Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 10:02 PM EDT

PDB ID	:	7AAT
Title	:	X-RAY STRUCTURE REFINEMENT AND COMPARISON OF THREE FORMS OF MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE
Authors	:	Mcphalen, C.A.; Vincent, M.G.; Jansonius, J.N.
Deposited on	:	1991-12-02
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:

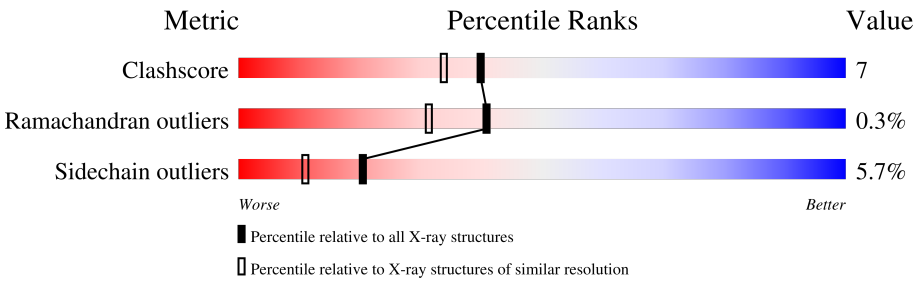
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	85% 13% •
1	B	401	79% 18% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7022 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.

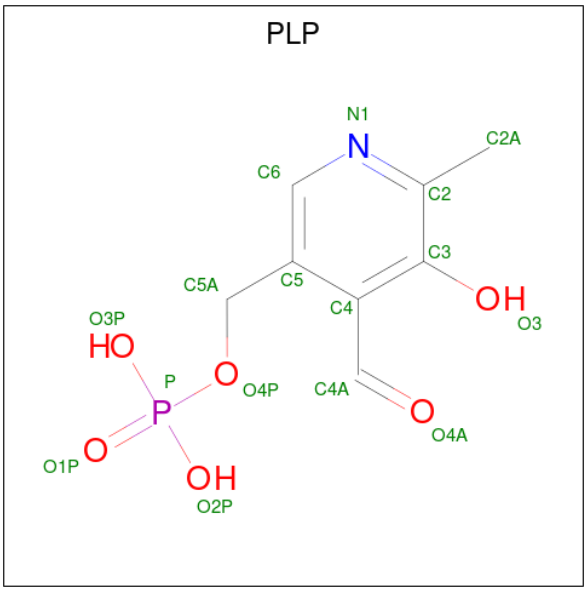
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3161	2004	558	581	18	0	0	0
1	B	401	3161	2004	558	581	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	SER	CONFLICT	UNP P00508
B	47	PRO	SER	CONFLICT	UNP P00508

- 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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	337	337	337	0	0
			Total	O		
3	B	333	333	333	0	0

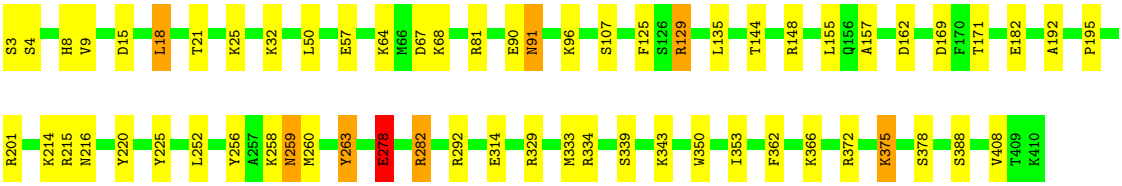
3 Residue-property plots (i)

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. 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.

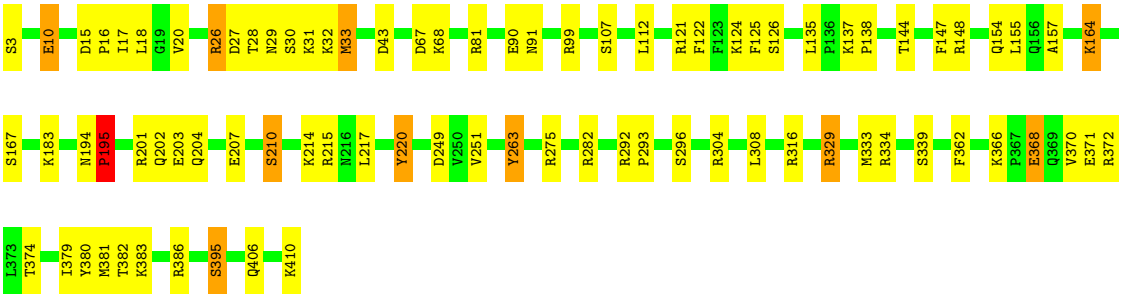
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A:



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.60Å 58.70Å 75.90Å 85.20° 109.20° 115.60°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7022	wwPDB-VP
Average B, all atoms ($Å^2$)	20.0	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: 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	0.67	0/3231	1.29	14/4360 (0.3%)
1	B	0.67	0/3231	1.29	21/4360 (0.5%)
All	All	0.67	0/6462	1.29	35/8720 (0.4%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	334	ARG	NE-CZ-NH1	12.05	126.32	120.30
1	A	278	GLU	CB-CG-CD	11.79	146.03	114.20
1	B	81	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	A	278	GLU	OE1-CD-OE2	-9.84	111.49	123.30
1	B	81	ARG	CD-NE-CZ	8.65	135.71	123.60
1	A	334	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	A	329	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	A	182	GLU	CA-CB-CG	8.20	131.44	113.40
1	B	316	ARG	NE-CZ-NH2	6.83	123.72	120.30
1	B	304	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	10	GLU	CB-CG-CD	6.25	131.06	114.20
1	A	278	GLU	CA-CB-CG	6.22	127.08	113.40
1	B	67	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	121	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	388	SER	N-CA-CB	6.05	119.58	110.50
1	B	121	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	195	PRO	N-CA-C	5.82	127.23	112.10
1	B	249	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	15	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	148	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	26	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	91	ASN	CB-CA-C	5.58	121.56	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	SER	N-CA-CB	-5.47	102.29	110.50
1	B	251	VAL	N-CA-CB	5.42	123.42	111.50
1	B	210	SER	CB-CA-C	5.41	120.38	110.10
1	A	282	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	304	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	216	ASN	N-CA-CB	-5.25	101.15	110.60
1	B	334	ARG	CD-NE-CZ	5.23	130.92	123.60
1	B	33	MET	CB-CA-C	5.19	120.78	110.40
1	A	278	GLU	CG-CD-OE1	5.12	128.54	118.30
1	A	192	ALA	CB-CA-C	5.11	117.76	110.10
1	B	329	ARG	CD-NE-CZ	5.08	130.71	123.60
1	B	81	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	252	LEU	N-CA-CB	-5.04	100.32	110.40

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	3161	0	3151	46	1
1	B	3161	0	3151	51	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	337	0	0	14	0
3	B	333	0	0	11	2
All	All	7022	0	6314	93	2

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 7.

All (93) 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:406:GLN:HE22	1:B:410:LYS:CE	1.55	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:GLN:HE22	1:B:410:LYS:HE2	1.00	1.16
1:B:406:GLN:NE2	1:B:410:LYS:HE2	1.70	1.05
1:B:406:GLN:NE2	1:B:410:LYS:CE	2.25	0.99
1:A:333:MET:HE3	3:A:671:HOH:O	1.66	0.96
1:B:201:ARG:H	1:B:204:GLN:HE21	1.17	0.91
1:B:374:THR:HG23	1:B:380:TYR:CE1	2.09	0.87
1:A:375:LYS:NZ	3:A:628:HOH:O	2.06	0.86
1:A:292:ARG:HD2	3:A:559:HOH:O	1.75	0.84
1:A:64:LYS:HD2	3:A:701:HOH:O	1.78	0.82
1:A:4:SER:HA	3:B:647:HOH:O	1.84	0.76
1:B:207:GLU:HG2	3:B:718:HOH:O	1.86	0.74
1:A:201:ARG:HG2	3:A:547:HOH:O	1.88	0.73
1:B:3:SER:O	3:B:662:HOH:O	2.08	0.72
1:A:278:GLU:OE1	1:A:282:ARG:NH2	2.21	0.72
1:A:8:HIS:H	1:A:8:HIS:CD2	2.06	0.72
1:B:154:GLN:NE2	3:B:620:HOH:O	2.24	0.71
1:A:148:ARG:NH2	3:A:727:HOH:O	2.25	0.70
1:B:26:ARG:O	1:B:26:ARG:HG3	1.91	0.69
1:A:372:ARG:HG2	1:A:408:VAL:HG12	1.75	0.68
1:B:406:GLN:NE2	1:B:410:LYS:HE3	2.08	0.68
1:A:57:GLU:OE2	3:A:517:HOH:O	2.11	0.67
1:B:201:ARG:HD2	1:B:203:GLU:OE2	1.96	0.66
1:A:91:ASN:HA	1:A:96:LYS:HE2	1.76	0.66
1:A:64:LYS:HA	3:A:701:HOH:O	1.96	0.65
1:A:68:LYS:O	1:B:263:TYR:HB2	1.99	0.62
1:A:278:GLU:OE1	1:A:282:ARG:NE	2.36	0.59
1:A:129:ARG:HA	1:A:129:ARG:HE	1.67	0.58
1:A:263:TYR:HB2	1:B:68:LYS:O	2.05	0.57
1:B:374:THR:CG2	1:B:380:TYR:CE1	2.86	0.56
1:A:81:ARG:HB3	1:A:81:ARG:NH1	2.21	0.56
1:B:29:ASN:OD1	1:B:31:LYS:HB2	2.06	0.55
1:B:275:ARG:HH11	1:B:275:ARG:HG2	1.72	0.55
1:A:162:ASP:HB2	1:A:169:ASP:HB2	1.89	0.54
1:A:372:ARG:HG2	1:A:408:VAL:CG1	2.38	0.54
1:B:195:PRO:HB3	3:B:707:HOH:O	2.08	0.52
1:B:144:THR:HG23	1:B:155:LEU:HD13	1.91	0.52
1:B:214:LYS:HG3	3:B:686:HOH:O	2.09	0.52
1:A:135:LEU:O	1:A:157:ALA:HA	2.10	0.52
1:B:167:SER:HB2	3:B:511:HOH:O	2.09	0.52
1:B:201:ARG:H	1:B:204:GLN:NE2	1.98	0.51
1:A:8:HIS:HE1	1:B:122:PHE:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LYS:NZ	3:B:720:HOH:O	2.44	0.51
1:A:18:LEU:HA	1:A:21:THR:HG22	1.93	0.50
1:A:259:ASN:HD22	1:A:260:MET:N	2.09	0.50
1:A:278:GLU:CD	1:A:282:ARG:HE	2.15	0.50
1:A:8:HIS:H	1:A:8:HIS:HD2	1.56	0.50
1:A:9:VAL:O	1:B:282:ARG:HD2	2.11	0.49
1:B:33:MET:HG2	1:B:379:ILE:HG12	1.93	0.49
1:B:27:ASP:HB3	1:B:32:LYS:HD3	1.95	0.49
1:B:374:THR:HG23	1:B:380:TYR:CD1	2.47	0.49
1:B:292:ARG:HB3	1:B:293:PRO:HD3	1.95	0.49
1:A:18:LEU:C	1:A:18:LEU:HD23	2.33	0.48
1:B:164:LYS:HB2	1:B:164:LYS:HE2	1.50	0.48
1:B:329:ARG:O	1:B:333:MET:HG2	2.13	0.48
1:B:183:LYS:HE2	3:B:651:HOH:O	2.11	0.48
1:A:129:ARG:HE	1:A:129:ARG:CA	2.26	0.48
1:B:386:ARG:NH1	3:B:470:HOH:O	2.39	0.48
1:B:395:SER:OG	3:B:695:HOH:O	2.10	0.47
1:A:292:ARG:NH2	3:A:542:HOH:O	2.47	0.47
1:A:25:LYS:HE2	3:A:625:HOH:O	2.13	0.47
1:B:215:ARG:HB2	1:B:217:LEU:HG	1.96	0.47
1:B:135:LEU:O	1:B:157:ALA:HA	2.15	0.47
1:B:370:VAL:HG13	1:B:381:MET:HG3	1.97	0.47
1:A:171:THR:HG22	3:A:652:HOH:O	2.15	0.47
1:A:50:LEU:N	1:A:50:LEU:HD12	2.30	0.46
1:A:18:LEU:HA	1:A:21:THR:CG2	2.46	0.46
1:A:256:TYR:HA	1:A:259:ASN:HD21	1.81	0.46
1:A:350:TRP:HB3	1:A:353:ILE:HD12	1.98	0.46
1:B:194:ASN:HA	1:B:195:PRO:HA	1.72	0.46
1:B:112:LEU:HA	1:B:220:TYR:OH	2.16	0.45
1:B:99:ARG:O	1:B:99:ARG:HG3	2.16	0.45
1:A:201:ARG:CG	3:A:547:HOH:O	2.57	0.45
1:A:278:GLU:OE1	1:A:282:ARG:CZ	2.64	0.45
1:B:27:ASP:HB3	1:B:32:LYS:CD	2.47	0.44
1:A:225:TYR:CE1	1:A:258:LYS:HD3	2.52	0.44
1:B:275:ARG:HG2	1:B:275:ARG:NH1	2.33	0.44
1:B:15:ASP:HA	1:B:16:PRO:HD3	1.77	0.43
1:B:371:GLU:HG3	1:B:383:LYS:HE3	2.00	0.43
1:A:3:SER:HB2	3:A:747:HOH:O	2.17	0.43
1:A:57:GLU:HG2	3:A:517:HOH:O	2.18	0.42
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.78	0.42
1:A:129:ARG:HA	1:A:129:ARG:NE	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:GLN:NE2	1:B:406:GLN:HA	2.33	0.42
1:A:32:LYS:HA	1:A:378:SER:O	2.18	0.42
1:A:81:ARG:HB3	1:A:81:ARG:CZ	2.50	0.42
1:A:67:ASP:C	1:A:67:ASP:OD1	2.59	0.42
1:B:27:ASP:OD1	1:B:28:THR:N	2.53	0.41
1:B:17:ILE:O	1:B:20:VAL:HG22	2.20	0.41
1:B:147:PHE:HB2	1:B:155:LEU:HD21	2.02	0.41
1:A:144:THR:HG23	1:A:155:LEU:HD13	2.03	0.41
1:B:17:ILE:HD13	1:B:382:THR:HG21	2.03	0.40
1:B:368:GLU:O	1:B:372:ARG:HG3	2.22	0.40

All (2) 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:B:474:HOH:O	3:B:733:HOH:O[1_545]	1.95	0.25
1:A:201:ARG:CD	3:B:670:HOH:O[1_444]	2.14	0.06

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%)	389 (98%)	9 (2%)	1 (0%)	41	31
1	B	399/401 (100%)	385 (96%)	13 (3%)	1 (0%)	41	31
All	All	798/802 (100%)	774 (97%)	22 (3%)	2 (0%)	41	31

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%)	318 (95%)	17 (5%)	24 14
1	B	335/335 (100%)	314 (94%)	21 (6%)	18 8
All	All	670/670 (100%)	632 (94%)	38 (6%)	20 11

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	90	GLU
1	A	107	SER
1	A	125	PHE
1	A	129	ARG
1	A	195	PRO
1	A	214	LYS
1	A	215	ARG
1	A	220	TYR
1	A	259	ASN
1	A	278	GLU
1	A	314	GLU
1	A	339	SER
1	A	343	LYS
1	A	362	PHE
1	A	366	LYS
1	A	375	LYS
1	B	10	GLU
1	B	18	LEU
1	B	30	SER
1	B	43	ASP
1	B	90	GLU
1	B	91	ASN
1	B	107	SER
1	B	124	LYS
1	B	125	PHE
1	B	138	PRO

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Mol	Chain	Res	Type
1	B	164	LYS
1	B	195	PRO
1	B	202	GLN
1	B	210	SER
1	B	220	TYR
1	B	296	SER
1	B	339	SER
1	B	362	PHE
1	B	366	LYS
1	B	368	GLU
1	B	395	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	44	ASN
1	A	259	ASN
1	A	340	ASN
1	A	351	GLN
1	B	154	GLN
1	B	202	GLN
1	B	204	GLN
1	B	216	ASN
1	B	226	GLN
1	B	406	GLN

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	B	411	1	15,15,16	1.69	4 (26%)	20,22,23	2.28	9 (45%)
2	PLP	A	411	1	15,15,16	1.69	3 (20%)	20,22,23	2.28	8 (40%)

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	B	411	1	-	3/6/6/8	0/1/1/1
2	PLP	A	411	1	-	3/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	PLP	C4A-C4	-3.34	1.44	1.51
2	A	411	PLP	C5-C4	3.23	1.44	1.40
2	B	411	PLP	C5-C4	3.18	1.44	1.40
2	B	411	PLP	C4A-C4	-3.11	1.45	1.51
2	B	411	PLP	C3-C2	2.74	1.43	1.40
2	A	411	PLP	C3-C2	2.46	1.43	1.40
2	B	411	PLP	P-O2P	-2.04	1.47	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	411	PLP	C2A-C2-C3	5.47	127.64	120.89
2	B	411	PLP	C6-C5-C4	4.44	121.65	118.16
2	B	411	PLP	C2A-C2-C3	4.30	126.20	120.89
2	A	411	PLP	C6-C5-C4	3.84	121.18	118.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	411	PLP	O3-C3-C4	3.70	127.85	118.10
2	A	411	PLP	O3-C3-C4	3.57	127.51	118.10
2	B	411	PLP	O4P-C5A-C5	3.48	115.97	109.35
2	A	411	PLP	C3-C2-N1	-2.99	116.90	120.77
2	A	411	PLP	C6-N1-C2	2.97	124.66	119.17
2	A	411	PLP	C5-C6-N1	-2.81	119.13	123.82
2	B	411	PLP	C5-C6-N1	-2.66	119.39	123.82
2	B	411	PLP	O3-C3-C2	-2.59	111.86	117.49
2	A	411	PLP	O4P-C5A-C5	2.55	114.21	109.35
2	A	411	PLP	O3-C3-C2	-2.45	112.15	117.49
2	B	411	PLP	C4A-C4-C5	2.45	123.45	120.94
2	B	411	PLP	C6-N1-C2	2.38	123.57	119.17
2	B	411	PLP	C3-C2-N1	-2.34	117.74	120.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	411	PLP	C4-C5-C5A-O4P
2	A	411	PLP	C6-C5-C5A-O4P
2	B	411	PLP	C4-C5-C5A-O4P
2	B	411	PLP	C6-C5-C5A-O4P
2	A	411	PLP	C5A-O4P-P-O2P
2	B	411	PLP	C5A-O4P-P-O2P

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.