



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2023 – 01:27 AM EDT

PDB ID : 3UAO  
Title : Structure and Catalytic Mechanism of the Vitamin B3 Degradative Enzyme  
Maleamate Amidohydrolase from Bordetella bronchiseptica RB50  
Authors : Kincaid, V.A.; Sullivan, E.D.; Klein, R.D.; Rowlett, R.S.; Snider, M.J.  
Deposited on : 2011-10-21  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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

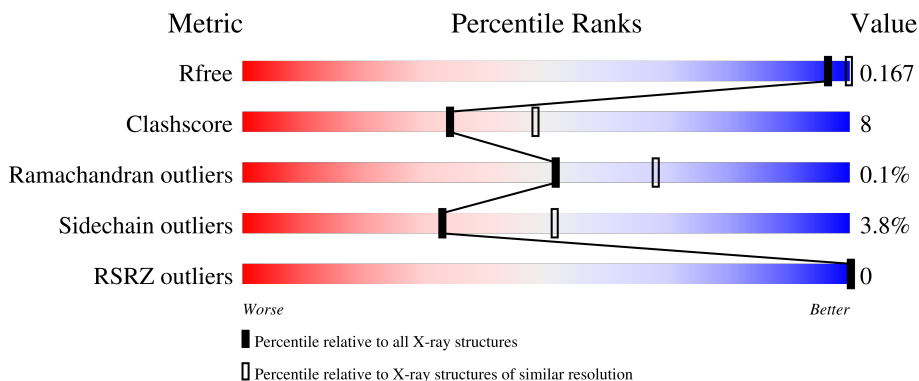
# 1 Overall quality at a glance i

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)
RSRZ outliers	127900	3811 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	236	71% 13% • 15%
1	B	236	76% 8% • 15%
1	C	236	74% 10% • 15%
1	D	236	74% 10% 15%
1	E	236	71% 13% • 15%

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Mol	Chain	Length	Quality of chain
1	F	236	 73% 9% 16%
1	G	236	 67% 16% 16%
1	H	236	 75% 8% 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
1	CSO	A	150	-	-	X	-
1	CSO	B	150	-	-	X	-
1	CSO	C	150	-	-	X	-
1	CSO	D	150	-	-	X	-
1	CSO	E	150	-	-	X	-
1	CSO	F	150	-	-	X	-
1	CSO	G	150	-	-	X	-
1	CSO	H	150	-	-	X	-
2	ACT	A	215	-	-	X	-
2	ACT	B	215	-	-	X	-
2	ACT	C	215	-	-	X	-
2	ACT	D	215	-	-	X	-
2	ACT	E	215	-	-	X	-
2	ACT	F	215	-	-	X	-
2	ACT	G	215	-	-	X	-
2	ACT	H	215	-	-	X	-

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 12462 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	200	1480	937	260	276	7	0	0	0
1	B	200	1479	937	260	275	7	0	0	0
1	C	201	1487	943	262	275	7	0	0	0
1	D	200	1479	937	261	274	7	0	0	0
1	E	201	1487	943	262	275	7	0	0	0
1	F	199	1476	935	260	274	7	0	0	0
1	G	198	1467	929	258	273	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

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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

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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

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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

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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

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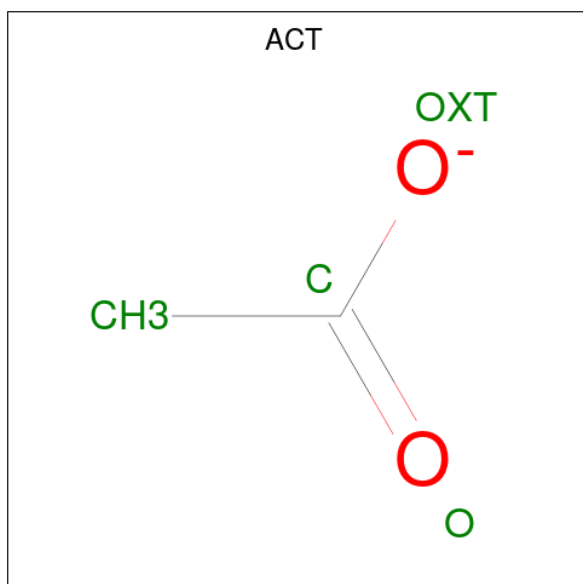
Chain	Residue	Modelled	Actual	Comment	Reference
F	210	HIS	-	expression tag	UNP Q7TTE5
F	211	HIS	-	expression tag	UNP Q7TTE5
F	212	HIS	-	expression tag	UNP Q7TTE5
F	213	HIS	-	expression tag	UNP Q7TTE5
F	214	HIS	-	expression tag	UNP Q7TTE5
G	-21	GLY	-	expression tag	UNP Q7TTE5
G	-20	SER	-	expression tag	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

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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 ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	51	Total O 51 51	0	0
3	B	72	Total O 72 72	0	0
3	C	74	Total O 74 74	0	0
3	D	84	Total O 84 84	0	0

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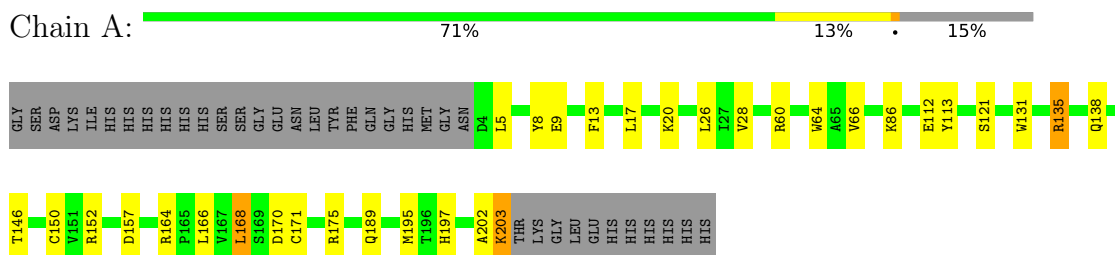
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	E	104	Total 104	O 104	0	0
3	F	61	Total 61	O 61	0	0
3	G	47	Total 47	O 47	0	0
3	H	83	Total 83	O 83	0	0

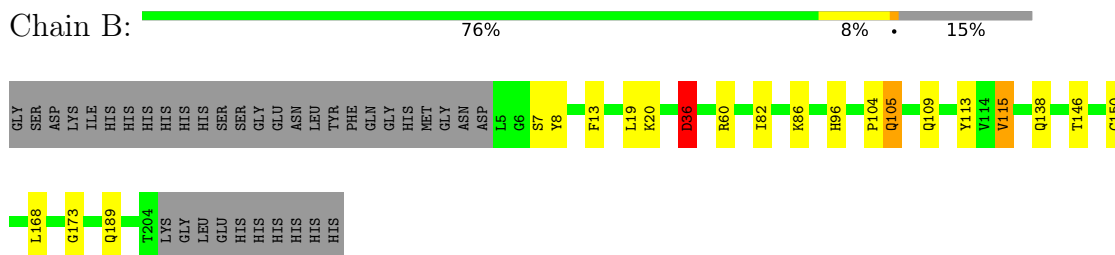
### 3 Residue-property plots [i](#)

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 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.

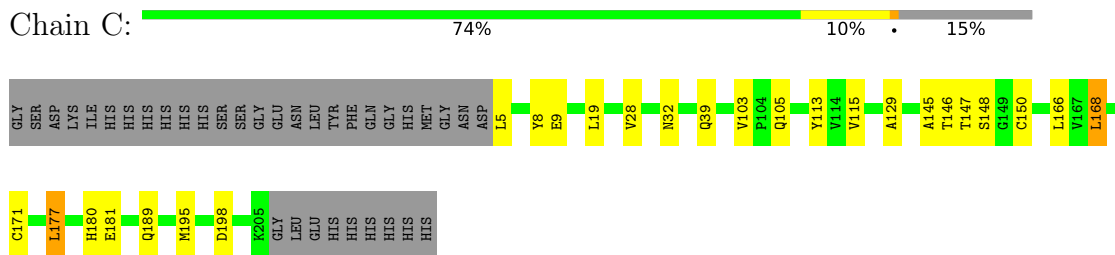
- Molecule 1: Putative isochorismatase



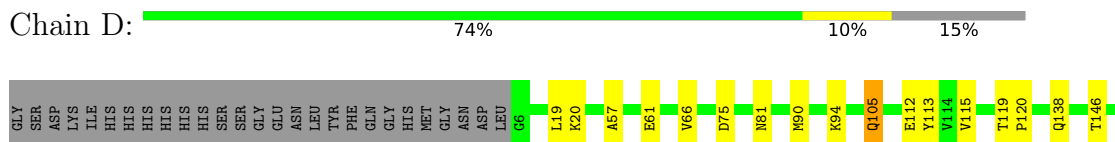
- Molecule 1: Putative isochorismatase



- Molecule 1: Putative isochorismatase



- Molecule 1: Putative isochorismatase

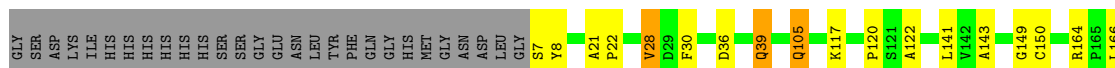




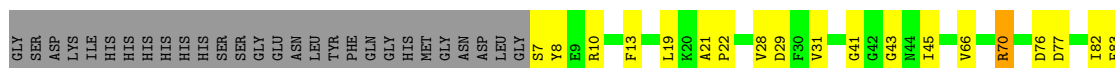
- Molecule 1: Putative isochorismatase



- Molecule 1: Putative isochorismatase



- Molecule 1: Putative isochorismatase



- Molecule 1: Putative isochorismatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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)	97.9 (12.01-2.40) 98.1 (12.01-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.127 , 0.173 0.125 , 0.167	Depositor DCC
$R_{free}$ test set	1400 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 4.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	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
Reported twinning fraction	0.611 for H, K, L 0.389 for -H-K, K, -L	Depositor
Outliers	0 of 69904 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12462	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

Xtrriage'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.*



## 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, ACT

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	0.77	1/1503 (0.1%)	0.82	3/2043 (0.1%)
1	B	0.85	1/1502 (0.1%)	0.85	1/2042 (0.0%)
1	C	0.84	1/1510 (0.1%)	0.80	0/2052
1	D	0.81	0/1502	0.80	0/2041
1	E	0.82	0/1510	0.86	1/2052 (0.0%)
1	F	0.87	0/1499	0.85	0/2037
1	G	0.77	0/1490	0.79	0/2026
1	H	0.83	0/1490	0.79	0/2026
All	All	0.82	3/12006 (0.0%)	0.82	5/16319 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	ASP	CB-CG	6.42	1.65	1.51
1	A	9	GLU	CG-CD	5.56	1.60	1.51
1	C	9	GLU	CG-CD	5.40	1.60	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	135	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	36	ASP	CB-CG-OD1	5.18	122.96	118.30
1	E	168	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	60	ARG	NE-CZ-NH2	-5.05	117.77	120.30

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	1480	0	1469	36	0
1	B	1479	0	1472	24	0
1	C	1487	0	1485	21	0
1	D	1479	0	1474	30	0
1	E	1487	0	1485	30	0
1	F	1476	0	1471	25	0
1	G	1467	0	1458	29	0
1	H	1467	0	1458	21	0
2	A	8	0	6	11	0
2	B	8	0	6	8	0
2	C	8	0	6	6	0
2	D	8	0	6	9	0
2	E	8	0	6	9	0
2	F	8	0	6	8	0
2	G	8	0	6	8	0
2	H	8	0	6	6	0
3	A	51	0	0	1	0
3	B	72	0	0	3	0
3	C	74	0	0	2	0
3	D	84	0	0	0	0
3	E	104	0	0	1	0
3	F	61	0	0	0	0
3	G	47	0	0	0	0
3	H	83	0	0	1	0
All	All	12462	0	11820	200	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 8.

The worst 5 of 200 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:F:150:CSO:OD	2:F:215:ACT:CH3	1.75	1.32
1:D:150:CSO:OD	2:D:215:ACT:H2	1.29	1.28
1:A:150:CSO:OD	2:A:215:ACT:H3	1.15	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:CSO:OD	2:A:215:ACT:CH3	1.80	1.27
1:D:150:CSO:OD	2:D:215:ACT:CH3	1.86	1.23

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	197/236 (84%)	191 (97%)	6 (3%)	0	100	100
1	B	197/236 (84%)	191 (97%)	6 (3%)	0	100	100
1	C	198/236 (84%)	194 (98%)	4 (2%)	0	100	100
1	D	197/236 (84%)	191 (97%)	6 (3%)	0	100	100
1	E	198/236 (84%)	194 (98%)	4 (2%)	0	100	100
1	F	196/236 (83%)	191 (97%)	5 (3%)	0	100	100
1	G	195/236 (83%)	187 (96%)	7 (4%)	1 (0%)	29	41
1	H	195/236 (83%)	191 (98%)	4 (2%)	0	100	100
All	All	1573/1888 (83%)	1530 (97%)	42 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	43	GLY

### 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	145/176 (82%)	142 (98%)	3 (2%)	53	72
1	B	145/176 (82%)	139 (96%)	6 (4%)	30	48
1	C	146/176 (83%)	140 (96%)	6 (4%)	30	48
1	D	145/176 (82%)	141 (97%)	4 (3%)	43	63
1	E	146/176 (83%)	141 (97%)	5 (3%)	37	56
1	F	145/176 (82%)	138 (95%)	7 (5%)	25	41
1	G	144/176 (82%)	136 (94%)	8 (6%)	21	34
1	H	144/176 (82%)	139 (96%)	5 (4%)	36	55
All	All	1160/1408 (82%)	1116 (96%)	44 (4%)	33	51

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	105	GLN
1	G	109	GLN
1	F	168	LEU
1	G	28	VAL
1	G	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	138	GLN
1	H	32	ASN
1	H	197	HIS
1	C	189	GLN
1	C	180	HIS

### 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	E	150	1	3,6,7	0.66	0	0,6,8	-	-
1	CSO	C	150	1	3,6,7	0.51	0	0,6,8	-	-
1	CSO	A	150	1	3,6,7	0.50	0	0,6,8	-	-
1	CSO	F	150	1	3,6,7	1.14	0	0,6,8	-	-
1	CSO	G	150	1	3,6,7	0.42	0	0,6,8	-	-
1	CSO	B	150	1	3,6,7	0.75	0	0,6,8	-	-
1	CSO	D	150	1	3,6,7	0.70	0	0,6,8	-	-
1	CSO	H	150	1	3,6,7	0.58	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	E	150	1	-	0/1/5/7	-
1	CSO	C	150	1	-	0/1/5/7	-
1	CSO	A	150	1	-	0/1/5/7	-
1	CSO	F	150	1	-	0/1/5/7	-
1	CSO	G	150	1	-	0/1/5/7	-
1	CSO	B	150	1	-	0/1/5/7	-
1	CSO	D	150	1	-	0/1/5/7	-
1	CSO	H	150	1	-	0/1/5/7	-

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.

8 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	150	CSO	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	150	CSO	6	0
1	A	150	CSO	7	0
1	F	150	CSO	8	0
1	G	150	CSO	4	0
1	B	150	CSO	4	0
1	D	150	CSO	6	0
1	H	150	CSO	4	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands 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	$\# Z  > 2$
2	ACT	E	216	-	3,3,3	1.30	0	3,3,3	1.15	0
2	ACT	A	216	-	3,3,3	1.12	0	3,3,3	1.53	0
2	ACT	C	216	-	3,3,3	1.08	0	3,3,3	0.98	0
2	ACT	E	215	-	3,3,3	0.84	0	3,3,3	1.63	1 (33%)
2	ACT	G	215	-	3,3,3	0.99	0	3,3,3	1.62	1 (33%)
2	ACT	F	216	-	3,3,3	1.83	1 (33%)	3,3,3	0.60	0
2	ACT	B	216	-	3,3,3	1.17	0	3,3,3	1.14	0
2	ACT	G	216	-	3,3,3	1.25	0	3,3,3	0.67	0
2	ACT	D	216	-	3,3,3	1.53	1 (33%)	3,3,3	1.09	0
2	ACT	H	216	-	3,3,3	1.09	0	3,3,3	1.36	0
2	ACT	C	215	-	3,3,3	0.72	0	3,3,3	1.51	1 (33%)
2	ACT	B	215	-	3,3,3	0.85	0	3,3,3	2.05	1 (33%)
2	ACT	D	215	-	3,3,3	0.73	0	3,3,3	2.08	2 (66%)
2	ACT	F	215	-	3,3,3	0.61	0	3,3,3	1.66	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ACT	H	215	-	3,3,3	0.88	0	3,3,3	2.16	2 (66%)
2	ACT	A	215	-	3,3,3	0.79	0	3,3,3	1.57	1 (33%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	216	ACT	O-C	2.96	1.35	1.22
2	D	216	ACT	O-C	2.12	1.32	1.22

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	215	ACT	OXT-C-O	-3.04	110.86	122.05
2	B	215	ACT	OXT-C-O	-2.89	111.39	122.05
2	D	215	ACT	OXT-C-CH3	2.59	125.87	115.18
2	D	215	ACT	OXT-C-O	-2.49	112.87	122.05
2	G	215	ACT	OXT-C-O	-2.29	113.61	122.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	215	ACT	9	0
2	G	215	ACT	8	0
2	C	215	ACT	6	0
2	B	215	ACT	8	0
2	D	215	ACT	9	0
2	F	215	ACT	8	0
2	H	215	ACT	6	0
2	A	215	ACT	11	0

## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	199/236 (84%)	-0.85	0 100 100	9, 20, 36, 46	0
1	B	199/236 (84%)	-0.90	0 100 100	9, 16, 32, 42	0
1	C	200/236 (84%)	-0.91	0 100 100	9, 17, 32, 40	0
1	D	199/236 (84%)	-0.94	0 100 100	9, 14, 31, 59	0
1	E	200/236 (84%)	-0.96	0 100 100	8, 13, 29, 56	0
1	F	198/236 (83%)	-0.98	0 100 100	9, 14, 27, 44	0
1	G	197/236 (83%)	-0.89	0 100 100	11, 21, 36, 51	0
1	H	197/236 (83%)	-0.97	0 100 100	9, 14, 27, 58	0
All	All	1589/1888 (84%)	-0.93	0 100 100	8, 16, 33, 59	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSO	A	150	7/8	0.99	0.08	11,11,13,14	0
1	CSO	B	150	7/8	0.99	0.06	9,9,13,14	0
1	CSO	C	150	7/8	0.99	0.08	10,10,11,12	0
1	CSO	D	150	7/8	0.99	0.06	9,10,10,14	0
1	CSO	E	150	7/8	0.99	0.07	8,8,9,9	0
1	CSO	F	150	7/8	0.99	0.06	9,9,10,12	0
1	CSO	G	150	7/8	0.99	0.07	12,14,17,18	0
1	CSO	H	150	7/8	0.99	0.06	8,9,11,11	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACT	C	216	4/4	0.90	0.11	22,23,24,24	0
2	ACT	D	216	4/4	0.90	0.11	16,18,19,20	0
2	ACT	B	216	4/4	0.94	0.08	20,21,21,22	0
2	ACT	E	216	4/4	0.94	0.09	15,17,17,18	0
2	ACT	F	216	4/4	0.94	0.10	14,16,16,18	0
2	ACT	H	216	4/4	0.95	0.09	24,25,25,26	0
2	ACT	G	216	4/4	0.96	0.11	18,20,20,21	0
2	ACT	A	216	4/4	0.96	0.07	15,16,17,18	0
2	ACT	D	215	4/4	0.97	0.12	18,18,19,19	0
2	ACT	H	215	4/4	0.97	0.09	8,8,8,9	0
2	ACT	E	215	4/4	0.97	0.10	15,16,17,18	0
2	ACT	G	215	4/4	0.98	0.08	19,19,20,20	0
2	ACT	A	215	4/4	0.98	0.09	8,9,9,10	0
2	ACT	F	215	4/4	0.98	0.10	8,9,10,10	0
2	ACT	C	215	4/4	0.98	0.14	12,12,13,13	0
2	ACT	B	215	4/4	0.99	0.07	6,7,8,8	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.