



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 10:32 AM BST

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](mailto: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.

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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 : 2.14.4.dev1  
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) : 2.14.4.dev1

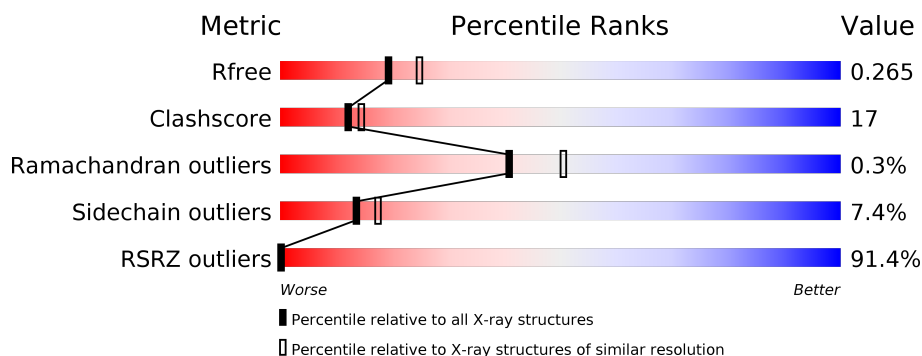
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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  $\geq 3$ , 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	425	<div> <div>85%</div> <div>61% 28% 7%</div> </div>

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
3	LYS	A	407	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	1003	-	-	-	X

## 2 Entry composition [i](#)

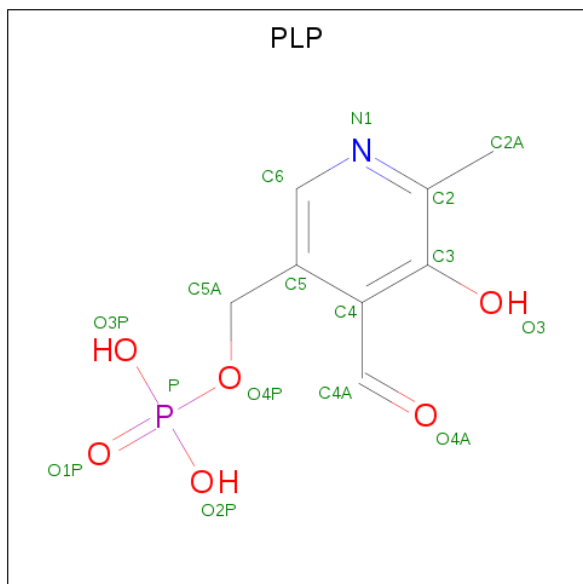
There are 5 unique types of molecules in this entry. The entry contains 3254 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

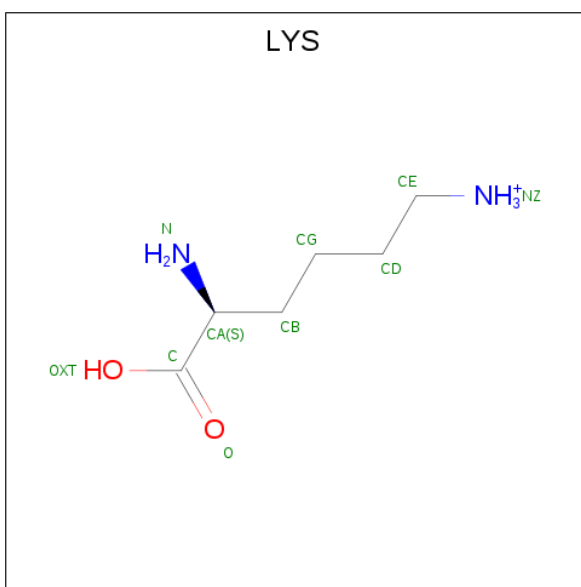
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3102	1999	515	579	9			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

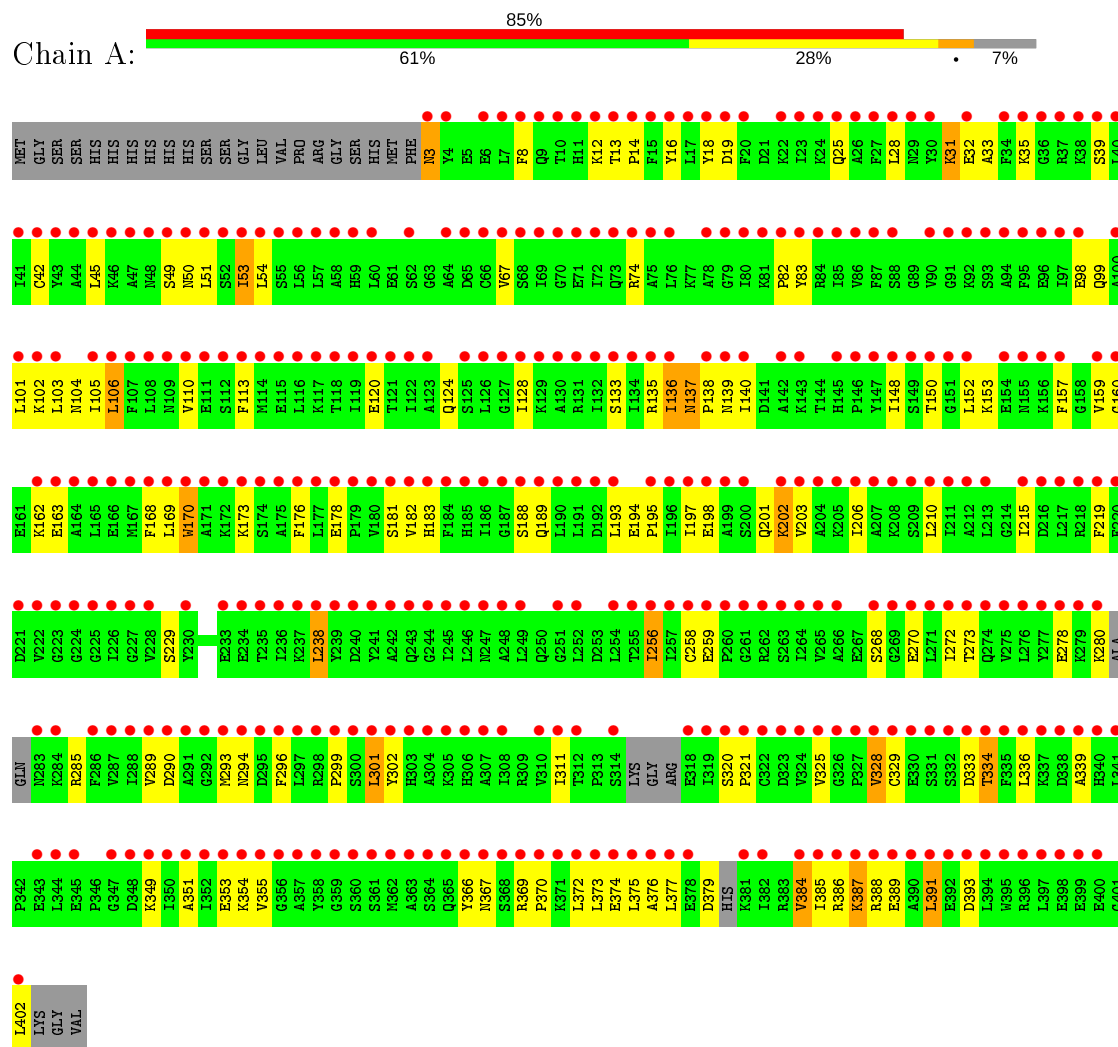
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total 121	O 121	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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.28 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.206 , 0.267 0.204 , 0.265	Depositor DCC
$R_{free}$ test set	2146 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: 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 [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	3102	0	3174	108	0
2	A	15	0	7	1	0
3	A	10	0	9	1	0
4	A	6	0	8	2	0
5	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	5: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	5: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	5: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	5: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	4: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:203:VAL:HG13	1:A:206:ILE:HD11	1.87	0.56
1:A:301:LEU:HD13	1:A:302:TYR:CZ	2.41	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:101:LEU:HB3	1:A:128:ILE:HD11	1.90	0.53
1:A:366:TYR:O	1:A:367:ASN:HB2	2.09	0.53
1:A:354:LYS:HE2	5: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:12:LYS:HD2	5:A:1061:HOH:O	2.13	0.48
1:A:159:VAL:CG1	1:A:163:GLU:HG2	2.24	0.48
1:A:270:GLU:OE1	1:A:353:GLU:HG2	2.13	0.48
1:A:120:GLU:OE2	1:A:170:TRP:CH2	2.66	0.48
1:A:203:VAL:HA	1:A:206:ILE:HG12	1.95	0.48
1:A:25:GLN:NE2	5:A:1113:HOH:O	2.46	0.48
1:A:387:LYS:CE	1:A:388:ARG:H	2.27	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:33:ALA:CB	1:A:238:LEU:HD12	2.44	0.47
1:A:14:PRO:HG2	1:A:372:LEU:HD22	1.94	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	5:A:1072:HOH:O	2.15	0.46
1:A:159:VAL:HG12	1:A:163:GLU:HB3	1.98	0.46
1:A:99:GLN:O	1:A:103:LEU:HG	2.16	0.46
1:A:82:PRO:O	1:A:105:ILE:HA	2.16	0.46
1:A:296:PHE:CE2	1:A:299:PRO:HD3	2.51	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:173:LYS:HB2	1:A:173:LYS:NZ	2.33	0.44
1:A:290:ASP:O	1:A:369:ARG:NH2	2.51	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:138:PRO:O	1:A:140:ILE:HG13	2.18	0.43
1:A:202:LYS:HD2	1:A:202:LYS:N	2.32	0.43
1:A:302:TYR:HH	3:A:407:LYS:N	2.17	0.43
1:A:376:ALA:HB2	1:A:385:ILE:HD13	2.00	0.43
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.91	0.43
1:A:136:ILE:HD13	1:A:183:HIS:O	2.19	0.42
1:A:31:LYS:HE2	5:A:1117:HOH:O	2.19	0.42
1:A:50:ASN:HB3	1:A:53:ILE:CG2	2.47	0.42
1:A:194:GLU:HB2	1:A:195:PRO:HD3	2.01	0.42
1:A:373:LEU:HB2	1:A:388:ARG:HB2	2.02	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:189:GLN:HG3	1:A:189:GLN:O	2.20	0.41
1:A:272:ILE:HD12	1:A:311:ILE:HD11	2.02	0.41
1:A:150:THR:HB	1:A:157:PHE:CD2	2.56	0.40
1:A:168:PHE:CE1	1:A:210:LEU:HD21	2.56	0.40
1:A:104:ASN:HA	4: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%)	41	50

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%)	13	17

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 monosaccharides 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	LYS	A	407	2	5,9,9	0.68	0	4,10,10	0.34	0
2	PLP	A	406	3	15,15,16	2.44	5 (33%)	20,22,23	1.94	7 (35%)
4	GOL	A	1003	-	5,5,5	0.18	0	5,5,5	0.31	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	LYS	A	407	2	-	0/5/9/9	-
2	PLP	A	406	3	-	2/6/6/8	0/1/1/1
4	GOL	A	1003	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	406	PLP	C3-C2	4.72	1.45	1.40
2	A	406	PLP	P-O4P	-4.15	1.46	1.60
2	A	406	PLP	C2-N1	4.06	1.41	1.33
2	A	406	PLP	C6-C5	3.58	1.45	1.37
2	A	406	PLP	C6-N1	2.95	1.40	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	406	PLP	O4P-P-O1P	4.59	119.34	106.47
2	A	406	PLP	C5A-C5-C6	-3.41	113.77	119.37
2	A	406	PLP	C4A-C4-C3	-3.20	115.07	120.50
2	A	406	PLP	C5-C6-N1	-2.55	119.57	123.82
2	A	406	PLP	C4A-C4-C5	2.14	123.14	120.94
2	A	406	PLP	C3-C2-N1	-2.09	118.06	120.77
2	A	406	PLP	C3-C4-C5	2.02	120.92	118.74

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	406	PLP	C5A-O4P-P-O3P
2	A	406	PLP	C5A-O4P-P-O2P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	407	LYS	1	0
2	A	406	PLP	1	0
4	A	1003	GOL	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	394/425 (92%)	6.40	360 (91%) 0 0	13, 25, 45, 57	0

All (360) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ILE	23.9
1	A	146	PRO	23.5
1	A	147	TYR	23.3
1	A	86	VAL	20.1
1	A	394	LEU	19.6
1	A	350	ILE	19.3
1	A	283	ASN	18.2
1	A	230	TYR	18.2
1	A	134	ILE	17.9
1	A	264	ILE	17.9
1	A	81	LYS	17.4
1	A	157	PHE	17.4
1	A	145	HIS	16.6
1	A	217	LEU	16.4
1	A	388	ARG	16.0
1	A	276	LEU	15.8
1	A	311	ILE	15.5
1	A	52	SER	15.4
1	A	16	TYR	15.1
1	A	297	LEU	15.0
1	A	51	LEU	14.9
1	A	402	LEU	14.9
1	A	277	TYR	14.7
1	A	152	LEU	14.5
1	A	143	LYS	14.3
1	A	324	VAL	14.2
1	A	43	TYR	13.9

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Mol	Chain	Res	Type	RSRZ
1	A	101	LEU	13.9
1	A	271	LEU	13.8
1	A	381	LYS	13.8
1	A	150	THR	13.7
1	A	219	PHE	13.6
1	A	159	VAL	13.2
1	A	117	LYS	13.2
1	A	106	LEU	13.2
1	A	41	ILE	13.1
1	A	382	ILE	13.1
1	A	362	MET	12.9
1	A	69	ILE	12.6
1	A	107	PHE	12.6
1	A	110	VAL	12.4
1	A	220	PHE	12.1
1	A	72	ILE	12.0
1	A	355	VAL	11.9
1	A	97	ILE	11.8
1	A	279	LYS	11.5
1	A	262	ARG	11.5
1	A	319	ILE	11.4
1	A	83	TYR	11.2
1	A	142	ALA	11.1
1	A	132	ILE	11.1
1	A	177	LEU	10.9
1	A	17	LEU	10.8
1	A	263	SER	10.8
1	A	351	ALA	10.8
1	A	44	ALA	10.8
1	A	211	ILE	10.7
1	A	56	LEU	10.7
1	A	119	ILE	10.7
1	A	329	CYS	10.6
1	A	292	GLY	10.6
1	A	296	PHE	10.6
1	A	384	VAL	10.4
1	A	45	LEU	10.4
1	A	76	LEU	10.2
1	A	34	PHE	10.1
1	A	265	VAL	9.8
1	A	85	ILE	9.8
1	A	239	TYR	9.8

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Mol	Chain	Res	Type	RSRZ
1	A	366	TYR	9.7
1	A	27	PHE	9.6
1	A	241	TYR	9.6
1	A	80	ILE	9.5
1	A	186	ILE	9.4
1	A	184	PHE	9.4
1	A	57	LEU	9.3
1	A	15	PHE	9.3
1	A	257	ILE	9.2
1	A	54	LEU	9.1
1	A	173	LYS	9.1
1	A	12	LYS	9.1
1	A	197	ILE	9.0
1	A	189	GLN	9.0
1	A	136	ILE	8.8
1	A	23	ILE	8.7
1	A	357	ALA	8.7
1	A	53	ILE	8.6
1	A	37	ARG	8.6
1	A	165	LEU	8.6
1	A	386	ARG	8.6
1	A	48	ASN	8.6
1	A	7	LEU	8.5
1	A	258	CYS	8.5
1	A	112	SER	8.4
1	A	246	LEU	8.4
1	A	249	LEU	8.4
1	A	35	LYS	8.4
1	A	369	ARG	8.4
1	A	126	LEU	8.4
1	A	206	ILE	8.4
1	A	135	ARG	8.3
1	A	395	TRP	8.3
1	A	358	TYR	8.3
1	A	40	LEU	8.2
1	A	193	LEU	8.2
1	A	252	LEU	8.2
1	A	127	GLY	8.2
1	A	169	LEU	8.1
1	A	259	GLU	8.1
1	A	288	ILE	8.1
1	A	323	ASP	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	191	LEU	8.0
1	A	24	LYS	8.0
1	A	373	LEU	7.9
1	A	325	VAL	7.9
1	A	67	VAL	7.8
1	A	284	LYS	7.8
1	A	30	TYR	7.8
1	A	8	PHE	7.8
1	A	308	ILE	7.7
1	A	190	LEU	7.6
1	A	287	VAL	7.6
1	A	345	GLU	7.5
1	A	46	LYS	7.5
1	A	130	ALA	7.4
1	A	167	MET	7.4
1	A	303	HIS	7.4
1	A	301	LEU	7.3
1	A	154	GLU	7.3
1	A	278	GLU	7.2
1	A	49	SER	7.2
1	A	270	GLU	7.1
1	A	62	SER	7.0
1	A	340	HIS	7.0
1	A	20	PHE	7.0
1	A	245	ILE	7.0
1	A	66	CYS	6.9
1	A	336	LEU	6.9
1	A	90	VAL	6.9
1	A	59	HIS	6.8
1	A	47	ALA	6.8
1	A	84	ARG	6.8
1	A	371	LYS	6.8
1	A	343	GLU	6.8
1	A	176	PHE	6.7
1	A	204	ALA	6.7
1	A	156	LYS	6.7
1	A	293	MET	6.7
1	A	187	GLY	6.7
1	A	375	LEU	6.7
1	A	42	CYS	6.6
1	A	128	ILE	6.6
1	A	354	LYS	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	4	TYR	6.6
1	A	349	LYS	6.6
1	A	108	LEU	6.5
1	A	180	VAL	6.5
1	A	310	VAL	6.5
1	A	74	ARG	6.4
1	A	185	HIS	6.4
1	A	188	SER	6.4
1	A	121	THR	6.4
1	A	327	PRO	6.3
1	A	116	LEU	6.2
1	A	228	VAL	6.2
1	A	151	GLY	6.2
1	A	335	PHE	6.2
1	A	122	ILE	6.2
1	A	365	GLN	6.2
1	A	328	VAL	6.1
1	A	344	LEU	6.1
1	A	203	VAL	6.1
1	A	289	VAL	6.1
1	A	352	ILE	6.0
1	A	65	ASP	6.0
1	A	103	LEU	6.0
1	A	272	ILE	5.9
1	A	171	ALA	5.6
1	A	10	THR	5.6
1	A	38	LYS	5.6
1	A	199	ALA	5.6
1	A	364	SER	5.6
1	A	28	LEU	5.5
1	A	370	PRO	5.5
1	A	227	GLY	5.4
1	A	212	ALA	5.4
1	A	168	PHE	5.4
1	A	148	ILE	5.4
1	A	254	LEU	5.4
1	A	195	PRO	5.3
1	A	261	GLY	5.3
1	A	374	GLU	5.3
1	A	359	GLY	5.3
1	A	114	MET	5.2
1	A	391	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	223	GLY	5.2
1	A	341	LEU	5.2
1	A	399	GLU	5.2
1	A	172	LYS	5.2
1	A	181	SER	5.1
1	A	60	LEU	5.1
1	A	109	ASN	5.1
1	A	133	SER	5.0
1	A	87	PHE	5.0
1	A	160	GLY	5.0
1	A	396	ARG	5.0
1	A	113	PHE	5.0
1	A	102	LYS	4.9
1	A	360	SER	4.9
1	A	334	THR	4.9
1	A	131	ARG	4.9
1	A	73	GLN	4.9
1	A	94	ALA	4.9
1	A	398	GLU	4.8
1	A	234	GLU	4.8
1	A	247	ASN	4.8
1	A	205	LYS	4.8
1	A	175	ALA	4.8
1	A	50	ASN	4.8
1	A	393	ASP	4.8
1	A	318	GLU	4.7
1	A	312	THR	4.7
1	A	275	VAL	4.7
1	A	376	ALA	4.7
1	A	170	TRP	4.6
1	A	25	GLN	4.6
1	A	367	ASN	4.6
1	A	368	SER	4.6
1	A	330	GLU	4.6
1	A	397	LEU	4.6
1	A	105	ILE	4.6
1	A	291	ALA	4.5
1	A	164	ALA	4.5
1	A	347	GLY	4.5
1	A	3	ASN	4.4
1	A	182	VAL	4.4
1	A	356	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	240	ASP	4.4
1	A	236	ILE	4.4
1	A	242	ALA	4.4
1	A	200	SER	4.3
1	A	11	HIS	4.3
1	A	377	LEU	4.3
1	A	123	ALA	4.3
1	A	273	THR	4.3
1	A	361	SER	4.3
1	A	302	TYR	4.3
1	A	389	GLU	4.3
1	A	238	LEU	4.2
1	A	166	GLU	4.2
1	A	226	ILE	4.2
1	A	215	ILE	4.2
1	A	9	GLN	4.2
1	A	298	ARG	4.1
1	A	337	LYS	4.1
1	A	36	GLY	4.1
1	A	70	GLY	4.1
1	A	18	TYR	4.1
1	A	268	SER	4.1
1	A	19	ASP	4.1
1	A	129	LYS	4.1
1	A	353	GLU	4.0
1	A	314	SER	4.0
1	A	306	HIS	4.0
1	A	118	THR	3.9
1	A	256	ILE	3.8
1	A	115	GLU	3.8
1	A	210	LEU	3.7
1	A	333	ASP	3.7
1	A	322	CYS	3.7
1	A	183	HIS	3.7
1	A	213	LEU	3.6
1	A	363	ALA	3.6
1	A	95	PHE	3.6
1	A	75	ALA	3.6
1	A	98	GLU	3.6
1	A	208	LYS	3.6
1	A	235	THR	3.6
1	A	111	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	255	THR	3.6
1	A	385	ILE	3.6
1	A	222	VAL	3.5
1	A	64	ALA	3.5
1	A	348	ASP	3.5
1	A	274	GLN	3.5
1	A	286	PHE	3.5
1	A	26	ALA	3.5
1	A	326	GLY	3.5
1	A	251	GLY	3.5
1	A	29	ASN	3.4
1	A	372	LEU	3.4
1	A	22	LYS	3.4
1	A	266	ALA	3.4
1	A	269	GLY	3.3
1	A	331	SER	3.3
1	A	207	ALA	3.3
1	A	155	ASN	3.3
1	A	6	GLU	3.3
1	A	91	GLY	3.2
1	A	300	SER	3.2
1	A	68	SER	3.2
1	A	82	PRO	3.2
1	A	96	GLU	3.2
1	A	55	SER	3.2
1	A	88	SER	3.1
1	A	221	ASP	3.1
1	A	78	ALA	3.1
1	A	192	ASP	3.1
1	A	295	ASP	3.1
1	A	290	ASP	3.1
1	A	233	GLU	3.0
1	A	179	PRO	3.0
1	A	100	ALA	3.0
1	A	339	ALA	3.0
1	A	79	GLY	3.0
1	A	93	SER	3.0
1	A	218	ARG	2.9
1	A	280	LYS	2.9
1	A	198	GLU	2.9
1	A	305	LYS	2.9
1	A	338	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	244	GLY	2.9
1	A	248	ALA	2.9
1	A	307	ALA	2.9
1	A	260	PRO	2.9
1	A	138	PRO	2.8
1	A	378	GLU	2.8
1	A	13	THR	2.8
1	A	320	SER	2.7
1	A	162	LYS	2.7
1	A	202	LYS	2.7
1	A	387	LYS	2.7
1	A	92	LYS	2.7
1	A	14	PRO	2.7
1	A	39	SER	2.7
1	A	332	SER	2.7
1	A	224	GLY	2.7
1	A	174	SER	2.6
1	A	237	LYS	2.6
1	A	390	ALA	2.6
1	A	125	SER	2.6
1	A	304	ALA	2.6
1	A	139	ASN	2.5
1	A	209	SER	2.5
1	A	299	PRO	2.5
1	A	392	GLU	2.4
1	A	149	SER	2.4
1	A	243	GLN	2.4
1	A	120	GLU	2.4
1	A	71	GLU	2.4
1	A	178	GLU	2.3
1	A	216	ASP	2.3
1	A	225	GLY	2.3
1	A	58	ALA	2.2
1	A	294	ASN	2.2
1	A	140	ILE	2.2
1	A	32	GLU	2.1
1	A	321	PRO	2.1
1	A	163	GLU	2.0
1	A	400	GLU	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 monosaccharides 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	1003	6/6	0.01	0.71	36,36,38,42	0
3	LYS	A	407	10/10	0.35	0.69	18,20,23,24	0
2	PLP	A	406	15/16	0.42	0.42	16,17,19,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.