



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:30 PM UTC

PDB ID : 5X7M / pdb_00005x7m
Title : Crystal structure of meso-diaminopimelate decarboxylase (DAPDC) from
Corynebacterium glutamicum
Authors : Son, H.-F.; Kim, K.-J.
Deposited on : 2017-02-27
Resolution : 2.40 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
Mogul : 2022.3.0, CSD as543be (2022)
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

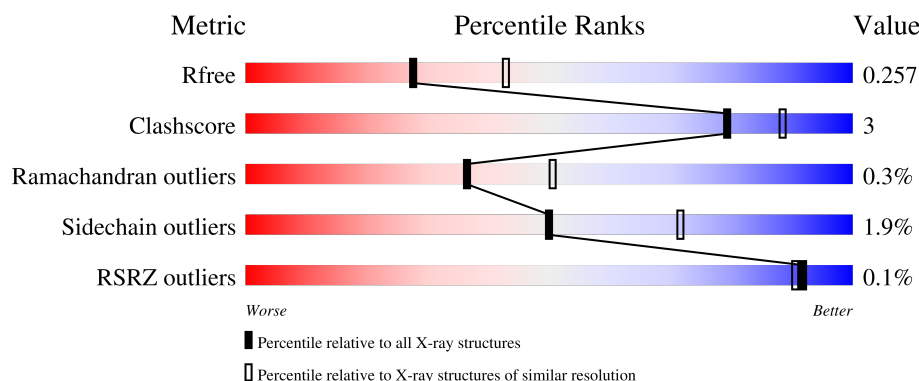
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	453	
1	B	453	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6813 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 Diaminopimelate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3326	2087	572	658	9			
1	B	443	Total	C	N	O	S	0	0	0
			3326	2087	572	658	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	LEU	-	expression tag	UNP P09890
A	447	GLU	-	expression tag	UNP P09890
A	448	HIS	-	expression tag	UNP P09890
A	449	HIS	-	expression tag	UNP P09890
A	450	HIS	-	expression tag	UNP P09890
A	451	HIS	-	expression tag	UNP P09890
A	452	HIS	-	expression tag	UNP P09890
A	453	HIS	-	expression tag	UNP P09890
B	446	LEU	-	expression tag	UNP P09890
B	447	GLU	-	expression tag	UNP P09890
B	448	HIS	-	expression tag	UNP P09890
B	449	HIS	-	expression tag	UNP P09890
B	450	HIS	-	expression tag	UNP P09890
B	451	HIS	-	expression tag	UNP P09890
B	452	HIS	-	expression tag	UNP P09890
B	453	HIS	-	expression tag	UNP P09890

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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		

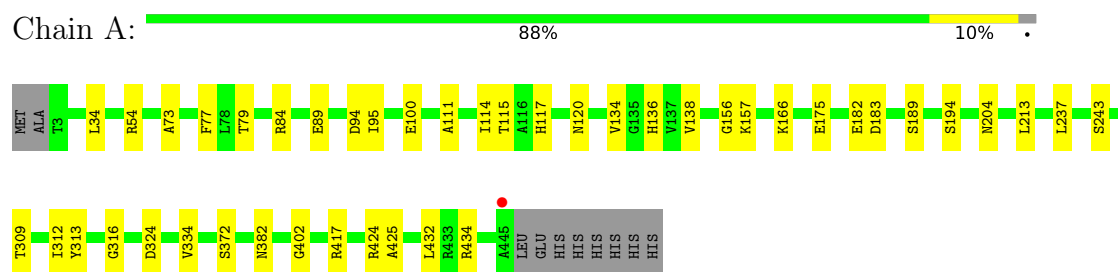
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	63	Total	O	0	0
			63	63		

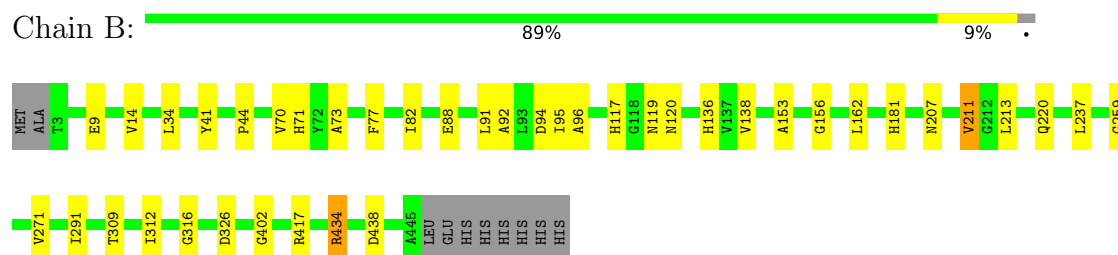
3 Residue-property plots

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: Diaminopimelate decarboxylase



• Molecule 1: Diaminopimelate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.65Å 92.01Å 94.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.71 – 2.40 23.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (23.71-2.40) 95.5 (23.71-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.65 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.186 , 0.253 0.192 , 0.257	Depositor DCC
R_{free} test set	1898 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.030 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6813	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 74.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6443e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.97	1/3388 (0.0%)	1.07	5/4609 (0.1%)
1	B	0.96	0/3388	1.08	4/4609 (0.1%)
All	All	0.97	1/6776 (0.0%)	1.07	9/9218 (0.1%)

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	B	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	A	183	ASP	C-O	-5.55	1.17	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	LYS	N-CA-C	7.62	121.34	110.14
1	B	211	VAL	N-CA-CB	-6.58	104.97	112.21
1	B	434	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	A	382	ASN	N-CA-C	5.79	117.67	111.36
1	B	14	VAL	CB-CA-C	-5.66	106.07	111.44
1	A	100	GLU	N-CA-C	-5.32	105.56	111.36
1	B	88	GLU	N-CA-C	5.13	116.87	111.28
1	A	434	ARG	NE-CZ-NH1	-5.08	116.42	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	SER	CB-CA-C	-5.07	101.30	109.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	GLY	Peptide
1	B	156	GLY	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	3326	0	3237	20	0
1	B	3326	0	3236	20	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
3	A	68	0	0	0	0
3	B	63	0	0	0	0
All	All	6813	0	6487	35	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 (35) 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:B:44:PRO:O	1:B:434:ARG:NH1	2.11	0.83
1:A:34:LEU:HD22	1:A:312:ILE:HD11	1.84	0.59
1:B:213:LEU:CD1	1:B:237:LEU:HD23	2.35	0.57
1:A:117:HIS:CE1	1:A:138:VAL:HG21	2.40	0.56
1:A:54:ARG:NH2	1:A:89:GLU:OE2	2.39	0.53
1:B:73:ALA:HA	1:B:94:ASP:HB2	1.90	0.53
1:B:162:LEU:N	1:B:162:LEU:HD12	2.24	0.53
1:B:96:ALA:HA	1:B:117:HIS:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:HIS:CD2	1:B:162:LEU:HD11	2.44	0.52
1:A:115:THR:HG23	1:A:136:HIS:HB2	1.91	0.52
1:A:213:LEU:CD1	1:A:237:LEU:HD23	2.40	0.51
1:B:117:HIS:CE1	1:B:138:VAL:HG21	2.46	0.51
1:B:34:LEU:HD22	1:B:312:ILE:HD11	1.93	0.51
1:A:316:GLY:HA3	1:B:120:ASN:HD21	1.78	0.48
1:A:120:ASN:HD21	1:B:316:GLY:HA3	1.79	0.48
1:A:166:LYS:HD2	1:A:182:GLU:HB2	1.96	0.48
1:A:111:ALA:O	1:A:134:VAL:HA	2.14	0.47
1:B:309:THR:HB	1:B:402:GLY:CA	2.45	0.47
1:A:309:THR:HB	1:A:402:GLY:CA	2.45	0.46
1:A:213:LEU:HD13	1:A:237:LEU:HD23	1.98	0.46
1:A:417:ARG:HH22	1:B:417:ARG:NH2	2.15	0.45
1:B:153:ALA:HB2	1:B:207:ASN:ND2	2.32	0.45
1:A:73:ALA:HA	1:A:94:ASP:OD1	2.19	0.43
1:B:309:THR:HB	1:B:402:GLY:HA3	2.00	0.43
1:A:79:THR:CG2	1:A:432:LEU:HD11	2.48	0.43
1:B:41:TYR:O	1:B:434:ARG:NH2	2.52	0.42
1:A:111:ALA:HA	1:A:114:ILE:HD12	2.02	0.42
1:A:79:THR:HG22	1:A:432:LEU:HD11	2.02	0.42
1:B:71:HIS:CD2	1:B:92:ALA:HB3	2.55	0.42
1:A:424:ARG:O	1:A:425:ALA:C	2.64	0.41
1:B:70:VAL:HB	1:B:91:LEU:HD22	2.02	0.41
1:A:313:TYR:HB3	1:A:334:VAL:HB	2.02	0.41
1:A:324:ASP:HA	1:B:181:HIS:CD2	2.56	0.40
1:A:372:SER:HA	1:B:119:ASN:HD21	1.86	0.40
1:B:220:GLN:OE1	1:B:259:GLY:HA2	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	441/453 (97%)	425 (96%)	14 (3%)	2 (0%)	24	37
1	B	441/453 (97%)	428 (97%)	12 (3%)	1 (0%)	43	58
All	All	882/906 (97%)	853 (97%)	26 (3%)	3 (0%)	36	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	B	77	PHE
1	A	77	PHE

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	345/354 (98%)	340 (99%)	5 (1%)	59	79
1	B	345/354 (98%)	337 (98%)	8 (2%)	44	66
All	All	690/708 (98%)	677 (98%)	13 (2%)	50	71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	95	ILE
1	A	175	GLU
1	A	194	SER
1	A	243	SER
1	B	9	GLU
1	B	82	ILE
1	B	95	ILE
1	B	211	VAL
1	B	271	VAL
1	B	291	ILE
1	B	326	ASP
1	B	438	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	71	HIS
1	A	99	ASN
1	A	117	HIS
1	A	120	ASN
1	A	131	GLN
1	A	143	GLN
1	A	159	GLN
1	A	216	HIS
1	A	382	ASN
1	A	413	ASN
1	B	22	GLN
1	B	71	HIS
1	B	119	ASN
1	B	120	ASN
1	B	131	GLN
1	B	136	HIS
1	B	181	HIS
1	B	240	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](#)

2 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	A	501	1	15,15,16	4.02	5 (33%)	21,22,23	2.06	4 (19%)
2	PLP	B	501	1	15,15,16	4.16	4 (26%)	21,22,23	2.12	7 (33%)

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	A	501	1	-	4/6/6/8	0/1/1/1
2	PLP	B	501	1	-	2/6/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PLP	C5-C4	12.13	1.54	1.40
2	A	501	PLP	C5-C4	11.61	1.53	1.40
2	A	501	PLP	C3-C2	7.63	1.48	1.41
2	B	501	PLP	C3-C2	7.58	1.48	1.41
2	B	501	PLP	C3-C4	6.46	1.52	1.40
2	A	501	PLP	C3-C4	5.86	1.51	1.40
2	B	501	PLP	C6-C5	2.24	1.42	1.37
2	A	501	PLP	C6-C5	2.18	1.42	1.37
2	A	501	PLP	C5A-C5	2.10	1.56	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	O4P-C5A-C5	7.47	123.35	109.36
2	B	501	PLP	O4P-C5A-C5	6.42	121.38	109.36
2	B	501	PLP	C4A-C4-C5	2.82	123.85	120.94
2	B	501	PLP	C6-N1-C2	2.66	124.02	119.20
2	B	501	PLP	O3P-P-O4P	-2.45	100.27	106.67
2	A	501	PLP	C6-C5-C4	-2.35	116.17	118.10
2	B	501	PLP	O3-C3-C4	2.24	123.95	118.10
2	B	501	PLP	C5A-C5-C4	2.23	127.04	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PLP	C5A-C5-C6	-2.08	115.97	119.36
2	A	501	PLP	C4A-C4-C5	2.07	123.07	120.94
2	A	501	PLP	C6-N1-C2	2.00	122.83	119.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLP	C4-C5-C5A-O4P
2	A	501	PLP	C6-C5-C5A-O4P
2	A	501	PLP	C5A-O4P-P-O1P
2	A	501	PLP	C5A-O4P-P-O2P
2	B	501	PLP	C4-C5-C5A-O4P
2	B	501	PLP	C6-C5-C5A-O4P

There are no ring outliers.

No monomer is involved in short contacts.

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	443/453 (97%)	-0.39	1 (0%) 91 89	21, 33, 53, 79	0
1	B	443/453 (97%)	-0.36	0 100 100	22, 35, 56, 72	0
All	All	886/906 (97%)	-0.37	1 (0%) 92 90	21, 34, 55, 79	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	ALA	2.5

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](#)

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	A	501	15/16	0.95	0.11	24,56,67,67	0
2	PLP	B	501	15/16	0.95	0.13	24,57,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.