



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:21 PM UTC

PDB ID : 1ARS / pdb_00001ars
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

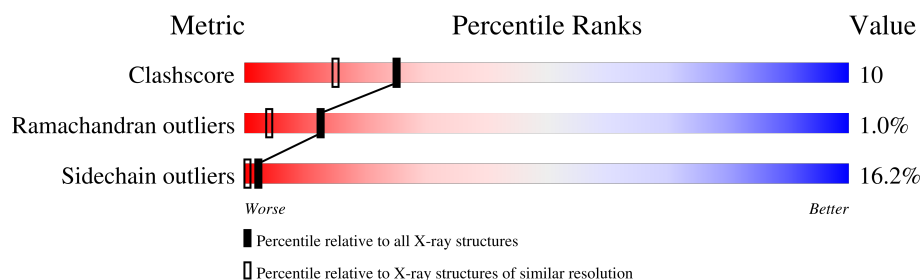
1 Overall quality at a glance

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](#)

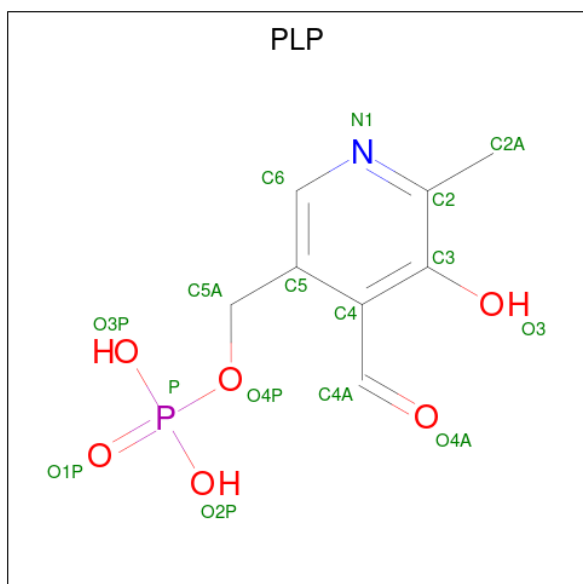
There are 3 unique types of molecules in this entry. The entry contains 3211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	396	Total	C	N	O	S	0	0	0
			3069	1936	536	584	13			

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



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

- Molecule 3 is water.

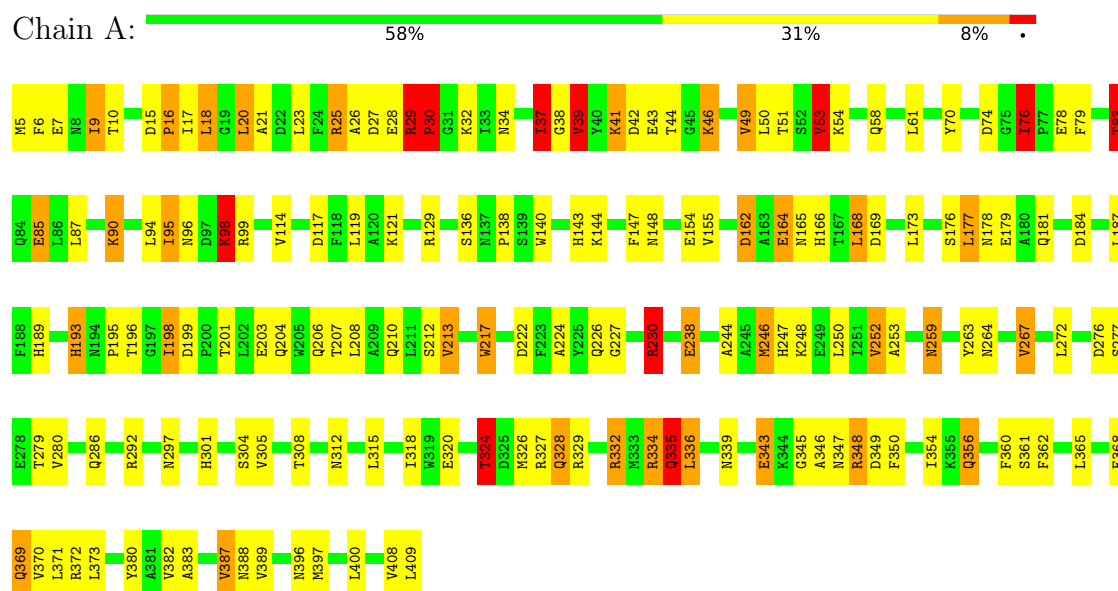
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		

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	155.42Å 87.13Å 79.40Å 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}	0.213 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3211	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.16	16/3130 (0.5%)	1.96	103/4240 (2.4%)

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	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	ILE	CA-CB	8.86	1.65	1.54
1	A	198	ILE	CA-CB	8.06	1.64	1.54
1	A	247	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	143	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	267	VAL	CA-CB	6.52	1.62	1.54
1	A	193	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	230	ARG	CA-CB	-6.25	1.43	1.53
1	A	301	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	189	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	53	VAL	CA-CB	5.92	1.62	1.54
1	A	252	VAL	CA-CB	5.84	1.62	1.54
1	A	114	VAL	CA-CB	5.59	1.62	1.54
1	A	166	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	324	THR	CA-CB	5.41	1.62	1.53
1	A	280	VAL	CA-CB	5.37	1.61	1.54
1	A	83	THR	CA-CB	5.24	1.61	1.53

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ILE	N-CA-C	11.45	126.97	111.17
1	A	230	ARG	CB-CG-CD	-10.97	86.06	111.30
1	A	29	ARG	CA-CB-CG	10.93	135.96	114.10
1	A	29	ARG	O-C-N	-10.61	111.71	121.36
1	A	9	ILE	N-CA-CB	-9.56	100.24	110.95
1	A	335	GLN	OE1-CD-NE2	-8.35	114.25	122.60
1	A	198	ILE	N-CA-CB	8.14	120.76	110.99
1	A	29	ARG	CB-CG-CD	8.07	129.87	111.30
1	A	343	GLU	N-CA-C	-8.05	103.05	113.12
1	A	286	GLN	OE1-CD-NE2	-7.83	114.77	122.60
1	A	320	GLU	CA-CB-CG	-7.70	98.70	114.10
1	A	312	ASN	OD1-CG-ND2	-7.69	114.91	122.60
1	A	335	GLN	CG-CD-NE2	7.69	127.93	116.40
1	A	148	ASN	CB-CG-ND2	7.68	127.92	116.40
1	A	54	LYS	CA-CB-CG	-7.60	98.89	114.10
1	A	9	ILE	CB-CA-C	7.55	119.92	111.08
1	A	37	ILE	O-C-N	-7.52	114.30	121.90
1	A	178	ASN	OD1-CG-ND2	-7.51	115.09	122.60
1	A	34	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	A	147	PHE	CA-CB-CG	-7.37	106.43	113.80
1	A	98	LYS	CG-CD-CE	7.26	127.99	111.30
1	A	246	MET	N-CA-CB	-7.25	99.87	110.53
1	A	396	ASN	CA-CB-CG	7.20	119.80	112.60
1	A	140	TRP	CG-CD2-CE3	7.19	141.09	133.90
1	A	43	GLU	CB-CG-CD	6.77	124.11	112.60
1	A	148	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	A	356	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	A	37	ILE	CA-C-O	-6.66	113.39	120.64
1	A	196	THR	N-CA-C	6.65	121.14	112.89
1	A	259	ASN	CA-CB-CG	6.65	119.25	112.60
1	A	297	ASN	OD1-CG-ND2	-6.63	115.97	122.60
1	A	53	VAL	N-CA-C	-6.54	103.13	112.35
1	A	39	VAL	N-CA-CB	-6.53	100.41	112.43
1	A	259	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	A	226	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	A	29	ARG	NH1-CZ-NH2	-6.49	110.87	119.30
1	A	184	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	279	THR	N-CA-C	-6.42	104.36	111.36
1	A	6	PHE	CA-CB-CG	6.41	120.21	113.80
1	A	162	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	206	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	A	372	ARG	CA-CB-CG	6.30	126.70	114.10
1	A	143	HIS	CB-CG-CD2	-6.27	123.04	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	NH1-CZ-NH2	-6.25	111.18	119.30
1	A	30	PRO	N-CA-C	6.14	125.11	112.47
1	A	301	HIS	N-CA-C	6.11	118.47	111.02
1	A	349	ASP	O-C-N	6.10	130.70	122.59
1	A	129	ARG	CA-CB-CG	6.09	126.28	114.10
1	A	29	ARG	N-CA-CB	-6.06	101.23	111.30
1	A	230	ARG	CD-NE-CZ	-6.04	115.94	124.40
1	A	179	GLU	CA-CB-CG	6.02	126.14	114.10
1	A	74	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	29	ARG	CA-C-O	-5.96	112.47	120.64
1	A	347	ASN	N-CA-C	-5.93	100.61	109.15
1	A	224	ALA	N-CA-C	5.89	120.46	113.28
1	A	217	TRP	CE2-CD2-CE3	5.88	124.68	118.80
1	A	264	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	A	140	TRP	CB-CG-CD1	-5.85	118.12	126.90
1	A	292	ARG	CA-CB-CG	-5.85	102.41	114.10
1	A	42	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	154	GLU	CB-CG-CD	5.80	122.46	112.60
1	A	217	TRP	CA-CB-CG	5.79	124.60	113.60
1	A	276	ASP	CA-C-O	5.70	127.54	121.45
1	A	347	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	204	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	A	349	ASP	N-CA-C	-5.62	98.82	110.80
1	A	267	VAL	CB-CA-C	5.62	118.74	110.77
1	A	238	GLU	CA-CB-CG	5.61	125.32	114.10
1	A	339	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	70	TYR	N-CA-C	5.60	118.47	110.24
1	A	53	VAL	CA-C-O	-5.59	114.05	119.92
1	A	198	ILE	CB-CA-C	-5.51	103.34	110.84
1	A	329	ARG	CA-CB-CG	-5.51	103.09	114.10
1	A	222	ASP	N-CA-C	-5.45	98.87	108.20
1	A	247	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	A	166	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	A	98	LYS	CB-CG-CD	5.42	123.76	111.30
1	A	140	TRP	CE2-CD2-CG	-5.38	100.74	107.20
1	A	334	ARG	NE-CZ-NH2	-5.37	114.37	119.20
1	A	206	GLN	CG-CD-NE2	5.35	124.43	116.40
1	A	369	GLN	CA-C-O	-5.32	114.92	120.55
1	A	252	VAL	CA-C-O	5.31	125.99	120.36
1	A	387	VAL	N-CA-CB	-5.31	102.15	111.39
1	A	328	GLN	CA-CB-CG	-5.29	103.52	114.10
1	A	267	VAL	N-CA-CB	-5.29	104.77	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	THR	CA-CB-OG1	-5.28	101.68	109.60
1	A	96	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	30	PRO	CA-CB-CG	-5.26	94.50	104.50
1	A	213	VAL	N-CA-C	-5.26	105.58	110.53
1	A	29	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	A	230	ARG	N-CA-C	5.23	121.95	110.80
1	A	301	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	A	41	LYS	CA-CB-CG	-5.17	103.77	114.10
1	A	387	VAL	CB-CA-C	5.14	118.28	110.62
1	A	253	ALA	O-C-N	-5.12	116.95	123.05
1	A	226	GLN	CG-CD-NE2	5.12	124.08	116.40
1	A	83	THR	CA-C-O	-5.11	114.56	120.24
1	A	199	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	95	ILE	N-CA-C	-5.08	105.89	110.82
1	A	349	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	332	ARG	CG-CD-NE	5.07	123.15	112.00
1	A	335	GLN	CB-CG-CD	5.07	121.21	112.60
1	A	6	PHE	O-C-N	-5.01	116.13	122.19

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	ARG	Sidechain
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	3016	59	2
2	A	15	0	6	0	0
3	A	127	0	0	3	2
All	All	3211	0	3022	59	3

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 10.

All (59) 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:98:LYS:HA	1:A:98:LYS:HZ2	1.45	0.80
1:A:370:VAL:HG21	1:A:383:ALA:HA	1.65	0.77
1:A:50:LEU:HB2	1:A:53:VAL:HG13	1.69	0.74
1:A:27:ASP:HB3	1:A:32:LYS:HD3	1.72	0.70
1:A:95:ILE:O	1:A:98:LYS:HD2	1.93	0.68
1:A:20:LEU:HD12	1:A:380:TYR:HD2	1.59	0.68
1:A:203:GLU:O	1:A:207:THR:HG23	1.95	0.67
1:A:304:SER:O	1:A:308:THR:HG23	1.95	0.66
1:A:37:ILE:HD13	1:A:41:LYS:HD2	1.78	0.65
1:A:334:ARG:HH22	1:A:361:SER:HB3	1.64	0.62
1:A:94:LEU:HD11	1:A:244:ALA:HB1	1.82	0.60
1:A:346:ALA:N	1:A:348:ARG:NH1	2.49	0.60
1:A:44:THR:HG22	1:A:46:LYS:HE3	1.84	0.58
1:A:117:ASP:O	1:A:121:LYS:HG2	2.04	0.58
1:A:335:GLN:HA	1:A:354:ILE:HD11	1.86	0.56
1:A:348:ARG:HB2	1:A:350:PHE:CD2	2.41	0.55
1:A:49:VAL:HG23	1:A:53:VAL:HG22	1.89	0.54
1:A:164:GLU:HG3	1:A:165:ASN:N	2.22	0.54
1:A:168:LEU:HD21	1:A:173:LEU:HD12	1.89	0.54
1:A:90:LYS:H	1:A:90:LYS:HD2	1.73	0.53
1:A:136:SER:OG	1:A:193:HIS:HE1	1.91	0.53
1:A:76:ILE:HD11	1:A:78:GLU:HB2	1.90	0.53
1:A:212:SER:HA	1:A:217:TRP:CD1	2.43	0.53
1:A:17:ILE:HG13	1:A:18:LEU:N	2.24	0.53
1:A:324:THR:HB	1:A:327:ARG:NH2	2.24	0.52
1:A:328:GLN:O	1:A:332:ARG:HD3	2.10	0.51
1:A:227:GLY:O	1:A:327:ARG:HD3	2.11	0.51
1:A:308:THR:HB	3:A:504:HOH:O	2.10	0.50
1:A:38:GLY:HA2	1:A:360:PHE:CZ	2.47	0.50
1:A:79:PHE:O	1:A:83:THR:HG23	2.11	0.49
1:A:334:ARG:HG2	1:A:389:VAL:HG11	1.93	0.49
1:A:356:GLN:NE2	1:A:361:SER:HB2	2.26	0.49
1:A:98:LYS:HA	1:A:98:LYS:NZ	2.22	0.49
1:A:144:LYS:HA	1:A:155:VAL:HG21	1.95	0.49
1:A:85:GLU:HG2	1:A:90:LYS:HA	1.94	0.48
1:A:58:GLN:HE22	1:A:61:LEU:HD23	1.79	0.47
1:A:336:LEU:HB3	1:A:397:MET:HE3	1.96	0.47
1:A:37:ILE:HD12	1:A:39:VAL:O	2.15	0.47
1:A:324:THR:HB	1:A:327:ARG:HH22	1.80	0.47
1:A:38:GLY:HA2	1:A:360:PHE:HZ	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:HB2	3:A:539:HOH:O	2.15	0.46
1:A:51:THR:HG23	3:A:433:HOH:O	2.15	0.46
1:A:373:LEU:CD1	1:A:408:VAL:HG21	2.46	0.45
1:A:21:ALA:O	1:A:25:ARG:HG2	2.16	0.45
1:A:17:ILE:HG13	1:A:18:LEU:H	1.82	0.44
1:A:53:VAL:HB	1:A:305:VAL:HG11	1.99	0.44
1:A:15:ASP:HA	1:A:16:PRO:HD2	1.85	0.43
1:A:50:LEU:HD21	1:A:326:MET:HE3	2.01	0.43
1:A:346:ALA:HB3	1:A:348:ARG:CZ	2.49	0.43
1:A:138:PRO:HG3	1:A:362:PHE:HE2	1.83	0.42
1:A:369:GLN:NE2	1:A:409:LEU:HA	2.34	0.42
1:A:28:GLU:HG3	1:A:29:ARG:CZ	2.49	0.42
1:A:162:ASP:HB2	1:A:169:ASP:HB2	2.00	0.42
1:A:38:GLY:N	1:A:388:ASN:HD22	2.19	0.41
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.90	0.41
1:A:230:ARG:HH12	1:A:238:GLU:CD	2.28	0.41
1:A:348:ARG:HE	1:A:350:PHE:HD2	1.68	0.41
1:A:39:VAL:HG22	1:A:263:TYR:CE1	2.56	0.40
1:A:318:ILE:HG21	1:A:318:ILE:HD13	1.92	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:437:HOH:O	3:A:495:HOH:O[6_555]	1.37	0.83
1:A:5:MET:SD	1:A:368:GLU:CG[6_555]	1.65	0.55
1:A:368:GLU:OE2	3:A:462:HOH:O[6_554]	2.19	0.01

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%)	373 (95%)	17 (4%)	4 (1%)	12 4

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	345	GLY
1	A	26	ALA
1	A	16	PRO

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%)	268 (84%)	52 (16%)	2 0

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	9	ILE
1	A	10	THR
1	A	18	LEU
1	A	20	LEU
1	A	23	LEU
1	A	25	ARG
1	A	29	ARG
1	A	30	PRO
1	A	37	ILE
1	A	39	VAL
1	A	46	LYS
1	A	49	VAL
1	A	53	VAL
1	A	76	ILE
1	A	83	THR
1	A	85	GLU

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Mol	Chain	Res	Type
1	A	87	LEU
1	A	90	LYS
1	A	98	LYS
1	A	99	ARG
1	A	119	LEU
1	A	164	GLU
1	A	168	LEU
1	A	176	SER
1	A	177	LEU
1	A	181	GLN
1	A	187	LEU
1	A	195	PRO
1	A	198	ILE
1	A	208	LEU
1	A	210	GLN
1	A	213	VAL
1	A	246	MET
1	A	248	LYS
1	A	250	LEU
1	A	252	VAL
1	A	259	ASN
1	A	267	VAL
1	A	272	LEU
1	A	277	SER
1	A	315	LEU
1	A	324	THR
1	A	335	GLN
1	A	336	LEU
1	A	343	GLU
1	A	348	ARG
1	A	365	LEU
1	A	371	LEU
1	A	382	VAL
1	A	387	VAL
1	A	400	LEU

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	58	GLN
1	A	63	ASN
1	A	69	ASN

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Mol	Chain	Res	Type
1	A	84	GLN
1	A	96	ASN
1	A	122	ASN
1	A	166	HIS
1	A	181	GLN
1	A	193	HIS
1	A	210	GLN
1	A	259	ASN
1	A	321	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 ⓘ

1 ligand is 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	1	15,15,16	1.62	2 (13%)	21,22,23	2.05	4 (19%)

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	1	-	2/6/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	413	PLP	C3-C2	-4.65	1.36	1.41
2	A	413	PLP	C2A-C2	2.10	1.53	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	413	PLP	O4P-C5A-C5	6.99	122.45	109.36
2	A	413	PLP	O3P-P-O4P	-2.73	99.55	106.67
2	A	413	PLP	C5A-C5-C6	-2.29	115.63	119.36
2	A	413	PLP	C5-C6-N1	-2.10	120.42	123.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	413	PLP	C4-C5-C5A-O4P
2	A	413	PLP	C6-C5-C5A-O4P

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.