wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 04:25 AM EDT

PDB ID	:	3OT4
Title	:	Structure and Catalytic Mechanism of Bordetella bronchiseptica nicF
Authors	:	Rowlett, R.S.; Snider, M.J.
Deposited on	:	2010-09-10
Resolution	:	2.40 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:

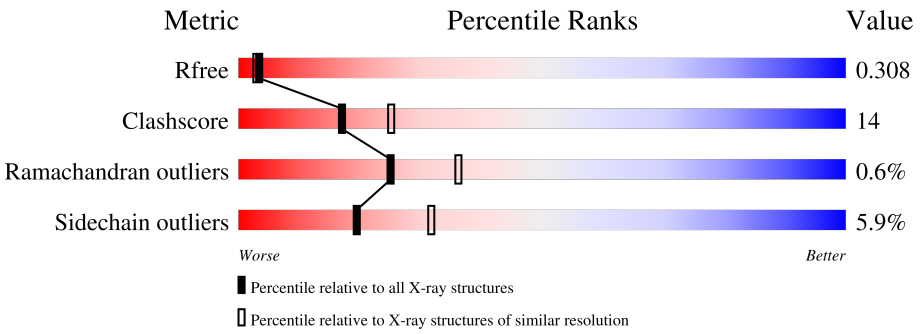
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Mol	Chain	Length	Quality of chain
1	A	236	61% 20% • 16%
1	B	236	64% 18% • 16%
1	C	236	61% 20% • 16%
1	D	236	56% 25% • 16%
1	E	236	67% 16% • 15%
1	F	236	65% 16% • 17%
1	G	236	65% 17% • 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	236	59% 21% • 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12175 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 Putative isochorismatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	198	1463	927	257	272	7	0	0	0
1	B	198	1463	927	257	272	7	0	0	0
1	C	198	1469	932	259	271	7	0	0	0
1	D	198	1469	932	259	271	7	0	0	0
1	E	201	1487	943	262	275	7	0	0	0
1	F	197	1461	926	257	271	7	0	0	0
1	G	197	1461	926	257	271	7	0	0	0
1	H	198	1467	929	258	273	7	0	0	0

There are 248 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	GLY	-	expression tag	UNP Q7TTE5
A	-20	SER	-	expression tag	UNP Q7TTE5
A	-19	ASP	-	expression tag	UNP Q7TTE5
A	-18	LYS	-	expression tag	UNP Q7TTE5
A	-17	ILE	-	expression tag	UNP Q7TTE5
A	-16	HIS	-	expression tag	UNP Q7TTE5
A	-15	HIS	-	expression tag	UNP Q7TTE5
A	-14	HIS	-	expression tag	UNP Q7TTE5
A	-13	HIS	-	expression tag	UNP Q7TTE5
A	-12	HIS	-	expression tag	UNP Q7TTE5
A	-11	HIS	-	expression tag	UNP Q7TTE5
A	-10	SER	-	expression tag	UNP Q7TTE5
A	-9	SER	-	expression tag	UNP Q7TTE5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP Q7TTE5
A	-7	GLU	-	expression tag	UNP Q7TTE5
A	-6	ASN	-	expression tag	UNP Q7TTE5
A	-5	LEU	-	expression tag	UNP Q7TTE5
A	-4	TYR	-	expression tag	UNP Q7TTE5
A	-3	PHE	-	expression tag	UNP Q7TTE5
A	-2	GLN	-	expression tag	UNP Q7TTE5
A	-1	GLY	-	expression tag	UNP Q7TTE5
A	0	HIS	-	expression tag	UNP Q7TTE5
A	206	GLY	-	expression tag	UNP Q7TTE5
A	207	LEU	-	expression tag	UNP Q7TTE5
A	208	GLU	-	expression tag	UNP Q7TTE5
A	209	HIS	-	expression tag	UNP Q7TTE5
A	210	HIS	-	expression tag	UNP Q7TTE5
A	211	HIS	-	expression tag	UNP Q7TTE5
A	212	HIS	-	expression tag	UNP Q7TTE5
A	213	HIS	-	expression tag	UNP Q7TTE5
A	214	HIS	-	expression tag	UNP Q7TTE5
B	-21	GLY	-	expression tag	UNP Q7TTE5
B	-20	SER	-	expression tag	UNP Q7TTE5
B	-19	ASP	-	expression tag	UNP Q7TTE5
B	-18	LYS	-	expression tag	UNP Q7TTE5
B	-17	ILE	-	expression tag	UNP Q7TTE5
B	-16	HIS	-	expression tag	UNP Q7TTE5
B	-15	HIS	-	expression tag	UNP Q7TTE5
B	-14	HIS	-	expression tag	UNP Q7TTE5
B	-13	HIS	-	expression tag	UNP Q7TTE5
B	-12	HIS	-	expression tag	UNP Q7TTE5
B	-11	HIS	-	expression tag	UNP Q7TTE5
B	-10	SER	-	expression tag	UNP Q7TTE5
B	-9	SER	-	expression tag	UNP Q7TTE5
B	-8	GLY	-	expression tag	UNP Q7TTE5
B	-7	GLU	-	expression tag	UNP Q7TTE5
B	-6	ASN	-	expression tag	UNP Q7TTE5
B	-5	LEU	-	expression tag	UNP Q7TTE5
B	-4	TYR	-	expression tag	UNP Q7TTE5
B	-3	PHE	-	expression tag	UNP Q7TTE5
B	-2	GLN	-	expression tag	UNP Q7TTE5
B	-1	GLY	-	expression tag	UNP Q7TTE5
B	0	HIS	-	expression tag	UNP Q7TTE5
B	206	GLY	-	expression tag	UNP Q7TTE5
B	207	LEU	-	expression tag	UNP Q7TTE5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	208	GLU	-	expression tag	UNP Q7TTE5
B	209	HIS	-	expression tag	UNP Q7TTE5
B	210	HIS	-	expression tag	UNP Q7TTE5
B	211	HIS	-	expression tag	UNP Q7TTE5
B	212	HIS	-	expression tag	UNP Q7TTE5
B	213	HIS	-	expression tag	UNP Q7TTE5
B	214	HIS	-	expression tag	UNP Q7TTE5
C	-21	GLY	-	expression tag	UNP Q7TTE5
C	-20	SER	-	expression tag	UNP Q7TTE5
C	-19	ASP	-	expression tag	UNP Q7TTE5
C	-18	LYS	-	expression tag	UNP Q7TTE5
C	-17	ILE	-	expression tag	UNP Q7TTE5
C	-16	HIS	-	expression tag	UNP Q7TTE5
C	-15	HIS	-	expression tag	UNP Q7TTE5
C	-14	HIS	-	expression tag	UNP Q7TTE5
C	-13	HIS	-	expression tag	UNP Q7TTE5
C	-12	HIS	-	expression tag	UNP Q7TTE5
C	-11	HIS	-	expression tag	UNP Q7TTE5
C	-10	SER	-	expression tag	UNP Q7TTE5
C	-9	SER	-	expression tag	UNP Q7TTE5
C	-8	GLY	-	expression tag	UNP Q7TTE5
C	-7	GLU	-	expression tag	UNP Q7TTE5
C	-6	ASN	-	expression tag	UNP Q7TTE5
C	-5	LEU	-	expression tag	UNP Q7TTE5
C	-4	TYR	-	expression tag	UNP Q7TTE5
C	-3	PHE	-	expression tag	UNP Q7TTE5
C	-2	GLN	-	expression tag	UNP Q7TTE5
C	-1	GLY	-	expression tag	UNP Q7TTE5
C	0	HIS	-	expression tag	UNP Q7TTE5
C	206	GLY	-	expression tag	UNP Q7TTE5
C	207	LEU	-	expression tag	UNP Q7TTE5
C	208	GLU	-	expression tag	UNP Q7TTE5
C	209	HIS	-	expression tag	UNP Q7TTE5
C	210	HIS	-	expression tag	UNP Q7TTE5
C	211	HIS	-	expression tag	UNP Q7TTE5
C	212	HIS	-	expression tag	UNP Q7TTE5
C	213	HIS	-	expression tag	UNP Q7TTE5
C	214	HIS	-	expression tag	UNP Q7TTE5
D	-21	GLY	-	expression tag	UNP Q7TTE5
D	-20	SER	-	expression tag	UNP Q7TTE5
D	-19	ASP	-	expression tag	UNP Q7TTE5
D	-18	LYS	-	expression tag	UNP Q7TTE5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	ILE	-	expression tag	UNP Q7TTE5
D	-16	HIS	-	expression tag	UNP Q7TTE5
D	-15	HIS	-	expression tag	UNP Q7TTE5
D	-14	HIS	-	expression tag	UNP Q7TTE5
D	-13	HIS	-	expression tag	UNP Q7TTE5
D	-12	HIS	-	expression tag	UNP Q7TTE5
D	-11	HIS	-	expression tag	UNP Q7TTE5
D	-10	SER	-	expression tag	UNP Q7TTE5
D	-9	SER	-	expression tag	UNP Q7TTE5
D	-8	GLY	-	expression tag	UNP Q7TTE5
D	-7	GLU	-	expression tag	UNP Q7TTE5
D	-6	ASN	-	expression tag	UNP Q7TTE5
D	-5	LEU	-	expression tag	UNP Q7TTE5
D	-4	TYR	-	expression tag	UNP Q7TTE5
D	-3	PHE	-	expression tag	UNP Q7TTE5
D	-2	GLN	-	expression tag	UNP Q7TTE5
D	-1	GLY	-	expression tag	UNP Q7TTE5
D	0	HIS	-	expression tag	UNP Q7TTE5
D	206	GLY	-	expression tag	UNP Q7TTE5
D	207	LEU	-	expression tag	UNP Q7TTE5
D	208	GLU	-	expression tag	UNP Q7TTE5
D	209	HIS	-	expression tag	UNP Q7TTE5
D	210	HIS	-	expression tag	UNP Q7TTE5
D	211	HIS	-	expression tag	UNP Q7TTE5
D	212	HIS	-	expression tag	UNP Q7TTE5
D	213	HIS	-	expression tag	UNP Q7TTE5
D	214	HIS	-	expression tag	UNP Q7TTE5
E	-21	GLY	-	expression tag	UNP Q7TTE5
E	-20	SER	-	expression tag	UNP Q7TTE5
E	-19	ASP	-	expression tag	UNP Q7TTE5
E	-18	LYS	-	expression tag	UNP Q7TTE5
E	-17	ILE	-	expression tag	UNP Q7TTE5
E	-16	HIS	-	expression tag	UNP Q7TTE5
E	-15	HIS	-	expression tag	UNP Q7TTE5
E	-14	HIS	-	expression tag	UNP Q7TTE5
E	-13	HIS	-	expression tag	UNP Q7TTE5
E	-12	HIS	-	expression tag	UNP Q7TTE5
E	-11	HIS	-	expression tag	UNP Q7TTE5
E	-10	SER	-	expression tag	UNP Q7TTE5
E	-9	SER	-	expression tag	UNP Q7TTE5
E	-8	GLY	-	expression tag	UNP Q7TTE5
E	-7	GLU	-	expression tag	UNP Q7TTE5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	ASN	-	expression tag	UNP Q7TTE5
E	-5	LEU	-	expression tag	UNP Q7TTE5
E	-4	TYR	-	expression tag	UNP Q7TTE5
E	-3	PHE	-	expression tag	UNP Q7TTE5
E	-2	GLN	-	expression tag	UNP Q7TTE5
E	-1	GLY	-	expression tag	UNP Q7TTE5
E	0	HIS	-	expression tag	UNP Q7TTE5
E	206	GLY	-	expression tag	UNP Q7TTE5
E	207	LEU	-	expression tag	UNP Q7TTE5
E	208	GLU	-	expression tag	UNP Q7TTE5
E	209	HIS	-	expression tag	UNP Q7TTE5
E	210	HIS	-	expression tag	UNP Q7TTE5
E	211	HIS	-	expression tag	UNP Q7TTE5
E	212	HIS	-	expression tag	UNP Q7TTE5
E	213	HIS	-	expression tag	UNP Q7TTE5
E	214	HIS	-	expression tag	UNP Q7TTE5
F	-21	GLY	-	expression tag	UNP Q7TTE5
F	-20	SER	-	expression tag	UNP Q7TTE5
F	-19	ASP	-	expression tag	UNP Q7TTE5
F	-18	LYS	-	expression tag	UNP Q7TTE5
F	-17	ILE	-	expression tag	UNP Q7TTE5
F	-16	HIS	-	expression tag	UNP Q7TTE5
F	-15	HIS	-	expression tag	UNP Q7TTE5
F	-14	HIS	-	expression tag	UNP Q7TTE5
F	-13	HIS	-	expression tag	UNP Q7TTE5
F	-12	HIS	-	expression tag	UNP Q7TTE5
F	-11	HIS	-	expression tag	UNP Q7TTE5
F	-10	SER	-	expression tag	UNP Q7TTE5
F	-9	SER	-	expression tag	UNP Q7TTE5
F	-8	GLY	-	expression tag	UNP Q7TTE5
F	-7	GLU	-	expression tag	UNP Q7TTE5
F	-6	ASN	-	expression tag	UNP Q7TTE5
F	-5	LEU	-	expression tag	UNP Q7TTE5
F	-4	TYR	-	expression tag	UNP Q7TTE5
F	-3	PHE	-	expression tag	UNP Q7TTE5
F	-2	GLN	-	expression tag	UNP Q7TTE5
F	-1	GLY	-	expression tag	UNP Q7TTE5
F	0	HIS	-	expression tag	UNP Q7TTE5
F	206	GLY	-	expression tag	UNP Q7TTE5
F	207	LEU	-	expression tag	UNP Q7TTE5
F	208	GLU	-	expression tag	UNP Q7TTE5
F	209	HIS	-	expression tag	UNP Q7TTE5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	210	HIS	-	expression tag	UNP Q7TTE5
F	211	HIS	-	expression tag	UNP Q7TTE5
F	212	HIS	-	expression tag	UNP Q7TTE5
F	213	HIS	-	expression tag	UNP Q7TTE5
F	214	HIS	-	expression tag	UNP Q7TTE5
G	-21	GLY	-	expression tag	UNP Q7TTE5
G	-20	SER	-	expression tag	UNP Q7TTE5
G	-19	ASP	-	expression tag	UNP Q7TTE5
G	-18	LYS	-	expression tag	UNP Q7TTE5
G	-17	ILE	-	expression tag	UNP Q7TTE5
G	-16	HIS	-	expression tag	UNP Q7TTE5
G	-15	HIS	-	expression tag	UNP Q7TTE5
G	-14	HIS	-	expression tag	UNP Q7TTE5
G	-13	HIS	-	expression tag	UNP Q7TTE5
G	-12	HIS	-	expression tag	UNP Q7TTE5
G	-11	HIS	-	expression tag	UNP Q7TTE5
G	-10	SER	-	expression tag	UNP Q7TTE5
G	-9	SER	-	expression tag	UNP Q7TTE5
G	-8	GLY	-	expression tag	UNP Q7TTE5
G	-7	GLU	-	expression tag	UNP Q7TTE5
G	-6	ASN	-	expression tag	UNP Q7TTE5
G	-5	LEU	-	expression tag	UNP Q7TTE5
G	-4	TYR	-	expression tag	UNP Q7TTE5
G	-3	PHE	-	expression tag	UNP Q7TTE5
G	-2	GLN	-	expression tag	UNP Q7TTE5
G	-1	GLY	-	expression tag	UNP Q7TTE5
G	0	HIS	-	expression tag	UNP Q7TTE5
G	206	GLY	-	expression tag	UNP Q7TTE5
G	207	LEU	-	expression tag	UNP Q7TTE5
G	208	GLU	-	expression tag	UNP Q7TTE5
G	209	HIS	-	expression tag	UNP Q7TTE5
G	210	HIS	-	expression tag	UNP Q7TTE5
G	211	HIS	-	expression tag	UNP Q7TTE5
G	212	HIS	-	expression tag	UNP Q7TTE5
G	213	HIS	-	expression tag	UNP Q7TTE5
G	214	HIS	-	expression tag	UNP Q7TTE5
H	-21	GLY	-	expression tag	UNP Q7TTE5
H	-20	SER	-	expression tag	UNP Q7TTE5
H	-19	ASP	-	expression tag	UNP Q7TTE5
H	-18	LYS	-	expression tag	UNP Q7TTE5
H	-17	ILE	-	expression tag	UNP Q7TTE5
H	-16	HIS	-	expression tag	UNP Q7TTE5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-15	HIS	-	expression tag	UNP Q7TTE5
H	-14	HIS	-	expression tag	UNP Q7TTE5
H	-13	HIS	-	expression tag	UNP Q7TTE5
H	-12	HIS	-	expression tag	UNP Q7TTE5
H	-11	HIS	-	expression tag	UNP Q7TTE5
H	-10	SER	-	expression tag	UNP Q7TTE5
H	-9	SER	-	expression tag	UNP Q7TTE5
H	-8	GLY	-	expression tag	UNP Q7TTE5
H	-7	GLU	-	expression tag	UNP Q7TTE5
H	-6	ASN	-	expression tag	UNP Q7TTE5
H	-5	LEU	-	expression tag	UNP Q7TTE5
H	-4	TYR	-	expression tag	UNP Q7TTE5
H	-3	PHE	-	expression tag	UNP Q7TTE5
H	-2	GLN	-	expression tag	UNP Q7TTE5
H	-1	GLY	-	expression tag	UNP Q7TTE5
H	0	HIS	-	expression tag	UNP Q7TTE5
H	206	GLY	-	expression tag	UNP Q7TTE5
H	207	LEU	-	expression tag	UNP Q7TTE5
H	208	GLU	-	expression tag	UNP Q7TTE5
H	209	HIS	-	expression tag	UNP Q7TTE5
H	210	HIS	-	expression tag	UNP Q7TTE5
H	211	HIS	-	expression tag	UNP Q7TTE5
H	212	HIS	-	expression tag	UNP Q7TTE5
H	213	HIS	-	expression tag	UNP Q7TTE5
H	214	HIS	-	expression tag	UNP Q7TTE5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	37	37	37	0	0
			Total	O		
2	B	46	46	46	0	0
			Total	O		
2	C	63	63	63	0	0
			Total	O		
2	D	69	69	69	0	0
			Total	O		
2	E	82	82	82	0	0
			Total	O		
2	F	38	38	38	0	0
			Total	O		
2	G	37	37	37	0	0

Continued on next page...

Continued from previous page...

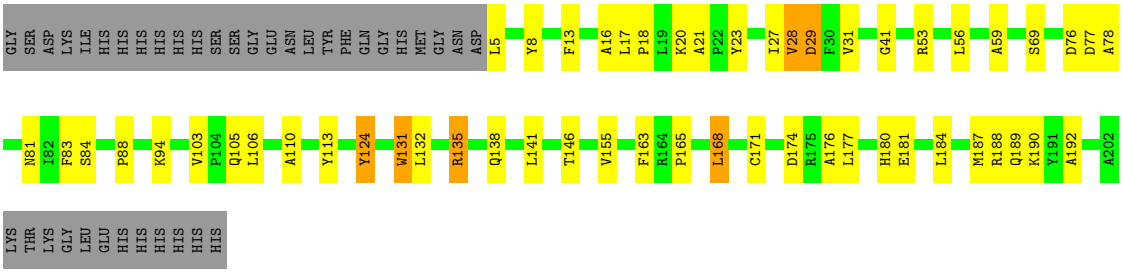
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	H	63	63	63	0	0

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.

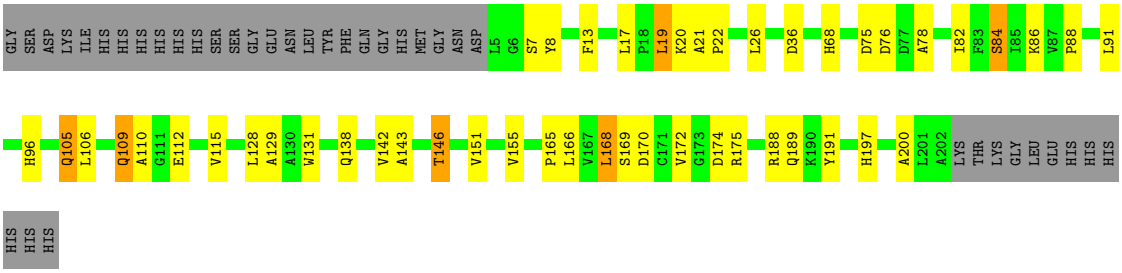
• Molecule 1: Putative isochorismatase

Chain A:



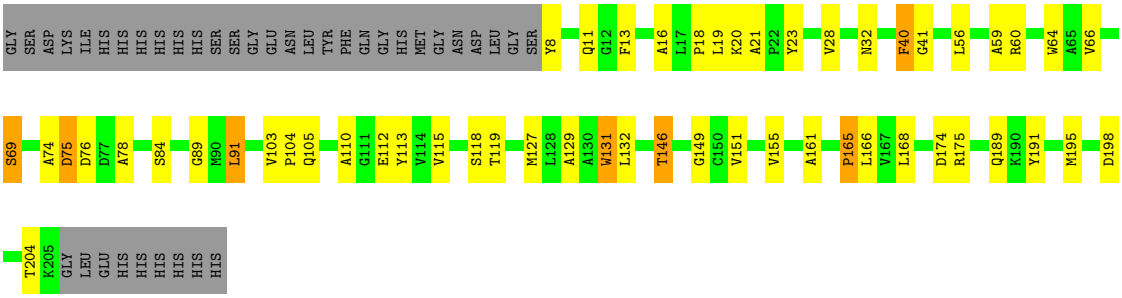
• Molecule 1: Putative isochorismatase

Chain B:



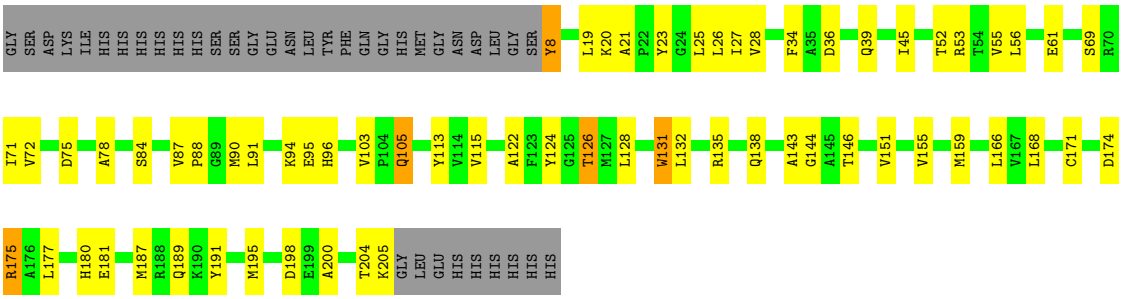
• Molecule 1: Putative isochorismatase

Chain C:



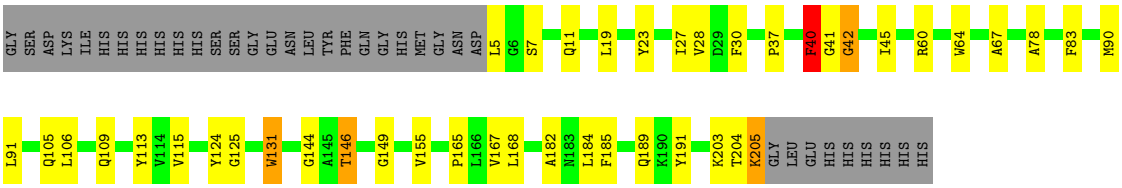
• Molecule 1: Putative isochorismatase

Chain D:



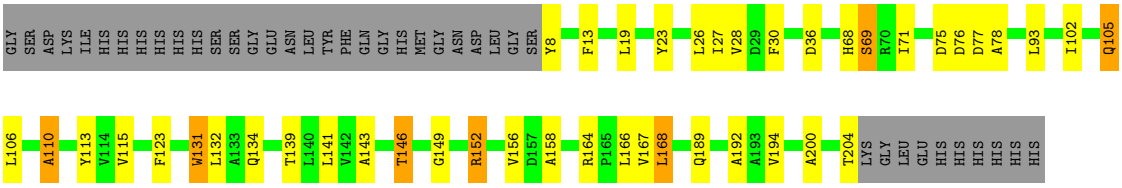
- Molecule 1: Putative isochorismatase

Chain E:



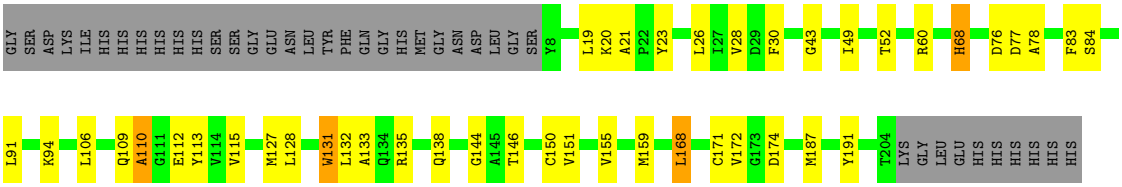
- Molecule 1: Putative isochorismatase

Chain F:



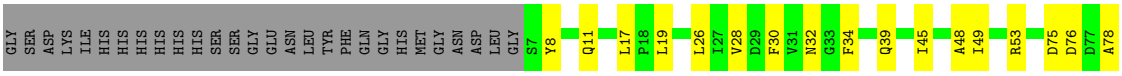
- Molecule 1: Putative isochorismatase

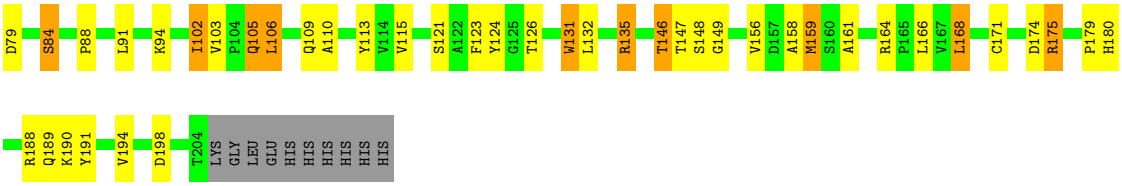
Chain G:



- Molecule 1: Putative isochorismatase

Chain H:




D79
S84
P88
L91
K94
I102
V103
P104
Q105
L106
Q109
A110
Y113
V114
V115
S121
A122
F123
Y124
G125
T126
W131
L132
R135
T146
T147
S148
G149
V156
D157
A158
M159
S160
A161
R164
P165
L166
V167
L168
C171
D174
R175
P179
H180
R188
Q189
K190
Y191
V194
D198
T204
LYS
GLY
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	157.56Å 157.56Å 198.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.01 – 2.40 12.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (12.01-2.40) 98.1 (12.01-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.241 , 0.311 0.241 , 0.308	Depositor DCC
R_{free} test set	1400 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , -1.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.105 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.095 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.095 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.094 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.096 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.105 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.380 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12175	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CSO

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	0.69	0/1486	0.80	0/2021
1	B	0.74	0/1486	0.80	0/2021
1	C	0.71	0/1492	0.78	0/2028
1	D	0.70	0/1492	0.78	0/2028
1	E	0.74	0/1510	0.81	0/2052
1	F	0.74	0/1484	0.81	0/2018
1	G	0.67	0/1484	0.76	1/2018 (0.0%)
1	H	0.73	0/1490	0.80	1/2026 (0.0%)
All	All	0.72	0/11924	0.79	2/16212 (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	B	0	1
1	C	0	1
1	E	0	2
1	G	0	1
1	H	0	1
All	All	0	6

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	H	175	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	G	60	ARG	NE-CZ-NH1	5.36	122.98	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	109	GLN	Peptide
1	C	40	PHE	Peptide
1	E	125	GLY	Peptide
1	E	40	PHE	Peptide
1	G	109	GLN	Peptide

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	1463	0	1452	56	0
1	B	1463	0	1452	34	0
1	C	1469	0	1466	44	0
1	D	1469	0	1466	63	0
1	E	1487	0	1485	42	0
1	F	1461	0	1453	36	0
1	G	1461	0	1453	37	0
1	H	1467	0	1458	58	0
2	A	37	0	0	1	0
2	B	46	0	0	4	0
2	C	63	0	0	3	0
2	D	69	0	0	6	0
2	E	82	0	0	2	0
2	F	38	0	0	3	0
2	G	37	0	0	0	0
2	H	63	0	0	1	0
All	All	12175	0	11685	327	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 14.

The worst 5 of 327 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:D:159:MET:CE	1:G:83:PHE:HA	1.84	1.06
1:D:159:MET:HE2	1:G:83:PHE:HA	1.42	0.98
1:A:83:PHE:HA	1:H:159:MET:HE2	1.46	0.97
1:F:105:GLN:H	1:F:105:GLN:HE21	1.12	0.96
1:C:84:SER:HB2	1:C:91:LEU:HD12	1.49	0.93

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	195/236 (83%)	179 (92%)	14 (7%)	2 (1%)	15	23
1	B	195/236 (83%)	183 (94%)	10 (5%)	2 (1%)	15	23
1	C	195/236 (83%)	185 (95%)	9 (5%)	1 (0%)	29	41
1	D	195/236 (83%)	185 (95%)	9 (5%)	1 (0%)	29	41
1	E	198/236 (84%)	192 (97%)	5 (2%)	1 (0%)	29	41
1	F	194/236 (82%)	184 (95%)	9 (5%)	1 (0%)	29	41
1	G	194/236 (82%)	181 (93%)	12 (6%)	1 (0%)	29	41
1	H	195/236 (83%)	191 (98%)	4 (2%)	0	100	100
All	All	1561/1888 (83%)	1480 (95%)	72 (5%)	9 (1%)	25	36

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	D	175	ARG
1	F	110	ALA
1	C	75	ASP
1	B	7	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	143/176 (81%)	139 (97%)	4 (3%)	43	63
1	B	143/176 (81%)	133 (93%)	10 (7%)	15	24
1	C	144/176 (82%)	134 (93%)	10 (7%)	15	25
1	D	144/176 (82%)	136 (94%)	8 (6%)	21	34
1	E	146/176 (83%)	138 (94%)	8 (6%)	21	35
1	F	143/176 (81%)	135 (94%)	8 (6%)	21	34
1	G	143/176 (81%)	137 (96%)	6 (4%)	30	47
1	H	144/176 (82%)	130 (90%)	14 (10%)	8	12
All	All	1150/1408 (82%)	1082 (94%)	68 (6%)	19	32

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	102	ILE
1	H	106	LEU
1	H	168	LEU
1	D	8	TYR
1	C	198	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	11	GLN
1	H	189	GLN
1	E	138	GLN
1	H	105	GLN
1	E	109	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)

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	B	150	1	3,6,7	0.55	0	0,6,8	-	-
1	CSO	F	150	1	3,6,7	0.76	0	0,6,8	-	-
1	CSO	H	150	1	3,6,7	0.62	0	0,6,8	-	-
1	CSO	G	150	1	3,6,7	0.94	0	0,6,8	-	-
1	CSO	E	150	1	3,6,7	0.68	0	0,6,8	-	-
1	CSO	D	150	1	3,6,7	0.69	0	0,6,8	-	-
1	CSO	C	150	1	3,6,7	0.85	0	0,6,8	-	-
1	CSO	A	150	1	3,6,7	0.57	0	0,6,8	-	-

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
1	CSO	B	150	1	-	0/1/5/7	-
1	CSO	F	150	1	-	1/1/5/7	-
1	CSO	H	150	1	-	0/1/5/7	-
1	CSO	G	150	1	-	0/1/5/7	-
1	CSO	E	150	1	-	0/1/5/7	-
1	CSO	D	150	1	-	0/1/5/7	-
1	CSO	C	150	1	-	0/1/5/7	-
1	CSO	A	150	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	150	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	150	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.