



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:15 AM UTC

PDB ID : 5GP4 / pdb_00005gp4
Title : Lactobacillus brevis CGMCC 1306 Glutamate decarboxylase
Authors : Mei, L.; Huang, J.
Deposited on : 2016-07-31
Resolution : 2.16 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

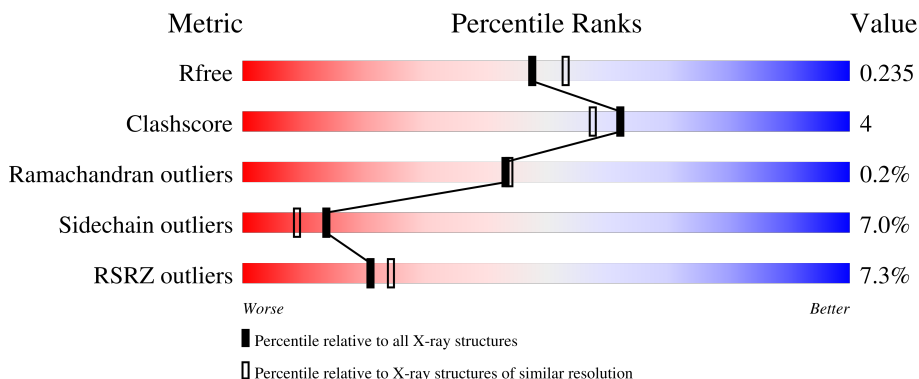
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 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	468	7% 81% 11% 6%
1	B	468	6% 75% 14% 9%
1	C	468	7% 79% 12% 6%

2 Entry composition [i](#)

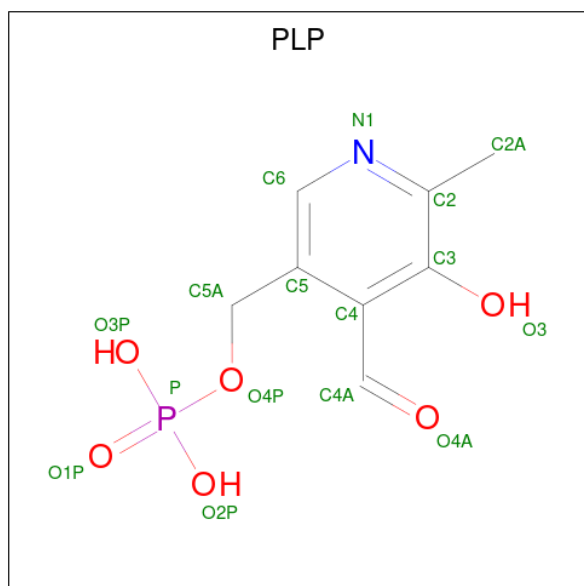
There are 3 unique types of molecules in this entry. The entry contains 10728 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	439	Total	C	N	O	S	0	0	0
			3534	2258	596	661	19			
1	A	441	Total	C	N	O	S	0	0	0
			3549	2269	598	663	19			
1	B	424	Total	C	N	O	S	0	0	0
			3415	2183	573	640	19			

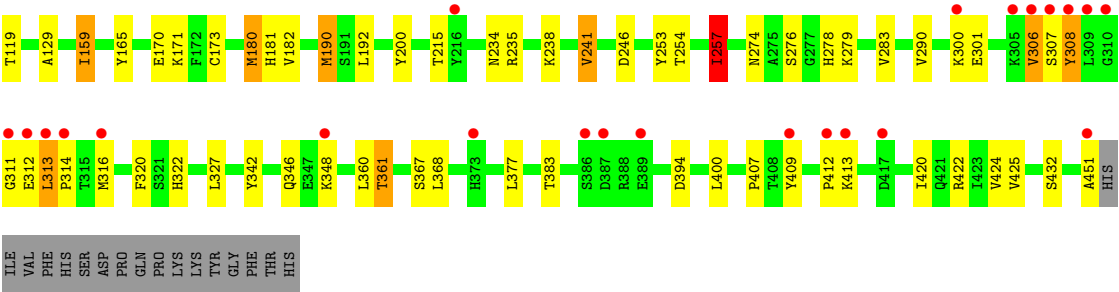
- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
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	C	57	Total 57	O 57	0	0
3	A	72	Total 72	O 72	0	0
3	B	56	Total 56	O 56	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.33Å 170.13Å 164.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 2.16 48.54 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.54-2.16) 99.6 (48.54-2.16)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.187 , 0.230 0.195 , 0.235	Depositor DCC
R_{free} test set	4290 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10728	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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

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	1.22	0/3639	1.18	15/4943 (0.3%)
1	B	1.25	3/3501 (0.1%)	1.24	13/4756 (0.3%)
1	C	1.22	5/3624 (0.1%)	1.20	12/4922 (0.2%)
All	All	1.23	8/10764 (0.1%)	1.21	40/14621 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	432	SER	CA-C	-5.83	1.45	1.52
1	B	412	PRO	C-O	5.29	1.30	1.23
1	C	313	LEU	CA-C	5.29	1.57	1.52
1	B	170	GLU	CA-C	5.27	1.59	1.52
1	B	257	ILE	C-O	-5.22	1.19	1.24
1	C	253	TYR	CA-C	5.17	1.57	1.52
1	C	317	ALA	CA-C	-5.15	1.45	1.52
1	C	88	ASP	CA-C	5.03	1.59	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	SER	N-CA-C	11.49	126.86	113.19
1	B	308	TYR	N-CA-C	9.90	124.79	110.24
1	B	311	GLY	N-CA-C	7.96	122.80	112.13
1	C	425	VAL	CB-CA-C	7.67	121.49	110.98
1	C	413	LYS	CA-C-N	7.10	133.69	122.61
1	C	413	LYS	C-N-CA	7.10	133.69	122.61
1	C	403	GLY	N-CA-C	6.95	123.35	115.08
1	C	119	THR	CB-CA-C	-6.89	94.92	110.07
1	A	159	ILE	CB-CA-C	-6.45	100.37	110.69
1	C	409	TYR	N-CA-C	6.40	113.98	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ARG	CB-CG-CD	6.28	125.75	111.30
1	B	413	LYS	O-C-N	6.24	130.10	123.11
1	A	309	LEU	N-CA-C	-6.15	102.75	111.24
1	C	94	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	A	425	VAL	CB-CA-C	5.89	119.56	110.96
1	A	144	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	A	316	MET	N-CA-C	-5.80	98.82	108.34
1	A	50	ASP	N-CA-C	5.64	117.43	111.28
1	B	432	SER	CB-CA-C	-5.63	101.44	110.79
1	B	159	ILE	CB-CA-C	-5.58	101.77	110.69
1	C	159	ILE	CB-CA-C	-5.54	101.83	110.69
1	B	413	LYS	CA-C-N	5.54	132.11	121.54
1	B	413	LYS	C-N-CA	5.54	132.11	121.54
1	C	46	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	A	424	VAL	CB-CA-C	5.44	118.24	110.84
1	C	144	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	A	413	LYS	O-C-N	5.44	129.78	122.82
1	A	203	ASP	N-CA-C	5.43	117.95	111.71
1	B	306	VAL	N-CA-C	5.41	116.69	108.80
1	B	235	ARG	CB-CG-CD	5.39	123.70	111.30
1	B	171	LYS	CG-CD-CE	5.30	123.49	111.30
1	A	409	TYR	N-CA-C	5.29	114.39	108.25
1	C	127	SER	N-CA-CB	5.28	117.85	109.82
1	B	361	THR	N-CA-CB	5.28	117.98	110.16
1	A	173	CYS	N-CA-C	5.27	117.03	111.28
1	B	91	GLU	CB-CG-CD	5.15	121.36	112.60
1	A	232	ARG	CA-CB-CG	-5.09	103.92	114.10
1	A	156	GLN	CA-C-N	-5.03	114.54	119.92
1	A	156	GLN	C-N-CA	-5.03	114.54	119.92
1	C	46	ARG	NE-CZ-NH2	5.01	123.71	119.20

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	3549	0	3448	30	1
1	B	3415	0	3312	34	0
1	C	3534	0	3427	32	1
2	A	15	0	7	1	0
2	B	15	0	7	1	0
2	C	15	0	7	1	0
3	A	72	0	0	1	0
3	B	56	0	0	1	0
3	C	57	0	0	1	0
All	All	10728	0	10208	84	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 4.

All (84) 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:61:ASN:OD1	1:A:91:GLU:OE1	2.05	0.74
1:A:308:TYR:CE2	1:A:309:LEU:HD13	2.23	0.73
1:A:246:ASP:HA	1:A:274:ASN:HD21	1.55	0.70
1:A:253:TYR:CE2	1:A:257:ILE:HD11	2.30	0.67
1:A:215:THR:HG22	2:A:501:PLP:O3	1.95	0.65
1:B:165:TYR:CE2	1:B:180:MET:HE1	2.31	0.65
1:B:246:ASP:HA	1:B:274:ASN:HD21	1.62	0.65
1:A:215:THR:HG23	3:A:609:HOH:O	1.98	0.62
1:B:246:ASP:HA	1:B:274:ASN:ND2	2.14	0.62
1:C:215:THR:HG22	2:C:501:PLP:O3	2.00	0.61
1:C:246:ASP:HA	1:C:274:ASN:HD21	1.65	0.60
1:A:353:ALA:O	1:A:378:ILE:HD11	2.02	0.59
1:B:313:LEU:HD23	1:B:314:PRO:HD2	1.84	0.58
1:B:65:PHE:HB2	1:B:279:LYS:HG2	1.85	0.58
1:B:367:SER:HB2	1:B:383:THR:HG22	1.85	0.58
1:C:63:ALA:O	1:C:422:ARG:NH2	2.37	0.58
1:C:91:GLU:OE1	1:A:63:ALA:HB3	2.05	0.57
1:B:65:PHE:CB	1:B:279:LYS:HG2	2.35	0.57
1:B:215:THR:HG22	2:B:501:PLP:O3	2.05	0.56
1:A:246:ASP:HA	1:A:274:ASN:ND2	2.21	0.56
1:A:309:LEU:O	1:A:310:GLY:C	2.49	0.56
1:B:63:ALA:HB2	1:B:407:PRO:HD3	1.87	0.55
1:C:173:CYS:SG	1:C:180:MET:HG2	2.47	0.55
1:A:181:HIS:HD2	1:A:200:TYR:O	1.89	0.55
1:B:276:SER:HB2	1:B:279:LYS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ALA:O	1:C:248:ALA:C	2.51	0.54
1:C:181:HIS:HD2	1:C:200:TYR:O	1.90	0.53
1:B:308:TYR:CD2	1:B:313:LEU:HD12	2.43	0.53
1:B:180:MET:HE2	1:B:182:VAL:HG22	1.90	0.53
1:B:89:LYS:HB3	1:B:308:TYR:HB2	1.91	0.53
1:B:165:TYR:CZ	1:B:180:MET:HE1	2.44	0.53
1:C:246:ASP:HA	1:C:274:ASN:ND2	2.25	0.51
1:B:173:CYS:SG	1:B:180:MET:HG3	2.50	0.51
1:A:129:ALA:HB1	1:A:290:VAL:HB	1.93	0.51
1:B:234:ASN:HD21	1:B:241:VAL:H	1.60	0.50
1:B:306:VAL:O	1:B:312:GLU:HA	2.12	0.50
1:C:361:THR:HG22	1:C:368:LEU:HD21	1.94	0.49
1:C:88:ASP:OD2	1:C:91:GLU:OE2	2.29	0.49
1:C:357:ALA:O	1:C:361:THR:HG23	2.13	0.49
1:A:173:CYS:SG	1:A:180:MET:HG2	2.53	0.49
1:B:181:HIS:HD2	1:B:200:TYR:O	1.96	0.49
1:B:165:TYR:CD2	1:B:180:MET:HE1	2.48	0.48
1:C:234:ASN:HD21	1:C:241:VAL:H	1.61	0.48
1:C:54:ASP:OD2	1:A:94:ARG:NH2	2.46	0.48
1:C:342:TYR:O	1:C:346:GLN:HG2	2.14	0.48
1:C:215:THR:HG23	3:C:638:HOH:O	2.13	0.48
1:A:88:ASP:OD1	1:A:91:GLU:HG3	2.14	0.48
1:A:402:LYS:O	1:B:54:ASP:OD1	2.31	0.47
1:A:88:ASP:OD2	1:A:91:GLU:OE2	2.32	0.47
1:A:278:HIS:HA	1:A:283:VAL:O	2.15	0.47
1:B:190:MET:HA	1:B:190:MET:HE2	1.96	0.47
1:A:144:ARG:HD3	1:A:240:PRO:HD2	1.96	0.47
1:C:29:LEU:HD21	1:C:47:LEU:HB3	1.98	0.46
1:B:253:TYR:CE2	1:B:257:ILE:HD12	2.51	0.46
1:C:52:LEU:HD21	1:A:98:ILE:HD12	1.97	0.46
1:C:320:PHE:O	1:C:322:HIS:HD2	1.99	0.46
1:A:453:ILE:HD11	1:B:394:ASP:OD1	2.16	0.46
1:C:124:ILE:HD12	1:A:124:ILE:HD12	1.98	0.45
1:C:106:ILE:HG22	1:C:291:ILE:HD12	1.98	0.45
1:C:192:LEU:HB2	1:C:221:ASP:CG	2.42	0.45
1:B:88:ASP:OD1	1:B:91:GLU:HG3	2.17	0.45
1:C:51:GLN:O	1:A:94:ARG:HG2	2.18	0.44
1:B:342:TYR:O	1:B:346:GLN:HG2	2.18	0.44
1:C:65:PHE:HB2	1:C:279:LYS:HE2	2.00	0.44
1:B:320:PHE:O	1:B:322:HIS:HD2	2.01	0.43
1:C:65:PHE:HB3	1:C:279:LYS:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ILE:HG21	1:C:46:ARG:HG2	2.00	0.43
1:B:215:THR:HG23	3:B:608:HOH:O	2.18	0.43
1:C:94:ARG:CG	1:A:51:GLN:O	2.67	0.43
1:A:253:TYR:CE2	1:A:257:ILE:CD1	3.01	0.42
1:B:377:LEU:HD21	1:B:422:ARG:HG3	2.01	0.42
1:A:454:VAL:HB	1:B:451:ALA:C	2.45	0.42
1:C:63:ALA:HB3	1:A:91:GLU:OE1	2.19	0.41
1:B:409:TYR:CE2	1:B:420:ILE:HD11	2.56	0.41
1:C:79:LYS:HB2	1:A:79:LYS:HG3	2.02	0.41
1:C:361:THR:HG22	1:C:368:LEU:CD2	2.50	0.41
1:A:388:ARG:HD2	1:A:390:TRP:CD2	2.56	0.41
1:B:129:ALA:HB1	1:B:290:VAL:HB	2.03	0.41
1:B:234:ASN:ND2	1:B:241:VAL:H	2.17	0.41
1:C:308:TYR:CD2	1:C:313:LEU:HD13	2.56	0.41
1:B:313:LEU:HA	1:B:314:PRO:HD2	1.91	0.41
1:C:88:ASP:OD1	1:C:91:GLU:HG3	2.21	0.40
1:A:65:PHE:HB2	1:A:279:LYS:HE2	2.03	0.40
1:B:278:HIS:HA	1:B:283:VAL:O	2.20	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)
1:C:443:GLN:OE1	1:A:309:LEU:CD2[3_654]	2.11	0.09

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	439/468 (94%)	422 (96%)	16 (4%)	1 (0%)	43 44
1	B	422/468 (90%)	400 (95%)	22 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	437/468 (93%)	416 (95%)	20 (5%)	1 (0%)	43	44
All	All	1298/1404 (92%)	1238 (95%)	58 (4%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	413	LYS
1	A	295	GLN

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	380/404 (94%)	353 (93%)	27 (7%)	13	8
1	B	366/404 (91%)	338 (92%)	28 (8%)	12	7
1	C	378/404 (94%)	354 (94%)	24 (6%)	16	11
All	All	1124/1212 (93%)	1045 (93%)	79 (7%)	14	9

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	THR
1	C	34	LEU
1	C	59	ARG
1	C	77	LEU
1	C	79	LYS
1	C	94	ARG
1	C	119	THR
1	C	159	ILE
1	C	190	MET
1	C	192	LEU
1	C	238	LYS
1	C	254	THR
1	C	257	ILE

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Mol	Chain	Res	Type
1	C	313	LEU
1	C	316	MET
1	C	327	LEU
1	C	348	LYS
1	C	361	THR
1	C	369	ILE
1	C	400	LEU
1	C	414	ASN
1	C	424	VAL
1	C	425	VAL
1	C	450	GLN
1	A	26	ARG
1	A	30	PRO
1	A	33	LYS
1	A	77	LEU
1	A	79	LYS
1	A	94	ARG
1	A	119	THR
1	A	135	LEU
1	A	159	ILE
1	A	190	MET
1	A	192	LEU
1	A	238	LYS
1	A	241	VAL
1	A	254	THR
1	A	257	ILE
1	A	300	LYS
1	A	316	MET
1	A	335	ILE
1	A	346	GLN
1	A	360	LEU
1	A	368	LEU
1	A	422	ARG
1	A	424	VAL
1	A	425	VAL
1	A	452	HIS
1	A	453	ILE
1	A	454	VAL
1	B	28	ASP
1	B	34	LEU
1	B	46	ARG
1	B	77	LEU

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Mol	Chain	Res	Type
1	B	79	LYS
1	B	94	ARG
1	B	108	ASN
1	B	119	THR
1	B	159	ILE
1	B	180	MET
1	B	190	MET
1	B	192	LEU
1	B	238	LYS
1	B	241	VAL
1	B	254	THR
1	B	257	ILE
1	B	300	LYS
1	B	301	GLU
1	B	313	LEU
1	B	316	MET
1	B	327	LEU
1	B	348	LYS
1	B	360	LEU
1	B	361	THR
1	B	368	LEU
1	B	400	LEU
1	B	424	VAL
1	B	425	VAL

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

Mol	Chain	Res	Type
1	C	158	ASN
1	C	181	HIS
1	C	234	ASN
1	C	274	ASN
1	C	322	HIS
1	C	443	GLN
1	A	108	ASN
1	A	158	ASN
1	A	181	HIS
1	A	234	ASN
1	A	274	ASN
1	A	452	HIS
1	B	158	ASN
1	B	181	HIS

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Mol	Chain	Res	Type
1	B	234	ASN
1	B	274	ASN
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](#)

3 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	2.00	3 (20%)	21,22,23	1.99	8 (38%)
2	PLP	C	501	1	15,15,16	2.08	4 (26%)	21,22,23	2.54	9 (42%)
2	PLP	B	501	1	15,15,16	3.01	5 (33%)	21,22,23	1.86	5 (23%)

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	-	0/6/6/8	0/1/1/1
2	PLP	C	501	1	-	0/6/6/8	0/1/1/1
2	PLP	B	501	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	B	501	PLP	C3-C2	8.21	1.49	1.41
2	A	501	PLP	C3-C2	5.10	1.46	1.41
2	B	501	PLP	C3-C4	5.04	1.49	1.40
2	B	501	PLP	C5-C4	5.00	1.46	1.40
2	C	501	PLP	C3-C2	4.47	1.45	1.41
2	C	501	PLP	C3-C4	4.40	1.48	1.40
2	A	501	PLP	C3-C4	3.72	1.47	1.40
2	C	501	PLP	C5-C4	3.37	1.44	1.40
2	C	501	PLP	C2-N1	3.00	1.39	1.33
2	B	501	PLP	P-O2P	-2.52	1.45	1.54
2	B	501	PLP	C2-N1	2.33	1.38	1.33
2	A	501	PLP	C6-C5	2.11	1.41	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	PLP	C4A-C4-C5	-4.87	115.92	120.94
2	C	501	PLP	C2A-C2-N1	4.22	125.59	117.64
2	B	501	PLP	O3-C3-C2	4.15	126.18	117.58
2	C	501	PLP	C6-N1-C2	4.08	126.60	119.20
2	A	501	PLP	C2A-C2-C3	-3.37	116.85	120.80
2	B	501	PLP	O4P-C5A-C5	-3.25	103.27	109.36
2	C	501	PLP	C2A-C2-C3	-3.24	117.00	120.80
2	A	501	PLP	O4P-P-O1P	-3.23	97.71	106.44
2	C	501	PLP	C3-C4-C5	3.23	122.46	118.59
2	A	501	PLP	C2A-C2-N1	3.13	123.55	117.64
2	B	501	PLP	C4-C3-C2	-3.11	115.24	119.89
2	A	501	PLP	C5A-C5-C6	3.04	124.32	119.36
2	C	501	PLP	C4-C3-C2	-3.03	115.36	119.89
2	A	501	PLP	C5A-C5-C4	-2.83	117.06	122.64
2	C	501	PLP	C3-C2-N1	-2.82	117.41	120.96
2	A	501	PLP	C6-N1-C2	2.81	124.29	119.20
2	B	501	PLP	C6-N1-C2	2.70	124.09	119.20
2	A	501	PLP	O3-C3-C2	2.50	122.76	117.58
2	C	501	PLP	C5A-C5-C6	2.49	123.42	119.36
2	B	501	PLP	O3P-P-O2P	2.48	117.10	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	PLP	O3P-P-O4P	-2.48	100.21	106.67
2	A	501	PLP	C4-C3-C2	-2.15	116.67	119.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PLP	1	0
2	C	501	PLP	1	0
2	B	501	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

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	441/468 (94%)	0.21	33 (7%) 20 23	14, 28, 64, 108	0
1	B	424/468 (90%)	0.16	30 (7%) 22 25	14, 26, 57, 115	0
1	C	439/468 (93%)	0.19	32 (7%) 21 24	13, 26, 61, 125	0
All	All	1304/1404 (92%)	0.19	95 (7%) 21 24	13, 27, 63, 125	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	309	LEU	8.8
1	A	454	VAL	8.0
1	B	29	LEU	7.9
1	A	309	LEU	7.2
1	B	310	GLY	7.2
1	A	310	GLY	6.7
1	B	309	LEU	6.4
1	B	311	GLY	6.1
1	B	413	LYS	6.1
1	C	311	GLY	5.8
1	C	310	GLY	5.6
1	A	384	ALA	5.3
1	C	313	LEU	5.0
1	A	311	GLY	5.0
1	B	308	TYR	5.0
1	C	308	TYR	4.8
1	B	32	TYR	4.8
1	C	452	HIS	4.7
1	B	28	ASP	4.7
1	B	30	PRO	4.6
1	A	453	ILE	4.4
1	A	452	HIS	4.3
1	C	314	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	313	LEU	4.0
1	B	306	VAL	3.9
1	C	306	VAL	3.9
1	B	312	GLU	3.8
1	C	384	ALA	3.8
1	C	307	SER	3.6
1	C	15	THR	3.5
1	A	216	TYR	3.5
1	A	300	LYS	3.5
1	A	413	LYS	3.3
1	B	56	GLY	3.3
1	C	446	HIS	3.3
1	A	15	THR	3.2
1	A	14	GLU	3.2
1	C	300	LYS	3.2
1	C	56	GLY	3.2
1	B	115	ALA	3.1
1	C	238	LYS	3.1
1	C	383	THR	3.1
1	B	386	SER	3.1
1	C	312	GLU	3.1
1	C	305	LYS	3.1
1	A	313	LEU	3.1
1	A	362	LYS	3.0
1	B	108	ASN	3.0
1	C	14	GLU	3.0
1	C	451	ALA	3.0
1	B	451	ALA	2.9
1	A	412	PRO	2.9
1	C	386	SER	2.9
1	A	446	HIS	2.8
1	A	451	ALA	2.8
1	B	307	SER	2.8
1	A	189	HIS	2.8
1	A	308	TYR	2.8
1	C	368	LEU	2.7
1	C	257	ILE	2.7
1	A	416	THR	2.7
1	A	297	TYR	2.7
1	B	300	LYS	2.6
1	B	305	LYS	2.6
1	A	361	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	54	ASP	2.6
1	A	56	GLY	2.6
1	C	348	LYS	2.6
1	C	413	LYS	2.6
1	A	363	LEU	2.5
1	C	16	LEU	2.4
1	B	389	GLU	2.4
1	C	216	TYR	2.4
1	A	407	PRO	2.4
1	A	188	ASP	2.4
1	B	387	ASP	2.4
1	B	412	PRO	2.4
1	B	373	HIS	2.4
1	C	450	GLN	2.3
1	A	187	ASP	2.3
1	C	315	THR	2.2
1	B	348	LYS	2.2
1	A	383	THR	2.2
1	B	409	TYR	2.2
1	A	386	SER	2.2
1	A	316	MET	2.2
1	A	307	SER	2.2
1	A	42	ARG	2.1
1	C	114	GLU	2.1
1	C	402	LYS	2.1
1	B	417	ASP	2.1
1	B	316	MET	2.0
1	A	411	LEU	2.0
1	B	314	PRO	2.0
1	B	216	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

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	C	501	15/16	0.98	0.05	15,17,19,23	0
2	PLP	A	501	15/16	0.98	0.05	14,17,20,22	0
2	PLP	B	501	15/16	0.99	0.05	15,18,21,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.