wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 06:52 AM EDT

PDB ID	:	2POZ
Title	:	Crystal structure of a putative dehydratase from Mesorhizobium loti
Authors	:	Sugadev, R.; Eswaramoorthy, S.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-04-27
Resolution	:	2.04 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:

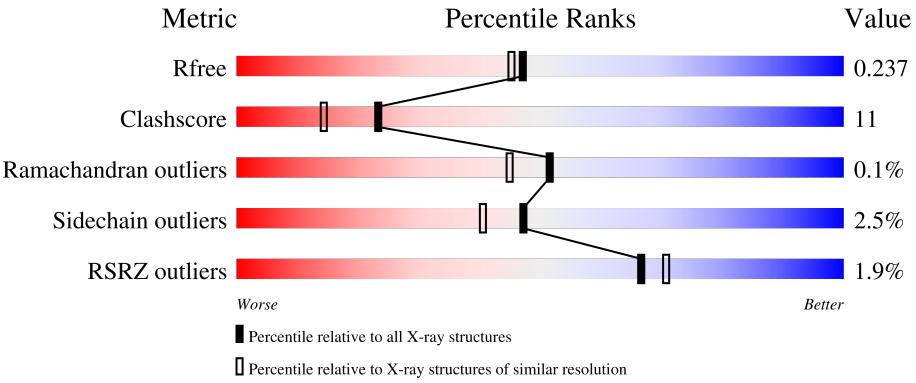
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 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	392	79% 18%
1	B	392	79% 16%
1	C	392	3% 79% 16%
1	D	392	74% 20%
1	E	392	3% 78% 19%

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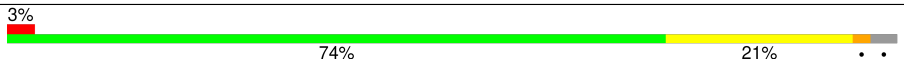
Mol	Chain	Length	Quality of chain
1	F	392	
1	G	392	
1	H	392	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24043 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 dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	Se	0	0	0
			2932	1873	497	545	8	9			
1	B	377	Total	C	N	O	S	Se	0	0	0
			2899	1854	489	539	8	9			
1	C	376	Total	C	N	O	S	Se	0	0	0
			2890	1849	487	537	8	9			
1	D	377	Total	C	N	O	S	Se	0	0	0
			2899	1854	489	539	8	9			
1	E	382	Total	C	N	O	S	Se	0	0	0
			2932	1873	497	545	8	9			
1	F	382	Total	C	N	O	S	Se	0	0	0
			2932	1873	497	545	8	9			
1	G	377	Total	C	N	O	S	Se	0	0	0
			2899	1854	489	539	8	9			
1	H	379	Total	C	N	O	S	Se	0	0	0
			2917	1865	494	541	8	9			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP Q981H6
A	2	SER	-	cloning artifact	UNP Q981H6
A	3	LEU	-	cloning artifact	UNP Q981H6
A	51	MSE	MET	modified residue	UNP Q981H6
A	75	MSE	MET	modified residue	UNP Q981H6
A	177	MSE	MET	modified residue	UNP Q981H6
A	203	MSE	MET	modified residue	UNP Q981H6
A	288	MSE	MET	modified residue	UNP Q981H6
A	296	MSE	MET	modified residue	UNP Q981H6
A	302	MSE	MET	modified residue	UNP Q981H6
A	329	MSE	MET	modified residue	UNP Q981H6
A	360	MSE	MET	modified residue	UNP Q981H6
A	385	GLU	-	cloning artifact	UNP Q981H6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	386	GLY	-	cloning artifact	UNP Q981H6
A	387	HIS	-	cloning artifact	UNP Q981H6
A	388	HIS	-	cloning artifact	UNP Q981H6
A	389	HIS	-	cloning artifact	UNP Q981H6
A	390	HIS	-	cloning artifact	UNP Q981H6
A	391	HIS	-	cloning artifact	UNP Q981H6
A	392	HIS	-	cloning artifact	UNP Q981H6
B	1	MSE	-	cloning artifact	UNP Q981H6
B	2	SER	-	cloning artifact	UNP Q981H6
B	3	LEU	-	cloning artifact	UNP Q981H6
B	51	MSE	MET	modified residue	UNP Q981H6
B	75	MSE	MET	modified residue	UNP Q981H6
B	177	MSE	MET	modified residue	UNP Q981H6
B	203	MSE	MET	modified residue	UNP Q981H6
B	288	MSE	MET	modified residue	UNP Q981H6
B	296	MSE	MET	modified residue	UNP Q981H6
B	302	MSE	MET	modified residue	UNP Q981H6
B	329	MSE	MET	modified residue	UNP Q981H6
B	360	MSE	MET	modified residue	UNP Q981H6
B	385	GLU	-	cloning artifact	UNP Q981H6
B	386	GLY	-	cloning artifact	UNP Q981H6
B	387	HIS	-	cloning artifact	UNP Q981H6
B	388	HIS	-	cloning artifact	UNP Q981H6
B	389	HIS	-	cloning artifact	UNP Q981H6
B	390	HIS	-	cloning artifact	UNP Q981H6
B	391	HIS	-	cloning artifact	UNP Q981H6
B	392	HIS	-	cloning artifact	UNP Q981H6
C	1	MSE	-	cloning artifact	UNP Q981H6
C	2	SER	-	cloning artifact	UNP Q981H6
C	3	LEU	-	cloning artifact	UNP Q981H6
C	51	MSE	MET	modified residue	UNP Q981H6
C	75	MSE	MET	modified residue	UNP Q981H6
C	177	MSE	MET	modified residue	UNP Q981H6
C	203	MSE	MET	modified residue	UNP Q981H6
C	288	MSE	MET	modified residue	UNP Q981H6
C	296	MSE	MET	modified residue	UNP Q981H6
C	302	MSE	MET	modified residue	UNP Q981H6
C	329	MSE	MET	modified residue	UNP Q981H6
C	360	MSE	MET	modified residue	UNP Q981H6
C	385	GLU	-	cloning artifact	UNP Q981H6
C	386	GLY	-	cloning artifact	UNP Q981H6
C	387	HIS	-	cloning artifact	UNP Q981H6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	388	HIS	-	cloning artifact	UNP Q981H6
C	389	HIS	-	cloning artifact	UNP Q981H6
C	390	HIS	-	cloning artifact	UNP Q981H6
C	391	HIS	-	cloning artifact	UNP Q981H6
C	392	HIS	-	cloning artifact	UNP Q981H6
D	1	MSE	-	cloning artifact	UNP Q981H6
D	2	SER	-	cloning artifact	UNP Q981H6
D	3	LEU	-	cloning artifact	UNP Q981H6
D	51	MSE	MET	modified residue	UNP Q981H6
D	75	MSE	MET	modified residue	UNP Q981H6
D	177	MSE	MET	modified residue	UNP Q981H6
D	203	MSE	MET	modified residue	UNP Q981H6
D	288	MSE	MET	modified residue	UNP Q981H6
D	296	MSE	MET	modified residue	UNP Q981H6
D	302	MSE	MET	modified residue	UNP Q981H6
D	329	MSE	MET	modified residue	UNP Q981H6
D	360	MSE	MET	modified residue	UNP Q981H6
D	385	GLU	-	cloning artifact	UNP Q981H6
D	386	GLY	-	cloning artifact	UNP Q981H6
D	387	HIS	-	cloning artifact	UNP Q981H6
D	388	HIS	-	cloning artifact	UNP Q981H6
D	389	HIS	-	cloning artifact	UNP Q981H6
D	390	HIS	-	cloning artifact	UNP Q981H6
D	391	HIS	-	cloning artifact	UNP Q981H6
D	392	HIS	-	cloning artifact	UNP Q981H6
E	1	MSE	-	cloning artifact	UNP Q981H6
E	2	SER	-	cloning artifact	UNP Q981H6
E	3	LEU	-	cloning artifact	UNP Q981H6
E	51	MSE	MET	modified residue	UNP Q981H6
E	75	MSE	MET	modified residue	UNP Q981H6
E	177	MSE	MET	modified residue	UNP Q981H6
E	203	MSE	MET	modified residue	UNP Q981H6
E	288	MSE	MET	modified residue	UNP Q981H6
E	296	MSE	MET	modified residue	UNP Q981H6
E	302	MSE	MET	modified residue	UNP Q981H6
E	329	MSE	MET	modified residue	UNP Q981H6
E	360	MSE	MET	modified residue	UNP Q981H6
E	385	GLU	-	cloning artifact	UNP Q981H6
E	386	GLY	-	cloning artifact	UNP Q981H6
E	387	HIS	-	cloning artifact	UNP Q981H6
E	388	HIS	-	cloning artifact	UNP Q981H6
E	389	HIS	-	cloning artifact	UNP Q981H6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	390	HIS	-	cloning artifact	UNP Q981H6
E	391	HIS	-	cloning artifact	UNP Q981H6
E	392	HIS	-	cloning artifact	UNP Q981H6
F	1	MSE	-	cloning artifact	UNP Q981H6
F	2	SER	-	cloning artifact	UNP Q981H6
F	3	LEU	-	cloning artifact	UNP Q981H6
F	51	MSE	MET	modified residue	UNP Q981H6
F	75	MSE	MET	modified residue	UNP Q981H6
F	177	MSE	MET	modified residue	UNP Q981H6
F	203	MSE	MET	modified residue	UNP Q981H6
F	288	MSE	MET	modified residue	UNP Q981H6
F	296	MSE	MET	modified residue	UNP Q981H6
F	302	MSE	MET	modified residue	UNP Q981H6
F	329	MSE	MET	modified residue	UNP Q981H6
F	360	MSE	MET	modified residue	UNP Q981H6
F	385	GLU	-	cloning artifact	UNP Q981H6
F	386	GLY	-	cloning artifact	UNP Q981H6
F	387	HIS	-	cloning artifact	UNP Q981H6
F	388	HIS	-	cloning artifact	UNP Q981H6
F	389	HIS	-	cloning artifact	UNP Q981H6
F	390	HIS	-	cloning artifact	UNP Q981H6
F	391	HIS	-	cloning artifact	UNP Q981H6
F	392	HIS	-	cloning artifact	UNP Q981H6
G	1	MSE	-	cloning artifact	UNP Q981H6
G	2	SER	-	cloning artifact	UNP Q981H6
G	3	LEU	-	cloning artifact	UNP Q981H6
G	51	MSE	MET	modified residue	UNP Q981H6
G	75	MSE	MET	modified residue	UNP Q981H6
G	177	MSE	MET	modified residue	UNP Q981H6
G	203	MSE	MET	modified residue	UNP Q981H6
G	288	MSE	MET	modified residue	UNP Q981H6
G	296	MSE	MET	modified residue	UNP Q981H6
G	302	MSE	MET	modified residue	UNP Q981H6
G	329	MSE	MET	modified residue	UNP Q981H6
G	360	MSE	MET	modified residue	UNP Q981H6
G	385	GLU	-	cloning artifact	UNP Q981H6
G	386	GLY	-	cloning artifact	UNP Q981H6
G	387	HIS	-	cloning artifact	UNP Q981H6
G	388	HIS	-	cloning artifact	UNP Q981H6
G	389	HIS	-	cloning artifact	UNP Q981H6
G	390	HIS	-	cloning artifact	UNP Q981H6
G	391	HIS	-	cloning artifact	UNP Q981H6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	392	HIS	-	cloning artifact	UNP Q981H6
H	1	MSE	-	cloning artifact	UNP Q981H6
H	2	SER	-	cloning artifact	UNP Q981H6
H	3	LEU	-	cloning artifact	UNP Q981H6
H	51	MSE	MET	modified residue	UNP Q981H6
H	75	MSE	MET	modified residue	UNP Q981H6
H	177	MSE	MET	modified residue	UNP Q981H6
H	203	MSE	MET	modified residue	UNP Q981H6
H	288	MSE	MET	modified residue	UNP Q981H6
H	296	MSE	MET	modified residue	UNP Q981H6
H	302	MSE	MET	modified residue	UNP Q981H6
H	329	MSE	MET	modified residue	UNP Q981H6
H	360	MSE	MET	modified residue	UNP Q981H6
H	385	GLU	-	cloning artifact	UNP Q981H6
H	386	GLY	-	cloning artifact	UNP Q981H6
H	387	HIS	-	cloning artifact	UNP Q981H6
H	388	HIS	-	cloning artifact	UNP Q981H6
H	389	HIS	-	cloning artifact	UNP Q981H6
H	390	HIS	-	cloning artifact	UNP Q981H6
H	391	HIS	-	cloning artifact	UNP Q981H6
H	392	HIS	-	cloning artifact	UNP Q981H6

- Molecule 2 is water.

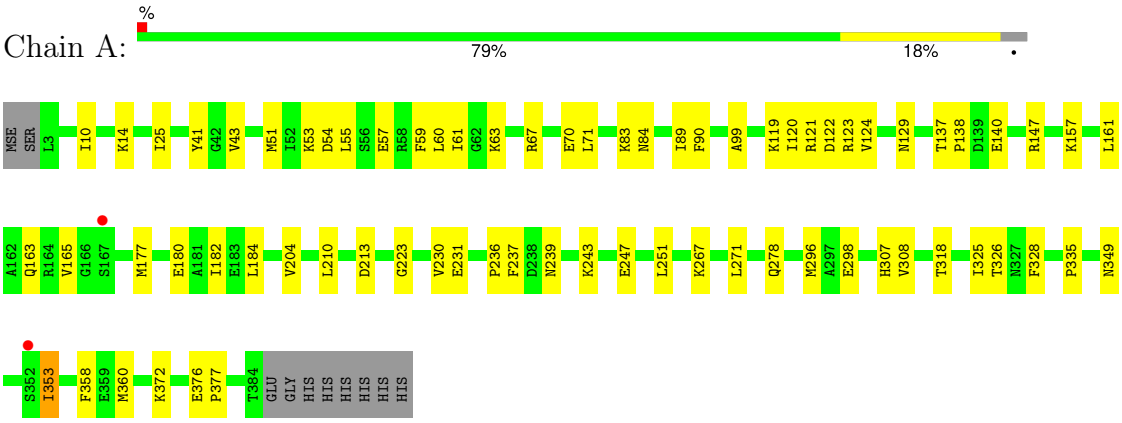
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	137	Total O 137 137	0	0
2	B	111	Total O 111 111	0	0
2	C	66	Total O 66 66	0	0
2	D	70	Total O 70 70	0	0
2	E	81	Total O 81 81	0	0
2	F	138	Total O 138 138	0	0
2	G	50	Total O 50 50	0	0
2	H	90	Total O 90 90	0	0

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.

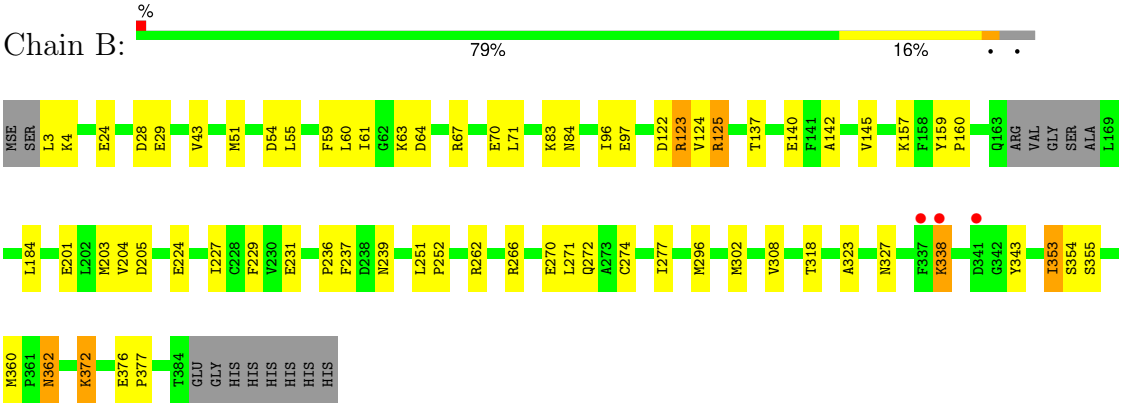
• Molecule 1: Putative dehydratase

Chain A:



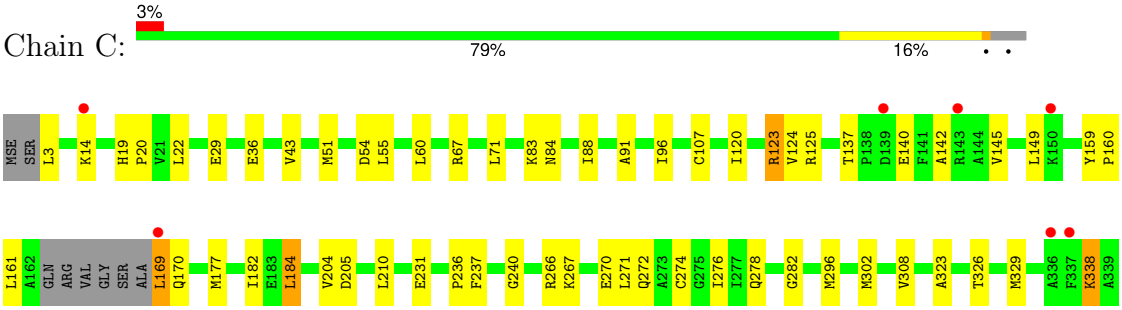
• Molecule 1: Putative dehydratase

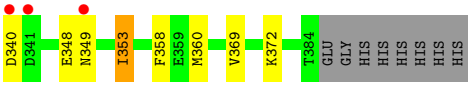
Chain B:



• Molecule 1: Putative dehydratase

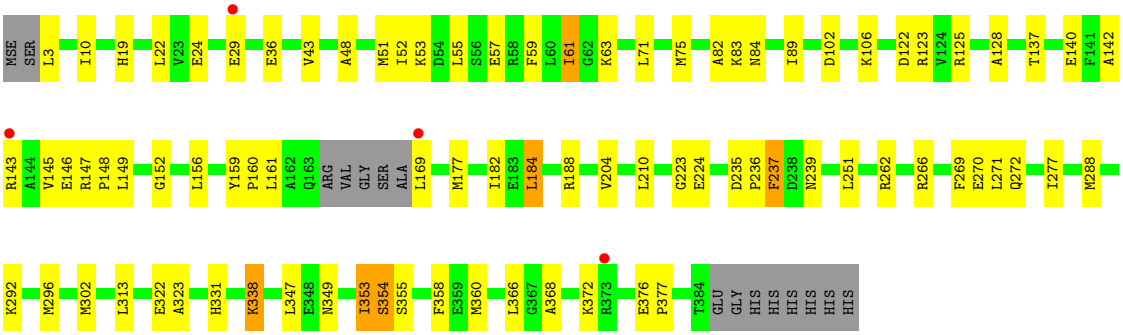
Chain C:





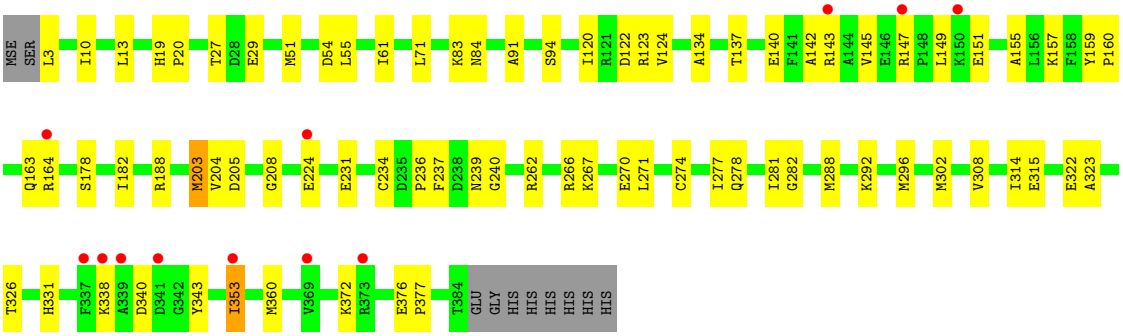
• Molecule 1: Putative dehydratase

Chain D:



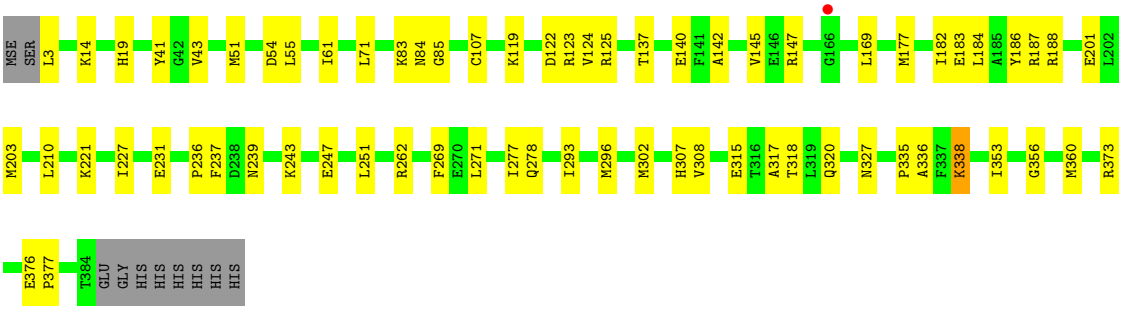
• Molecule 1: Putative dehydratase

Chain E:



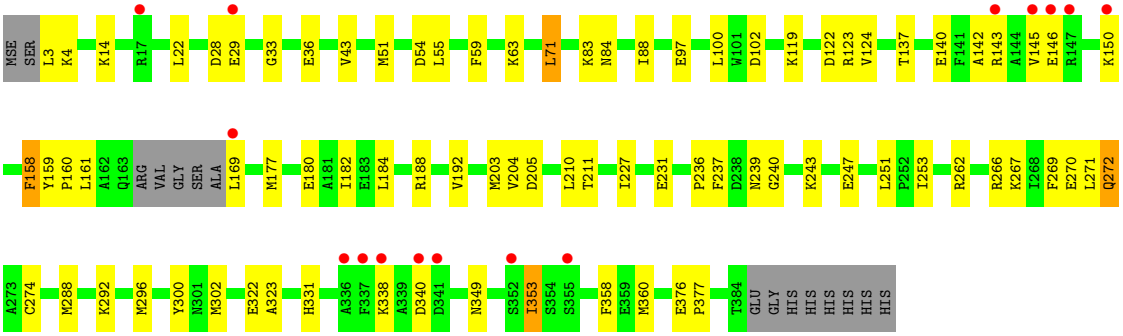
• Molecule 1: Putative dehydratase

Chain F:



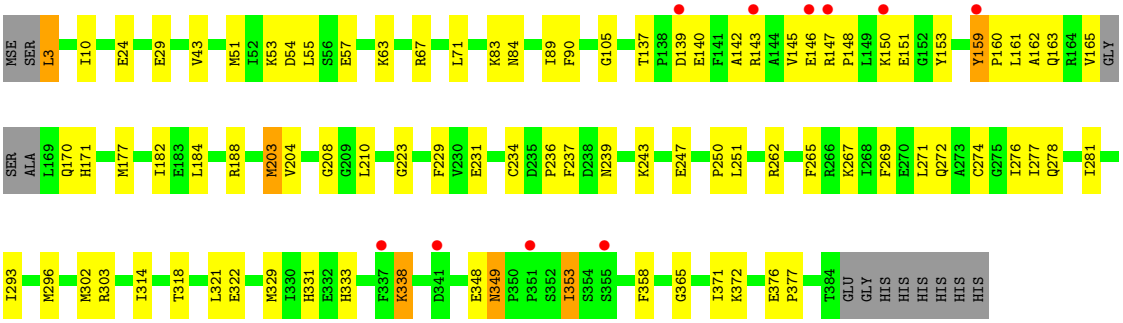
• Molecule 1: Putative dehydratase

Chain G:



- Molecule 1: Putative dehydratase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.27Å 189.82Å 192.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.94 – 2.04 46.07 – 2.04	Depositor EDS
% Data completeness (in resolution range)	91.2 (42.94-2.04) 91.4 (46.07-2.04)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.34 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.237 0.202 , 0.237	Depositor DCC
R_{free} test set	9769 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24043	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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

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	0.36	0/2987	0.62	2/4030 (0.0%)
1	B	0.33	0/2953	0.61	0/3983
1	C	0.31	0/2944	0.58	0/3971
1	D	0.30	0/2953	0.57	0/3983
1	E	0.32	0/2987	0.59	0/4030
1	F	0.35	0/2987	0.62	1/4030 (0.0%)
1	G	0.30	0/2953	0.57	0/3983
1	H	0.32	0/2971	0.59	0/4007
All	All	0.33	0/23735	0.60	3/32017 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	LYS	N-CA-C	-5.37	96.50	111.00
1	A	60	LEU	N-CA-C	5.09	124.74	111.00
1	F	14	LYS	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2932	0	2923	56	0
1	B	2899	0	2887	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2890	0	2879	67	0
1	D	2899	0	2887	89	0
1	E	2932	0	2923	72	0
1	F	2932	0	2923	54	0
1	G	2899	0	2887	82	0
1	H	2917	0	2909	84	0
2	A	137	0	0	3	0
2	B	111	0	0	0	0
2	C	66	0	0	2	0
2	D	70	0	0	0	0
2	E	81	0	0	1	0
2	F	138	0	0	3	0
2	G	50	0	0	0	0
2	H	90	0	0	2	0
All	All	24043	0	23218	526	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 11.

The worst 5 of 526 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:A:51:MSE:HE2	1:A:55:LEU:HG	1.19	1.14
1:C:51:MSE:HE2	1:C:55:LEU:HG	1.28	1.12
1:D:3:LEU:HD22	1:D:29:GLU:HG3	1.34	1.09
1:H:51:MSE:HE2	1:H:55:LEU:HG	1.29	1.08
1:G:3:LEU:HD22	1:G:29:GLU:HG3	1.28	1.08

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	380/392 (97%)	367 (97%)	13 (3%)	0	100 100
1	B	373/392 (95%)	356 (95%)	17 (5%)	0	100 100
1	C	372/392 (95%)	354 (95%)	18 (5%)	0	100 100
1	D	373/392 (95%)	351 (94%)	19 (5%)	3 (1%)	19 10
1	E	380/392 (97%)	361 (95%)	19 (5%)	0	100 100
1	F	380/392 (97%)	365 (96%)	15 (4%)	0	100 100
1	G	373/392 (95%)	352 (94%)	21 (6%)	0	100 100
1	H	375/392 (96%)	360 (96%)	15 (4%)	0	100 100
All	All	3006/3136 (96%)	2866 (95%)	137 (5%)	3 (0%)	51 45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	354	SER
1	D	61	ILE
1	D	353	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	302/301 (100%)	298 (99%)	4 (1%)	69 67
1	B	299/301 (99%)	288 (96%)	11 (4%)	34 27
1	C	298/301 (99%)	289 (97%)	9 (3%)	41 34
1	D	299/301 (99%)	293 (98%)	6 (2%)	55 50
1	E	302/301 (100%)	297 (98%)	5 (2%)	60 57
1	F	302/301 (100%)	296 (98%)	6 (2%)	55 50
1	G	299/301 (99%)	290 (97%)	9 (3%)	41 34
1	H	301/301 (100%)	291 (97%)	10 (3%)	38 31
All	All	2402/2408 (100%)	2342 (98%)	60 (2%)	47 40

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	338	LYS
1	H	237	PHE
1	F	71	LEU
1	H	203	MSE
1	H	353	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	163	GLN
1	H	349	ASN
1	F	9	ASN
1	H	163	GLN
1	E	362	ASN

5.3.3 RNA (i)

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 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

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	373/392 (95%)	-0.49	2 (0%)	91	92	9, 15, 29, 44	0
1	B	368/392 (93%)	-0.26	3 (0%)	86	88	10, 20, 38, 48	0
1	C	367/392 (93%)	-0.19	10 (2%)	54	59	15, 25, 44, 57	0
1	D	368/392 (93%)	-0.02	4 (1%)	80	82	13, 28, 46, 54	0
1	E	373/392 (95%)	-0.06	12 (3%)	47	52	12, 24, 43, 56	0
1	F	373/392 (95%)	-0.53	1 (0%)	94	94	8, 16, 30, 44	0
1	G	368/392 (93%)	-0.01	15 (4%)	37	40	17, 30, 48, 56	0
1	H	370/392 (94%)	-0.10	10 (2%)	54	59	13, 23, 41, 49	0
All	All	2960/3136 (94%)	-0.21	57 (1%)	66	71	8, 23, 42, 57	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	169	LEU	5.4
1	H	159	TYR	5.0
1	H	143	ARG	4.7
1	C	337	PHE	4.1
1	G	355	SER	4.0

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.