



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:06 am GMT

PDB ID : 1N3T
Title : Biosynthesis of pteridins. Reaction mechanism of GTP cyclohydrolase I
Authors : Rebelo, J.; Auerbach, G.; Bader, G.; Bracher, A.; Nar, H.; Hoesl, C.; Schramek, N.; Kaiser, J.; Bacher, A.; Huber, R.; Fischer, M.
Deposited on : 2002-10-29
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

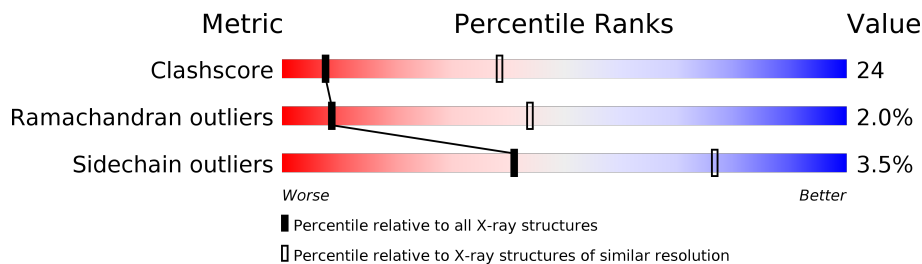
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)


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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	
1	B	221	
1	C	221	
1	D	221	
1	E	221	
1	F	221	
1	G	221	

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Mol	Chain	Length	Quality of chain
1	H	221	
1	I	221	
1	J	221	
1	K	221	
1	L	221	
1	M	221	
1	N	221	
1	O	221	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26475 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.

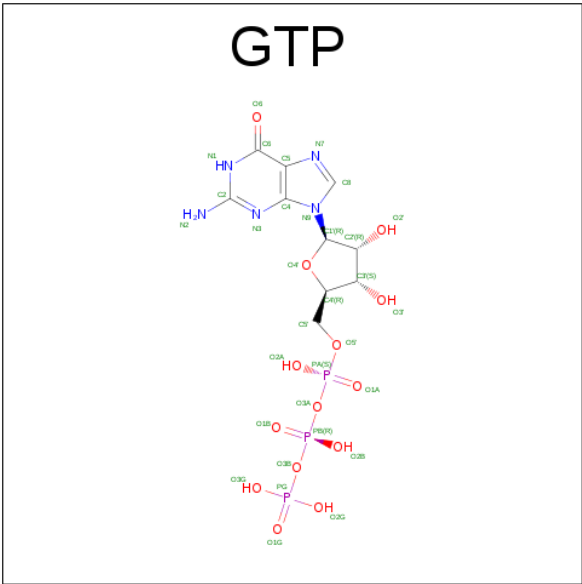
- Molecule 1 is a protein called GTP cyclohydrolase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	G	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	H	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	I	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	J	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	K	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	L	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	M	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	N	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	O	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	A	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	B	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	C	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	D	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			
1	E	221	Total	C	N	O	S	0	0	0
			1733	1088	309	328	8			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	SER	CYS	ENGINEERED	UNP P0A6T5
B	181	SER	CYS	ENGINEERED	UNP P0A6T5
C	181	SER	CYS	ENGINEERED	UNP P0A6T5
D	181	SER	CYS	ENGINEERED	UNP P0A6T5
E	181	SER	CYS	ENGINEERED	UNP P0A6T5
F	181	SER	CYS	ENGINEERED	UNP P0A6T5
G	181	SER	CYS	ENGINEERED	UNP P0A6T5
H	181	SER	CYS	ENGINEERED	UNP P0A6T5
I	181	SER	CYS	ENGINEERED	UNP P0A6T5
J	181	SER	CYS	ENGINEERED	UNP P0A6T5
K	181	SER	CYS	ENGINEERED	UNP P0A6T5
L	181	SER	CYS	ENGINEERED	UNP P0A6T5
M	181	SER	CYS	ENGINEERED	UNP P0A6T5
N	181	SER	CYS	ENGINEERED	UNP P0A6T5
O	181	SER	CYS	ENGINEERED	UNP P0A6T5

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	I	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	J	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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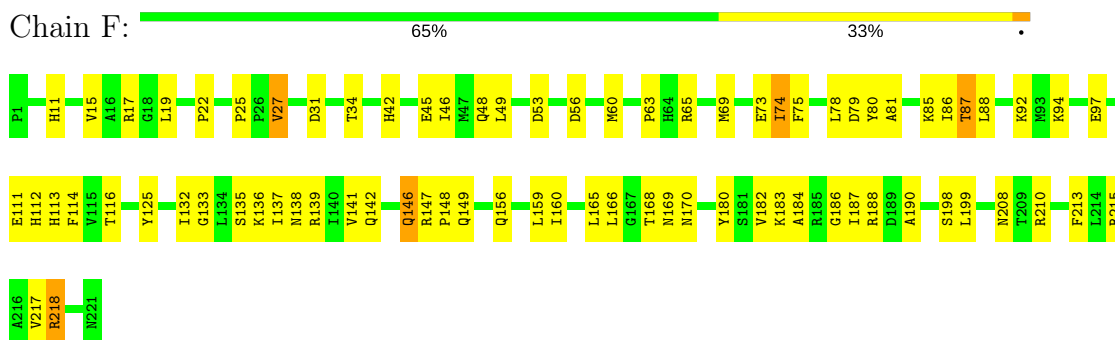
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	L	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	M	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	N	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	O	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	K	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	B	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	C	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	D	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	E	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	A	1	Total 32	C 10	N 5	O 14	P 3	0	0

3 Residue-property plots

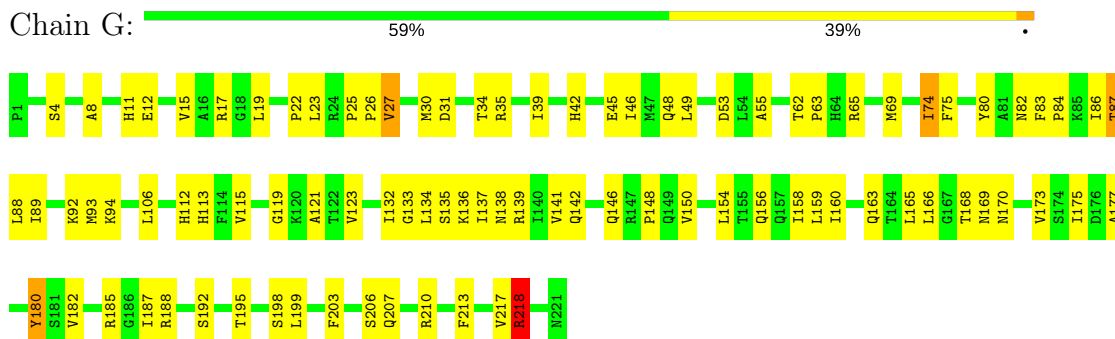
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

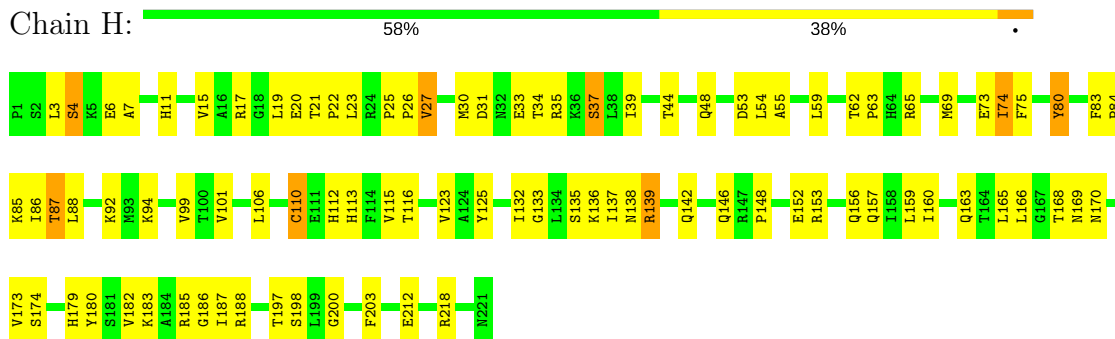
• Molecule 1: GTP cyclohydrolase I



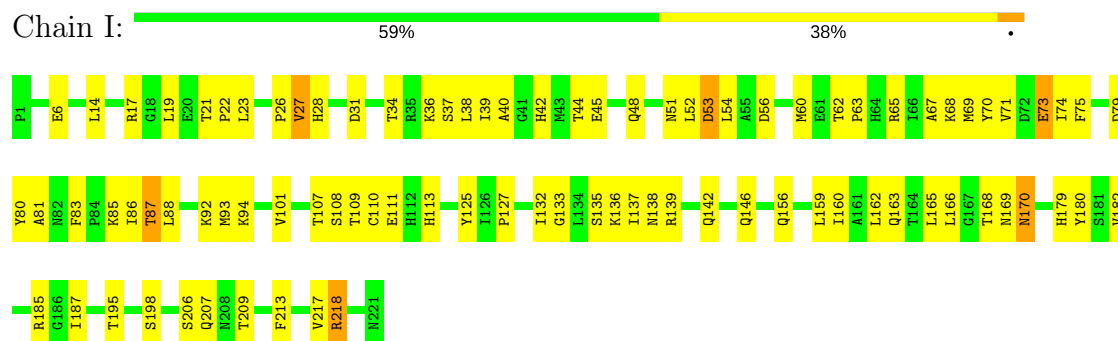
• Molecule 1: GTP cyclohydrolase I



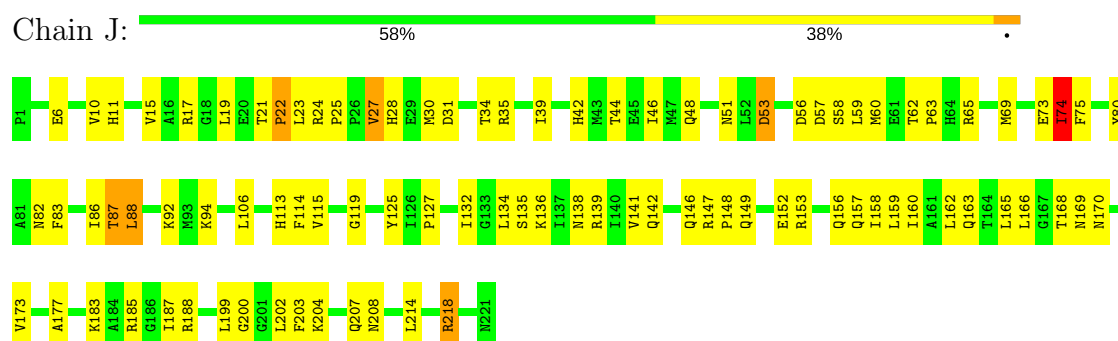
• Molecule 1: GTP cyclohydrolase I



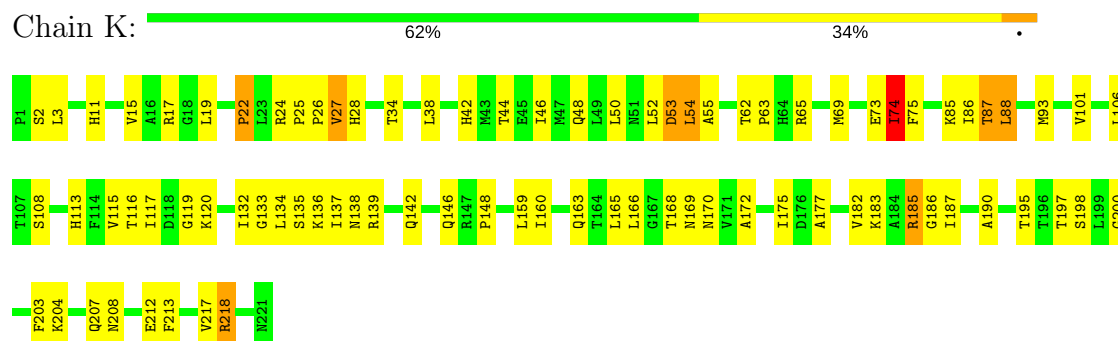
● Molecule 1: GTP cyclohydrolase I



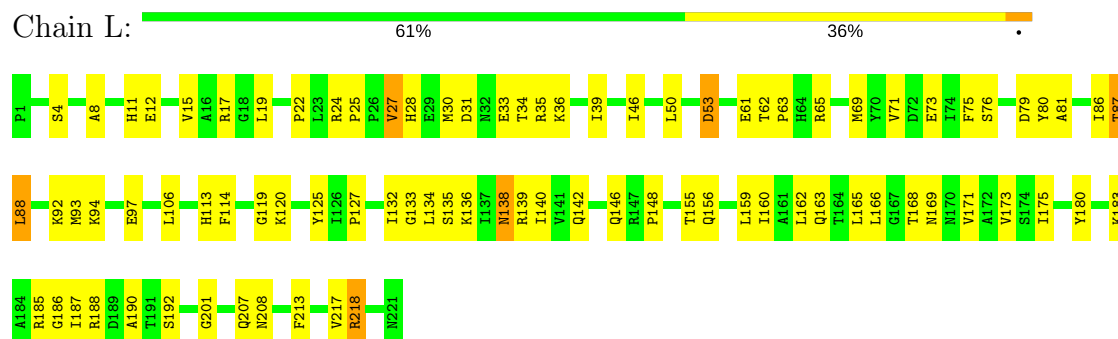
● Molecule 1: GTP cyclohydrolase I



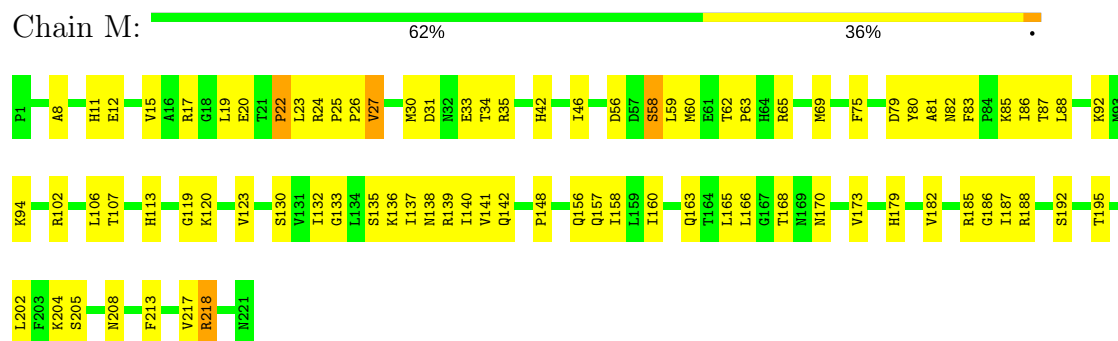
● Molecule 1: GTP cyclohydrolase I



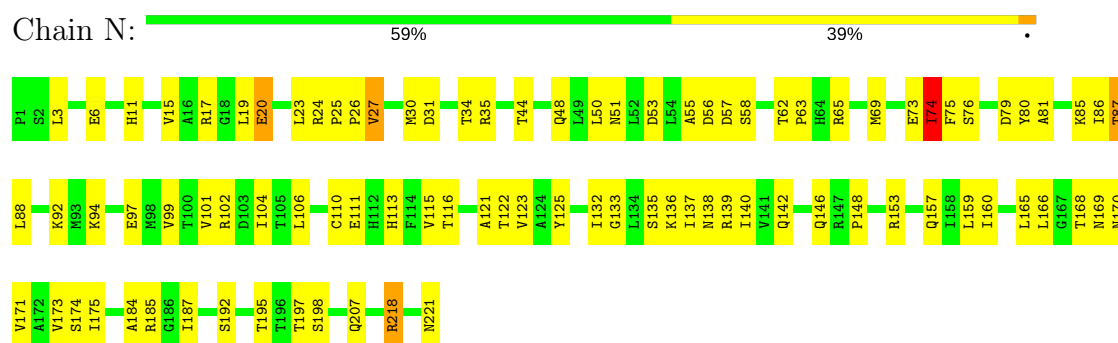
● Molecule 1: GTP cyclohydrolase I



● Molecule 1: GTP cyclohydrolase I



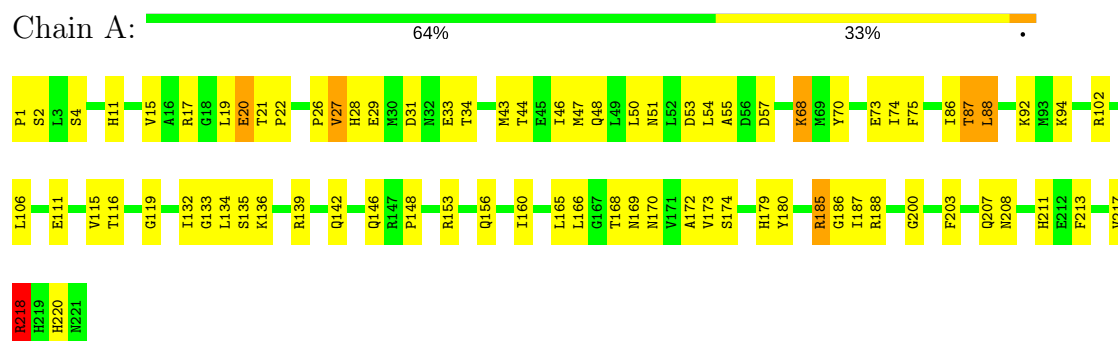
● Molecule 1: GTP cyclohydrolase I



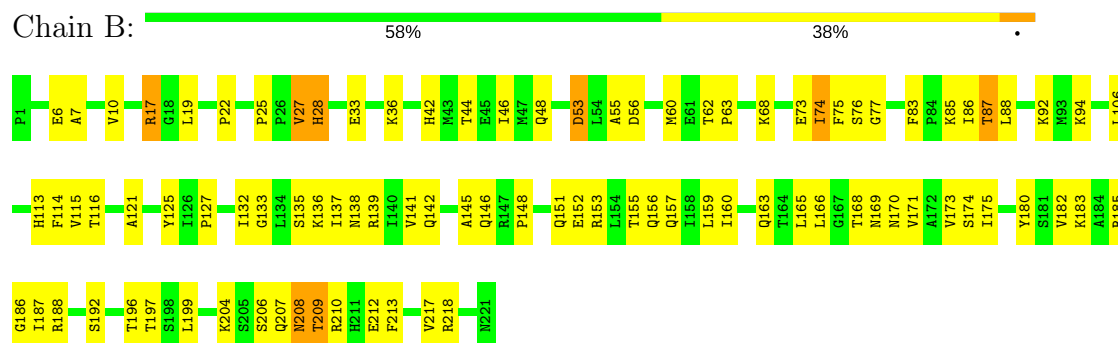
● Molecule 1: GTP cyclohydrolase I



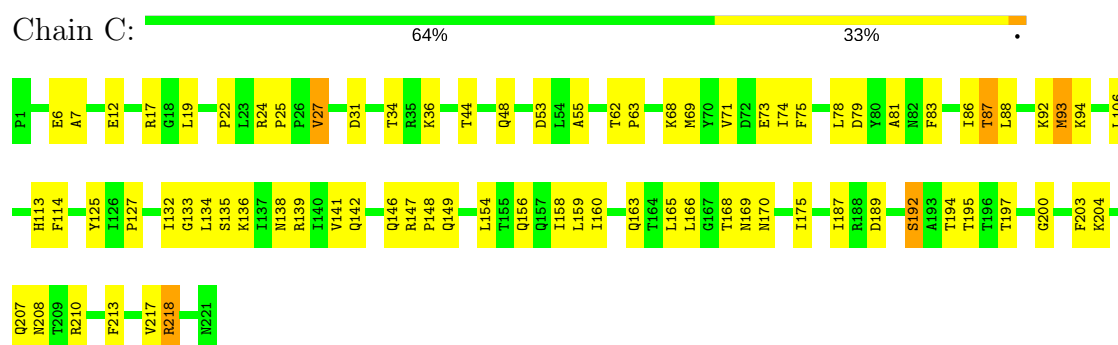
● Molecule 1: GTP cyclohydrolase I



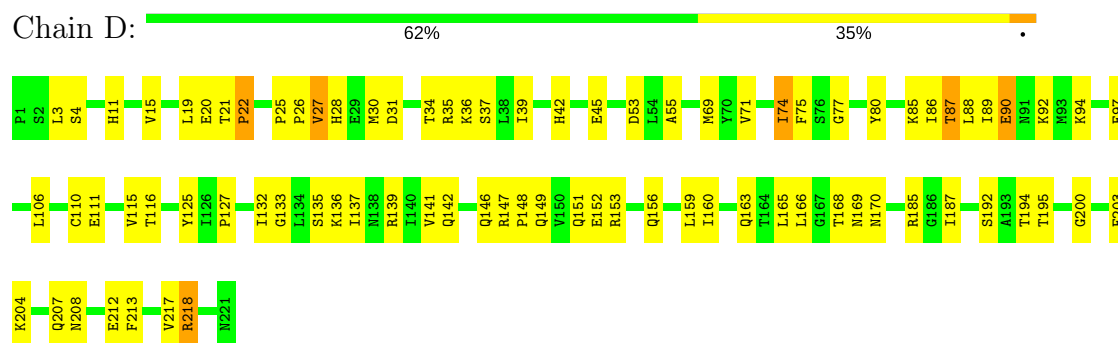
- Molecule 1: GTP cyclohydrolase I



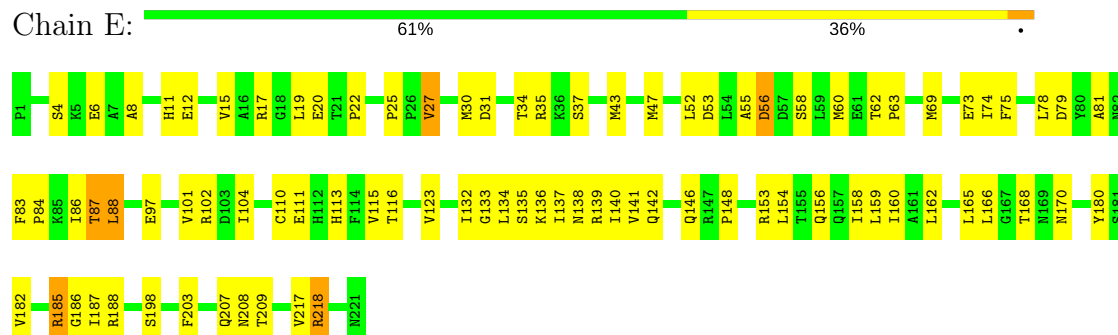
- Molecule 1: GTP cyclohydrolase I



- Molecule 1: GTP cyclohydrolase I



- Molecule 1: GTP cyclohydrolase I



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	223.14Å 317.81Å 132.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.185 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26475	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.49	0/1761	0.82	3/2384 (0.1%)
1	B	0.44	0/1761	0.70	0/2384
1	C	0.40	0/1761	0.68	0/2384
1	D	0.42	0/1761	0.68	1/2384 (0.0%)
1	E	0.43	0/1761	0.70	0/2384
1	F	0.39	0/1761	0.68	0/2384
1	G	0.38	0/1761	0.67	0/2384
1	H	0.38	0/1761	0.67	0/2384
1	I	0.39	0/1761	0.67	0/2384
1	J	0.40	0/1761	0.69	0/2384
1	K	0.39	0/1761	0.68	0/2384
1	L	0.39	0/1761	0.68	0/2384
1	M	0.40	0/1761	0.68	0/2384
1	N	0.40	0/1761	0.69	0/2384
1	O	0.38	0/1761	0.66	1/2384 (0.0%)
All	All	0.41	0/26415	0.69	5/35760 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	I	0	1
1	L	0	1
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PRO	O-C-N	6.81	133.59	122.70
1	A	218	ARG	O-C-N	5.82	132.00	122.70
1	A	218	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	D	149	GLN	N-CA-C	5.14	124.87	111.00
1	O	148	PRO	N-CA-C	-5.05	98.96	112.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	TYR	Sidechain
1	G	180	TYR	Sidechain
1	I	180	TYR	Sidechain
1	L	180	TYR	Sidechain

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	1733	0	1768	79	0
1	B	1733	0	1768	88	0
1	C	1733	0	1768	85	0
1	D	1733	0	1768	87	0
1	E	1733	0	1768	93	0
1	F	1733	0	1768	103	0
1	G	1733	0	1768	111	0
1	H	1733	0	1768	111	0
1	I	1733	0	1768	112	0
1	J	1733	0	1768	118	0
1	K	1733	0	1768	106	0
1	L	1733	0	1768	106	0
1	M	1733	0	1768	102	0
1	N	1733	0	1768	113	0
1	O	1733	0	1768	116	0
2	A	32	0	11	3	0
2	B	32	0	11	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	32	0	11	2	0
2	D	32	0	11	1	0
2	E	32	0	11	3	0
2	F	32	0	11	2	0
2	G	32	0	11	4	0
2	H	32	0	11	4	0
2	I	32	0	11	3	0
2	J	32	0	11	6	0
2	K	32	0	11	4	0
2	L	32	0	11	4	0
2	M	32	0	11	4	0
2	N	32	0	11	6	0
2	O	32	0	11	3	0
All	All	26475	0	26685	1290	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 1290 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:H:168:THR:HG22	1:H:170:ASN:H	1.14	1.06
1:A:86:ILE:HD13	1:A:165:LEU:HD13	1.37	1.05
1:O:168:THR:HG22	1:O:170:ASN:H	1.23	1.03
1:D:187:ILE:HD11	1:E:139:ARG:HG2	1.41	1.03
1:F:168:THR:HG22	1:F:170:ASN:H	1.21	1.02

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	219/221 (99%)	193 (88%)	22 (10%)	4 (2%)	10	47
1	B	219/221 (99%)	187 (85%)	25 (11%)	7 (3%)	5	30
1	C	219/221 (99%)	192 (88%)	25 (11%)	2 (1%)	20	64
1	D	219/221 (99%)	196 (90%)	20 (9%)	3 (1%)	13	53
1	E	219/221 (99%)	196 (90%)	18 (8%)	5 (2%)	7	40
1	F	219/221 (99%)	193 (88%)	20 (9%)	6 (3%)	6	35
1	G	219/221 (99%)	196 (90%)	19 (9%)	4 (2%)	10	47
1	H	219/221 (99%)	194 (89%)	22 (10%)	3 (1%)	13	53
1	I	219/221 (99%)	195 (89%)	19 (9%)	5 (2%)	7	40
1	J	219/221 (99%)	192 (88%)	23 (10%)	4 (2%)	10	47
1	K	219/221 (99%)	191 (87%)	23 (10%)	5 (2%)	7	40
1	L	219/221 (99%)	196 (90%)	18 (8%)	5 (2%)	7	40
1	M	219/221 (99%)	187 (85%)	29 (13%)	3 (1%)	13	53
1	N	219/221 (99%)	187 (85%)	27 (12%)	5 (2%)	7	40
1	O	219/221 (99%)	187 (85%)	26 (12%)	6 (3%)	6	35
All	All	3285/3315 (99%)	2882 (88%)	336 (10%)	67 (2%)	9	44

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	53	ASP
1	F	53	ASP
1	F	80	TYR
1	F	116	THR
1	G	27	VAL

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	194/194 (100%)	183 (94%)	11 (6%)	24	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	194/194 (100%)	188 (97%)	6 (3%)	45	79
1	C	194/194 (100%)	189 (97%)	5 (3%)	51	83
1	D	194/194 (100%)	187 (96%)	7 (4%)	40	76
1	E	194/194 (100%)	187 (96%)	7 (4%)	40	76
1	F	194/194 (100%)	190 (98%)	4 (2%)	59	85
1	G	194/194 (100%)	187 (96%)	7 (4%)	40	76
1	H	194/194 (100%)	185 (95%)	9 (5%)	31	70
1	I	194/194 (100%)	189 (97%)	5 (3%)	51	83
1	J	194/194 (100%)	188 (97%)	6 (3%)	45	79
1	K	194/194 (100%)	186 (96%)	8 (4%)	35	72
1	L	194/194 (100%)	186 (96%)	8 (4%)	35	72
1	M	194/194 (100%)	188 (97%)	6 (3%)	45	79
1	N	194/194 (100%)	188 (97%)	6 (3%)	45	79
1	O	194/194 (100%)	188 (97%)	6 (3%)	45	79
All	All	2910/2910 (100%)	2809 (96%)	101 (4%)	41	76

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	168	THR
1	N	87	THR
1	D	218	ARG
1	M	17	ARG
1	M	195	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	211	HIS
1	N	138	ASN
1	E	138	ASN
1	N	51	ASN
1	N	163	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

15 ligands 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	$\# Z > 2$
2	GTP	A	425	-	27,34,34	3.88	12 (44%)	27,54,54	3.02	10 (37%)
2	GTP	B	421	-	27,34,34	4.07	13 (48%)	27,54,54	3.06	10 (37%)
2	GTP	C	422	-	27,34,34	3.96	10 (37%)	27,54,54	3.25	9 (33%)
2	GTP	D	423	-	27,34,34	3.86	11 (40%)	27,54,54	3.10	9 (33%)
2	GTP	E	424	-	27,34,34	3.81	11 (40%)	27,54,54	2.89	9 (33%)
2	GTP	F	415	-	27,34,34	3.98	11 (40%)	27,54,54	3.16	10 (37%)
2	GTP	G	411	-	27,34,34	3.82	11 (40%)	27,54,54	3.19	10 (37%)
2	GTP	H	412	-	27,34,34	3.80	12 (44%)	27,54,54	3.21	10 (37%)
2	GTP	I	413	-	27,34,34	3.82	13 (48%)	27,54,54	3.21	9 (33%)
2	GTP	J	414	-	27,34,34	3.77	11 (40%)	27,54,54	3.11	10 (37%)
2	GTP	K	420	-	27,34,34	3.89	12 (44%)	27,54,54	3.20	9 (33%)
2	GTP	L	416	-	27,34,34	3.85	11 (40%)	27,54,54	3.16	10 (37%)
2	GTP	M	417	-	27,34,34	3.79	11 (40%)	27,54,54	3.22	10 (37%)
2	GTP	N	418	-	27,34,34	3.88	12 (44%)	27,54,54	3.15	9 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GTP	O	419	-	27,34,34	3.83	10 (37%)	27,54,54	3.15	9 (33%)

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
2	GTP	A	425	-	-	0/18/38/38	0/3/3/3
2	GTP	B	421	-	-	0/18/38/38	0/3/3/3
2	GTP	C	422	-	-	0/18/38/38	0/3/3/3
2	GTP	D	423	-	-	0/18/38/38	0/3/3/3
2	GTP	E	424	-	-	0/18/38/38	0/3/3/3
2	GTP	F	415	-	-	0/18/38/38	0/3/3/3
2	GTP	G	411	-	-	0/18/38/38	0/3/3/3
2	GTP	H	412	-	-	0/18/38/38	0/3/3/3
2	GTP	I	413	-	-	0/18/38/38	0/3/3/3
2	GTP	J	414	-	-	0/18/38/38	0/3/3/3
2	GTP	K	420	-	-	0/18/38/38	0/3/3/3
2	GTP	L	416	-	-	0/18/38/38	0/3/3/3
2	GTP	M	417	-	-	0/18/38/38	0/3/3/3
2	GTP	N	418	-	-	0/18/38/38	0/3/3/3
2	GTP	O	419	-	-	0/18/38/38	0/3/3/3

The worst 5 of 171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	415	GTP	C6-C5	-7.56	1.27	1.41
2	O	419	GTP	C6-C5	-6.83	1.28	1.41
2	B	421	GTP	C6-C5	-6.79	1.28	1.41
2	I	413	GTP	C6-C5	-6.71	1.28	1.41
2	M	417	GTP	C6-C5	-6.62	1.28	1.41

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	413	GTP	C5-C6-N1	-8.76	111.02	123.48
2	C	422	GTP	C5-C6-N1	-8.72	111.06	123.48
2	H	412	GTP	C5-C6-N1	-8.70	111.09	123.48
2	A	425	GTP	C5-C6-N1	-8.65	111.17	123.48
2	K	420	GTP	C5-C6-N1	-8.60	111.23	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	425	GTP	3	0
2	B	421	GTP	2	0
2	C	422	GTP	2	0
2	D	423	GTP	1	0
2	E	424	GTP	3	0
2	F	415	GTP	2	0
2	G	411	GTP	4	0
2	H	412	GTP	4	0
2	I	413	GTP	3	0
2	J	414	GTP	6	0
2	K	420	GTP	4	0
2	L	416	GTP	4	0
2	M	417	GTP	4	0
2	N	418	GTP	6	0
2	O	419	GTP	3	0

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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.