



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:21 pm BST

PDB ID : 5LL3
Title : Structure of the Isoleucine 2-epimerase from *Lactobacillus buchneri* (PLP complex form)
Authors : Reiser, J.-B.; Awad, R.; Gans, P.
Deposited on : 2016-07-26
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

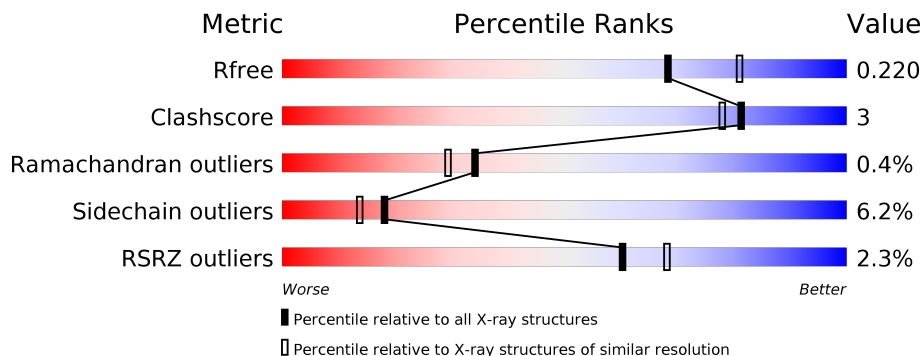
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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	 2% 77% 9% • 13%
1	B	480	 2% 76% 10% • 13%
1	C	480	 2% 77% 9% • 13%
1	D	480	 2% 78% 8% • 13%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13699 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
			Total	C	N	O	S			
1	A	417	3217	2052	537	612	16	0	1	0
1	B	417	3214	2050	537	611	16	0	0	0
1	C	417	3214	2050	537	611	16	0	0	0
1	D	417	3214	2050	537	611	16	0	0	0

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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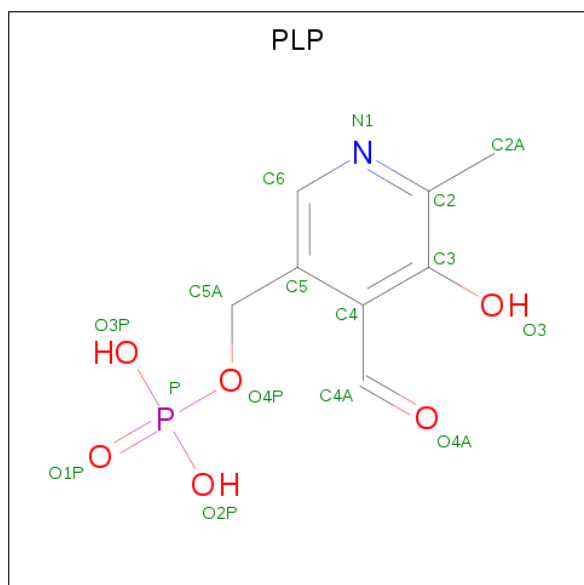
Chain	Residue	Modelled	Actual	Comment	Reference
C	-26	SER	-	expression tag	UNP M1GRN3
C	-25	HIS	-	expression tag	UNP M1GRN3
C	-24	HIS	-	expression tag	UNP M1GRN3
C	-23	HIS	-	expression tag	UNP M1GRN3
C	-22	HIS	-	expression tag	UNP M1GRN3
C	-21	HIS	-	expression tag	UNP M1GRN3
C	-20	HIS	-	expression tag	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 PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

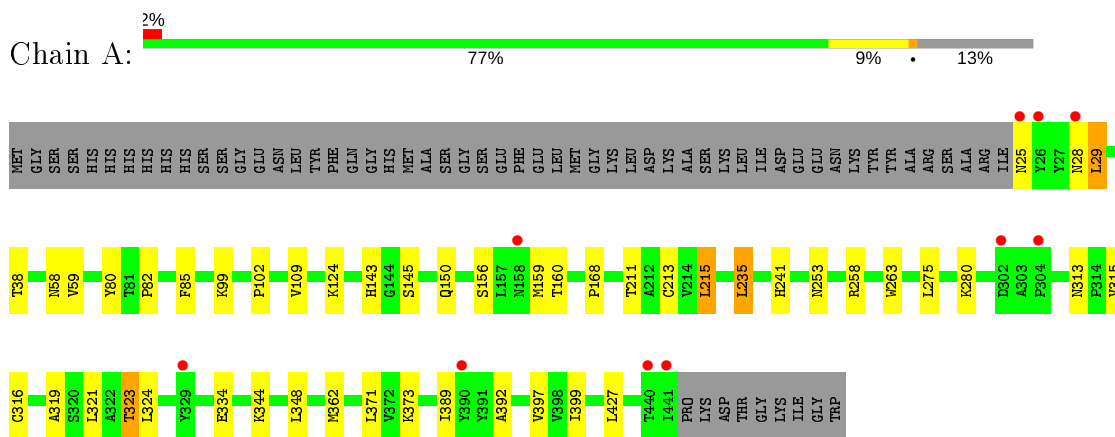
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	196	Total 196	O 196	0	0
3	B	184	Total 184	O 184	0	0
3	C	185	Total 185	O 185	0	0
3	D	215	Total 215	O 215	0	0

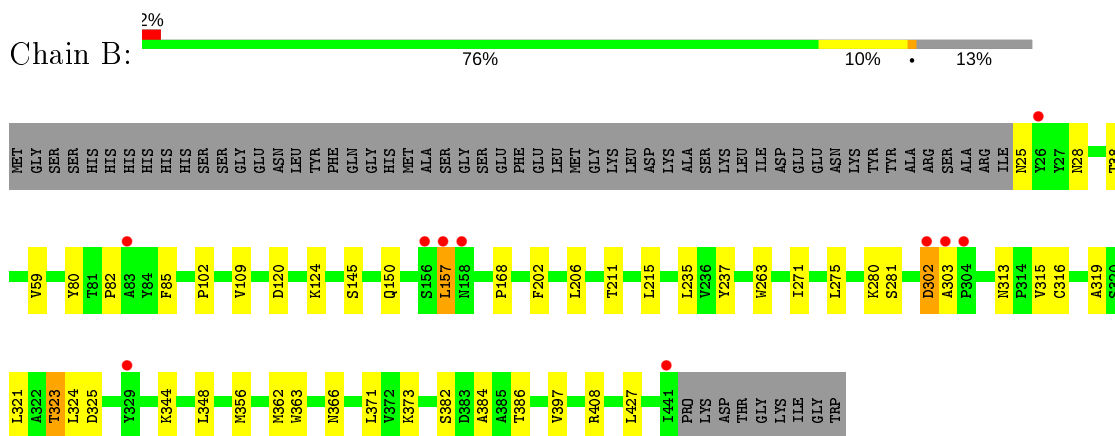
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

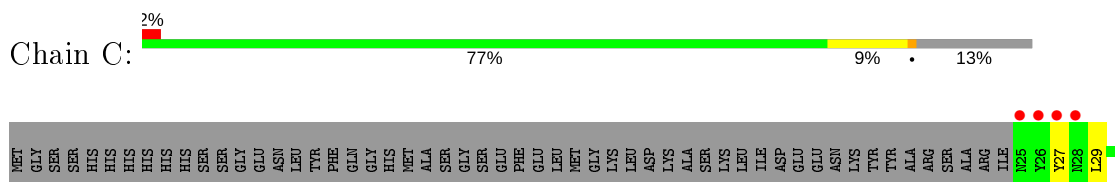
- Molecule 1: Isoleucine 2-epimerase

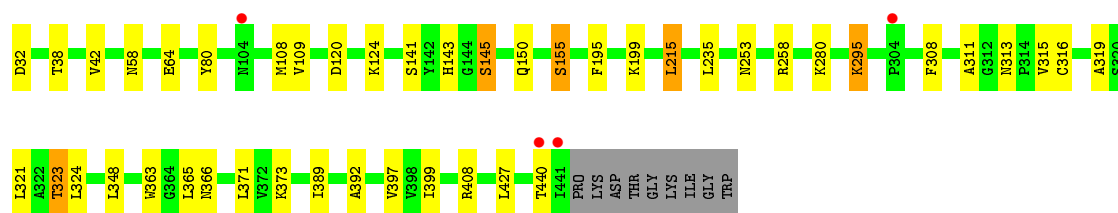


- Molecule 1: Isoleucine 2-epimerase

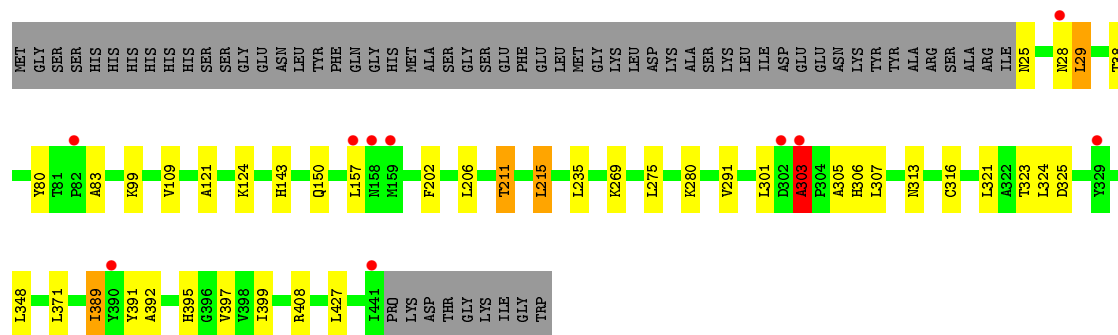
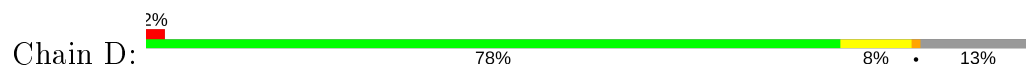


- Molecule 1: Isoleucine 2-epimerase





• 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	57.46Å 165.40Å 188.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 19.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.15) 99.6 (19.99-2.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.15Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.177 , 0.218 0.180 , 0.220	Depositor DCC
R_{free} test set	4953 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13699	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

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	0.50	0/3296	0.70	2/4474 (0.0%)
1	B	0.51	0/3290	0.69	1/4466 (0.0%)
1	C	0.51	0/3290	0.68	0/4466
1	D	0.51	0/3290	0.71	2/4466 (0.0%)
All	All	0.51	0/13166	0.69	5/17872 (0.0%)

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	29	LEU	CA-CB-CG	5.88	128.82	115.30
1	D	29	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	157	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	235	LEU	CA-CB-CG	5.01	126.83	115.30
1	B	157	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	302	ASP	Peptide
1	D	303	ALA	Peptide

5.2 Too-close contacts [i](#)

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	3217	0	3171	18	0
1	B	3214	0	3166	19	0
1	C	3214	0	3166	19	0
1	D	3214	0	3166	16	0
2	A	15	0	6	1	0
2	B	15	0	6	0	0
2	C	15	0	6	1	0
2	D	15	0	6	0	0
3	A	196	0	0	1	0
3	B	184	0	0	1	0
3	C	185	0	0	0	0
3	D	215	0	0	0	0
All	All	13699	0	12693	66	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 3.

All (66) 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:313:ASN:HD22	1:C:316:CYS:H	1.33	0.76
1:C:145:SER:HA	1:C:150:GLN:HE21	1.49	0.76
1:B:313:ASN:HD22	1:B:316:CYS:H	1.34	0.74
1:A:313:ASN:HD22	1:A:316:CYS:H	1.36	0.73
1:A:124:LYS:HZ3	1:B:150:GLN:HE22	1.41	0.69
1:D:313:ASN:HD22	1:D:316:CYS:H	1.42	0.68
1:A:25:ASN:HD22	1:A:28:ASN:H	1.44	0.65
1:D:202:PHE:HE1	1:D:211:THR:HG21	1.61	0.64
1:A:124:LYS:NZ	1:B:150:GLN:HE22	1.95	0.63
1:C:195:PHE:CE2	1:C:199:LYS:HD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:ALA:HB1	1:C:397:VAL:HG22	1.84	0.59
1:D:121:ALA:HB3	1:D:291:VAL:HG21	1.87	0.56
1:A:102:PRO:HD3	1:A:263:TRP:CD1	2.42	0.55
1:D:121:ALA:HB2	1:D:306:HIS:CE1	2.41	0.54
1:D:143:HIS:CE1	1:D:215:LEU:HD13	2.43	0.54
1:C:319:ALA:O	1:C:323:THR:HG23	2.07	0.53
1:A:392:ALA:HB1	1:A:397:VAL:HG22	1.90	0.53
1:C:319:ALA:O	1:C:323:THR:CG2	2.58	0.52
1:D:202:PHE:CE1	1:D:211:THR:HG21	2.42	0.52
1:A:313:ASN:HD21	1:A:315:VAL:HB	1.74	0.52
1:A:82:PRO:HA	1:A:85:PHE:O	2.10	0.51
1:B:313:ASN:HD21	1:B:315:VAL:HB	1.76	0.51
1:B:344:LYS:HD3	1:B:362:MET:HB3	1.91	0.51
1:D:392:ALA:HB1	1:D:397:VAL:HG22	1.92	0.51
1:C:32:ASP:HB2	1:C:42:VAL:HA	1.93	0.51
1:D:25:ASN:HD22	1:D:28:ASN:H	1.59	0.51
1:B:102:PRO:HD3	1:B:263:TRP:CD1	2.46	0.50
1:B:319:ALA:O	1:B:323:THR:HG23	2.11	0.50
1:C:124:LYS:NZ	1:D:150:GLN:HE22	2.10	0.50
1:D:124:LYS:HB3	1:D:301:LEU:HD11	1.93	0.50
1:B:356:MET:HE1	1:B:384:ALA:HB1	1.94	0.50
1:C:313:ASN:HD21	1:C:315:VAL:HB	1.77	0.50
1:A:319:ALA:O	1:A:323:THR:HG23	2.13	0.49
1:A:168:PRO:HG3	1:B:168:PRO:HG3	1.96	0.48
1:B:363:TRP:O	1:B:366:ASN:HB3	2.14	0.48
1:A:344:LYS:HB2	1:A:362:MET:HG2	1.96	0.47
1:B:382:SER:O	1:B:386:THR:HG23	2.14	0.47
1:C:253:ASN:HB2	2:C:1000:PLP:O3	2.14	0.47
1:C:363:TRP:O	1:C:366:ASN:HB3	2.15	0.47
1:A:58:ASN:ND2	1:A:258:ARG:HH21	2.12	0.46
1:B:386:THR:HG22	3:B:1107:HOH:O	2.15	0.46
1:A:253:ASN:HB2	2:A:1000:PLP:O3	2.16	0.46
1:C:58:ASN:ND2	1:C:258:ARG:HH21	2.13	0.46
1:A:344:LYS:HD2	3:A:1271:HOH:O	2.15	0.45
1:D:202:PHE:HA	1:D:206:LEU:O	2.16	0.45
1:A:143:HIS:CE1	1:A:215:LEU:HD13	2.52	0.45
1:A:389:ILE:HG22	1:A:399:ILE:HG23	1.99	0.45
1:D:303:ALA:HA	1:D:305:ALA:N	2.32	0.45
1:C:389:ILE:HG22	1:C:399:ILE:HG23	1.98	0.45
1:C:143:HIS:CE1	1:C:215:LEU:HD13	2.52	0.44
1:D:391:TYR:O	1:D:395:HIS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:TYR:CE1	1:B:271:ILE:HG23	2.53	0.44
1:A:150:GLN:HE22	1:B:124:LYS:NZ	2.16	0.44
1:C:124:LYS:HZ3	1:D:150:GLN:HE22	1.64	0.44
1:D:389:ILE:HD12	1:D:399:ILE:HG23	2.00	0.43
1:B:356:MET:CE	1:B:384:ALA:HB1	2.49	0.43
1:C:308:PHE:HB2	1:C:311:ALA:HB2	2.01	0.43
1:D:83:ALA:HB2	1:D:307:LEU:HD13	2.00	0.43
1:B:82:PRO:HA	1:B:85:PHE:O	2.19	0.42
1:C:108:MET:HG3	1:C:295:LYS:HD3	2.01	0.42
1:C:258:ARG:NH1	1:C:365:LEU:O	2.48	0.42
1:B:202:PHE:HA	1:B:206:LEU:O	2.20	0.41
1:B:313:ASN:ND2	1:B:316:CYS:H	2.10	0.41
1:A:156[A]:SER:HB3	1:A:159:MET:HG3	2.02	0.41
1:B:25:ASN:HD22	1:B:28:ASN:HA	1.86	0.41
1:C:141:SER:O	1:C:155:SER:HB2	2.20	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	416/480 (87%)	400 (96%)	15 (4%)	1 (0%)	47	46
1	B	415/480 (86%)	397 (96%)	16 (4%)	2 (0%)	29	22
1	C	415/480 (86%)	395 (95%)	19 (5%)	1 (0%)	47	46
1	D	415/480 (86%)	397 (96%)	16 (4%)	2 (0%)	29	22
All	All	1661/1920 (86%)	1589 (96%)	66 (4%)	6 (0%)	34	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	LYS
1	A	280	LYS
1	C	280	LYS
1	D	280	LYS
1	B	303	ALA
1	D	303	ALA

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	345/396 (87%)	323 (94%)	22 (6%)	17	12
1	B	344/396 (87%)	321 (93%)	23 (7%)	16	11
1	C	344/396 (87%)	323 (94%)	21 (6%)	18	14
1	D	344/396 (87%)	325 (94%)	19 (6%)	21	17
All	All	1377/1584 (87%)	1292 (94%)	85 (6%)	18	14

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	38	THR
1	A	59	VAL
1	A	80	TYR
1	A	99	LYS
1	A	109	VAL
1	A	145	SER
1	A	160	THR
1	A	211	THR
1	A	213	CYS
1	A	215	LEU
1	A	235	LEU
1	A	241	HIS
1	A	275	LEU
1	A	321	LEU
1	A	323	THR

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Mol	Chain	Res	Type
1	A	324	LEU
1	A	334	GLU
1	A	348	LEU
1	A	371	LEU
1	A	373	LYS
1	A	427	LEU
1	B	38	THR
1	B	59	VAL
1	B	80	TYR
1	B	109	VAL
1	B	120	ASP
1	B	145	SER
1	B	157	LEU
1	B	211	THR
1	B	215	LEU
1	B	235	LEU
1	B	275	LEU
1	B	281	SER
1	B	302	ASP
1	B	321	LEU
1	B	323	THR
1	B	324	LEU
1	B	325	ASP
1	B	348	LEU
1	B	371	LEU
1	B	373	LYS
1	B	397	VAL
1	B	408	ARG
1	B	427	LEU
1	C	27	TYR
1	C	29	LEU
1	C	38	THR
1	C	64	GLU
1	C	80	TYR
1	C	109	VAL
1	C	120	ASP
1	C	145	SER
1	C	155	SER
1	C	215	LEU
1	C	235	LEU
1	C	295	LYS
1	C	321	LEU

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Mol	Chain	Res	Type
1	C	323	THR
1	C	324	LEU
1	C	348	LEU
1	C	371	LEU
1	C	373	LYS
1	C	408	ARG
1	C	427	LEU
1	C	440	THR
1	D	29	LEU
1	D	38	THR
1	D	80	TYR
1	D	99	LYS
1	D	109	VAL
1	D	211	THR
1	D	215	LEU
1	D	235	LEU
1	D	269	LYS
1	D	275	LEU
1	D	321	LEU
1	D	323	THR
1	D	324	LEU
1	D	325	ASP
1	D	348	LEU
1	D	371	LEU
1	D	389	ILE
1	D	408	ARG
1	D	427	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	58	ASN
1	A	150	GLN
1	A	313	ASN
1	B	25	ASN
1	B	58	ASN
1	B	150	GLN
1	B	243	HIS
1	B	266	GLN
1	B	313	ASN
1	B	395	HIS

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Mol	Chain	Res	Type
1	C	25	ASN
1	C	35	HIS
1	C	58	ASN
1	C	113	ASN
1	C	150	GLN
1	C	241	HIS
1	C	243	HIS
1	C	266	GLN
1	C	313	ASN
1	C	395	HIS
1	D	25	ASN
1	D	58	ASN
1	D	79	HIS
1	D	133	GLN
1	D	150	GLN
1	D	241	HIS
1	D	266	GLN
1	D	313	ASN
1	D	395	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PLP	C	1000	1	15,15,16	3.33	3 (20%)	20,22,23	1.50	3 (15%)
2	PLP	D	1000	1	15,15,16	2.94	3 (20%)	20,22,23	1.55	4 (20%)
2	PLP	A	1000	1	15,15,16	3.25	3 (20%)	20,22,23	1.54	4 (20%)
2	PLP	B	1000	1	15,15,16	3.32	3 (20%)	20,22,23	1.46	3 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	C	1000	1	-	0/6/6/8	0/1/1/1
2	PLP	D	1000	1	-	0/6/6/8	0/1/1/1
2	PLP	A	1000	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1000	1	-	0/6/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	PLP	C5-C4	9.40	1.50	1.40
2	A	1000	PLP	C5-C4	8.33	1.49	1.40
2	B	1000	PLP	C5-C4	8.33	1.49	1.40
2	B	1000	PLP	C3-C2	8.21	1.49	1.40
2	A	1000	PLP	C3-C2	7.97	1.48	1.40
2	D	1000	PLP	C5-C4	7.29	1.48	1.40
2	C	1000	PLP	C3-C2	7.26	1.48	1.40
2	D	1000	PLP	C3-C2	6.92	1.47	1.40
2	B	1000	PLP	C3-C4	4.57	1.49	1.40
2	D	1000	PLP	C3-C4	4.33	1.49	1.40
2	C	1000	PLP	C3-C4	4.25	1.49	1.40
2	A	1000	PLP	C3-C4	4.06	1.48	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	PLP	C4A-C4-C5	3.41	124.45	120.94
2	C	1000	PLP	C6-N1-C2	3.23	125.14	119.17
2	B	1000	PLP	C6-N1-C2	2.86	124.47	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1000	PLP	C6-N1-C2	2.85	124.44	119.17
2	C	1000	PLP	C4A-C4-C5	2.81	123.83	120.94
2	D	1000	PLP	O4P-C5A-C5	2.70	114.50	109.35
2	B	1000	PLP	O4P-C5A-C5	2.51	114.13	109.35
2	D	1000	PLP	C4A-C4-C5	2.42	123.43	120.94
2	A	1000	PLP	O3P-P-O2P	2.34	116.58	107.64
2	A	1000	PLP	C6-N1-C2	2.31	123.44	119.17
2	C	1000	PLP	O4P-C5A-C5	2.27	113.69	109.35
2	B	1000	PLP	O2P-P-O4P	-2.13	101.05	106.73
2	D	1000	PLP	O3P-P-O2P	2.10	115.66	107.64
2	A	1000	PLP	O3-C3-C2	2.05	121.95	117.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1000	PLP	1	0
2	A	1000	PLP	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	417/480 (86%)	-0.31	10 (2%) 59 67	17, 27, 51, 74	0
1	B	417/480 (86%)	-0.20	10 (2%) 59 67	18, 30, 54, 75	0
1	C	417/480 (86%)	-0.25	8 (1%) 66 74	16, 28, 48, 140	0
1	D	417/480 (86%)	-0.33	10 (2%) 59 67	15, 27, 50, 71	0
All	All	1668/1920 (86%)	-0.27	38 (2%) 60 68	15, 28, 51, 140	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	25	ASN	7.6
1	B	157	LEU	5.6
1	C	26	TYR	4.9
1	C	28	ASN	4.9
1	A	302	ASP	3.9
1	C	27	TYR	3.8
1	B	302	ASP	3.7
1	B	441	ILE	3.6
1	D	329	TYR	3.5
1	A	329	TYR	2.9
1	B	156	SER	2.9
1	D	157	LEU	2.9
1	D	441	ILE	2.8
1	A	390	TYR	2.8
1	A	304	PRO	2.7
1	A	28	ASN	2.7
1	B	304	PRO	2.7
1	B	329	TYR	2.6
1	A	441	ILE	2.6
1	B	158	ASN	2.6
1	D	302	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	104	ASN	2.5
1	A	26	TYR	2.5
1	D	390	TYR	2.5
1	A	440	THR	2.3
1	B	83	ALA	2.2
1	D	158	ASN	2.2
1	B	303	ALA	2.2
1	D	82	PRO	2.2
1	C	440	THR	2.1
1	C	304	PRO	2.1
1	C	441	ILE	2.1
1	A	158	ASN	2.1
1	D	28	ASN	2.1
1	D	159	MET	2.1
1	A	25	ASN	2.0
1	D	303	ALA	2.0
1	B	26	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PLP	C	1000	15/16	0.97	0.10	21,23,25,27	0
2	PLP	B	1000	15/16	0.97	0.07	24,27,29,30	0
2	PLP	A	1000	15/16	0.98	0.07	21,22,24,25	0
2	PLP	D	1000	15/16	0.98	0.07	21,22,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.