



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:18 PM UTC

PDB ID : 1FB1 / pdb_00001fb1
Title : CRYSTAL STRUCTURE OF HUMAN GTP CYCLOHYDROLASE I
Authors : Auerbach, G.; Herrmann, A.; Bracher, A.; Bader, G.; Gutlich, M.; Fischer, M.; Neukamm, M.; Nar, H.; Garrido-Franco, M.; Richardson, J.; Huber, R.; Bacher, A.
Deposited on : 2000-07-14
Resolution : 3.10 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

<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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

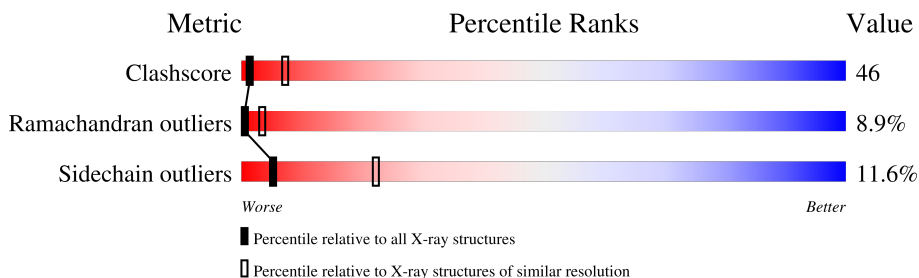
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	196	37% 49% 12% .
1	B	196	32% 49% 17% .
1	C	196	34% 51% 15% .
1	D	196	36% 48% 14% .
1	E	196	31% 51% 16% .

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
3	IPA	B	303	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7750 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.

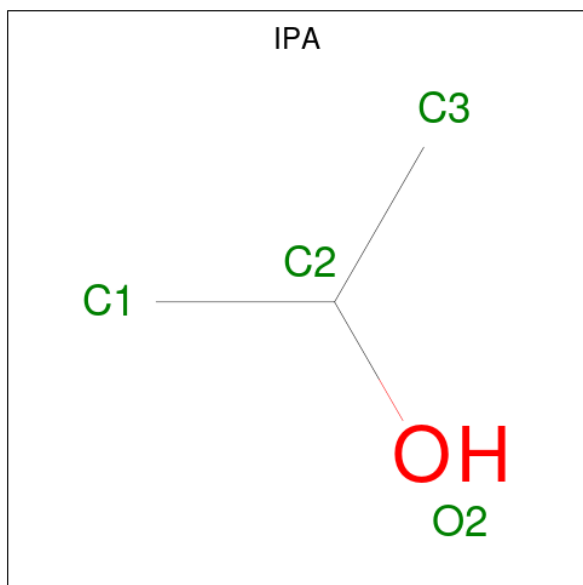
- Molecule 1 is a protein called GTP CYCLOHYDROLASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	196	1545	972	272	290	11	120	0	0
1	B	196	1545	972	272	290	11	119	0	0
1	C	196	1545	972	272	290	11	182	0	0
1	D	196	1545	972	272	290	11	143	0	0
1	E	196	1545	972	272	290	11	119	0	0

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

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

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



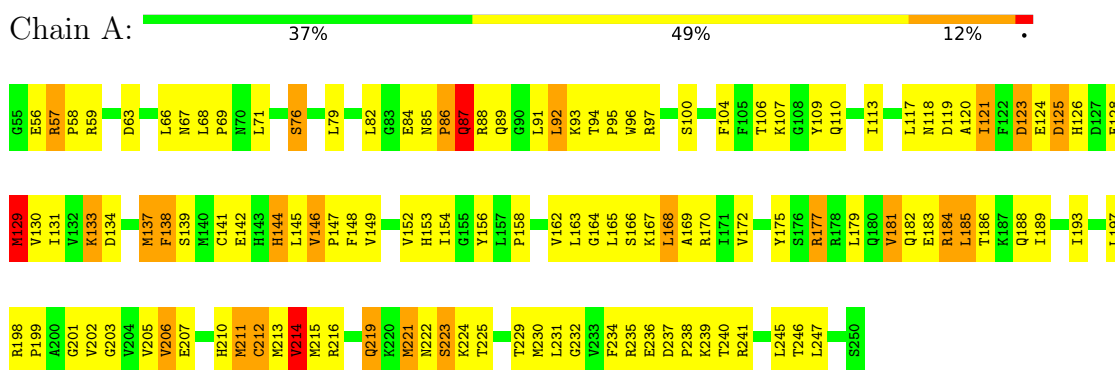
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		
3	B	1	Total	C	O	0	0
			4	3	1		
3	B	1	Total	C	O	0	0
			4	3	1		
3	D	1	Total	C	O	0	0
			4	3	1		
3	D	1	Total	C	O	0	0
			4	3	1		

3 Residue-property plots [i](#)

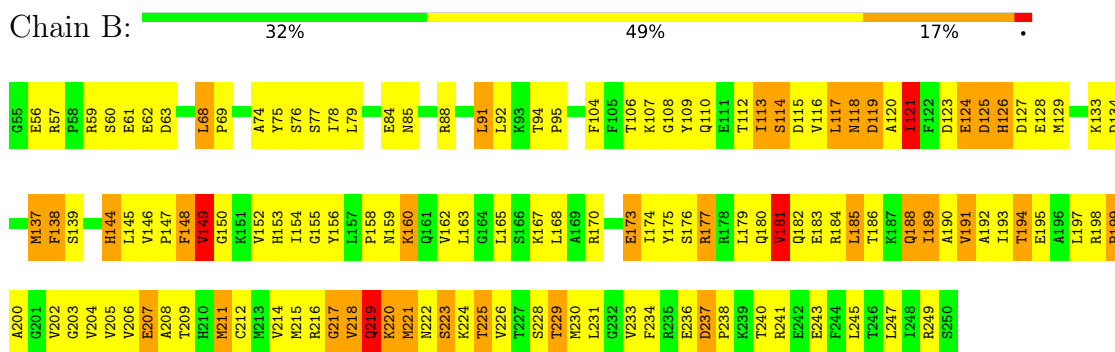
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



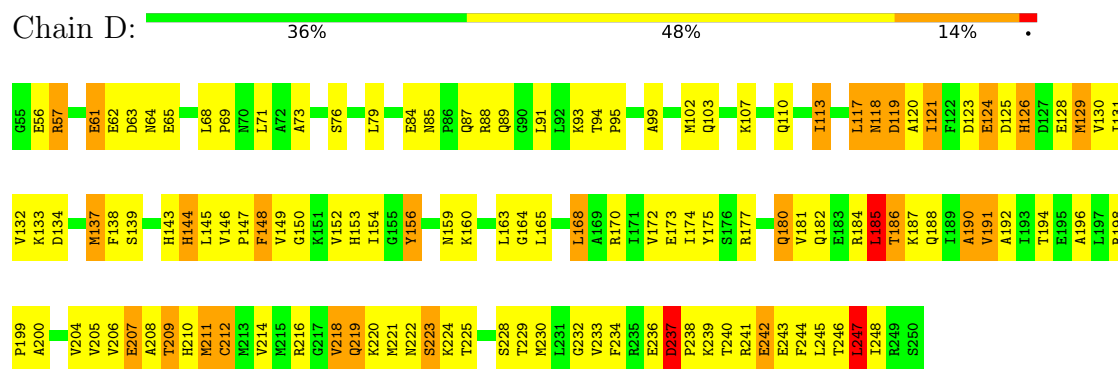
• Molecule 1: GTP CYCLOHYDROLASE I



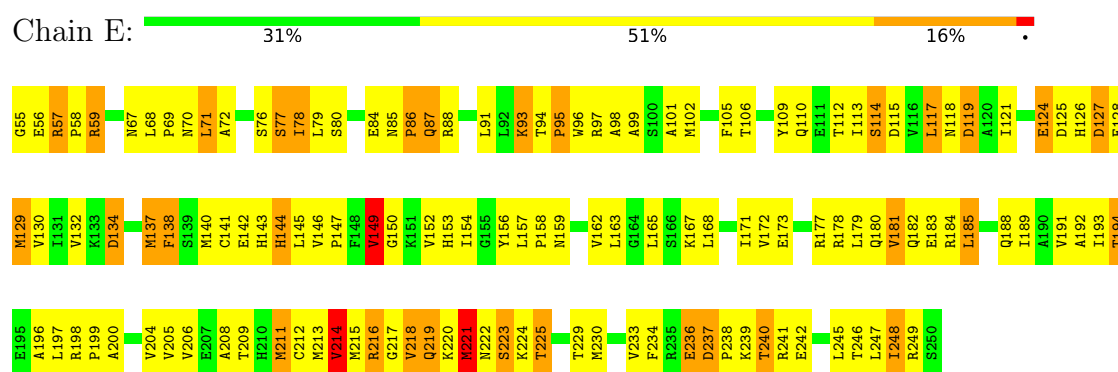
• Molecule 1: GTP CYCLOHYDROLASE I



- Molecule 1: GTP CYCLOHYDROLASE I



- Molecule 1: GTP CYCLOHYDROLASE I



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	115.11Å 115.11Å 387.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.97 – 3.10	Depositor
% Data completeness (in resolution range)	84.2 (14.97-3.10)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7750	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

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: ZN, IPA

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	0.72	0/1570	1.15	12/2119 (0.6%)
1	B	0.69	0/1570	1.13	13/2119 (0.6%)
1	C	0.62	0/1570	1.11	12/2119 (0.6%)
1	D	0.66	0/1570	1.19	17/2119 (0.8%)
1	E	0.71	1/1570 (0.1%)	1.16	15/2119 (0.7%)
All	All	0.68	1/7850 (0.0%)	1.15	69/10595 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	102	MET	SD-CE	5.38	1.93	1.79

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	VAL	N-CA-C	-9.22	93.84	108.86
1	C	180	GLN	N-CA-C	8.65	122.14	109.69
1	D	65	GLU	N-CA-C	-8.51	103.33	114.31
1	B	249	ARG	N-CA-C	-8.09	101.21	112.45
1	D	180	GLN	N-CA-C	7.88	119.96	108.86

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	1545	0	1565	115	0
1	B	1545	0	1565	154	0
1	C	1545	0	1565	149	0
1	D	1545	0	1565	119	0
1	E	1545	0	1565	119	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
2	E	1	0	0	0	0
3	A	4	0	7	1	0
3	B	8	0	15	5	0
3	D	8	0	16	3	0
All	All	7750	0	7863	642	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 46.

The worst 5 of 642 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:211:MET:HA	1:A:214:VAL:HG12	1.33	1.11
1:B:230:MET:HG3	1:B:241:ARG:HD3	1.38	1.05
1:B:113:ILE:H	1:B:113:ILE:HD12	1.20	1.03
1:C:235:ARG:HH11	1:C:235:ARG:HB2	1.24	0.99
1:C:235:ARG:HH11	1:C:235:ARG:CB	1.78	0.96

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	194/196 (99%)	154 (79%)	26 (13%)	14 (7%)	1	5
1	B	194/196 (99%)	147 (76%)	29 (15%)	18 (9%)	0	3
1	C	194/196 (99%)	149 (77%)	27 (14%)	18 (9%)	0	3
1	D	194/196 (99%)	151 (78%)	27 (14%)	16 (8%)	0	4
1	E	194/196 (99%)	145 (75%)	29 (15%)	20 (10%)	0	2
All	All	970/980 (99%)	746 (77%)	138 (14%)	86 (9%)	0	3

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	A	117	LEU
1	A	125	ASP
1	A	214	VAL
1	A	223	SER

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	172/172 (100%)	152 (88%)	20 (12%)	5	22
1	B	172/172 (100%)	144 (84%)	28 (16%)	2	11
1	C	172/172 (100%)	154 (90%)	18 (10%)	6	26
1	D	172/172 (100%)	156 (91%)	16 (9%)	8	31
1	E	172/172 (100%)	154 (90%)	18 (10%)	6	26
All	All	860/860 (100%)	760 (88%)	100 (12%)	5	22

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	205	VAL
1	D	156	TYR
1	E	240	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	213	MET
1	C	240	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	153	HIS
1	E	143	HIS
1	E	144	HIS
1	D	188	GLN
1	B	219	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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\# Z > 2$
3	IPA	D	304	2	3,3,3	0.76	0	3,3,3	0.23	0
3	IPA	B	302	2	3,3,3	0.83	0	3,3,3	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IPA	D	305	2	3,3,3	0.66	0	3,3,3	0.28	0
3	IPA	A	306	2	3,3,3	0.37	0	3,3,3	0.54	0
3	IPA	B	303	2	3,3,3	0.70	0	3,3,3	0.55	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	304	IPA	1	0
3	D	305	IPA	2	0
3	A	306	IPA	1	0
3	B	303	IPA	5	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.