



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 06:09 am BST

PDB ID : 2ZY3
Title : dodecameric L-aspartate beta-decarboxylase
Authors : Chen, H.-J.; Ko, T.-P.; Lee, C.-Y.; Wang, N.-C.; Wang, A.H.-J.
Deposited on : 2009-01-13
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

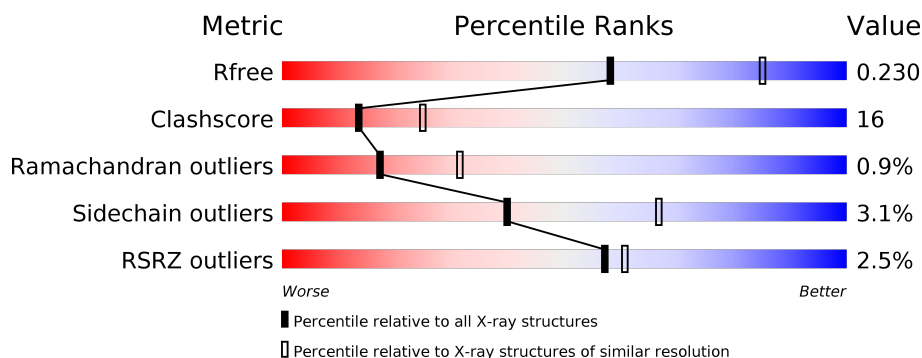
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	546	<div> <div>3%</div> <div>67% 25% • 7%</div> </div>
1	B	546	<div> <div>%</div> <div>66% 27% • 6%</div> </div>
1	C	546	<div> <div>3%</div> <div>71% 22% • 5%</div> </div>
1	D	546	<div> <div>2%</div> <div>69% 23% • 6%</div> </div>
1	E	546	<div> <div>3%</div> <div>62% 29% • 6%</div> </div>
1	F	546	<div> <div>2%</div> <div>64% 30% • •</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26599 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 L-aspartate beta-decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4011	2553	684	757	17			
1	B	515	Total	C	N	O	S	0	0	0
			4054	2579	691	767	17			
1	C	516	Total	C	N	O	S	0	0	0
			4065	2588	692	768	17			
1	D	514	Total	C	N	O	S	0	0	0
			4042	2571	692	762	17			
1	E	512	Total	C	N	O	S	0	0	0
			4028	2563	687	761	17			
1	F	523	Total	C	N	O	S	0	0	0
			4116	2620	701	778	17			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	LYS	-	EXPRESSION TAG	UNP Q93QX0
A	535	LEU	-	EXPRESSION TAG	UNP Q93QX0
A	536	ALA	-	EXPRESSION TAG	UNP Q93QX0
A	537	ALA	-	EXPRESSION TAG	UNP Q93QX0
A	538	ALA	-	EXPRESSION TAG	UNP Q93QX0
A	539	LEU	-	EXPRESSION TAG	UNP Q93QX0
A	540	GLU	-	EXPRESSION TAG	UNP Q93QX0
A	541	HIS	-	EXPRESSION TAG	UNP Q93QX0
A	542	HIS	-	EXPRESSION TAG	UNP Q93QX0
A	543	HIS	-	EXPRESSION TAG	UNP Q93QX0
A	544	HIS	-	EXPRESSION TAG	UNP Q93QX0
A	545	HIS	-	EXPRESSION TAG	UNP Q93QX0
A	546	HIS	-	EXPRESSION TAG	UNP Q93QX0
B	534	LYS	-	EXPRESSION TAG	UNP Q93QX0
B	535	LEU	-	EXPRESSION TAG	UNP Q93QX0
B	536	ALA	-	EXPRESSION TAG	UNP Q93QX0
B	537	ALA	-	EXPRESSION TAG	UNP Q93QX0

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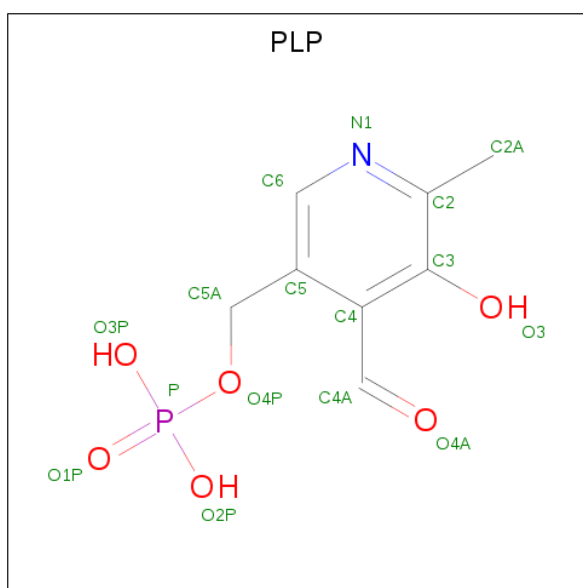
Chain	Residue	Modelled	Actual	Comment	Reference
B	538	ALA	-	EXPRESSION TAG	UNP Q93QX0
B	539	LEU	-	EXPRESSION TAG	UNP Q93QX0
B	540	GLU	-	EXPRESSION TAG	UNP Q93QX0
B	541	HIS	-	EXPRESSION TAG	UNP Q93QX0
B	542	HIS	-	EXPRESSION TAG	UNP Q93QX0
B	543	HIS	-	EXPRESSION TAG	UNP Q93QX0
B	544	HIS	-	EXPRESSION TAG	UNP Q93QX0
B	545	HIS	-	EXPRESSION TAG	UNP Q93QX0
B	546	HIS	-	EXPRESSION TAG	UNP Q93QX0
C	534	LYS	-	EXPRESSION TAG	UNP Q93QX0
C	535	LEU	-	EXPRESSION TAG	UNP Q93QX0
C	536	ALA	-	EXPRESSION TAG	UNP Q93QX0
C	537	ALA	-	EXPRESSION TAG	UNP Q93QX0
C	538	ALA	-	EXPRESSION TAG	UNP Q93QX0
C	539	LEU	-	EXPRESSION TAG	UNP Q93QX0
C	540	GLU	-	EXPRESSION TAG	UNP Q93QX0
C	541	HIS	-	EXPRESSION TAG	UNP Q93QX0
C	542	HIS	-	EXPRESSION TAG	UNP Q93QX0
C	543	HIS	-	EXPRESSION TAG	UNP Q93QX0
C	544	HIS	-	EXPRESSION TAG	UNP Q93QX0
C	545	HIS	-	EXPRESSION TAG	UNP Q93QX0
C	546	HIS	-	EXPRESSION TAG	UNP Q93QX0
D	534	LYS	-	EXPRESSION TAG	UNP Q93QX0
D	535	LEU	-	EXPRESSION TAG	UNP Q93QX0
D	536	ALA	-	EXPRESSION TAG	UNP Q93QX0
D	537	ALA	-	EXPRESSION TAG	UNP Q93QX0
D	538	ALA	-	EXPRESSION TAG	UNP Q93QX0
D	539	LEU	-	EXPRESSION TAG	UNP Q93QX0
D	540	GLU	-	EXPRESSION TAG	UNP Q93QX0
D	541	HIS	-	EXPRESSION TAG	UNP Q93QX0
D	542	HIS	-	EXPRESSION TAG	UNP Q93QX0
D	543	HIS	-	EXPRESSION TAG	UNP Q93QX0
D	544	HIS	-	EXPRESSION TAG	UNP Q93QX0
D	545	HIS	-	EXPRESSION TAG	UNP Q93QX0
D	546	HIS	-	EXPRESSION TAG	UNP Q93QX0
E	534	LYS	-	EXPRESSION TAG	UNP Q93QX0
E	535	LEU	-	EXPRESSION TAG	UNP Q93QX0
E	536	ALA	-	EXPRESSION TAG	UNP Q93QX0
E	537	ALA	-	EXPRESSION TAG	UNP Q93QX0
E	538	ALA	-	EXPRESSION TAG	UNP Q93QX0
E	539	LEU	-	EXPRESSION TAG	UNP Q93QX0
E	540	GLU	-	EXPRESSION TAG	UNP Q93QX0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	541	HIS	-	EXPRESSION TAG	UNP Q93QX0
E	542	HIS	-	EXPRESSION TAG	UNP Q93QX0
E	543	HIS	-	EXPRESSION TAG	UNP Q93QX0
E	544	HIS	-	EXPRESSION TAG	UNP Q93QX0
E	545	HIS	-	EXPRESSION TAG	UNP Q93QX0
E	546	HIS	-	EXPRESSION TAG	UNP Q93QX0
F	534	LYS	-	EXPRESSION TAG	UNP Q93QX0
F	535	LEU	-	EXPRESSION TAG	UNP Q93QX0
F	536	ALA	-	EXPRESSION TAG	UNP Q93QX0
F	537	ALA	-	EXPRESSION TAG	UNP Q93QX0
F	538	ALA	-	EXPRESSION TAG	UNP Q93QX0
F	539	LEU	-	EXPRESSION TAG	UNP Q93QX0
F	540	GLU	-	EXPRESSION TAG	UNP Q93QX0
F	541	HIS	-	EXPRESSION TAG	UNP Q93QX0
F	542	HIS	-	EXPRESSION TAG	UNP Q93QX0
F	543	HIS	-	EXPRESSION TAG	UNP Q93QX0
F	544	HIS	-	EXPRESSION TAG	UNP Q93QX0
F	545	HIS	-	EXPRESSION TAG	UNP Q93QX0
F	546	HIS	-	EXPRESSION TAG	UNP Q93QX0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

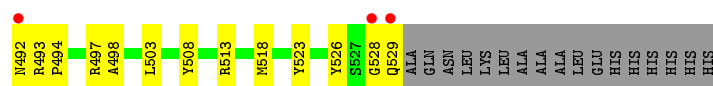
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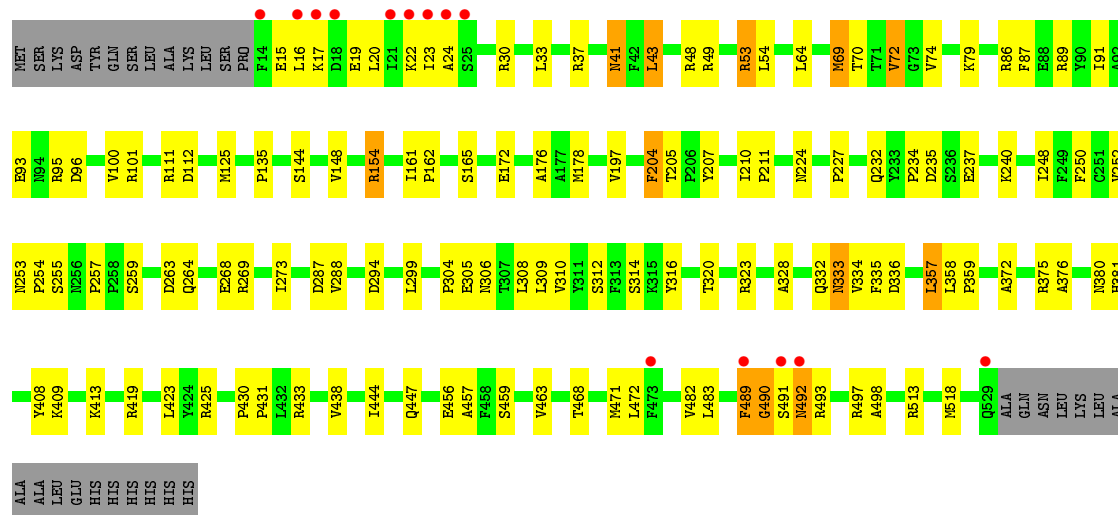
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

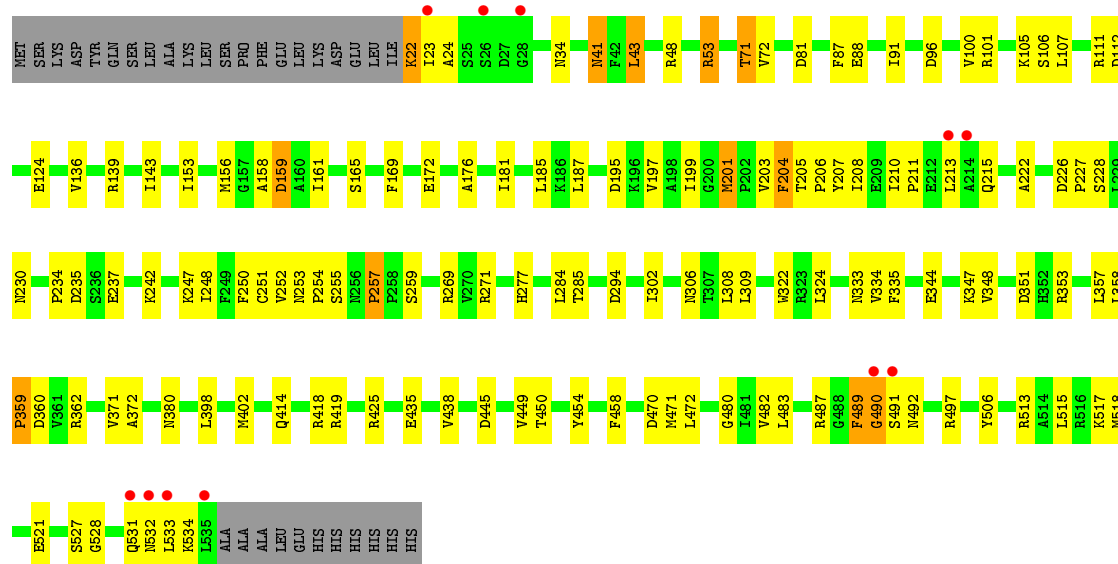
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	369	Total	O	0	0
			369	369		
3	B	431	Total	O	0	0
			431	431		
3	C	403	Total	O	0	0
			403	403		
3	D	353	Total	O	0	0
			353	353		
3	E	329	Total	O	0	0
			329	329		
3	F	308	Total	O	0	0
			308	308		



• Molecule 1: L-aspartate beta-decarboxylase

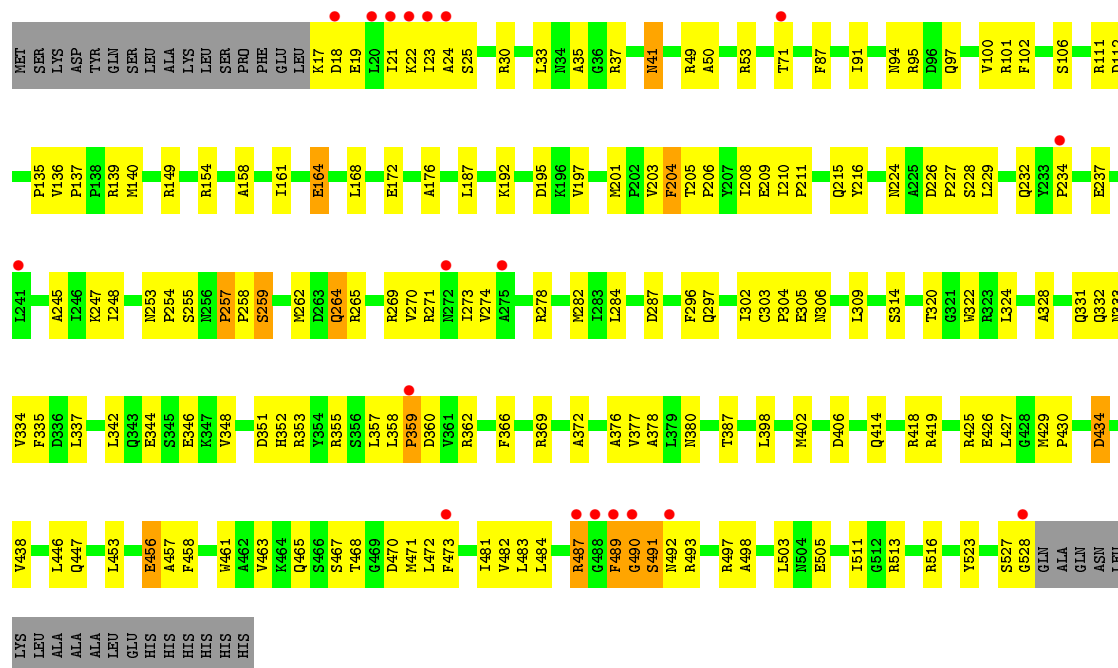


• Molecule 1: L-aspartate beta-decarboxylase

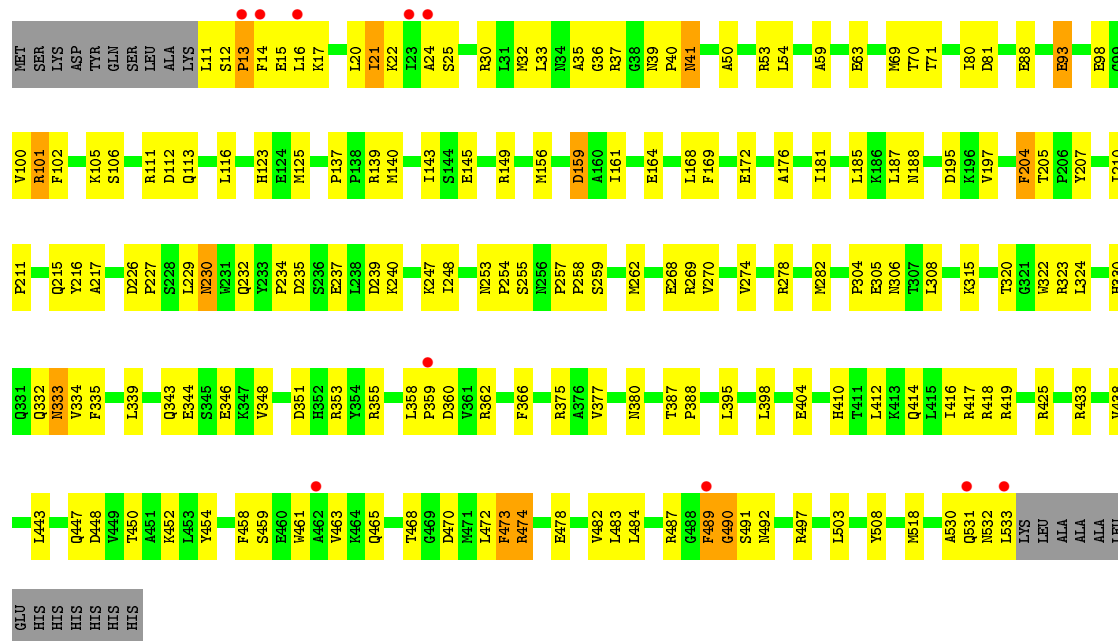


• Molecule 1: L-aspartate beta-decarboxylase





• Molecule 1: L-aspartate beta-decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	149.73Å 216.14Å 208.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 44.08 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.8 (50.00-2.50) 92.6 (44.08-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.175 , 0.234 0.172 , 0.230	Depositor DCC
R_{free} test set	5444 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26599	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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	0.56	0/4093	0.71	0/5543
1	B	0.56	0/4136	0.72	0/5600
1	C	0.56	0/4148	0.73	1/5616 (0.0%)
1	D	0.54	0/4124	0.71	1/5584 (0.0%)
1	E	0.53	0/4110	0.70	1/5565 (0.0%)
1	F	0.56	1/4200 (0.0%)	0.70	0/5688
All	All	0.55	1/24811 (0.0%)	0.71	3/33596 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	315	LYS	CE-NZ	-5.25	1.35	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	PRO	N-CA-C	6.18	128.18	112.10
1	C	257	PRO	N-CA-C	5.78	127.12	112.10
1	E	257	PRO	N-CA-C	5.13	125.45	112.10

There are no chirality outliers.

There are no planarity outliers.

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	4011	0	3978	126	0
1	B	4054	0	4021	140	0
1	C	4065	0	4029	104	1
1	D	4042	0	4013	128	0
1	E	4028	0	3996	146	0
1	F	4116	0	4082	162	0
2	A	15	0	7	0	0
2	B	15	0	7	1	0
2	C	15	0	7	0	0
2	D	15	0	7	0	0
2	E	15	0	7	0	0
2	F	15	0	6	0	0
3	A	369	0	0	12	0
3	B	431	0	0	15	0
3	C	403	0	0	10	0
3	D	353	0	0	14	0
3	E	329	0	0	16	1
3	F	308	0	0	18	0
All	All	26599	0	24160	776	1

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 16.

The worst 5 of 776 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:D:105:LYS:HE3	3:D:1343:HOH:O	1.46	1.13
1:E:447:GLN:HE21	1:E:463:VAL:HG21	1.14	1.10
1:B:425:ARG:HH12	1:D:159:ASP:HA	1.21	1.02
1:F:530:ALA:O	1:F:533:LEU:HG	1.65	0.97
1:B:333:ASN:HD22	1:B:335:PHE:H	1.17	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ARG:NH2	3:E:1708:HOH:O[4_566]	2.17	0.03

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	508/546 (93%)	484 (95%)	19 (4%)	5 (1%)	15	28
1	B	513/546 (94%)	485 (94%)	25 (5%)	3 (1%)	25	43
1	C	514/546 (94%)	491 (96%)	18 (4%)	5 (1%)	15	28
1	D	512/546 (94%)	484 (94%)	24 (5%)	4 (1%)	19	35
1	E	510/546 (93%)	479 (94%)	27 (5%)	4 (1%)	19	35
1	F	521/546 (95%)	487 (94%)	28 (5%)	6 (1%)	13	24
All	All	3078/3276 (94%)	2910 (94%)	141 (5%)	27 (1%)	17	31

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	SER
1	B	491	SER
1	C	491	SER
1	D	491	SER
1	D	534	LYS

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	424/455 (93%)	415 (98%)	9 (2%)	53	78
1	B	429/455 (94%)	414 (96%)	15 (4%)	36	62
1	C	430/455 (94%)	414 (96%)	16 (4%)	34	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	427/455 (94%)	415 (97%)	12 (3%)	43	70
1	E	426/455 (94%)	413 (97%)	13 (3%)	40	67
1	F	436/455 (96%)	421 (97%)	15 (3%)	37	63
All	All	2572/2730 (94%)	2492 (97%)	80 (3%)	40	67

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	332	GLN
1	D	71	THR
1	F	230	ASN
1	C	333	ASN
1	D	22	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	333	ASN
1	D	150	GLN
1	F	332	GLN
1	C	380	ASN
1	C	504	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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	F	900	1	15,15,16	1.49	3 (20%)	20,22,23	1.20	2 (10%)
2	PLP	A	900	1	15,15,16	2.35	5 (33%)	20,22,23	1.70	3 (15%)
2	PLP	C	900	1	15,15,16	2.13	5 (33%)	20,22,23	1.79	4 (20%)
2	PLP	B	900	1	15,15,16	1.73	4 (26%)	20,22,23	1.62	2 (10%)
2	PLP	E	900	1	15,15,16	2.14	6 (40%)	20,22,23	1.39	2 (10%)
2	PLP	D	900	1	15,15,16	2.31	7 (46%)	20,22,23	1.64	2 (10%)

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	F	900	1	-	1/6/6/8	0/1/1/1
2	PLP	A	900	1	-	1/6/6/8	0/1/1/1
2	PLP	C	900	1	-	0/6/6/8	0/1/1/1
2	PLP	B	900	1	-	0/6/6/8	0/1/1/1
2	PLP	E	900	1	-	1/6/6/8	0/1/1/1
2	PLP	D	900	1	-	0/6/6/8	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	PLP	C2A-C2	5.74	1.60	1.50
2	A	900	PLP	C2A-C2	5.15	1.59	1.50
2	C	900	PLP	C2A-C2	4.86	1.58	1.50
2	D	900	PLP	C2-N1	4.08	1.41	1.33
2	A	900	PLP	C5A-C5	3.93	1.61	1.50

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	900	PLP	O4P-C5A-C5	6.02	120.83	109.35
2	D	900	PLP	O4P-C5A-C5	5.63	120.09	109.35
2	A	900	PLP	O4P-C5A-C5	5.57	119.96	109.35
2	C	900	PLP	O4P-C5A-C5	5.14	119.14	109.35
2	E	900	PLP	O4P-C5A-C5	3.75	116.50	109.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	900	PLP	C6-C5-C5A-O4P
2	A	900	PLP	C6-C5-C5A-O4P
2	E	900	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	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	510/546 (93%)	-0.17	16 (3%) 49 52	14, 34, 77, 110	0
1	B	515/546 (94%)	-0.34	8 (1%) 72 74	10, 31, 70, 105	0
1	C	516/546 (94%)	-0.29	14 (2%) 54 58	13, 33, 65, 120	0
1	D	514/546 (94%)	-0.26	11 (2%) 63 66	14, 34, 71, 115	0
1	E	512/546 (93%)	0.01	19 (3%) 41 45	16, 41, 76, 110	0
1	F	523/546 (95%)	-0.23	10 (1%) 66 69	16, 35, 70, 118	0
All	All	3090/3276 (94%)	-0.21	78 (2%) 57 61	10, 34, 74, 120	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	ALA	11.9
1	E	490	GLY	8.0
1	A	23	ILE	8.0
1	D	535	LEU	7.8
1	C	14	PHE	6.9

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(Å ²)	Q<0.9
2	PLP	F	900	15/16	0.97	0.15	26,30,32,32	0
2	PLP	E	900	15/16	0.97	0.18	25,37,39,39	0
2	PLP	C	900	15/16	0.98	0.16	23,25,29,31	0
2	PLP	B	900	15/16	0.98	0.15	26,28,30,31	0
2	PLP	A	900	15/16	0.98	0.15	24,32,35,35	0
2	PLP	D	900	15/16	0.98	0.15	25,28,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.