



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:53 am BST

PDB ID : 4RXO
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

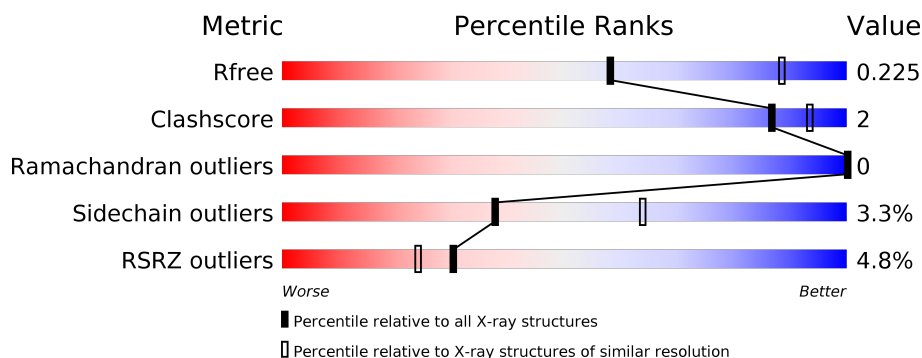
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>7%</div> <div>15%</div> </div> </div>
1	B	539	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>•</div> <div>20%</div> </div> </div>
1	C	539	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>•</div> <div>19%</div> </div> </div>
1	D	539	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>5%</div> <div>•</div> <div>18%</div> </div> </div>

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

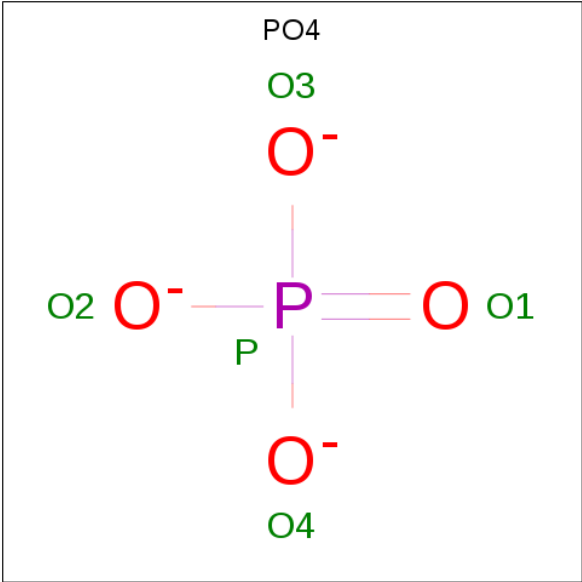
Continued from previous page...

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 (three-letter code: ZN) (formula: Zn).

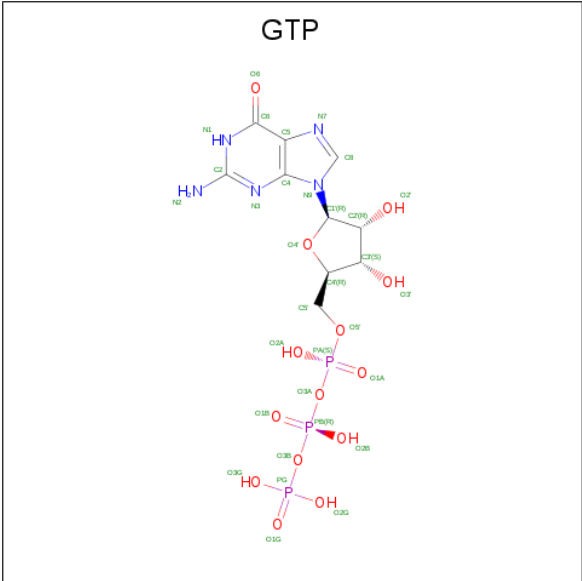
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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		

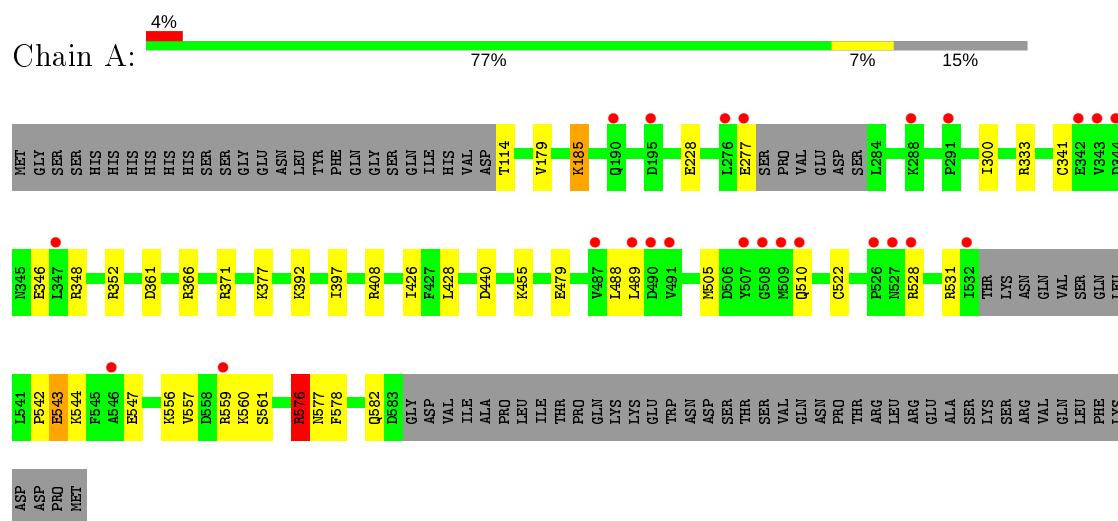
- Molecule 5 is water.

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		

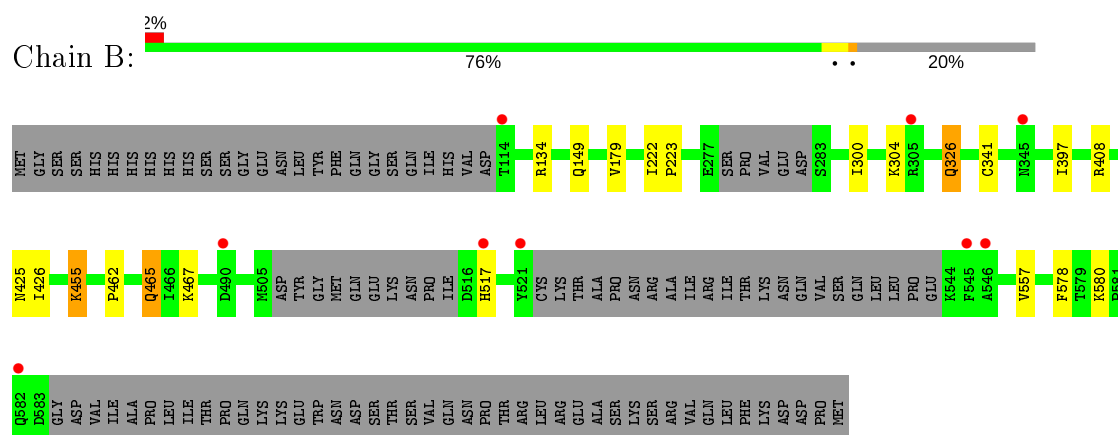
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

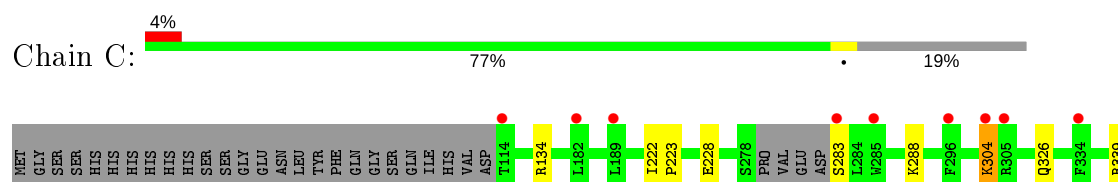
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

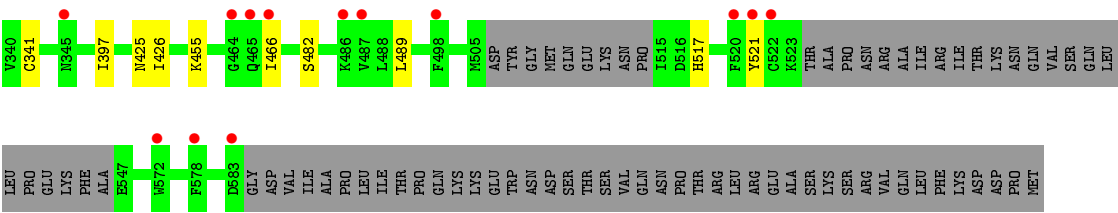


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

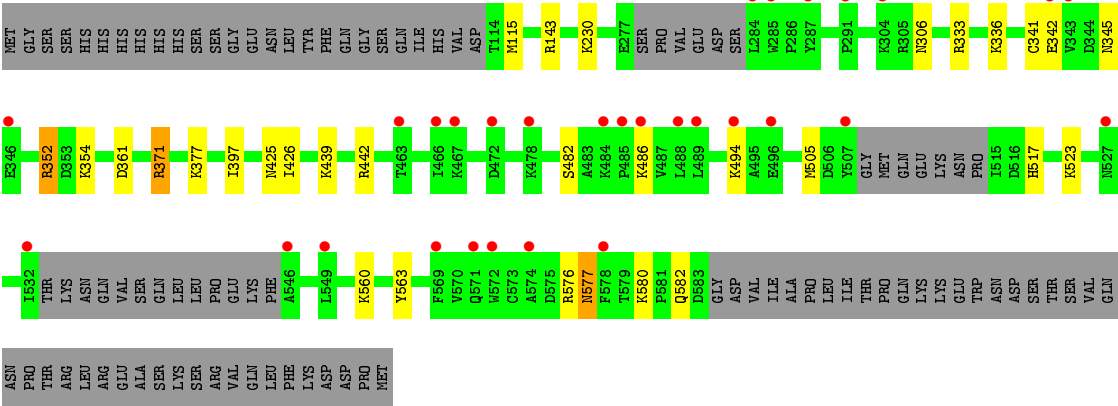


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



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 48.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.60) 96.7 (48.74-2.60)	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 0.188 , 0.225	Depositor DCC
R_{free} test set	3257 reflections (4.95%)	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)	0.32 , 45.8	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 [i](#)

5.1 Standard geometry [i](#)

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	0.46	0/3826	0.67	1/5161 (0.0%)
1	B	0.46	0/3639	0.65	0/4906
1	C	0.45	0/3642	0.64	0/4910
1	D	0.44	0/3727	0.64	0/5027
All	All	0.45	0/14834	0.65	1/20004 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	ARG	CG-CD-NE	-5.39	100.48	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3737	0	3703	22	0
1	B	3555	0	3520	14	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	60	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 (60) 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: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:D:371:ARG:HH11	1:D:505:MET:HE2	1.62	0.64
1:D:371:ARG:NH1	1:D:505:MET:HE2	2.11	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:A:366:ARG:HH12	1:A:505:MET:HE1	1.67	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:HE2	1:C:304:LYS:HA	1.87	0.55
1:A:346:GLU:OE1	1:A:348:ARG:NH2	2.39	0.55
1:A:366:ARG:NH1	1:A:505:MET:HE1	2.22	0.55
1:A:542:PRO:HB3	1:A:543:GLU:OE1	2.08	0.54
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:560:LYS:HD2	1:D:560:LYS:H	1.76	0.50
1:D:371:ARG:HH11	1:D:505:MET:CE	2.23	0.49
1:A:582:GLN:NE2	5:A:851:HOH:O	2.35	0.47
1:D:560:LYS:H	1:D:560:LYS:CD	2.28	0.47
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.95	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:A:543:GLU:CD	1:A:543:GLU:N	2.70	0.46
1:C:339:ARG:HD3	1:C:521:TYR:CZ	2.50	0.45
1:A:556:LYS:NZ	5:A:850:HOH:O	2.43	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:C:228:GLU:CD	1:C:228:GLU:H	2.22	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:HB2	1:D:580:LYS:HE2	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: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: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
1:D:352:ARG:CZ	1:D:523:LYS:HD3	2.51	0.41
1:A:377:LYS:HB2	1:A:377:LYS:HE3	1.81	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

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	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

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%)	384 (95%)	19 (5%)	26	50
1	B	384/481 (80%)	375 (98%)	9 (2%)	50	75
1	C	386/481 (80%)	377 (98%)	9 (2%)	50	75
1	D	393/481 (82%)	379 (96%)	14 (4%)	35	61
All	All	1566/1924 (81%)	1515 (97%)	51 (3%)	38	64

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

Mol	Chain	Res	Type
1	A	114	THR
1	A	185	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	228	GLU
1	A	277	GLU
1	A	341	CYS
1	A	352	ARG
1	A	371	ARG
1	A	408	ARG
1	A	488	LEU
1	A	489	LEU
1	A	510	GLN
1	A	522	CYS
1	A	528	ARG
1	A	531	ARG
1	A	543	GLU
1	A	544	LYS
1	A	559	ARG
1	A	576	ARG
1	A	577	ASN
1	B	134	ARG
1	B	149	GLN
1	B	304	LYS
1	B	326	GLN
1	B	341	CYS
1	B	455	LYS
1	B	465	GLN
1	B	517	HIS
1	B	580	LYS
1	C	134	ARG
1	C	283	SER
1	C	288	LYS
1	C	304	LYS
1	C	341	CYS
1	C	466	ILE
1	C	482	SER
1	C	489	LEU
1	C	517	HIS
1	D	230	LYS
1	D	336	LYS
1	D	341	CYS
1	D	342	GLU
1	D	345	ASN
1	D	352	ARG
1	D	371	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	377	LYS
1	D	482	SER
1	D	486	LYS
1	D	494	LYS
1	D	563	TYR
1	D	577	ASN
1	D	582	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	577	ASN
1	B	326	GLN
1	B	345	ASN
1	D	210	HIS
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 carbohydrates 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	-	26,34,34	1.09	2 (7%)	33,54,54	2.03	8 (24%)
4	GTP	C	702	-	26,34,34	1.09	3 (11%)	33,54,54	1.85	9 (27%)
3	PO4	B	804	2	4,4,4	1.04	0	6,6,6	0.18	0
4	GTP	D	702	-	26,34,34	1.04	2 (7%)	33,54,54	1.84	7 (21%)
3	PO4	D	703	2	4,4,4	1.15	0	6,6,6	0.61	0
4	GTP	B	801	-	26,34,34	1.11	2 (7%)	33,54,54	1.89	8 (24%)
3	PO4	C	703	2	4,4,4	1.21	0	6,6,6	0.32	0
3	PO4	A	702	2	4,4,4	1.25	0	6,6,6	0.85	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	B	801	-	-	6/18/38/38	0/3/3/3
4	GTP	B	803	-	-	5/18/38/38	0/3/3/3
4	GTP	C	702	-	-	7/18/38/38	0/3/3/3
4	GTP	D	702	-	-	6/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	GTP	C6-C5	4.25	1.48	1.41
4	B	801	GTP	C6-C5	3.98	1.48	1.41
4	D	702	GTP	C6-C5	3.58	1.47	1.41
4	C	702	GTP	C6-C5	3.44	1.47	1.41
4	C	702	GTP	C5-C4	2.62	1.47	1.40
4	D	702	GTP	C5-C4	2.44	1.47	1.40
4	C	702	GTP	O4'-C1'	2.42	1.44	1.41
4	B	803	GTP	C5-C4	2.19	1.46	1.40
4	B	801	GTP	C5-C4	2.15	1.46	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	GTP	C2-N3-C4	5.28	121.38	115.36
4	D	702	GTP	C5-C6-N1	-4.45	117.35	123.43
4	B	801	GTP	C2-N3-C4	4.43	120.42	115.36
4	D	702	GTP	C6-N1-C2	4.29	122.75	115.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	702	GTP	C6-N1-C2	4.25	122.69	115.93
4	B	803	GTP	C6-N1-C2	4.22	122.64	115.93
4	B	803	GTP	C5-C6-N1	-4.20	117.69	123.43
4	C	702	GTP	C2-N3-C4	4.16	120.10	115.36
4	B	801	GTP	C5-C6-N1	-4.14	117.77	123.43
4	C	702	GTP	C5-C6-N1	-4.10	117.82	123.43
4	D	702	GTP	C2-N3-C4	4.08	120.02	115.36
4	B	801	GTP	C6-N1-C2	3.98	122.26	115.93
4	B	803	GTP	C6-C5-C4	-3.82	117.15	120.80
4	D	702	GTP	PB-O3B-PG	-3.67	120.22	132.83
4	B	803	GTP	N3-C2-N1	-3.65	122.35	127.22
4	B	801	GTP	C6-C5-C4	-3.58	117.38	120.80
4	C	702	GTP	C6-C5-C4	-3.57	117.39	120.80
4	B	801	GTP	C3'-C2'-C1'	3.13	105.68	100.98
4	D	702	GTP	N3-C2-N1	-3.11	123.07	127.22
4	B	801	GTP	N3-C2-N1	-3.08	123.12	127.22
4	C	702	GTP	N3-C2-N1	-3.03	123.18	127.22
4	B	803	GTP	C4-C5-N7	-2.99	106.28	109.40
4	D	702	GTP	C6-C5-C4	-2.92	118.01	120.80
4	B	803	GTP	C3'-C2'-C1'	2.75	105.12	100.98
4	C	702	GTP	C3'-C2'-C1'	2.65	104.97	100.98
4	B	801	GTP	C4-C5-N7	-2.40	106.90	109.40
4	C	702	GTP	PB-O3B-PG	-2.35	124.76	132.83
4	B	801	GTP	PB-O3B-PG	-2.27	125.04	132.83
4	B	803	GTP	PB-O3B-PG	-2.06	125.75	132.83
4	C	702	GTP	O2A-PA-O1A	2.05	122.37	112.24
4	D	702	GTP	C3'-C2'-C1'	2.04	104.05	100.98
4	C	702	GTP	O3G-PG-O2G	2.01	115.33	107.64

There are no chirality outliers.

All (24) 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-O3A
4	B	803	GTP	C5'-O5'-PA-O1A
4	B	803	GTP	C5'-O5'-PA-O2A
4	C	702	GTP	C5'-O5'-PA-O3A
4	D	702	GTP	C5'-O5'-PA-O3A
4	D	702	GTP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

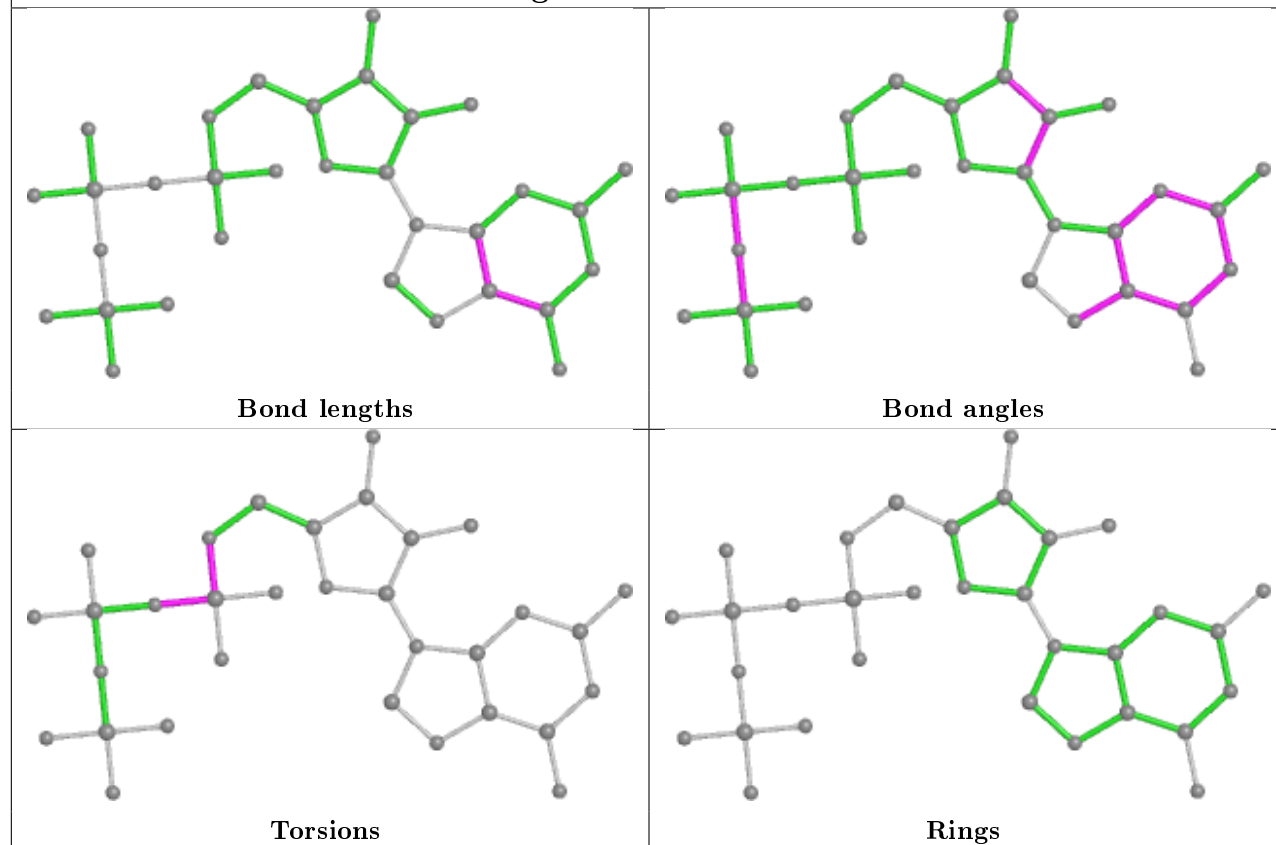
Mol	Chain	Res	Type	Atoms
4	D	702	GTP	C5'-O5'-PA-O2A
4	B	801	GTP	PG-O3B-PB-O1B
4	C	702	GTP	PG-O3B-PB-O1B
4	B	801	GTP	C4'-C5'-O5'-PA
4	C	702	GTP	C5'-O5'-PA-O1A
4	C	702	GTP	C5'-O5'-PA-O2A
4	B	801	GTP	PG-O3B-PB-O2B
4	B	803	GTP	PB-O3A-PA-O2A
4	C	702	GTP	PG-O3B-PB-O2B
4	D	702	GTP	C4'-C5'-O5'-PA
4	C	702	GTP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

There are no ring outliers.

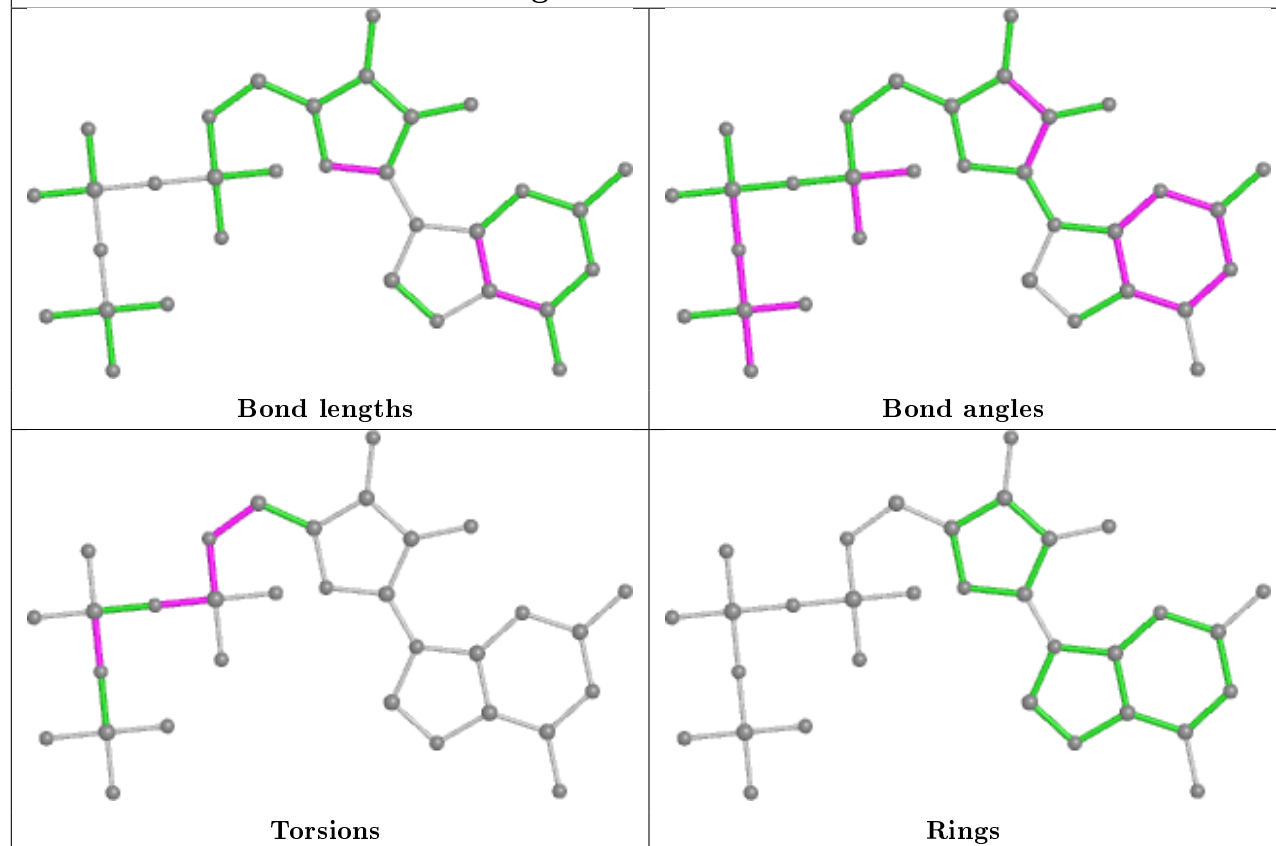
No monomer is involved in short contacts.

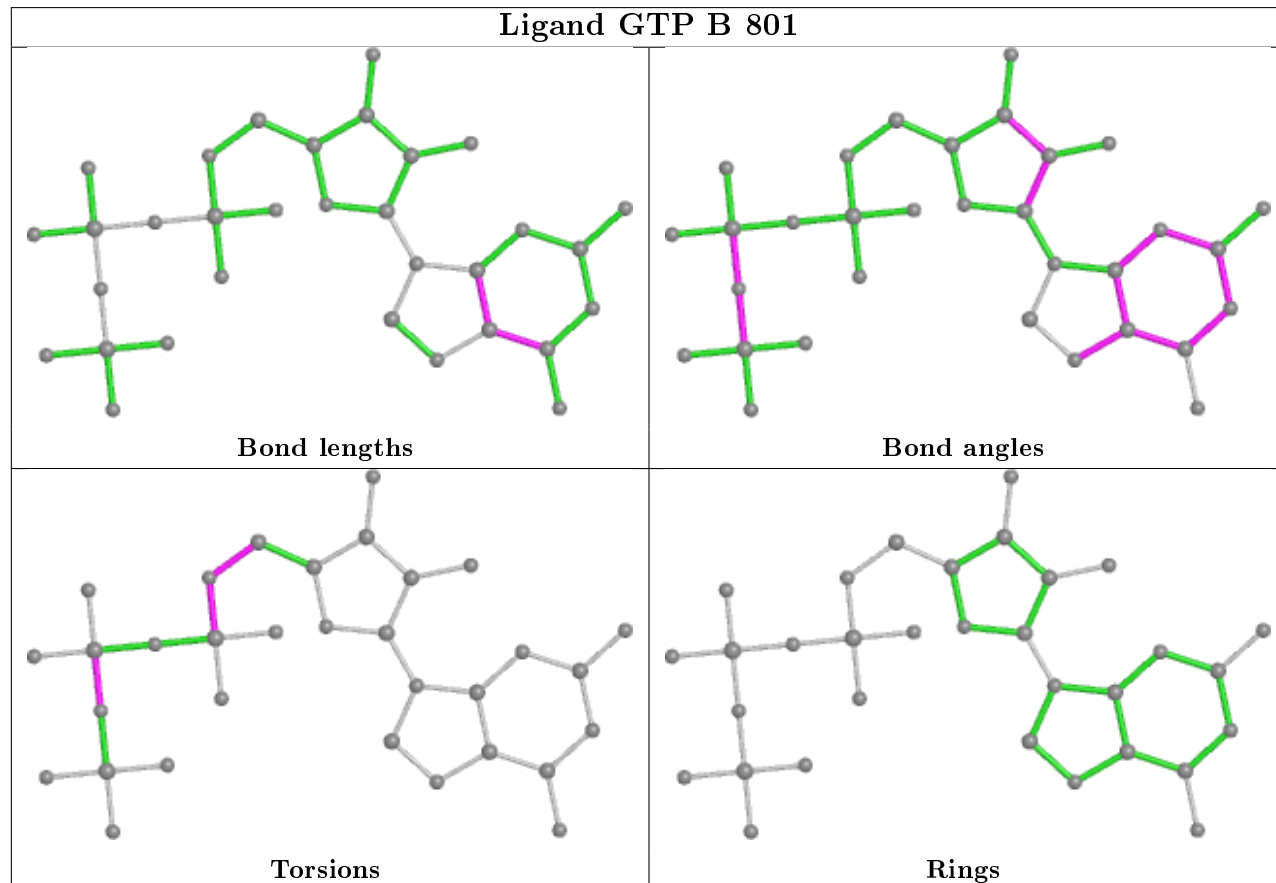
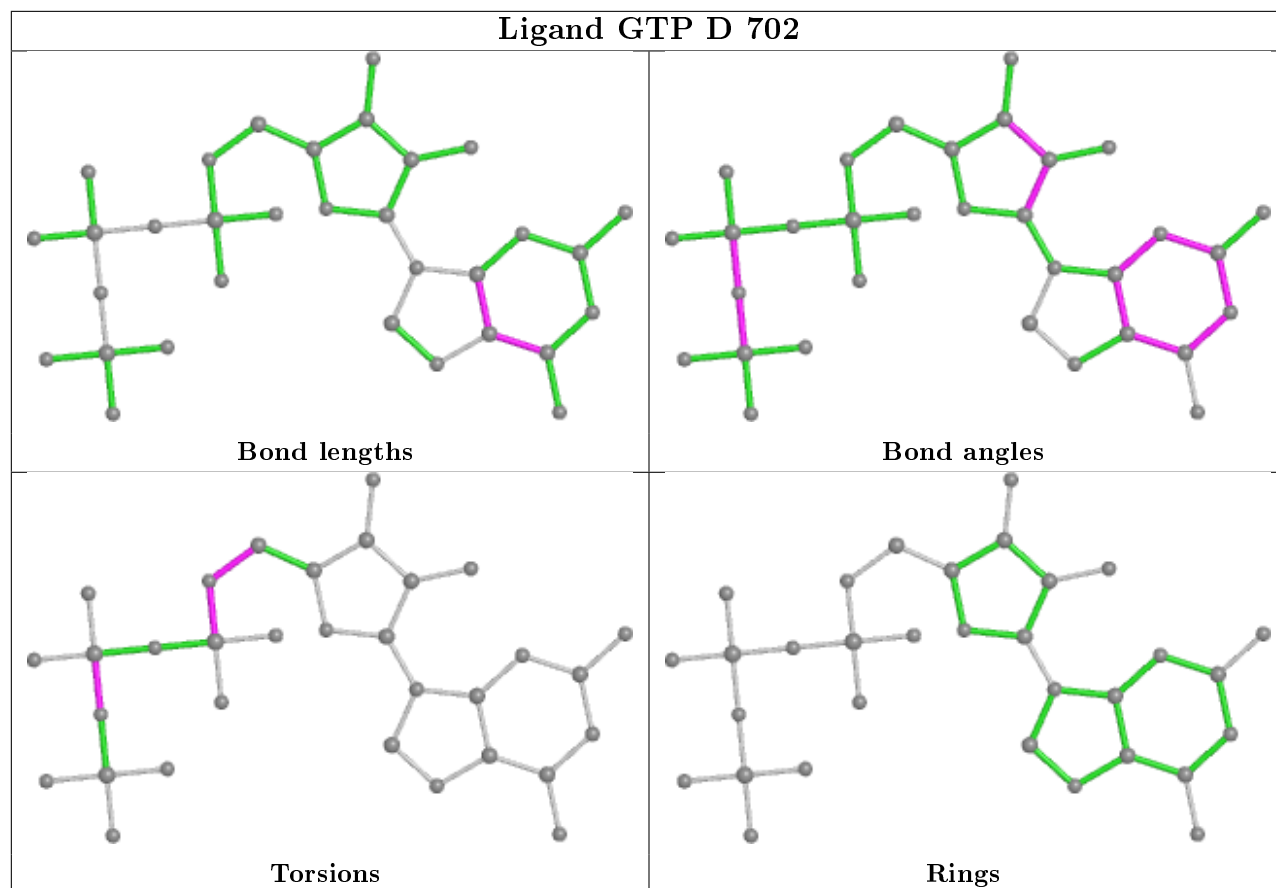
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 C 702





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 ⓘ

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%)	0.18	24 (5%)	26 20	33, 59, 115, 143	0
1	B	433/539 (80%)	0.05	9 (2%)	63 58	30, 55, 112, 150	0
1	C	434/539 (80%)	0.17	22 (5%)	28 22	33, 60, 117, 143	0
1	D	444/539 (82%)	0.31	30 (6%)	17 12	36, 63, 119, 145	0
All	All	1767/2156 (81%)	0.18	85 (4%)	30 24	30, 59, 117, 150	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	114	THR	5.3
1	D	488	LEU	5.0
1	A	532	ILE	4.8
1	D	346	GLU	4.8
1	C	465	GLN	4.4
1	D	489	LEU	4.3
1	A	487	VAL	4.1
1	A	276	LEU	4.0
1	A	508	GLY	3.9
1	C	304	LYS	3.9
1	B	490	ASP	3.8
1	D	494	LYS	3.8
1	B	545	PHE	3.6
1	C	521	TYR	3.6
1	B	521	TYR	3.6
1	D	578	PHE	3.4
1	A	347	LEU	3.3
1	C	498	PHE	3.3
1	A	190	GLN	3.3
1	C	283	SER	3.2
1	B	517	HIS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	549	LEU	3.2
1	B	546	ALA	3.2
1	A	546	ALA	3.1
1	C	466	ILE	3.1
1	A	490	ASP	3.0
1	C	464	GLY	3.0
1	B	345	ASN	2.9
1	A	489	LEU	2.9
1	A	277	GLU	2.9
1	D	304	LYS	2.9
1	C	345	ASN	2.9
1	D	546	ALA	2.9
1	A	507	TYR	2.8
1	D	472	ASP	2.8
1	C	305	ARG	2.8
1	A	527	ASN	2.8
1	D	284	LEU	2.7
1	D	342	GLU	2.7
1	A	526	PRO	2.7
1	D	291	PRO	2.6
1	D	478	LYS	2.6
1	A	342	GLU	2.6
1	B	305	ARG	2.6
1	A	559	ARG	2.6
1	B	114	THR	2.5
1	D	496	GLU	2.5
1	D	532	ILE	2.5
1	C	487	VAL	2.4
1	D	285	TRP	2.4
1	D	343	VAL	2.4
1	B	582	GLN	2.4
1	C	572	TRP	2.4
1	D	527	ASN	2.4
1	A	509	MET	2.4
1	D	572	TRP	2.4
1	A	510	GLN	2.4
1	C	285	TRP	2.3
1	C	522	CYS	2.3
1	C	334	PHE	2.3
1	C	583	ASP	2.3
1	C	578	PHE	2.3
1	D	463	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	466	ILE	2.3
1	A	491	VAL	2.2
1	C	189	LEU	2.2
1	A	344	ASP	2.2
1	C	520	PHE	2.2
1	D	569	PHE	2.2
1	A	195	ASP	2.2
1	D	287	TYR	2.2
1	A	291	PRO	2.2
1	D	484	LYS	2.1
1	D	507	TYR	2.1
1	C	296	PHE	2.1
1	D	486	LYS	2.1
1	A	528	ARG	2.1
1	D	574	ALA	2.0
1	A	288	LYS	2.0
1	D	467	LYS	2.0
1	D	571	GLN	2.0
1	C	182	LEU	2.0
1	A	343	VAL	2.0
1	D	485	PRO	2.0
1	C	486	LYS	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 carbohydrates 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.

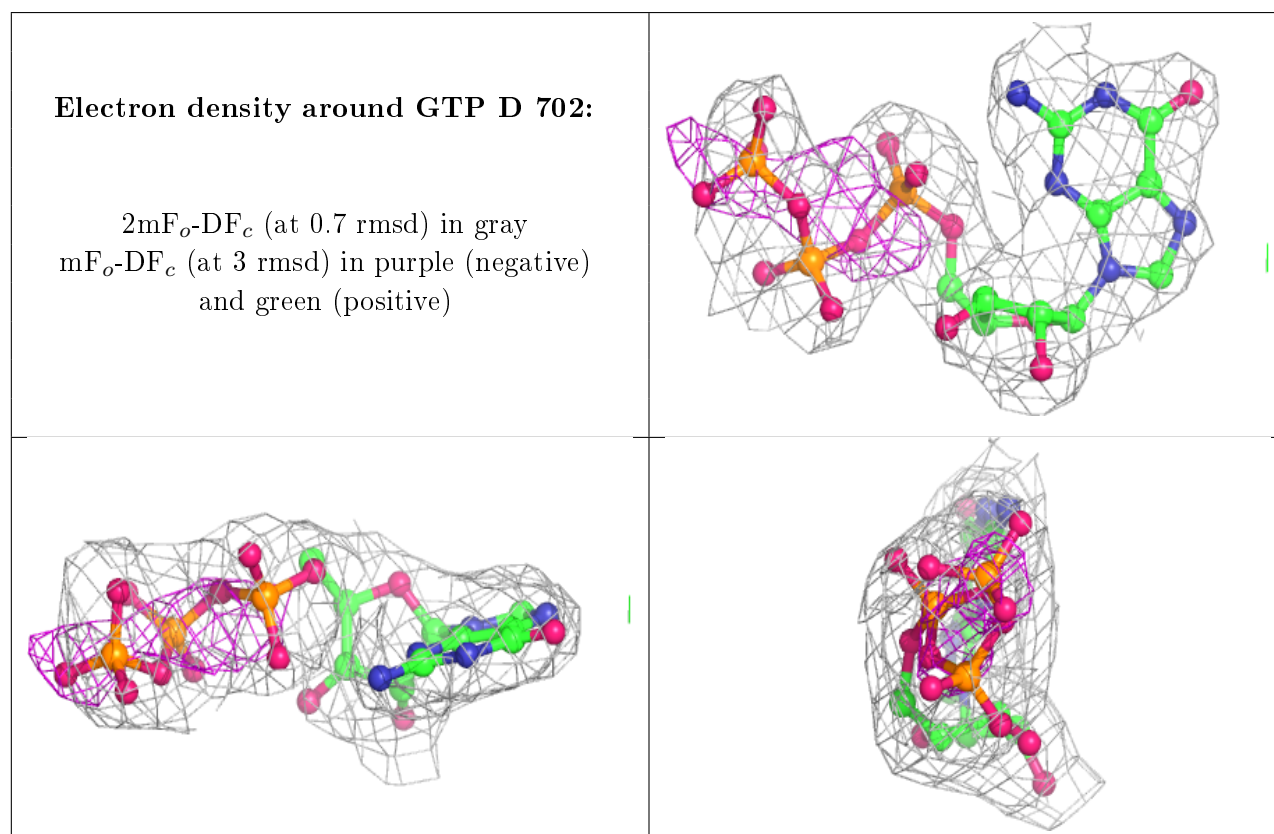
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GTP	D	702	32/32	0.94	0.13	52,66,102,110	0

Continued on next page...

Continued from previous page...

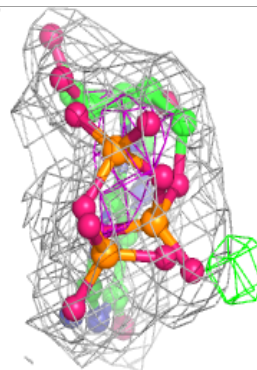
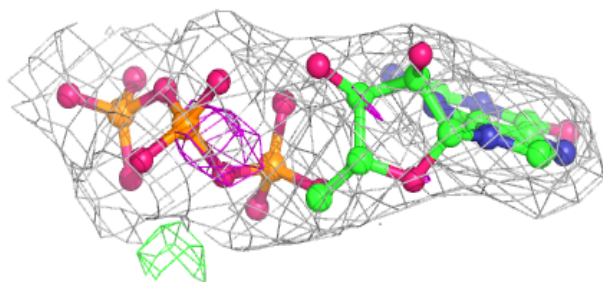
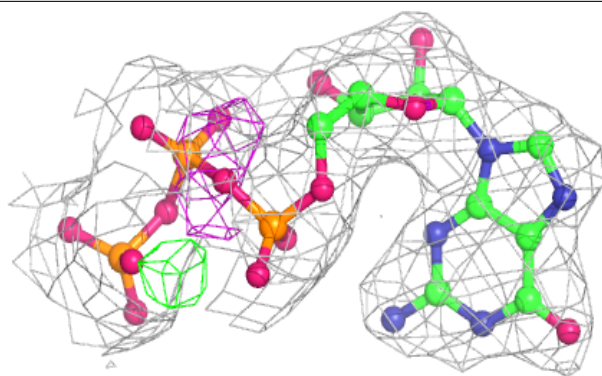
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GTP	B	803	32/32	0.95	0.13	50,55,92,97	0
4	GTP	B	801	32/32	0.95	0.13	47,63,103,104	0
3	PO4	D	703	5/5	0.95	0.12	65,69,75,75	0
2	ZN	C	701	1/1	0.96	0.10	62,62,62,62	0
3	PO4	B	804	5/5	0.97	0.13	63,65,67,72	0
4	GTP	C	702	32/32	0.97	0.11	46,54,109,116	0
3	PO4	A	702	5/5	0.97	0.16	53,57,63,63	0
3	PO4	C	703	5/5	0.98	0.11	62,66,75,81	0
2	ZN	D	701	1/1	0.99	0.07	64,64,64,64	0
2	ZN	A	701	1/1	0.99	0.12	58,58,58,58	0
2	ZN	B	802	1/1	1.00	0.08	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.

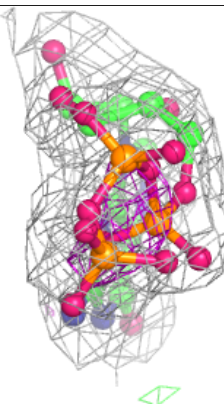
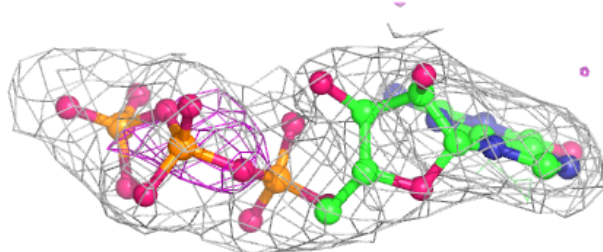
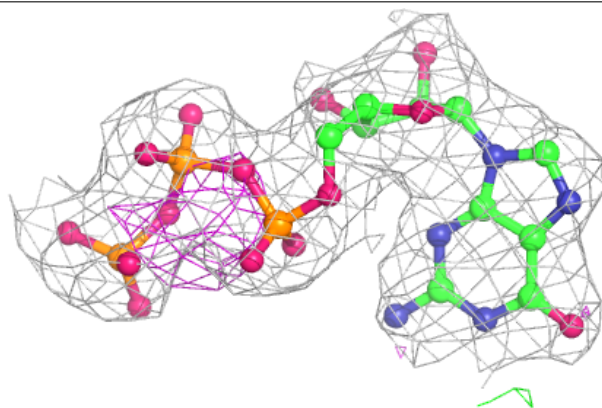


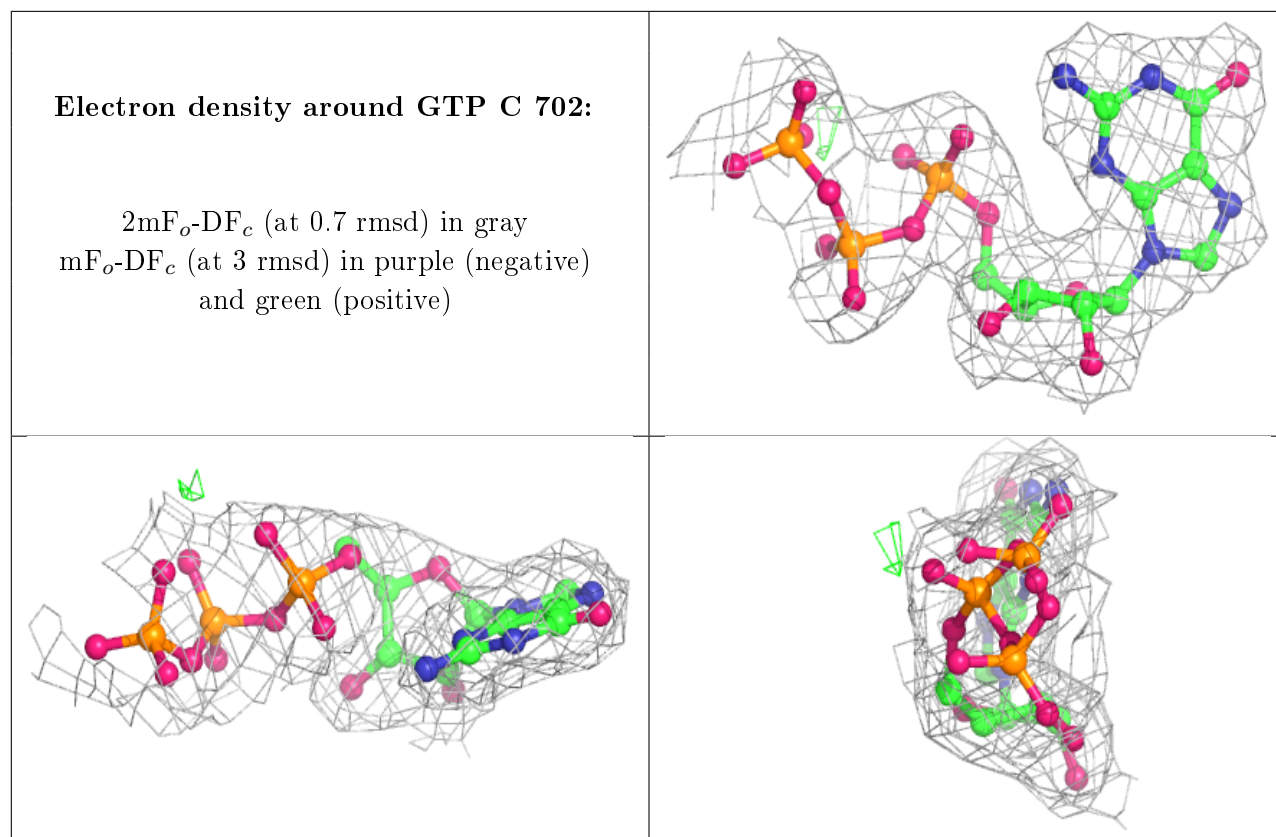
Electron density around GTP B 803:

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

**Electron density around GTP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.