



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:39 PM UTC

PDB ID : 1ART / pdb_00001art
Title : X-RAY CRYSTALLOGRAPHIC STUDY OF PYRIDOXAL 5'-
PHOSPHATE-TYPE ASPARTATE AMINOTRANSFERASES FROM
ESCHERICHIA COLI IN OPEN AND CLOSED FORM
Authors : Okamoto, A.; Higuchi, T.; Hirotsu, K.
Deposited on : 1993-08-02
Resolution : 1.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

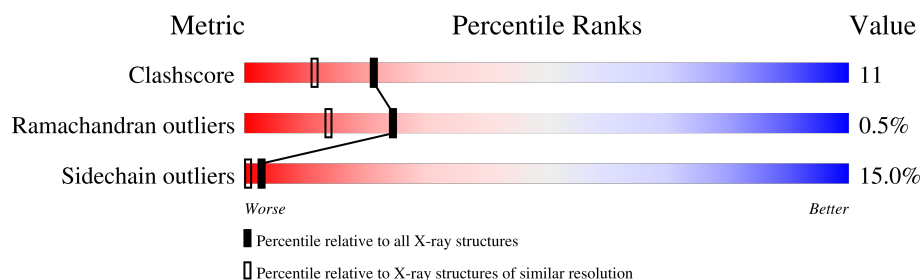
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3226 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 ASPARTATE AMINOTRANSFERASE.

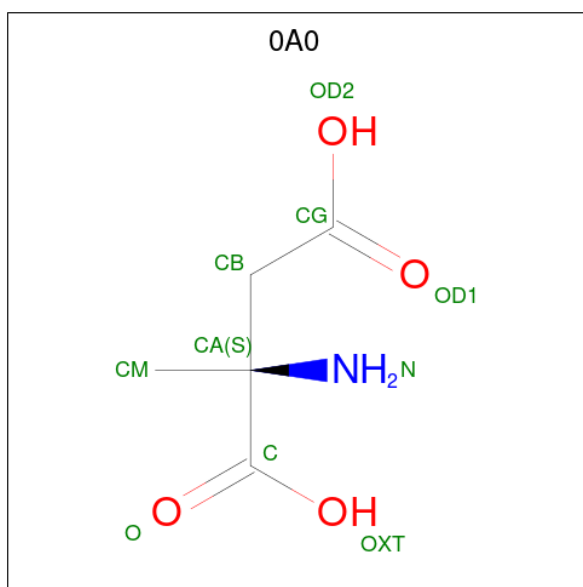
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3069	1936	536	584	13	0	0	0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 3 is 2-methyl-L-aspartic acid (CCD ID: 0A0) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is water.

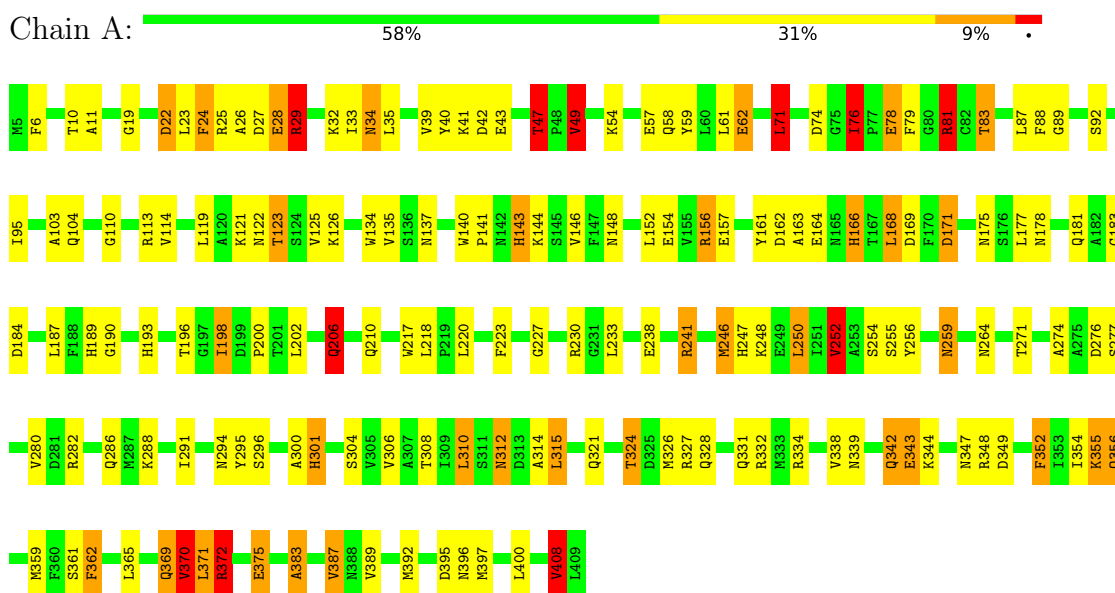
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	157.14Å 85.51Å 78.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.217 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3226	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

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: 0A0, 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	1.17	13/3130 (0.4%)	1.96	96/4240 (2.3%)

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	A	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	THR	CA-CB	8.02	1.64	1.53
1	A	76	ILE	CA-CB	7.46	1.64	1.53
1	A	49	VAL	CA-CB	7.25	1.63	1.54
1	A	247	HIS	CD2-NE2	-7.17	1.29	1.37
1	A	143	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	166	HIS	CD2-NE2	-6.89	1.30	1.37
1	A	301	HIS	CD2-NE2	-6.78	1.30	1.37
1	A	146	VAL	CA-CB	6.52	1.62	1.54
1	A	193	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	189	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	370	VAL	CA-CB	5.45	1.61	1.54
1	A	252	VAL	CA-CB	5.32	1.61	1.54
1	A	166	HIS	CG-ND1	-5.07	1.32	1.38

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ASP	CA-CB-CG	11.26	123.86	112.60
1	A	288	LYS	CB-CG-CD	-8.86	90.93	111.30
1	A	348	ARG	CB-CG-CD	-8.84	90.98	111.30
1	A	140	TRP	CG-CD2-CE3	8.83	142.73	133.90
1	A	342	GLN	OE1-CD-NE2	-8.28	114.32	122.60
1	A	137	ASN	CA-CB-CG	-8.23	104.37	112.60
1	A	359	MET	N-CA-C	7.89	122.95	113.16
1	A	42	ASP	CA-CB-CG	7.89	120.49	112.60
1	A	301	HIS	N-CA-C	7.83	120.51	111.11
1	A	175	ASN	CA-CB-CG	-7.81	104.79	112.60
1	A	286	GLN	OE1-CD-NE2	-7.71	114.89	122.60
1	A	396	ASN	CA-CB-CG	7.52	120.12	112.60
1	A	47	THR	CA-C-O	7.21	127.15	120.09
1	A	78	GLU	CA-CB-CG	7.17	128.43	114.10
1	A	250	LEU	CB-CA-C	-7.11	97.40	110.62
1	A	22	ASP	N-CA-C	7.06	118.63	111.07
1	A	22	ASP	CA-C-O	-7.05	113.42	120.82
1	A	76	ILE	CB-CA-C	7.04	117.48	110.94
1	A	22	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	58	GLN	CA-CB-CG	-6.93	100.25	114.10
1	A	259	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	A	206	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	34	ASN	CB-CG-ND2	6.69	126.43	116.40
1	A	259	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	183	GLY	CA-C-N	-6.60	111.24	123.05
1	A	183	GLY	C-N-CA	-6.60	111.24	123.05
1	A	206	GLN	CB-CG-CD	6.54	123.71	112.60
1	A	11	ALA	N-CA-C	-6.41	98.45	108.90
1	A	342	GLN	CB-CG-CD	6.38	123.45	112.60
1	A	29	ARG	N-CA-CB	6.38	121.72	110.37
1	A	113	ARG	CA-C-O	-6.36	114.15	120.70
1	A	383	ALA	N-CA-C	6.22	119.97	112.38
1	A	71	LEU	O-C-N	-6.20	113.90	122.46
1	A	28	GLU	N-CA-C	-6.14	101.37	110.46
1	A	408	VAL	N-CA-CB	-6.14	101.10	111.23
1	A	321	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	A	122	ASN	CA-CB-CG	-6.11	106.49	112.60
1	A	154	GLU	CB-CG-CD	6.10	122.97	112.60
1	A	162	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	123	THR	N-CA-CB	-6.06	101.80	111.62
1	A	163	ALA	N-CA-C	6.06	118.38	111.11
1	A	300	ALA	N-CA-C	5.97	117.46	111.07
1	A	387	VAL	N-CA-CB	-5.93	103.22	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	A	372	ARG	CA-C-O	-5.89	113.70	120.24
1	A	148	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	375	GLU	N-CA-C	5.85	117.66	111.28
1	A	103	ALA	N-CA-C	-5.83	99.39	108.90
1	A	89	GLY	N-CA-C	-5.82	104.38	112.18
1	A	29	ARG	N-CA-C	-5.80	96.99	109.81
1	A	359	MET	CA-CB-CG	5.80	125.70	114.10
1	A	41	LYS	CA-CB-CG	-5.80	102.50	114.10
1	A	343	GLU	CA-CB-CG	5.77	125.63	114.10
1	A	81	ARG	CG-CD-NE	5.76	124.68	112.00
1	A	246	MET	CG-SD-CE	5.75	113.54	100.90
1	A	395	ASP	N-CA-C	5.74	118.75	111.69
1	A	348	ARG	N-CA-CB	-5.74	101.57	110.29
1	A	140	TRP	CB-CG-CD1	-5.73	118.31	126.90
1	A	134	TRP	CE2-CD2-CG	-5.69	100.37	107.20
1	A	247	HIS	CB-CG-CD2	-5.64	123.86	131.20
1	A	342	GLN	O-C-N	-5.64	115.72	122.15
1	A	294	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	276	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	78	GLU	CB-CA-C	-5.49	101.67	110.79
1	A	348	ARG	CD-NE-CZ	-5.49	116.72	124.40
1	A	74	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	339	ASN	N-CA-C	5.43	116.88	111.07
1	A	22	ASP	O-C-N	-5.40	116.51	122.07
1	A	6	PHE	N-CA-C	5.39	119.86	113.28
1	A	169	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	241	ARG	CG-CD-NE	5.36	123.80	112.00
1	A	39	VAL	N-CA-C	-5.36	100.35	108.17
1	A	328	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	A	29	ARG	CA-CB-CG	5.31	124.72	114.10
1	A	171	ASP	N-CA-C	5.30	117.49	111.02
1	A	230	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	A	24	PHE	N-CA-C	-5.28	105.60	111.36
1	A	259	ASN	CB-CG-ND2	5.23	124.25	116.40
1	A	372	ARG	CB-CG-CD	-5.22	99.29	111.30
1	A	178	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	217	TRP	CG-CD1-NE1	-5.20	103.44	110.20
1	A	356	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	88	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	241	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	A	371	LEU	N-CA-C	-5.17	105.73	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	GLN	CA-C-O	-5.16	114.95	120.42
1	A	250	LEU	N-CA-CB	5.15	119.55	111.56
1	A	276	ASP	O-C-N	-5.12	117.94	123.42
1	A	264	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	352	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	157	GLU	N-CA-C	5.08	117.69	109.40
1	A	371	LEU	CA-C-N	-5.08	111.89	120.58
1	A	371	LEU	C-N-CA	-5.08	111.89	120.58
1	A	104	GLN	N-CA-C	-5.06	101.71	109.76
1	A	392	MET	CG-SD-CE	-5.05	89.78	100.90
1	A	156	ARG	CA-CB-CG	-5.05	104.00	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	ARG	Sidechain

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	3069	0	3018	67	0
2	A	15	0	6	0	0
3	A	10	0	6	0	0
4	A	132	0	0	7	0
All	All	3226	0	3030	67	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 11.

All (67) 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:372:ARG:HD2	1:A:408:VAL:HG22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASN:ND2	1:A:315:LEU:H	1.91	0.67
1:A:143:HIS:HB2	1:A:144:LYS:HD3	1.78	0.65
1:A:397:MET:HE3	1:A:397:MET:HA	1.78	0.65
1:A:123:THR:HG22	1:A:125:VAL:H	1.62	0.65
1:A:76:ILE:HD13	1:A:79:PHE:H	1.63	0.63
1:A:78:GLU:HG3	4:A:541:HOH:O	1.99	0.62
1:A:28:GLU:O	1:A:29:ARG:HB3	2.00	0.61
1:A:356:GLN:NE2	1:A:361:SER:HA	2.16	0.60
1:A:202:LEU:HD13	1:A:238:GLU:HG2	1.84	0.59
1:A:23:LEU:HB2	4:A:540:HOH:O	2.01	0.59
1:A:352:PHE:HA	1:A:355:LYS:HE2	1.85	0.58
1:A:327:ARG:HG2	1:A:331:GLN:HE21	1.67	0.58
1:A:370:VAL:HG21	1:A:383:ALA:HA	1.86	0.58
1:A:40:TYR:O	1:A:47:THR:HB	2.04	0.57
1:A:141:PRO:O	1:A:144:LYS:HG2	2.05	0.57
1:A:356:GLN:HE22	1:A:362:PHE:H	1.51	0.56
1:A:166:HIS:HB3	4:A:511:HOH:O	2.06	0.55
1:A:190:GLY:HA3	1:A:223:PHE:CD1	2.42	0.55
1:A:375:GLU:HG2	4:A:464:HOH:O	2.06	0.55
1:A:92:SER:HB3	1:A:95:ILE:HD12	1.88	0.55
1:A:19:GLY:O	1:A:22:ASP:HB3	2.08	0.54
1:A:338:VAL:O	1:A:342:GLN:HG2	2.07	0.54
1:A:371:LEU:O	1:A:375:GLU:HG3	2.08	0.53
1:A:312:ASN:HD22	1:A:315:LEU:H	1.55	0.53
1:A:57:GLU:OE2	1:A:301:HIS:HE1	1.93	0.52
1:A:327:ARG:O	1:A:331:GLN:HG3	2.11	0.51
1:A:356:GLN:HE22	1:A:361:SER:HA	1.76	0.51
1:A:210:GLN:OE1	1:A:246:MET:HE2	2.11	0.50
1:A:24:PHE:CE1	1:A:34:ASN:HB2	2.47	0.50
1:A:29:ARG:O	1:A:32:LYS:HG3	2.13	0.49
1:A:71:LEU:HB2	4:A:524:HOH:O	2.12	0.49
1:A:314:ALA:HB3	4:A:429:HOH:O	2.13	0.49
1:A:334:ARG:HB3	1:A:389:VAL:HG11	1.95	0.49
1:A:306:VAL:O	1:A:310:LEU:HB2	2.12	0.49
1:A:304:SER:O	1:A:308:THR:HG23	2.12	0.49
1:A:227:GLY:O	1:A:327:ARG:HD3	2.12	0.48
1:A:397:MET:CE	1:A:400:LEU:HD22	2.43	0.48
1:A:312:ASN:HD21	1:A:314:ALA:HB3	1.79	0.47
1:A:202:LEU:O	1:A:206:GLN:HG2	2.13	0.47
1:A:33:ILE:HG22	1:A:35:LEU:HD13	1.96	0.47
1:A:83:THR:HB	1:A:256:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HG22	1:A:54:LYS:HG2	1.97	0.46
1:A:119:LEU:O	1:A:123:THR:HB	2.15	0.45
1:A:81:ARG:HH11	1:A:81:ARG:HG3	1.82	0.45
1:A:143:HIS:CB	1:A:144:LYS:HD3	2.47	0.45
1:A:144:LYS:HD3	1:A:144:LYS:N	2.32	0.44
1:A:223:PHE:O	1:A:254:SER:HA	2.17	0.44
1:A:277:SER:HA	1:A:280:VAL:HG12	1.99	0.43
1:A:252:VAL:HG13	1:A:271:THR:HB	2.00	0.42
1:A:324:THR:HB	1:A:327:ARG:NH2	2.34	0.42
1:A:312:ASN:HD22	1:A:315:LEU:N	2.16	0.42
1:A:27:ASP:HB3	1:A:32:LYS:HD3	2.01	0.42
1:A:59:TYR:O	1:A:62:GLU:HG2	2.19	0.42
1:A:40:TYR:CD2	1:A:326:MET:HE2	2.55	0.41
1:A:291:ILE:HG23	1:A:295:TYR:CE1	2.55	0.41
1:A:349:ASP:HB3	4:A:537:HOH:O	2.20	0.41
1:A:144:LYS:N	1:A:144:LYS:CD	2.83	0.41
1:A:196:THR:O	1:A:198:ILE:HD12	2.19	0.41
1:A:274:ALA:HB3	1:A:280:VAL:HB	2.03	0.41
1:A:87:LEU:O	1:A:241:ARG:NH1	2.54	0.41
1:A:161:TYR:CE1	1:A:198:ILE:HD13	2.56	0.41
1:A:168:LEU:HD11	1:A:200:PRO:HG3	2.02	0.41
1:A:177:LEU:HA	1:A:177:LEU:HD23	1.78	0.40
1:A:25:ARG:HG3	1:A:26:ALA:N	2.34	0.40
1:A:110:GLY:O	1:A:114:VAL:HG13	2.21	0.40
1:A:369:GLN:HG2	1:A:408:VAL:HG13	2.03	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	394/396 (100%)	371 (94%)	21 (5%)	2 (0%)	24 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	43	GLU

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	320/320 (100%)	272 (85%)	48 (15%)	3 0

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	29	ARG
1	A	47	THR
1	A	49	VAL
1	A	61	LEU
1	A	62	GLU
1	A	71	LEU
1	A	76	ILE
1	A	81	ARG
1	A	83	THR
1	A	121	LYS
1	A	126	LYS
1	A	135	VAL
1	A	152	LEU
1	A	156	ARG
1	A	164	GLU
1	A	168	LEU
1	A	171	ASP
1	A	181	GLN
1	A	187	LEU
1	A	198	ILE
1	A	206	GLN
1	A	218	LEU

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Mol	Chain	Res	Type
1	A	220	LEU
1	A	233	LEU
1	A	248	LYS
1	A	250	LEU
1	A	252	VAL
1	A	255	SER
1	A	259	ASN
1	A	282	ARG
1	A	296	SER
1	A	310	LEU
1	A	312	ASN
1	A	315	LEU
1	A	324	THR
1	A	332	ARG
1	A	343	GLU
1	A	344	LYS
1	A	347	ASN
1	A	354	ILE
1	A	355	LYS
1	A	362	PHE
1	A	365	LEU
1	A	370	VAL
1	A	372	ARG
1	A	387	VAL
1	A	408	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	84	GLN
1	A	148	ASN
1	A	166	HIS
1	A	204	GLN
1	A	247	HIS
1	A	259	ASN
1	A	297	ASN
1	A	301	HIS
1	A	312	ASN
1	A	321	GLN
1	A	331	GLN
1	A	356	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	413	3	15,15,16	1.59	2 (13%)	21,22,23	1.40	4 (19%)
3	0A0	A	414	2	6,9,9	1.38	1 (16%)	9,13,13	1.88	5 (55%)

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	413	3	-	0/6/6/8	0/1/1/1
3	0A0	A	414	2	-	4/11/11/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	413	PLP	C3-C2	-3.90	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	413	PLP	C3-C4	-2.14	1.36	1.40
3	A	414	0A0	OD2-CG	-2.13	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	414	0A0	CM-CA-CB	-3.60	105.77	110.82
2	A	413	PLP	O2P-P-O4P	-2.92	99.05	106.67
2	A	413	PLP	C5-C6-N1	-2.82	119.24	123.83
2	A	413	PLP	C6-C5-C4	2.54	120.18	118.10
3	A	414	0A0	CB-CA-C	2.23	112.16	109.10
2	A	413	PLP	O4P-P-O1P	2.19	112.36	106.44
3	A	414	0A0	CA-CB-CG	2.05	118.01	114.31
3	A	414	0A0	OXT-C-CA	2.03	119.85	113.77
3	A	414	0A0	O-C-CA	-2.01	119.17	122.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	414	0A0	O-C-CA-CB
3	A	414	0A0	OXT-C-CA-CB
3	A	414	0A0	N-CA-CB-CG
3	A	414	0A0	C-CA-CB-CG

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.