



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 03:01 PM GMT

PDB ID : 3GCH
Title : CHEMISTRY OF CAGED ENZYMES. BINDING OF PHOTOREVERSIBLE CINNAMATES TO CHYMOTRYPSIN
Authors : Stoddard, B.L.; Ringe, D.; Petsko, G.A.
Deposited on : 1989-09-25
Resolution : 1.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

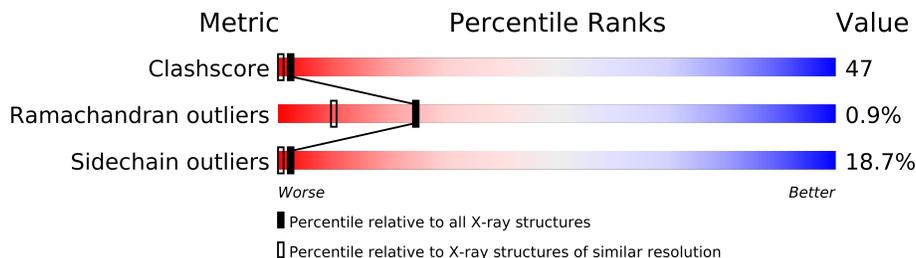
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	13	
2	B	131	
3	C	97	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	OAC	C	246	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1824 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GAMMA-CHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	11	69	45	12	11	1	0	0	1

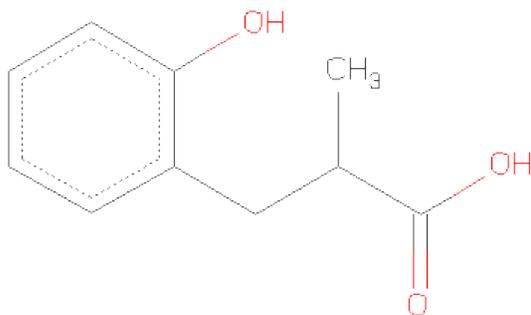
- Molecule 2 is a protein called GAMMA-CHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	131	979	618	162	195	4	0	0	0

- Molecule 3 is a protein called GAMMA-CHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	95	688	429	120	132	7	0	0	0

- Molecule 4 is TRANS-O-HYDROXY-ALPHA-METHYLCINNAMATE (three-letter code: OAC) (formula: C₁₀H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			12	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	52	Total	O	0	0
			52	52		
5	C	20	Total	O	0	0
			20	20		

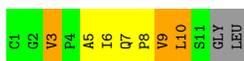
3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

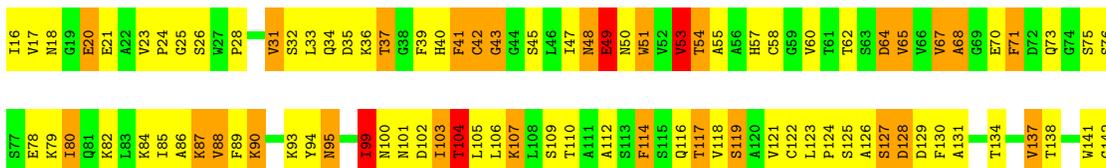
- Molecule 1: GAMMA-CHYMOTRYPSIN

Chain A: 



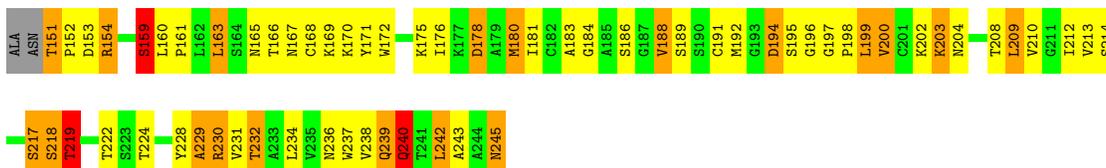
- Molecule 2: GAMMA-CHYMOTRYPSIN

Chain B: 



- Molecule 3: GAMMA-CHYMOTRYPSIN

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.70Å 69.70Å 97.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1824	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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: OAC

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	1.06	0/70	2.23	4/97 (4.1%)
2	B	1.19	4/999 (0.4%)	2.38	59/1361 (4.3%)
3	C	1.15	2/701 (0.3%)	2.12	28/955 (2.9%)
All	All	1.17	6/1770 (0.3%)	2.27	91/2413 (3.8%)

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
2	B	0	1
3	C	0	1
All	All	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	49	GLU	CD-OE2	6.64	1.32	1.25
2	B	78	GLU	CD-OE2	5.98	1.32	1.25
3	C	184	GLY	N-CA	-5.88	1.37	1.46
2	B	70	GLU	CD-OE2	5.73	1.31	1.25
3	C	198	PRO	N-CD	5.63	1.55	1.47

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	154	ARG	NE-CZ-NH1	12.43	126.52	120.30
2	B	146	TYR	CB-CG-CD1	-12.34	113.60	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	128	ASP	CB-CG-OD2	-10.50	108.85	118.30
3	C	154	ARG	NE-CZ-NH2	-10.48	115.06	120.30
2	B	94	TYR	CB-CG-CD2	10.38	127.23	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LEU	Mainchain
2	B	145	ARG	Sidechain
3	C	200	VAL	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	69	0	76	9	0
2	B	979	0	950	112	1
3	C	688	0	685	79	3
4	C	12	0	10	3	0
5	A	4	0	0	1	3
5	B	52	0	0	12	4
5	C	20	0	0	7	1
All	All	1824	0	1721	163	7

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 47.

The worst 5 of 163 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:31:VAL:HG12	2:B:68:ALA:HB2	1.30	1.07
3:C:172:TRP:HB2	3:C:176:ILE:HD11	1.36	1.02
2:B:90:LYS:HA	2:B:104:THR:HG22	1.38	1.01
2:B:58:CYS:HB2	5:B:271:HOH:O	1.61	1.01
3:C:230:ARG:NE	5:C:316:HOH:O	1.93	1.00

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:240:GLN:NE2	5:A:251:HOH:O[5_646]	0.51	1.69
5:B:273:HOH:O	5:B:273:HOH:O[2_675]	0.78	1.42
3:C:240:GLN:CD	5:A:251:HOH:O[5_646]	1.29	0.91
5:B:274:HOH:O	5:B:286:HOH:O[2_675]	1.64	0.56
2:B:82:LYS:NZ	5:B:302:HOH:O[6_476]	1.75	0.45

5.3 Torsion angles

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	9/13 (69%)	7 (78%)	2 (22%)	0	100	100
2	B	129/131 (98%)	116 (90%)	11 (8%)	2 (2%)	14	3
3	C	93/97 (96%)	87 (94%)	6 (6%)	0	100	100
All	All	231/241 (96%)	210 (91%)	19 (8%)	2 (1%)	25	10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	79	LYS
2	B	99	ILE

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	8/10 (80%)	8 (100%)	0	100	100
2	B	109/109 (100%)	91 (84%)	18 (16%)	3	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	76/77 (99%)	58 (76%)	18 (24%)	1	0
All	All	193/196 (98%)	157 (81%)	36 (19%)	2	0

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	127	SER
3	C	163	LEU
3	C	232	THR
3	C	151	THR
3	C	166	THR

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

Mol	Chain	Res	Type
2	B	48	ASN
2	B	100	ASN
2	B	116	GLN
3	C	165	ASN
3	C	239	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

1 ligand is 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
4	OAC	C	246	3	12,12,13	10.47	5 (41%)	14,15,17	11.21	9 (64%)

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	OAC	C	246	3	1/1/1/2	0/4/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	246	OAC	O-C	34.80	1.35	1.11
4	C	246	OAC	CE2-CD2	7.32	1.53	1.39
4	C	246	OAC	CZ-CE2	4.02	1.48	1.39
4	C	246	OAC	OH-CD2	3.95	1.44	1.36
4	C	246	OAC	CB1-CG	3.50	1.56	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	246	OAC	O-C-CA	-38.69	133.46	176.50
4	C	246	OAC	CB2-CA-C	-11.64	103.27	108.46
4	C	246	OAC	CG-CB1-CA	5.24	131.87	113.69
4	C	246	OAC	CB2-CA-CB1	5.15	138.91	112.75
4	C	246	OAC	CE2-CD2-CG	-4.58	116.07	120.45

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	246	OAC	CA

There are no torsion outliers.

There are no ring outliers.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.