



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:22 AM GMT

PDB ID : 2QGH
Title : Crystal structure of diaminopimelate decarboxylase from *Helicobacter pylori* complexed with L-lysine
Authors : Hu, T.; Wu, D.; Jiang, H.; Shen, X.
Deposited on : 2007-06-28
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

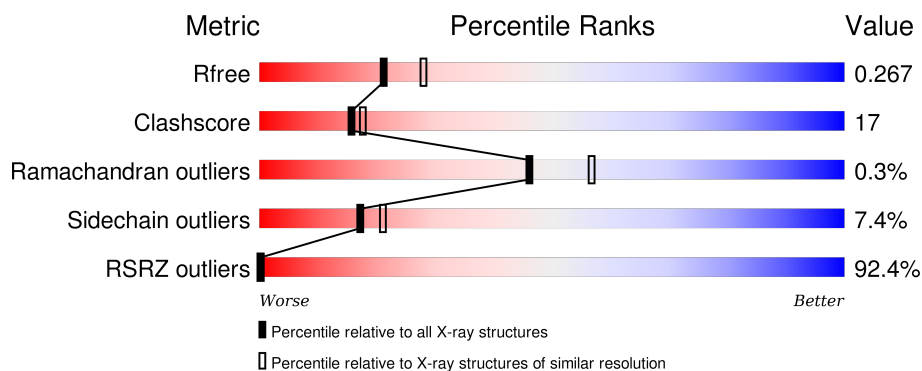
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	425	

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	PLP	A	406	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LYS	A	407	-	-	-	X
3	GOL	A	1003	-	-	-	X

2 Entry composition [i](#)

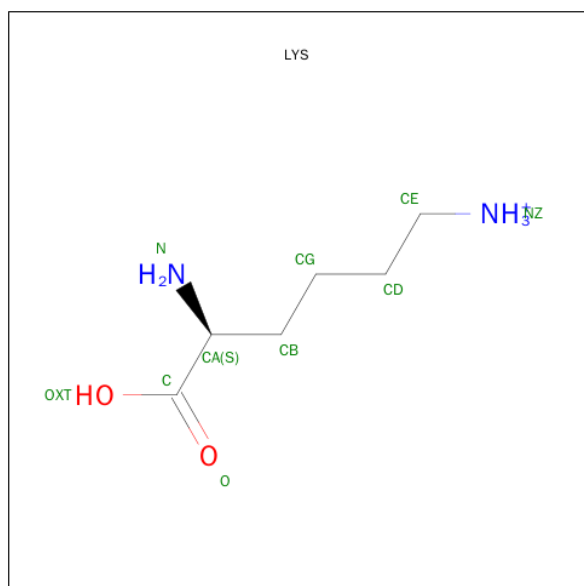
There are 4 unique types of molecules in this entry. The entry contains 3254 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	394	Total	C	N	O	S	0	0	0
			3102	1999	515	579	9			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: LYS, PLP) (formula: $C_6H_{15}N_2O_2$, $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	2	Total	C	N	O	P	0	0
			25	14	3	7	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		

3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	79.25Å 79.25Å 134.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.30 19.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (15.00-2.30) 96.6 (19.00-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.28 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.267 0.206 , 0.267	Depositor DCC
R_{free} test set	2136 reflections (9.94%)	DCC
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.5	EDS
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 21599 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3254	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 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	0.36	0/3156	0.60	0/4251

There are no bond length outliers.

There are no bond angle outliers.

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	3102	0	3174	108	0
2	A	25	0	16	2	0
3	A	6	0	8	2	0
4	A	121	0	0	9	0
All	All	3254	0	3198	108	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 17.

All (108) 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:A:159:VAL:HG11	1:A:163:GLU:HG2	1.34	1.04
1:A:159:VAL:HB	4:A:1107:HOH:O	1.67	0.94
1:A:387:LYS:HA	1:A:387:LYS:HE2	1.54	0.88
1:A:325:VAL:HG12	1:A:334:THR:HB	1.57	0.86
1:A:53:ILE:HG21	4:A:1122:HOH:O	1.79	0.81
1:A:198:GLU:O	1:A:202:LYS:HD3	1.81	0.80
1:A:311:ILE:HD11	1:A:351:ALA:HB2	1.65	0.79
1:A:273:THR:OG1	1:A:289:VAL:HG13	1.81	0.79
1:A:137:ASN:HD22	1:A:139:ASN:H	1.33	0.73
1:A:256:ILE:HD11	1:A:258:CYS:SG	2.30	0.70
1:A:16:TYR:HB2	1:A:374:GLU:HG2	1.77	0.67
1:A:386:ARG:HD2	4:A:1100:HOH:O	1.95	0.67
1:A:159:VAL:HG11	1:A:163:GLU:CG	2.20	0.67
1:A:8:PHE:CE1	1:A:349:LYS:HG3	2.30	0.67
1:A:328:VAL:HG22	1:A:333:ASP:HB2	1.78	0.65
1:A:102:LYS:HE2	4:A:1124:HOH:O	1.97	0.65
1:A:39:SER:HB3	1:A:256:ILE:HG23	1.79	0.64
1:A:104:ASN:HA	3:A:1003:GOL:O1	1.98	0.63
1:A:387:LYS:NZ	1:A:388:ARG:H	1.95	0.63
1:A:328:VAL:HG22	1:A:333:ASP:CB	2.29	0.62
1:A:336:LEU:HD22	1:A:339:ALA:HB2	1.82	0.61
1:A:370:PRO:HB3	1:A:389:GLU:HB3	1.84	0.59
1:A:374:GLU:HB2	1:A:386:ARG:HB3	1.83	0.59
1:A:256:ILE:HD13	1:A:256:ILE:C	2.23	0.59
1:A:3:ASN:HD22	1:A:3:ASN:N	2.01	0.58
1:A:278:GLU:OE2	1:A:285:ARG:HD2	2.04	0.57
1:A:229:SER:O	1:A:354:LYS:HE3	2.03	0.57
1:A:375:LEU:HD23	1:A:384:VAL:HA	1.86	0.57
1:A:32:GLU:O	1:A:35:LYS:HG3	2.06	0.56
1:A:50:ASN:HB3	1:A:53:ILE:HG23	1.87	0.56
1:A:301:LEU:HD13	1:A:302:TYR:CZ	2.41	0.56
1:A:203:VAL:HG13	1:A:206:ILE:HD11	1.87	0.56
1:A:168:PHE:HB3	1:A:215:ILE:CD1	2.36	0.55
1:A:137:ASN:ND2	1:A:139:ASN:H	2.03	0.55
1:A:377:LEU:HD23	1:A:379:ASP:H	1.71	0.54
1:A:148:ILE:HB	1:A:188:SER:HB3	1.90	0.54
1:A:49:SER:HB3	1:A:74:ARG:HD3	1.88	0.54
1:A:366:TYR:O	1:A:367:ASN:HB2	2.09	0.53
1:A:101:LEU:HB3	1:A:128:ILE:HD11	1.90	0.53
1:A:354:LYS:HE2	4:A:1078:HOH:O	2.09	0.53
1:A:294:ASN:OD1	1:A:369:ARG:NH1	2.42	0.53
1:A:320:SER:HB2	1:A:321:PRO:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LYS:CA	1:A:387:LYS:HE2	2.33	0.52
1:A:124:GLN:HG3	1:A:176:PHE:CZ	2.45	0.52
1:A:136:ILE:HD11	1:A:203:VAL:CG2	2.40	0.52
1:A:181:SER:HB2	1:A:219:PHE:HB2	1.92	0.52
1:A:124:GLN:HA	1:A:176:PHE:CD2	2.45	0.51
1:A:293:MET:HG2	1:A:328:VAL:HG21	1.92	0.51
1:A:137:ASN:C	1:A:137:ASN:HD22	2.15	0.50
1:A:197:ILE:O	1:A:201:GLN:HG3	2.12	0.50
1:A:206:ILE:O	1:A:210:LEU:HD13	2.10	0.50
1:A:259:GLU:O	2:A:406:PLP:H6	2.11	0.50
1:A:12:LYS:HE2	1:A:13:THR:O	2.11	0.50
1:A:203:VAL:O	1:A:206:ILE:HG12	2.12	0.49
1:A:159:VAL:HG12	1:A:160:GLY:N	2.28	0.49
1:A:168:PHE:HB3	1:A:215:ILE:HD13	1.95	0.49
1:A:159:VAL:CG1	1:A:163:GLU:HG2	2.24	0.48
1:A:12:LYS:HD2	4:A:1061:HOH:O	2.13	0.48
1:A:270:GLU:OE1	1:A:353:GLU:HG2	2.13	0.48
1:A:203:VAL:HA	1:A:206:ILE:HG12	1.95	0.48
1:A:120:GLU:OE2	1:A:170:TRP:CH2	2.66	0.48
1:A:387:LYS:CE	1:A:388:ARG:H	2.27	0.48
1:A:25:GLN:NE2	4:A:1113:HOH:O	2.46	0.48
1:A:12:LYS:HD2	1:A:13:THR:H	1.78	0.48
1:A:193:LEU:O	1:A:197:ILE:HG12	2.14	0.48
1:A:14:PRO:HG2	1:A:372:LEU:HD22	1.94	0.47
1:A:33:ALA:CB	1:A:238:LEU:HD12	2.44	0.47
1:A:270:GLU:HA	1:A:355:VAL:HG22	1.96	0.47
1:A:136:ILE:H	1:A:136:ILE:HD13	1.79	0.47
1:A:321:PRO:HA	1:A:339:ALA:O	2.14	0.47
1:A:13:THR:HB	1:A:14:PRO:HA	1.97	0.47
1:A:178:GLU:HG3	4:A:1072:HOH:O	2.15	0.46
1:A:159:VAL:HG12	1:A:163:GLU:HB3	1.98	0.46
1:A:296:PHE:CE2	1:A:299:PRO:HD3	2.51	0.46
1:A:82:PRO:O	1:A:105:ILE:HA	2.16	0.46
1:A:99:GLN:O	1:A:103:LEU:HG	2.16	0.46
1:A:18:TYR:HA	1:A:268:SER:O	2.17	0.45
1:A:136:ILE:HD11	1:A:203:VAL:HG22	1.99	0.45
1:A:45:LEU:HG	1:A:54:LEU:HD21	1.99	0.44
1:A:83:TYR:O	1:A:106:LEU:HG	2.17	0.44
1:A:290:ASP:O	1:A:369:ARG:NH2	2.51	0.44
1:A:173:LYS:NZ	1:A:173:LYS:HB2	2.33	0.44
1:A:98:GLU:HG2	1:A:102:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PHE:HB3	1:A:215:ILE:HD11	1.99	0.43
1:A:202:LYS:HD2	1:A:202:LYS:N	2.32	0.43
1:A:302:TYR:HH	2:A:407:LYS:N	2.17	0.43
1:A:138:PRO:O	1:A:140:ILE:HG13	2.18	0.43
1:A:376:ALA:HB2	1:A:385:ILE:HD13	2.00	0.43
1:A:152:LEU:HA	1:A:152:LEU:HD12	1.91	0.43
1:A:136:ILE:HD13	1:A:183:HIS:O	2.19	0.42
1:A:31:LYS:HE2	4:A:1117:HOH:O	2.19	0.42
1:A:50:ASN:HB3	1:A:53:ILE:CG2	2.47	0.42
1:A:373:LEU:HB2	1:A:388:ARG:HB2	2.02	0.42
1:A:194:GLU:HB2	1:A:195:PRO:HD3	2.01	0.42
1:A:12:LYS:HD2	1:A:13:THR:N	2.34	0.42
1:A:19:ASP:O	1:A:268:SER:HB2	2.20	0.42
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.91	0.42
1:A:133:SER:HB2	1:A:181:SER:HB3	2.02	0.42
1:A:42:CYS:O	1:A:259:GLU:HA	2.20	0.42
1:A:67:VAL:O	1:A:67:VAL:HG22	2.19	0.42
1:A:169:LEU:O	1:A:173:LYS:HG3	2.21	0.41
1:A:135:ARG:CZ	1:A:157:PHE:HB3	2.51	0.41
1:A:389:GLU:HG2	1:A:393:ASP:HB2	2.02	0.41
1:A:272:ILE:HD12	1:A:311:ILE:HD11	2.02	0.41
1:A:189:GLN:HG3	1:A:189:GLN:O	2.20	0.41
1:A:168:PHE:CE1	1:A:210:LEU:HD21	2.56	0.40
1:A:150:THR:HB	1:A:157:PHE:CD2	2.56	0.40
1:A:104:ASN:HA	3:A:1003:GOL:C1	2.52	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	386/425 (91%)	369 (96%)	16 (4%)	1 (0%)	46 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	CYS

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	336/361 (93%)	311 (93%)	25 (7%)	17	21

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	28	LEU
1	A	31	LYS
1	A	51	LEU
1	A	53	ILE
1	A	106	LEU
1	A	110	VAL
1	A	113	PHE
1	A	136	ILE
1	A	137	ASN
1	A	153	LYS
1	A	162	LYS
1	A	170	TRP
1	A	182	VAL
1	A	202	LYS
1	A	238	LEU
1	A	256	ILE
1	A	280	LYS
1	A	301	LEU
1	A	328	VAL
1	A	334	THR
1	A	384	VAL
1	A	387	LYS
1	A	391	LEU

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Mol	Chain	Res	Type
1	A	402	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	73	GLN
1	A	99	GLN
1	A	124	GLN
1	A	137	ASN
1	A	243	GLN
1	A	274	GLN
1	A	303	HIS
1	A	367	ASN

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](#)

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
3	GOL	A	1003	-	5,5,5	0.13	0	5,5,5	0.28	0
2	PLP	A	406	2	15,15,16	2.68	5 (33%)	21,22,23	1.98	6 (28%)
2	LYS	A	407	2	6,9,9	0.34	0	4,10,10	0.41	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	GOL	A	1003	-	-	0/4/4/4	0/0/0/0
2	PLP	A	406	2	-	0/6/6/8	0/1/1/1
2	LYS	A	407	2	-	0/5/9/9	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	406	PLP	P-O4P	-4.00	1.46	1.60
2	A	406	PLP	C6-N1	2.88	1.40	1.34
2	A	406	PLP	C6-C5	3.41	1.45	1.37
2	A	406	PLP	C2-N1	3.50	1.41	1.34
2	A	406	PLP	C3-C2	7.02	1.45	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	406	PLP	C4A-C4-C3	-2.92	115.07	120.36
2	A	406	PLP	C5A-C5-C6	-2.91	113.77	119.28
2	A	406	PLP	C5-C6-N1	-2.47	119.57	123.86
2	A	406	PLP	C4A-C4-C5	2.17	123.14	120.88
2	A	406	PLP	C5A-C5-C4	3.55	126.35	121.65
2	A	406	PLP	O4P-P-O1P	4.79	119.34	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	406	PLP	1	0
2	A	407	LYS	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	394/425 (92%)	6.63	364 (92%) 0 0	13, 25, 45, 57	0

All (364) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	TYR	27.4
1	A	196	ILE	26.1
1	A	146	PRO	23.2
1	A	350	ILE	22.0
1	A	394	LEU	21.1
1	A	86	VAL	20.9
1	A	230	TYR	20.1
1	A	264	ILE	19.8
1	A	16	TYR	18.4
1	A	52	SER	18.3
1	A	157	PHE	18.0
1	A	134	ILE	17.1
1	A	217	LEU	17.0
1	A	81	LYS	17.0
1	A	277	TYR	17.0
1	A	51	LEU	16.6
1	A	150	THR	16.5
1	A	145	HIS	16.3
1	A	388	ARG	16.1
1	A	41	ILE	15.8
1	A	271	LEU	15.6
1	A	143	LYS	15.5
1	A	152	LEU	15.4
1	A	276	LEU	15.3
1	A	101	LEU	15.0
1	A	297	LEU	14.9
1	A	311	ILE	14.9

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Mol	Chain	Res	Type	RSRZ
1	A	219	PHE	14.8
1	A	107	PHE	14.8
1	A	43	TYR	14.6
1	A	324	VAL	14.4
1	A	402	LEU	14.3
1	A	362	MET	14.1
1	A	106	LEU	14.0
1	A	220	PHE	13.9
1	A	159	VAL	13.8
1	A	97	ILE	13.3
1	A	355	VAL	13.3
1	A	69	ILE	13.3
1	A	382	ILE	12.9
1	A	72	ILE	12.8
1	A	329	CYS	12.6
1	A	117	LYS	12.6
1	A	262	ARG	12.4
1	A	265	VAL	12.3
1	A	142	ALA	12.2
1	A	283	ASN	12.0
1	A	56	LEU	12.0
1	A	384	VAL	12.0
1	A	110	VAL	11.9
1	A	85	ILE	11.6
1	A	17	LEU	11.4
1	A	44	ALA	11.1
1	A	292	GLY	11.1
1	A	258	CYS	11.1
1	A	132	ILE	11.0
1	A	119	ILE	11.0
1	A	80	ILE	11.0
1	A	12	LYS	10.9
1	A	45	LEU	10.9
1	A	186	ILE	10.8
1	A	177	LEU	10.7
1	A	263	SER	10.7
1	A	279	LYS	10.6
1	A	34	PHE	10.6
1	A	197	ILE	10.5
1	A	296	PHE	10.4
1	A	351	ALA	10.4
1	A	76	LEU	10.0

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Mol	Chain	Res	Type	RSRZ
1	A	366	TYR	10.0
1	A	27	PHE	10.0
1	A	184	PHE	10.0
1	A	57	LEU	10.0
1	A	83	TYR	9.8
1	A	206	ILE	9.5
1	A	189	GLN	9.5
1	A	211	ILE	9.5
1	A	369	ARG	9.4
1	A	319	ILE	9.4
1	A	259	GLU	9.3
1	A	257	ILE	9.3
1	A	241	TYR	9.3
1	A	165	LEU	9.3
1	A	249	LEU	9.3
1	A	239	TYR	9.2
1	A	40	LEU	9.2
1	A	23	ILE	9.2
1	A	37	ARG	9.1
1	A	193	LEU	9.1
1	A	395	TRP	8.9
1	A	53	ILE	8.9
1	A	15	PHE	8.8
1	A	48	ASN	8.8
1	A	246	LEU	8.7
1	A	386	ARG	8.7
1	A	325	VAL	8.6
1	A	8	PHE	8.5
1	A	54	LEU	8.5
1	A	323	ASP	8.5
1	A	7	LEU	8.4
1	A	278	GLU	8.4
1	A	381	LYS	8.4
1	A	112	SER	8.4
1	A	30	TYR	8.3
1	A	136	ILE	8.3
1	A	173	LYS	8.2
1	A	126	LEU	8.2
1	A	67	VAL	8.1
1	A	90	VAL	8.1
1	A	358	TYR	8.1
1	A	47	ALA	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	167	MET	8.0
1	A	303	HIS	8.0
1	A	66	CYS	7.9
1	A	135	ARG	7.9
1	A	357	ALA	7.9
1	A	127	GLY	7.8
1	A	288	ILE	7.8
1	A	375	LEU	7.8
1	A	46	LYS	7.8
1	A	130	ALA	7.7
1	A	252	LEU	7.7
1	A	108	LEU	7.6
1	A	287	VAL	7.6
1	A	190	LEU	7.6
1	A	154	GLU	7.6
1	A	327	PRO	7.5
1	A	24	LYS	7.5
1	A	373	LEU	7.5
1	A	308	ILE	7.5
1	A	171	ALA	7.4
1	A	128	ILE	7.4
1	A	62	SER	7.4
1	A	301	LEU	7.3
1	A	336	LEU	7.3
1	A	151	GLY	7.3
1	A	49	SER	7.3
1	A	84	ARG	7.3
1	A	349	LYS	7.2
1	A	185	HIS	7.2
1	A	270	GLU	7.2
1	A	245	ILE	7.2
1	A	121	THR	7.2
1	A	191	LEU	7.2
1	A	35	LYS	7.1
1	A	169	LEU	7.0
1	A	116	LEU	7.0
1	A	335	PHE	6.9
1	A	343	GLU	6.8
1	A	293	MET	6.8
1	A	20	PHE	6.7
1	A	74	ARG	6.7
1	A	328	VAL	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	42	CYS	6.6
1	A	345	GLU	6.6
1	A	168	PHE	6.6
1	A	344	LEU	6.6
1	A	228	VAL	6.6
1	A	354	LYS	6.6
1	A	156	LYS	6.5
1	A	284	LYS	6.5
1	A	188	SER	6.5
1	A	291	ALA	6.4
1	A	371	LYS	6.4
1	A	352	ILE	6.4
1	A	4	TYR	6.3
1	A	65	ASP	6.3
1	A	59	HIS	6.3
1	A	364	SER	6.3
1	A	187	GLY	6.2
1	A	365	GLN	6.2
1	A	340	HIS	6.2
1	A	370	PRO	6.2
1	A	204	ALA	6.1
1	A	376	ALA	6.1
1	A	10	THR	6.1
1	A	122	ILE	6.1
1	A	289	VAL	6.0
1	A	310	VAL	6.0
1	A	374	GLU	5.9
1	A	199	ALA	5.9
1	A	272	ILE	5.9
1	A	398	GLU	5.9
1	A	227	GLY	5.8
1	A	28	LEU	5.8
1	A	148	ILE	5.8
1	A	176	PHE	5.8
1	A	212	ALA	5.7
1	A	172	LYS	5.7
1	A	254	LEU	5.6
1	A	341	LEU	5.6
1	A	114	MET	5.6
1	A	103	LEU	5.5
1	A	102	LYS	5.5
1	A	181	SER	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	360	SER	5.4
1	A	60	LEU	5.4
1	A	180	VAL	5.4
1	A	377	LEU	5.4
1	A	19	ASP	5.4
1	A	73	GLN	5.4
1	A	223	GLY	5.3
1	A	261	GLY	5.3
1	A	391	LEU	5.3
1	A	273	THR	5.3
1	A	203	VAL	5.2
1	A	200	SER	5.1
1	A	18	TYR	5.1
1	A	131	ARG	5.0
1	A	226	ILE	5.0
1	A	38	LYS	5.0
1	A	50	ASN	5.0
1	A	133	SER	4.9
1	A	109	ASN	4.9
1	A	182	VAL	4.9
1	A	9	GLN	4.9
1	A	87	PHE	4.9
1	A	170	TRP	4.9
1	A	334	THR	4.9
1	A	105	ILE	4.9
1	A	330	GLU	4.8
1	A	393	ASP	4.8
1	A	195	PRO	4.8
1	A	368	SER	4.8
1	A	113	PHE	4.8
1	A	399	GLU	4.7
1	A	367	ASN	4.7
1	A	286	PHE	4.7
1	A	302	TYR	4.6
1	A	359	GLY	4.6
1	A	129	LYS	4.6
1	A	242	ALA	4.6
1	A	347	GLY	4.6
1	A	298	ARG	4.6
1	A	247	ASN	4.6
1	A	25	GLN	4.6
1	A	205	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	389	GLU	4.5
1	A	64	ALA	4.5
1	A	361	SER	4.5
1	A	11	HIS	4.5
1	A	123	ALA	4.5
1	A	160	GLY	4.5
1	A	164	ALA	4.5
1	A	312	THR	4.5
1	A	175	ALA	4.4
1	A	397	LEU	4.4
1	A	238	LEU	4.4
1	A	215	ILE	4.3
1	A	236	ILE	4.3
1	A	70	GLY	4.3
1	A	356	GLY	4.3
1	A	275	VAL	4.3
1	A	268	SER	4.2
1	A	353	GLU	4.2
1	A	318	GLU	4.1
1	A	314	SER	4.1
1	A	118	THR	4.1
1	A	183	HIS	4.1
1	A	306	HIS	4.1
1	A	75	ALA	4.1
1	A	234	GLU	4.1
1	A	94	ALA	4.0
1	A	115	GLU	4.0
1	A	3	ASN	3.9
1	A	166	GLU	3.9
1	A	235	THR	3.9
1	A	333	ASP	3.9
1	A	6	GLU	3.9
1	A	240	ASP	3.8
1	A	337	LYS	3.8
1	A	348	ASP	3.7
1	A	95	PHE	3.7
1	A	363	ALA	3.7
1	A	256	ILE	3.7
1	A	221	ASP	3.7
1	A	269	GLY	3.7
1	A	396	ARG	3.7
1	A	98	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	322	CYS	3.6
1	A	248	ALA	3.6
1	A	111	GLU	3.6
1	A	179	PRO	3.6
1	A	266	ALA	3.6
1	A	326	GLY	3.6
1	A	26	ALA	3.5
1	A	207	ALA	3.5
1	A	155	ASN	3.5
1	A	210	LEU	3.5
1	A	251	GLY	3.5
1	A	82	PRO	3.5
1	A	222	VAL	3.4
1	A	385	ILE	3.4
1	A	300	SER	3.4
1	A	29	ASN	3.4
1	A	79	GLY	3.4
1	A	216	ASP	3.4
1	A	22	LYS	3.4
1	A	372	LEU	3.3
1	A	55	SER	3.3
1	A	290	ASP	3.3
1	A	100	ALA	3.3
1	A	387	LYS	3.3
1	A	68	SER	3.3
1	A	96	GLU	3.2
1	A	125	SER	3.2
1	A	331	SER	3.2
1	A	39	SER	3.2
1	A	213	LEU	3.1
1	A	88	SER	3.1
1	A	91	GLY	3.1
1	A	244	GLY	3.1
1	A	320	SER	3.1
1	A	339	ALA	3.0
1	A	255	THR	3.0
1	A	274	GLN	3.0
1	A	192	ASP	3.0
1	A	218	ARG	3.0
1	A	13	THR	3.0
1	A	332	SER	3.0
1	A	295	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	78	ALA	2.9
1	A	390	ALA	2.9
1	A	138	PRO	2.9
1	A	198	GLU	2.9
1	A	174	SER	2.8
1	A	224	GLY	2.8
1	A	338	ASP	2.8
1	A	208	LYS	2.8
1	A	209	SER	2.8
1	A	14	PRO	2.8
1	A	307	ALA	2.8
1	A	92	LYS	2.7
1	A	243	GLN	2.7
1	A	304	ALA	2.7
1	A	233	GLU	2.7
1	A	392	GLU	2.7
1	A	149	SER	2.7
1	A	202	LYS	2.6
1	A	260	PRO	2.6
1	A	36	GLY	2.5
1	A	299	PRO	2.5
1	A	71	GLU	2.5
1	A	225	GLY	2.5
1	A	77	LYS	2.5
1	A	178	GLU	2.5
1	A	89	GLY	2.4
1	A	93	SER	2.4
1	A	120	GLU	2.4
1	A	162	LYS	2.4
1	A	58	ALA	2.4
1	A	237	LYS	2.4
1	A	280	LYS	2.4
1	A	163	GLU	2.4
1	A	378	GLU	2.3
1	A	400	GLU	2.3
1	A	305	LYS	2.3
1	A	139	ASN	2.3
1	A	321	PRO	2.2
1	A	294	ASN	2.2
1	A	144	THR	2.2
1	A	140	ILE	2.1
1	A	32	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	63	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	LYS	A	407	10/10	0.35	0.73	0.62	18,20,23,24	0
3	GOL	A	1003	6/6	0.01	0.67	0.48	36,36,38,42	0
2	PLP	A	406	15/16	0.41	0.43	-0.65	16,17,19,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.