



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:24 PM GMT

PDB ID : 1AKA  
Title : STRUCTURAL BASIS FOR THE CATALYTIC ACTIVITY OF ASPARTATE AMINOTRANSFERASE K258H LACKING ITS PYRIDOXAL-5'-PHOSPHATE-BINDING LYSINE RESIDUE  
Authors : Malashkevich, V.N.; Jansonius, J.N.  
Deposited on : 1994-02-28  
Resolution : 2.10 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

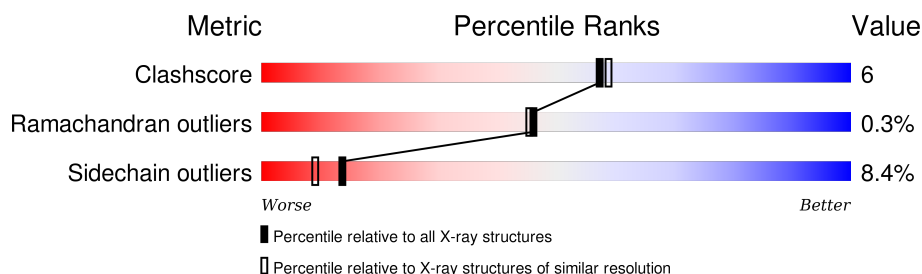
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	
1	B	401	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7011 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.

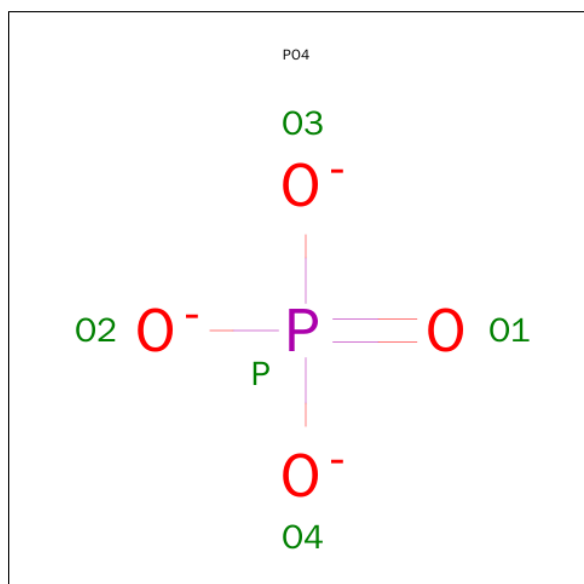
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3162	2004	559	581	18			
1	B	401	Total	C	N	O	S	0	0	0
			3162	2004	559	581	18			

There are 4 discrepancies between the modelled and reference sequences:

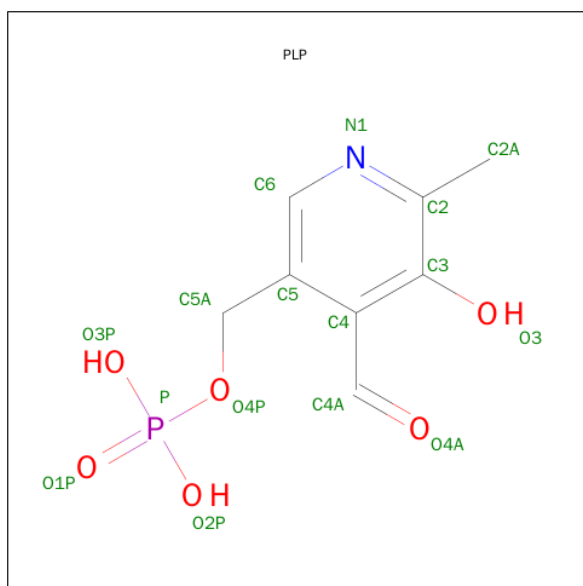
Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	SER	CONFLICT	UNP P00508
A	258	HIS	LYS	ENGINEERED MUTATION	UNP P00508
B	47	PRO	SER	CONFLICT	UNP P00508
B	258	HIS	LYS	ENGINEERED MUTATION	UNP P00508

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 4 is water.

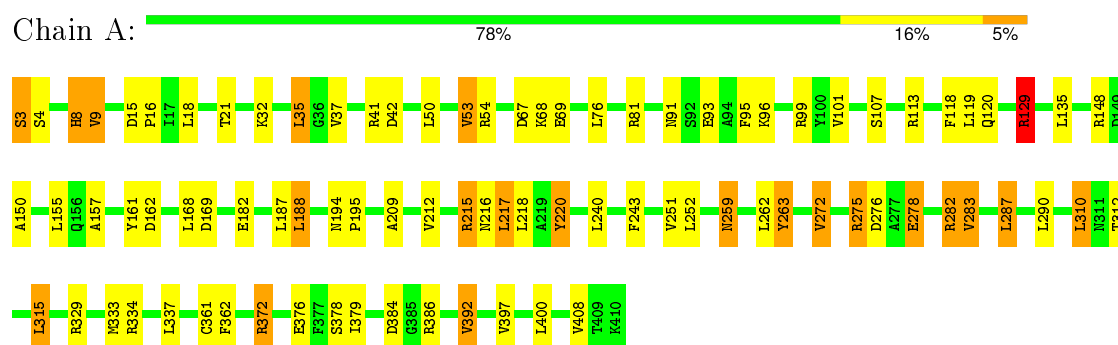
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	341	Total	O	0	0
			341	341		
4	B	325	Total	O	0	0
			325	325		

### 3 Residue-property plots

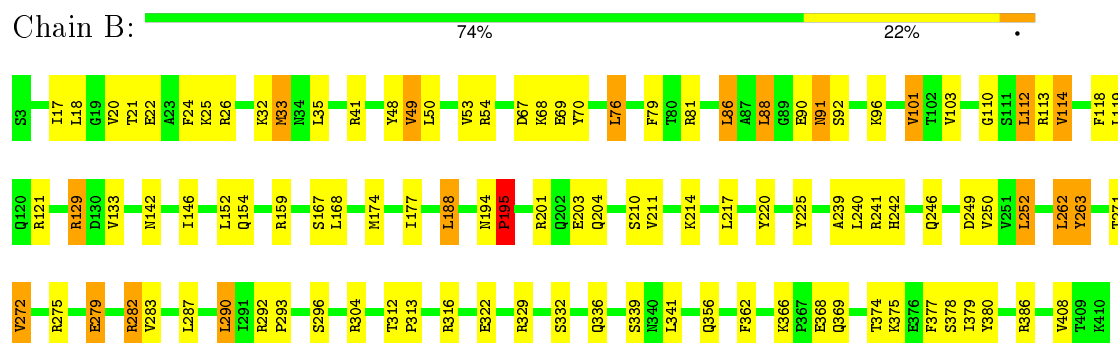
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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.

Note EDS was not executed.

#### • Molecule 1: ASPARTATE AMINOTRANSFERASE



#### • Molecule 1: ASPARTATE AMINOTRANSFERASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.87Å 58.80Å 75.81Å 85.26° 108.96° 115.57°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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: PO4, 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	0.82	0/3233	1.59	48/4364 (1.1%)
1	B	0.81	0/3233	1.53	44/4364 (1.0%)
All	All	0.81	0/6466	1.56	92/8728 (1.1%)

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ARG	NE-CZ-NH1	15.85	128.23	120.30
1	A	329	ARG	NE-CZ-NH1	12.61	126.60	120.30
1	A	54	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	B	54	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	A	329	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	B	54	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	334	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	A	41	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	B	33	MET	CA-CB-CG	9.21	128.96	113.30
1	B	81	ARG	CD-NE-CZ	9.12	136.37	123.60
1	A	148	ARG	NE-CZ-NH1	-8.95	115.82	120.30
1	B	329	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	A	67	ASP	CB-CG-OD2	-8.16	110.95	118.30
1	A	386	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	B	316	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	A	129	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	B	113	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	A	386	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	69	GLU	OE1-CD-OE2	7.64	132.46	123.30
1	B	250	VAL	N-CA-CB	-7.61	94.76	111.50
1	B	188	LEU	CA-CB-CG	7.45	132.44	115.30
1	B	282	ARG	NE-CZ-NH1	7.38	123.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	GLU	OE1-CD-OE2	-7.25	114.60	123.30
1	B	113	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	384	ASP	CB-CG-OD1	7.07	124.67	118.30
1	B	41	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	B	304	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	81	ARG	NE-CZ-NH2	6.77	123.69	120.30
1	A	69	GLU	CG-CD-OE1	-6.74	104.81	118.30
1	A	217	LEU	N-CA-CB	-6.65	97.09	110.40
1	B	49	VAL	CB-CA-C	6.50	123.75	111.40
1	A	278	GLU	CA-CB-CG	6.47	127.64	113.40
1	B	69	GLU	CG-CD-OE1	-6.46	105.38	118.30
1	B	121	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	113	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	187	LEU	CA-CB-CG	6.25	129.68	115.30
1	B	86	LEU	CA-CB-CG	6.25	129.66	115.30
1	A	41	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	239	ALA	CB-CA-C	6.14	119.31	110.10
1	A	220	TYR	CB-CG-CD1	6.12	124.67	121.00
1	B	112	LEU	CA-CB-CG	6.07	129.26	115.30
1	B	129	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	252	LEU	CA-CB-CG	6.03	129.18	115.30
1	A	278	GLU	CG-CD-OE1	5.99	130.27	118.30
1	A	93	GLU	OE1-CD-OE2	5.95	130.44	123.30
1	A	372	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	216	ASN	N-CA-CB	-5.90	99.98	110.60
1	B	81	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	B	70	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	A	53	VAL	CA-CB-CG2	5.85	119.67	110.90
1	B	356	GLN	O-C-N	5.85	132.06	122.70
1	B	159	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	81	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	B	241	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	26	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	282	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	42	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	B	121	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	322	GLU	CG-CD-OE1	5.54	129.39	118.30
1	B	67	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	8	HIS	CA-CB-CG	-5.51	104.24	113.60
1	A	182	GLU	CA-CB-CG	5.47	125.43	113.40
1	B	101	VAL	CB-CA-C	-5.45	101.05	111.40
1	A	275	ARG	NE-CZ-NH1	5.45	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	VAL	CA-CB-CG2	5.40	119.00	110.90
1	A	372	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	95	PHE	CB-CG-CD1	-5.39	117.03	120.80
1	A	278	GLU	CB-CG-CD	5.36	128.66	114.20
1	A	99	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	101	VAL	CA-CB-CG2	5.32	118.88	110.90
1	B	103	VAL	N-CA-CB	-5.30	99.83	111.50
1	A	218	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	161	TYR	CB-CG-CD2	5.29	124.17	121.00
1	B	272	VAL	CA-CB-CG1	5.29	118.83	110.90
1	B	282	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	70	TYR	CA-CB-CG	5.24	123.36	113.40
1	A	386	ARG	CD-NE-CZ	5.23	130.92	123.60
1	B	195	PRO	N-CA-C	5.23	125.70	112.10
1	A	392	VAL	CB-CA-C	5.20	121.28	111.40
1	A	67	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	279	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	A	220	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	54	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	250	VAL	CA-CB-CG1	5.08	118.52	110.90
1	B	290	LEU	CA-CB-CG	5.04	126.90	115.30
1	B	225	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	A	310	LEU	CA-CB-CG	5.03	126.88	115.30
1	A	188	LEU	CA-CB-CG	5.03	126.87	115.30
1	A	259	ASN	CB-CA-C	5.02	120.44	110.40
1	A	252	LEU	N-CA-CB	-5.02	100.36	110.40
1	B	70	TYR	CB-CG-CD1	5.02	124.01	121.00
1	B	249	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	3162	0	3148	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3162	0	3148	44	0
2	B	5	0	0	0	0
3	A	16	0	7	1	0
4	A	341	0	0	1	0
4	B	325	0	0	4	0
All	All	7011	0	6303	76	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 6.

All (76) 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:B:91:ASN:HA	1:B:96:LYS:HE2	1.59	0.84
1:B:201:ARG:H	1:B:204:GLN:HE21	1.27	0.80
1:B:292:ARG:HB3	1:B:293:PRO:HD3	1.73	0.71
1:A:50:LEU:HB2	1:A:53:VAL:HG13	1.75	0.69
1:A:8:HIS:CD2	1:A:8:HIS:H	2.08	0.68
1:A:18:LEU:HA	1:A:21:THR:HG22	1.77	0.66
1:A:101:VAL:HG11	1:A:283:VAL:HG22	1.79	0.65
1:A:68:LYS:O	1:B:263:TYR:HB2	1.99	0.63
1:B:101:VAL:HG21	1:B:283:VAL:HG22	1.81	0.62
1:B:203:GLU:HB3	4:B:660:HOH:O	2.00	0.61
1:B:201:ARG:H	1:B:204:GLN:NE2	1.96	0.60
1:A:162:ASP:HB2	1:A:169:ASP:HB2	1.82	0.60
1:B:167:SER:HB2	4:B:422:HOH:O	2.02	0.60
1:A:333:MET:HB3	1:A:392:VAL:HG22	1.85	0.58
1:A:263:TYR:HB2	1:B:68:LYS:O	2.06	0.56
1:A:215:ARG:HB2	1:A:217:LEU:HD13	1.88	0.55
1:B:154:GLN:NE2	4:B:636:HOH:O	2.39	0.55
1:A:251:VAL:HG12	1:A:272:VAL:HB	1.90	0.54
1:B:33:MET:HG2	1:B:379:ILE:HG12	1.89	0.54
1:B:22:GLU:HA	1:B:25:LYS:HD3	1.90	0.53
1:B:32:LYS:HA	1:B:378:SER:HB3	1.91	0.52
1:B:17:ILE:O	1:B:20:VAL:HG22	2.10	0.51
1:A:276:ASP:OD1	1:A:278:GLU:HB3	2.11	0.51
1:B:33:MET:HE2	1:B:35:LEU:HD21	1.93	0.51
1:B:88:LEU:O	1:B:92:SER:HB2	2.10	0.51
1:A:91:ASN:HA	1:A:96:LYS:NZ	2.25	0.51
1:A:91:ASN:HA	1:A:96:LYS:HZ3	1.75	0.51
1:B:374:THR:HG23	1:B:380:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:PHE:O	1:B:378:SER:HB2	2.10	0.50
1:A:8:HIS:CD2	1:A:8:HIS:N	2.80	0.49
1:A:194:ASN:HB3	3:A:411:PLP:H2A1	1.94	0.49
1:B:386:ARG:NH1	4:B:607:HOH:O	2.35	0.48
1:B:76:LEU:HB3	1:B:79:PHE:HB3	1.96	0.47
1:A:372:ARG:HG2	1:A:408:VAL:HG12	1.97	0.47
1:B:48:TYR:CE2	1:B:50:LEU:HD22	2.50	0.47
1:A:15:ASP:HA	1:A:16:PRO:HD3	1.81	0.46
1:B:194:ASN:HA	1:B:195:PRO:HA	1.76	0.46
1:B:174:MET:HE3	1:B:211:VAL:HG21	1.98	0.46
1:A:8:HIS:H	1:A:8:HIS:HD2	1.59	0.46
1:A:278:GLU:OE1	1:A:282:ARG:NH2	2.43	0.46
1:A:275:ARG:HD3	4:A:557:HOH:O	2.15	0.45
1:A:3:SER:OG	1:A:4:SER:N	2.50	0.45
1:B:242:HIS:O	1:B:246:GLN:HG2	2.17	0.44
1:B:279:GLU:O	1:B:283:VAL:HG13	2.17	0.44
1:B:110:GLY:O	1:B:114:VAL:HG13	2.16	0.44
1:B:177:ILE:HG22	1:B:211:VAL:HG12	2.00	0.44
1:A:120:GLN:HG3	1:A:150:ALA:O	2.18	0.44
1:A:129:ARG:HA	1:A:129:ARG:HE	1.82	0.44
1:B:332:SER:O	1:B:336:GLN:HG3	2.18	0.44
1:B:369:GLN:HB3	1:B:408:VAL:CG1	2.48	0.43
1:A:18:LEU:HA	1:A:21:THR:CG2	2.45	0.43
1:B:101:VAL:O	1:B:271:THR:HA	2.19	0.43
1:B:142:ASN:O	1:B:146:ILE:HG13	2.18	0.43
1:A:9:VAL:O	1:B:282:ARG:HD2	2.18	0.43
1:B:375:LYS:HD2	1:B:375:LYS:N	2.32	0.43
1:B:210:SER:O	1:B:214:LYS:HG3	2.19	0.43
1:A:135:LEU:O	1:A:157:ALA:HA	2.19	0.43
1:A:209:ALA:HB2	1:A:243:PHE:CE1	2.54	0.43
1:B:312:THR:HA	1:B:313:PRO:HD3	1.82	0.42
1:A:215:ARG:HH11	1:A:215:ARG:HD2	1.67	0.42
1:A:135:LEU:HD11	1:A:155:LEU:HD22	2.01	0.42
1:B:129:ARG:HA	1:B:129:ARG:HE	1.84	0.42
1:B:118:PHE:CD1	1:B:287:LEU:HD13	2.54	0.42
1:B:275:ARG:HG2	1:B:275:ARG:HH11	1.84	0.42
1:B:262:LEU:O	1:B:263:TYR:C	2.58	0.42
1:A:278:GLU:CD	1:A:282:ARG:HE	2.22	0.42
1:A:35:LEU:HD22	1:A:379:ILE:HG23	2.01	0.42
1:A:32:LYS:HA	1:A:378:SER:O	2.20	0.42
1:A:312:THR:HB	1:A:315:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PHE:CD1	1:A:287:LEU:HD13	2.55	0.41
1:B:341:LEU:HA	1:B:341:LEU:HD23	1.91	0.41
1:B:275:ARG:HG2	1:B:275:ARG:NH1	2.36	0.41
1:A:372:ARG:HG3	1:A:376:GLU:CD	2.41	0.41
1:B:33:MET:CG	1:B:379:ILE:HG12	2.51	0.41
1:B:21:THR:O	1:B:24:PHE:HB3	2.21	0.41
1:B:129:ARG:HA	1:B:129:ARG:NE	2.36	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	399/401 (100%)	387 (97%)	11 (3%)	1 (0%)	46	45
1	B	399/401 (100%)	384 (96%)	14 (4%)	1 (0%)	46	45
All	All	798/802 (100%)	771 (97%)	25 (3%)	2 (0%)	46	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR
1	B	263	TYR

### 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	335/335 (100%)	307 (92%)	28 (8%)	14	9
1	B	335/335 (100%)	307 (92%)	28 (8%)	14	9
All	All	670/670 (100%)	614 (92%)	56 (8%)	14	9

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	9	VAL
1	A	35	LEU
1	A	37	VAL
1	A	76	LEU
1	A	107	SER
1	A	119	LEU
1	A	129	ARG
1	A	168	LEU
1	A	188	LEU
1	A	195	PRO
1	A	212	VAL
1	A	215	ARG
1	A	220	TYR
1	A	240	LEU
1	A	259	ASN
1	A	262	LEU
1	A	272	VAL
1	A	283	VAL
1	A	287	LEU
1	A	290	LEU
1	A	310	LEU
1	A	315	LEU
1	A	337	LEU
1	A	361	CYS
1	A	362	PHE
1	A	397	VAL
1	A	400	LEU
1	B	18	LEU
1	B	49	VAL
1	B	53	VAL
1	B	76	LEU
1	B	86	LEU
1	B	88	LEU
1	B	90	GLU

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Mol	Chain	Res	Type
1	B	91	ASN
1	B	112	LEU
1	B	114	VAL
1	B	119	LEU
1	B	133	VAL
1	B	152	LEU
1	B	168	LEU
1	B	188	LEU
1	B	195	PRO
1	B	217	LEU
1	B	220	TYR
1	B	240	LEU
1	B	252	LEU
1	B	262	LEU
1	B	272	VAL
1	B	290	LEU
1	B	296	SER
1	B	339	SER
1	B	362	PHE
1	B	366	LYS
1	B	368	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	44	ASN
1	A	259	ASN
1	A	336	GLN
1	A	348	HIS
1	B	154	GLN
1	B	202	GLN
1	B	204	GLN
1	B	226	GLN
1	B	351	GLN

### 5.3.3 RNA ⓘ

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](#)

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	$\# Z  > 2$
3	PLP	A	411	-	16,16,16	2.89	2 (12%)	21,23,23	4.03	10 (47%)
2	PO4	B	411	-	4,4,4	1.51	1 (25%)	6,6,6	0.30	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	PLP	A	411	-	-	0/8/8/8	0/1/1/1
2	PO4	B	411	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	PO4	P-O4	2.28	1.61	1.53
3	A	411	PLP	C3-C2	6.07	1.45	1.40
3	A	411	PLP	O4A-C4A	8.87	1.49	1.21

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	411	PLP	C3-C4-C5	-10.12	110.53	118.11
3	A	411	PLP	C3-C2-N1	-5.62	112.85	120.61
3	A	411	PLP	O4A-C4A-C4	-4.98	115.05	125.11
3	A	411	PLP	O3-C3-C2	-4.77	109.36	117.66
3	A	411	PLP	C5A-C5-C6	-2.24	115.04	119.28
3	A	411	PLP	C6-C5-C4	2.31	123.29	118.17
3	A	411	PLP	O3P-P-O2P	2.49	116.85	107.38
3	A	411	PLP	C5-C4-C4A	3.34	129.98	122.35
3	A	411	PLP	C2A-C2-C3	6.90	129.36	121.04
3	A	411	PLP	O4P-C5A-C5	8.65	123.29	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	411	PLP	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.