Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 05:25 AM EDT

PDB ID	:	3DOD
Title	:	Crystal Structure of PLP Bound 7,8-Diaminopelargonic Acid Synthase in Bacillus subtilis
Authors	:	Dey, S.; Sacchettini, J.C.
Deposited on	:	2008-07-03
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

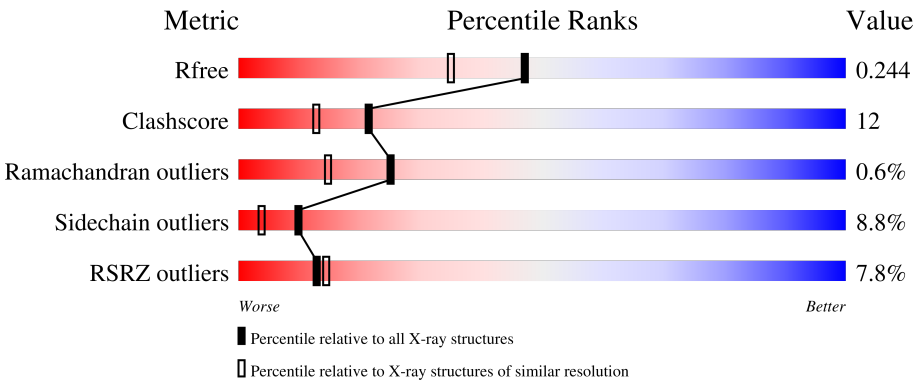
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	448	2%, 72%, 17%, •, 7%
1	B	448	12%, 72%, 17%, •, 7%

2 Entry composition (i)

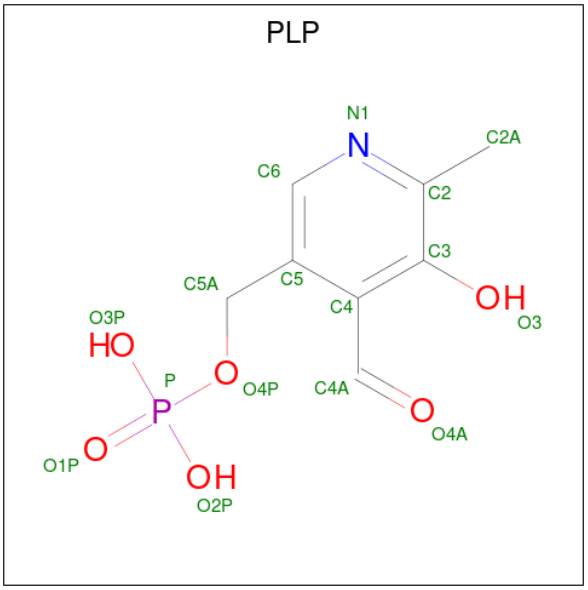
There are 3 unique types of molecules in this entry. The entry contains 6987 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosylmethionine-8-amino-7-oxononanoate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	3295	2107	544	622	22	0	2	0
1	B	416	3278	2094	541	621	22	0	1	0

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



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

- Molecule 3 is water.

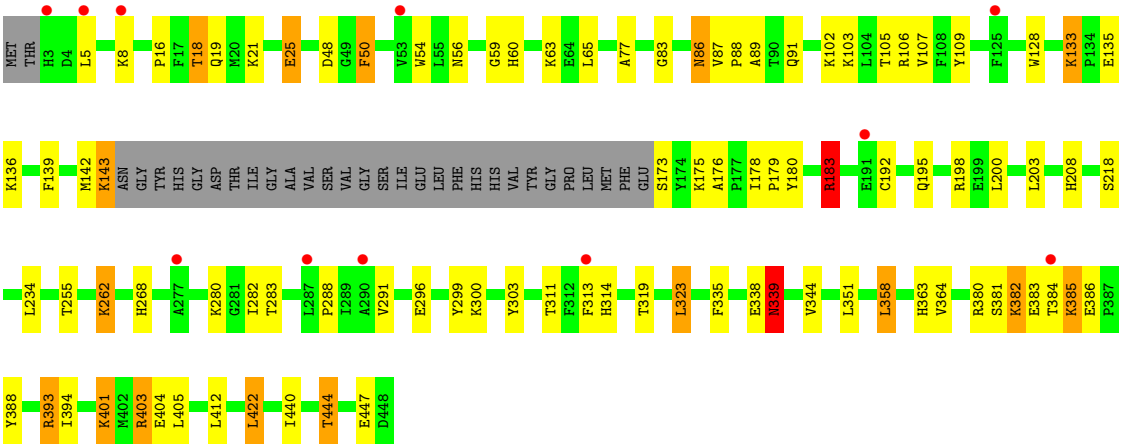
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	199	199	199	0	0
			Total	O		
3	B	185	185	185	0	0

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.

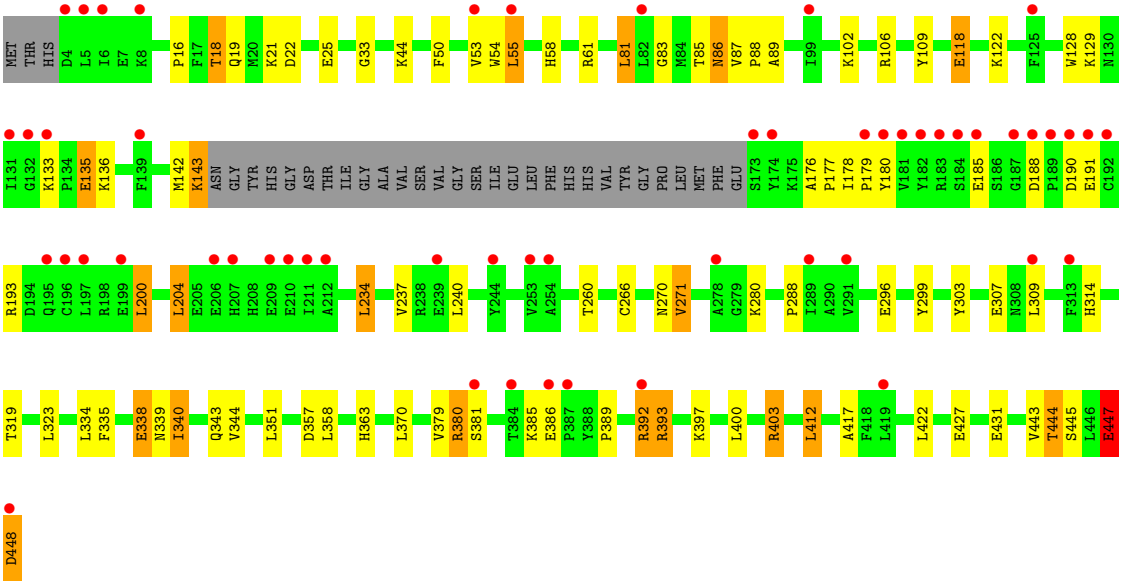
• Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase

Chain A:



• Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.67Å 104.03Å 73.87Å 90.00° 105.38° 90.00°	Depositor
Resolution (Å)	35.00 – 1.90 37.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (35.00-1.90) 98.4 (37.99-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.240 0.204 , 0.244	Depositor DCC
R_{free} test set	3331 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6987	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.46	0/3372	0.64	2/4548 (0.0%)
1	B	0.45	1/3349 (0.0%)	0.63	5/4517 (0.1%)
All	All	0.46	1/6721 (0.0%)	0.64	7/9065 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	447	GLU	C-N	5.14	1.45	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	447	GLU	CA-C-N	6.51	131.53	117.20
1	B	393	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	55	LEU	CA-CB-CG	6.20	129.57	115.30
1	A	393	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	447	GLU	C-N-CA	-5.85	107.06	121.70
1	B	447	GLU	O-C-N	-5.84	113.36	122.70
1	A	183	ARG	NE-CZ-NH1	5.74	123.17	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	447	GLU	Mainchain

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	3295	0	3280	82	0
1	B	3278	0	3268	82	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
3	A	199	0	0	12	0
3	B	185	0	0	11	0
All	All	6987	0	6562	158	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 12.

All (158) 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:383:GLU:HB3	3:A:699:HOH:O	1.58	1.02
1:B:443:VAL:HG13	1:B:448:ASP:OD1	1.64	0.96
1:B:234:LEU:HD13	1:B:271:VAL:HG11	1.46	0.94
1:B:397:LYS:HD3	1:B:448:ASP:HB2	1.53	0.91
1:B:447:GLU:HG3	3:B:682:HOH:O	1.72	0.88
1:B:363:HIS:CD2	1:B:444:THR:HG23	2.16	0.81
1:B:19:GLN:HE21	1:B:21:LYS:H	1.27	0.80
1:A:16:PRO:O	1:A:18:THR:HG22	1.86	0.75
1:B:335:PHE:HA	1:B:340:ILE:HG13	1.69	0.74
1:B:363:HIS:HD2	1:B:444:THR:HG23	1.52	0.74
1:A:393:ARG:CD	3:A:599:HOH:O	2.35	0.74
1:B:447:GLU:HA	1:B:447:GLU:OE1	1.87	0.73
1:B:447:GLU:O	1:B:448:ASP:C	2.27	0.73
1:A:83:GLY:H	1:B:18:THR:HG21	1.51	0.72
1:B:190:ASP:HB2	1:B:193:ARG:CZ	2.21	0.71
1:A:363:HIS:CD2	1:A:444:THR:HG23	2.26	0.70
1:A:195:GLN:OE1	1:A:198:ARG:NH2	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HA	1:A:103:LYS:HE2	1.72	0.70
1:B:190:ASP:HB2	1:B:193:ARG:NH2	2.05	0.69
1:A:393:ARG:HD3	3:A:599:HOH:O	1.92	0.67
1:A:363:HIS:HB2	1:A:444:THR:HG21	1.76	0.67
1:A:21:LYS:O	1:A:25:GLU:HG2	1.95	0.67
1:A:19:GLN:HE21	1:A:21:LYS:H	1.42	0.67
1:A:56:ASN:HD21	1:A:59:GLY:CA	2.09	0.64
1:A:16:PRO:O	1:A:18:THR:CG2	2.44	0.64
1:B:188:ASP:HB3	1:B:191:GLU:HB2	1.78	0.64
1:A:208:HIS:HD2	3:A:683:HOH:O	1.80	0.64
1:A:56:ASN:HD21	1:A:59:GLY:H	1.46	0.63
1:B:381:SER:O	1:B:385:LYS:HA	1.98	0.63
1:A:183:ARG:HH11	1:A:183:ARG:HG3	1.64	0.62
1:B:397:LYS:CD	1:B:448:ASP:HB2	2.28	0.62
1:A:18:THR:HG21	1:B:83:GLY:H	1.66	0.61
1:A:86:ASN:ND2	1:A:89:ALA:H	1.99	0.61
1:A:384:THR:CG2	1:A:386:GLU:HB2	2.30	0.61
1:B:380:ARG:HD2	1:B:386:GLU:OE2	2.01	0.60
1:A:384:THR:HG21	1:A:386:GLU:HB2	1.83	0.60
1:A:393:ARG:HD2	3:A:599:HOH:O	1.99	0.60
1:A:56:ASN:HD21	1:A:59:GLY:N	1.99	0.60
1:B:44:LYS:HE2	3:B:573:HOH:O	2.00	0.60
1:B:427:GLU:O	1:B:431:GLU:HG3	2.01	0.60
1:A:403:ARG:CD	3:A:611:HOH:O	2.50	0.60
1:B:380:ARG:HD2	1:B:386:GLU:CD	2.22	0.59
1:A:403:ARG:HD2	3:A:611:HOH:O	2.03	0.59
1:B:25:GLU:HG2	3:B:588:HOH:O	2.02	0.59
1:A:87:VAL:HB	1:A:88:PRO:HD3	1.84	0.58
1:B:266:CYS:HB2	1:B:271:VAL:HG13	1.86	0.58
1:B:133:LYS:HA	1:B:135:GLU:OE2	2.03	0.58
1:B:447:GLU:CG	3:B:682:HOH:O	2.41	0.58
1:B:86:ASN:ND2	1:B:89:ALA:H	2.01	0.58
1:A:143:LYS:HE3	1:A:175:LYS:HB3	1.86	0.58
1:A:91:GLN:NE2	3:A:633:HOH:O	2.37	0.57
1:B:33:GLY:O	1:B:61:ARG:HD3	2.05	0.56
1:B:109:TYR:HB2	1:B:319:THR:HG23	1.88	0.56
1:B:106:ARG:HD3	1:B:296:GLU:OE1	2.06	0.56
1:A:83:GLY:N	1:B:18:THR:HG21	2.21	0.56
1:A:314:HIS:HE1	3:A:561:HOH:O	1.88	0.55
1:B:143:LYS:HE2	1:B:177:PRO:HA	1.88	0.55
1:A:63:LYS:HD3	3:A:628:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASN:ND2	1:A:59:GLY:H	2.05	0.55
1:B:393:ARG:HD2	3:B:622:HOH:O	2.07	0.55
1:B:19:GLN:NE2	1:B:21:LYS:H	2.03	0.54
1:B:200:LEU:HD22	1:B:204:LEU:HD22	1.90	0.53
1:A:335:PHE:O	1:A:339:ASN:HA	2.08	0.53
1:A:106:ARG:HD3	1:A:296:GLU:OE1	2.09	0.53
1:A:139:PHE:CE2	1:A:173:SER:HB3	2.44	0.53
1:B:16:PRO:O	1:B:18:THR:CG2	2.57	0.52
1:B:86:ASN:HD21	1:B:89:ALA:H	1.57	0.52
1:B:363:HIS:CD2	1:B:444:THR:CG2	2.91	0.52
1:B:58:HIS:CE1	1:B:340:ILE:CD1	2.93	0.52
1:B:204:LEU:HD23	1:B:240:LEU:HB3	1.90	0.52
1:A:60:HIS:HD2	3:B:599:HOH:O	1.92	0.52
1:A:86:ASN:HD21	1:A:89:ALA:H	1.58	0.52
1:A:128:TRP:CD2	1:A:136:LYS:HD2	2.45	0.51
1:A:440:ILE:O	1:A:444:THR:HB	2.10	0.51
1:B:443:VAL:CG1	1:B:448:ASP:OD1	2.47	0.50
1:B:86:ASN:HD22	1:B:86:ASN:C	2.14	0.50
1:A:86:ASN:C	1:A:86:ASN:HD22	2.14	0.50
1:B:393:ARG:CD	3:B:622:HOH:O	2.59	0.50
1:B:86:ASN:ND2	1:B:88:PRO:HD2	2.26	0.50
1:B:338:GLU:HB3	1:B:340:ILE:HG12	1.94	0.50
1:A:311:THR:HB	1:A:313[A]:PHE:CZ	2.47	0.49
1:A:19:GLN:HE22	1:B:303:TYR:HA	1.77	0.49
1:B:58:HIS:HE1	1:B:340:ILE:CD1	2.25	0.49
1:B:87:VAL:HB	1:B:88:PRO:HD3	1.95	0.49
1:B:338:GLU:O	1:B:343:GLN:NE2	2.42	0.49
1:A:86:ASN:ND2	1:A:88:PRO:HD2	2.28	0.49
1:A:106:ARG:HG3	1:A:299:TYR:CD1	2.48	0.49
1:A:178:ILE:CG2	1:A:179:PRO:HD2	2.43	0.49
1:A:183:ARG:HH11	1:A:183:ARG:CG	2.26	0.48
1:B:334:LEU:O	1:B:338:GLU:HB2	2.13	0.48
1:B:389:PRO:HD2	1:B:392:ARG:HD3	1.95	0.48
1:A:344:VAL:HG21	1:A:422:LEU:HG	1.95	0.48
1:A:383:GLU:HG3	1:A:383:GLU:O	2.12	0.48
1:B:128:TRP:CZ2	1:B:136:LYS:HE2	2.49	0.48
1:A:363:HIS:CE1	1:A:388:TYR:OH	2.67	0.47
1:A:48:ASP:OD2	1:A:60:HIS:HE1	1.97	0.47
1:B:58:HIS:CE1	1:B:340:ILE:HD12	2.50	0.47
1:B:81:LEU:HD22	1:B:85:THR:HA	1.97	0.47
1:A:142:MET:CE	1:A:176:ALA:HB3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:O	1:A:255:THR:HG21	2.14	0.46
1:A:403:ARG:HD3	3:A:611:HOH:O	2.13	0.46
1:A:77:ALA:HA	1:A:323:LEU:HD13	1.98	0.46
1:A:282:ILE:HG23	1:A:283:THR:HG23	1.97	0.46
1:A:303:TYR:HA	1:B:19:GLN:HE22	1.79	0.46
1:A:383:GLU:O	1:A:383:GLU:CG	2.63	0.46
1:B:142:MET:SD	1:B:176:ALA:HB3	2.55	0.46
1:A:178:ILE:CG2	1:A:179:PRO:CD	2.94	0.46
1:B:270:ASN:ND2	3:B:642:HOH:O	2.48	0.46
1:A:105:THR:O	1:A:106:ARG:HD2	2.16	0.46
1:B:118:GLU:O	1:B:122:LYS:HD2	2.16	0.46
1:B:445:SER:C	1:B:447:GLU:H	2.19	0.45
1:A:358:LEU:HD22	1:A:364:VAL:HG21	1.99	0.45
1:A:54:TRP:N	1:A:54:TRP:CD1	2.84	0.45
1:A:107:VAL:HG13	1:A:291:VAL:HG13	1.98	0.45
1:B:16:PRO:O	1:B:18:THR:HG23	2.16	0.45
1:A:50:PHE:HD2	1:A:50:PHE:H	1.64	0.45
1:A:364:VAL:O	1:A:382:LYS:NZ	2.49	0.45
1:B:178:ILE:CG2	1:B:179:PRO:HD2	2.47	0.44
1:B:314:HIS:HE1	3:B:613:HOH:O	2.00	0.44
1:A:338:GLU:O	1:A:339:ASN:C	2.55	0.44
1:B:412:LEU:HD22	1:B:417:ALA:HB2	1.99	0.44
1:A:288:PRO:HG2	1:B:288:PRO:HG2	1.98	0.44
1:A:394:ILE:CD1	1:A:447:GLU:HG3	2.47	0.44
1:A:86:ASN:HD22	1:A:88:PRO:HD2	1.83	0.44
1:A:296:GLU:HG3	1:A:300:LYS:HE3	1.98	0.44
1:B:16:PRO:O	1:B:18:THR:HG22	2.18	0.44
1:B:86:ASN:HD22	1:B:88:PRO:HD2	1.81	0.44
1:B:118:GLU:HG3	1:B:122:LYS:HD2	2.00	0.43
1:A:106:ARG:HG3	1:A:299:TYR:HB2	2.00	0.43
1:B:381:SER:HB2	1:B:386:GLU:HG2	2.01	0.43
1:B:397:LYS:HD3	1:B:448:ASP:CB	2.36	0.43
1:B:54:TRP:CD1	1:B:54:TRP:N	2.85	0.43
1:B:403:ARG:CD	3:B:623:HOH:O	2.66	0.43
1:A:179:PRO:HB3	1:A:192:CYS:SG	2.59	0.43
1:A:128:TRP:HE3	1:A:133:LYS:HG3	1.84	0.42
1:B:344:VAL:HG21	1:B:422:LEU:HG	2.00	0.42
1:B:307:GLU:O	1:B:309:LEU:HD12	2.18	0.42
1:B:443:VAL:O	1:B:448:ASP:OD1	2.37	0.42
1:A:109:TYR:HB2	1:A:319:THR:HG23	2.02	0.42
1:B:381:SER:O	1:B:385:LYS:CA	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASN:HD21	1:A:59:GLY:HA2	1.83	0.41
1:A:381:SER:O	1:A:385:LYS:HA	2.19	0.41
1:B:260:THR:HB	1:B:370:LEU:HG	2.01	0.41
1:B:106:ARG:HG3	1:B:299:TYR:HB2	2.02	0.41
1:A:18:THR:HB	3:A:517:HOH:O	2.20	0.41
1:A:105:THR:C	1:A:106:ARG:HD2	2.40	0.41
1:B:190:ASP:HA	1:B:193:ARG:HB3	2.03	0.41
1:B:403:ARG:HD3	3:B:623:HOH:O	2.19	0.41
1:A:50:PHE:N	1:A:50:PHE:CD2	2.89	0.41
1:B:22:ASP:CG	1:B:393:ARG:HH22	2.23	0.41
1:A:401:LYS:HE3	1:A:404:GLU:OE1	2.21	0.41
1:B:58:HIS:CE1	1:B:340:ILE:HD11	2.54	0.41
1:B:363:HIS:HB2	1:B:444:THR:HG21	2.03	0.41
1:A:142:MET:HB2	1:A:178:ILE:HD11	2.04	0.40
1:B:178:ILE:HG22	1:B:179:PRO:HD2	2.03	0.40
1:A:262:LYS:HG2	1:A:268:HIS:CE1	2.57	0.40
1:A:300:LYS:HE2	1:A:300:LYS:HB3	1.45	0.40

There are no symmetry-related clashes.

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	415/448 (93%)	399 (96%)	14 (3%)	2 (0%)	29 18
1	B	413/448 (92%)	397 (96%)	13 (3%)	3 (1%)	22 12
All	All	828/896 (92%)	796 (96%)	27 (3%)	5 (1%)	25 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	ASN

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Mol	Chain	Res	Type
1	A	280	LYS
1	B	447	GLU
1	B	280	LYS
1	B	53	VAL

5.3.2 Protein sidechains (i)

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	355/378 (94%)	325 (92%)	30 (8%)	10 4
1	B	353/378 (93%)	321 (91%)	32 (9%)	9 3
All	All	708/756 (94%)	646 (91%)	62 (9%)	10 4

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	8	LYS
1	A	18	THR
1	A	25	GLU
1	A	50	PHE
1	A	65	LEU
1	A	86	ASN
1	A	102	LYS
1	A	133	LYS
1	A	135	GLU
1	A	143	LYS
1	A	180	TYR
1	A	183	ARG
1	A	200	LEU
1	A	203	LEU
1	A	234	LEU
1	A	262	LYS
1	A	323	LEU
1	A	339	ASN

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Mol	Chain	Res	Type
1	A	351	LEU
1	A	358	LEU
1	A	380	ARG
1	A	382	LYS
1	A	385	LYS
1	A	401	LYS
1	A	403	ARG
1	A	405	LEU
1	A	412	LEU
1	A	422	LEU
1	A	444	THR
1	B	18	THR
1	B	50	PHE
1	B	55	LEU
1	B	81	LEU
1	B	86	ASN
1	B	102	LYS
1	B	118	GLU
1	B	129	LYS
1	B	135	GLU
1	B	143	LYS
1	B	180	TYR
1	B	185	GLU
1	B	200	LEU
1	B	204	LEU
1	B	234	LEU
1	B	237	VAL
1	B	271	VAL
1	B	323	LEU
1	B	338	GLU
1	B	339	ASN
1	B	340	ILE
1	B	351	LEU
1	B	357	ASP
1	B	358	LEU
1	B	379	VAL
1	B	380	ARG
1	B	392	ARG
1	B	400	LEU
1	B	403	ARG
1	B	412	LEU
1	B	444	THR

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Mol	Chain	Res	Type
1	B	448	ASP

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	19	GLN
1	A	42	ASN
1	A	56	ASN
1	A	60	HIS
1	A	86	ASN
1	A	91	GLN
1	A	126	GLN
1	A	321	ASN
1	A	363	HIS
1	B	19	GLN
1	B	42	ASN
1	B	86	ASN
1	B	137	GLN
1	B	331	ASN
1	B	339	ASN
1	B	359	HIS
1	B	363	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLP	A	501	1	15,15,16	0.94	2 (13%)	20,22,23	1.17	1 (5%)
2	PLP	B	502	1	15,15,16	1.02	1 (6%)	20,22,23	1.09	2 (10%)

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	B	502	1	-	0/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	PLP	C2-N1	2.46	1.38	1.33
2	A	501	PLP	C2-N1	2.15	1.37	1.33
2	A	501	PLP	C6-N1	2.01	1.38	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	PLP	O4P-C5A-C5	3.36	115.75	109.35
2	B	502	PLP	C6-C5-C4	2.14	119.84	118.16
2	B	502	PLP	O4P-C5A-C5	2.06	113.27	109.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	417/448 (93%)	0.26	11 (2%) 56 58	34, 44, 60, 81	4 (0%)
1	B	416/448 (92%)	0.73	54 (12%) 3 3	35, 47, 70, 85	2 (0%)
All	All	833/896 (92%)	0.49	65 (7%) 13 14	34, 46, 65, 85	6 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	CYS	7.3
1	A	5	LEU	4.9
1	B	190	ASP	4.4
1	B	4	ASP	4.2
1	A	313[A]	PHE	4.2
1	B	196	CYS	4.2
1	B	125	PHE	4.1
1	B	5	LEU	4.0
1	B	392	ARG	3.8
1	B	188	ASP	3.8
1	B	381	SER	3.8
1	B	191	GLU	3.7
1	A	384	THR	3.7
1	B	448	ASP	3.6
1	B	187	GLY	3.5
1	B	185	GLU	3.5
1	A	3	HIS	3.4
1	B	197	LEU	3.4
1	B	173	SER	3.4
1	B	180	TYR	3.3
1	B	384	THR	3.2
1	B	183	ARG	3.2
1	B	207	HIS	3.2
1	B	195	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	181	VAL	3.2
1	B	253	VAL	3.1
1	B	132	GLY	3.1
1	B	309	LEU	3.1
1	B	313[A]	PHE	3.0
1	B	184	SER	3.0
1	B	139	PHE	3.0
1	B	131	ILE	3.0
1	B	174	TYR	2.9
1	B	211	ILE	2.9
1	B	210	GLU	2.8
1	B	387	PRO	2.8
1	A	290	ALA	2.8
1	B	206	GLU	2.8
1	B	289	ILE	2.8
1	B	189	PRO	2.7
1	B	179	PRO	2.7
1	B	133	LYS	2.6
1	A	125[A]	PHE	2.5
1	B	53	VAL	2.5
1	B	82	LEU	2.4
1	A	277	ALA	2.4
1	B	419	LEU	2.4
1	B	278	ALA	2.4
1	B	55	LEU	2.3
1	B	254	ALA	2.3
1	B	199	GLU	2.3
1	B	386	GLU	2.3
1	A	8	LYS	2.3
1	B	209	GLU	2.3
1	B	291	VAL	2.2
1	B	182	TYR	2.2
1	B	244	TYR	2.2
1	B	239	GLU	2.2
1	A	287	LEU	2.1
1	B	99	ILE	2.1
1	B	212	ALA	2.1
1	A	191	GLU	2.1
1	A	53	VAL	2.0
1	B	6	ILE	2.0
1	B	8	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLP	A	501	15/16	0.94	0.13	38,42,46,47	0
2	PLP	B	502	15/16	0.95	0.13	37,42,45,46	0

6.5 Other polymers (i)

There are no such residues in this entry.