Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:22 AM GMT

PDB ID	:	2QDE
Title	:	Crystal structure of mandelate racemase/muconate lactonizing family protein from Azoarcus sp. EbN1
Authors	:	Agarwal, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-06-20
Resolution	:	1.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

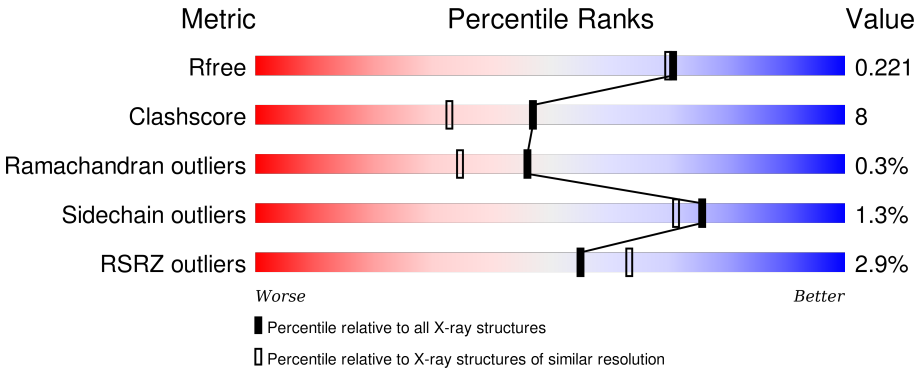
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.93 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	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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	397	3% 79% 15% • 6%
1	B	397	6% 77% 17% • 6%
1	C	397	3% 78% 16% • 6%
1	D	397	2% 79% 15% • 6%
1	E	397	% 79% 15% • 6%

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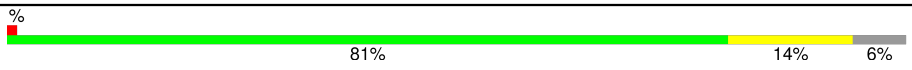
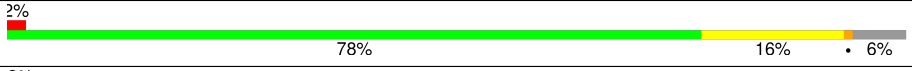
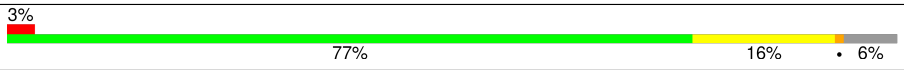
Mol	Chain	Length	Quality of chain
1	F	397	
1	G	397	
1	H	397	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24451 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 Mandelate racemase/muconate lactonizing enzyme family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2853	1814	495	533	11			
1	B	375	Total	C	N	O	S	0	0	0
			2853	1814	495	533	11			
1	C	375	Total	C	N	O	S	0	0	0
			2853	1814	495	533	11			
1	D	375	Total	C	N	O	S	0	0	0
			2853	1814	495	533	11			
1	E	375	Total	C	N	O	S	0	0	0
			2853	1814	495	533	11			
1	F	375	Total	C	N	O	S	0	0	0
			2853	1814	495	533	11			
1	G	375	Total	C	N	O	S	0	0	0
			2853	1814	495	533	11			
1	H	375	Total	C	N	O	S	0	0	0
			2853	1814	495	533	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP Q5P025
A	2	SER	-	CLONING ARTIFACT	UNP Q5P025
A	3	LEU	-	CLONING ARTIFACT	UNP Q5P025
A	390	GLU	-	CLONING ARTIFACT	UNP Q5P025
A	391	GLY	-	CLONING ARTIFACT	UNP Q5P025
A	392	HIS	-	CLONING ARTIFACT	UNP Q5P025
A	393	HIS	-	CLONING ARTIFACT	UNP Q5P025
A	394	HIS	-	CLONING ARTIFACT	UNP Q5P025
A	395	HIS	-	CLONING ARTIFACT	UNP Q5P025
A	396	HIS	-	CLONING ARTIFACT	UNP Q5P025
A	397	HIS	-	CLONING ARTIFACT	UNP Q5P025
B	1	MET	-	CLONING ARTIFACT	UNP Q5P025

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	CLONING ARTIFACT	UNP Q5P025
B	3	LEU	-	CLONING ARTIFACT	UNP Q5P025
B	390	GLU	-	CLONING ARTIFACT	UNP Q5P025
B	391	GLY	-	CLONING ARTIFACT	UNP Q5P025
B	392	HIS	-	CLONING ARTIFACT	UNP Q5P025
B	393	HIS	-	CLONING ARTIFACT	UNP Q5P025
B	394	HIS	-	CLONING ARTIFACT	UNP Q5P025
B	395	HIS	-	CLONING ARTIFACT	UNP Q5P025
B	396	HIS	-	CLONING ARTIFACT	UNP Q5P025
B	397	HIS	-	CLONING ARTIFACT	UNP Q5P025
C	1	MET	-	CLONING ARTIFACT	UNP Q5P025
C	2	SER	-	CLONING ARTIFACT	UNP Q5P025
C	3	LEU	-	CLONING ARTIFACT	UNP Q5P025
C	390	GLU	-	CLONING ARTIFACT	UNP Q5P025
C	391	GLY	-	CLONING ARTIFACT	UNP Q5P025
C	392	HIS	-	CLONING ARTIFACT	UNP Q5P025
C	393	HIS	-	CLONING ARTIFACT	UNP Q5P025
C	394	HIS	-	CLONING ARTIFACT	UNP Q5P025
C	395	HIS	-	CLONING ARTIFACT	UNP Q5P025
C	396	HIS	-	CLONING ARTIFACT	UNP Q5P025
C	397	HIS	-	CLONING ARTIFACT	UNP Q5P025
D	1	MET	-	CLONING ARTIFACT	UNP Q5P025
D	2	SER	-	CLONING ARTIFACT	UNP Q5P025
D	3	LEU	-	CLONING ARTIFACT	UNP Q5P025
D	390	GLU	-	CLONING ARTIFACT	UNP Q5P025
D	391	GLY	-	CLONING ARTIFACT	UNP Q5P025
D	392	HIS	-	CLONING ARTIFACT	UNP Q5P025
D	393	HIS	-	CLONING ARTIFACT	UNP Q5P025
D	394	HIS	-	CLONING ARTIFACT	UNP Q5P025
D	395	HIS	-	CLONING ARTIFACT	UNP Q5P025
D	396	HIS	-	CLONING ARTIFACT	UNP Q5P025
D	397	HIS	-	CLONING ARTIFACT	UNP Q5P025
E	1	MET	-	CLONING ARTIFACT	UNP Q5P025
E	2	SER	-	CLONING ARTIFACT	UNP Q5P025
E	3	LEU	-	CLONING ARTIFACT	UNP Q5P025
E	390	GLU	-	CLONING ARTIFACT	UNP Q5P025
E	391	GLY	-	CLONING ARTIFACT	UNP Q5P025
E	392	HIS	-	CLONING ARTIFACT	UNP Q5P025
E	393	HIS	-	CLONING ARTIFACT	UNP Q5P025
E	394	HIS	-	CLONING ARTIFACT	UNP Q5P025
E	395	HIS	-	CLONING ARTIFACT	UNP Q5P025
E	396	HIS	-	CLONING ARTIFACT	UNP Q5P025

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Chain	Residue	Modelled	Actual	Comment	Reference
E	397	HIS	-	CLONING ARTIFACT	UNP Q5P025
F	1	MET	-	CLONING ARTIFACT	UNP Q5P025
F	2	SER	-	CLONING ARTIFACT	UNP Q5P025
F	3	LEU	-	CLONING ARTIFACT	UNP Q5P025
F	390	GLU	-	CLONING ARTIFACT	UNP Q5P025
F	391	GLY	-	CLONING ARTIFACT	UNP Q5P025
F	392	HIS	-	CLONING ARTIFACT	UNP Q5P025
F	393	HIS	-	CLONING ARTIFACT	UNP Q5P025
F	394	HIS	-	CLONING ARTIFACT	UNP Q5P025
F	395	HIS	-	CLONING ARTIFACT	UNP Q5P025
F	396	HIS	-	CLONING ARTIFACT	UNP Q5P025
F	397	HIS	-	CLONING ARTIFACT	UNP Q5P025
G	1	MET	-	CLONING ARTIFACT	UNP Q5P025
G	2	SER	-	CLONING ARTIFACT	UNP Q5P025
G	3	LEU	-	CLONING ARTIFACT	UNP Q5P025
G	390	GLU	-	CLONING ARTIFACT	UNP Q5P025
G	391	GLY	-	CLONING ARTIFACT	UNP Q5P025
G	392	HIS	-	CLONING ARTIFACT	UNP Q5P025
G	393	HIS	-	CLONING ARTIFACT	UNP Q5P025
G	394	HIS	-	CLONING ARTIFACT	UNP Q5P025
G	395	HIS	-	CLONING ARTIFACT	UNP Q5P025
G	396	HIS	-	CLONING ARTIFACT	UNP Q5P025
G	397	HIS	-	CLONING ARTIFACT	UNP Q5P025
H	1	MET	-	CLONING ARTIFACT	UNP Q5P025
H	2	SER	-	CLONING ARTIFACT	UNP Q5P025
H	3	LEU	-	CLONING ARTIFACT	UNP Q5P025
H	390	GLU	-	CLONING ARTIFACT	UNP Q5P025
H	391	GLY	-	CLONING ARTIFACT	UNP Q5P025
H	392	HIS	-	CLONING ARTIFACT	UNP Q5P025
H	393	HIS	-	CLONING ARTIFACT	UNP Q5P025
H	394	HIS	-	CLONING ARTIFACT	UNP Q5P025
H	395	HIS	-	CLONING ARTIFACT	UNP Q5P025
H	396	HIS	-	CLONING ARTIFACT	UNP Q5P025
H	397	HIS	-	CLONING ARTIFACT	UNP Q5P025

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ba 1 1	0	0
2	D	1	Total Ba 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Ba 1 1	0	0
2	H	1	Total Ba 1 1	0	0
2	B	1	Total Ba 1 1	0	0
2	C	1	Total Ba 1 1	0	0
2	A	1	Total Ba 1 1	0	0
2	F	1	Total Ba 1 1	0	0

- Molecule 3 is water.

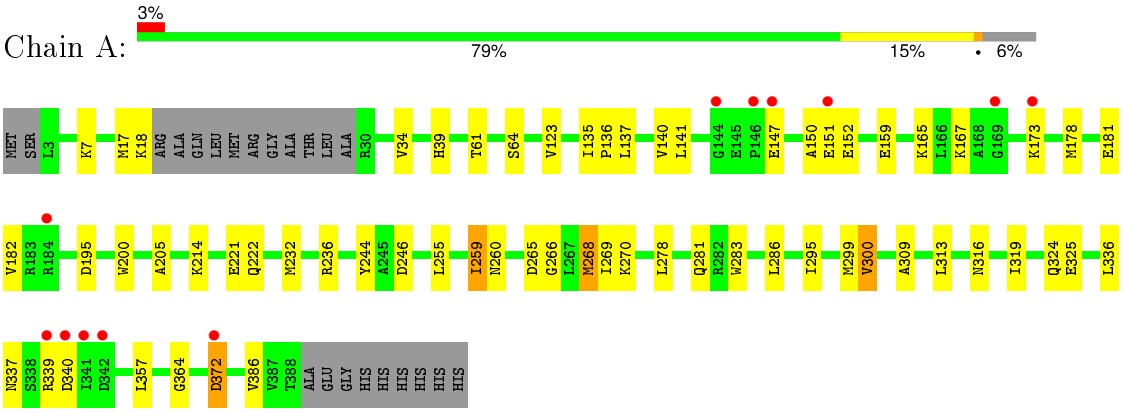
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	194	Total O 194 194	0	0
3	B	156	Total O 156 156	0	0
3	C	205	Total O 205 205	0	0
3	D	210	Total O 210 210	0	0
3	E	211	Total O 211 211	0	0
3	F	248	Total O 248 248	0	0
3	G	226	Total O 226 226	0	0
3	H	169	Total O 169 169	0	0

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.

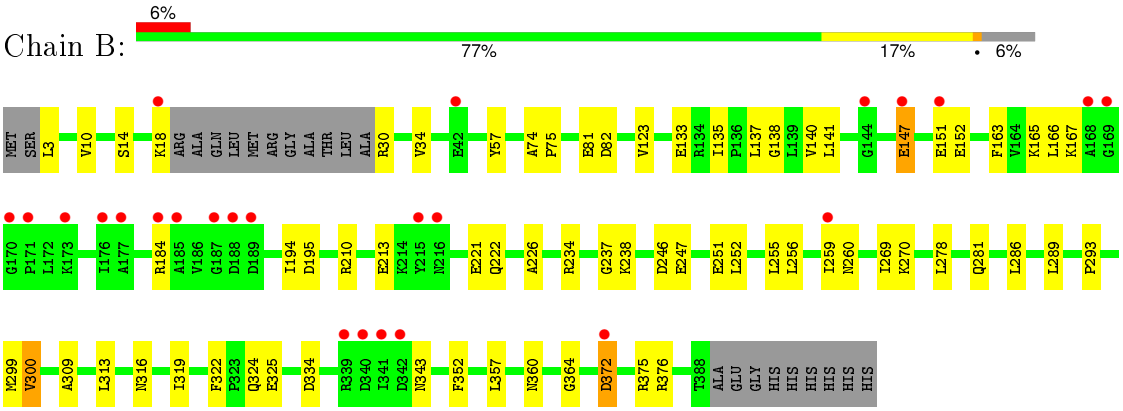
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

Chain A:



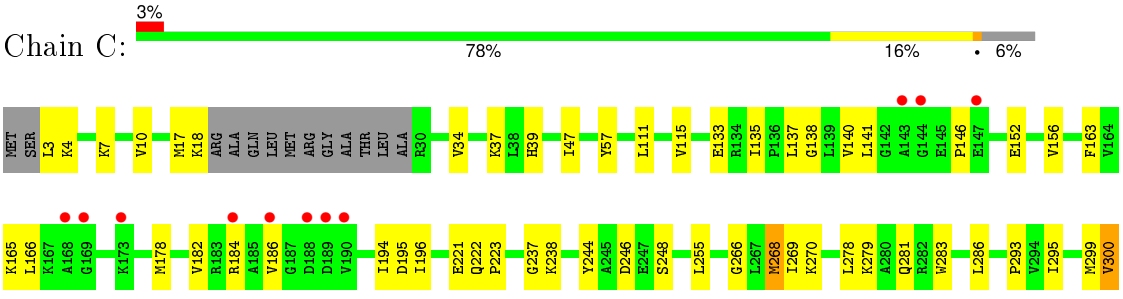
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

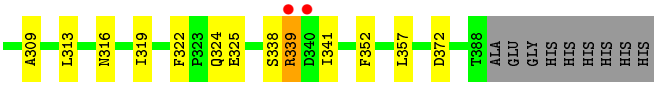
Chain B:



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

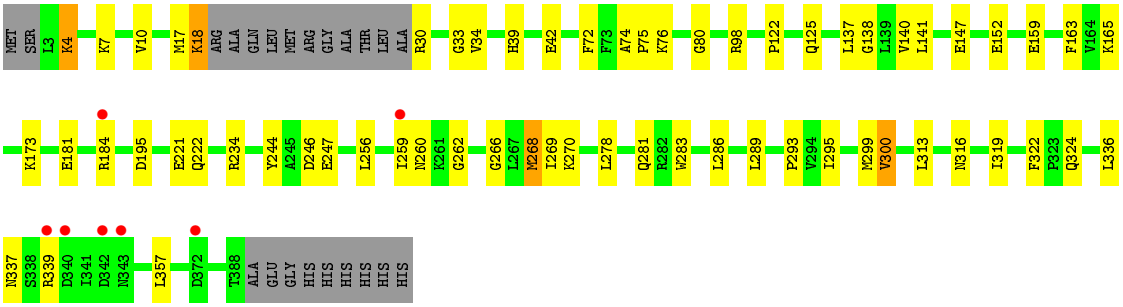
Chain C:





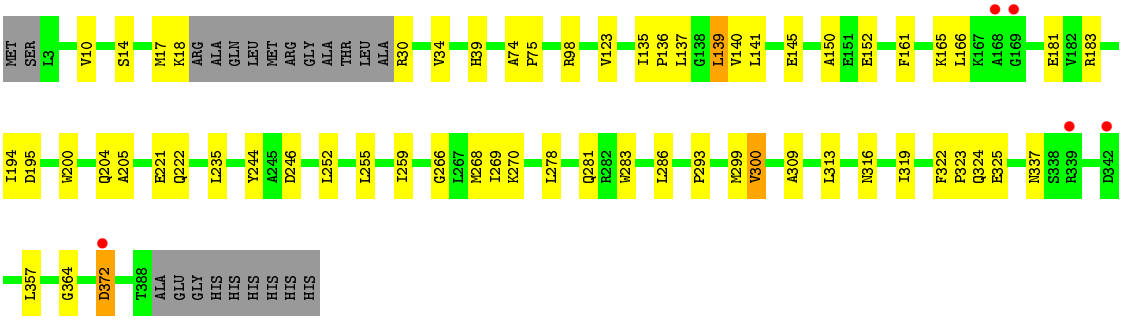
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

Chain D:



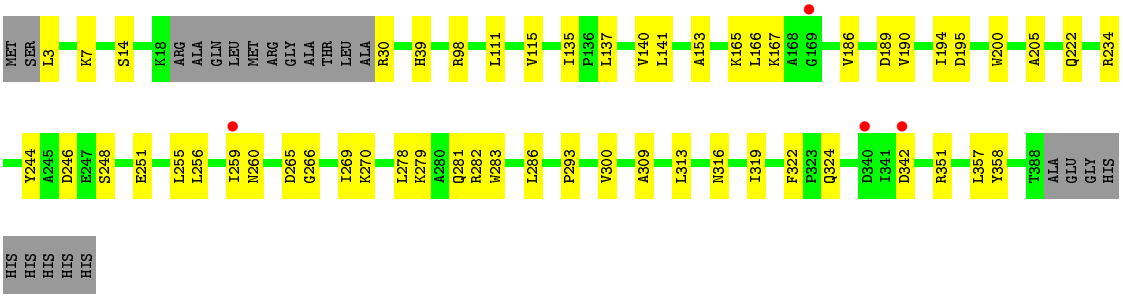
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

Chain E:



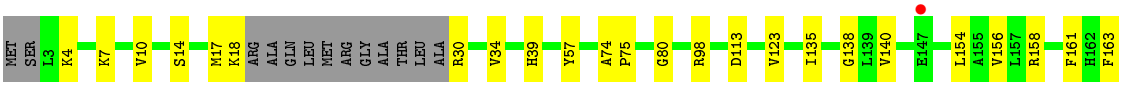
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

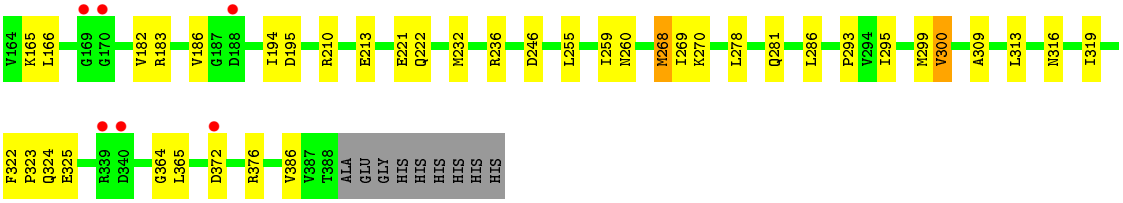
Chain F:



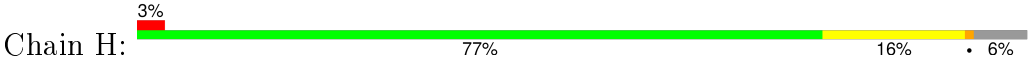
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein

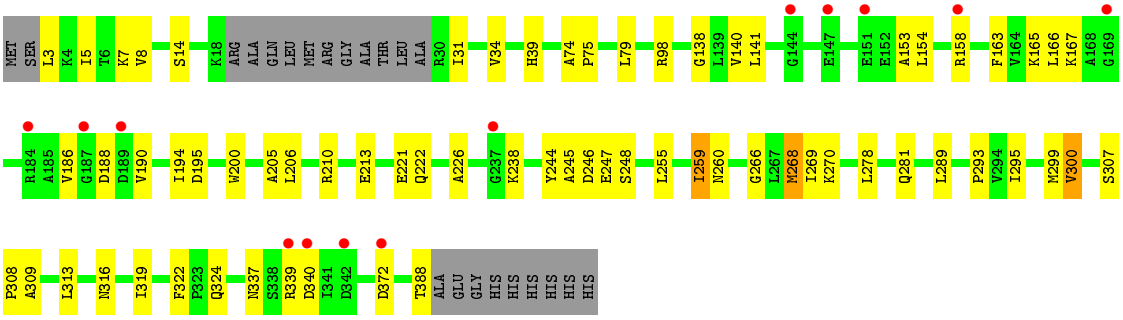
Chain G:





• Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.06Å 114.59Å 146.23Å 90.00° 101.45° 90.00°	Depositor
Resolution (Å)	46.14 – 1.93 47.65 – 1.93	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.14-1.93) 95.8 (47.65-1.93)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.66 (at 1.92Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.225 0.195 , 0.221	Depositor DCC
R_{free} test set	8163 reflections (3.05%)	DCC
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 285400 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24451	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.52% 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: BA

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	0.33	0/2903	0.61	0/3939
1	B	0.34	0/2903	0.61	0/3939
1	C	0.34	0/2903	0.62	0/3939
1	D	0.34	0/2903	0.61	0/3939
1	E	0.34	0/2903	0.61	0/3939
1	F	0.35	0/2903	0.62	0/3939
1	G	0.34	0/2903	0.62	0/3939
1	H	0.34	0/2903	0.61	0/3939
All	All	0.34	0/23224	0.61	0/31512

There are no bond length outliers.

There are no bond angle outliers.

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	2853	0	2909	43	0
1	B	2853	0	2909	49	0
1	C	2853	0	2909	49	0
1	D	2853	0	2909	45	0
1	E	2853	0	2909	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2853	0	2909	38	0
1	G	2853	0	2909	43	0
1	H	2853	0	2909	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	194	0	0	6	0
3	B	156	0	0	4	0
3	C	205	0	0	8	0
3	D	210	0	0	5	0
3	E	211	0	0	6	0
3	F	248	0	0	8	0
3	G	226	0	0	6	0
3	H	169	0	0	7	0
All	All	24451	0	23272	347	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.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:372:ASP:HB3	3:H:496:HOH:O	1.71	0.89
1:C:222:GLN:HE21	1:C:246:ASP:H	1.20	0.85
1:G:222:GLN:HE21	1:G:246:ASP:H	1.25	0.82
1:F:234:ARG:HD3	3:G:577:HOH:O	1.79	0.81
1:H:222:GLN:HE21	1:H:246:ASP:H	1.27	0.81
1:H:140:VAL:HG22	1:H:165:LYS:HD3	1.62	0.81
1:A:165:LYS:HE3	1:A:195:ASP:HB2	1.62	0.80
1:A:265:ASP:HA	3:A:510:HOH:O	1.81	0.79
1:B:18:LYS:HG2	1:B:334:ASP:HB2	1.65	0.78
1:F:222:GLN:HE21	1:F:246:ASP:H	1.31	0.78
1:B:222:GLN:HE21	1:B:246:ASP:H	1.29	0.78
1:E:222:GLN:HE21	1:E:246:ASP:H	1.31	0.78
1:F:7:LYS:HG2	1:F:39:HIS:HB2	1.66	0.77
1:G:140:VAL:HG22	1:G:165:LYS:HD3	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLN:HE21	1:A:246:ASP:H	1.29	0.77
1:D:140:VAL:HG22	1:D:165:LYS:HD3	1.68	0.76
1:D:222:GLN:HE21	1:D:246:ASP:H	1.31	0.76
1:C:140:VAL:HG22	1:C:165:LYS:HD3	1.66	0.75
1:D:165:LYS:HE3	1:D:195:ASP:HB2	1.69	0.75
1:E:141:LEU:HD22	1:E:152:GLU:HG2	1.70	0.73
1:H:337:ASN:OD1	1:H:339:ARG:HG2	1.89	0.73
1:F:309:ALA:O	1:F:313:LEU:HG	1.89	0.72
1:E:313:LEU:HD13	1:E:324:GLN:HG3	1.71	0.72
1:C:3:LEU:HD22	3:C:594:HOH:O	1.89	0.71
1:B:309:ALA:O	1:B:313:LEU:HG	1.90	0.71
1:C:313:LEU:HD13	1:C:324:GLN:HG3	1.73	0.70
1:C:222:GLN:NE2	1:C:246:ASP:H	1.89	0.69
1:C:309:ALA:O	1:C:313:LEU:HG	1.92	0.69
1:B:313:LEU:HD13	1:B:324:GLN:HG3	1.75	0.68
1:B:140:VAL:HG22	1:B:165:LYS:HD3	1.74	0.68
1:A:222:GLN:NE2	1:A:246:ASP:H	1.93	0.67
1:C:341:ILE:HG13	3:C:557:HOH:O	1.95	0.67
1:H:222:GLN:NE2	1:H:246:ASP:H	1.93	0.65
1:B:222:GLN:NE2	1:B:246:ASP:H	1.96	0.64
1:C:3:LEU:HD23	1:C:4:LYS:HG3	1.79	0.64
1:H:255:LEU:O	1:H:259:ILE:HG23	1.97	0.64
1:H:268:MET:HE3	1:H:295:ILE:HB	1.79	0.64
1:A:255:LEU:O	1:A:259:ILE:HG23	1.98	0.64
1:A:7:LYS:HB3	1:A:39:HIS:HB2	1.80	0.64
1:B:140:VAL:HG11	1:B:167:LYS:HE3	1.79	0.63
1:E:309:ALA:O	1:E:313:LEU:HG	1.98	0.63
1:F:279:LYS:HD2	1:F:282:ARG:HD2	1.81	0.63
1:H:165:LYS:HE3	1:H:195:ASP:HB2	1.81	0.62
1:F:313:LEU:HD13	1:F:324:GLN:HG3	1.81	0.62
1:D:316:ASN:HB3	1:D:319:ILE:HG22	1.80	0.62
1:A:313:LEU:HD13	1:A:324:GLN:HG3	1.82	0.62
1:A:268:MET:HE3	1:A:295:ILE:HB	1.80	0.62
1:G:259:ILE:HG13	1:G:260:ASN:N	2.14	0.62
1:E:165:LYS:HE3	1:E:195:ASP:HB2	1.81	0.62
1:H:8:VAL:HG23	3:H:520:HOH:O	1.99	0.62
1:B:147:GLU:O	1:B:151:GLU:HG3	1.99	0.62
1:F:255:LEU:HB2	1:F:286:LEU:HD23	1.82	0.62
1:B:316:ASN:HB3	1:B:319:ILE:HG22	1.81	0.61
1:F:3:LEU:HA	3:F:555:HOH:O	1.99	0.61
1:G:17:MET:O	1:G:18:LYS:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:LYS:HE2	1:G:386:VAL:HG11	1.81	0.61
1:G:222:GLN:NE2	1:G:246:ASP:H	1.96	0.61
1:H:5:ILE:HG22	3:H:520:HOH:O	2.00	0.61
1:H:195:ASP:HA	1:H:221:GLU:HB3	1.81	0.61
1:F:140:VAL:HG22	1:F:165:LYS:HD3	1.82	0.60
1:F:165:LYS:HE3	1:F:195:ASP:HB2	1.82	0.60
1:D:173:LYS:HE3	3:D:605:HOH:O	2.02	0.60
1:H:309:ALA:O	1:H:313:LEU:HG	2.01	0.60
1:H:259:ILE:HG13	1:H:260:ASN:N	2.16	0.60
1:C:184:ARG:HG2	1:C:184:ARG:HH11	1.67	0.59
1:B:137:LEU:HD11	1:B:357:LEU:HB2	1.85	0.59
1:F:135:ILE:HD13	1:F:313:LEU:HB2	1.83	0.59
1:G:309:ALA:O	1:G:313:LEU:HG	2.02	0.59
1:D:234:ARG:HD3	3:F:581:HOH:O	2.03	0.59
1:C:165:LYS:HE3	1:C:195:ASP:HB2	1.85	0.59
1:B:141:LEU:HD22	1:B:152:GLU:HG2	1.84	0.58
1:H:7:LYS:HB3	1:H:39:HIS:HB2	1.85	0.58
1:G:268:MET:HE3	1:G:295:ILE:HB	1.85	0.58
1:D:137:LEU:HD11	1:D:357:LEU:HB2	1.85	0.58
1:C:111:LEU:O	1:C:115:VAL:HG23	2.03	0.58
1:A:17:MET:O	1:A:18:LYS:HB2	2.03	0.58
1:A:140:VAL:HG11	1:A:167:LYS:HE3	1.84	0.58
1:G:323:PRO:HB2	3:G:564:HOH:O	2.03	0.57
1:C:141:LEU:HD22	1:C:152:GLU:HG2	1.85	0.57
1:B:372:ASP:HB3	1:B:375:ARG:HH21	1.70	0.57
1:G:210:ARG:HA	1:G:213:GLU:HG3	1.86	0.57
1:E:278:LEU:HA	1:E:281:GLN:HE21	1.69	0.57
1:D:195:ASP:HA	1:D:221:GLU:HB3	1.87	0.57
1:G:165:LYS:HE3	1:G:195:ASP:HB2	1.85	0.57
1:D:222:GLN:NE2	1:D:246:ASP:H	1.98	0.57
1:F:98:ARG:HD3	3:F:482:HOH:O	2.05	0.57
1:C:255:LEU:HB2	1:C:286:LEU:HD23	1.86	0.56
1:A:147:GLU:O	1:A:151:GLU:HG3	2.04	0.56
1:C:316:ASN:HB3	1:C:319:ILE:HG22	1.88	0.56
1:G:313:LEU:HD13	1:G:324:GLN:HG3	1.87	0.56
1:G:98:ARG:HD3	3:G:458:HOH:O	2.05	0.56
1:E:140:VAL:HG22	1:E:165:LYS:HD3	1.87	0.56
1:D:262:GLY:HA2	3:D:553:HOH:O	2.05	0.56
1:A:135:ILE:HD13	1:A:313:LEU:HB2	1.88	0.55
1:E:235:LEU:HA	3:E:587:HOH:O	2.06	0.55
1:C:135:ILE:HD13	1:C:313:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:ILE:HD13	1:E:313:LEU:HB2	1.89	0.54
1:H:186:VAL:HB	1:H:190:VAL:HG21	1.90	0.54
1:A:140:VAL:HG22	1:A:165:LYS:HD3	1.90	0.54
1:G:7:LYS:HB3	1:G:39:HIS:HB2	1.89	0.54
1:G:316:ASN:HB3	1:G:319:ILE:HG22	1.89	0.54
1:E:222:GLN:NE2	1:E:246:ASP:H	2.02	0.54
1:H:269:ILE:HG12	1:H:270:LYS:N	2.22	0.54
1:D:184:ARG:HG2	1:D:184:ARG:HH11	1.73	0.54
1:B:135:ILE:HD13	1:B:313:LEU:HB2	1.90	0.54
1:F:351:ARG:HB3	1:F:358:TYR:HB2	1.90	0.53
1:H:210:ARG:HA	1:H:213:GLU:HG3	1.91	0.53
1:A:195:ASP:HA	1:A:221:GLU:HB3	1.90	0.53
1:C:339:ARG:HA	3:C:575:HOH:O	2.08	0.53
1:A:165:LYS:HD3	1:A:325:GLU:OE2	2.09	0.53
1:D:246:ASP:HB2	1:D:268:MET:HG3	1.91	0.53
1:D:268:MET:HE3	1:D:295:ILE:HB	1.90	0.53
1:F:222:GLN:NE2	1:F:246:ASP:H	2.02	0.52
1:F:279:LYS:HG3	3:F:611:HOH:O	2.09	0.52
1:H:140:VAL:HG11	1:H:167:LYS:HE3	1.91	0.52
1:E:39:HIS:HD2	3:E:585:HOH:O	1.92	0.52
1:D:278:LEU:HA	1:D:281:GLN:HE21	1.73	0.52
1:H:3:LEU:HA	3:H:543:HOH:O	2.09	0.52
1:G:4:LYS:HE3	1:G:80:GLY:O	2.10	0.51
1:A:340:ASP:HA	3:A:593:HOH:O	2.08	0.51
1:G:182:VAL:O	1:G:186:VAL:HG22	2.10	0.51
1:D:313:LEU:HD13	1:D:324:GLN:HG3	1.91	0.51
1:C:182:VAL:O	1:C:186:VAL:HG22	2.10	0.51
1:C:138:GLY:HA3	1:C:163:PHE:CE2	2.45	0.51
1:A:137:LEU:HD11	1:A:357:LEU:HB2	1.92	0.51
1:H:166:LEU:HB2	1:H:194:ILE:HG22	1.92	0.51
1:B:289:LEU:HD22	1:D:286:LEU:HD21	1.93	0.51
1:E:337:ASN:HB3	3:E:592:HOH:O	2.10	0.51
1:F:342:ASP:HA	3:F:590:HOH:O	2.11	0.51
1:F:14:SER:HB3	1:F:30:ARG:HD2	1.93	0.51
1:B:234:ARG:HD3	3:H:462:HOH:O	2.12	0.50
1:C:17:MET:O	1:C:18:LYS:HB2	2.11	0.50
1:E:372:ASP:OD2	1:E:372:ASP:N	2.42	0.50
1:E:325:GLU:HG2	1:E:325:GLU:O	2.12	0.50
1:C:341:ILE:N	3:C:460:HOH:O	2.44	0.50
1:C:137:LEU:HD11	1:C:357:LEU:HB2	1.93	0.50
1:G:195:ASP:HA	1:G:221:GLU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:LEU:HA	1:F:281:GLN:HE21	1.77	0.50
1:E:195:ASP:HA	1:E:221:GLU:HB3	1.93	0.49
1:C:166:LEU:HB2	1:C:194:ILE:HG22	1.94	0.49
1:C:237:GLY:O	1:C:238:LYS:HD2	2.12	0.49
1:H:313:LEU:HD13	1:H:324:GLN:HG3	1.95	0.49
1:E:204:GLN:HB3	3:E:515:HOH:O	2.11	0.49
1:H:226:ALA:HB2	1:H:247:GLU:HB3	1.94	0.49
1:D:138:GLY:HA3	1:D:163:PHE:CZ	2.48	0.49
1:B:226:ALA:HB2	1:B:247:GLU:HB3	1.95	0.49
1:A:309:ALA:O	1:A:313:LEU:HG	2.13	0.49
1:G:156:VAL:HG12	1:G:161:PHE:HB2	1.95	0.49
1:B:278:LEU:HA	1:B:281:GLN:HE21	1.77	0.49
1:H:154:LEU:O	1:H:158:ARG:HG3	2.13	0.48
1:A:316:ASN:HB3	1:A:319:ILE:HG22	1.95	0.48
1:G:232:MET:O	1:G:236:ARG:HG3	2.14	0.48
1:E:10:VAL:HG13	1:E:34:VAL:CG1	2.42	0.48
1:A:159:GLU:HG2	1:A:336:LEU:HB3	1.96	0.48
1:G:269:ILE:HG12	1:G:270:LYS:N	2.29	0.48
1:G:246:ASP:HB2	1:G:268:MET:HG3	1.94	0.48
1:A:259:ILE:HG13	1:A:260:ASN:N	2.28	0.48
1:D:244:TYR:CE2	1:D:266:GLY:HA3	2.48	0.48
1:D:141:LEU:HD22	1:D:152:GLU:HG2	1.96	0.48
1:D:259:ILE:HG13	1:D:260:ASN:N	2.28	0.48
1:A:246:ASP:HB2	1:A:268:MET:HG3	1.96	0.48
1:H:293:PRO:HA	1:H:322:PHE:CZ	2.49	0.48
1:B:3:LEU:N	3:B:508:HOH:O	2.46	0.48
1:A:339:ARG:HG2	3:A:499:HOH:O	2.13	0.48
1:C:195:ASP:HA	1:C:221:GLU:HB3	1.95	0.47
1:C:269:ILE:HG12	1:C:270:LYS:N	2.29	0.47
1:B:123:VAL:HG23	1:B:364:GLY:C	2.34	0.47
1:A:123:VAL:HG23	1:A:364:GLY:C	2.34	0.47
1:C:10:VAL:HG13	1:C:34:VAL:CG1	2.45	0.47
1:B:10:VAL:HG13	1:B:34:VAL:HG13	1.96	0.47
1:C:268:MET:HE3	1:C:295:ILE:HB	1.97	0.47
1:H:299:MET:O	1:H:300:VAL:C	2.52	0.47
1:E:269:ILE:HG12	1:E:270:LYS:N	2.29	0.47
1:D:234:ARG:CD	3:F:581:HOH:O	2.61	0.47
1:D:122:PRO:HD2	1:D:125:GLN:HG3	1.96	0.47
1:B:286:LEU:HD21	1:D:289:LEU:HD22	1.95	0.47
1:G:325:GLU:O	1:G:325:GLU:HG2	2.14	0.47
1:F:265:ASP:HA	3:F:581:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:LYS:HE2	3:C:535:HOH:O	2.14	0.47
1:E:137:LEU:HD11	1:E:357:LEU:HB2	1.96	0.47
1:B:269:ILE:HG12	1:B:270:LYS:N	2.30	0.47
1:G:293:PRO:HA	1:G:322:PHE:CZ	2.50	0.47
1:E:14:SER:HB3	1:E:30:ARG:HD2	1.97	0.47
1:H:244:TYR:CE2	1:H:266:GLY:HA3	2.50	0.47
1:E:255:LEU:HB2	1:E:286:LEU:HD23	1.97	0.47
1:C:138:GLY:HA3	1:C:163:PHE:CZ	2.50	0.47
1:A:173:LYS:HG2	3:A:552:HOH:O	2.14	0.47
1:G:138:GLY:HA3	1:G:163:PHE:CE2	2.50	0.47
1:H:278:LEU:HA	1:H:281:GLN:HE21	1.80	0.47
1:D:299:MET:O	1:D:300:VAL:C	2.53	0.47
1:B:313:LEU:HD22	1:B:319:ILE:HD13	1.97	0.46
1:G:135:ILE:HD13	1:G:313:LEU:HB2	1.98	0.46
1:G:183:ARG:CZ	3:G:444:HOH:O	2.62	0.46
1:H:141:LEU:HD11	1:H:153:ALA:HB2	1.96	0.46
1:E:252:LEU:HD22	1:E:286:LEU:HD22	1.98	0.46
1:F:269:ILE:HD12	1:F:283:TRP:CE3	2.51	0.46
1:F:269:ILE:HG12	1:F:270:LYS:N	2.30	0.46
1:F:259:ILE:HG13	1:F:260:ASN:N	2.30	0.46
1:B:3:LEU:HD11	3:B:542:HOH:O	2.15	0.46
1:B:299:MET:O	1:B:300:VAL:C	2.54	0.46
1:A:150:ALA:HB2	1:A:181:GLU:HG3	1.97	0.46
1:D:7:LYS:HB3	1:D:39:HIS:HB2	1.98	0.46
1:E:244:TYR:CE2	1:E:266:GLY:HA3	2.50	0.46
1:A:141:LEU:HD22	1:A:152:GLU:HG2	1.97	0.46
1:B:184:ARG:HG2	1:B:184:ARG:HH11	1.81	0.46
1:D:269:ILE:HD12	1:D:283:TRP:CE3	2.51	0.46
1:F:137:LEU:HD11	1:F:357:LEU:HB2	1.97	0.46
1:A:7:LYS:HE3	1:A:386:VAL:HG11	1.97	0.46
1:F:293:PRO:HA	1:F:322:PHE:CZ	2.51	0.46
1:A:178:MET:O	1:A:182:VAL:HG23	2.16	0.46
1:C:244:TYR:CE2	1:C:266:GLY:HA3	2.50	0.46
1:E:293:PRO:HA	1:E:322:PHE:CZ	2.51	0.45
1:F:244:TYR:CE2	1:F:266:GLY:HA3	2.51	0.45
1:G:299:MET:O	1:G:300:VAL:C	2.54	0.45
1:D:337:ASN:OD1	1:D:339:ARG:HG2	2.16	0.45
1:C:313:LEU:HD13	1:C:324:GLN:CG	2.45	0.45
1:C:57:TYR:CE2	1:C:270:LYS:HD2	2.52	0.45
1:H:98:ARG:NH1	3:H:429:HOH:O	2.35	0.45
1:F:189:ASP:HB2	3:F:614:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:222:GLN:NE2	1:H:248:SER:H	2.14	0.45
1:C:279:LYS:CE	3:C:535:HOH:O	2.64	0.45
1:A:244:TYR:CE2	1:A:266:GLY:HA3	2.51	0.45
1:E:98:ARG:HD3	3:E:444:HOH:O	2.15	0.45
1:D:17:MET:O	1:D:18:LYS:HB2	2.15	0.45
1:E:17:MET:O	1:E:18:LYS:HB2	2.15	0.45
1:D:98:ARG:HD3	3:D:445:HOH:O	2.16	0.45
1:F:200:TRP:CE3	1:F:205:ALA:HA	2.52	0.45
1:B:251:GLU:O	1:B:255:LEU:HD13	2.17	0.45
1:G:255:LEU:HD23	1:G:286:LEU:HB2	1.98	0.45
1:A:372:ASP:HB2	3:A:571:HOH:O	2.16	0.45
1:A:286:LEU:HD21	1:H:289:LEU:HD22	1.98	0.45
1:H:165:LYS:HE3	1:H:195:ASP:CB	2.47	0.45
1:A:246:ASP:HB2	1:A:268:MET:CG	2.47	0.45
1:B:313:LEU:HD13	1:B:324:GLN:CG	2.44	0.45
1:E:255:LEU:O	1:E:259:ILE:HG23	2.16	0.45
1:C:146:PRO:HB3	1:C:178:MET:HA	1.99	0.45
1:E:74:ALA:HB3	1:E:75:PRO:HD3	1.99	0.45
1:F:316:ASN:HB3	1:F:319:ILE:HG22	1.99	0.45
1:C:299:MET:O	1:C:300:VAL:C	2.56	0.44
1:G:278:LEU:HA	1:G:281:GLN:HE21	1.81	0.44
1:E:123:VAL:HG23	1:E:364:GLY:C	2.38	0.44
1:C:184:ARG:NH1	1:C:184:ARG:HG2	2.31	0.44
1:D:184:ARG:NH1	1:D:184:ARG:HG2	2.33	0.44
1:H:200:TRP:CE3	1:H:205:ALA:HA	2.52	0.44
1:D:138:GLY:HA3	1:D:163:PHE:CE1	2.53	0.44
1:C:293:PRO:HA	1:C:322:PHE:CZ	2.52	0.44
1:F:141:LEU:HD11	1:F:153:ALA:HB2	2.00	0.44
1:C:152:GLU:O	1:C:156:VAL:HG23	2.17	0.44
1:B:166:LEU:HB2	1:B:194:ILE:HG22	2.00	0.44
1:B:14:SER:HB3	1:B:30:ARG:HD2	2.00	0.44
1:A:299:MET:O	1:A:300:VAL:C	2.56	0.44
1:E:299:MET:O	1:E:300:VAL:C	2.56	0.44
1:A:61:THR:H	1:A:64:SER:HB2	1.83	0.44
1:G:123:VAL:HG23	1:G:364:GLY:C	2.38	0.44
1:D:293:PRO:HA	1:D:322:PHE:CZ	2.53	0.43
1:D:147:GLU:HG2	1:D:181:GLU:OE2	2.18	0.43
1:D:74:ALA:HB3	1:D:75:PRO:CD	2.47	0.43
1:A:269:ILE:HG12	1:A:270:LYS:N	2.32	0.43
1:G:10:VAL:HG13	1:G:34:VAL:CG1	2.48	0.43
1:C:18:LYS:HG3	3:C:587:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:LYS:HG3	3:C:535:HOH:O	2.17	0.43
1:B:57:TYR:CE2	1:B:270:LYS:HD2	2.53	0.43
1:D:269:ILE:HG12	1:D:270:LYS:N	2.33	0.43
1:G:154:LEU:O	1:G:158:ARG:HG3	2.17	0.43
1:G:14:SER:HB3	1:G:30:ARG:HD2	2.00	0.43
1:F:140:VAL:HG22	1:F:165:LYS:CD	2.48	0.43
1:B:372:ASP:O	1:B:376:ARG:HG3	2.17	0.43
1:G:138:GLY:HA3	1:G:163:PHE:CZ	2.54	0.43
1:D:4:LYS:HD2	1:D:80:GLY:O	2.19	0.43
1:B:138:GLY:HA3	1:B:163:PHE:CZ	2.54	0.43
1:B:360:ASN:HB3	3:B:532:HOH:O	2.18	0.43
1:D:10:VAL:HG13	1:D:34:VAL:HG13	2.01	0.43
1:H:316:ASN:HB3	1:H:319:ILE:HG22	2.00	0.43
1:G:98:ARG:NH1	3:G:458:HOH:O	2.51	0.43
1:A:337:ASN:OD1	1:A:339:ARG:HG3	2.19	0.43
1:G:246:ASP:HB2	1:G:268:MET:CG	2.48	0.43
1:D:246:ASP:HB3	1:D:247:GLU:OE1	2.19	0.43
1:B:256:LEU:O	1:B:259:ILE:HG12	2.18	0.43
1:B:195:ASP:HA	1:B:221:GLU:HB3	2.00	0.43
1:H:79:LEU:HD23	3:H:520:HOH:O	2.18	0.43
1:G:57:TYR:O	1:H:98:ARG:CZ	2.67	0.43
1:F:186:VAL:HB	1:F:190:VAL:HG21	1.99	0.43
1:A:278:LEU:HA	1:A:281:GLN:HE21	1.84	0.43
1:G:372:ASP:OD1	1:G:376:ARG:NH1	2.52	0.43
1:F:256:LEU:O	1:F:259:ILE:HG12	2.19	0.42
1:H:138:GLY:HA3	1:H:163:PHE:CZ	2.54	0.42
1:D:159:GLU:HG2	1:D:336:LEU:HB3	2.01	0.42
1:F:140:VAL:HG11	1:F:167:LYS:HE3	2.01	0.42
1:B:252:LEU:HD22	1:B:286:LEU:HD22	2.00	0.42
1:A:269:ILE:HD12	1:A:283:TRP:CE3	2.54	0.42
1:H:206:LEU:HD11	1:H:238:LYS:HB3	2.01	0.42
1:F:279:LYS:HD2	1:F:279:LYS:HA	1.95	0.42
1:G:324:GLN:N	3:G:564:HOH:O	2.51	0.42
1:E:300:VAL:HG23	3:E:550:HOH:O	2.20	0.42
1:C:7:LYS:HB3	1:C:39:HIS:HB2	2.01	0.42
1:D:72:PHE:O	1:D:76:LYS:HB2	2.20	0.42
1:E:316:ASN:HB3	1:E:319:ILE:HG22	2.00	0.42
1:A:136:PRO:HD2	3:A:416:HOH:O	2.18	0.42
1:D:256:LEU:O	1:D:259:ILE:HG12	2.19	0.42
1:B:138:GLY:HA3	1:B:163:PHE:CE2	2.55	0.42
1:B:74:ALA:HB3	1:B:75:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:PRO:HG2	1:E:323:PRO:HA	2.01	0.41
1:C:278:LEU:HA	1:C:281:GLN:HE21	1.84	0.41
1:B:352:PHE:CE1	1:B:357:LEU:HD13	2.55	0.41
1:C:196:ILE:HB	1:C:223:PRO:HA	2.02	0.41
1:F:166:LEU:HB2	1:F:194:ILE:HG22	2.02	0.41
1:B:237:GLY:O	1:B:238:LYS:HD2	2.20	0.41
1:G:166:LEU:HB2	1:G:194:ILE:HG22	2.01	0.41
1:B:74:ALA:HB3	1:B:75:PRO:CD	2.50	0.41
1:E:200:TRP:CE3	1:E:205:ALA:HA	2.55	0.41
1:A:232:MET:O	1:A:236:ARG:HG3	2.20	0.41
1:A:200:TRP:CE3	1:A:205:ALA:HA	2.56	0.41
1:H:246:ASP:HB2	1:H:268:MET:HG3	2.02	0.41
1:C:138:GLY:HA3	1:C:163:PHE:CD2	2.55	0.41
1:B:30:ARG:N	3:B:526:HOH:O	2.54	0.41
1:D:246:ASP:HB2	1:D:268:MET:CG	2.49	0.41
1:F:251:GLU:O	1:F:255:LEU:HD13	2.21	0.41
1:D:138:GLY:HA3	1:D:163:PHE:CE2	2.55	0.41
1:H:138:GLY:HA3	1:H:163:PHE:CE2	2.56	0.41
1:G:113:ASP:HB2	1:G:365:LEU:HG	2.03	0.41
1:E:166:LEU:HB2	1:E:194:ILE:HG22	2.01	0.41
1:E:269:ILE:HD12	1:E:283:TRP:CE3	2.56	0.41
1:H:74:ALA:HB3	1:H:75:PRO:CD	2.50	0.41
1:B:210:ARG:HA	1:B:213:GLU:HG3	2.01	0.41
1:C:222:GLN:NE2	1:C:248:SER:H	2.19	0.41
1:B:259:ILE:HG13	1:B:260:ASN:N	2.35	0.41
1:C:338:SER:HB3	1:C:352:PHE:HB2	2.03	0.41
1:A:214:LYS:HB3	1:A:214:LYS:HE2	1.92	0.41
1:D:30:ARG:N	3:D:580:HOH:O	2.53	0.41
1:D:33:GLY:HA3	3:D:519:HOH:O	2.21	0.41
1:H:245:ALA:O	1:H:268:MET:HG2	2.21	0.41
1:B:165:LYS:HE3	1:B:195:ASP:HB2	2.03	0.41
1:E:74:ALA:HB3	1:E:75:PRO:CD	2.50	0.41
1:H:14:SER:HA	1:H:31:ILE:O	2.21	0.41
1:E:150:ALA:HB2	1:E:181:GLU:HG3	2.03	0.41
1:F:111:LEU:O	1:F:115:VAL:HG23	2.21	0.41
1:F:222:GLN:NE2	1:F:248:SER:H	2.20	0.41
1:B:81:GLU:HG3	1:B:82:ASP:N	2.36	0.41
1:C:269:ILE:HD12	1:C:283:TRP:CE3	2.57	0.40
1:H:307:SER:HB2	1:H:308:PRO:HD3	2.03	0.40
1:E:10:VAL:HG13	1:E:34:VAL:HG13	2.04	0.40
1:C:10:VAL:HG13	1:C:34:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:74:ALA:HB3	1:G:75:PRO:HD3	2.04	0.40
1:B:140:VAL:CG1	1:B:167:LYS:HE3	2.49	0.40
1:B:293:PRO:HA	1:B:322:PHE:CZ	2.57	0.40
1:C:37:LYS:HG2	1:C:47:ILE:HG22	2.03	0.40
1:E:139:LEU:HD13	1:E:161:PHE:CE2	2.57	0.40

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	371/397 (94%)	359 (97%)	11 (3%)	1 (0%)	46	35
1	B	371/397 (94%)	355 (96%)	15 (4%)	1 (0%)	46	35
1	C	371/397 (94%)	356 (96%)	14 (4%)	1 (0%)	46	35
1	D	371/397 (94%)	356 (96%)	14 (4%)	1 (0%)	46	35
1	E	371/397 (94%)	357 (96%)	13 (4%)	1 (0%)	46	35
1	F	371/397 (94%)	362 (98%)	8 (2%)	1 (0%)	46	35
1	G	371/397 (94%)	359 (97%)	11 (3%)	1 (0%)	46	35
1	H	371/397 (94%)	358 (96%)	12 (3%)	1 (0%)	46	35
All	All	2968/3176 (94%)	2862 (96%)	98 (3%)	8 (0%)	46	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	VAL
1	B	300	VAL
1	C	300	VAL
1	D	300	VAL
1	E	300	VAL

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Mol	Chain	Res	Type
1	F	300	VAL
1	G	300	VAL
1	H	300	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/315 (95%)	295 (99%)	4 (1%)	76	71
1	B	299/315 (95%)	294 (98%)	5 (2%)	68	61
1	C	299/315 (95%)	294 (98%)	5 (2%)	68	61
1	D	299/315 (95%)	295 (99%)	4 (1%)	76	71
1	E	299/315 (95%)	294 (98%)	5 (2%)	68	61
1	F	299/315 (95%)	299 (100%)	0	100	100
1	G	299/315 (95%)	298 (100%)	1 (0%)	94	94
1	H	299/315 (95%)	293 (98%)	6 (2%)	63	53
All	All	2392/2520 (95%)	2362 (99%)	30 (1%)	76	71

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	259	ILE
1	A	268	MET
1	A	372	ASP
1	B	133	GLU
1	B	147	GLU
1	B	325	GLU
1	B	343	ASN
1	B	372	ASP
1	C	133	GLU
1	C	268	MET
1	C	325	GLU

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Mol	Chain	Res	Type
1	C	339	ARG
1	C	372	ASP
1	D	4	LYS
1	D	18	LYS
1	D	42	GLU
1	D	268	MET
1	E	139	LEU
1	E	145	GLU
1	E	183	ARG
1	E	268	MET
1	E	372	ASP
1	G	268	MET
1	H	34	VAL
1	H	188	ASP
1	H	259	ILE
1	H	268	MET
1	H	340	ASP
1	H	388	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	162	HIS
1	A	222	GLN
1	A	281	GLN
1	A	321	GLN
1	A	331	HIS
1	A	360	ASN
1	B	222	GLN
1	B	281	GLN
1	B	321	GLN
1	B	331	HIS
1	B	343	ASN
1	B	360	ASN
1	C	162	HIS
1	C	222	GLN
1	C	281	GLN
1	C	321	GLN
1	C	360	ASN
1	D	222	GLN
1	D	281	GLN

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Mol	Chain	Res	Type
1	D	321	GLN
1	D	360	ASN
1	E	39	HIS
1	E	162	HIS
1	E	222	GLN
1	E	281	GLN
1	E	321	GLN
1	E	331	HIS
1	E	360	ASN
1	F	162	HIS
1	F	222	GLN
1	F	281	GLN
1	F	321	GLN
1	F	331	HIS
1	F	360	ASN
1	G	39	HIS
1	G	162	HIS
1	G	222	GLN
1	G	281	GLN
1	G	321	GLN
1	G	331	HIS
1	G	360	ASN
1	H	162	HIS
1	H	222	GLN
1	H	281	GLN
1	H	360	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	375/397 (94%)	0.11	12 (3%)	51	60	12, 21, 32, 37	0
1	B	375/397 (94%)	0.15	25 (6%)	21	29	13, 23, 34, 38	0
1	C	375/397 (94%)	0.01	13 (3%)	48	57	10, 20, 33, 41	0
1	D	375/397 (94%)	0.01	7 (1%)	70	77	13, 21, 32, 37	0
1	E	375/397 (94%)	-0.01	5 (1%)	79	84	11, 19, 30, 37	0
1	F	375/397 (94%)	-0.11	4 (1%)	82	87	10, 17, 28, 34	0
1	G	375/397 (94%)	-0.22	7 (1%)	70	77	10, 19, 30, 38	0
1	H	375/397 (94%)	0.07	13 (3%)	48	57	14, 23, 34, 38	0
All	All	3000/3176 (94%)	0.00	86 (2%)	55	63	10, 20, 33, 41	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	340	ASP	5.1
1	A	340	ASP	4.7
1	A	339	ARG	4.4
1	B	169	GLY	4.3
1	H	340	ASP	4.0
1	C	168	ALA	3.8
1	B	189	ASP	3.8
1	H	339	ARG	3.7
1	C	173	LYS	3.6
1	B	144	GLY	3.6
1	D	342	ASP	3.4
1	A	169	GLY	3.4
1	G	340	ASP	3.4
1	E	339	ARG	3.2
1	B	170	GLY	3.1
1	A	342	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	340	ASP	3.1
1	G	169	GLY	3.0
1	D	372	ASP	3.0
1	B	340	ASP	3.0
1	D	339	ARG	2.9
1	H	237	GLY	2.9
1	H	151	GLU	2.9
1	C	189	ASP	2.9
1	A	144	GLY	2.9
1	C	190	VAL	2.9
1	C	184	ARG	2.8
1	H	184	ARG	2.8
1	A	151	GLU	2.8
1	B	168	ALA	2.7
1	B	173	LYS	2.7
1	B	176	ILE	2.7
1	H	187	GLY	2.7
1	E	342	ASP	2.7
1	A	146	PRO	2.6
1	B	151	GLU	2.6
1	B	188	ASP	2.6
1	H	342	ASP	2.6
1	B	184	ARG	2.6
1	B	342	ASP	2.6
1	F	340	ASP	2.6
1	B	185	ALA	2.6
1	G	339	ARG	2.5
1	A	147	GLU	2.5
1	B	372	ASP	2.5
1	D	343	ASN	2.4
1	H	169	GLY	2.4
1	C	169	GLY	2.4
1	H	158	ARG	2.4
1	G	372	ASP	2.4
1	H	144	GLY	2.4
1	D	259	ILE	2.4
1	B	215	TYR	2.4
1	C	147	GLU	2.4
1	E	168	ALA	2.4
1	H	372	ASP	2.3
1	C	143	ALA	2.3
1	E	372	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	341	ILE	2.3
1	A	173	LYS	2.3
1	A	372	ASP	2.3
1	F	342	ASP	2.3
1	E	169	GLY	2.3
1	F	169	GLY	2.3
1	A	341	ILE	2.2
1	B	147	GLU	2.2
1	G	188	ASP	2.2
1	B	177	ALA	2.2
1	C	339	ARG	2.2
1	B	259	ILE	2.2
1	B	42	GLU	2.1
1	B	18	LYS	2.1
1	G	170	GLY	2.1
1	B	339	ARG	2.1
1	A	184	ARG	2.1
1	B	216	ASN	2.0
1	F	259	ILE	2.0
1	B	171	PRO	2.0
1	D	184	ARG	2.0
1	B	187	GLY	2.0
1	G	147	GLU	2.0
1	H	147	GLU	2.0
1	C	188	ASP	2.0
1	C	186	VAL	2.0
1	C	144	GLY	2.0
1	H	189	ASP	2.0

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

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	BA	C	401	1/1	0.98	0.09	-0.36	66,66,66,66	0
2	BA	A	401	1/1	0.99	0.06	-1.99	50,50,50,50	0
2	BA	F	401	1/1	0.99	0.04	-2.59	39,39,39,39	0
2	BA	H	401	1/1	0.99	0.05	-2.75	47,47,47,47	0
2	BA	E	401	1/1	0.99	0.04	-3.02	42,42,42,42	0
2	BA	D	401	1/1	0.99	0.03	-3.38	38,38,38,38	0
2	BA	B	401	1/1	0.98	0.04	-3.55	47,47,47,47	0
2	BA	G	401	1/1	0.97	0.04	-3.63	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.