wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:20 AM GMT

PDB ID	:	3OOQ
Title	:	CRYSTAL STRUCTURE OF amidohydrolase from Thermotoga maritima MSB8
Authors	:	Malashkevich, V.N.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-08-31
Resolution	:	2.06 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

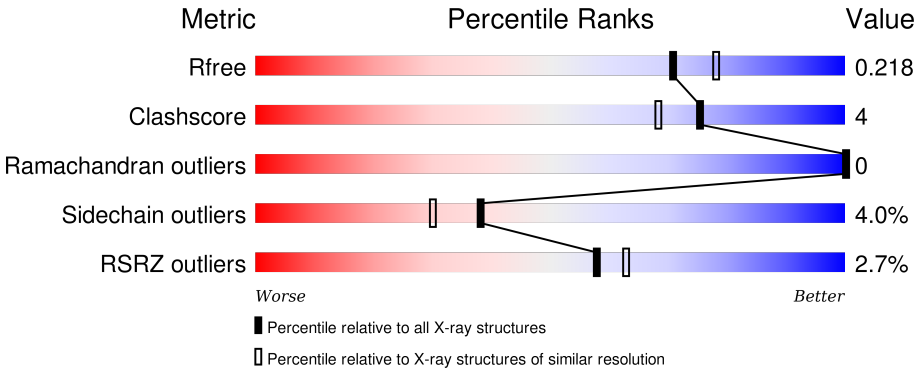
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.06 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}	91344	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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. 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	396	2% 86% 9%
1	B	396	3% 88% 8%
1	C	396	% 87% 8%
1	D	396	3% 88% 7%
1	E	396	2% 86% 10%

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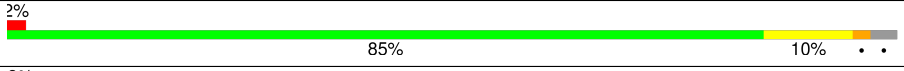
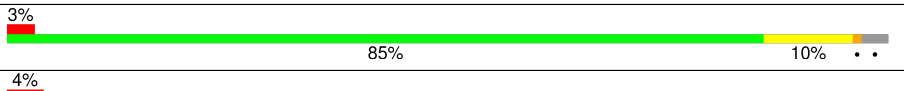
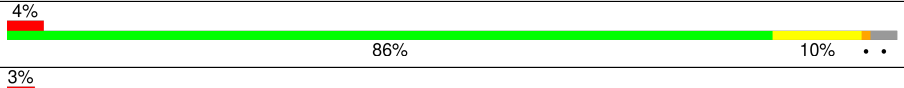
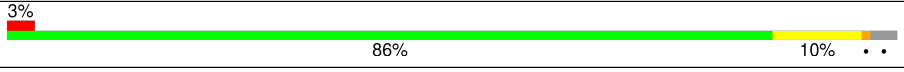
Mol	Chain	Length	Quality of chain
1	F	396	
1	G	396	
1	H	396	
1	I	396	
1	J	396	

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
2	GOL	C	500	-	-	-	X
2	GOL	E	500	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31584 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 amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	Se	0	1	0
			2985	1914	502	556	2	11			
1	B	383	Total	C	N	O	S	Se	0	0	0
			2970	1905	501	551	2	11			
1	C	384	Total	C	N	O	S	Se	0	3	0
			2996	1921	503	559	2	11			
1	D	384	Total	C	N	O	S	Se	0	0	0
			2979	1910	502	554	2	11			
1	E	383	Total	C	N	O	S	Se	0	0	0
			2970	1905	501	551	2	11			
1	F	385	Total	C	N	O	S	Se	0	0	0
			2986	1915	503	555	2	11			
1	G	383	Total	C	N	O	S	Se	0	1	0
			2974	1908	501	552	2	11			
1	H	383	Total	C	N	O	S	Se	0	1	0
			2976	1909	502	552	2	11			
1	I	383	Total	C	N	O	S	Se	0	1	0
			2976	1909	501	553	2	11			
1	J	383	Total	C	N	O	S	Se	0	0	0
			2970	1905	501	551	2	11			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q9X247
A	2	SER	-	expression tag	UNP Q9X247
A	3	LEU	-	expression tag	UNP Q9X247
A	389	GLU	-	expression tag	UNP Q9X247
A	390	GLY	-	expression tag	UNP Q9X247
A	391	HIS	-	expression tag	UNP Q9X247
A	392	HIS	-	expression tag	UNP Q9X247
A	393	HIS	-	expression tag	UNP Q9X247
A	394	HIS	-	expression tag	UNP Q9X247

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Chain	Residue	Modelled	Actual	Comment	Reference
A	395	HIS	-	expression tag	UNP Q9X247
A	396	HIS	-	expression tag	UNP Q9X247
B	1	MSE	-	expression tag	UNP Q9X247
B	2	SER	-	expression tag	UNP Q9X247
B	3	LEU	-	expression tag	UNP Q9X247
B	389	GLU	-	expression tag	UNP Q9X247
B	390	GLY	-	expression tag	UNP Q9X247
B	391	HIS	-	expression tag	UNP Q9X247
B	392	HIS	-	expression tag	UNP Q9X247
B	393	HIS	-	expression tag	UNP Q9X247
B	394	HIS	-	expression tag	UNP Q9X247
B	395	HIS	-	expression tag	UNP Q9X247
B	396	HIS	-	expression tag	UNP Q9X247
C	1	MSE	-	expression tag	UNP Q9X247
C	2	SER	-	expression tag	UNP Q9X247
C	3	LEU	-	expression tag	UNP Q9X247
C	389	GLU	-	expression tag	UNP Q9X247
C	390	GLY	-	expression tag	UNP Q9X247
C	391	HIS	-	expression tag	UNP Q9X247
C	392	HIS	-	expression tag	UNP Q9X247
C	393	HIS	-	expression tag	UNP Q9X247
C	394	HIS	-	expression tag	UNP Q9X247
C	395	HIS	-	expression tag	UNP Q9X247
C	396	HIS	-	expression tag	UNP Q9X247
D	1	MSE	-	expression tag	UNP Q9X247
D	2	SER	-	expression tag	UNP Q9X247
D	3	LEU	-	expression tag	UNP Q9X247
D	389	GLU	-	expression tag	UNP Q9X247
D	390	GLY	-	expression tag	UNP Q9X247
D	391	HIS	-	expression tag	UNP Q9X247
D	392	HIS	-	expression tag	UNP Q9X247
D	393	HIS	-	expression tag	UNP Q9X247
D	394	HIS	-	expression tag	UNP Q9X247
D	395	HIS	-	expression tag	UNP Q9X247
D	396	HIS	-	expression tag	UNP Q9X247
E	1	MSE	-	expression tag	UNP Q9X247
E	2	SER	-	expression tag	UNP Q9X247
E	3	LEU	-	expression tag	UNP Q9X247
E	389	GLU	-	expression tag	UNP Q9X247
E	390	GLY	-	expression tag	UNP Q9X247
E	391	HIS	-	expression tag	UNP Q9X247
E	392	HIS	-	expression tag	UNP Q9X247

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Chain	Residue	Modelled	Actual	Comment	Reference
E	393	HIS	-	expression tag	UNP Q9X247
E	394	HIS	-	expression tag	UNP Q9X247
E	395	HIS	-	expression tag	UNP Q9X247
E	396	HIS	-	expression tag	UNP Q9X247
F	1	MSE	-	expression tag	UNP Q9X247
F	2	SER	-	expression tag	UNP Q9X247
F	3	LEU	-	expression tag	UNP Q9X247
F	389	GLU	-	expression tag	UNP Q9X247
F	390	GLY	-	expression tag	UNP Q9X247
F	391	HIS	-	expression tag	UNP Q9X247
F	392	HIS	-	expression tag	UNP Q9X247
F	393	HIS	-	expression tag	UNP Q9X247
F	394	HIS	-	expression tag	UNP Q9X247
F	395	HIS	-	expression tag	UNP Q9X247
F	396	HIS	-	expression tag	UNP Q9X247
G	1	MSE	-	expression tag	UNP Q9X247
G	2	SER	-	expression tag	UNP Q9X247
G	3	LEU	-	expression tag	UNP Q9X247
G	389	GLU	-	expression tag	UNP Q9X247
G	390	GLY	-	expression tag	UNP Q9X247
G	391	HIS	-	expression tag	UNP Q9X247
G	392	HIS	-	expression tag	UNP Q9X247
G	393	HIS	-	expression tag	UNP Q9X247
G	394	HIS	-	expression tag	UNP Q9X247
G	395	HIS	-	expression tag	UNP Q9X247
G	396	HIS	-	expression tag	UNP Q9X247
H	1	MSE	-	expression tag	UNP Q9X247
H	2	SER	-	expression tag	UNP Q9X247
H	3	LEU	-	expression tag	UNP Q9X247
H	389	GLU	-	expression tag	UNP Q9X247
H	390	GLY	-	expression tag	UNP Q9X247
H	391	HIS	-	expression tag	UNP Q9X247
H	392	HIS	-	expression tag	UNP Q9X247
H	393	HIS	-	expression tag	UNP Q9X247
H	394	HIS	-	expression tag	UNP Q9X247
H	395	HIS	-	expression tag	UNP Q9X247
H	396	HIS	-	expression tag	UNP Q9X247
I	1	MSE	-	expression tag	UNP Q9X247
I	2	SER	-	expression tag	UNP Q9X247
I	3	LEU	-	expression tag	UNP Q9X247
I	389	GLU	-	expression tag	UNP Q9X247
I	390	GLY	-	expression tag	UNP Q9X247

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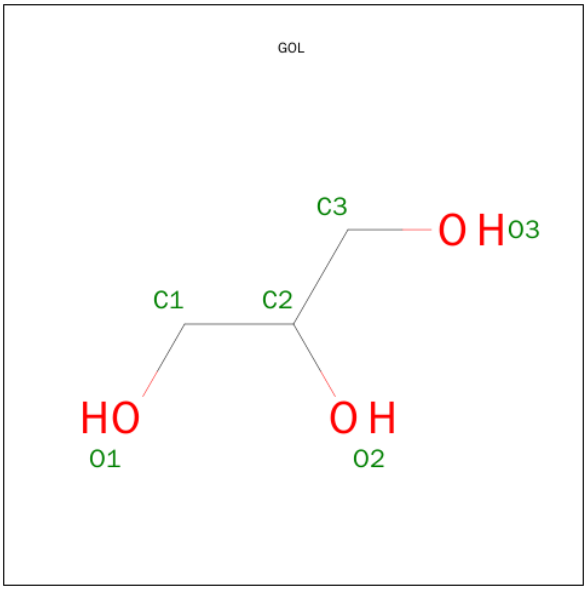
Chain	Residue	Modelled	Actual	Comment	Reference
I	391	HIS	-	expression tag	UNP Q9X247
I	392	HIS	-	expression tag	UNP Q9X247
I	393	HIS	-	expression tag	UNP Q9X247
I	394	HIS	-	expression tag	UNP Q9X247
I	395	HIS	-	expression tag	UNP Q9X247
I	396	HIS	-	expression tag	UNP Q9X247
J	1	MSE	-	expression tag	UNP Q9X247
J	2	SER	-	expression tag	UNP Q9X247
J	3	LEU	-	expression tag	UNP Q9X247
J	389	GLU	-	expression tag	UNP Q9X247
J	390	GLY	-	expression tag	UNP Q9X247
J	391	HIS	-	expression tag	UNP Q9X247
J	392	HIS	-	expression tag	UNP Q9X247
J	393	HIS	-	expression tag	UNP Q9X247
J	394	HIS	-	expression tag	UNP Q9X247
J	395	HIS	-	expression tag	UNP Q9X247
J	396	HIS	-	expression tag	UNP Q9X247

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

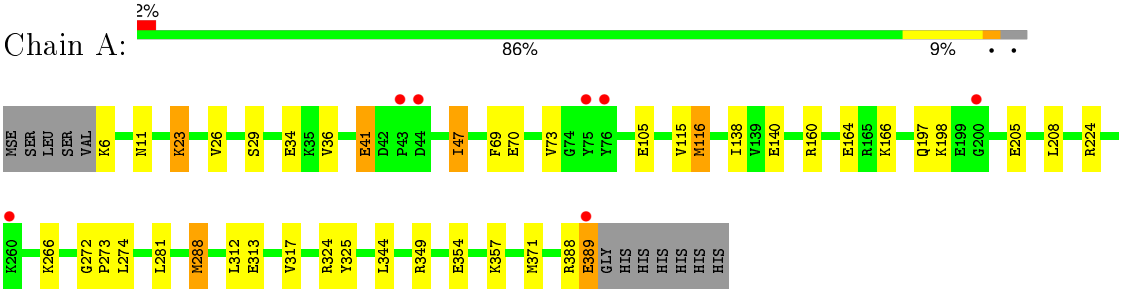
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	229	Total O 229 229	0	0
3	B	179	Total O 179 179	0	0
3	C	213	Total O 213 213	0	0
3	D	188	Total O 188 188	0	0
3	E	167	Total O 167 167	0	0
3	F	199	Total O 199 199	0	0
3	G	170	Total O 170 170	0	0
3	H	149	Total O 149 149	0	0
3	I	136	Total O 136 136	0	0
3	J	142	Total O 142 142	0	0

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.

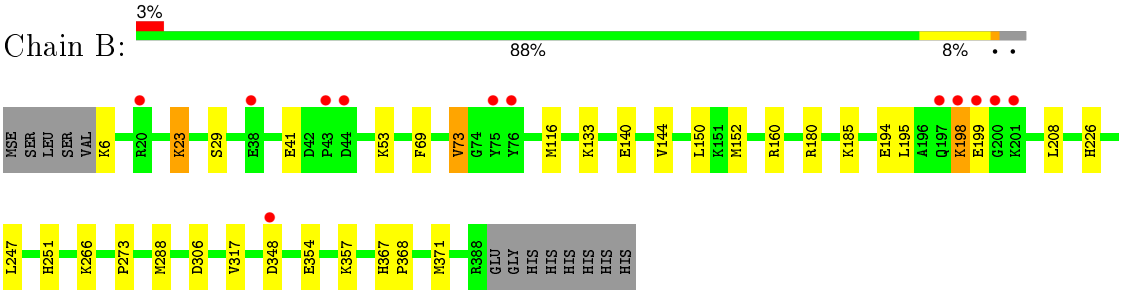
- Molecule 1: amidohydrolase

Chain A:



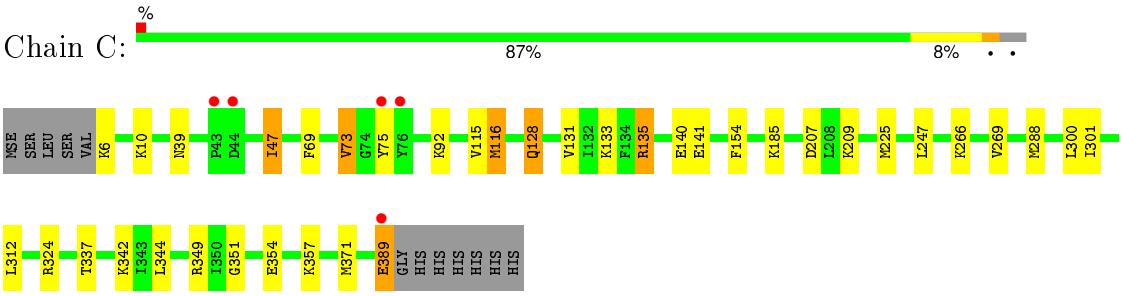
- Molecule 1: amidohydrolase

Chain B:



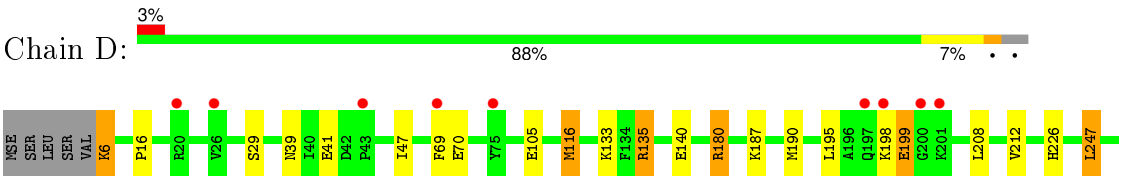
- Molecule 1: amidohydrolase

Chain C:



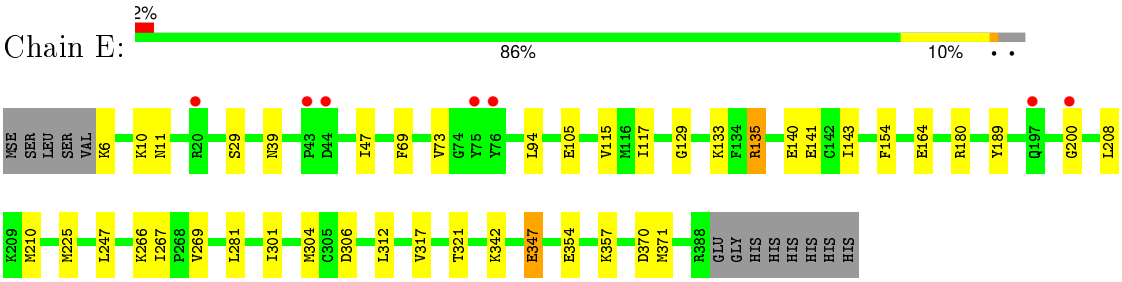
- Molecule 1: amidohydrolase

Chain D:



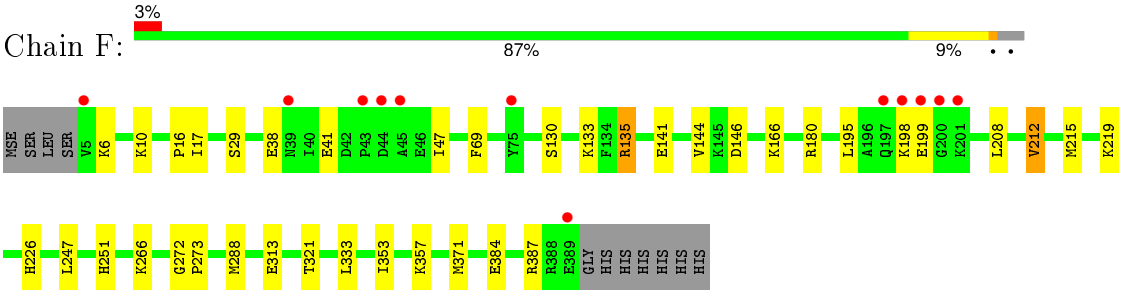
• Molecule 1: amidohydrolase

Chain E:



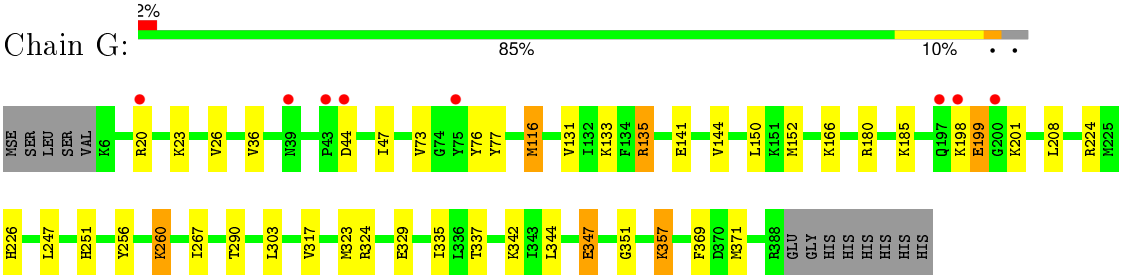
• Molecule 1: amidohydrolase

Chain F:



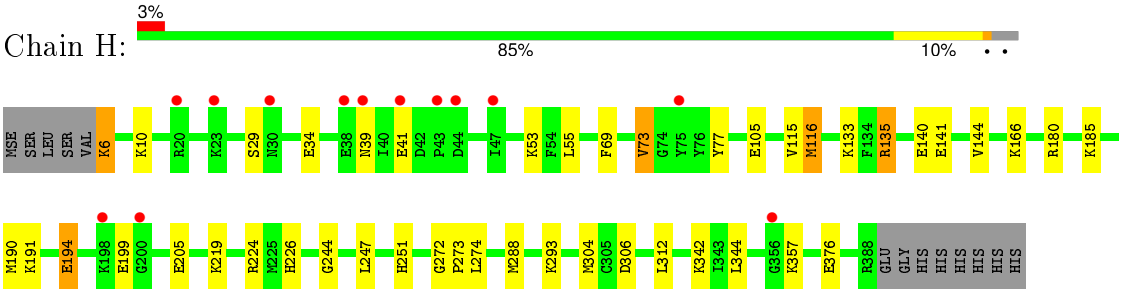
• Molecule 1: amidohydrolase

Chain G:



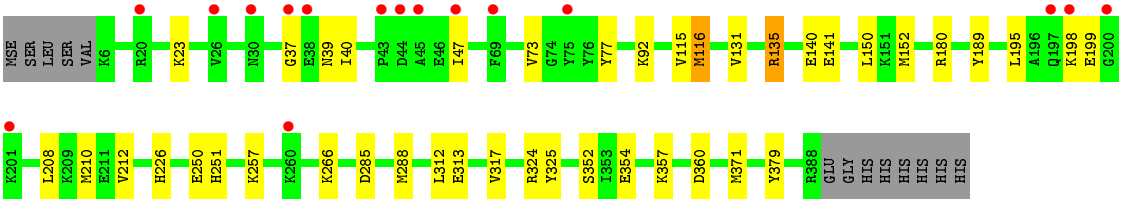
• Molecule 1: amidohydrolase

Chain H:

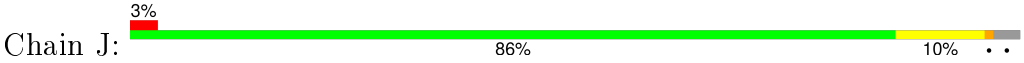


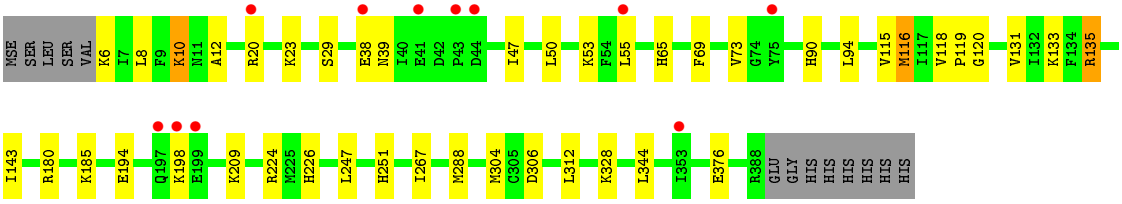
• Molecule 1: amidohydrolase

Chain I:



- Molecule 1: amidohydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.45Å 148.30Å 195.02Å 90.00° 105.31° 90.00°	Depositor
Resolution (Å)	19.92 – 2.06 19.92 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.92-2.06) 98.4 (19.92-2.06)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.167 , 0.213 0.173 , 0.218	Depositor DCC
R_{free} test set	12737 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 252990 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	31584	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.57	0/3034	0.68	0/4078
1	B	0.53	0/3016	0.64	0/4054
1	C	0.58	0/3051	0.67	1/4101 (0.0%)
1	D	0.56	0/3025	0.63	0/4066
1	E	0.56	0/3016	0.65	0/4054
1	F	0.57	0/3032	0.64	0/4076
1	G	0.54	0/3023	0.65	0/4064
1	H	0.53	0/3025	0.65	0/4066
1	I	0.53	0/3025	0.62	0/4066
1	J	0.52	0/3016	0.61	0/4054
All	All	0.55	0/30263	0.65	1/40679 (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	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	207	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	200	GLY	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	2985	0	3061	30	0
1	B	2970	0	3049	22	0
1	C	2996	0	3073	26	0
1	D	2979	0	3055	22	0
1	E	2970	0	3049	24	0
1	F	2986	0	3064	20	0
1	G	2974	0	3056	39	0
1	H	2976	0	3057	24	0
1	I	2976	0	3055	26	0
1	J	2970	0	3049	25	0
2	A	6	0	8	0	0
2	C	6	0	8	2	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
2	H	6	0	8	0	0
3	A	229	0	0	6	0
3	B	179	0	0	5	0
3	C	213	0	0	6	0
3	D	188	0	0	3	0
3	E	167	0	0	5	0
3	F	199	0	0	3	0
3	G	170	0	0	3	0
3	H	149	0	0	1	0
3	I	136	0	0	4	0
3	J	142	0	0	2	0
All	All	31584	0	30608	238	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 4.

The worst 5 of 238 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:B:195:LEU:O	1:B:199:GLU:HG2	1.68	0.94
1:I:195:LEU:O	1:I:199:GLU:HG2	1.68	0.92
1:F:135:ARG:HD2	1:F:141:GLU:O	1.71	0.89
3:E:426:HOH:O	1:H:205:GLU:HG2	1.71	0.89
1:A:388:ARG:O	1:A:389:GLU:HB2	1.76	0.83

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	383/396 (97%)	373 (97%)	10 (3%)	0	100	100
1	B	381/396 (96%)	369 (97%)	12 (3%)	0	100	100
1	C	385/396 (97%)	372 (97%)	13 (3%)	0	100	100
1	D	382/396 (96%)	370 (97%)	12 (3%)	0	100	100
1	E	381/396 (96%)	367 (96%)	14 (4%)	0	100	100
1	F	383/396 (97%)	369 (96%)	14 (4%)	0	100	100
1	G	382/396 (96%)	372 (97%)	10 (3%)	0	100	100
1	H	382/396 (96%)	370 (97%)	12 (3%)	0	100	100
1	I	382/396 (96%)	369 (97%)	13 (3%)	0	100	100
1	J	381/396 (96%)	370 (97%)	11 (3%)	0	100	100
All	All	3822/3960 (96%)	3701 (97%)	121 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	323/321 (101%)	309 (96%)	14 (4%)	35	27
1	B	321/321 (100%)	311 (97%)	10 (3%)	47	41
1	C	325/321 (101%)	314 (97%)	11 (3%)	44	37
1	D	322/321 (100%)	306 (95%)	16 (5%)	30	20
1	E	321/321 (100%)	310 (97%)	11 (3%)	44	37
1	F	323/321 (101%)	310 (96%)	13 (4%)	38	30
1	G	322/321 (100%)	309 (96%)	13 (4%)	38	30
1	H	322/321 (100%)	305 (95%)	17 (5%)	28	18
1	I	322/321 (100%)	313 (97%)	9 (3%)	51	45
1	J	321/321 (100%)	307 (96%)	14 (4%)	35	26
All	All	3222/3210 (100%)	3094 (96%)	128 (4%)	38	30

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	105	GLU
1	F	247	LEU
1	J	39	ASN
1	E	164	GLU
1	F	47	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	30	ASN
1	G	63	HIS
1	I	226	HIS
1	E	39	ASN
1	F	226	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	GOL	A	500	-	5,5,5	0.41	0	5,5,5	0.34	0
2	GOL	C	500	-	5,5,5	0.39	0	5,5,5	0.59	0
2	GOL	E	500	-	5,5,5	0.33	0	5,5,5	0.65	0
2	GOL	F	500	-	5,5,5	0.33	0	5,5,5	0.48	0
2	GOL	H	500	-	5,5,5	0.30	0	5,5,5	0.48	0

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
2	GOL	A	500	-	-	0/4/4/4	0/0/0/0
2	GOL	C	500	-	-	0/4/4/4	0/0/0/0
2	GOL	E	500	-	-	0/4/4/4	0/0/0/0
2	GOL	F	500	-	-	0/4/4/4	0/0/0/0
2	GOL	H	500	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	373/396 (94%)	-0.42	7 (1%) 70 73	15, 21, 40, 54	0
1	B	372/396 (93%)	-0.23	12 (3%) 51 56	16, 25, 53, 73	0
1	C	373/396 (94%)	-0.41	5 (1%) 79 81	16, 23, 37, 53	0
1	D	373/396 (94%)	-0.29	10 (2%) 58 63	17, 24, 47, 68	0
1	E	372/396 (93%)	-0.37	7 (1%) 70 73	17, 26, 42, 65	0
1	F	374/396 (94%)	-0.31	12 (3%) 51 56	16, 24, 46, 67	0
1	G	372/396 (93%)	-0.25	8 (2%) 65 69	17, 26, 48, 69	0
1	H	372/396 (93%)	-0.25	13 (3%) 48 53	17, 28, 52, 71	0
1	I	372/396 (93%)	-0.13	16 (4%) 39 43	18, 29, 56, 81	0
1	J	372/396 (93%)	-0.16	11 (2%) 54 59	19, 30, 55, 78	0
All	All	3725/3960 (94%)	-0.28	101 (2%) 58 63	15, 26, 49, 81	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	200	GLY	7.6
1	D	200	GLY	6.5
1	G	75	TYR	6.3
1	H	44	ASP	5.9
1	I	43	PRO	5.9

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 (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	E	500	6/6	0.79	0.19	3.13	38,41,42,42	0
2	GOL	C	500	6/6	0.78	0.24	2.54	50,52,56,56	0
2	GOL	H	500	6/6	0.85	0.15	1.89	54,54,56,56	0
2	GOL	A	500	6/6	0.87	0.12	1.15	36,37,37,38	0
2	GOL	F	500	6/6	0.94	0.12	1.12	27,28,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.