



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:13 AM UTC

PDB ID : 8AAT / pdb_00008aat
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 : 2.30 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)
Xtrriage (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

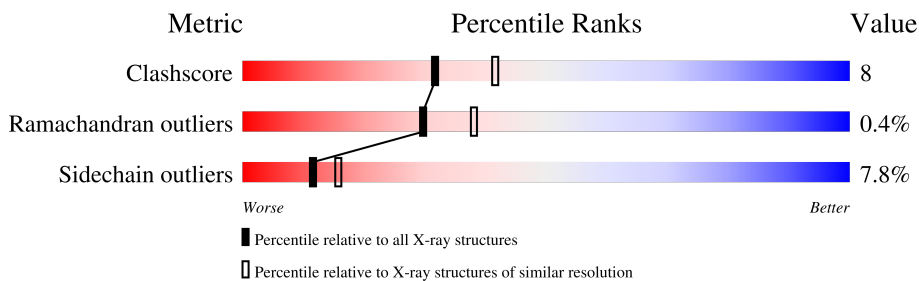
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	401	
1	B	401	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6952 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.

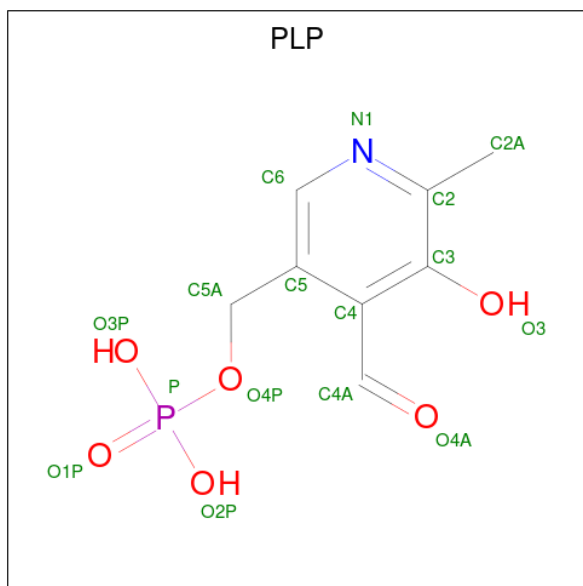
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	Total 3161	C 2004	N 558	O 581	S 18	0	0	0
1	B	401	Total 3161	C 2004	N 558	O 581	S 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 (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is water.

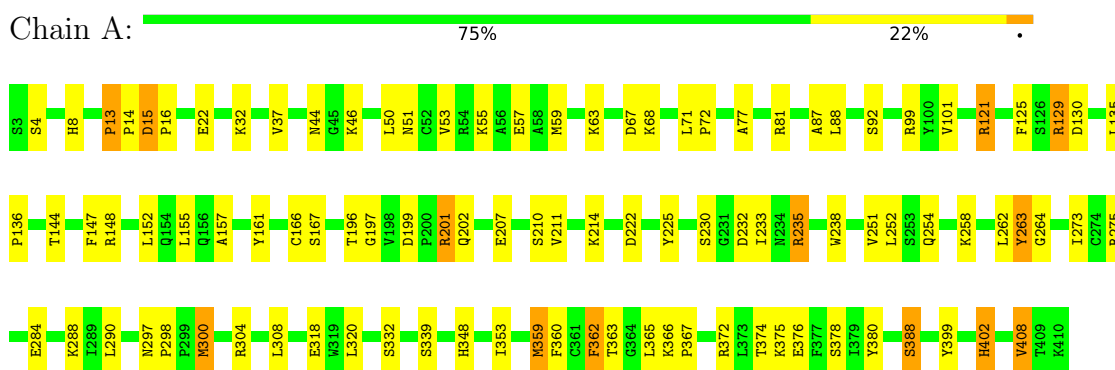
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	297	Total	O	0	0
			297	297		
3	B	303	Total	O	0	0
			303	303		

3 Residue-property plots [i](#)

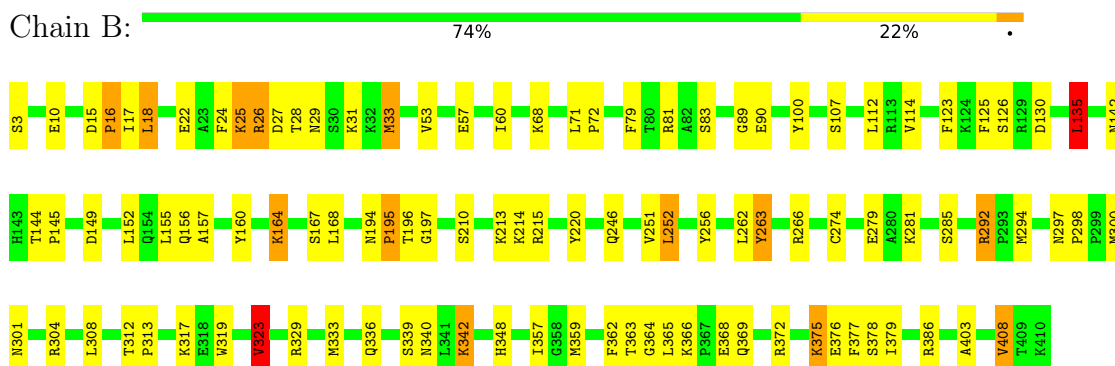
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



- Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

Xtrriage (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	55.53Å 58.68Å 75.77Å 85.10° 109.20° 115.90°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.130 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6952	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	0.82	0/3231	1.68	40/4360 (0.9%)
1	B	0.82	0/3231	1.69	33/4360 (0.8%)
All	All	0.82	0/6462	1.69	73/8720 (0.8%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	ARG	CD-NE-CZ	7.73	135.22	124.40
1	A	300	MET	N-CA-C	7.46	121.63	112.23
1	B	301	ASN	N-CA-C	7.38	119.02	110.97
1	A	15	ASP	CB-CA-C	7.30	119.90	109.38
1	B	297	ASN	CB-CA-C	7.30	119.85	110.22
1	A	13	PRO	O-C-N	7.24	124.55	121.15
1	A	196	THR	N-CA-C	7.17	121.27	112.23
1	A	297	ASN	CB-CA-C	7.07	120.93	109.97
1	B	215	ARG	CD-NE-CZ	-7.06	114.52	124.40
1	A	53	VAL	CB-CA-C	6.96	121.13	112.02
1	A	298	PRO	N-CA-C	6.91	119.13	110.70
1	B	71	LEU	N-CA-C	-6.89	101.12	110.36
1	A	8	HIS	CA-CB-CG	-6.74	107.06	113.80
1	B	323	VAL	N-CA-CB	6.64	118.32	110.55
1	A	251	VAL	CB-CA-C	6.62	121.01	110.82
1	B	300	MET	N-CA-C	6.36	120.25	112.23
1	A	252	LEU	N-CA-CB	-6.35	99.71	111.52
1	B	256	TYR	CA-C-N	6.20	128.50	120.44
1	B	256	TYR	C-N-CA	6.20	128.50	120.44
1	B	196	THR	N-CA-C	6.17	120.99	112.90
1	B	126	SER	N-CA-CB	-6.13	102.24	111.56
1	B	149	ASP	CA-CB-CG	6.12	118.72	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	PHE	CA-CB-CG	-6.12	107.68	113.80
1	B	251	VAL	N-CA-C	-6.00	99.60	108.85
1	B	130	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	251	VAL	N-CA-C	-5.90	99.76	108.85
1	B	123	PHE	CA-CB-CG	-5.88	107.92	113.80
1	A	376	GLU	N-CA-C	5.81	120.52	112.90
1	A	264	GLY	N-CA-C	5.81	121.06	114.67
1	A	199	ASP	O-C-N	5.79	127.18	121.57
1	B	197	GLY	N-CA-C	-5.78	107.78	115.40
1	A	71	LEU	N-CA-C	-5.77	102.63	110.36
1	A	254	GLN	OE1-CD-NE2	5.70	128.29	122.60
1	A	210	SER	O-C-N	5.65	128.11	122.12
1	B	298	PRO	N-CA-C	5.65	117.59	110.70
1	B	252	LEU	N-CA-CB	-5.64	101.02	111.52
1	A	130	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	362	PHE	N-CA-C	-5.64	99.33	108.41
1	B	89	GLY	CA-C-N	5.63	128.10	120.38
1	B	89	GLY	C-N-CA	5.63	128.10	120.38
1	B	72	PRO	N-CA-C	-5.61	102.64	111.34
1	A	121	ARG	N-CA-C	5.55	118.17	111.40
1	A	360	PHE	CA-CB-CG	-5.45	108.35	113.80
1	A	37	VAL	CB-CA-C	5.44	120.46	111.59
1	A	44	ASN	CB-CA-C	5.44	119.75	110.56
1	B	156	GLN	OE1-CD-NE2	5.41	128.01	122.60
1	A	402	HIS	CA-CB-CG	-5.41	108.39	113.80
1	B	215	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	B	375	LYS	N-CA-C	5.34	116.79	111.07
1	B	114	VAL	CA-C-N	5.30	125.82	119.94
1	B	114	VAL	C-N-CA	5.30	125.82	119.94
1	B	266	ARG	N-CA-C	5.27	117.07	110.91
1	A	129	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	A	87	ALA	N-CA-C	5.25	116.81	111.14
1	B	135	LEU	O-C-N	5.24	127.57	121.39
1	A	363	THR	N-CA-C	5.21	118.10	111.69
1	A	99	ARG	CD-NE-CZ	5.20	131.69	124.40
1	A	144	THR	CA-CB-OG1	-5.19	101.81	109.60
1	A	211	VAL	CB-CA-C	5.18	119.18	112.24
1	A	72	PRO	N-CA-C	-5.16	103.34	111.34
1	A	388	SER	N-CA-C	-5.15	100.78	108.96
1	A	77	ALA	N-CA-C	5.13	117.54	111.33
1	A	348	HIS	CA-CB-CG	-5.12	108.68	113.80
1	A	359	MET	N-CA-C	5.11	117.74	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ILE	N-CA-CB	5.08	116.79	111.00
1	A	196	THR	CA-CB-OG1	-5.07	101.99	109.60
1	B	256	TYR	CA-C-O	5.07	125.46	119.48
1	A	136	PRO	N-CA-C	-5.07	103.81	111.41
1	B	364	GLY	N-CA-C	-5.06	108.34	114.92
1	A	197	GLY	N-CA-C	-5.06	108.63	115.36
1	A	51	ASN	OD1-CG-ND2	5.02	127.62	122.60
1	B	33	MET	CB-CA-C	5.01	119.27	109.35
1	B	251	VAL	CB-CA-C	5.01	118.53	110.82

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	3152	54	0
1	B	3161	0	3152	48	0
2	A	15	0	6	2	0
2	B	15	0	6	1	0
3	A	297	0	0	9	0
3	B	303	0	0	14	0
All	All	6952	0	6316	102	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 8.

All (102) 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:201:ARG:HH11	1:A:201:ARG:HG3	1.01	1.14
1:A:129:ARG:HA	1:A:129:ARG:HE	1.16	1.05
1:B:26:ARG:HH11	1:B:26:ARG:HG3	1.20	1.03
1:A:22:GLU:HG3	3:A:690:HOH:O	1.67	0.94
1:A:4:SER:HA	3:B:639:HOH:O	1.66	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ARG:HH11	1:A:201:ARG:CG	1.82	0.92
1:A:201:ARG:HG3	1:A:201:ARG:NH1	1.81	0.87
1:B:33:MET:HG2	1:B:379:ILE:HG12	1.55	0.86
1:A:167:SER:HB2	3:A:491:HOH:O	1.77	0.83
1:B:26:ARG:HH11	1:B:26:ARG:CG	1.91	0.83
1:A:129:ARG:HE	1:A:129:ARG:CA	1.90	0.80
1:A:22:GLU:HA	1:A:22:GLU:OE1	1.84	0.78
1:A:81:ARG:HD3	3:A:614:HOH:O	1.83	0.78
1:A:129:ARG:HA	1:A:129:ARG:NE	1.99	0.76
1:B:15:ASP:OD2	1:B:18:LEU:HB2	1.85	0.76
1:B:376:GLU:OE1	3:B:687:HOH:O	2.06	0.73
1:B:292:ARG:NH1	3:B:679:HOH:O	2.23	0.72
1:A:125:PHE:CE1	3:B:634:HOH:O	2.44	0.70
1:B:3:SER:O	3:B:691:HOH:O	2.09	0.70
1:B:363:THR:OG1	1:B:365:LEU:HD12	1.93	0.68
1:B:33:MET:CG	1:B:379:ILE:HG12	2.24	0.67
1:A:57:GLU:HG2	3:A:508:HOH:O	1.93	0.67
1:A:232:ASP:HB3	1:A:235:ARG:HH11	1.60	0.67
1:B:26:ARG:HG3	1:B:26:ARG:NH1	1.99	0.67
1:A:202:GLN:HG3	1:A:238:TRP:CH2	2.30	0.66
1:B:29:ASN:OD1	1:B:31:LYS:HB2	1.95	0.66
1:A:232:ASP:HB3	1:A:235:ARG:NH1	2.11	0.66
1:B:213:LYS:HE3	1:B:246:GLN:O	1.97	0.65
1:B:368:GLU:OE2	3:B:705:HOH:O	2.15	0.64
1:B:377:PHE:O	1:B:378:SER:HB2	1.95	0.64
1:A:101:VAL:HG21	1:A:284:GLU:HB2	1.81	0.61
1:A:125:PHE:HE1	3:B:634:HOH:O	1.83	0.61
1:B:22:GLU:HG3	3:B:441:HOH:O	2.00	0.61
1:A:22:GLU:CG	3:A:690:HOH:O	2.37	0.60
1:A:225:TYR:CE1	1:A:258:LYS:HD3	2.38	0.58
1:B:27:ASP:OD1	1:B:28:THR:N	2.37	0.57
1:B:79:PHE:O	1:B:83:SER:HB2	2.05	0.57
1:B:386:ARG:NH1	3:B:465:HOH:O	2.36	0.57
1:A:201:ARG:CG	1:A:201:ARG:NH1	2.48	0.56
1:B:329:ARG:O	1:B:333:MET:HG2	2.05	0.56
1:A:68:LYS:O	1:B:263:TYR:HB2	2.04	0.56
1:A:129:ARG:CA	1:A:129:ARG:NE	2.64	0.55
1:A:46:LYS:NZ	3:A:538:HOH:O	2.39	0.54
1:B:160:TYR:O	1:B:168:LEU:HD12	2.07	0.54
1:B:142:ASN:O	1:B:145:PRO:HD2	2.08	0.53
3:A:703:HOH:O	1:B:294:MET:HE3	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:CG	1:B:26:ARG:NH1	2.58	0.51
1:A:262:LEU:O	1:A:263:TYR:C	2.54	0.50
1:A:88:LEU:O	1:A:92:SER:HB2	2.12	0.50
1:A:372:ARG:HG2	1:A:408:VAL:HG12	1.93	0.50
1:B:167:SER:HB2	3:B:500:HOH:O	2.12	0.50
2:B:411:PLP:C4A	2:B:411:PLP:O4P	2.59	0.50
1:A:359:MET:HE3	1:A:388:SER:OG	2.11	0.49
1:B:262:LEU:O	1:B:263:TYR:C	2.55	0.49
1:B:10:GLU:OE1	3:B:414:HOH:O	2.19	0.49
1:B:25:LYS:C	1:B:27:ASP:H	2.19	0.49
1:B:53:VAL:O	1:B:57:GLU:HG3	2.13	0.48
1:B:342:LYS:NZ	3:B:700:HOH:O	2.47	0.48
1:B:274:CYS:HB3	1:B:279:GLU:HG2	1.95	0.48
1:A:13:PRO:HA	1:A:14:PRO:HD3	1.76	0.47
1:A:135:LEU:O	1:A:157:ALA:HA	2.15	0.47
1:A:230:SER:OG	1:A:235:ARG:HD2	2.14	0.47
1:A:67:ASP:C	1:A:67:ASP:OD1	2.58	0.47
1:A:263:TYR:HB2	1:B:68:LYS:O	2.15	0.47
1:A:202:GLN:HG3	1:A:238:TRP:CZ3	2.50	0.47
1:B:308:LEU:HA	1:B:308:LEU:HD23	1.73	0.46
1:A:233:ILE:HD13	1:A:320:LEU:HD21	1.98	0.46
1:B:144:THR:HB	1:B:145:PRO:HD3	1.98	0.46
1:A:32:LYS:HA	1:A:378:SER:O	2.16	0.46
1:A:59:MET:O	1:A:63:LYS:HG3	2.15	0.46
1:B:112:LEU:HA	1:B:220:TYR:OH	2.16	0.45
1:B:135:LEU:O	1:B:157:ALA:HA	2.16	0.45
1:A:50:LEU:N	1:A:50:LEU:HD12	2.32	0.45
1:A:15:ASP:HA	1:A:16:PRO:HD3	1.77	0.45
1:A:300:MET:HE2	1:A:304:ARG:CZ	2.47	0.45
1:B:164:LYS:HB2	1:B:164:LYS:HE2	1.60	0.45
1:B:319:TRP:O	1:B:323:VAL:HG22	2.16	0.45
1:A:101:VAL:CG2	1:A:284:GLU:HB2	2.47	0.45
1:A:148:ARG:HD2	3:A:486:HOH:O	2.15	0.45
1:A:284:GLU:O	1:A:288:LYS:HG3	2.16	0.45
1:A:399:TYR:O	1:A:402:HIS:HB3	2.17	0.44
1:A:374:THR:HG23	1:A:380:TYR:CE1	2.54	0.43
1:B:336:GLN:O	1:B:340:ASN:ND2	2.51	0.43
1:B:348:HIS:CG	3:B:636:HOH:O	2.71	0.43
1:B:366:LYS:HE2	3:B:705:HOH:O	2.18	0.43
1:B:15:ASP:HA	1:B:16:PRO:HD3	1.73	0.43
1:B:100:TYR:CD1	1:B:100:TYR:C	2.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ILE:HD13	1:B:304:ARG:HB3	2.01	0.43
1:B:363:THR:CB	1:B:365:LEU:HD12	2.49	0.42
1:A:366:LYS:HB3	1:A:367:PRO:HD2	2.02	0.42
1:A:359:MET:HE2	1:A:359:MET:HB3	1.97	0.42
1:A:372:ARG:HG2	1:A:408:VAL:CG1	2.50	0.41
2:A:411:PLP:C4A	2:A:411:PLP:O4P	2.68	0.41
1:A:147:PHE:HD1	1:A:152:LEU:HD12	1.84	0.41
1:A:55:LYS:NZ	1:A:318:GLU:OE1	2.44	0.41
1:A:121:ARG:HD3	3:A:469:HOH:O	2.21	0.41
1:B:403:ALA:O	1:B:408:VAL:HG13	2.21	0.41
1:A:161:TYR:OH	1:A:166:CYS:HA	2.22	0.40
1:A:101:VAL:HG21	1:A:284:GLU:CB	2.51	0.40
1:A:222:ASP:OD2	2:A:411:PLP:N1	2.54	0.40
1:B:194:ASN:HA	1:B:195:PRO:HA	1.78	0.40
1:B:312:THR:HA	1:B:313:PRO:HD3	1.94	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%)	391 (98%)	7 (2%)	1 (0%)	36	46
1	B	399/401 (100%)	384 (96%)	13 (3%)	2 (0%)	24	31
All	All	798/802 (100%)	775 (97%)	20 (2%)	3 (0%)	30	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR
1	B	263	TYR
1	B	16	PRO

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	230/335 (69%)	215 (94%)	15 (6%)	15	22
1	B	335/335 (100%)	306 (91%)	29 (9%)	9	12
All	All	565/670 (84%)	521 (92%)	44 (8%)	11	16

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LEU
1	A	201	ARG
1	A	207	GLU
1	A	214	LYS
1	A	235	ARG
1	A	275	ARG
1	A	290	LEU
1	A	308	LEU
1	A	332	SER
1	A	339	SER
1	A	353	ILE
1	A	362	PHE
1	A	365	LEU
1	A	375	LYS
1	A	408	VAL
1	B	17	ILE
1	B	18	LEU
1	B	25	LYS
1	B	26	ARG
1	B	90	GLU
1	B	107	SER
1	B	125	PHE
1	B	135	LEU
1	B	152	LEU
1	B	155	LEU
1	B	164	LYS
1	B	195	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	210	SER
1	B	214	LYS
1	B	252	LEU
1	B	281	LYS
1	B	285	SER
1	B	292	ARG
1	B	317	LYS
1	B	323	VAL
1	B	339	SER
1	B	342	LYS
1	B	357	ILE
1	B	359	MET
1	B	362	PHE
1	B	369	GLN
1	B	372	ARG
1	B	375	LYS
1	B	408	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	226	GLN
1	A	297	ASN
1	A	336	GLN
1	A	349	ASN
1	A	351	GLN
1	B	91	ASN
1	B	120	GLN
1	B	216	ASN
1	B	226	GLN
1	B	297	ASN
1	B	336	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 oligosaccharides 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	1.32	1 (6%)	21,22,23	2.14	6 (28%)
2	PLP	A	411	1	15,15,16	1.20	1 (6%)	21,22,23	2.23	8 (38%)

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	-	2/6/6/8	0/1/1/1
2	PLP	A	411	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	B	411	PLP	C4A-C4	-3.53	1.44	1.51
2	A	411	PLP	C4A-C4	-3.33	1.45	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PLP	C6-C5-C4	4.54	121.82	118.10
2	B	411	PLP	C6-C5-C4	4.46	121.75	118.10
2	A	411	PLP	C2A-C2-C3	4.34	125.88	120.80
2	B	411	PLP	C2A-C2-C3	4.02	125.51	120.80
2	B	411	PLP	O4P-C5A-C5	3.77	116.43	109.36
2	A	411	PLP	O4P-C5A-C5	3.72	116.32	109.36
2	A	411	PLP	C3-C2-N1	-3.34	116.75	120.96
2	A	411	PLP	C5-C6-N1	-3.11	118.78	123.83
2	B	411	PLP	C5-C6-N1	-3.06	118.86	123.83
2	B	411	PLP	C3-C2-N1	-2.89	117.31	120.96
2	A	411	PLP	C6-N1-C2	2.88	124.42	119.20
2	B	411	PLP	C6-N1-C2	2.62	123.96	119.20
2	A	411	PLP	C5A-C5-C6	-2.20	115.77	119.36
2	A	411	PLP	C3-C4-C5	-2.00	116.19	118.59

There are no chirality outliers.

All (4) 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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	411	PLP	1	0
2	A	411	PLP	2	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 [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.