WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 20, 2023 – 07:48 PM EDT

PDB ID	:	5HY4
Title	:	Structure-function analysis of functionally diverse members of the cyclic amide hydrolase family of Toblerone fold enzymes
Authors	:	Peat, T.S.; Balotra, S.; Wilding, M.; Newman, J.; Scott, C.
Deposited on	:	2016-02-01
Resolution	:	2.56 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 (i) 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 (i)) were used in the production of this report:

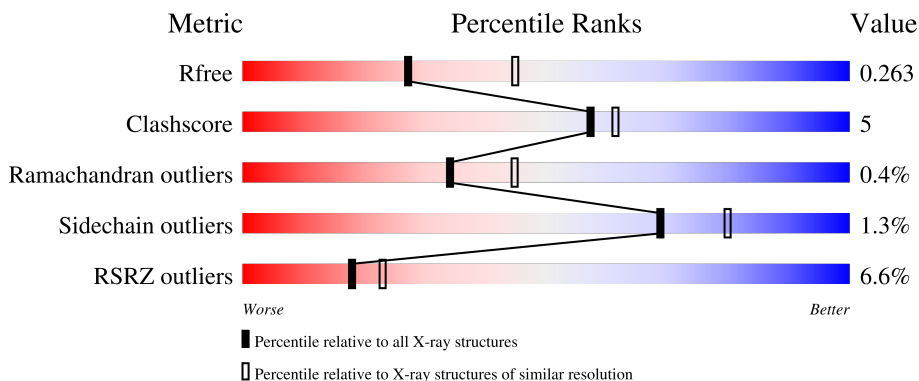|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.56 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.
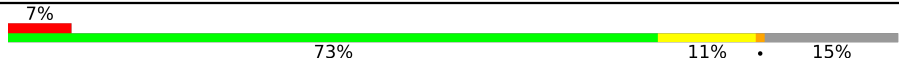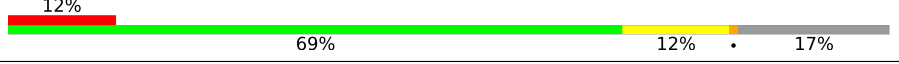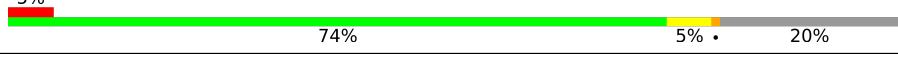
Metric	Percentile Ranks	Value
Rfree		0.263
Clashscore		5
Ramachandran outliers		0.4%
Sidechain outliers		1.3%
RSRZ outliers		6.6%

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))
R$_{free}$	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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% 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	410	5% / 80% / 8% / 12%
1	B	410	3% / 80% / 6% · 12%
1	C	410	4% / 74% / 9% · 15%
1	D	410	5% / 74% / 7% · 19%
1	E	410	3% / 80% / 5% / 15%

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Mol	Chain	Length	Quality of chain
1	F	410	7% ... 73% ... 11% ... 15%
1	G	410	12% ... 69% ... 12% ... 17%
1	H	410	5% ... 74% ... 5% ... 20%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 19841 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 Ring-opening amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	1	0
			2565	1590	463	501	11			
1	B	360	Total	C	N	O	S	0	2	0
			2586	1606	472	497	11			
1	C	348	Total	C	N	O	S	0	2	0
			2430	1509	437	473	11			
1	D	333	Total	C	N	O	S	0	2	0
			2349	1457	423	459	10			
1	E	349	Total	C	N	O	S	0	3	0
			2482	1538	451	483	10			
1	F	350	Total	C	N	O	S	0	1	0
			2461	1529	439	482	11			
1	G	340	Total	C	N	O	S	0	1	0
			2371	1472	421	467	11			
1	H	328	Total	C	N	O	S	0	2	0
			2341	1454	424	452	11			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E3JD18
A	-18	GLY	-	expression tag	UNP E3JD18
A	-17	SER	-	expression tag	UNP E3JD18
A	-16	SER	-	expression tag	UNP E3JD18
A	-15	HIS	-	expression tag	UNP E3JD18
A	-14	HIS	-	expression tag	UNP E3JD18
A	-13	HIS	-	expression tag	UNP E3JD18
A	-12	HIS	-	expression tag	UNP E3JD18
A	-11	HIS	-	expression tag	UNP E3JD18
A	-10	HIS	-	expression tag	UNP E3JD18
A	-9	SER	-	expression tag	UNP E3JD18
A	-8	SER	-	expression tag	UNP E3JD18
A	-7	GLY	-	expression tag	UNP E3JD18

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP E3JD18
A	-5	VAL	-	expression tag	UNP E3JD18
A	-4	PRO	-	expression tag	UNP E3JD18
A	-3	ARG	-	expression tag	UNP E3JD18
A	-2	GLY	-	expression tag	UNP E3JD18
A	-1	SER	-	expression tag	UNP E3JD18
A	0	HIS	-	expression tag	UNP E3JD18
B	-19	MET	-	initiating methionine	UNP E3JD18
B	-18	GLY	-	expression tag	UNP E3JD18
B	-17	SER	-	expression tag	UNP E3JD18
B	-16	SER	-	expression tag	UNP E3JD18
B	-15	HIS	-	expression tag	UNP E3JD18
B	-14	HIS	-	expression tag	UNP E3JD18
B	-13	HIS	-	expression tag	UNP E3JD18
B	-12	HIS	-	expression tag	UNP E3JD18
B	-11	HIS	-	expression tag	UNP E3JD18
B	-10	HIS	-	expression tag	UNP E3JD18
B	-9	SER	-	expression tag	UNP E3JD18
B	-8	SER	-	expression tag	UNP E3JD18
B	-7	GLY	-	expression tag	UNP E3JD18
B	-6	LEU	-	expression tag	UNP E3JD18
B	-5	VAL	-	expression tag	UNP E3JD18
B	-4	PRO	-	expression tag	UNP E3JD18
B	-3	ARG	-	expression tag	UNP E3JD18
B	-2	GLY	-	expression tag	UNP E3JD18
B	-1	SER	-	expression tag	UNP E3JD18
B	0	HIS	-	expression tag	UNP E3JD18
C	-19	MET	-	initiating methionine	UNP E3JD18
C	-18	GLY	-	expression tag	UNP E3JD18
C	-17	SER	-	expression tag	UNP E3JD18
C	-16	SER	-	expression tag	UNP E3JD18
C	-15	HIS	-	expression tag	UNP E3JD18
C	-14	HIS	-	expression tag	UNP E3JD18
C	-13	HIS	-	expression tag	UNP E3JD18
C	-12	HIS	-	expression tag	UNP E3JD18
C	-11	HIS	-	expression tag	UNP E3JD18
C	-10	HIS	-	expression tag	UNP E3JD18
C	-9	SER	-	expression tag	UNP E3JD18
C	-8	SER	-	expression tag	UNP E3JD18
C	-7	GLY	-	expression tag	UNP E3JD18
C	-6	LEU	-	expression tag	UNP E3JD18
C	-5	VAL	-	expression tag	UNP E3JD18

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP E3JD18
C	-3	ARG	-	expression tag	UNP E3JD18
C	-2	GLY	-	expression tag	UNP E3JD18
C	-1	SER	-	expression tag	UNP E3JD18
C	0	HIS	-	expression tag	UNP E3JD18
D	-19	MET	-	initiating methionine	UNP E3JD18
D	-18	GLY	-	expression tag	UNP E3JD18
D	-17	SER	-	expression tag	UNP E3JD18
D	-16	SER	-	expression tag	UNP E3JD18
D	-15	HIS	-	expression tag	UNP E3JD18
D	-14	HIS	-	expression tag	UNP E3JD18
D	-13	HIS	-	expression tag	UNP E3JD18
D	-12	HIS	-	expression tag	UNP E3JD18
D	-11	HIS	-	expression tag	UNP E3JD18
D	-10	HIS	-	expression tag	UNP E3JD18
D	-9	SER	-	expression tag	UNP E3JD18
D	-8	SER	-	expression tag	UNP E3JD18
D	-7	GLY	-	expression tag	UNP E3JD18
D	-6	LEU	-	expression tag	UNP E3JD18
D	-5	VAL	-	expression tag	UNP E3JD18
D	-4	PRO	-	expression tag	UNP E3JD18
D	-3	ARG	-	expression tag	UNP E3JD18
D	-2	GLY	-	expression tag	UNP E3JD18
D	-1	SER	-	expression tag	UNP E3JD18
D	0	HIS	-	expression tag	UNP E3JD18
E	-19	MET	-	initiating methionine	UNP E3JD18
E	-18	GLY	-	expression tag	UNP E3JD18
E	-17	SER	-	expression tag	UNP E3JD18
E	-16	SER	-	expression tag	UNP E3JD18
E	-15	HIS	-	expression tag	UNP E3JD18
E	-14	HIS	-	expression tag	UNP E3JD18
E	-13	HIS	-	expression tag	UNP E3JD18
E	-12	HIS	-	expression tag	UNP E3JD18
E	-11	HIS	-	expression tag	UNP E3JD18
E	-10	HIS	-	expression tag	UNP E3JD18
E	-9	SER	-	expression tag	UNP E3JD18
E	-8	SER	-	expression tag	UNP E3JD18
E	-7	GLY	-	expression tag	UNP E3JD18
E	-6	LEU	-	expression tag	UNP E3JD18
E	-5	VAL	-	expression tag	UNP E3JD18
E	-4	PRO	-	expression tag	UNP E3JD18
E	-3	ARG	-	expression tag	UNP E3JD18

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP E3JD18
E	-1	SER	-	expression tag	UNP E3JD18
E	0	HIS	-	expression tag	UNP E3JD18
F	-19	MET	-	initiating methionine	UNP E3JD18
F	-18	GLY	-	expression tag	UNP E3JD18
F	-17	SER	-	expression tag	UNP E3JD18
F	-16	SER	-	expression tag	UNP E3JD18
F	-15	HIS	-	expression tag	UNP E3JD18
F	-14	HIS	-	expression tag	UNP E3JD18
F	-13	HIS	-	expression tag	UNP E3JD18
F	-12	HIS	-	expression tag	UNP E3JD18
F	-11	HIS	-	expression tag	UNP E3JD18
F	-10	HIS	-	expression tag	UNP E3JD18
F	-9	SER	-	expression tag	UNP E3JD18
F	-8	SER	-	expression tag	UNP E3JD18
F	-7	GLY	-	expression tag	UNP E3JD18
F	-6	LEU	-	expression tag	UNP E3JD18
F	-5	VAL	-	expression tag	UNP E3JD18
F	-4	PRO	-	expression tag	UNP E3JD18
F	-3	ARG	-	expression tag	UNP E3JD18
F	-2	GLY	-	expression tag	UNP E3JD18
F	-1	SER	-	expression tag	UNP E3JD18
F	0	HIS	-	expression tag	UNP E3JD18
G	-19	MET	-	initiating methionine	UNP E3JD18
G	-18	GLY	-	expression tag	UNP E3JD18
G	-17	SER	-	expression tag	UNP E3JD18
G	-16	SER	-	expression tag	UNP E3JD18
G	-15	HIS	-	expression tag	UNP E3JD18
G	-14	HIS	-	expression tag	UNP E3JD18
G	-13	HIS	-	expression tag	UNP E3JD18
G	-12	HIS	-	expression tag	UNP E3JD18
G	-11	HIS	-	expression tag	UNP E3JD18
G	-10	HIS	-	expression tag	UNP E3JD18
G	-9	SER	-	expression tag	UNP E3JD18
G	-8	SER	-	expression tag	UNP E3JD18
G	-7	GLY	-	expression tag	UNP E3JD18
G	-6	LEU	-	expression tag	UNP E3JD18
G	-5	VAL	-	expression tag	UNP E3JD18
G	-4	PRO	-	expression tag	UNP E3JD18
G	-3	ARG	-	expression tag	UNP E3JD18
G	-2	GLY	-	expression tag	UNP E3JD18
G	-1	SER	-	expression tag	UNP E3JD18

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP E3JD18
H	-19	MET	-	initiating methionine	UNP E3JD18
H	-18	GLY	-	expression tag	UNP E3JD18
H	-17	SER	-	expression tag	UNP E3JD18
H	-16	SER	-	expression tag	UNP E3JD18
H	-15	HIS	-	expression tag	UNP E3JD18
H	-14	HIS	-	expression tag	UNP E3JD18
H	-13	HIS	-	expression tag	UNP E3JD18
H	-12	HIS	-	expression tag	UNP E3JD18
H	-11	HIS	-	expression tag	UNP E3JD18
H	-10	HIS	-	expression tag	UNP E3JD18
H	-9	SER	-	expression tag	UNP E3JD18
H	-8	SER	-	expression tag	UNP E3JD18
H	-7	GLY	-	expression tag	UNP E3JD18
H	-6	LEU	-	expression tag	UNP E3JD18
H	-5	VAL	-	expression tag	UNP E3JD18
H	-4	PRO	-	expression tag	UNP E3JD18
H	-3	ARG	-	expression tag	UNP E3JD18
H	-2	GLY	-	expression tag	UNP E3JD18
H	-1	SER	-	expression tag	UNP E3JD18
H	0	HIS	-	expression tag	UNP E3JD18

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	50	Total 50	O 50	0	0
2	B	27	Total 27	O 27	0	0
2	C	25	Total 25	O 25	0	0
2	D	21	Total 21	O 21	0	0
2	E	53	Total 53	O 53	0	0
2	F	37	Total 37	O 37	0	0
2	G	11	Total 11	O 11	0	0
2	H	32	Total 32	O 32	0	0

3 Residue-property plots ⓘ

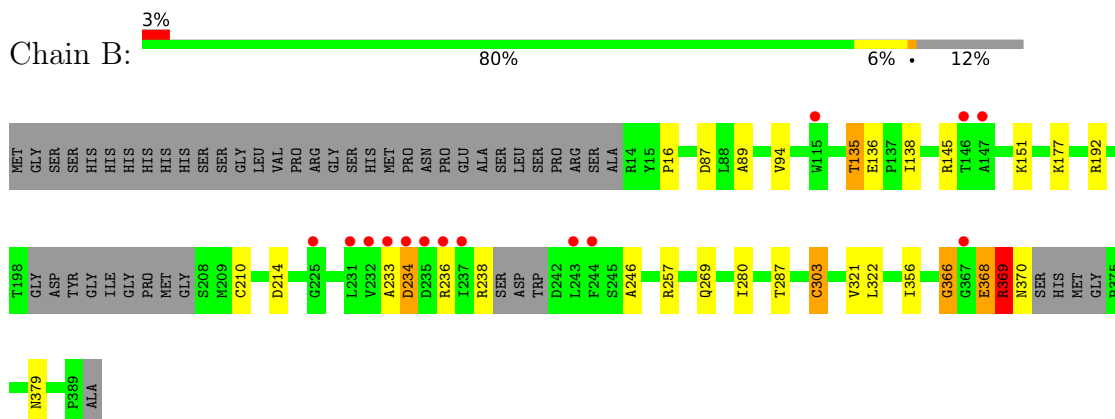These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.
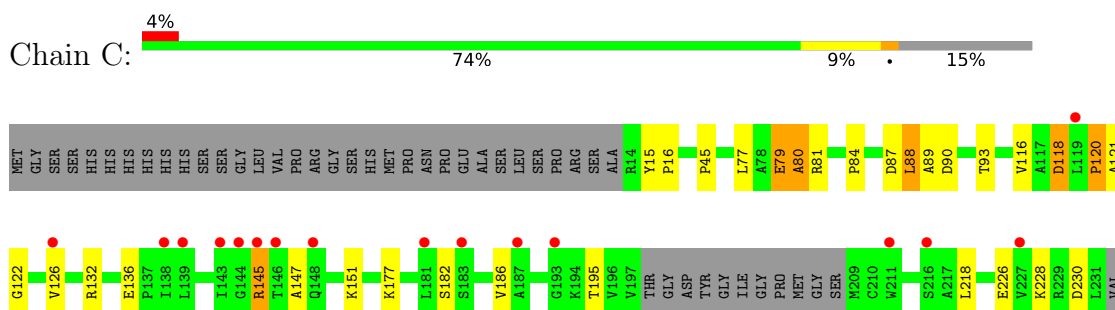
- Molecule 1: Ring-opening amidohydrolase

Chain A:

- Molecule 1: Ring-opening amidohydrolase

Chain B:

- Molecule 1: Ring-opening amidohydrolase

Chain C:

ALA ASP ASP ARG ILE ARG SER ASP TRP D242 L243 F244 S245 A246 E255 Q269 S270 I280 T281 R282 D286 T287 C303 V321 K346 I356 E368 R369 N370 SER HIS MET GLY PRO G377 R387 L388 PRO ALA

● Molecule 1: Ring-opening amidohydrolase

Chain D:

5%

74%   7% ·   19%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET PRO ASN PRO GLU ALA LEU SER PRO ARG SER ALA R14 Y15 P16 V49 A76 D87 L88 A89 V92 E114 W115 V116 A117 D118 L119 P120 L123 V126 R132

L139 G144 R145 T146 A147 A157 M160 L173 V174 M175 A180 L181 SER SER ARG ALA VAL ALA ASP ALA LEU SER ARG LYS THR VAL VAL THR GLY ASP TYR GLY ILE GLY GLY MET GLY SER M209 C210 W211 V227 D230 L231 V232 A233 D234 D235 ARG ILE ARG

SER ASP TRP ASP LEU PHE S245 A246 Q269 R275 I280 T281 R282 T287 V299 C303 Q312 G324 I356 N370 SER HIS MET GLY P376 G377 V385 R386 R387 LEU PRO ALA

● Molecule 1: Ring-opening amidohydrolase

Chain E:

3%

80%   5%   15%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET PRO ASN PRO GLU ALA LEU SER PRO ARG SER ALA R14 Y15 P16 F68 E86 D87 L88 A89 L123 P124 G125 R145 L181 S182 S183 R184 A185 V186 A187 G193 K194

T195 V196 V197 THR GLY ASP TYR GLY ILE GLY PRO MET GLY SER M209 D230 L231 V232 ALA ASP ASP ARG ILE SER ASP TRP D242 L243 F244 S245 A246 Q269 I280 T281 T287 C303 K346 I356 N370 SER HIS MET GLY PRO PRO G377 G378 L388 PRO ALA
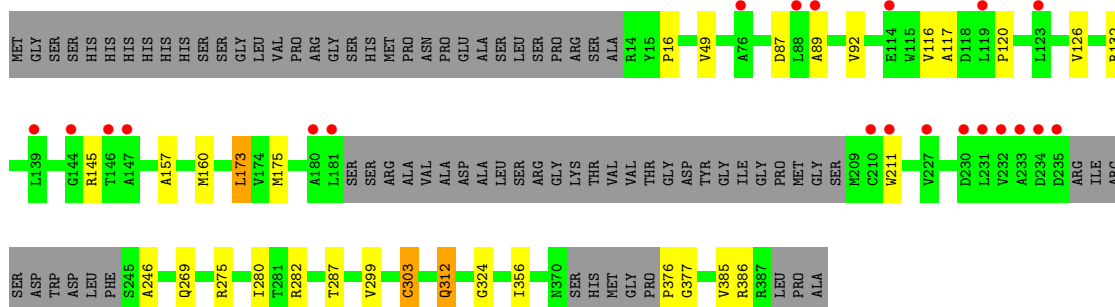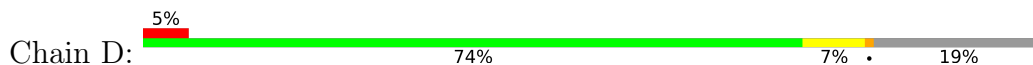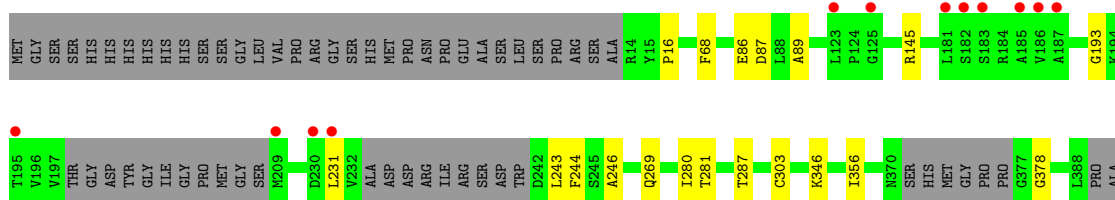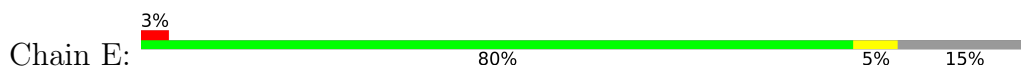
● Molecule 1: Ring-opening amidohydrolase

Chain F:

7%

73%   11%   ·   15%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET PRO ASN PRO GLU ALA LEU SER PRO ARG SER ALA A13 P16 K17 R66 P84 D87 L88 A89 D90 T93 L119 R132 D142 I143 G144 R145 T146 A147 Q148 V149

D150 K151 V152 L161 L181 S182 S183 R184 A185 V186 A187 D188 A189 L190 S191 R192 G193 K194 T195 V196 VAL THR GLY ASP TYR GLY ILE GLY PRO MET GLY S208 M209 C210 W211 V222 L218 V227 K228 R229 D230 L231 V232 A233 D234 D235 R236 ILE ARG SER ASP TRP ASP LEU PHE

S245 A246 G253 GLY GLU LYS ARG GLY G259 Q269 I280 T281 R282 T287 F301 D302 C303 V321 H342 I356 G367 E368 R369 N370 SER HIS MET GLY P375 P376 G377 G378 N379 A390
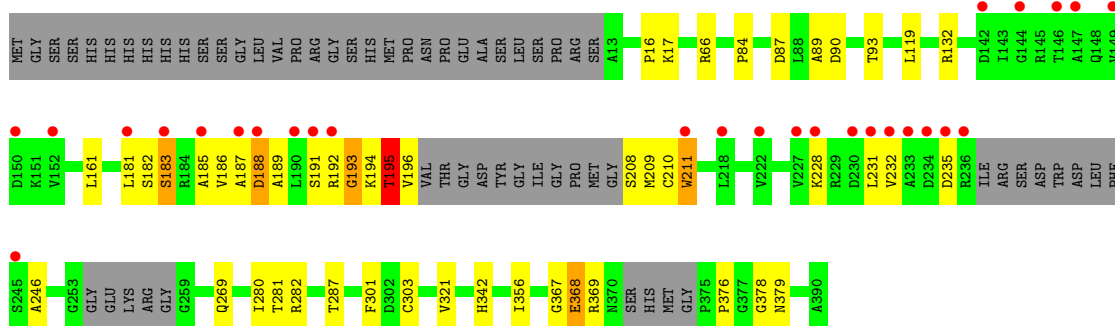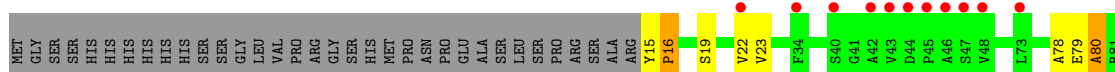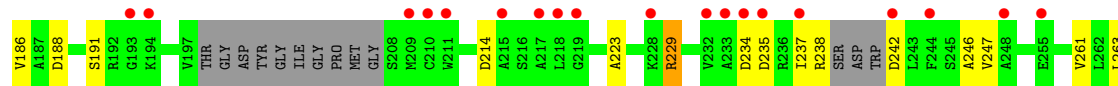
● Molecule 1: Ring-opening amidohydrolase

Chain G:

12%

69%   12% ·   17%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET PRO ASN PRO GLU ALA LEU SER PRO ARG SER ALA ARG Y15 P16 S19 V22 V23 F34 S40 G41 A42 V43 D44 P45 A46 S47 V48 L73 A78 E79 A80 R81

G82 V85 E86 D87 L88 A89 D90 S91 V92 T112 Q113 GLU TRP VAL ALA ASP LEU PRO ALA GLY LEU P124 G131 R132 G133 I138 L139 P140 E141 D142 R145 D150 D154 A155 V156 L161 D162 A163 G164 V165 P168 V171 H172 P179 A180 L181 S182 A185

V186 A187 D188 S191 R192 G193 K194 V197 THR GLY ASP TYR GLY ILE GLY PRO MET GLY S208 M209 C210 W211 D214 A215 S216 A217 L218 G219 A223 K228 R229 V232 A233 D234 D235 R236 I237 R238 SER ASP TRP D242 L243 F244 S245 A246 V247 A248 E255 V261 L262 L263

L264 A265 ASN SER A268 S272 E273 I276 I280 T281 T287 D300 C303 V321 I356 G367 E368 R369 N370 SER HIS MET GLY PRO PRO GLY G378 R386 ARG LEU PRO ALA

• Molecule 1: Ring-opening amidohydrolase

Chain H:

5%

74%   5% •   20%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET PRO ASN PRO GLU ALA SER LEU SER PRO ARG SER ALA R14 Y15 P16 R35 F68 T75 E79 D87 L88 A89 E114 W115 I138 I143 G144 R145 T146 A147 Q148

V149 D150 K151 P179 ALA LEU SER SER ARG ALA VAL ALA ASP ALA LEU SER ARG GLY LYS T195 V196 VAL THR GLY ASP TYR GLY ILE GLY PRO MET GLY S208 M209 C210 W211 A215 L218 G219 V220 V227 K228 R229 ASP LEU VAL ALA ASP ASP ARG ILE ARG SER ASP TRP ASP

LEU PHE S245 A246 G253 G254 Q269 I280 T281 T287 C303 V321 L322 I356 G367 E368 R369 N370 SER HIS MET GLY PRO PRO GLY G378 P389 ALA

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.76Å 105.80Å 299.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.56 45.95 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.70-2.56) 99.4 (45.95-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.229 , 0.263 0.232 , 0.263	Depositor DCC
R_{free} test set	4666 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.5	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19841	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2675e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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	0.65	0/2604	0.83	6/3550 (0.2%)
1	B	0.67	0/2627	0.83	6/3578 (0.2%)
1	C	0.68	1/2466 (0.0%)	0.85	7/3366 (0.2%)
1	D	0.63	0/2385	0.81	4/3254 (0.1%)
1	E	0.64	0/2517	0.82	2/3429 (0.1%)
1	F	0.68	0/2500	0.80	2/3413 (0.1%)
1	G	0.70	0/2402	0.86	4/3273 (0.1%)
1	H	0.66	1/2377 (0.0%)	0.79	1/3239 (0.0%)
All	All	0.66	2/19878 (0.0%)	0.82	32/27102 (0.1%)

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	B	0	2
1	C	0	8
1	D	0	4
1	F	0	4
1	G	0	4
All	All	0	22

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	211	TRP	CB-CG	-5.59	1.40	1.50
1	C	226	GLU	CD-OE1	-5.34	1.19	1.25

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	145	ARG	NE-CZ-NH1	9.01	124.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	145	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	G	235	ASP	CB-CG-OD1	8.14	125.63	118.30
1	G	154	ASP	CB-CG-OD2	7.80	125.32	118.30
1	G	79	GLU	CB-CA-C	7.65	125.70	110.40

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	366	GLY	Peptide
1	B	369	ARG	Peptide
1	C	79	GLU	Peptide
1	C	80	ALA	Mainchain
1	C	88	LEU	Peptide

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	2565	0	2528	16	0
1	B	2586	0	2575	22	1
1	C	2430	0	2359	27	0
1	D	2349	0	2306	17	0
1	E	2482	0	2451	10	1
1	F	2461	0	2414	39	0
1	G	2371	0	2318	43	0
1	H	2341	0	2317	20	0
2	A	50	0	0	1	0
2	B	27	0	0	0	0
2	C	25	0	0	1	0
2	D	21	0	0	0	0
2	E	53	0	0	1	0
2	F	37	0	0	2	0
2	G	11	0	0	0	0
2	H	32	0	0	0	0
All	All	19841	0	19268	189	1

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 5.

The worst 5 of 189 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:35[B]:ARG:NH2	1:H:79[B]:GLU:OE1	1.62	1.31
1:G:172:HIS:O	1:G:247:VAL:HG13	1.43	1.15
1:G:150:ASP:OD1	1:G:229:ARG:NH1	1.82	1.12
1:C:87:ASP:O	1:C:89:ALA:N	1.97	0.97
1:H:35[B]:ARG:HH21	1:H:79[B]:GLU:CD	1.73	0.91

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASP:OD1	1:E:193:GLY:O[4_445]	2.13	0.07

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	356/410 (87%)	343 (96%)	13 (4%)	0	100	100
1	B	354/410 (86%)	343 (97%)	10 (3%)	1 (0%)	41	50
1	C	342/410 (83%)	322 (94%)	18 (5%)	2 (1%)	25	33
1	D	327/410 (80%)	316 (97%)	11 (3%)	0	100	100
1	E	344/410 (84%)	335 (97%)	9 (3%)	0	100	100
1	F	341/410 (83%)	324 (95%)	13 (4%)	4 (1%)	13	17
1	G	329/410 (80%)	310 (94%)	15 (5%)	4 (1%)	13	17
1	H	320/410 (78%)	312 (98%)	8 (2%)	0	100	100
All	All	2713/3280 (83%)	2605 (96%)	97 (4%)	11 (0%)	34	45

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	80	ALA
1	C	88	LEU
1	G	141	GLU
1	G	368	GLU
1	B	368	GLU

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	263/310 (85%)	261 (99%)	2 (1%)	81	88
1	B	268/310 (86%)	266 (99%)	2 (1%)	84	90
1	C	241/310 (78%)	239 (99%)	2 (1%)	81	88
1	D	240/310 (77%)	237 (99%)	3 (1%)	69	80
1	E	254/310 (82%)	252 (99%)	2 (1%)	81	88
1	F	252/310 (81%)	246 (98%)	6 (2%)	49	63
1	G	241/310 (78%)	236 (98%)	5 (2%)	53	67
1	H	242/310 (78%)	238 (98%)	4 (2%)	60	74
All	All	2001/2480 (81%)	1975 (99%)	26 (1%)	69	80

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	235	ASP
1	G	141	GLU
1	H	369	ARG
1	F	303	CYS
1	G	229	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	134	HIS
1	G	172	HIS
1	G	370	ASN
1	H	370	ASN

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 ⓘ

There are no ligands in this entry.

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	361/410 (88%)	0.15	20 (5%)	25	32	19, 41, 99, 140	0
1	B	360/410 (87%)	0.14	14 (3%)	39	48	22, 47, 86, 130	0
1	C	348/410 (84%)	0.31	18 (5%)	27	34	20, 57, 107, 144	0
1	D	333/410 (81%)	0.46	21 (6%)	20	25	24, 58, 106, 134	0
1	E	349/410 (85%)	0.12	12 (3%)	45	54	20, 42, 105, 137	0
1	F	350/410 (85%)	0.38	28 (8%)	12	17	22, 48, 99, 122	0
1	G	340/410 (82%)	0.77	49 (14%)	2	3	25, 70, 111, 138	0
1	H	328/410 (80%)	0.24	22 (6%)	17	22	22, 49, 95, 139	0
All	All	2769/3280 (84%)	0.32	184 (6%)	18	23	19, 51, 104, 144	0

The worst 5 of 184 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ILE	7.7
1	F	235	ASP	7.5
1	F	191	SER	6.9
1	D	235	ASP	6.3
1	G	233	ALA	6.2

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

There are no ligands in this entry.

6.5　Other polymers ⓘ

There are no such residues in this entry.