wwPDB X-ray Structure Validation Summary Report (i)

Jan 29, 2024 – 08:05 PM EST

PDB ID	:	1FB1
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)

The following versions of software and data (see references (i)) were used in the production of this report:

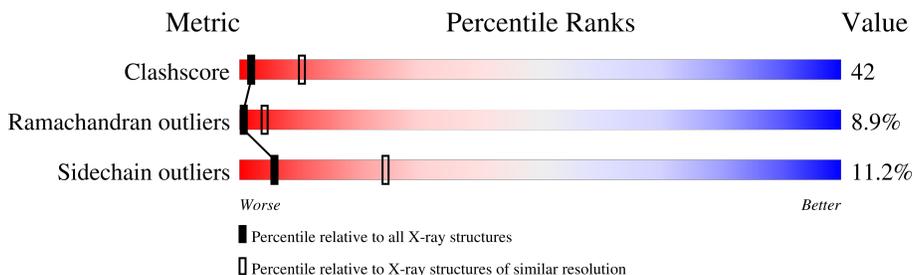|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Clashscore		42
Ramachandran outliers		8.9%
Sidechain outliers		11.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	196	43% 46% 9% •
1	B	196	37% 49% 13% •
1	C	196	38% 48% 13% •
1	D	196	41% 47% 11%
1	E	196	35% 52% 13% •

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 ⓘ

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.
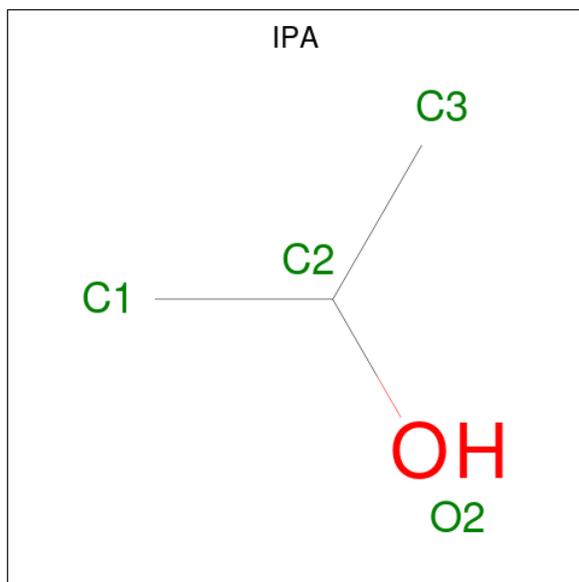
- Molecule 1 is a protein called GTP CYCLOHYDROLASE I.

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

- Molecule 2 is ZINC ION (three-letter code: 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 (three-letter code: IPA) (formula: C_3H_8O).

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

IPA

C3

C2

C1

OH

O2

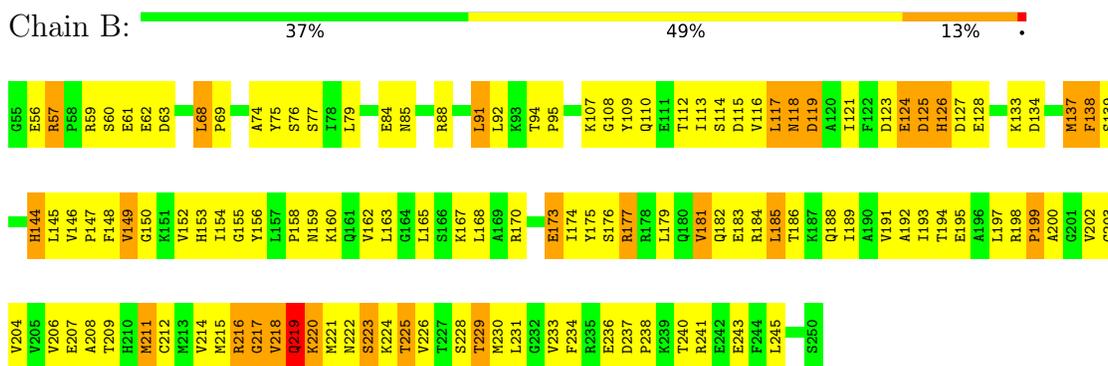| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 3	O 1	0	0
3	B	1	Total 4	C 3	O 1	0	0
3	B	1	Total 4	C 3	O 1	0	0
3	D	1	Total 4	C 3	O 1	0	0
3	D	1	Total 4	C 3	O 1	0	0

3 Residue-property plots ⓘ

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

Chain A:

• Molecule 1: GTP CYCLOHYDROLASE I

Chain B:

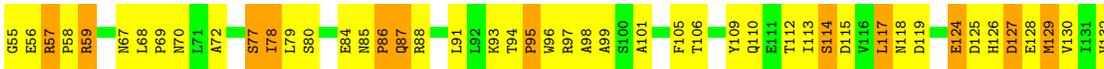• Molecule 1: GTP CYCLOHYDROLASE I

Chain C:

P199 A200 G201 V202 G203 V204 V205 V206 E207 A208 T209 H210 M211 C212 M213 V214 M215 R216 G217 V218 Q219 K220 M221 N222 S223 K224 T225 V226 T227 S228 T229 M230 V233 F234 R235 E236 D237 P238 K239 T240 R241 F244 L245 I248 R249 S250

• Molecule 1: GTP CYCLOHYDROLASE I

Chain D:

41%   47%   11%

G55 E56 R57 P58 R59 S60 E61 N64 L68 P69 N70 L71 A72 A73 S76 L79 E84 N85 P86 Q87 R88 Q89 G90 L91 L92 K93 T94 P95 A99 M102 Q103 K107 Q110 I113 L117 N118 D119 A120 I121 F122 D123 E124 D125 H126 D127 E128 M129 V130 I131

V132 K133 D134 M137 F138 H143 H144 L145 V146 P147 F148 V149 G150 K151 V152 H153 I154 G155 Y156 N159 K160 L163 G164 L165 L168 A169 R170 I171 V172 E173 I174 Y175 S176 R177 Q180 V181 Q182 E183 R184 L185 T186 K187 Q188 I189 A190 V191 A192 I193 T194 E195 A196 L197 R198 P199

A200 V205 V206 E207 A208 T209 H210 M211 C212 M213 V214 M215 R216 G217 V218 Q219 K220 M221 N222 S223 K224 T225 S228 T229 V233 E236 D237 P238 K239 T240 R241 E242 E243 F244 L245 T246 L247 I248 R249 S250

• Molecule 1: GTP CYCLOHYDROLASE I

Chain E:

35%   52%   13%   •

G55 E56 R57 P58 R59 N67 L68 P69 N70 L71 A72 S77 I78 L79 S80 E84 N85 P86 Q87 R88 L91 L92 K93 T94 P95 W96 R97 A98 A99 S100 A101 F105 T106 Y109 Q110 E111 T112 I113 S114 D115 V116 L117 N118 D119 E124 D125 H126 D127 E128 M129 V130 I131 V132

K133 D134 M137 F138 S139 M140 C141 E142 H143 H144 L145 V146 P147 F148 V149 G150 K151 V152 H153 I154 G155 Y156 L157 P158 V162 L163 G164 L165 S166 K167 L168 I171 V172 E173 R177 R178 L179 Q180 V181 Q182 E183 R184 L185 Q188 I189 A190 V191 A192 I193 T194 E195 A196 L197 R198 P199

A200 V204 V205 V206 E207 A208 T209 H210 M211 C212 M213 V214 M215 R216 G217 V218 Q219 K220 M221 N222 S223 K224 T225 T229 M230 V233 F234 R235 E236 D237 P238 K239 T240 R241 E242 L245 T246 L247 I248 R249 S250

4 Data and refinement statistics ⓘ

Xtriage (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.	Xtriage
Total number of atoms	7750	wwPDB-VP
Average B, all atoms (Å^2)	93.0	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: 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	0.56	0/1570	0.78	1/2119 (0.0%)
1	B	0.52	0/1570	0.78	0/2119
1	C	0.46	0/1570	0.71	0/2119
1	D	0.48	0/1570	0.77	1/2119 (0.0%)
1	E	0.52	0/1570	0.76	0/2119
All	All	0.51	0/7850	0.76	2/10595 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	VAL	N-CA-C	-6.36	93.84	111.00
1	D	148	PHE	N-CA-C	-5.39	96.45	111.00

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	1545	0	1565	104	0
1	B	1545	0	1565	142	0
1	C	1545	0	1565	138	0
1	D	1545	0	1565	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1545	0	1565	111	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	586	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 42.

The worst 5 of 586 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 ⓘ

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	194/196 (99%)	154 (79%)	26 (13%)	14 (7%)	1	6
1	B	194/196 (99%)	147 (76%)	29 (15%)	18 (9%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	C	194/196 (99%)	149 (77%)	27 (14%)	18 (9%)	0	3	
1	D	194/196 (99%)	151 (78%)	27 (14%)	16 (8%)	1	5	
1	E	194/196 (99%)	145 (75%)	29 (15%)	20 (10%)	0	3	
All	All	970/980 (99%)	746 (77%)	138 (14%)	86 (9%)	1	4	

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 ⓘ

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%)	148 (86%)	24 (14%)	3	15
1	C	172/172 (100%)	152 (88%)	20 (12%)	5	22
1	D	172/172 (100%)	156 (91%)	16 (9%)	9	32
1	E	172/172 (100%)	156 (91%)	16 (9%)	9	32
All	All	860/860 (100%)	764 (89%)	96 (11%)	6	24

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	213	MET
1	D	168	LEU
1	C	219	GLN
1	D	89	GLN
1	D	209	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	144	HIS
1	E	143	HIS
1	C	153	HIS
1	D	153	HIS
1	B	219	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	306	2	3,3,3	0.38	0	3,3,3	0.54	0
3	IPA	B	302	2	3,3,3	0.82	0	3,3,3	0.28	0
3	IPA	D	304	2	3,3,3	0.76	0	3,3,3	0.24	0
3	IPA	B	303	2	3,3,3	0.70	0	3,3,3	0.54	0
3	IPA	D	305	2	3,3,3	0.66	0	3,3,3	0.29	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	A	306	IPA	1	0
3	D	304	IPA	1	0
3	B	303	IPA	5	0
3	D	305	IPA	2	0

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.