



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:04 PM UTC

PDB ID : 5LL2 / pdb_00005ll2
Title : Structure of Isoleucine 2-epimerase from *Lactobacillus buchneri* (apo form)
Authors : Reiser, J.-B.; Awad, R.; Gans, P.
Deposited on : 2016-07-26
Resolution : 2.60 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)
Validation Pipeline (wwPDB-VP)	:	2.49

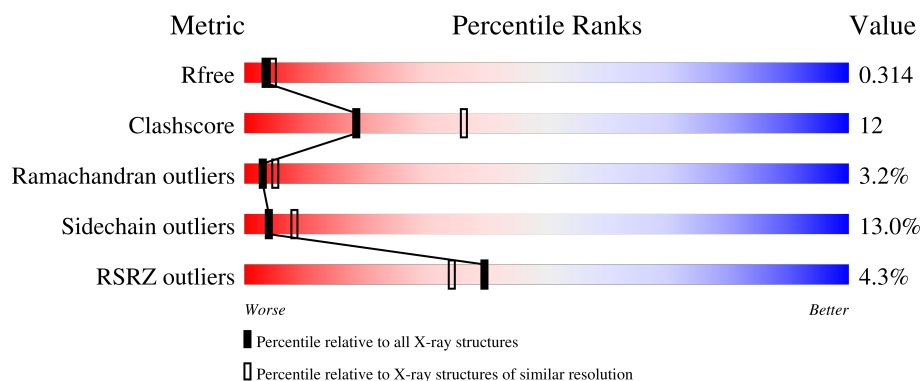
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	480	
1	B	480	
1	C	480	
1	D	480	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12578 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 Isoleucine 2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	1	0
			3151	2007	526	602	16			
1	B	409	Total	C	N	O	S	0	0	0
			3146	2005	526	599	16			
1	C	407	Total	C	N	O	S	0	0	0
			3134	1997	524	597	16			
1	D	405	Total	C	N	O	S	0	0	0
			3121	1990	522	593	16			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	initiating methionine	UNP M1GRN3
A	-28	GLY	-	expression tag	UNP M1GRN3
A	-27	SER	-	expression tag	UNP M1GRN3
A	-26	SER	-	expression tag	UNP M1GRN3
A	-25	HIS	-	expression tag	UNP M1GRN3
A	-24	HIS	-	expression tag	UNP M1GRN3
A	-23	HIS	-	expression tag	UNP M1GRN3
A	-22	HIS	-	expression tag	UNP M1GRN3
A	-21	HIS	-	expression tag	UNP M1GRN3
A	-20	HIS	-	expression tag	UNP M1GRN3
A	-19	SER	-	expression tag	UNP M1GRN3
A	-18	SER	-	expression tag	UNP M1GRN3
A	-17	GLY	-	expression tag	UNP M1GRN3
A	-16	GLU	-	expression tag	UNP M1GRN3
A	-15	ASN	-	expression tag	UNP M1GRN3
A	-14	LEU	-	expression tag	UNP M1GRN3
A	-13	TYR	-	expression tag	UNP M1GRN3
A	-12	PHE	-	expression tag	UNP M1GRN3
A	-11	GLN	-	expression tag	UNP M1GRN3
A	-10	GLY	-	expression tag	UNP M1GRN3
A	-9	HIS	-	expression tag	UNP M1GRN3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP M1GRN3
A	-7	ALA	-	expression tag	UNP M1GRN3
A	-6	SER	-	expression tag	UNP M1GRN3
A	-5	GLY	-	expression tag	UNP M1GRN3
A	-4	SER	-	expression tag	UNP M1GRN3
A	-3	GLU	-	expression tag	UNP M1GRN3
A	-2	PHE	-	expression tag	UNP M1GRN3
A	-1	GLU	-	expression tag	UNP M1GRN3
A	0	LEU	-	expression tag	UNP M1GRN3
B	-29	MET	-	initiating methionine	UNP M1GRN3
B	-28	GLY	-	expression tag	UNP M1GRN3
B	-27	SER	-	expression tag	UNP M1GRN3
B	-26	SER	-	expression tag	UNP M1GRN3
B	-25	HIS	-	expression tag	UNP M1GRN3
B	-24	HIS	-	expression tag	UNP M1GRN3
B	-23	HIS	-	expression tag	UNP M1GRN3
B	-22	HIS	-	expression tag	UNP M1GRN3
B	-21	HIS	-	expression tag	UNP M1GRN3
B	-20	HIS	-	expression tag	UNP M1GRN3
B	-19	SER	-	expression tag	UNP M1GRN3
B	-18	SER	-	expression tag	UNP M1GRN3
B	-17	GLY	-	expression tag	UNP M1GRN3
B	-16	GLU	-	expression tag	UNP M1GRN3
B	-15	ASN	-	expression tag	UNP M1GRN3
B	-14	LEU	-	expression tag	UNP M1GRN3
B	-13	TYR	-	expression tag	UNP M1GRN3
B	-12	PHE	-	expression tag	UNP M1GRN3
B	-11	GLN	-	expression tag	UNP M1GRN3
B	-10	GLY	-	expression tag	UNP M1GRN3
B	-9	HIS	-	expression tag	UNP M1GRN3
B	-8	MET	-	expression tag	UNP M1GRN3
B	-7	ALA	-	expression tag	UNP M1GRN3
B	-6	SER	-	expression tag	UNP M1GRN3
B	-5	GLY	-	expression tag	UNP M1GRN3
B	-4	SER	-	expression tag	UNP M1GRN3
B	-3	GLU	-	expression tag	UNP M1GRN3
B	-2	PHE	-	expression tag	UNP M1GRN3
B	-1	GLU	-	expression tag	UNP M1GRN3
B	0	LEU	-	expression tag	UNP M1GRN3
C	-29	MET	-	initiating methionine	UNP M1GRN3
C	-28	GLY	-	expression tag	UNP M1GRN3
C	-27	SER	-	expression tag	UNP M1GRN3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-26	SER	-	expression tag	UNP M1GRN3
C	-25	HIS	-	expression tag	UNP M1GRN3
C	-24	HIS	-	expression tag	UNP M1GRN3
C	-23	HIS	-	expression tag	UNP M1GRN3
C	-22	HIS	-	expression tag	UNP M1GRN3
C	-21	HIS	-	expression tag	UNP M1GRN3
C	-20	HIS	-	expression tag	UNP M1GRN3
C	-19	SER	-	expression tag	UNP M1GRN3
C	-18	SER	-	expression tag	UNP M1GRN3
C	-17	GLY	-	expression tag	UNP M1GRN3
C	-16	GLU	-	expression tag	UNP M1GRN3
C	-15	ASN	-	expression tag	UNP M1GRN3
C	-14	LEU	-	expression tag	UNP M1GRN3
C	-13	TYR	-	expression tag	UNP M1GRN3
C	-12	PHE	-	expression tag	UNP M1GRN3
C	-11	GLN	-	expression tag	UNP M1GRN3
C	-10	GLY	-	expression tag	UNP M1GRN3
C	-9	HIS	-	expression tag	UNP M1GRN3
C	-8	MET	-	expression tag	UNP M1GRN3
C	-7	ALA	-	expression tag	UNP M1GRN3
C	-6	SER	-	expression tag	UNP M1GRN3
C	-5	GLY	-	expression tag	UNP M1GRN3
C	-4	SER	-	expression tag	UNP M1GRN3
C	-3	GLU	-	expression tag	UNP M1GRN3
C	-2	PHE	-	expression tag	UNP M1GRN3
C	-1	GLU	-	expression tag	UNP M1GRN3
C	0	LEU	-	expression tag	UNP M1GRN3
D	-29	MET	-	initiating methionine	UNP M1GRN3
D	-28	GLY	-	expression tag	UNP M1GRN3
D	-27	SER	-	expression tag	UNP M1GRN3
D	-26	SER	-	expression tag	UNP M1GRN3
D	-25	HIS	-	expression tag	UNP M1GRN3
D	-24	HIS	-	expression tag	UNP M1GRN3
D	-23	HIS	-	expression tag	UNP M1GRN3
D	-22	HIS	-	expression tag	UNP M1GRN3
D	-21	HIS	-	expression tag	UNP M1GRN3
D	-20	HIS	-	expression tag	UNP M1GRN3
D	-19	SER	-	expression tag	UNP M1GRN3
D	-18	SER	-	expression tag	UNP M1GRN3
D	-17	GLY	-	expression tag	UNP M1GRN3
D	-16	GLU	-	expression tag	UNP M1GRN3
D	-15	ASN	-	expression tag	UNP M1GRN3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	LEU	-	expression tag	UNP M1GRN3
D	-13	TYR	-	expression tag	UNP M1GRN3
D	-12	PHE	-	expression tag	UNP M1GRN3
D	-11	GLN	-	expression tag	UNP M1GRN3
D	-10	GLY	-	expression tag	UNP M1GRN3
D	-9	HIS	-	expression tag	UNP M1GRN3
D	-8	MET	-	expression tag	UNP M1GRN3
D	-7	ALA	-	expression tag	UNP M1GRN3
D	-6	SER	-	expression tag	UNP M1GRN3
D	-5	GLY	-	expression tag	UNP M1GRN3
D	-4	SER	-	expression tag	UNP M1GRN3
D	-3	GLU	-	expression tag	UNP M1GRN3
D	-2	PHE	-	expression tag	UNP M1GRN3
D	-1	GLU	-	expression tag	UNP M1GRN3
D	0	LEU	-	expression tag	UNP M1GRN3

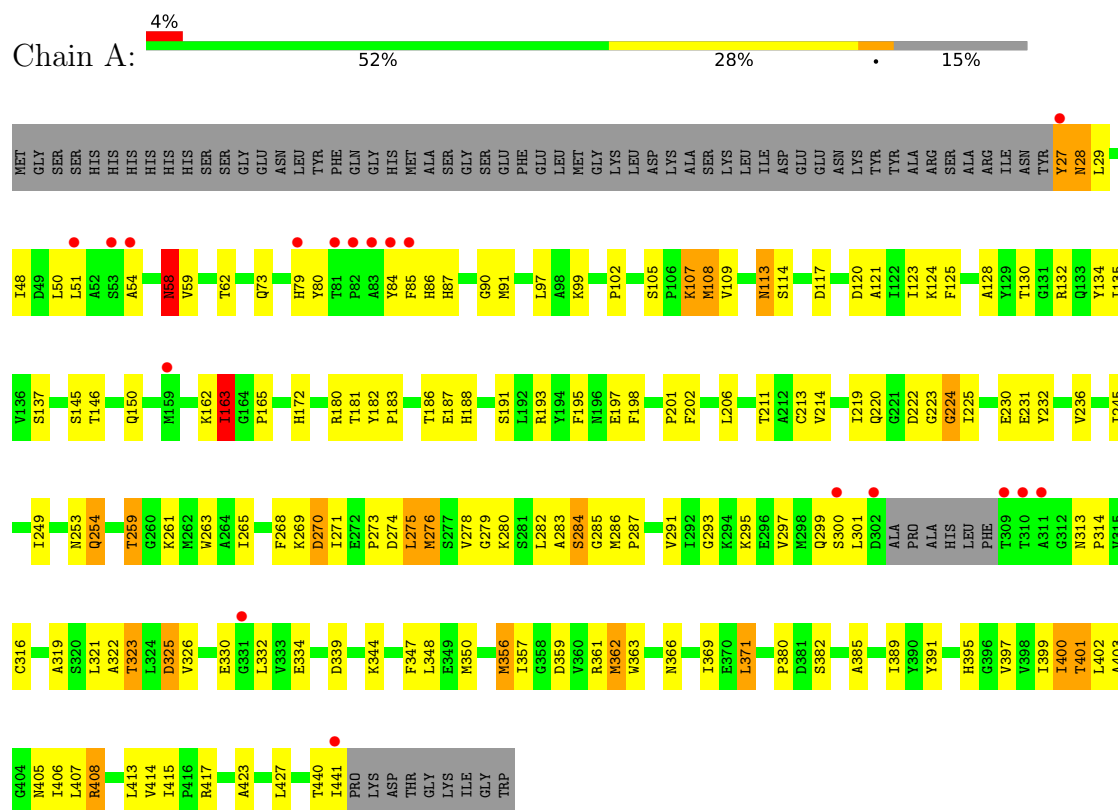
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	3	Total O 3 3	0	0
2	C	8	Total O 8 8	0	0
2	D	5	Total O 5 5	0	0

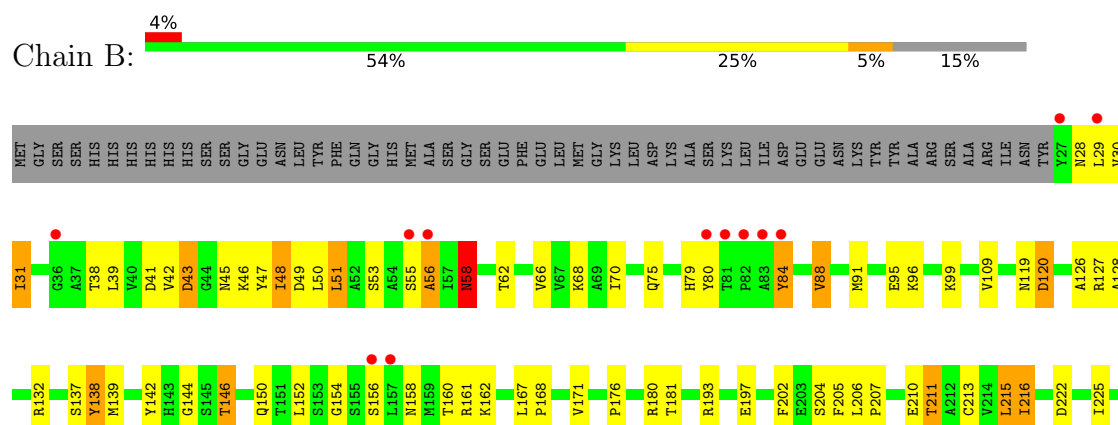
3 Residue-property plots [i](#)

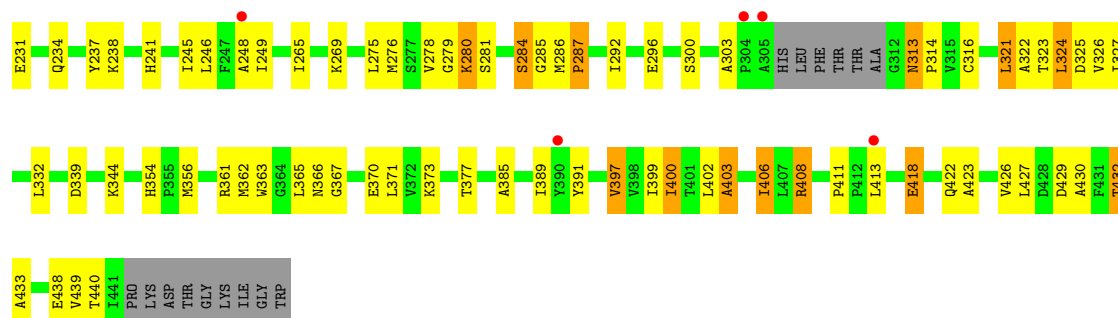
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Isoleucine 2-epimerase

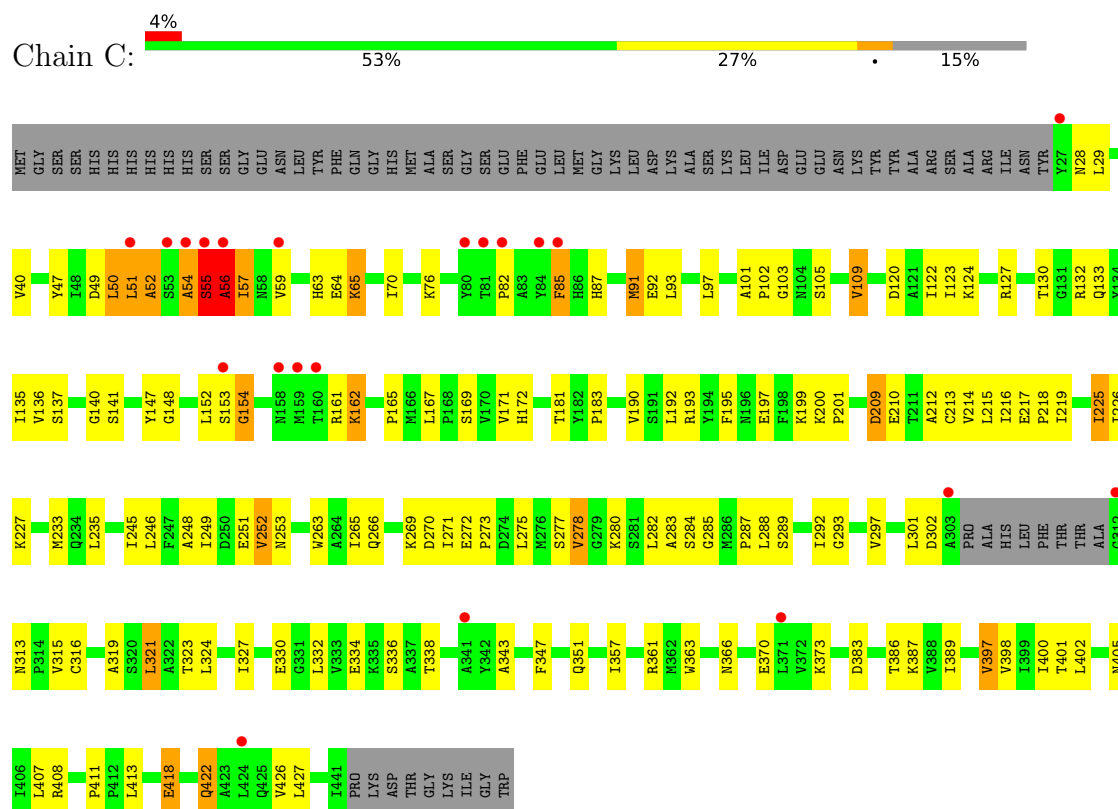


• Molecule 1: Isoleucine 2-epimerase

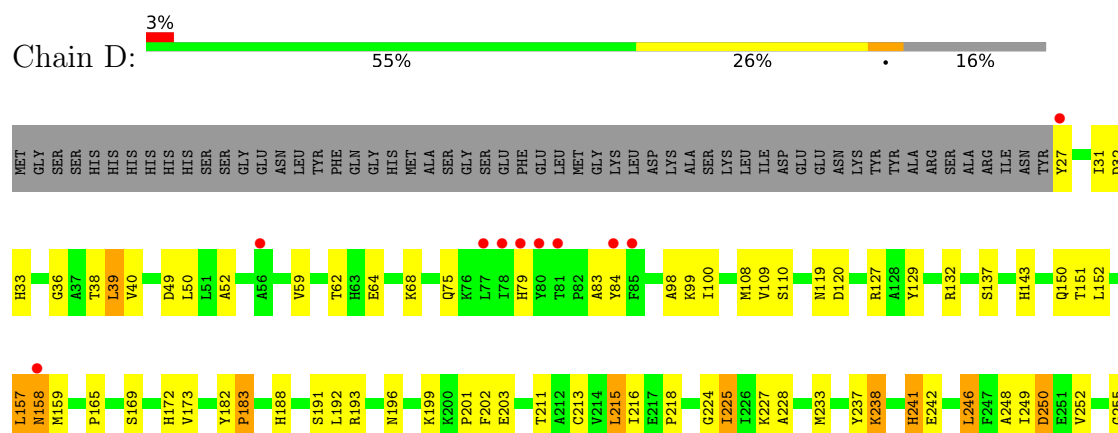


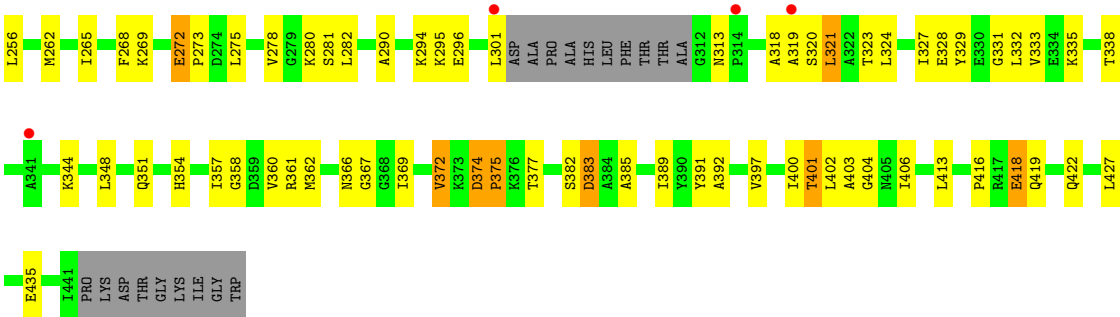


• Molecule 1: Isoleucine 2-epimerase



• Molecule 1: Isoleucine 2-epimerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.16Å 161.78Å 186.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.60 19.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.93-2.60) 98.6 (19.93-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	33.57 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.244 , 0.316 0.243 , 0.314	Depositor DCC
R_{free} test set	2752 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12578	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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.

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	0.92	0/3225	1.27	9/4374 (0.2%)
1	B	0.89	1/3218 (0.0%)	1.26	8/4365 (0.2%)
1	C	0.85	0/3205	1.20	9/4346 (0.2%)
1	D	0.91	0/3192	1.24	14/4328 (0.3%)
All	All	0.89	1/12840 (0.0%)	1.24	40/17413 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	31	ILE	N-CA	5.14	1.52	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	VAL	N-CA-C	-8.88	101.32	111.00
1	B	138	TYR	N-CA-C	8.60	123.49	109.72
1	B	144	GLY	N-CA-C	8.55	121.23	110.29
1	B	313	ASN	CA-C-N	8.38	127.68	118.97
1	B	313	ASN	C-N-CA	8.38	127.68	118.97
1	B	31	ILE	N-CA-C	7.97	120.06	109.21
1	A	405	ASN	N-CA-C	7.38	121.19	112.93
1	D	374	ASP	CA-C-N	7.34	129.01	119.84
1	D	374	ASP	C-N-CA	7.34	129.01	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	GLN	N-CA-C	7.27	121.25	112.38
1	C	147	TYR	N-CA-C	6.90	120.59	111.75
1	C	169	SER	N-CA-C	6.76	120.87	111.74
1	B	79	HIS	N-CA-C	6.15	119.58	108.69
1	A	332	LEU	N-CA-C	5.92	118.52	111.71
1	C	252	VAL	N-CA-C	-5.86	104.61	110.30
1	B	269	LYS	N-CA-C	5.75	118.59	109.96
1	A	254	GLN	N-CA-C	5.74	120.40	113.17
1	D	203	GLU	N-CA-C	-5.74	106.14	113.02
1	A	58	ASN	N-CA-C	-5.63	106.54	113.41
1	D	372	VAL	N-CA-C	5.61	116.81	108.46
1	A	274	ASP	N-CA-C	-5.54	105.16	111.14
1	C	133	GLN	N-CA-C	5.53	117.11	111.14
1	D	199	LYS	N-CA-C	5.46	118.74	111.75
1	D	272	GLU	CA-C-N	5.46	125.40	119.78
1	D	272	GLU	C-N-CA	5.46	125.40	119.78
1	C	56	ALA	N-CA-C	5.42	122.34	110.80
1	D	228	ALA	CA-C-N	5.36	125.36	119.89
1	D	228	ALA	C-N-CA	5.36	125.36	119.89
1	D	313	ASN	CA-C-N	5.30	126.47	119.84
1	D	313	ASN	C-N-CA	5.30	126.47	119.84
1	B	146	THR	N-CA-C	-5.18	102.39	110.42
1	C	405	ASN	N-CA-C	5.14	118.02	111.69
1	D	64	GLU	N-CA-C	5.14	116.89	111.28
1	C	101	ALA	CA-C-N	5.14	125.38	119.83
1	C	101	ALA	C-N-CA	5.14	125.38	119.83
1	A	285	GLY	N-CA-C	5.08	120.74	114.69
1	D	52	ALA	N-CA-C	5.06	118.72	112.24
1	A	163	ILE	N-CA-C	5.05	117.08	112.43
1	A	356	MET	N-CA-C	5.03	118.56	112.23
1	C	91	MET	N-CA-C	5.00	116.74	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	GLY	Peptide
1	D	159	MET	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3151	0	3114	85	0
1	B	3146	0	3107	80	0
1	C	3134	0	3095	100	0
1	D	3121	0	3086	61	0
2	A	10	0	0	4	0
2	B	3	0	0	0	0
2	C	8	0	0	1	0
2	D	5	0	0	0	0
All	All	12578	0	12402	299	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 12.

All (299) 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:C:52:ALA:CB	1:C:408:ARG:HD2	1.69	1.23
1:C:52:ALA:HB2	1:C:408:ARG:HD2	1.28	1.10
1:C:52:ALA:HB1	1:C:408:ARG:HD2	1.51	0.91
1:C:54:ALA:HB1	1:C:280:LYS:NZ	1.84	0.91
1:C:52:ALA:HB2	1:C:408:ARG:CD	2.01	0.89
1:D:319:ALA:O	1:D:323:THR:HG23	1.72	0.89
1:D:416:PRO:HD2	1:D:419:GLN:OE1	1.78	0.84
1:C:54:ALA:HB1	1:C:280:LYS:HZ3	1.43	0.83
1:C:252:VAL:HG12	1:C:280:LYS:HE3	1.60	0.81
1:C:397:VAL:HG11	1:C:426:VAL:HG11	1.63	0.80
1:B:344:LYS:HD3	1:B:362:MET:HB3	1.66	0.77
1:C:130:THR:HB	1:C:132:ARG:HD2	1.66	0.77
1:C:285:GLY:HA3	1:D:79:HIS:HB3	1.65	0.77
1:B:56:ALA:HA	1:B:281:SER:HA	1.69	0.74
1:B:222:ASP:HA	1:B:402:LEU:HD22	1.67	0.74
1:A:51:LEU:HD13	1:A:400:ILE:HG12	1.71	0.73
1:C:56:ALA:HA	1:C:280:LYS:HB3	1.70	0.72
1:A:389:ILE:HG22	1:A:399:ILE:HG23	1.69	0.72
1:C:124:LYS:NZ	1:D:150:GLN:HE22	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD12	1:B:399:ILE:HB	1.72	0.71
1:C:123:ILE:HD11	1:C:152:LEU:HD11	1.73	0.71
1:C:402:LEU:HD11	1:C:408:ARG:HE	1.54	0.71
1:D:278:VAL:HB	1:D:290:ALA:HB3	1.72	0.70
1:A:195:PHE:O	1:A:198:PHE:HB3	1.92	0.69
1:C:397:VAL:CG1	1:C:426:VAL:HG11	2.21	0.69
1:A:283:ALA:CB	2:A:507:HOH:O	2.42	0.67
1:C:52:ALA:CB	1:C:408:ARG:CD	2.60	0.67
1:A:249:ILE:HG21	1:A:265:ILE:HD13	1.78	0.66
1:B:422:GLN:O	1:B:426:VAL:HG23	1.96	0.66
1:C:55:SER:HB2	1:C:253:ASN:HA	1.76	0.65
1:B:249:ILE:HD13	1:B:265:ILE:HB	1.78	0.65
1:B:322:ALA:O	1:B:326:VAL:HG23	1.96	0.65
1:A:124:LYS:HE2	1:B:150:GLN:HE22	1.62	0.64
1:C:52:ALA:HB3	1:C:400:ILE:HD11	1.79	0.64
1:C:418:GLU:O	1:C:422:GLN:HB2	1.97	0.64
1:B:202:PHE:HE1	1:B:211:THR:HG21	1.64	0.63
1:C:54:ALA:HB1	1:C:280:LYS:CE	2.28	0.63
1:B:234:GLN:O	1:B:238:LYS:HG3	1.99	0.63
1:C:386:THR:HA	1:C:389:ILE:HG12	1.80	0.63
1:C:327:ILE:HG12	1:C:332:LEU:HD12	1.81	0.62
1:B:51:LEU:HD13	1:B:400:ILE:HD11	1.81	0.62
1:D:143:HIS:HD2	1:D:152:LEU:HB3	1.64	0.61
1:C:252:VAL:HG12	1:C:280:LYS:CE	2.31	0.61
1:C:51:LEU:O	1:C:52:ALA:CB	2.49	0.61
1:A:97:LEU:HD21	1:A:282:LEU:HD11	1.81	0.61
1:C:161:ARG:HG2	1:C:162:LYS:HG3	1.82	0.61
1:A:326:VAL:O	1:A:330:GLU:HB2	2.01	0.60
1:B:126:ALA:HA	1:B:246:LEU:HD12	1.83	0.59
1:B:249:ILE:HG21	1:B:265:ILE:HD13	1.83	0.59
1:A:283:ALA:HB1	2:A:507:HOH:O	2.02	0.59
1:D:237:TYR:CE1	1:D:241:HIS:CE1	2.91	0.59
1:C:97:LEU:CD2	1:C:324:LEU:HD21	2.34	0.58
1:A:102:PRO:HD2	1:A:276:MET:HE1	1.86	0.58
1:B:385:ALA:O	1:B:389:ILE:HG12	2.04	0.58
1:A:165:PRO:HG3	1:C:165:PRO:HB3	1.86	0.58
1:C:136:VAL:HB	1:C:214:VAL:HG22	1.87	0.57
1:B:126:ALA:HB1	1:B:213:CYS:HB2	1.87	0.56
1:A:369:ILE:HB	1:A:407:LEU:HB2	1.87	0.56
1:C:50:LEU:HA	1:C:411:PRO:HA	1.86	0.56
1:C:263:TRP:HB2	1:C:266:GLN:HE21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:ASN:HD22	1:D:143:HIS:HB3	1.70	0.56
1:B:43:ASP:HB2	1:B:45:ASN:OD1	2.06	0.56
1:C:283:ALA:C	1:C:285:GLY:H	2.14	0.56
1:A:322:ALA:O	1:A:325:ASP:HB2	2.05	0.56
1:B:58:ASN:O	1:B:413:LEU:HB2	2.06	0.56
1:A:58:ASN:HB3	1:A:413:LEU:HG	1.87	0.56
1:B:276:MET:HE2	1:B:292:ILE:HB	1.88	0.56
1:B:137:SER:HB3	1:B:152:LEU:HD22	1.86	0.55
1:C:361:ARG:NH1	1:C:370:GLU:OE1	2.36	0.55
1:B:211:THR:O	1:B:245:ILE:HG12	2.05	0.55
1:B:120:ASP:OD1	1:B:146:THR:OG1	2.24	0.55
1:A:230:GLU:HA	1:A:268:PHE:CD2	2.42	0.55
1:C:313:ASN:HB3	1:C:316:CYS:HB2	1.88	0.55
1:B:202:PHE:CE1	1:B:211:THR:HG21	2.42	0.54
1:C:54:ALA:CB	1:C:280:LYS:HE2	2.37	0.54
1:A:87:HIS:CE1	1:A:90:GLY:HA3	2.43	0.54
1:A:193:ARG:O	1:A:197:GLU:HG2	2.07	0.54
1:A:385:ALA:HB1	1:A:401:THR:HG21	1.88	0.54
1:B:150:GLN:HG2	1:B:160:THR:CG2	2.38	0.54
1:A:86:HIS:O	1:B:31:ILE:HG22	2.08	0.53
1:B:204:SER:OG	1:B:205:PHE:N	2.41	0.53
1:B:248:ALA:HA	1:B:275:LEU:O	2.08	0.53
1:C:132:ARG:O	1:C:212:ALA:HB2	2.08	0.53
1:C:193:ARG:O	1:C:197:GLU:HG2	2.09	0.53
1:B:402:LEU:HG	1:B:408:ARG:HG2	1.90	0.53
1:B:365:LEU:HD13	1:B:411:PRO:HG2	1.91	0.53
1:A:150:GLN:HE21	1:A:163:ILE:HD11	1.74	0.52
1:B:171:VAL:HG21	1:B:206:LEU:HD22	1.91	0.52
1:B:354:HIS:HE1	1:B:432:THR:HG23	1.74	0.52
1:C:97:LEU:HD23	1:C:324:LEU:HD21	1.91	0.52
1:D:392:ALA:HB1	1:D:397:VAL:HG23	1.92	0.52
1:D:39:LEU:HD21	1:D:49:ASP:CG	2.35	0.52
1:D:249:ILE:HG12	1:D:273:PRO:HB3	1.92	0.52
1:C:282:LEU:HG	1:C:288:LEU:HD23	1.90	0.52
1:A:128:ALA:HA	1:B:162:LYS:HB3	1.92	0.52
1:C:87:HIS:O	1:C:91:MET:HG3	2.09	0.52
1:A:230:GLU:HA	1:A:268:PHE:CE2	2.45	0.52
1:C:213:CYS:HA	1:C:245:ILE:CG2	2.40	0.52
1:D:216:ILE:O	1:D:249:ILE:HA	2.09	0.51
1:A:123:ILE:HG23	1:A:135:ILE:HD11	1.92	0.51
1:B:49:ASP:OD1	1:B:50:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:OD1	1:A:254:GLN:NE2	2.42	0.51
1:C:319:ALA:O	1:C:323:THR:HG23	2.10	0.51
1:B:344:LYS:HB2	1:B:362:MET:HG2	1.92	0.51
1:C:141:SER:HB2	1:C:217:GLU:OE1	2.11	0.51
1:D:385:ALA:HB1	1:D:401:THR:HG21	1.93	0.51
1:A:344:LYS:HG3	1:A:362:MET:HB3	1.92	0.51
1:B:193:ARG:O	1:B:197:GLU:HG2	2.10	0.50
1:B:284:SER:OG	1:B:323:THR:CG2	2.60	0.50
1:B:402:LEU:O	1:B:403:ALA:C	2.54	0.50
1:D:127:ARG:HG2	1:D:132:ARG:O	2.11	0.50
1:B:286:MET:HB3	1:B:316:CYS:SG	2.52	0.50
1:B:339:ASP:HB3	1:B:365:LEU:HD21	1.94	0.50
1:C:54:ALA:HB1	1:C:280:LYS:HE2	1.93	0.50
1:C:123:ILE:HG23	1:C:135:ILE:HG13	1.92	0.50
1:A:193:ARG:HG3	1:D:182:TYR:OH	2.10	0.50
1:C:124:LYS:HZ3	1:D:150:GLN:HE22	1.59	0.50
1:C:363:TRP:O	1:C:366:ASN:HB3	2.12	0.50
1:B:119:ASN:OD1	1:B:215:LEU:HD11	2.12	0.49
1:A:313:ASN:HB3	1:A:316:CYS:SG	2.52	0.49
1:A:403:ALA:HB3	1:A:406:ILE:HD12	1.94	0.49
1:D:108:MET:HG3	1:D:295:LYS:HG3	1.93	0.49
1:A:124:LYS:CE	1:B:150:GLN:HE22	2.26	0.49
1:C:213:CYS:HA	1:C:245:ILE:HG22	1.94	0.49
1:A:339:ASP:OD1	1:A:417:ARG:NH2	2.45	0.49
1:B:370:GLU:HA	1:B:406:ILE:HA	1.94	0.49
1:D:49:ASP:O	1:D:50:LEU:HD23	2.12	0.49
1:C:76:LYS:HE2	1:D:33:HIS:HB3	1.95	0.49
1:B:279:GLY:O	1:B:280:LYS:C	2.56	0.49
1:A:108:MET:SD	1:A:295:LYS:HG3	2.53	0.48
1:D:129:TYR:CD2	1:D:246:LEU:HD21	2.47	0.48
1:A:220:GLN:HE21	1:A:223:GLY:HA3	1.77	0.48
1:C:102:PRO:HD3	1:C:263:TRP:CD1	2.48	0.48
1:C:54:ALA:O	1:C:56:ALA:N	2.46	0.48
1:C:275:LEU:HD23	1:C:293:GLY:HA3	1.94	0.48
1:A:85:PHE:HB3	1:B:31:ILE:HB	1.95	0.48
1:A:59:VAL:HG13	1:A:326:VAL:HG11	1.96	0.48
1:C:124:LYS:HB3	1:C:301:LEU:HD11	1.96	0.48
1:C:127:ARG:CZ	1:D:165:PRO:HD2	2.44	0.48
1:D:225:ILE:HG21	1:D:367:GLY:HA2	1.95	0.48
1:A:319:ALA:O	1:A:323:THR:HG22	2.14	0.48
1:B:161:ARG:HD3	1:C:209:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:MET:HA	1:D:366:ASN:O	2.14	0.48
1:B:397:VAL:HG11	1:B:426:VAL:HB	1.95	0.47
1:C:70:ILE:HG23	1:C:315:VAL:HG13	1.96	0.47
1:A:347:PHE:HA	1:A:350:MET:HB2	1.96	0.47
1:B:138:TYR:CZ	1:B:216:ILE:HD12	2.49	0.47
1:D:278:VAL:HG11	1:D:282:LEU:HD13	1.95	0.47
1:C:233:MET:HG3	1:C:271:ILE:HD13	1.96	0.47
1:A:180:ARG:HH21	1:A:380:PRO:HD3	1.79	0.47
1:B:237:TYR:CZ	1:B:241:HIS:HE1	2.33	0.47
1:D:335:LYS:HD3	1:D:413:LEU:O	2.15	0.47
1:C:219:ILE:HG12	1:C:227:LYS:HB2	1.96	0.47
1:B:180:ARG:NH1	1:B:370:GLU:OE2	2.34	0.47
1:D:255:GLY:O	1:D:256:LEU:C	2.57	0.46
1:A:79:HIS:CB	1:B:285:GLY:HA3	2.46	0.46
1:A:414:VAL:O	1:A:415:ILE:C	2.59	0.46
1:A:222:ASP:HA	1:A:402:LEU:HD22	1.96	0.46
1:D:182:TYR:O	1:D:183:PRO:C	2.59	0.46
1:D:282:LEU:O	1:D:320:SER:OG	2.31	0.46
1:A:213:CYS:HA	1:A:245:ILE:HG22	1.98	0.46
1:A:322:ALA:O	1:A:326:VAL:HG23	2.16	0.46
1:C:336:SER:HB2	1:C:413:LEU:HD22	1.98	0.46
1:A:202:PHE:HE1	1:A:211:THR:HG21	1.81	0.46
1:B:237:TYR:CZ	1:B:241:HIS:CE1	3.04	0.46
1:B:313:ASN:HA	1:B:314:PRO:HD3	1.71	0.46
1:B:356:MET:HE2	1:B:371:LEU:HD23	1.98	0.46
1:C:54:ALA:CB	1:C:280:LYS:HZ3	2.23	0.46
1:C:109:VAL:HG12	1:C:292:ILE:HG23	1.98	0.46
1:C:389:ILE:HG21	1:C:401:THR:HG23	1.97	0.46
1:A:249:ILE:HG12	1:A:273:PRO:HB3	1.99	0.45
1:B:361:ARG:HB3	1:B:363:TRP:CZ3	2.52	0.45
1:A:54:ALA:O	1:A:280:LYS:HD3	2.17	0.45
1:A:105:SER:O	1:A:107:LYS:HG2	2.16	0.45
1:B:362:MET:HE2	1:B:362:MET:HB2	1.80	0.45
1:C:51:LEU:HD22	1:C:51:LEU:HA	1.62	0.45
1:B:204:SER:OG	1:B:205:PHE:HD1	1.99	0.45
1:C:278:VAL:O	1:C:289:SER:HA	2.16	0.45
1:A:219:ILE:O	1:A:254:GLN:HG3	2.17	0.45
1:C:93:LEU:HB2	1:C:321:LEU:HD13	1.98	0.45
1:C:195:PHE:CE2	1:C:199:LYS:HD2	2.51	0.45
1:D:329:TYR:C	1:D:331:GLY:H	2.24	0.45
1:A:48:ILE:HG21	1:A:423:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:THR:HG21	1:B:75:GLN:O	2.17	0.45
1:A:300:SER:O	1:A:301:LEU:HD23	2.16	0.45
1:B:207:PRO:HB3	1:C:161:ARG:HH12	1.82	0.45
1:C:327:ILE:HG23	1:C:332:LEU:HB2	1.99	0.45
1:C:402:LEU:HD11	1:C:408:ARG:NE	2.27	0.45
1:D:385:ALA:HB1	1:D:401:THR:CG2	2.47	0.45
1:D:227:LYS:HE2	1:D:268:PHE:CZ	2.52	0.45
1:D:294:LYS:HD3	1:D:296:GLU:OE1	2.17	0.45
1:C:137:SER:O	1:C:172:HIS:HA	2.16	0.45
1:B:167:LEU:HD12	1:B:168:PRO:HD2	1.99	0.44
1:C:135:ILE:HG21	1:C:152:LEU:HD21	2.00	0.44
1:D:351:GLN:NE2	1:D:357:ILE:O	2.50	0.44
1:D:382:SER:HA	1:D:404:GLY:O	2.16	0.44
1:A:113:ASN:HD22	1:B:287:PRO:HB3	1.82	0.44
1:B:96:LYS:HG2	1:B:324:LEU:HD23	1.98	0.44
1:D:215:LEU:HD23	1:D:248:ALA:HB1	2.00	0.44
1:D:374:ASP:HA	1:D:375:PRO:HD2	1.62	0.44
1:A:273:PRO:HB2	1:A:275:LEU:O	2.18	0.44
1:B:48:ILE:HG21	1:B:423:ALA:HB2	1.98	0.44
1:B:88:VAL:O	1:B:91:MET:HB2	2.17	0.44
1:B:365:LEU:HD12	1:B:413:LEU:HD23	2.00	0.44
1:B:139:MET:HE1	1:C:201:PRO:HD3	1.99	0.44
1:B:225:ILE:HG13	1:B:367:GLY:O	2.18	0.44
1:D:137:SER:O	1:D:172:HIS:HA	2.17	0.44
1:D:143:HIS:CD2	1:D:152:LEU:HB3	2.50	0.44
1:A:206:LEU:HD11	1:A:211:THR:HG22	2.00	0.44
1:A:284:SER:HB2	1:A:323:THR:HG21	1.99	0.44
1:B:41:ASP:OD1	1:B:47:TYR:HE2	2.01	0.43
1:B:132:ARG:HB3	1:B:210:GLU:O	2.18	0.43
1:D:157:LEU:C	1:D:158:ASN:HD22	2.26	0.43
1:D:202:PHE:HE1	1:D:211:THR:HG21	1.82	0.43
1:B:127:ARG:HG2	1:B:132:ARG:O	2.18	0.43
1:A:391:TYR:CE2	1:A:395:HIS:CD2	3.07	0.43
1:B:237:TYR:CE1	1:B:241:HIS:CE1	3.05	0.43
1:B:391:TYR:CD1	1:B:430:ALA:HB2	2.54	0.43
1:C:402:LEU:HD11	1:C:408:ARG:HH21	1.84	0.43
1:D:157:LEU:HD21	1:D:403:ALA:HA	2.00	0.43
1:D:224:GLY:O	1:D:361:ARG:NH2	2.38	0.43
1:C:82:PRO:HA	1:C:85:PHE:O	2.19	0.43
1:C:402:LEU:CD1	1:C:408:ARG:HE	2.26	0.43
1:D:31:ILE:HD11	1:D:39:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:MET:HE1	1:B:286:MET:CE	2.49	0.43
1:A:73:GLN:HG2	1:A:314:PRO:O	2.18	0.43
1:A:224:GLY:O	1:A:361:ARG:NH2	2.44	0.43
1:B:142:TYR:O	1:B:142:TYR:CD2	2.71	0.43
1:C:97:LEU:HD21	1:C:324:LEU:HD21	2.00	0.43
1:C:422:GLN:O	1:C:426:VAL:HG23	2.19	0.43
1:D:357:ILE:HG23	1:D:369:ILE:HG22	2.01	0.42
1:A:120:ASP:OD1	1:A:146:THR:OG1	2.34	0.42
1:A:186:THR:O	1:A:188:HIS:N	2.52	0.42
1:C:63:HIS:ND1	1:C:65:LYS:HB2	2.34	0.42
1:A:137:SER:O	1:A:172:HIS:HA	2.19	0.42
1:A:283:ALA:HB1	1:A:286:MET:HB2	2.01	0.42
1:A:87:HIS:CE1	1:A:90:GLY:CA	3.02	0.42
1:A:182:TYR:OH	1:D:193:ARG:HG3	2.19	0.42
1:C:278:VAL:O	1:C:289:SER:HB2	2.20	0.42
1:D:250:ASP:OD1	1:D:250:ASP:C	2.62	0.42
1:C:51:LEU:O	1:C:52:ALA:HB3	2.19	0.42
1:D:418:GLU:O	1:D:422:GLN:HG3	2.20	0.42
1:A:344:LYS:HA	1:A:362:MET:HE3	2.01	0.42
1:C:63:HIS:NE2	1:C:330:GLU:OE1	2.47	0.42
1:C:127:ARG:NH1	1:D:165:PRO:HD2	2.34	0.42
1:A:275:LEU:HD13	1:A:293:GLY:HA2	2.01	0.42
1:A:357:ILE:HA	1:A:371:LEU:HD12	2.00	0.42
1:B:429:ASP:O	1:B:433:ALA:N	2.48	0.42
1:C:47:TYR:HB3	1:C:398:VAL:HG23	2.02	0.42
1:C:55:SER:O	1:C:57:ILE:N	2.53	0.42
1:C:216:ILE:HG22	1:C:248:ALA:O	2.19	0.42
1:C:103:GLY:HA3	1:C:272:GLU:HG3	2.01	0.42
1:C:148:GLY:HA2	1:C:167:LEU:HD22	2.01	0.42
1:C:343:ALA:O	1:C:347:PHE:HB2	2.20	0.42
1:D:344:LYS:HB2	1:D:362:MET:HG2	2.00	0.42
1:A:27:TYR:HB2	1:B:84:TYR:O	2.20	0.41
1:A:165:PRO:HG2	1:B:168:PRO:HG2	2.02	0.41
1:A:224:GLY:HA3	1:A:406:ILE:HD13	2.02	0.41
1:A:263:TRP:HZ3	1:A:278:VAL:HG21	1.85	0.41
1:A:402:LEU:HD21	1:A:408:ARG:HH11	1.85	0.41
1:C:140:GLY:N	1:C:154:GLY:O	2.52	0.41
1:D:318:ALA:HA	1:D:321:LEU:HD22	2.02	0.41
1:A:162:LYS:HB3	1:B:128:ALA:HA	2.02	0.41
1:A:259:THR:O	1:A:363:TRP:C	2.63	0.41
1:C:122:ILE:HD11	1:C:277:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ILE:HG12	1:C:273:PRO:HB3	2.02	0.41
1:D:358:GLY:HA3	1:D:372:VAL:HG22	2.02	0.41
1:D:374:ASP:OD2	1:D:377:THR:N	2.51	0.41
1:A:399:ILE:HG22	2:A:502:HOH:O	2.20	0.41
1:A:130:THR:C	1:A:132:ARG:H	2.29	0.41
1:D:332:LEU:O	1:D:333:VAL:C	2.64	0.41
1:D:348:LEU:HD12	1:D:360:VAL:HG11	2.03	0.41
1:B:370:GLU:HB2	1:B:406:ILE:HG23	2.02	0.41
1:C:400:ILE:HD13	1:D:84:TYR:CZ	2.55	0.41
1:A:102:PRO:HD3	1:A:263:TRP:CD1	2.56	0.41
1:A:286:MET:HB2	2:A:507:HOH:O	2.20	0.41
1:B:138:TYR:CE1	1:B:216:ILE:HD12	2.56	0.41
1:C:76:LYS:NZ	1:D:32:ASP:OD1	2.49	0.41
1:C:218:PRO:O	1:C:219:ILE:HG13	2.20	0.41
1:C:383:ASP:OD1	1:C:387:LYS:HE3	2.21	0.41
1:D:218:PRO:HA	1:D:233:MET:HE1	2.03	0.41
1:A:121:ALA:O	1:A:125:PHE:HD2	2.04	0.41
1:A:202:PHE:HA	1:A:206:LEU:O	2.20	0.41
1:A:275:LEU:HD11	1:A:297:VAL:HG11	2.03	0.41
1:C:59:VAL:HG21	1:C:323:THR:HB	2.02	0.41
1:C:253:ASN:HA	1:C:280:LYS:HZ2	1.86	0.41
1:D:391:TYR:O	1:D:392:ALA:C	2.64	0.41
1:A:134:TYR:HB2	1:A:211:THR:HA	2.03	0.40
1:A:232:TYR:O	1:A:236:VAL:HG23	2.21	0.40
1:A:287:PRO:HG2	1:B:287:PRO:HG2	2.03	0.40
1:C:351:GLN:HG3	1:C:357:ILE:HB	2.02	0.40
1:D:173:VAL:HG12	1:D:201:PRO:HG2	2.03	0.40
1:D:278:VAL:HG12	1:D:282:LEU:HD22	2.03	0.40
1:C:210:GLU:HG2	2:C:503:HOH:O	2.21	0.40
1:B:150:GLN:HG2	1:B:160:THR:HG21	2.02	0.40
1:C:251:GLU:OE1	1:C:251:GLU:HA	2.21	0.40
1:A:211:THR:O	1:A:245:ILE:HG23	2.22	0.40
1:C:200:LYS:HB2	1:C:201:PRO:HD2	2.03	0.40
1:D:402:LEU:O	1:D:406:ILE:HB	2.21	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	406/480 (85%)	347 (86%)	50 (12%)	9 (2%)	5	10
1	B	405/480 (84%)	339 (84%)	49 (12%)	17 (4%)	2	3
1	C	403/480 (84%)	336 (83%)	55 (14%)	12 (3%)	3	6
1	D	401/480 (84%)	326 (81%)	62 (16%)	13 (3%)	3	5
All	All	1615/1920 (84%)	1348 (84%)	216 (13%)	51 (3%)	3	5

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLU
1	B	62	THR
1	B	280	LYS
1	B	403	ALA
1	C	52	ALA
1	C	55	SER
1	C	56	ALA
1	D	62	THR
1	D	98	ALA
1	D	383	ASP
1	A	270	ASP
1	A	284	SER
1	B	58	ASN
1	B	156	SER
1	C	183	PRO
1	C	270	ASP
1	C	284	SER
1	D	375	PRO
1	A	224	GLY
1	A	366	ASN
1	A	408	ARG
1	B	158	ASN

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Mol	Chain	Res	Type
1	B	287	PRO
1	B	366	ASN
1	D	83	ALA
1	D	188	HIS
1	D	262	MET
1	A	183	PRO
1	B	55	SER
1	B	56	ALA
1	B	321	LEU
1	B	418	GLU
1	C	54	ALA
1	D	238	LYS
1	D	280	LYS
1	A	28	ASN
1	B	438	GLU
1	C	181	THR
1	A	225	ILE
1	B	176	PRO
1	B	303	ALA
1	C	49	ASP
1	D	183	PRO
1	D	354	HIS
1	B	70	ILE
1	B	154	GLY
1	C	154	GLY
1	C	225	ILE
1	D	36	GLY
1	D	225	ILE
1	C	287	PRO

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	339/396 (86%)	293 (86%)	46 (14%)	3 7
1	B	337/396 (85%)	291 (86%)	46 (14%)	3 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	336/396 (85%)	297 (88%)	39 (12%)	5	11
1	D	335/396 (85%)	291 (87%)	44 (13%)	4	8
All	All	1347/1584 (85%)	1172 (87%)	175 (13%)	4	8

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	TYR
1	A	28	ASN
1	A	29	LEU
1	A	50	LEU
1	A	58	ASN
1	A	80	TYR
1	A	84	TYR
1	A	91	MET
1	A	99	LYS
1	A	107	LYS
1	A	108	MET
1	A	109	VAL
1	A	113	ASN
1	A	114	SER
1	A	117	ASP
1	A	145	SER
1	A	163	ILE
1	A	181	THR
1	A	191	SER
1	A	201	PRO
1	A	214	VAL
1	A	231	GLU
1	A	259	THR
1	A	261	LYS
1	A	269	LYS
1	A	270	ASP
1	A	271	ILE
1	A	275	LEU
1	A	276	MET
1	A	291	VAL
1	A	321	LEU
1	A	323	THR
1	A	325	ASP
1	A	334	GLU

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Mol	Chain	Res	Type
1	A	348	LEU
1	A	356	MET
1	A	359	ASP
1	A	362	MET
1	A	371	LEU
1	A	382	SER
1	A	397	VAL
1	A	400	ILE
1	A	401	THR
1	A	427	LEU
1	A	440	THR
1	A	441	ILE
1	B	28	ASN
1	B	29	LEU
1	B	30	VAL
1	B	38	THR
1	B	39	LEU
1	B	42	VAL
1	B	43	ASP
1	B	46	LYS
1	B	48	ILE
1	B	51	LEU
1	B	53	SER
1	B	58	ASN
1	B	66	VAL
1	B	68	LYS
1	B	80	TYR
1	B	84	TYR
1	B	88	VAL
1	B	95	GLU
1	B	99	LYS
1	B	109	VAL
1	B	120	ASP
1	B	181	THR
1	B	211	THR
1	B	215	LEU
1	B	216	ILE
1	B	231	GLU
1	B	278	VAL
1	B	284	SER
1	B	296	GLU
1	B	300	SER

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Mol	Chain	Res	Type
1	B	321	LEU
1	B	324	LEU
1	B	325	ASP
1	B	327	ILE
1	B	332	LEU
1	B	373	LYS
1	B	377	THR
1	B	397	VAL
1	B	400	ILE
1	B	406	ILE
1	B	408	ARG
1	B	418	GLU
1	B	427	LEU
1	B	432	THR
1	B	439	VAL
1	B	440	THR
1	C	28	ASN
1	C	29	LEU
1	C	40	VAL
1	C	50	LEU
1	C	51	LEU
1	C	55	SER
1	C	57	ILE
1	C	64	GLU
1	C	65	LYS
1	C	85	PHE
1	C	92	GLU
1	C	105	SER
1	C	109	VAL
1	C	120	ASP
1	C	153	SER
1	C	162	LYS
1	C	171	VAL
1	C	190	VAL
1	C	192	LEU
1	C	209	ASP
1	C	215	LEU
1	C	225	ILE
1	C	226	ILE
1	C	235	LEU
1	C	246	LEU
1	C	265	ILE

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Mol	Chain	Res	Type
1	C	269	LYS
1	C	278	VAL
1	C	297	VAL
1	C	302	ASP
1	C	321	LEU
1	C	334	GLU
1	C	338	THR
1	C	373	LYS
1	C	397	VAL
1	C	407	LEU
1	C	418	GLU
1	C	422	GLN
1	C	427	LEU
1	D	27	TYR
1	D	38	THR
1	D	39	LEU
1	D	40	VAL
1	D	59	VAL
1	D	68	LYS
1	D	75	GLN
1	D	99	LYS
1	D	100	ILE
1	D	109	VAL
1	D	110	SER
1	D	120	ASP
1	D	151	THR
1	D	157	LEU
1	D	158	ASN
1	D	169	SER
1	D	191	SER
1	D	192	LEU
1	D	196	ASN
1	D	213	CYS
1	D	215	LEU
1	D	238	LYS
1	D	241	HIS
1	D	242	GLU
1	D	246	LEU
1	D	250	ASP
1	D	265	ILE
1	D	269	LYS
1	D	272	GLU

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Mol	Chain	Res	Type
1	D	275	LEU
1	D	281	SER
1	D	301	LEU
1	D	321	LEU
1	D	324	LEU
1	D	327	ILE
1	D	328	GLU
1	D	338	THR
1	D	383	ASP
1	D	389	ILE
1	D	400	ILE
1	D	401	THR
1	D	418	GLU
1	D	427	LEU
1	D	435	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	58	ASN
1	A	75	GLN
1	A	113	ASN
1	A	188	HIS
1	A	220	GLN
1	A	366	ASN
1	A	395	HIS
1	A	422	GLN
1	B	79	HIS
1	B	87	HIS
1	B	143	HIS
1	B	241	HIS
1	B	243	HIS
1	B	313	ASN
1	B	422	GLN
1	B	425	GLN
1	C	58	ASN
1	C	61	HIS
1	C	104	ASN
1	C	220	GLN
1	C	241	HIS
1	C	266	GLN

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Mol	Chain	Res	Type
1	C	267	GLN
1	C	395	HIS
1	C	419	GLN
1	D	33	HIS
1	D	58	ASN
1	D	61	HIS
1	D	63	HIS
1	D	75	GLN
1	D	133	GLN
1	D	150	GLN
1	D	158	ASN
1	D	172	HIS
1	D	220	GLN
1	D	241	HIS
1	D	299	GLN
1	D	425	GLN

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 ⓘ

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	409/480 (85%)	0.33	18 (4%) 39 33	21, 38, 63, 92	8 (1%)
1	B	409/480 (85%)	0.30	17 (4%) 40 35	24, 39, 65, 98	7 (1%)
1	C	407/480 (84%)	0.38	21 (5%) 33 27	23, 43, 68, 134	1 (0%)
1	D	405/480 (84%)	0.25	14 (3%) 47 41	20, 40, 64, 129	1 (0%)
All	All	1630/1920 (84%)	0.32	70 (4%) 40 34	20, 41, 66, 134	17 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	THR	9.5
1	C	303	ALA	7.9
1	A	302	ASP	6.7
1	B	305	ALA	6.5
1	B	156	SER	6.1
1	D	301	LEU	6.0
1	B	82	PRO	6.0
1	B	157	LEU	5.7
1	C	85	PHE	5.3
1	D	78	ILE	5.2
1	A	82	PRO	5.0
1	A	83	ALA	4.5
1	C	312	GLY	4.3
1	C	27	TYR	4.2
1	C	53	SER	3.9
1	A	84	TYR	3.9
1	C	84	TYR	3.9
1	D	80	TYR	3.9
1	D	79	HIS	3.8
1	A	85	PHE	3.7
1	B	390	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	81	THR	3.3
1	C	56	ALA	3.3
1	B	29	LEU	3.3
1	A	54	ALA	3.1
1	C	55	SER	3.1
1	B	27	TYR	3.1
1	A	159	MET	3.1
1	B	84	TYR	3.0
1	A	441	ILE	3.0
1	A	51	LEU	3.0
1	D	314	PRO	3.0
1	D	158	ASN	2.9
1	C	51	LEU	2.9
1	D	77	LEU	2.8
1	B	248	ALA	2.7
1	B	55	SER	2.6
1	A	27	TYR	2.6
1	C	159	MET	2.6
1	C	82	PRO	2.6
1	C	80	TYR	2.5
1	C	81	THR	2.5
1	B	56	ALA	2.5
1	B	81	THR	2.5
1	D	81	THR	2.5
1	C	54	ALA	2.5
1	D	341	ALA	2.5
1	B	304	PRO	2.4
1	A	311	ALA	2.4
1	D	319	ALA	2.4
1	C	371	LEU	2.4
1	C	424	LEU	2.3
1	A	300	SER	2.3
1	C	59	VAL	2.3
1	D	85	PHE	2.3
1	A	310	THR	2.3
1	B	80	TYR	2.3
1	D	84	TYR	2.3
1	C	153	SER	2.2
1	C	341	ALA	2.1
1	D	56	ALA	2.1
1	C	158	ASN	2.1
1	A	79	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	83	ALA	2.1
1	B	413	LEU	2.1
1	D	27	TYR	2.0
1	A	53	SER	2.0
1	C	160	THR	2.0
1	A	331	GLY	2.0
1	B	36	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.