Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:41 PM GMT

PDB ID	:	4J3Z
Title	:	Crystal structure of mandelate racemase/muconate lactonizing enzyme from Jannaschia sp. CCS1
Authors	:	Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Lafluer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Zenchek, W.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2013-02-06
Resolution	:	2.50 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:

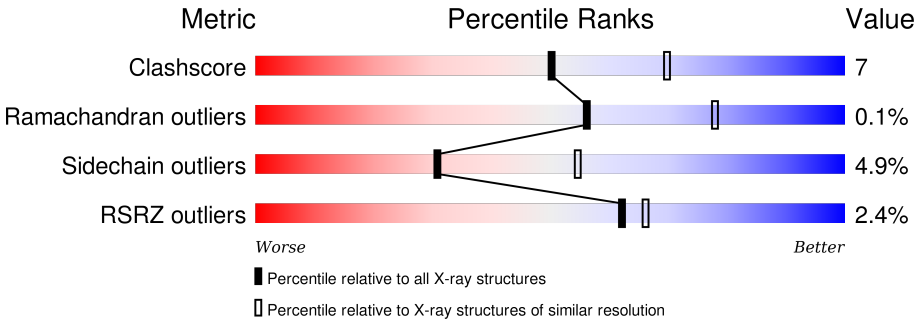
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	429	3% 74% 15% • 10%
1	B	429	2% 73% 16% • 10%
1	C	429	2% 76% 13% • 10%
1	D	429	3% 74% 16% • 8%
1	E	429	2% 74% 14% • 10%
1	F	429	2% 73% 17% • 10%
1	G	429	2% 74% 15% 10%

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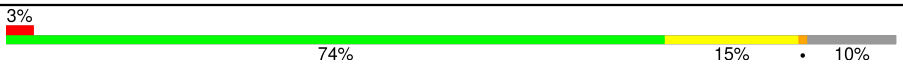
Mol	Chain	Length	Quality of chain
1	H	429	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24704 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			2939	1871	518	535	15			
1	B	386	Total	C	N	O	S	0	0	0
			2922	1861	515	532	14			
1	C	386	Total	C	N	O	S	0	0	0
			2922	1861	515	532	14			
1	D	393	Total	C	N	O	S	0	2	0
			2987	1901	527	542	17			
1	E	388	Total	C	N	O	S	0	0	0
			2938	1871	517	534	16			
1	F	386	Total	C	N	O	S	0	0	0
			2922	1861	515	532	14			
1	G	386	Total	C	N	O	S	0	2	0
			2935	1870	518	533	14			
1	H	388	Total	C	N	O	S	0	0	0
			2938	1871	517	534	16			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q28RT0
A	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
A	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
A	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
A	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
A	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
A	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
A	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
A	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
A	415	SER	-	EXPRESSION TAG	UNP Q28RT0
A	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	418	HIS	-	EXPRESSION TAG	UNP Q28RT0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
A	423	SER	-	EXPRESSION TAG	UNP Q28RT0
A	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
A	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
A	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
A	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
A	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
A	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
B	1	MET	-	EXPRESSION TAG	UNP Q28RT0
B	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
B	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
B	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
B	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
B	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
B	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
B	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
B	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
B	415	SER	-	EXPRESSION TAG	UNP Q28RT0
B	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
B	423	SER	-	EXPRESSION TAG	UNP Q28RT0
B	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
B	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
B	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
B	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
B	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
B	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
C	1	MET	-	EXPRESSION TAG	UNP Q28RT0
C	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
C	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
C	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
C	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
C	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
C	412	TYR	-	EXPRESSION TAG	UNP Q28RT0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
C	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
C	415	SER	-	EXPRESSION TAG	UNP Q28RT0
C	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
C	423	SER	-	EXPRESSION TAG	UNP Q28RT0
C	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
C	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
C	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
C	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
C	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
C	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
D	1	MET	-	EXPRESSION TAG	UNP Q28RT0
D	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
D	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
D	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
D	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
D	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
D	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
D	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
D	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
D	415	SER	-	EXPRESSION TAG	UNP Q28RT0
D	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
D	423	SER	-	EXPRESSION TAG	UNP Q28RT0
D	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
D	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
D	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
D	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
D	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
D	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
E	1	MET	-	EXPRESSION TAG	UNP Q28RT0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
E	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
E	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
E	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
E	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
E	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
E	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
E	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
E	415	SER	-	EXPRESSION TAG	UNP Q28RT0
E	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
E	423	SER	-	EXPRESSION TAG	UNP Q28RT0
E	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
E	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
E	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
E	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
E	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
E	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
F	1	MET	-	EXPRESSION TAG	UNP Q28RT0
F	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
F	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
F	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
F	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
F	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
F	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
F	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
F	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
F	415	SER	-	EXPRESSION TAG	UNP Q28RT0
F	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
F	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
F	423	SER	-	EXPRESSION TAG	UNP Q28RT0
F	424	HIS	-	EXPRESSION TAG	UNP Q28RT0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
F	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
F	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
F	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
F	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
G	1	MET	-	EXPRESSION TAG	UNP Q28RT0
G	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
G	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
G	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
G	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
G	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
G	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
G	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
G	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
G	415	SER	-	EXPRESSION TAG	UNP Q28RT0
G	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	418	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
G	423	SER	-	EXPRESSION TAG	UNP Q28RT0
G	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
G	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
G	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
G	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
G	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
G	429	LYS	-	EXPRESSION TAG	UNP Q28RT0
H	1	MET	-	EXPRESSION TAG	UNP Q28RT0
H	2	VAL	-	EXPRESSION TAG	UNP Q28RT0
H	408	ALA	-	EXPRESSION TAG	UNP Q28RT0
H	409	GLU	-	EXPRESSION TAG	UNP Q28RT0
H	410	ASN	-	EXPRESSION TAG	UNP Q28RT0
H	411	LEU	-	EXPRESSION TAG	UNP Q28RT0
H	412	TYR	-	EXPRESSION TAG	UNP Q28RT0
H	413	PHE	-	EXPRESSION TAG	UNP Q28RT0
H	414	GLN	-	EXPRESSION TAG	UNP Q28RT0
H	415	SER	-	EXPRESSION TAG	UNP Q28RT0
H	416	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	417	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	418	HIS	-	EXPRESSION TAG	UNP Q28RT0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	419	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	420	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	421	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	422	TRP	-	EXPRESSION TAG	UNP Q28RT0
H	423	SER	-	EXPRESSION TAG	UNP Q28RT0
H	424	HIS	-	EXPRESSION TAG	UNP Q28RT0
H	425	PRO	-	EXPRESSION TAG	UNP Q28RT0
H	426	GLN	-	EXPRESSION TAG	UNP Q28RT0
H	427	PHE	-	EXPRESSION TAG	UNP Q28RT0
H	428	GLU	-	EXPRESSION TAG	UNP Q28RT0
H	429	LYS	-	EXPRESSION TAG	UNP Q28RT0

- Molecule 2 is water.

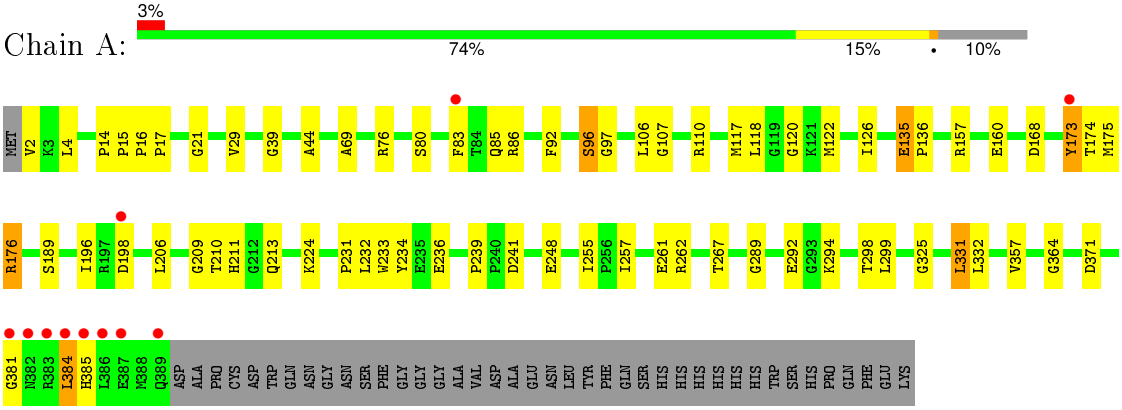
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	157	Total O 157 157	0	0
2	B	147	Total O 147 147	0	0
2	C	157	Total O 157 157	0	0
2	D	145	Total O 145 145	0	0
2	E	157	Total O 157 157	0	0
2	F	141	Total O 141 141	0	0
2	G	139	Total O 139 139	0	0
2	H	158	Total O 158 158	0	0

3 Residue-property plots

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.

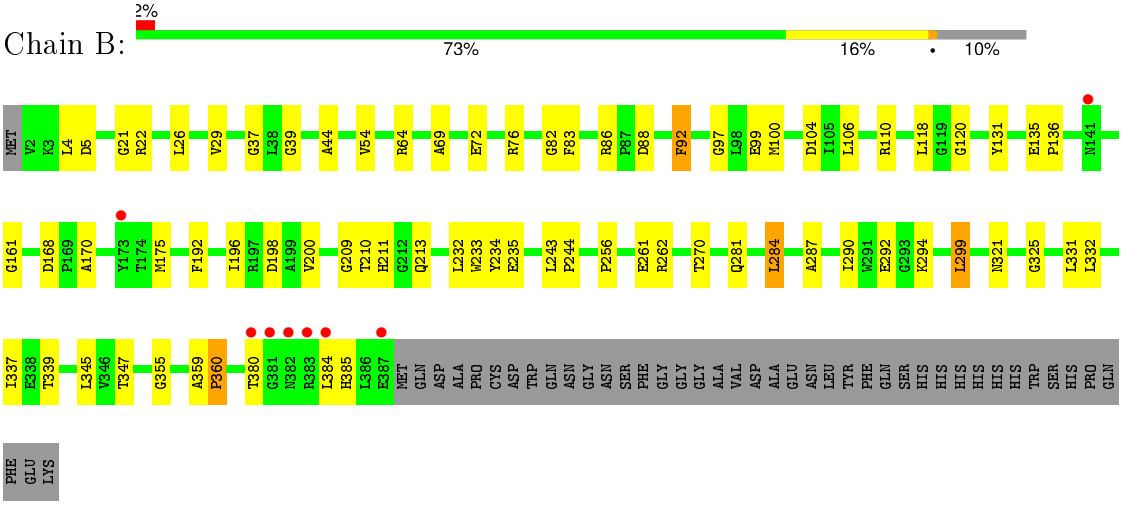
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain A:



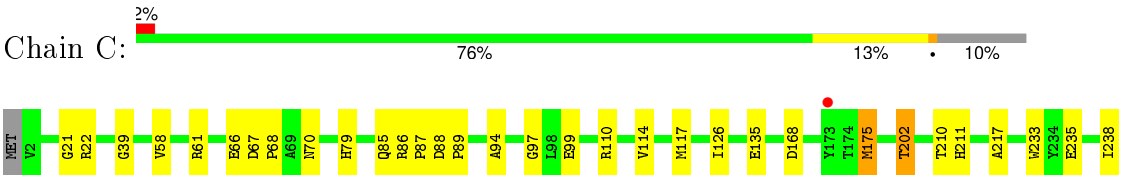
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

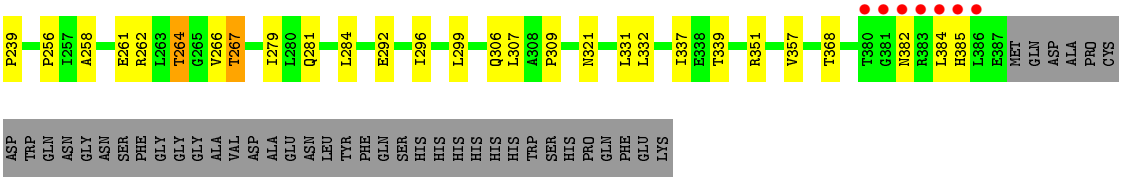
Chain B:



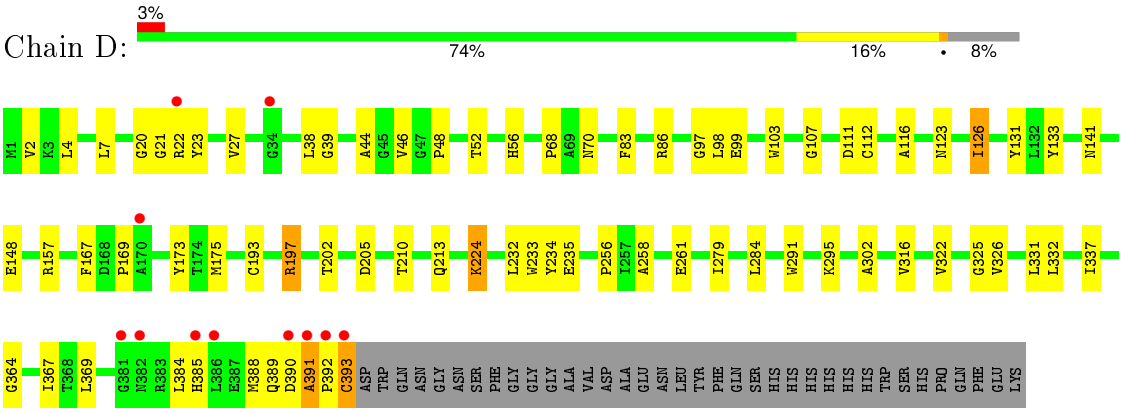
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain C:

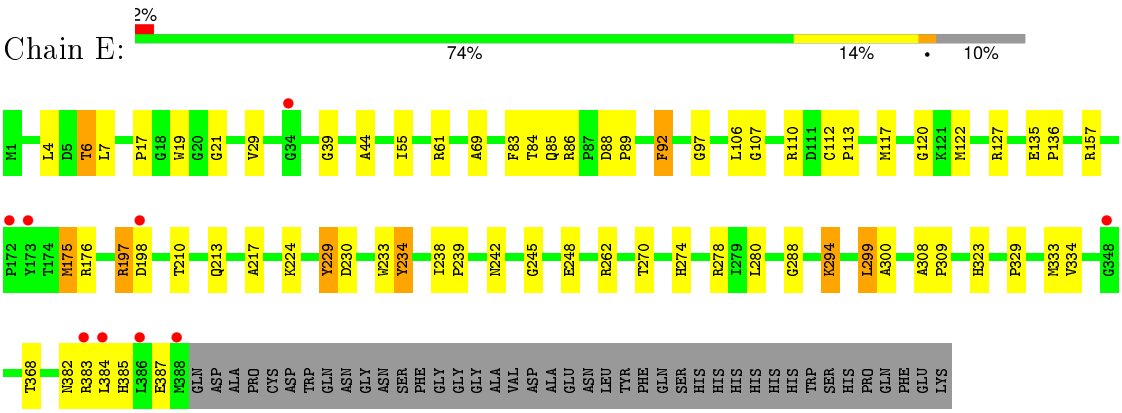




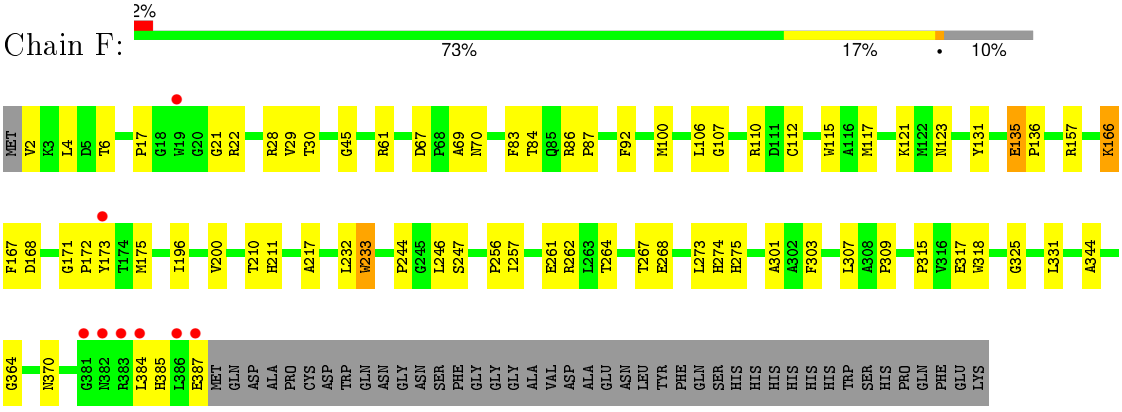
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

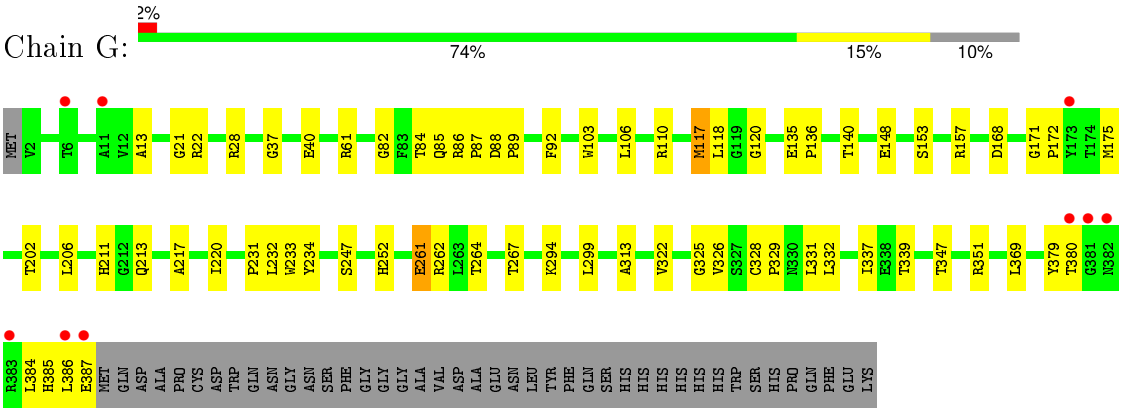


• Molecule 1: Mandelate racemase/muconate lactonizing enzyme



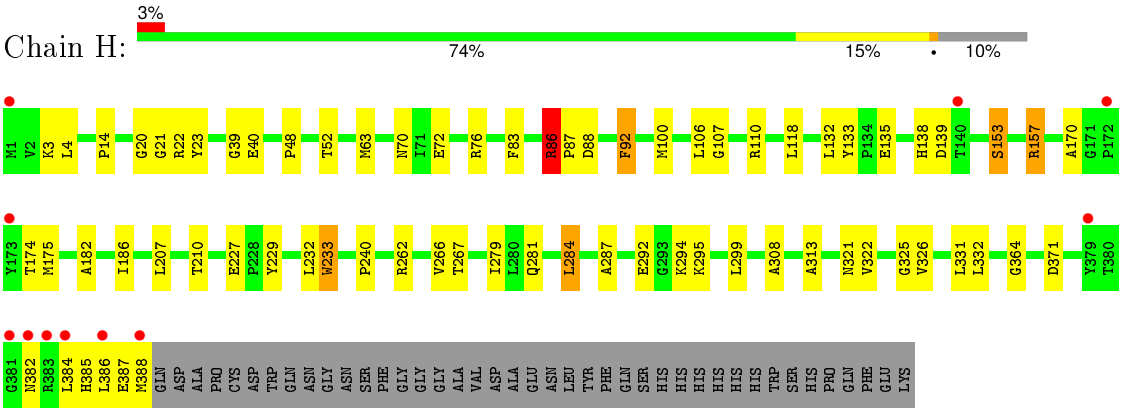
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain G:



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	126.91Å 126.63Å 126.78Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	44.88 – 2.50 44.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.88-2.50) 98.7 (44.88-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.41 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.211 , 0.245 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.0	EDS
Estimated twinning fraction	0.747 for H, K, L 0.091 for H, -K, -L 0.083 for -H, -L, -K 0.079 for -H, L, K 0.000 for -l,k,h 0.000 for -k,-h,-l 0.000 for k,h,-l 0.248 for -h,l,k 0.259 for -h,-l,-k 0.000 for k,l,h 0.000 for l,h,k 0.000 for k,-l,-h 0.000 for l,-h,-k 0.260 for -h,-k,l 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.747 for H, K, L 0.091 for H, -K, -L 0.083 for -H, -L, -K 0.079 for -H, L, K	Depositor
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Outliers	2 of 138036 reflections (0.001%)	Xtriage

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[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.

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Property	Value	Source
F_o,F_c correlation	0.85	EDS
Total number of atoms	24704	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.55	2/3026 (0.1%)	0.62	0/4136
1	B	0.48	1/3009 (0.0%)	0.62	2/4114 (0.0%)
1	C	0.46	0/3009	0.59	0/4114
1	D	0.55	0/3083	0.66	4/4214 (0.1%)
1	E	0.49	1/3025 (0.0%)	0.62	2/4134 (0.0%)
1	F	0.55	0/3009	0.60	0/4114
1	G	0.48	0/3029	0.60	0/4141
1	H	0.52	1/3025 (0.0%)	0.61	3/4134 (0.1%)
All	All	0.51	5/24215 (0.0%)	0.62	11/33101 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	229	TYR	CE1-CZ	-5.61	1.31	1.38
1	A	16	PRO	N-CD	5.60	1.55	1.47
1	A	17	PRO	N-CD	5.50	1.55	1.47
1	B	360	PRO	N-CD	5.14	1.55	1.47
1	H	87	PRO	N-CD	5.13	1.55	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	157	ARG	NE-CZ-NH2	8.46	124.53	120.30
1	E	157	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	D	157	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	H	157	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	E	230	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	359	ALA	C-N-CD	5.54	140.03	128.40
1	D	391	ALA	C-N-CD	5.50	139.95	128.40
1	D	2	VAL	N-CA-C	-5.47	96.24	111.00
1	H	157	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	B	360	PRO	CA-N-CD	-5.16	104.28	111.50
1	H	86	ARG	C-N-CD	5.07	139.04	128.40

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	2939	0	2857	46	0
1	B	2922	0	2840	40	0
1	C	2922	0	2840	44	0
1	D	2987	0	2904	55	0
1	E	2938	0	2861	59	0
1	F	2922	0	2840	45	0
1	G	2935	0	2855	40	0
1	H	2938	0	2861	40	0
2	A	157	0	0	2	0
2	B	147	0	0	0	0
2	C	157	0	0	1	0
2	D	145	0	0	1	0
2	E	157	0	0	2	0
2	F	141	0	0	1	0
2	G	139	0	0	0	0
2	H	158	0	0	0	0
All	All	24704	0	22858	323	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 7.

All (323) 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:E:4:LEU:HD22	1:E:29:VAL:HG11	1.46	0.95
1:C:126:ILE:HG23	1:C:331:LEU:HD21	1.54	0.89
1:A:83:PHE:CZ	1:C:211:HIS:HD2	1.90	0.89
1:E:217:ALA:HB1	1:F:256:PRO:HB3	1.56	0.87
1:D:389:GLN:OE1	1:D:391:ALA:HB3	1.75	0.86
1:E:21:GLY:HA3	1:E:385:HIS:CE1	2.09	0.86
1:E:198:ASP:HB3	2:E:608:HOH:O	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:TYR:HD1	1:D:388:MET:HE2	1.43	0.83
1:A:384:LEU:HD11	1:C:61:ARG:HD3	1.62	0.79
1:B:44:ALA:O	1:B:384:LEU:HD22	1.85	0.77
1:E:112:CYS:SG	1:E:117:MET:CE	2.73	0.76
1:D:389:GLN:HG2	1:D:391:ALA:H	1.50	0.76
1:C:126:ILE:CG2	1:C:331:LEU:HD21	2.15	0.75
1:A:21:GLY:HA3	1:A:385:HIS:CE1	2.22	0.74
1:A:325:GLY:HA2	1:A:331:LEU:HD13	1.69	0.74
1:F:135:GLU:HG3	1:F:136:PRO:HD2	1.69	0.74
1:B:294:LYS:NZ	1:H:72:GLU:OE2	2.21	0.73
1:D:389:GLN:CD	1:D:391:ALA:HB3	2.09	0.73
1:D:232:LEU:O	1:D:256:PRO:HG2	1.89	0.73
1:A:44:ALA:O	1:A:384:LEU:HD22	1.88	0.73
1:G:261:GLU:HG3	1:G:262:ARG:HG3	1.71	0.72
1:B:135:GLU:HG3	1:B:136:PRO:HD2	1.71	0.72
1:G:135:GLU:HG3	1:G:136:PRO:HD2	1.70	0.71
1:B:232:LEU:O	1:B:256:PRO:HG2	1.90	0.71
1:F:107:GLY:HA3	1:F:364:GLY:HA2	1.73	0.71
1:E:112:CYS:SG	1:E:117:MET:HE2	2.31	0.70
1:F:168:ASP:OD2	1:F:211:HIS:HE1	1.73	0.70
1:C:126:ILE:HG23	1:C:331:LEU:CD2	2.23	0.69
1:F:69:ALA:HA	1:F:106:LEU:HD11	1.75	0.69
1:D:210:THR:HB	1:D:213:GLN:OE1	1.93	0.68
1:D:392:PRO:O	1:D:393:CYS:HB2	1.91	0.68
1:E:112:CYS:SG	1:E:117:MET:HE3	2.32	0.68
1:B:72:GLU:O	1:B:76:ARG:HG2	1.94	0.68
1:F:168:ASP:OD2	1:F:211:HIS:CE1	2.47	0.67
1:D:126:ILE:HD11	1:D:326:VAL:HA	1.76	0.67
1:A:231:PRO:HG2	1:A:255:ILE:HG12	1.76	0.67
1:C:261:GLU:HG3	1:C:262:ARG:HG3	1.77	0.66
1:A:2:VAL:N	2:A:585:HOH:O	2.29	0.66
1:A:83:PHE:HZ	1:C:211:HIS:HD2	1.37	0.65
1:D:48:PRO:O	1:D:52:THR:HG23	1.97	0.65
1:E:69:ALA:HA	1:E:106:LEU:HD11	1.79	0.65
1:A:80:SER:OG	1:A:85:GLN:NE2	2.29	0.64
1:H:384:LEU:HB2	1:H:387:GLU:HG2	1.79	0.64
1:A:126:ILE:HG22	1:A:357:VAL:O	1.97	0.64
1:E:384:LEU:HD11	1:G:61:ARG:HD3	1.81	0.63
1:D:21:GLY:HA3	1:D:385:HIS:CE1	2.33	0.63
1:A:168:ASP:OD2	1:A:211:HIS:ND1	2.32	0.62
1:A:168:ASP:OD2	1:A:211:HIS:CE1	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:THR:HB	1:B:213:GLN:OE1	1.99	0.62
1:E:210:THR:HG21	1:E:234:TYR:HE1	1.64	0.62
1:H:153:SER:O	1:H:157:ARG:HG2	1.99	0.62
1:F:22:ARG:HD2	1:F:384:LEU:O	1.99	0.62
1:B:337:ILE:HG22	1:B:339:THR:HG23	1.81	0.61
1:E:309:PRO:HG2	1:E:334:VAL:HG12	1.80	0.61
1:D:173:TYR:HB3	1:D:213:GLN:HG3	1.82	0.61
1:D:173:TYR:CD1	1:D:388:MET:CE	2.83	0.61
1:E:197:ARG:NH1	1:E:229:TYR:O	2.34	0.61
1:E:4:LEU:CD2	1:E:29:VAL:HG11	2.27	0.61
1:B:256:PRO:HB3	1:F:217:ALA:HB1	1.82	0.61
1:B:21:GLY:HA3	1:B:385:HIS:CE1	2.36	0.60
1:D:173:TYR:HD1	1:D:388:MET:CE	2.13	0.60
1:B:211:HIS:HB3	1:D:83:PHE:HZ	1.66	0.60
1:C:70:ASN:HA	1:E:120:GLY:HA3	1.82	0.60
1:C:307:LEU:HG	1:C:309:PRO:HD3	1.84	0.60
1:A:83:PHE:CZ	1:C:211:HIS:CD2	2.82	0.59
1:B:22:ARG:HD2	1:B:384:LEU:O	2.03	0.59
1:D:22:ARG:HB2	1:D:385:HIS:HA	1.85	0.59
1:A:4:LEU:HD22	1:A:29:VAL:HG11	1.84	0.59
1:C:266:VAL:HG23	1:C:296:ILE:HG13	1.84	0.58
1:C:21:GLY:HA3	1:C:385:HIS:CE1	2.38	0.58
1:B:325:GLY:HA2	1:B:331:LEU:HD13	1.84	0.58
1:E:175:MET:HE2	1:E:176:ARG:CG	2.34	0.58
1:A:173:TYR:N	1:A:173:TYR:CD1	2.70	0.58
1:C:114:VAL:HA	1:C:117:MET:CE	2.34	0.57
1:A:126:ILE:CG2	1:A:357:VAL:HB	2.33	0.57
1:B:4:LEU:HD22	1:B:29:VAL:HG11	1.85	0.57
1:G:211:HIS:N	1:G:213:GLN:OE1	2.35	0.57
1:G:118:LEU:O	1:G:294:LYS:HE3	2.05	0.56
1:D:173:TYR:CD1	1:D:388:MET:HE2	2.30	0.56
1:D:325:GLY:HA2	1:D:331:LEU:HD13	1.88	0.56
1:F:273:LEU:HD22	1:F:303:PHE:HB2	1.87	0.56
1:F:232:LEU:O	1:F:256:PRO:HG2	2.05	0.56
1:E:197:ARG:HG2	1:E:197:ARG:NH1	2.20	0.56
1:G:337:ILE:HG22	1:G:339:THR:HG23	1.88	0.56
1:C:168:ASP:OD2	1:C:211:HIS:ND1	2.37	0.56
1:E:44:ALA:O	1:G:82:GLY:HA3	2.06	0.55
1:H:133:TYR:O	1:H:153:SER:OG	2.24	0.55
1:H:132:LEU:HD22	1:H:153:SER:HB3	1.88	0.55
1:H:281:GLN:HA	1:H:308:ALA:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ILE:O	1:B:200:VAL:HG22	2.07	0.55
1:A:261:GLU:HG3	1:A:262:ARG:HG3	1.87	0.54
1:B:69:ALA:HA	1:B:106:LEU:HD11	1.88	0.54
1:H:118:LEU:HD22	1:H:294:LYS:HG3	1.88	0.54
1:F:261:GLU:HG3	1:F:262:ARG:HG3	1.89	0.54
1:B:170:ALA:HB3	1:B:210:THR:HG22	1.90	0.54
1:G:22:ARG:HH12	1:G:387:GLU:H	1.55	0.54
1:C:22:ARG:HD3	1:C:384:LEU:O	2.08	0.54
1:B:88:ASP:O	1:B:92:PHE:HB2	2.07	0.54
1:E:262:ARG:HD2	1:G:84:THR:O	2.08	0.54
1:D:258:ALA:HB2	1:D:279:ILE:HB	1.89	0.54
1:G:118:LEU:HD22	1:G:294:LYS:HG3	1.89	0.54
1:B:261:GLU:HG3	1:B:262:ARG:HG3	1.90	0.53
1:B:168:ASP:HB2	1:B:209:GLY:O	2.07	0.53
1:A:267:THR:HA	2:A:566:HOH:O	2.07	0.53
1:C:284:LEU:HD12	1:C:321:ASN:OD1	2.08	0.53
1:D:7:LEU:HD11	1:D:27:VAL:HB	1.89	0.53
1:B:161:GLY:O	1:B:355:GLY:HA3	2.08	0.53
1:C:89:PRO:HD3	1:C:264:THR:HG21	1.89	0.53
1:B:170:ALA:CB	1:B:210:THR:HG22	2.39	0.52
1:E:61:ARG:HD3	1:G:384:LEU:HD11	1.92	0.52
1:A:196:ILE:HG22	1:A:206:LEU:HD11	1.92	0.52
1:D:133:TYR:OH	1:D:337:ILE:HG23	2.09	0.52
1:F:325:GLY:HA2	1:F:331:LEU:HD13	1.92	0.52
1:G:384:LEU:HB2	1:G:387:GLU:HG3	1.92	0.52
1:G:21:GLY:HA3	1:G:385:HIS:CE1	2.44	0.52
1:C:217:ALA:HB1	1:D:256:PRO:HB3	1.92	0.52
1:D:193:CYS:O	1:D:197:ARG:HB2	2.09	0.52
1:F:244:PRO:HA	1:F:275:HIS:CD2	2.45	0.52
1:H:20:GLY:O	1:H:385:HIS:HE1	1.92	0.52
1:D:123:ASN:HB2	1:D:126:ILE:HD11	1.90	0.51
1:A:135:GLU:HG3	1:A:136:PRO:HD2	1.92	0.51
1:E:210:THR:OG1	1:E:213:GLN:OE1	2.28	0.51
1:F:384:LEU:HD12	1:F:387:GLU:HG2	1.90	0.51
1:A:118:LEU:O	1:A:294:LYS:HE3	2.10	0.51
1:F:233:TRP:CD1	1:F:233:TRP:C	2.84	0.51
1:A:298:THR:HG21	1:D:295:LYS:HB2	1.92	0.51
1:A:69:ALA:HA	1:A:106:LEU:HD11	1.93	0.51
1:E:88:ASP:OD2	1:G:89:PRO:HG2	2.11	0.51
1:A:239:PRO:HB2	1:A:241:ASP:OD1	2.11	0.51
1:C:110:ARG:HD2	1:E:110:ARG:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:ARG:HH11	1:E:197:ARG:HG2	1.75	0.51
1:B:82:GLY:HA3	1:D:44:ALA:O	2.11	0.51
1:H:325:GLY:HA2	1:H:331:LEU:HD13	1.92	0.51
1:A:239:PRO:HB3	1:C:85:GLN:OE1	2.10	0.50
1:C:202:THR:O	1:C:202:THR:CG2	2.60	0.50
1:A:44:ALA:O	1:A:384:LEU:CD2	2.57	0.50
1:F:344:ALA:O	1:F:370:ASN:ND2	2.43	0.50
1:G:40:GLU:OE2	1:G:313:ALA:HB1	2.10	0.50
1:D:322:VAL:O	1:D:326:VAL:HG23	2.12	0.50
1:E:175:MET:HE2	1:E:176:ARG:HG3	1.92	0.50
1:C:267:THR:HB	2:C:524:HOH:O	2.11	0.50
1:E:44:ALA:O	1:E:384:LEU:HD22	2.12	0.50
1:C:337:ILE:HG22	1:C:339:THR:HG23	1.92	0.50
1:H:135:GLU:HB2	1:H:138:HIS:CE1	2.46	0.50
1:D:4:LEU:HD21	1:D:68:PRO:HB3	1.94	0.49
1:D:112:CYS:SG	1:D:116:ALA:HB3	2.51	0.49
1:D:23:TYR:CZ	1:D:48:PRO:HD3	2.48	0.49
1:F:61:ARG:HD3	1:H:384:LEU:HD11	1.95	0.49
1:F:83:PHE:HA	1:H:388:MET:HG3	1.93	0.49
1:B:120:GLY:HA3	1:H:70:ASN:HA	1.94	0.49
1:D:39:GLY:HA3	1:D:97:GLY:O	2.13	0.49
1:A:232:LEU:HD21	1:A:332:LEU:HD21	1.94	0.49
1:G:325:GLY:HA2	1:G:331:LEU:HD13	1.94	0.49
1:A:299:LEU:HD21	1:D:302:ALA:CB	2.42	0.49
1:G:106:LEU:O	1:G:110:ARG:HG3	2.12	0.49
1:C:114:VAL:HA	1:C:117:MET:HE2	1.94	0.49
1:A:96:SER:HB3	1:A:289:GLY:N	2.28	0.48
1:B:235:GLU:HG3	1:B:281:GLN:OE1	2.12	0.48
1:G:103:TRP:HZ3	1:G:117:MET:HB3	1.78	0.48
1:H:40:GLU:OE2	1:H:313:ALA:HB1	2.14	0.48
1:E:384:LEU:HD12	1:E:387:GLU:HG2	1.94	0.48
1:A:224:LYS:HD3	1:A:224:LYS:HA	1.64	0.48
1:H:139:ASP:OD1	1:H:139:ASP:C	2.52	0.48
1:D:235:GLU:HA	1:D:258:ALA:O	2.13	0.48
1:C:88:ASP:C	1:C:88:ASP:OD1	2.52	0.48
1:G:220:ILE:HG12	1:G:252:HIS:HB2	1.95	0.48
1:D:258:ALA:HA	1:D:279:ILE:O	2.12	0.48
1:D:224:LYS:HA	1:D:224:LYS:HD3	1.52	0.48
1:E:6:THR:O	1:E:29:VAL:HA	2.13	0.48
1:H:4:LEU:HD12	1:H:63:MET:O	2.14	0.48
1:C:266:VAL:HG22	1:C:299:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:GLY:HA2	1:E:117:MET:HE3	1.96	0.48
1:D:232:LEU:O	1:D:232:LEU:HD23	2.13	0.48
1:F:262:ARG:HD3	1:H:83:PHE:O	2.14	0.48
1:F:100:MET:HE2	1:F:317:GLU:HA	1.96	0.47
1:D:232:LEU:HD21	1:D:332:LEU:HD21	1.97	0.47
1:B:287:ALA:O	1:B:292:GLU:HG2	2.14	0.47
1:E:383:ARG:HA	1:G:61:ARG:HH12	1.79	0.47
1:B:211:HIS:HB3	1:D:83:PHE:CZ	2.48	0.47
1:G:153:SER:O	1:G:157:ARG:HG2	2.14	0.47
1:D:27:VAL:HG21	1:D:98:LEU:HD23	1.97	0.47
1:A:210:THR:HB	1:A:213:GLN:OE1	2.14	0.47
1:F:112:CYS:SG	1:F:117:MET:CE	3.03	0.47
1:B:284:LEU:HD22	1:B:321:ASN:OD1	2.15	0.47
1:F:301:ALA:HA	2:F:553:HOH:O	2.15	0.46
1:G:322:VAL:O	1:G:326:VAL:HG23	2.15	0.46
1:E:113:PRO:HB3	1:E:323:HIS:HE1	1.80	0.46
1:H:284:LEU:HD22	1:H:321:ASN:OD1	2.15	0.46
1:F:70:ASN:HA	1:G:120:GLY:HA3	1.96	0.46
1:H:21:GLY:HA3	1:H:385:HIS:CE1	2.51	0.46
1:C:22:ARG:CD	1:C:384:LEU:O	2.63	0.46
1:A:39:GLY:HA3	1:A:97:GLY:O	2.14	0.46
1:G:13:ALA:HB2	1:G:379:TYR:HD1	1.79	0.46
1:F:246:LEU:HD22	1:F:257:ILE:HG21	1.96	0.46
1:H:233:TRP:HE3	1:H:279:ILE:HD13	1.80	0.46
1:C:110:ARG:CD	1:E:110:ARG:HD3	2.45	0.46
1:H:386:LEU:HA	1:H:386:LEU:HD23	1.83	0.46
1:B:118:LEU:O	1:B:294:LYS:HE3	2.15	0.46
1:H:72:GLU:O	1:H:76:ARG:HG2	2.15	0.46
1:D:38:LEU:HD11	1:D:369:LEU:HB2	1.97	0.46
1:F:168:ASP:CG	1:F:211:HIS:HE1	2.20	0.46
1:A:168:ASP:CG	1:A:209:GLY:O	2.55	0.46
1:F:107:GLY:HA3	1:F:364:GLY:CA	2.45	0.45
1:F:112:CYS:SG	1:F:117:MET:HE3	2.56	0.45
1:B:232:LEU:HD21	1:B:332:LEU:HD21	1.98	0.45
1:F:21:GLY:HA3	1:F:385:HIS:CE1	2.51	0.45
1:G:28:ARG:HH21	1:G:369:LEU:HB3	1.81	0.45
1:F:196:ILE:O	1:F:200:VAL:HG22	2.17	0.45
1:F:6:THR:OG1	1:F:30:THR:HB	2.17	0.45
1:E:110:ARG:HB2	1:E:117:MET:CE	2.47	0.45
1:E:210:THR:CG2	1:E:234:TYR:HE1	2.29	0.45
1:C:256:PRO:HB3	1:G:217:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:THR:O	1:H:262:ARG:NH1	2.50	0.44
1:C:258:ALA:HB2	1:C:279:ILE:HB	1.99	0.44
1:E:7:LEU:HD21	1:E:55:ILE:HG22	1.99	0.44
1:E:110:ARG:HB2	1:E:117:MET:HE1	1.99	0.44
1:E:197:ARG:HH11	1:E:197:ARG:CG	2.30	0.44
1:F:110:ARG:HD2	1:G:110:ARG:HD3	1.98	0.44
1:H:240:PRO:HD3	1:H:262:ARG:NH2	2.32	0.44
1:A:120:GLY:HA3	1:D:70:ASN:HA	2.00	0.44
1:D:103:TRP:CZ2	1:D:291:TRP:CE3	3.05	0.44
1:H:322:VAL:O	1:H:326:VAL:HG23	2.18	0.44
1:D:173:TYR:CD1	1:D:388:MET:HE3	2.51	0.44
1:D:20:GLY:O	1:D:385:HIS:HE1	2.01	0.44
1:C:66:GLU:OE2	1:C:70:ASN:ND2	2.50	0.44
1:A:76:ARG:HB3	1:C:175:MET:O	2.16	0.44
1:G:103:TRP:CZ3	1:G:117:MET:HB3	2.53	0.44
1:F:4:LEU:HD22	1:F:29:VAL:HG11	1.99	0.44
1:B:83:PHE:HA	1:D:388:MET:HG3	2.00	0.44
1:F:171:GLY:HA3	1:F:172:PRO:HD3	1.87	0.44
1:D:56:HIS:HB3	2:D:581:HOH:O	2.18	0.44
1:D:22:ARG:HD2	1:D:384:LEU:O	2.18	0.44
1:H:232:LEU:HD21	1:H:332:LEU:HD21	2.00	0.44
1:C:58:VAL:HG21	1:C:94:ALA:HB3	2.00	0.44
1:A:83:PHE:HZ	1:C:211:HIS:CD2	2.27	0.43
1:A:157:ARG:HD3	1:A:160:GLU:OE1	2.18	0.43
1:G:232:LEU:HD21	1:G:332:LEU:HD21	2.00	0.43
1:G:87:PRO:HB3	1:G:264:THR:HG23	2.01	0.43
1:B:26:LEU:HD11	1:B:345:LEU:HD21	2.00	0.43
1:H:207:LEU:HD21	1:H:232:LEU:HD22	2.00	0.43
1:C:238:ILE:HB	1:C:239:PRO:CD	2.49	0.43
1:H:14:PRO:HD2	1:H:22:ARG:O	2.18	0.43
1:B:209:GLY:HA2	1:B:235:GLU:HB3	2.01	0.43
1:B:5:ASP:O	1:B:64:ARG:NE	2.50	0.43
1:E:135:GLU:HG3	1:E:136:PRO:HD2	2.01	0.43
1:B:100:MET:HA	1:B:290:ILE:HD12	2.00	0.43
1:C:306:GLN:OE1	1:C:332:LEU:HD13	2.19	0.43
1:A:384:LEU:HD11	1:C:61:ARG:CD	2.41	0.42
1:D:316:VAL:HG22	1:D:367:ILE:HD12	2.01	0.42
1:F:307:LEU:HG	1:F:309:PRO:HD3	2.01	0.42
1:A:234:TYR:HB3	1:A:257:ILE:HD13	2.00	0.42
1:A:210:THR:OG1	1:A:236:GLU:O	2.33	0.42
1:E:83:PHE:CG	1:E:83:PHE:O	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:ARG:O	1:C:357:VAL:HG13	2.19	0.42
1:E:122:MET:HE2	1:E:329:PRO:HA	2.00	0.42
1:D:167:PHE:HD2	1:D:169:PRO:HD3	1.85	0.42
1:C:39:GLY:HA3	1:C:97:GLY:O	2.19	0.42
1:E:239:PRO:HB3	1:G:85:GLN:OE1	2.20	0.42
1:B:37:GLY:HA3	1:B:104:ASP:HB3	2.01	0.42
1:E:83:PHE:HB3	1:G:386:LEU:HB3	2.00	0.42
1:E:92:PHE:CD2	1:E:288:GLY:HA2	2.54	0.42
1:F:315:PRO:HA	1:F:318:TRP:HB3	2.02	0.42
1:E:224:LYS:HD3	1:E:224:LYS:HA	1.81	0.42
1:G:168:ASP:OD2	1:G:211:HIS:CE1	2.73	0.42
1:F:166:LYS:HG3	1:F:167:PHE:N	2.34	0.42
1:E:39:GLY:HA3	1:E:97:GLY:O	2.19	0.42
1:F:167:PHE:CD1	1:F:167:PHE:N	2.87	0.42
1:H:182:ALA:O	1:H:186:ILE:HG13	2.19	0.42
1:G:22:ARG:HD2	1:G:384:LEU:O	2.19	0.42
1:F:168:ASP:CG	1:F:211:HIS:CE1	2.94	0.42
1:D:205:ASP:CG	1:D:232:LEU:HD12	2.40	0.41
1:B:243:LEU:N	1:B:244:PRO:CD	2.82	0.41
1:F:87:PRO:HB3	1:F:264:THR:HG23	2.01	0.41
1:A:14:PRO:HA	1:A:15:PRO:HD2	1.93	0.41
1:D:389:GLN:CD	1:D:391:ALA:CB	2.86	0.41
1:E:175:MET:H	1:E:175:MET:HG3	1.67	0.41
1:E:127:ARG:NH1	2:E:573:HOH:O	2.51	0.41
1:E:83:PHE:O	1:E:83:PHE:CD2	2.73	0.41
1:A:107:GLY:HA3	1:A:364:GLY:HA2	2.02	0.41
1:D:148:GLU:H	1:D:148:GLU:CD	2.23	0.41
1:D:205:ASP:HB3	1:D:232:LEU:HB2	2.03	0.41
1:D:107:GLY:HA3	1:D:364:GLY:HA2	2.00	0.41
1:E:17:PRO:HB2	1:E:19:TRP:CE2	2.55	0.41
1:G:206:LEU:HB2	1:G:231:PRO:HA	2.02	0.41
1:A:110:ARG:HB2	1:A:117:MET:CE	2.50	0.41
1:C:79:HIS:HE1	1:C:87:PRO:HD3	1.85	0.41
1:F:84:THR:O	1:H:262:ARG:HD2	2.21	0.41
1:G:328:CYS:HA	1:G:329:PRO:HD3	1.90	0.41
1:B:192:PHE:O	1:B:196:ILE:HG13	2.20	0.41
1:E:294:LYS:HD2	1:E:294:LYS:HA	1.63	0.41
1:F:268:GLU:OE2	1:H:86:ARG:NH1	2.47	0.41
1:E:245:GLY:O	1:E:248:GLU:HG2	2.19	0.41
1:C:235:GLU:HG3	1:C:281:GLN:OE1	2.21	0.41
1:A:248:GLU:CD	1:E:278:ARG:HE	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:GLU:C	1:H:229:TYR:H	2.24	0.41
1:H:106:LEU:O	1:H:110:ARG:HG3	2.21	0.41
1:H:107:GLY:HA3	1:H:364:GLY:HA2	2.03	0.41
1:H:170:ALA:HB3	1:H:210:THR:HG22	2.02	0.41
1:B:54:VAL:HG13	1:D:46:VAL:HG11	2.03	0.41
1:B:39:GLY:HA3	1:B:97:GLY:O	2.20	0.41
1:A:298:THR:CG2	1:D:295:LYS:HB2	2.51	0.41
1:F:112:CYS:HG	1:F:117:MET:HE3	1.86	0.41
1:E:238:ILE:HB	1:E:239:PRO:CD	2.51	0.41
1:E:238:ILE:HD11	1:E:242:ASN:O	2.21	0.41
1:F:115:TRP:CZ3	1:F:121:LYS:HB2	2.56	0.41
1:H:287:ALA:O	1:H:292:GLU:HG2	2.21	0.41
1:H:88:ASP:O	1:H:92:PHE:HB2	2.21	0.41
1:C:110:ARG:CD	1:E:110:ARG:CD	2.99	0.40
1:G:28:ARG:HA	1:G:37:GLY:O	2.22	0.40
1:A:174:THR:OG1	1:A:176:ARG:HB2	2.20	0.40
1:H:266:VAL:HG21	1:H:295:LYS:HB3	2.02	0.40
1:E:308:ALA:HA	1:E:333:MET:O	2.21	0.40
1:C:67:ASP:HA	1:C:68:PRO:HD2	1.82	0.40
1:E:84:THR:O	1:G:262:ARG:HD2	2.21	0.40
1:G:171:GLY:HA3	1:G:172:PRO:HD3	1.80	0.40
1:E:89:PRO:HG2	1:G:88:ASP:OD2	2.21	0.40
1:B:270:THR:OG1	1:B:299:LEU:HD22	2.21	0.40
1:C:88:ASP:HA	1:C:89:PRO:HD2	1.88	0.40
1:E:280:LEU:HD12	1:E:300:ALA:HB2	2.03	0.40
1:H:39:GLY:HA2	1:H:100:MET:HE2	2.03	0.40
1:H:23:TYR:CZ	1:H:48:PRO:HD3	2.57	0.40
1:F:2:VAL:O	1:F:67:ASP:HA	2.22	0.40
1:E:270:THR:OG1	1:E:299:LEU:HD22	2.22	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	386/429 (90%)	362 (94%)	23 (6%)	1 (0%)	46 68
1	B	384/429 (90%)	362 (94%)	22 (6%)	0	100 100
1	C	384/429 (90%)	360 (94%)	24 (6%)	0	100 100
1	D	393/429 (92%)	381 (97%)	12 (3%)	0	100 100
1	E	386/429 (90%)	366 (95%)	20 (5%)	0	100 100
1	F	384/429 (90%)	368 (96%)	15 (4%)	1 (0%)	46 68
1	G	386/429 (90%)	368 (95%)	18 (5%)	0	100 100
1	H	386/429 (90%)	371 (96%)	15 (4%)	0	100 100
All	All	3089/3432 (90%)	2938 (95%)	149 (5%)	2 (0%)	56 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	GLY
1	F	45	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	293/327 (90%)	278 (95%)	15 (5%)	29 52
1	B	291/327 (89%)	277 (95%)	14 (5%)	31 55
1	C	291/327 (89%)	279 (96%)	12 (4%)	37 63
1	D	299/327 (91%)	283 (95%)	16 (5%)	27 49
1	E	293/327 (90%)	280 (96%)	13 (4%)	35 60
1	F	291/327 (89%)	275 (94%)	16 (6%)	27 48
1	G	293/327 (90%)	277 (94%)	16 (6%)	27 48
1	H	293/327 (90%)	280 (96%)	13 (4%)	35 60
All	All	2344/2616 (90%)	2229 (95%)	115 (5%)	31 55

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	92	PHE
1	A	96	SER
1	A	122	MET
1	A	135	GLU
1	A	173	TYR
1	A	175	MET
1	A	176	ARG
1	A	189	SER
1	A	198	ASP
1	A	233	TRP
1	A	292	GLU
1	A	331	LEU
1	A	371	ASP
1	A	384	LEU
1	B	86	ARG
1	B	92	PHE
1	B	99	GLU
1	B	110	ARG
1	B	131	TYR
1	B	175	MET
1	B	198	ASP
1	B	233	TRP
1	B	234	TYR
1	B	284	LEU
1	B	299	LEU
1	B	347	THR
1	B	360	PRO
1	B	380	THR
1	C	86	ARG
1	C	99	GLU
1	C	135	GLU
1	C	175	MET
1	C	202	THR
1	C	210	THR
1	C	233	TRP
1	C	264	THR
1	C	267	THR
1	C	292	GLU
1	C	368	THR
1	C	382	ASN
1	D	86	ARG
1	D	99	GLU

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Mol	Chain	Res	Type
1	D	111	ASP
1	D	126	ILE
1	D	131	TYR
1	D	141	ASN
1	D	175	MET
1	D	197	ARG
1	D	202	THR
1	D	224	LYS
1	D	233	TRP
1	D	234	TYR
1	D	261	GLU
1	D	284	LEU
1	D	390	ASP
1	D	393	CYS
1	E	6	THR
1	E	85	GLN
1	E	86	ARG
1	E	92	PHE
1	E	175	MET
1	E	197	ARG
1	E	233	TRP
1	E	234	TYR
1	E	274	HIS
1	E	294	LYS
1	E	299	LEU
1	E	368	THR
1	E	382	ASN
1	F	17	PRO
1	F	28	ARG
1	F	86	ARG
1	F	92	PHE
1	F	123	ASN
1	F	131	TYR
1	F	135	GLU
1	F	157	ARG
1	F	166	LYS
1	F	173	TYR
1	F	175	MET
1	F	210	THR
1	F	233	TRP
1	F	247	SER
1	F	267	THR

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Mol	Chain	Res	Type
1	F	274	HIS
1	G	86	ARG
1	G	92	PHE
1	G	117	MET
1	G	140	THR
1	G	148	GLU
1	G	175	MET
1	G	202	THR
1	G	233	TRP
1	G	234	TYR
1	G	247	SER
1	G	261	GLU
1	G	267	THR
1	G	299	LEU
1	G	347	THR
1	G	351	ARG
1	G	380	THR
1	H	3	LYS
1	H	52	THR
1	H	86	ARG
1	H	92	PHE
1	H	153	SER
1	H	174	THR
1	H	175	MET
1	H	233	TRP
1	H	267	THR
1	H	284	LEU
1	H	299	LEU
1	H	371	ASP
1	H	382	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	281	GLN
1	B	56	HIS
1	B	274	HIS
1	B	275	HIS
1	C	211	HIS
1	C	382	ASN
1	C	385	HIS

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Mol	Chain	Res	Type
1	D	211	HIS
1	D	385	HIS
1	E	56	HIS
1	E	271	GLN
1	G	310	HIS
1	H	274	HIS
1	H	385	HIS

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

There are no ligands in this entry.

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	388/429 (90%)	0.03	11 (2%)	56	61	21, 29, 42, 75	0
1	B	386/429 (89%)	-0.05	8 (2%)	67	71	20, 28, 39, 73	0
1	C	386/429 (89%)	-0.04	8 (2%)	67	71	20, 27, 39, 69	0
1	D	393/429 (91%)	0.07	11 (2%)	56	61	20, 28, 45, 86	0
1	E	388/429 (90%)	0.04	9 (2%)	64	67	21, 29, 41, 69	0
1	F	386/429 (89%)	-0.03	8 (2%)	67	71	21, 28, 41, 81	0
1	G	386/429 (89%)	-0.01	9 (2%)	64	67	19, 27, 39, 81	0
1	H	388/429 (90%)	0.02	11 (2%)	56	61	20, 28, 42, 64	0
All	All	3101/3432 (90%)	0.00	75 (2%)	62	66	19, 28, 41, 86	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	173	TYR	5.5
1	C	381	GLY	5.3
1	A	386	LEU	5.2
1	G	386	LEU	5.0
1	D	381	GLY	4.9
1	F	381	GLY	4.8
1	B	173	TYR	4.7
1	A	381	GLY	4.4
1	D	382	ASN	4.3
1	G	382	ASN	4.1
1	D	390	ASP	4.0
1	A	383	ARG	4.0
1	H	173	TYR	3.9
1	F	382	ASN	3.7
1	A	173	TYR	3.7
1	A	382	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	387	GLU	3.7
1	E	384	LEU	3.7
1	B	382	ASN	3.5
1	C	384	LEU	3.5
1	G	173	TYR	3.4
1	G	383	ARG	3.4
1	B	383	ARG	3.3
1	E	173	TYR	3.3
1	F	386	LEU	3.3
1	C	383	ARG	3.2
1	E	172	PRO	3.2
1	G	387	GLU	3.2
1	H	386	LEU	3.2
1	E	386	LEU	3.2
1	D	385	HIS	3.2
1	H	172	PRO	3.1
1	D	386	LEU	3.0
1	E	383	ARG	3.0
1	G	380	THR	3.0
1	F	383	ARG	2.9
1	F	384	LEU	2.9
1	A	389	GLN	2.9
1	D	393	CYS	2.8
1	A	83	PHE	2.8
1	C	382	ASN	2.8
1	E	388	MET	2.7
1	H	1	MET	2.7
1	H	379	TYR	2.7
1	D	392	PRO	2.6
1	H	381	GLY	2.6
1	D	170	ALA	2.6
1	H	382	ASN	2.6
1	D	391	ALA	2.5
1	F	173	TYR	2.5
1	G	381	GLY	2.5
1	H	388	MET	2.5
1	C	380	THR	2.5
1	H	383	ARG	2.5
1	B	384	LEU	2.4
1	E	348	GLY	2.4
1	G	11	ALA	2.4
1	E	34	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	19	TRP	2.3
1	D	34	GLY	2.3
1	A	198	ASP	2.3
1	B	380	THR	2.3
1	A	384	LEU	2.2
1	G	6	THR	2.2
1	E	198	ASP	2.2
1	C	386	LEU	2.2
1	A	385	HIS	2.2
1	B	141	ASN	2.2
1	D	22	ARG	2.2
1	A	387	GLU	2.1
1	H	384	LEU	2.1
1	C	385	HIS	2.1
1	B	381	GLY	2.1
1	B	387	GLU	2.1
1	H	140	THR	2.0

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 carbohydrates 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.