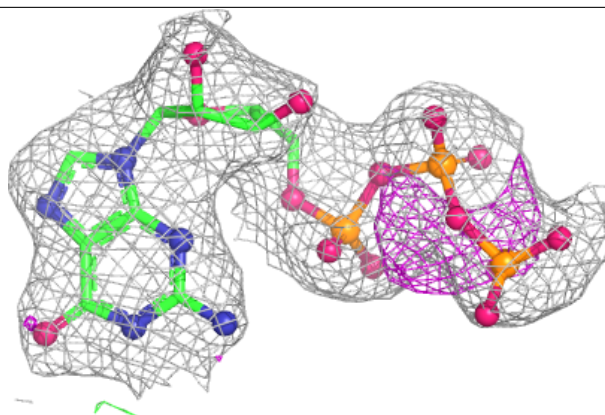
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	D	703	5/5	0.90	0.11	65,69,75,75	0
4	GTP	D	702	32/32	0.91	0.08	52,66,102,110	0
4	GTP	B	801	32/32	0.93	0.07	47,63,103,104	0
3	PO4	A	702	5/5	0.93	0.08	53,57,63,63	0
4	GTP	C	702	32/32	0.94	0.07	46,54,109,116	0
4	GTP	B	803	32/32	0.94	0.07	50,55,92,97	0
3	PO4	C	703	5/5	0.95	0.08	62,66,75,81	0
3	PO4	B	804	5/5	0.95	0.10	63,65,67,72	0
2	ZN	C	701	1/1	0.98	0.05	62,62,62,62	0
2	ZN	A	701	1/1	0.99	0.04	58,58,58,58	0
2	ZN	D	701	1/1	0.99	0.06	64,64,64,64	0
2	ZN	B	802	1/1	1.00	0.05	56,56,56,56	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.

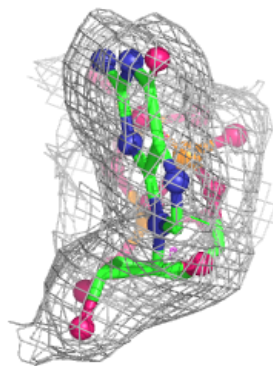
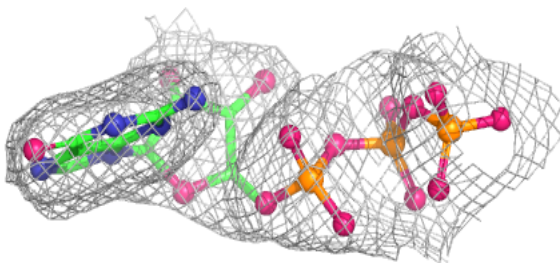
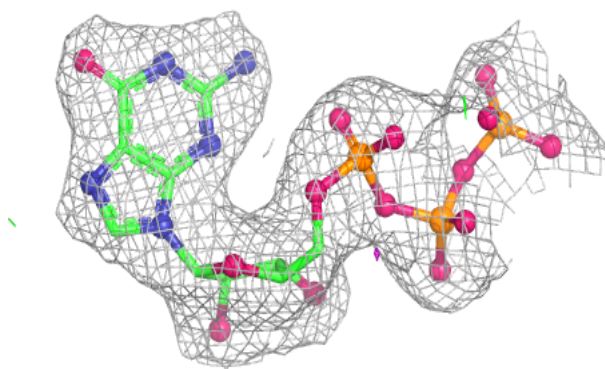


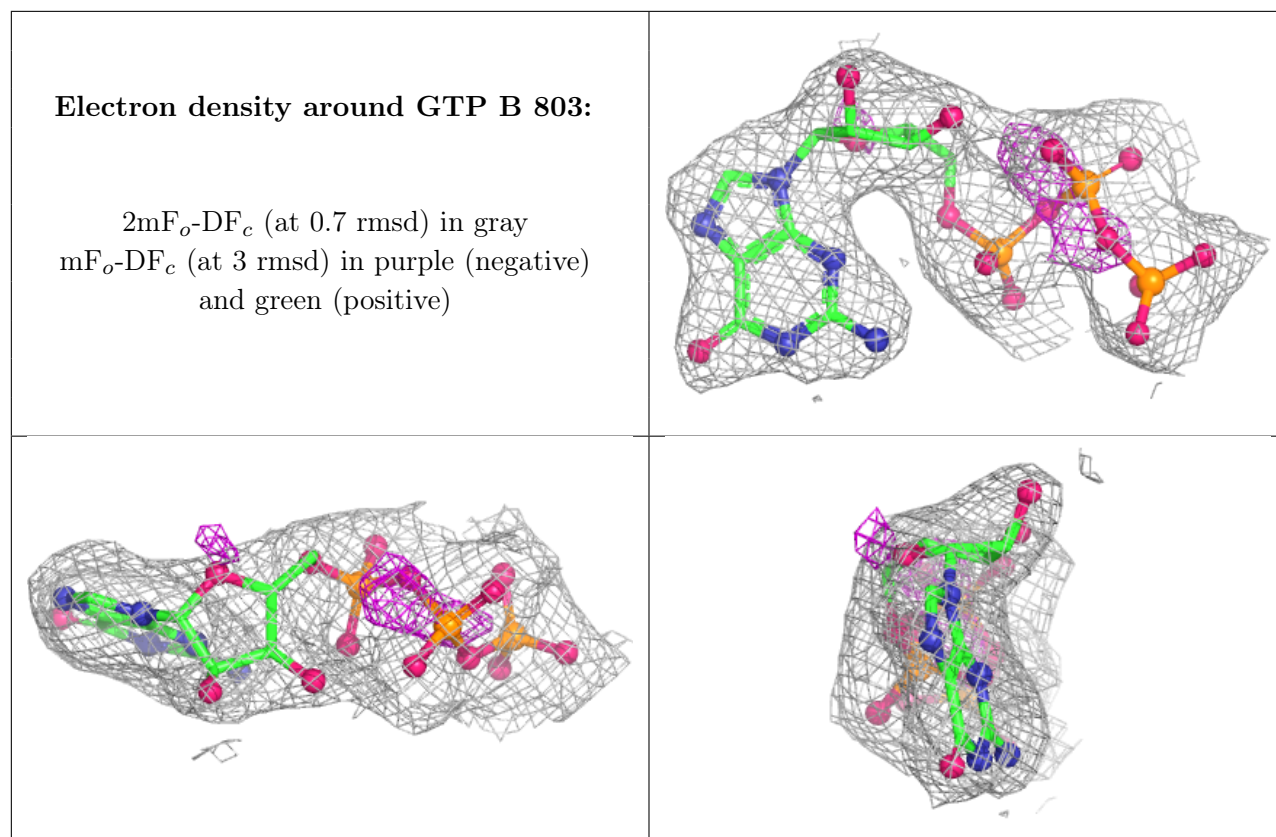
Electron density around GTP B 801:

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

**Electron density around GTP C 702:**

$2mF_o-DF_c$ (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.