



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:50 AM UTC

PDB ID : 5X7N / pdb_00005x7n
Title : Crystal structure of meso-diaminopimelate decarboxylase (DAPDC) from
Corynebacterium glutamicum
Authors : Son, H.-F.; Kim, K.-J.
Deposited on : 2017-02-27
Resolution : 1.72 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

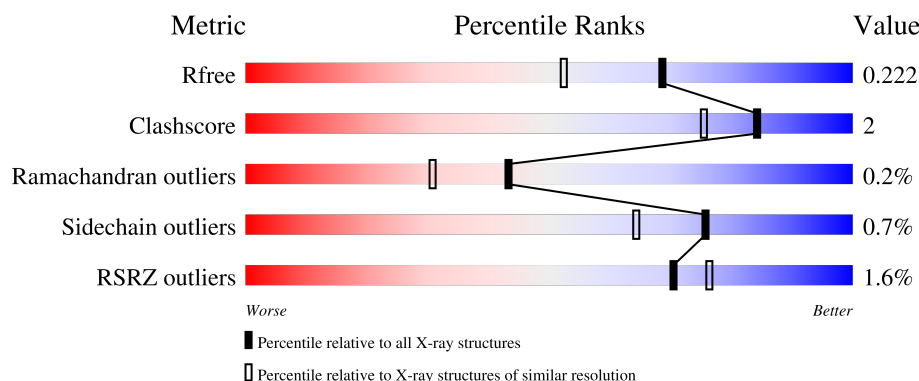
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	92% 6%
1	B	453	2% 90% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	503	-	X	-	-
3	PLP	A	504	-	X	-	-
3	PLP	B	506	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7608 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	442	Total	C	N	O	S	0	0	0
			3321	2084	571	657	9			
1	B	439	Total	C	N	O	S	0	0	0
			3297	2072	568	648	9			

There are 16 discrepancies between the modelled and reference sequences:

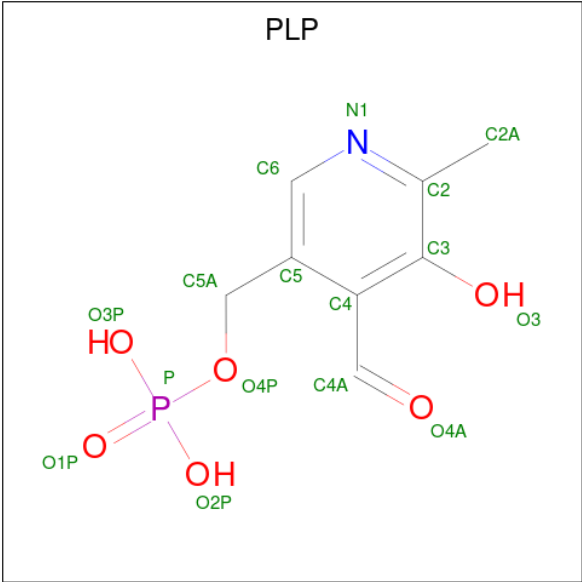
Chain	Residue	Modelled	Actual	Comment	Reference
A	446	LEU	-	expression tag	UNP P09890
A	447	GLU	-	expression tag	UNP P09890
A	448	HIS	-	expression tag	UNP P09890
A	449	HIS	-	expression tag	UNP P09890
A	450	HIS	-	expression tag	UNP P09890
A	451	HIS	-	expression tag	UNP P09890
A	452	HIS	-	expression tag	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 GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



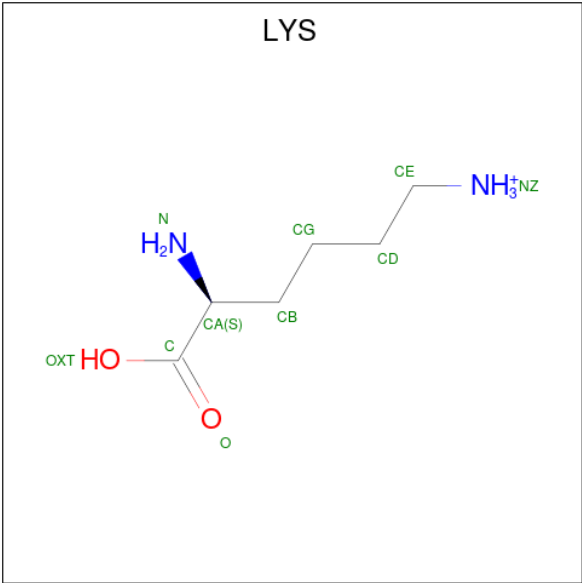
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 4 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	6	2	2		
4	B	1	Total	C	N	O	0	0
			10	6	2	2		

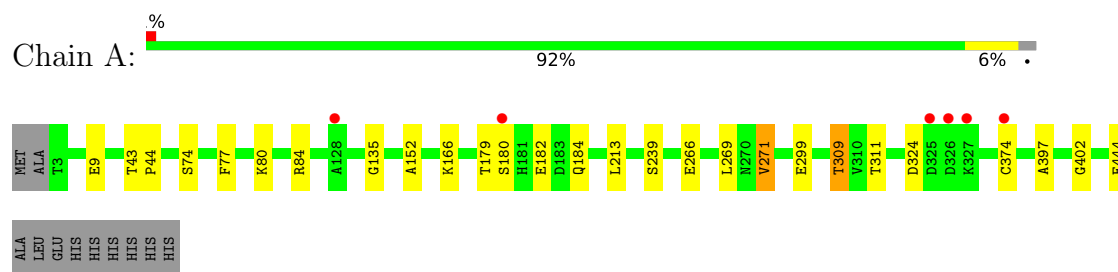
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	439	Total 439	O 439	0	0
5	B	453	Total 453	O 453	0	0

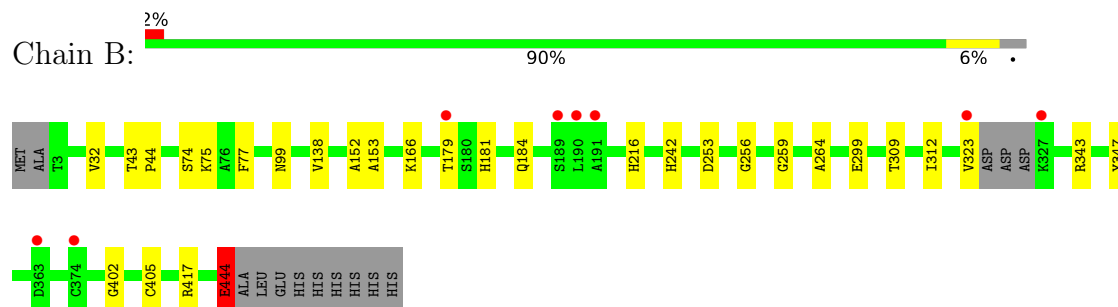
3 Residue-property plots [i](#)

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: 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	114.54Å 91.70Å 95.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.46 – 1.72 23.46 – 1.72	Depositor EDS
% Data completeness (in resolution range)	94.5 (23.46-1.72) 94.6 (23.46-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.44 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.171 , 0.211 0.185 , 0.222	Depositor DCC
R_{free} test set	5094 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7608	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 72.91 % 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 2.0248e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, GOL

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	1.44	8/3383 (0.2%)	1.20	2/4602 (0.0%)
1	B	1.43	12/3358 (0.4%)	1.23	9/4566 (0.2%)
All	All	1.43	20/6741 (0.3%)	1.22	11/9168 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	ALA	N-CA	6.58	1.54	1.46
1	A	74	SER	CB-OG	-6.57	1.29	1.42
1	A	213	LEU	N-CA	-6.34	1.38	1.45
1	A	239	SER	C-O	6.03	1.31	1.24
1	B	32	VAL	CA-C	5.98	1.57	1.53
1	B	99	ASN	C-O	5.92	1.31	1.24
1	B	253	ASP	C-O	-5.77	1.17	1.24
1	A	309	THR	CA-C	-5.67	1.45	1.52
1	B	74	SER	CA-CB	5.62	1.62	1.53
1	A	152	ALA	N-CA	-5.59	1.39	1.46
1	B	152	ALA	N-CA	-5.58	1.39	1.46
1	A	266	GLU	C-O	-5.52	1.16	1.23
1	A	180	SER	C-O	5.51	1.30	1.24
1	B	417	ARG	CZ-NH2	5.49	1.40	1.33
1	B	138	VAL	N-CA	5.46	1.52	1.46
1	B	312	ILE	C-O	-5.37	1.17	1.24
1	A	84	ARG	C-O	5.34	1.30	1.24
1	B	74	SER	CB-OG	-5.24	1.31	1.42
1	B	216	HIS	CA-C	-5.24	1.46	1.52
1	B	405	CYS	C-O	5.14	1.29	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	444	GLU	CA-C-O	-8.35	106.60	120.80
1	B	444	GLU	CG-CD-OE1	6.82	134.09	118.40
1	B	166	LYS	CA-C-N	-6.59	113.14	120.45
1	B	166	LYS	C-N-CA	-6.59	113.14	120.45
1	B	444	GLU	CG-CD-OE2	-6.32	103.86	118.40
1	A	444	GLU	CA-C-O	-5.62	111.24	120.80
1	B	417	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	A	135	GLY	N-CA-C	5.32	118.93	112.49
1	B	323	VAL	CA-C-O	-5.24	111.90	120.80
1	B	264	ALA	N-CA-C	5.21	116.96	111.28
1	B	259	GLY	N-CA-C	5.18	119.97	112.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3321	0	3232	15	0
1	B	3297	0	3218	17	0
2	A	18	0	24	0	0
2	B	30	0	40	0	0
3	A	15	0	7	4	0
3	B	15	0	7	5	0
4	A	10	0	12	0	0
4	B	10	0	12	5	0
5	A	439	0	0	3	1
5	B	453	0	0	3	1
All	All	7608	0	6552	31	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 2.

All (31) 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:343:ARG:NH2	4:B:507:LYS:OXT	2.10	0.84
1:A:271:VAL:HG13	5:A:913:HOH:O	1.80	0.82
1:B:347:TYR:CZ	4:B:507:LYS:HA	2.22	0.74
1:B:299:GLU:HB2	3:B:506:PLP:H6	1.82	0.60
1:A:269:LEU:CD2	1:A:271:VAL:HG12	2.36	0.56
3:B:506:PLP:C4A	3:B:506:PLP:O4P	2.54	0.55
1:B:444:GLU:HG2	5:B:943:HOH:O	2.05	0.55
1:A:9:GLU:HG3	5:A:959:HOH:O	2.09	0.53
3:A:504:PLP:C4A	3:A:504:PLP:O4P	2.58	0.52
1:B:179:THR:HG22	5:B:899:HOH:O	2.09	0.51
1:B:347:TYR:CE2	4:B:507:LYS:HA	2.45	0.51
1:A:299:GLU:HB2	3:A:504:PLP:H6	1.93	0.49
1:A:269:LEU:HD23	1:A:271:VAL:HG12	1.93	0.49
1:B:299:GLU:O	3:B:506:PLP:H6	2.13	0.48
1:B:343:ARG:NE	4:B:507:LYS:OXT	2.45	0.48
1:A:299:GLU:CB	3:A:504:PLP:H6	2.45	0.47
1:B:309:THR:HB	1:B:402:GLY:CA	2.44	0.47
1:A:179:THR:HG22	5:A:920:HOH:O	2.13	0.47
1:B:343:ARG:CZ	4:B:507:LYS:OXT	2.64	0.46
1:B:299:GLU:CB	3:B:506:PLP:H6	2.46	0.45
1:B:242:HIS:CD2	5:B:765:HOH:O	2.70	0.45
1:A:166:LYS:HD2	1:A:182:GLU:HB2	1.99	0.44
1:A:299:GLU:O	3:A:504:PLP:H6	2.17	0.44
1:A:43:THR:HA	1:A:44:PRO:C	2.42	0.44
1:A:311:THR:O	1:A:397:ALA:HA	2.19	0.42
1:B:256:GLY:HA3	3:B:506:PLP:H5A2	2.02	0.42
1:A:374:CYS:SG	1:B:75:LYS:HD3	2.59	0.42
1:B:43:THR:HA	1:B:44:PRO:C	2.45	0.41
1:A:309:THR:HB	1:A:402:GLY:CA	2.50	0.41
1:A:80:LYS:HE3	1:B:444:GLU:HG2	2.03	0.41
1:A:324:ASP:HA	1:B:181:HIS:CD2	2.56	0.40

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)
5:A:743:HOH:O	5:B:894:HOH:O[4_556]	2.16	0.04

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	440/453 (97%)	433 (98%)	6 (1%)	1 (0%)	43	31
1	B	435/453 (96%)	428 (98%)	6 (1%)	1 (0%)	43	31
All	All	875/906 (97%)	861 (98%)	12 (1%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	343 (99%)	2 (1%)	78	68
1	B	342/354 (97%)	340 (99%)	2 (1%)	78	68
All	All	687/708 (97%)	683 (99%)	4 (1%)	76	68

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	271	VAL
1	B	184	GLN
1	B	444	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	120	ASN
1	A	131	GLN
1	A	174	HIS
1	A	181	HIS
1	B	22	GLN
1	B	99	ASN
1	B	117	HIS
1	B	119	ASN
1	B	120	ASN
1	B	131	GLN
1	B	172	HIS
1	B	181	HIS
1	B	204	ASN
1	B	240	GLN
1	B	242	HIS
1	B	322	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
3	PLP	A	504	1	15,15,16	4.70	6 (40%)	21,22,23	4.01	12 (57%)
4	LYS	B	507	-	8,9,9	1.05	1 (12%)	7,10,10	1.41	1 (14%)
2	GOL	B	501	-	5,5,5	1.16	0	5,5,5	1.83	2 (40%)
2	GOL	A	503	-	5,5,5	0.48	0	5,5,5	1.43	1 (20%)
2	GOL	B	504	-	5,5,5	0.88	0	5,5,5	0.85	0
2	GOL	B	503	-	5,5,5	1.85	1 (20%)	5,5,5	2.18	3 (60%)
2	GOL	A	502	-	5,5,5	0.27	0	5,5,5	0.74	0
2	GOL	B	502	-	5,5,5	0.61	0	5,5,5	0.46	0
2	GOL	B	505	-	5,5,5	0.73	0	5,5,5	1.32	1 (20%)
4	LYS	A	505	-	8,9,9	0.55	0	7,10,10	1.07	0
3	PLP	B	506	1	15,15,16	4.94	8 (53%)	21,22,23	4.11	11 (52%)
2	GOL	A	501	-	5,5,5	1.33	0	5,5,5	1.06	0

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
3	PLP	A	504	1	-	5/6/6/8	0/1/1/1
4	LYS	B	507	-	-	5/9/9/9	-
2	GOL	B	501	-	-	0/4/4/4	-
2	GOL	A	503	-	-	3/4/4/4	-
2	GOL	B	504	-	-	0/4/4/4	-
2	GOL	B	503	-	-	2/4/4/4	-
2	GOL	A	502	-	-	0/4/4/4	-
2	GOL	B	502	-	-	0/4/4/4	-
2	GOL	B	505	-	-	0/4/4/4	-
4	LYS	A	505	-	-	5/9/9/9	-
3	PLP	B	506	1	-	5/6/6/8	0/1/1/1
2	GOL	A	501	-	-	0/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	506	PLP	C5-C4	16.05	1.58	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	PLP	C5-C4	14.63	1.57	1.40
3	A	504	PLP	C3-C4	7.34	1.54	1.40
3	B	506	PLP	C3-C4	6.22	1.52	1.40
3	A	504	PLP	C3-C2	5.02	1.46	1.41
3	B	506	PLP	C3-C2	4.51	1.45	1.41
2	B	503	GOL	O1-C1	3.53	1.57	1.42
3	B	506	PLP	C6-N1	3.51	1.41	1.34
3	A	504	PLP	C6-N1	3.42	1.41	1.34
3	A	504	PLP	P-O4P	-3.26	1.50	1.60
3	B	506	PLP	C2-N1	2.91	1.39	1.33
3	B	506	PLP	P-O4P	-2.82	1.51	1.60
4	B	507	LYS	OXT-C	-2.78	1.21	1.30
3	B	506	PLP	P-O2P	-2.58	1.45	1.54
3	A	504	PLP	O4P-C5A	2.42	1.53	1.44
3	B	506	PLP	O4P-C5A	2.38	1.53	1.44

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	PLP	C5A-C5-C6	10.14	135.89	119.36
3	B	506	PLP	C5A-C5-C6	9.87	135.46	119.36
3	A	504	PLP	C6-C5-C4	-7.33	112.09	118.10
3	B	506	PLP	C6-C5-C4	-7.33	112.09	118.10
3	B	506	PLP	C2A-C2-C3	-6.56	113.11	120.80
3	A	504	PLP	O4P-C5A-C5	6.30	121.17	109.36
3	B	506	PLP	O4P-C5A-C5	6.17	120.92	109.36
3	B	506	PLP	C2A-C2-N1	5.67	128.32	117.64
3	A	504	PLP	C5A-C5-C4	-5.42	111.95	122.64
3	B	506	PLP	C5A-C5-C4	-5.17	112.43	122.64
3	A	504	PLP	C2A-C2-N1	5.13	127.31	117.64
3	A	504	PLP	C6-N1-C2	4.64	127.61	119.20
3	A	504	PLP	C2A-C2-C3	-4.25	115.82	120.80
3	B	506	PLP	C6-N1-C2	3.80	126.08	119.20
3	B	506	PLP	C4A-C4-C3	-3.58	114.56	120.52
3	B	506	PLP	C3-C4-C5	3.51	122.80	118.59
3	A	504	PLP	C3-C2-N1	-3.32	116.78	120.96
2	B	503	GOL	O3-C3-C2	-3.27	95.66	110.38
3	A	504	PLP	O3-C3-C4	3.15	126.32	118.10
3	B	506	PLP	C4-C3-C2	-2.79	115.72	119.89
4	B	507	LYS	OXT-C-O	-2.72	117.91	124.08
3	A	504	PLP	C4A-C4-C3	-2.68	116.06	120.52
3	A	504	PLP	C3-C4-C5	2.66	121.78	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	506	PLP	O3-C3-C4	2.52	124.69	118.10
2	B	501	GOL	O2-C2-C1	2.32	118.78	109.18
2	B	503	GOL	O2-C2-C1	2.25	118.50	109.18
2	B	501	GOL	C3-C2-C1	-2.19	103.75	111.80
2	B	505	GOL	O2-C2-C1	2.16	118.11	109.18
3	A	504	PLP	C4-C3-C2	-2.14	116.69	119.89
2	B	503	GOL	O1-C1-C2	2.13	119.96	110.38
2	A	503	GOL	O1-C1-C2	-2.07	101.08	110.38

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	GOL	C1-C2-C3-O3
3	A	504	PLP	C4-C5-C5A-O4P
3	A	504	PLP	C6-C5-C5A-O4P
3	A	504	PLP	C5A-O4P-P-O3P
3	B	506	PLP	C4-C5-C5A-O4P
3	B	506	PLP	C6-C5-C5A-O4P
3	B	506	PLP	C5A-O4P-P-O3P
4	B	507	LYS	C-CA-CB-CG
4	A	505	LYS	OXT-C-CA-N
2	B	503	GOL	O2-C2-C3-O3
2	B	503	GOL	C1-C2-C3-O3
4	B	507	LYS	CA-CB-CG-CD
2	A	503	GOL	O2-C2-C3-O3
4	A	505	LYS	CE-CD-CG-CB
4	B	507	LYS	OXT-C-CA-N
3	B	506	PLP	C5A-O4P-P-O2P
3	A	504	PLP	C5A-O4P-P-O1P
3	B	506	PLP	C5A-O4P-P-O1P
2	A	503	GOL	O1-C1-C2-O2
4	A	505	LYS	O-C-CA-CB
4	B	507	LYS	OXT-C-CA-CB
4	B	507	LYS	O-C-CA-CB
3	A	504	PLP	C5A-O4P-P-O2P
4	A	505	LYS	OXT-C-CA-CB
4	A	505	LYS	O-C-CA-N

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	PLP	4	0
4	B	507	LYS	5	0
3	B	506	PLP	5	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	442/453 (97%)	0.03	6 (1%) 73 79	11, 16, 30, 59	0
1	B	439/453 (96%)	-0.02	8 (1%) 67 74	11, 16, 29, 49	0
All	All	881/906 (97%)	0.00	14 (1%) 70 76	11, 16, 29, 59	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	VAL	3.3
1	A	326	ASP	3.1
1	A	325	ASP	2.9
1	B	189	SER	2.7
1	B	363	ASP	2.3
1	B	374	CYS	2.3
1	A	128	ALA	2.2
1	B	327	LYS	2.2
1	B	190	LEU	2.1
1	B	191	ALA	2.1
1	A	180	SER	2.1
1	A	374	CYS	2.1
1	B	179	THR	2.1
1	A	327	LYS	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](#)

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
4	LYS	A	505	10/10	0.72	0.29	39,59,71,76	0
2	GOL	B	504	6/6	0.73	0.18	33,39,43,48	0
2	GOL	B	503	6/6	0.81	0.16	24,28,32,41	0
4	LYS	B	507	10/10	0.82	0.20	43,51,57,75	0
2	GOL	A	503	6/6	0.89	0.12	28,32,37,41	0
2	GOL	A	501	6/6	0.90	0.10	18,20,24,27	0
2	GOL	B	505	6/6	0.90	0.16	27,41,43,51	0
2	GOL	A	502	6/6	0.92	0.12	25,27,31,35	0
2	GOL	B	502	6/6	0.93	0.10	25,28,30,39	0
3	PLP	A	504	15/16	0.95	0.16	12,32,47,48	0
3	PLP	B	506	15/16	0.95	0.13	12,27,39,42	0
2	GOL	B	501	6/6	0.96	0.07	15,20,20,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.