



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:08 AM UTC

PDB ID : 4J3Z / pdb_00004j3z
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.; Laffuer, 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

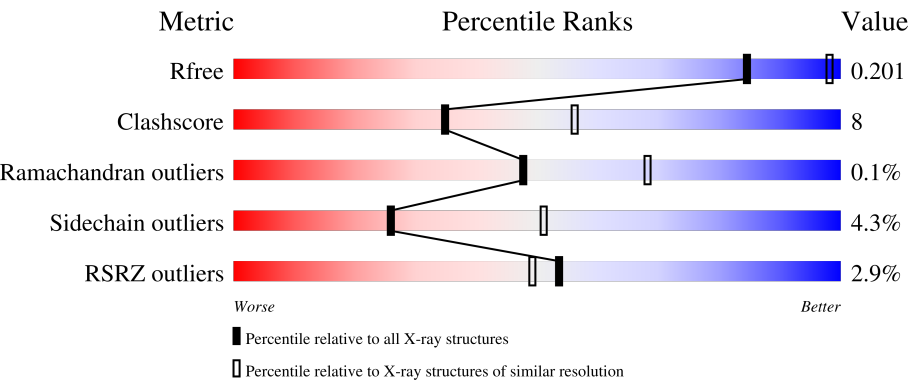
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	429	3% 71% 16% • 10%
1	B	429	2% 72% 16% • 10%
1	C	429	• 76% 13% • 10%
1	D	429	4% 72% 17% • 8%

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Mol	Chain	Length	Quality of chain
1	E	429	4% 73% 16% • 10%
1	F	429	3% 73% 17% 10%
1	G	429	2% 74% 15% • 10%
1	H	429	2% 74% 16% • 10%

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

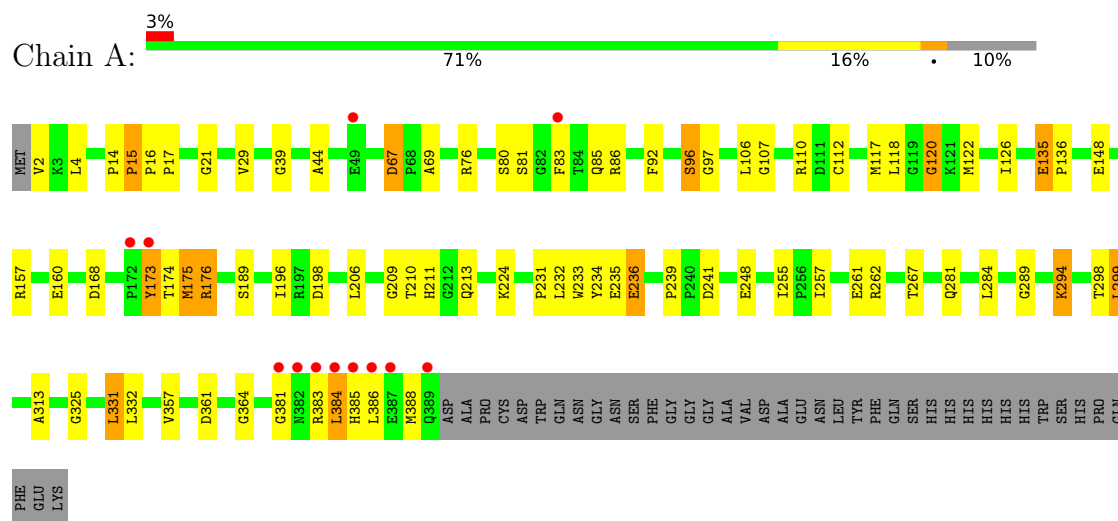
- Molecule 2 is water.

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

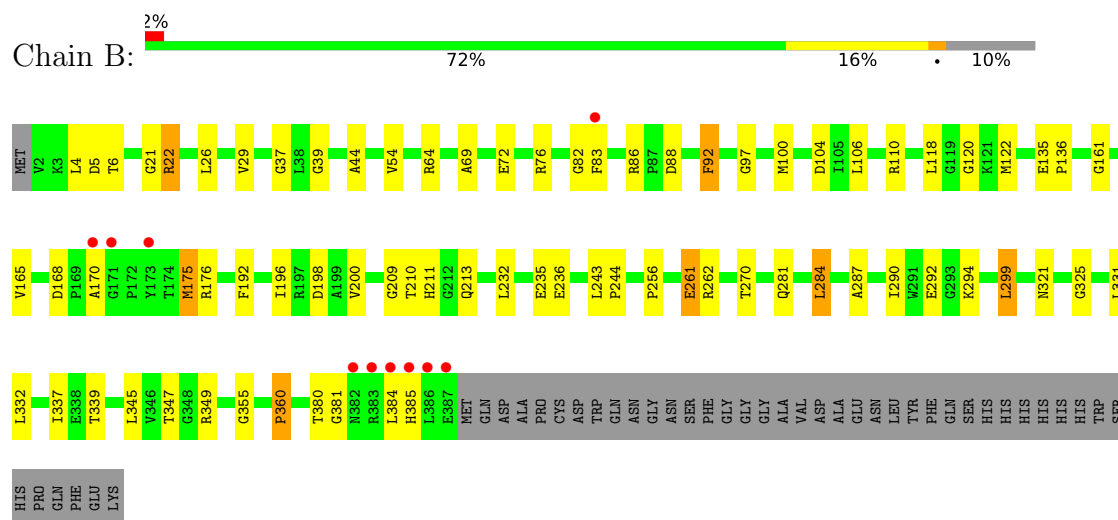
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

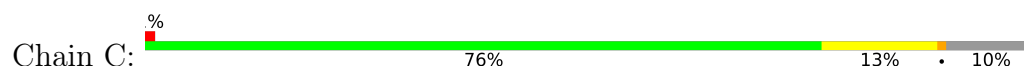
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

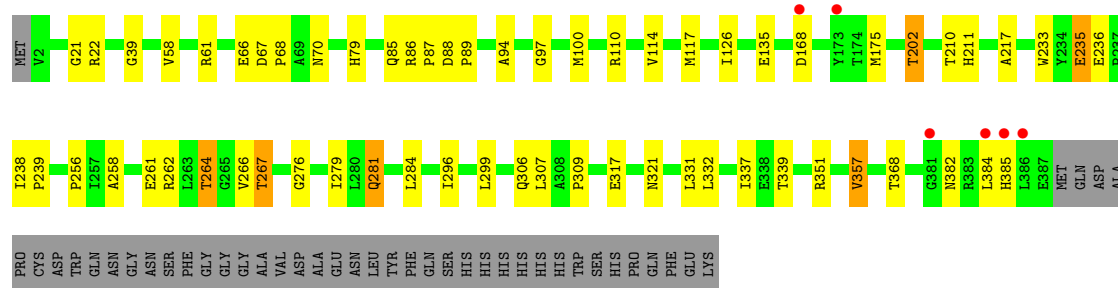


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

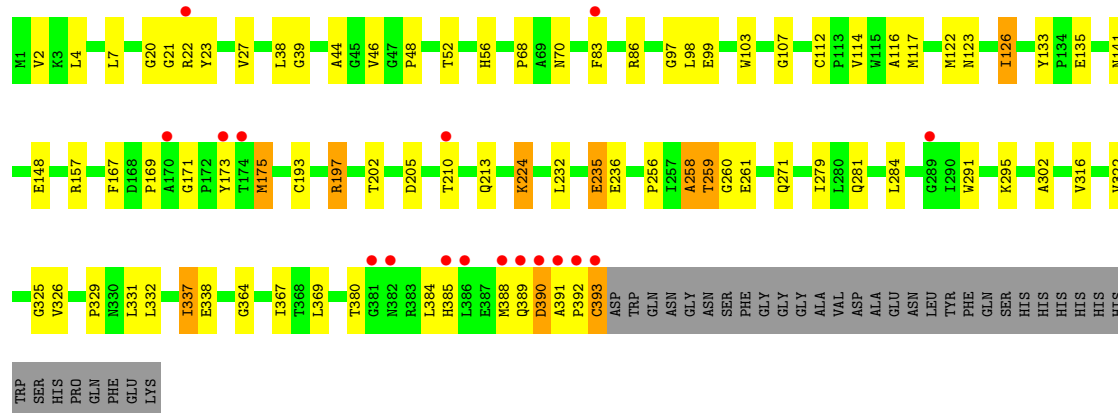


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

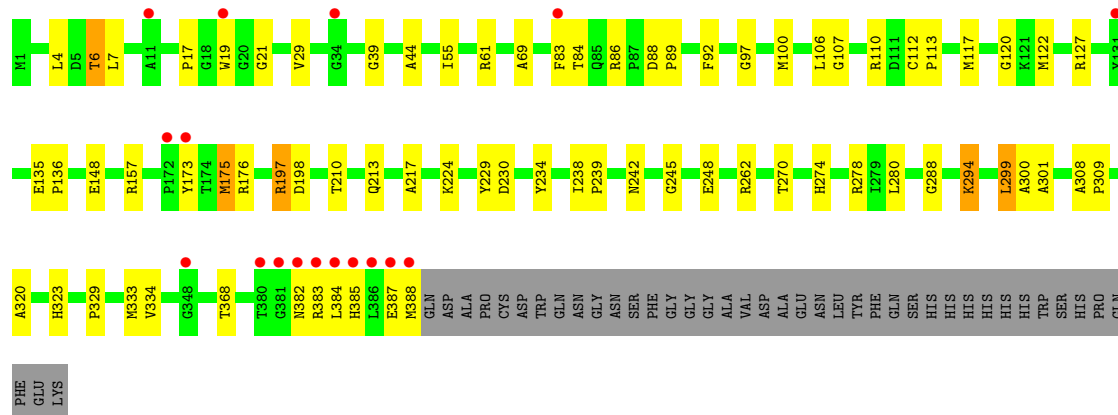




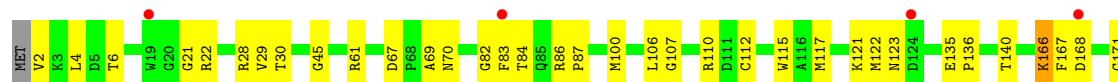
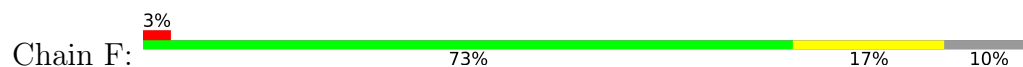
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

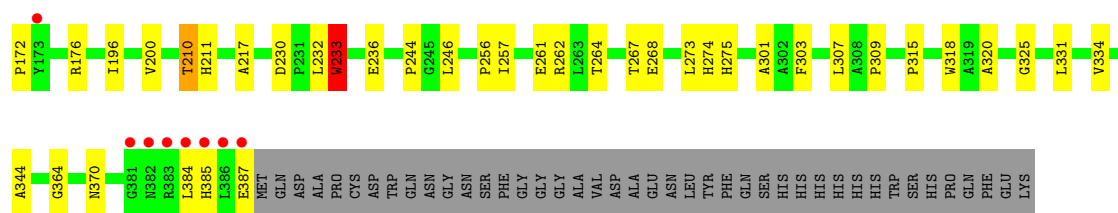


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

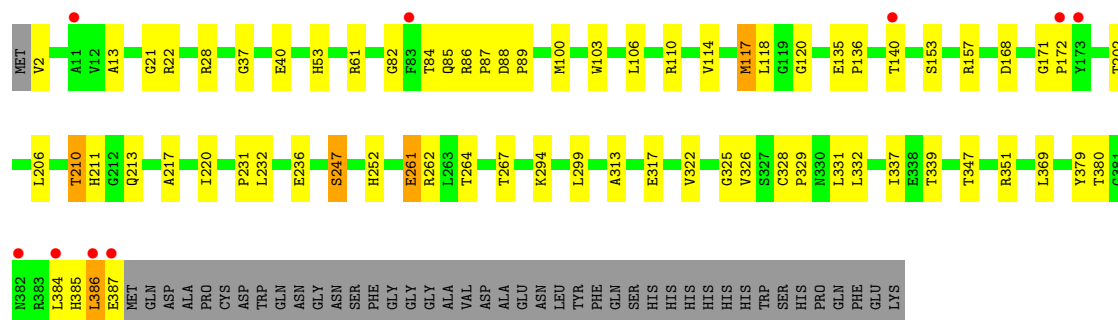
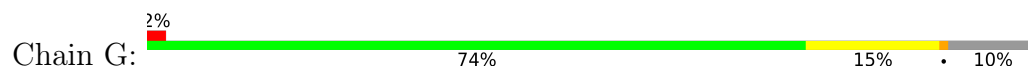


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

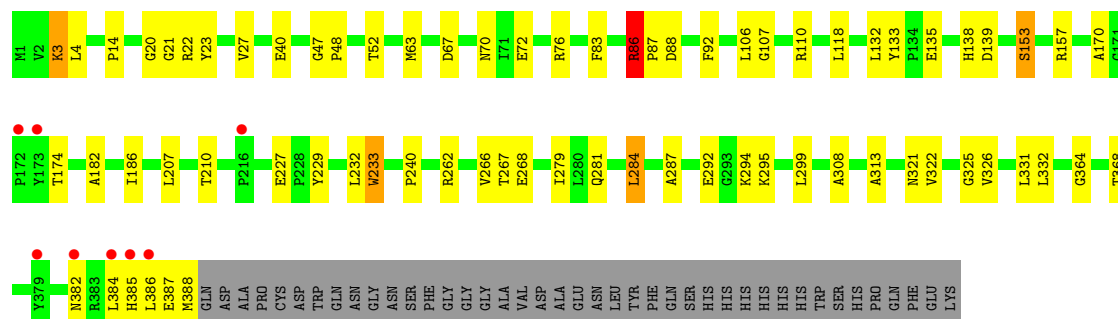
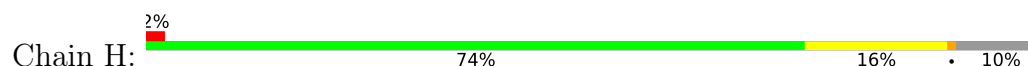




● Molecule 1: Mandelate racemase/muconate lactonizing enzyme



● Molecule 1: Mandelate racemase/muconate lactonizing enzyme



4 Data and refinement statistics

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) 98.9 (44.88-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.211 , 0.245 0.177 , 0.201	Depositor DCC
R_{free} test set	6950 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	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
Outliers	2 of 138036 reflections (0.001%)	Xtriage
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

¹Intensities estimated from amplitudes.

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

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 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	0.73	6/3026 (0.2%)	0.98	10/4136 (0.2%)
1	B	0.67	4/3009 (0.1%)	0.95	4/4114 (0.1%)
1	C	0.62	3/3009 (0.1%)	0.90	3/4114 (0.1%)
1	D	0.70	5/3083 (0.2%)	0.97	7/4214 (0.2%)
1	E	0.64	2/3025 (0.1%)	0.92	1/4134 (0.0%)
1	F	0.77	4/3009 (0.1%)	0.93	2/4114 (0.0%)
1	G	0.64	2/3029 (0.1%)	0.91	2/4141 (0.0%)
1	H	0.68	4/3025 (0.1%)	0.94	7/4134 (0.2%)
All	All	0.68	30/24215 (0.1%)	0.94	36/33101 (0.1%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	230	ASP	C-O	-13.65	1.17	1.23
1	A	313	ALA	C-O	-10.88	1.16	1.24
1	F	236	GLU	CA-C	-9.93	1.47	1.53
1	D	236	GLU	C-O	-9.37	1.19	1.23
1	B	236	GLU	C-O	-8.27	1.19	1.23
1	B	165	VAL	C-O	-7.82	1.16	1.24
1	G	236	GLU	C-O	-7.53	1.20	1.23
1	D	259	THR	C-O	-6.00	1.17	1.24
1	A	81	SER	C-O	-5.95	1.16	1.23
1	A	15	PRO	C-N	5.92	1.40	1.33
1	B	236	GLU	CA-C	-5.90	1.49	1.53
1	H	3	LYS	C-O	-5.87	1.16	1.23
1	D	258	ALA	C-O	-5.75	1.16	1.24
1	C	236	GLU	CA-C	-5.74	1.50	1.53
1	G	53	HIS	C-O	-5.72	1.17	1.24
1	F	236	GLU	C-O	-5.70	1.21	1.23
1	E	230	ASP	C-O	-5.68	1.21	1.23
1	A	16	PRO	N-CD	5.67	1.55	1.47
1	D	235	GLU	C-O	-5.61	1.17	1.24
1	A	17	PRO	N-CD	5.50	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLU	CA-C	-5.45	1.49	1.53
1	C	235	GLU	C-O	-5.38	1.17	1.24
1	C	236	GLU	C-O	-5.30	1.21	1.23
1	H	86	ARG	N-CA	-5.28	1.40	1.45
1	H	86	ARG	C-O	-5.24	1.18	1.24
1	B	360	PRO	N-CD	5.21	1.55	1.47
1	H	87	PRO	N-CD	5.20	1.55	1.47
1	D	260	GLY	C-O	-5.20	1.17	1.24
1	F	334	VAL	N-CA	-5.09	1.40	1.46
1	E	301	ALA	C-O	-5.08	1.18	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	VAL	N-CA-C	-8.38	96.24	108.23
1	A	16	PRO	C-N-CD	8.30	138.87	120.60
1	A	15	PRO	O-C-N	7.10	124.49	121.15
1	A	67	ASP	CA-C-N	6.79	127.34	119.47
1	A	67	ASP	C-N-CA	6.79	127.34	119.47
1	H	86	ARG	N-CA-C	-6.67	100.51	108.25
1	D	338	GLU	N-CA-C	6.56	118.91	110.65
1	B	381	GLY	N-CA-C	6.41	118.78	110.45
1	A	15	PRO	CA-C-N	-6.37	113.81	120.38
1	A	15	PRO	C-N-CA	-6.37	113.81	120.38
1	H	87	PRO	N-CA-C	6.30	121.22	111.21
1	D	281	GLN	CA-C-N	-6.28	113.51	119.85
1	D	281	GLN	C-N-CA	-6.28	113.51	119.85
1	G	247	SER	N-CA-C	6.26	117.91	111.14
1	H	67	ASP	CA-C-N	6.00	126.42	119.47
1	H	67	ASP	C-N-CA	6.00	126.42	119.47
1	H	47	GLY	CA-C-N	5.97	126.13	119.32
1	H	47	GLY	C-N-CA	5.97	126.13	119.32
1	D	157	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	C	276	GLY	N-CA-C	5.88	121.48	114.48
1	A	383	ARG	N-CA-C	5.76	118.14	110.53
1	B	360	PRO	N-CA-C	5.58	119.99	111.34
1	E	157	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	A	120	GLY	N-CA-C	5.54	118.79	111.70
1	B	360	PRO	CA-N-CD	-5.51	104.28	112.00
1	G	210	THR	N-CA-C	-5.50	102.06	110.14
1	D	171	GLY	CA-C-N	5.49	125.49	119.89
1	D	171	GLY	C-N-CA	5.49	125.49	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	210	THR	N-CA-C	-5.43	100.49	108.79
1	C	281	GLN	CA-C-N	-5.31	114.45	119.76
1	C	281	GLN	C-N-CA	-5.31	114.45	119.76
1	B	349	ARG	N-CA-C	5.14	115.89	109.57
1	H	87	PRO	CA-N-CD	-5.14	104.81	112.00
1	F	233	TRP	N-CA-C	5.11	116.57	108.96
1	A	16	PRO	CA-C-N	-5.06	114.85	127.00
1	A	16	PRO	C-N-CA	-5.06	114.85	127.00

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	2939	0	2857	54	0
1	B	2922	0	2840	42	0
1	C	2922	0	2840	46	0
1	D	2987	0	2904	59	0
1	E	2938	0	2861	63	0
1	F	2922	0	2840	50	0
1	G	2935	0	2855	44	0
1	H	2938	0	2861	41	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	349	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 (349) 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:112:CYS:SG	1:E:117:MET:HE3	1.95	1.06
1:E:4:LEU:HD22	1:E:29:VAL:HG11	1.46	0.95
1:F:112:CYS:SG	1:F:117:MET:HE3	2.07	0.94
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
1:D:173:TYR:CD1	1:D:388:MET:HE3	2.12	0.85
1:A:384:LEU:HD11	1:C:61:ARG:HD3	1.62	0.79
1:A:173:TYR:HB2	1:A:388:MET:HE3	1.65	0.78
1:D:389:GLN:CD	1:D:391:ALA:HB3	2.09	0.78
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: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:E:122:MET:HE2	1:E:329:PRO:HA	1.70	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: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:B:72:GLU:O	1:B:76:ARG:HG2	1.94	0.68
1:D:126:ILE:HD11	1:D:326:VAL:HA	1.76	0.67
1:F:168:ASP:OD2	1:F:211:HIS:CE1	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD1	1:D:388:MET:CE	2.13	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: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:D:122:MET:HE2	1:D:329:PRO:HA	1.83	0.60
1:D:173:TYR:CD1	1:D:388:MET:CE	2.83	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:E:175:MET:HE2	1:E:176:ARG:CG	2.33	0.59
1:D:22:ARG:HB2	1:D:385:HIS:HA	1.85	0.59
1:F:112:CYS:HG	1:F:117:MET:HE3	1.68	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: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:100:MET:HE1	1:G:317:GLU:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:LEU:O	1:G:294:LYS:HE3	2.05	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:E:197:ARG:NH1	1:E:197:ARG:HG2	2.20	0.56
1:F:232:LEU:O	1:F:256:PRO:HG2	2.05	0.56
1:F:233:TRP:CD1	1:F:233:TRP:C	2.84	0.56
1:E:107:GLY:HA2	1:E:117:MET:HE1	1.87	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
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:F:261:GLU:HG3	1:F:262:ARG:HG3	1.89	0.54
1:H:118:LEU:HD22	1:H:294:LYS:HG3	1.88	0.54
1:B:170:ALA:HB3	1:B:210:THR:HG22	1.90	0.54
1:B:88:ASP:O	1:B:92:PHE:HB2	2.07	0.54
1:C:22:ARG:HD3	1:C:384:LEU:O	2.08	0.54
1:E:262:ARG:HD2	1:G:84:THR:O	2.08	0.54
1:G:22:ARG:HH12	1:G:387:GLU:H	1.55	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:D:173:TYR:HD1	1:D:388:MET:HE3	1.64	0.53
1:A:112:CYS:HB2	1:A:117:MET:HE3	1.89	0.53
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:C:88:ASP:C	1:C:88:ASP:OD1	2.52	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:H:139:ASP:OD1	1:H:139:ASP:C	2.52	0.53
1:B:170:ALA:CB	1:B:210:THR:HG22	2.39	0.52
1:A:196:ILE:HG22	1:A:206:LEU:HD11	1.92	0.52
1:E:61:ARG:HD3	1:G:384: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:GLY:HA3	1:G:385:HIS:CE1	2.44	0.52
1:G:384:LEU:HB2	1:G:387:GLU:HG3	1.92	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:E:176:ARG:HG2	1:F:122:MET:HE1	1.91	0.52
1:F:244:PRO:HA	1:F:275:HIS:CD2	2.45	0.52
1:C:100:MET:HE1	1:C:317:GLU:HG3	1.92	0.52
1:H:20:GLY:O	1:H:385:HIS:HE1	1.92	0.52
1:A:135:GLU:HG3	1:A:136:PRO:HD2	1.92	0.51
1:D:123:ASN:HB2	1:D:126:ILE:HD11	1.90	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: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:D:114:VAL:HA	1:D:117:MET:HE2	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:B:82:GLY:HA3	1:D:44:ALA:O	2.11	0.51
1:C:110:ARG:HD2	1:E:110:ARG:HD3	1.91	0.51
1:E:197:ARG:HG2	1:E:197:ARG:HH11	1.75	0.51
1:H:325:GLY:HA2	1:H:331:LEU:HD13	1.92	0.51
1:E:175:MET:HE2	1:E:176:ARG:HG3	1.92	0.51
1:A:239:PRO:HB3	1:C:85:GLN:OE1	2.10	0.50
1:A:168:ASP:CG	1:A:209:GLY:O	2.55	0.50
1:C:202:THR:O	1:C:202:THR:CG2	2.60	0.50
1:F:168:ASP:CG	1:F:211:HIS:HE1	2.20	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:C:267:THR:HB	2:C:524:HOH:O	2.11	0.50
1:D:322:VAL:O	1:D:326:VAL:HG23	2.12	0.50
1:C:337:ILE:HG22	1:C:339:THR:HG23	1.92	0.50
1:E:44:ALA:O	1:E:384:LEU:HD22	2.12	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:B:120:GLY:HA3	1:H:70:ASN:HA	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:MET:HE2	1:F:320:ALA:HB3	1.94	0.49
1:A:232:LEU:HD21	1:A:332:LEU:HD21	1.94	0.49
1:D:39:GLY:HA3	1:D:97:GLY:O	2.13	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: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:A:224:LYS:HA	1:A:224:LYS:HD3	1.64	0.48
1:E:384:LEU:HD12	1:E:387:GLU:HG2	1.94	0.48
1:D:235:GLU:HA	1:D:258:ALA:O	2.13	0.48
1:G:220:ILE:HG12	1:G:252:HIS:HB2	1.95	0.48
1:D:224:LYS:HD3	1:D:224:LYS:HA	1.52	0.48
1:D:258:ALA:HA	1:D:279:ILE:O	2.12	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
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:B:287:ALA:O	1:B:292:GLU:HG2	2.14	0.47
1:D:232:LEU:HD21	1:D:332:LEU:HD21	1.97	0.47
1:B:211:HIS:HB3	1:D:83:PHE:CZ	2.48	0.47
1:E:383:ARG:HA	1:G:61:ARG:HH12	1.79	0.47
1:G:153:SER:O	1:G:157:ARG:HG2	2.14	0.47
1:A:210:THR:HB	1:A:213:GLN:OE1	2.14	0.47
1:D:27:VAL:HG21	1:D:98:LEU:HD23	1.97	0.47
1:B:284:LEU:HD22	1:B:321:ASN:OD1	2.15	0.47
1:F:168:ASP:CG	1:F:211:HIS:CE1	2.94	0.46
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:E:173:TYR:HD2	1:E:388:MET:HE3	1.80	0.46
1:H:284:LEU:HD22	1:H:321:ASN:OD1	2.15	0.46
1:D:205:ASP:CG	1:D:232:LEU:HD12	2.40	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:A:39:GLY:HA3	1:A:97:GLY:O	2.14	0.46
1:C:22:ARG:CD	1:C:384:LEU:O	2.63	0.46
1:D:148:GLU:CD	1:D:148:GLU:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:ALA:HB2	1:G:379:TYR:HD1	1.79	0.46
1:B:122:MET:HE3	1:F:176:ARG:NH1	2.31	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:HD23	1:H:386:LEU:HA	1.83	0.46
1:A:248:GLU:CD	1:E:278:ARG:HE	2.24	0.46
1:B:118:LEU:O	1:B:294:LYS:HE3	2.15	0.46
1:D:38:LEU:HD11	1:D:369:LEU:HB2	1.97	0.46
1:H:72:GLU:O	1:H:76:ARG:HG2	2.15	0.46
1:H:227:GLU:C	1:H:229:TYR:H	2.24	0.46
1:D:389:GLN:CD	1:D:391:ALA:CB	2.86	0.45
1:F:107:GLY:HA3	1:F:364:GLY:CA	2.45	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:A:110:ARG:HE	1:A:117:MET:HE2	1.81	0.45
1:G:28:ARG:HH21	1:G:369:LEU:HB3	1.81	0.45
1:G:117:MET:HE2	1:G:117:MET:HB2	1.83	0.45
1:F:6:THR:OG1	1:F:30:THR:HB	2.17	0.45
1:F:196:ILE:O	1:F:200:VAL:HG22	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
1:C:114:VAL:HA	1:C:117:MET:HE2	1.99	0.45
1:C:258:ALA:HB2	1:C:279:ILE:HB	1.99	0.44
1:E:110:ARG:HB2	1:E:117:MET:HE2	1.99	0.44
1:F:84:THR:O	1:H:262:ARG:NH1	2.50	0.44
1:E:7:LEU:HD21	1:E:55:ILE:HG22	1.99	0.44
1:E:197:ARG:HH11	1:E:197:ARG:CG	2.30	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: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:H:322:VAL:O	1:H:326:VAL:HG23	2.18	0.44
1:A:76:ARG:HB3	1:C:175:MET:O	2.16	0.44
1:C:66:GLU:OE2	1:C:70:ASN:ND2	2.50	0.44
1:D:20:GLY:O	1:D:385:HIS:HE1	2.01	0.44
1:E:173:TYR:CD2	1:E:388:MET:HE3	2.53	0.44
1:F:4:LEU:HD22	1:F:29:VAL:HG11	1.99	0.44
1:G:103:TRP:CZ3	1:G:117:MET:HB3	2.53	0.44
1:B:83:PHE:HA	1:D:388:MET:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:58:VAL:HG21	1:C:94:ALA:HB3	2.00	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: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:87:PRO:HB3	1:G:264:THR:HG23	2.01	0.43
1:G:232:LEU:HD21	1:G:332:LEU:HD21	2.00	0.43
1:A:235:GLU:CD	1:A:281:GLN:HE22	2.26	0.43
1:B:26:LEU:HD11	1:B:345:LEU:HD21	2.00	0.43
1:F:100:MET:HE2	1:F:320:ALA:CB	2.47	0.43
1:G:211:HIS:H	1:G:213:GLN:CD	2.25	0.43
1:C:238:ILE:HB	1:C:239:PRO:CD	2.49	0.43
1:H:207:LEU:HD21	1:H:232:LEU:HD22	2.00	0.43
1:H:14:PRO:HD2	1:H:22:ARG:O	2.18	0.43
1:B:5:ASP:O	1:B:64:ARG:NE	2.50	0.43
1:B:209:GLY:HA2	1:B:235:GLU:HB3	2.01	0.43
1:B:100:MET:HA	1:B:290:ILE:HD12	2.00	0.43
1:E:135:GLU:HG3	1:E:136:PRO:HD2	2.01	0.43
1:C:306:GLN:OE1	1:C:332:LEU:HD13	2.19	0.43
1:A:148:GLU:CD	1:A:148:GLU:H	2.27	0.42
1:A:384:LEU:HD11	1:C:61:ARG:CD	2.41	0.42
1:E:100:MET:HE3	1:E:320:ALA:HB2	2.01	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:B:37:GLY:HA3	1:B:104:ASP:HB3	2.01	0.42
1:C:39:GLY:HA3	1:C:97:GLY:O	2.19	0.42
1:C:351:ARG:O	1:C:357:VAL:HG13	2.19	0.42
1:D:167:PHE:HD2	1:D:169:PRO:HD3	1.85	0.42
1:E:83:PHE:O	1:E:83:PHE:CG	2.70	0.42
1:E:239:PRO:HB3	1:G:85:GLN:OE1	2.20	0.42
1:F:82:GLY:C	1:H:386:LEU:O	2.61	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:E:224:LYS:HA	1:E:224:LYS:HD3	1.81	0.42
1:F:315:PRO:HA	1:F:318:TRP:HB3	2.02	0.42
1:E:39:GLY:HA3	1:E:97:GLY:O	2.19	0.42
1:F:166:LYS:HG3	1:F:167:PHE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:168:ASP:OD2	1:G:211:HIS:CE1	2.73	0.42
1:F:167:PHE:N	1:F:167:PHE:CD1	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:B:175:MET:HE1	1:B:176:ARG:NH1	2.35	0.42
1:F:86:ARG:HH22	1:H:268:GLU:CD	2.28	0.42
1:A:14:PRO:HA	1:A:15:PRO:HD2	1.93	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:E:127:ARG:NH1	2:E:573:HOH:O	2.51	0.41
1:E:175:MET:H	1:E:175:MET:HG3	1.67	0.41
1:A:107:GLY:HA3	1:A:364:GLY:HA2	2.02	0.41
1:D:148:GLU:CD	1:D:148:GLU:N	2.78	0.41
1:E:83:PHE:O	1:E:83:PHE:CD2	2.73	0.41
1:D:107:GLY:HA3	1:D:364:GLY:HA2	2.00	0.41
1:D:205:ASP:HB3	1:D:232:LEU:HB2	2.03	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: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:175:MET:HE3	1:A:175:MET:C	2.46	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:HA	1:E:294:LYS:HD2	1.63	0.41
1:F:268:GLU:OE2	1:H:86:ARG:NH1	2.47	0.41
1:A:67:ASP:OD1	1:A:67:ASP:C	2.64	0.41
1:C:235:GLU:HG3	1:C:281:GLN:OE1	2.21	0.41
1:E:245:GLY:O	1:E:248:GLU:HG2	2.19	0.41
1:B:39:GLY:HA3	1:B:97:GLY:O	2.20	0.41
1:B:54:VAL:HG13	1:D:46:VAL:HG11	2.03	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:A:298:THR:CG2	1:D:295:LYS:HB2	2.51	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:88:ASP:O	1:H:92:PHE:HB2	2.21	0.41
1:H:287:ALA:O	1:H:292:GLU:HG2	2.21	0.41
1:A:174:THR:OG1	1:A:176:ARG:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ASP:HA	1:C:68:PRO:HD2	1.82	0.40
1:C:110:ARG:CD	1:E:110:ARG:CD	2.99	0.40
1:D:114:VAL:HG23	1:D:364:GLY:C	2.46	0.40
1:E:308:ALA:HA	1:E:333:MET:O	2.21	0.40
1:G:28:ARG:HA	1:G:37:GLY:O	2.22	0.40
1:G:114:VAL:HA	1:G:117:MET:HE2	2.02	0.40
1:H:266:VAL:HG21	1:H:295:LYS:HB3	2.02	0.40
1:B:270:THR:OG1	1:B:299:LEU:HD22	2.21	0.40
1:C:233:TRP:CD1	1:C:233:TRP:C	2.99	0.40
1:D:175:MET:HE2	1:D:390:ASP:OD1	2.22	0.40
1:E:84:THR:O	1:G:262:ARG:HD2	2.21	0.40
1:E:89:PRO:HG2	1:G:88:ASP:OD2	2.21	0.40
1:G:171:GLY:HA3	1:G:172:PRO:HD3	1.80	0.40
1:A:233:TRP:CD1	1:A:233:TRP:C	2.99	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:E:175:MET:HE2	1:E:176:ARG:HG2	2.04	0.40
1:F:106:LEU:O	1:F:117:MET:HE1	2.21	0.40
1:H:23:TYR:CZ	1:H:48:PRO:HD3	2.57	0.40
1:E:270:THR:OG1	1:E:299:LEU:HD22	2.22	0.40
1:F:2:VAL:O	1:F:67:ASP:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	36	55
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	386/429 (90%)	366 (95%)	20 (5%)	0	100	100
1	F	384/429 (90%)	368 (96%)	15 (4%)	1 (0%)	36	55
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%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	GLY
1	F	45	GLY

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	293/327 (90%)	276 (94%)	17 (6%)	18	38
1	B	291/327 (89%)	278 (96%)	13 (4%)	24	49
1	C	291/327 (89%)	282 (97%)	9 (3%)	35	62
1	D	299/327 (91%)	282 (94%)	17 (6%)	18	39
1	E	293/327 (90%)	283 (97%)	10 (3%)	32	60
1	F	291/327 (89%)	283 (97%)	8 (3%)	39	67
1	G	293/327 (90%)	279 (95%)	14 (5%)	23	46
1	H	293/327 (90%)	281 (96%)	12 (4%)	27	53
All	All	2344/2616 (90%)	2244 (96%)	100 (4%)	26	51

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	92	PHE

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Mol	Chain	Res	Type
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	284	LEU
1	A	294	LYS
1	A	299	LEU
1	A	331	LEU
1	A	361	ASP
1	A	384	LEU
1	A	386	LEU
1	B	6	THR
1	B	22	ARG
1	B	86	ARG
1	B	92	PHE
1	B	110	ARG
1	B	175	MET
1	B	198	ASP
1	B	261	GLU
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	135	GLU
1	C	202	THR
1	C	210	THR
1	C	264	THR
1	C	267	THR
1	C	357	VAL
1	C	368	THR
1	C	382	ASN
1	D	86	ARG
1	D	99	GLU
1	D	126	ILE
1	D	135	GLU
1	D	141	ASN

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Mol	Chain	Res	Type
1	D	175	MET
1	D	197	ARG
1	D	202	THR
1	D	224	LYS
1	D	259	THR
1	D	261	GLU
1	D	271	GLN
1	D	284	LEU
1	D	337	ILE
1	D	380	THR
1	D	390	ASP
1	D	393	CYS
1	E	6	THR
1	E	86	ARG
1	E	148	GLU
1	E	175	MET
1	E	197	ARG
1	E	274	HIS
1	E	294	LYS
1	E	299	LEU
1	E	368	THR
1	E	382	ASN
1	F	28	ARG
1	F	123	ASN
1	F	140	THR
1	F	166	LYS
1	F	210	THR
1	F	233	TRP
1	F	267	THR
1	F	274	HIS
1	G	2	VAL
1	G	86	ARG
1	G	117	MET
1	G	140	THR
1	G	202	THR
1	G	210	THR
1	G	247	SER
1	G	261	GLU
1	G	267	THR
1	G	299	LEU
1	G	347	THR
1	G	351	ARG

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Mol	Chain	Res	Type
1	G	380	THR
1	G	386	LEU
1	H	3	LYS
1	H	27	VAL
1	H	52	THR
1	H	86	ARG
1	H	153	SER
1	H	174	THR
1	H	233	TRP
1	H	267	THR
1	H	284	LEU
1	H	299	LEU
1	H	368	THR
1	H	382	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	137	HIS
1	A	179	HIS
1	A	203	GLN
1	A	275	HIS
1	A	281	GLN
1	A	310	HIS
1	A	370	ASN
1	A	382	ASN
1	A	385	HIS
1	B	56	HIS
1	B	137	HIS
1	B	274	HIS
1	B	275	HIS
1	B	370	ASN
1	C	79	HIS
1	C	211	HIS
1	C	275	HIS
1	C	281	GLN
1	C	385	HIS
1	D	56	HIS
1	D	385	HIS
1	E	56	HIS
1	E	271	GLN

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Mol	Chain	Res	Type
1	E	385	HIS
1	G	79	HIS
1	G	137	HIS
1	G	375	ASN
1	H	211	HIS
1	H	274	HIS
1	H	306	GLN
1	H	375	ASN
1	H	385	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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%)	0.44	12 (3%) 51 47	21, 29, 42, 75	0
1	B	386/429 (89%)	0.29	10 (2%) 57 52	20, 28, 39, 73	0
1	C	386/429 (89%)	0.25	6 (1%) 70 67	20, 27, 39, 69	0
1	D	393/429 (91%)	0.44	17 (4%) 40 35	14, 28, 45, 86	2 (0%)
1	E	388/429 (90%)	0.38	17 (4%) 39 34	21, 29, 41, 69	0
1	F	386/429 (89%)	0.35	12 (3%) 51 47	21, 28, 41, 81	0
1	G	386/429 (89%)	0.29	9 (2%) 61 57	12, 27, 39, 81	2 (0%)
1	H	388/429 (90%)	0.34	8 (2%) 63 59	20, 28, 42, 64	0
All	All	3101/3432 (90%)	0.35	91 (2%) 53 49	12, 28, 41, 86	4 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	LEU	5.8
1	G	386	LEU	5.7
1	F	386	LEU	5.6
1	D	386	LEU	5.4
1	D	392	PRO	5.2
1	H	173	TYR	4.8
1	B	173	TYR	4.6
1	D	390	ASP	4.6
1	E	386	LEU	4.4
1	C	173	TYR	4.3
1	A	173	TYR	4.2
1	D	170	ALA	3.9
1	D	385	HIS	3.8
1	D	381	GLY	3.7
1	C	386	LEU	3.7
1	F	384	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	173	TYR	3.6
1	A	83	PHE	3.6
1	A	383	ARG	3.5
1	A	384	LEU	3.5
1	H	379	TYR	3.5
1	E	388	MET	3.4
1	A	381	GLY	3.4
1	E	384	LEU	3.3
1	H	172	PRO	3.2
1	C	168	ASP	3.2
1	F	382	ASN	3.2
1	F	173	TYR	3.2
1	F	387	GLU	3.2
1	D	174	THR	3.2
1	E	173	TYR	3.1
1	C	384	LEU	3.0
1	G	83	PHE	3.0
1	H	386	LEU	3.0
1	E	383	ARG	3.0
1	B	170	ALA	2.9
1	F	19	TRP	2.9
1	E	385	HIS	2.9
1	D	173	TYR	2.9
1	G	384	LEU	2.9
1	F	381	GLY	2.9
1	A	385	HIS	2.8
1	B	384	LEU	2.8
1	E	380	THR	2.8
1	A	49	GLU	2.8
1	E	348	GLY	2.7
1	B	382	ASN	2.7
1	D	382	ASN	2.7
1	C	385	HIS	2.7
1	G	172	PRO	2.7
1	B	386	LEU	2.7
1	H	384	LEU	2.7
1	A	382	ASN	2.6
1	A	389	GLN	2.6
1	E	172	PRO	2.5
1	A	387	GLU	2.5
1	G	382	ASN	2.5
1	B	385	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	391	ALA	2.5
1	C	381	GLY	2.5
1	B	387	GLU	2.5
1	H	382	ASN	2.5
1	G	11	ALA	2.5
1	D	388	MET	2.5
1	G	387	GLU	2.4
1	E	382	ASN	2.4
1	E	381	GLY	2.4
1	F	383	ARG	2.4
1	D	393	CYS	2.4
1	F	168	ASP	2.3
1	E	83	PHE	2.3
1	B	383	ARG	2.3
1	D	389	GLN	2.3
1	E	387	GLU	2.3
1	F	83	PHE	2.3
1	D	289	GLY	2.2
1	F	385	HIS	2.2
1	B	171	GLY	2.2
1	E	19	TRP	2.2
1	D	210	THR	2.2
1	D	22	ARG	2.1
1	D	83	PHE	2.1
1	E	131	TYR	2.1
1	E	11	ALA	2.1
1	E	34	GLY	2.1
1	G	140	THR	2.1
1	A	172	PRO	2.1
1	B	83	PHE	2.0
1	H	216	PRO	2.0
1	H	385	HIS	2.0
1	F	124	ASP	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 oligosaccharides 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.