



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:35 AM UTC

PDB ID : 7AAT / pdb_00007aat
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 ⓘ 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

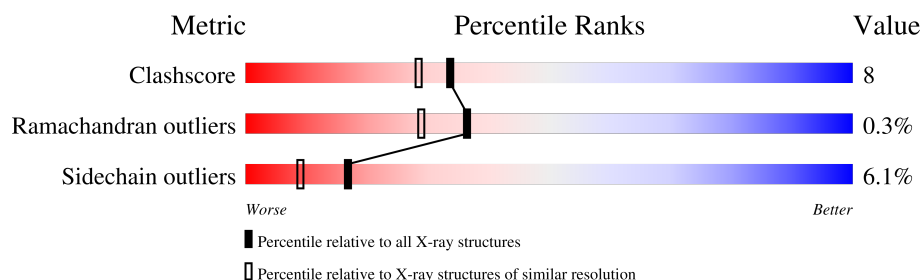
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	 78% 19% .
1	B	401	 73% 23% .

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.

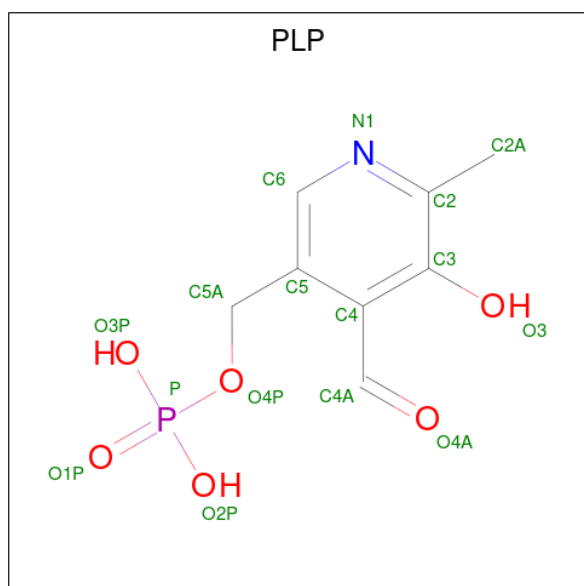
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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

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
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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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	337	Total	O	0	0
			337	337		
3	B	333	Total	O	0	0
			333	333		

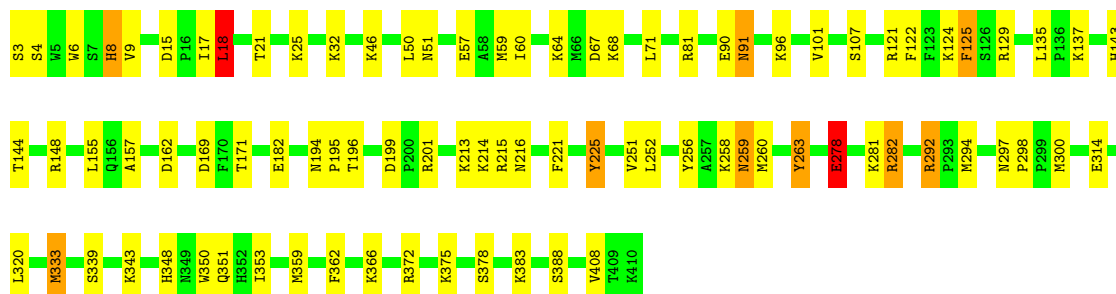
3 Residue-property plots [i](#)

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.

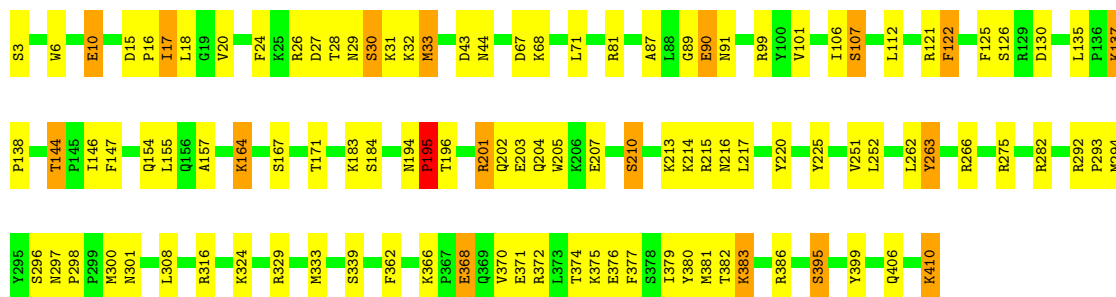
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A:  78% 19%



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain B:  73% 23%



4 Data and refinement statistics

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

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	0.84	0/3231	1.79	42/4360 (1.0%)
1	B	0.83	0/3231	1.76	54/4360 (1.2%)
All	All	0.83	0/6462	1.78	96/8720 (1.1%)

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	GLU	CB-CG-CD	19.66	146.03	112.60
1	B	10	GLU	CB-CG-CD	10.86	131.06	112.60
1	A	15	ASP	CA-CB-CG	9.44	122.04	112.60
1	A	182	GLU	CA-CB-CG	8.67	131.44	114.10
1	B	81	ARG	CD-NE-CZ	8.08	135.71	124.40
1	B	196	THR	N-CA-C	8.00	122.31	112.23
1	A	125	PHE	N-CA-C	7.83	120.71	111.71
1	A	298	PRO	N-CA-C	7.65	120.03	110.70
1	B	130	ASP	CA-CB-CG	7.42	120.02	112.60
1	A	194	ASN	CB-CA-C	7.09	118.31	110.15
1	B	301	ASN	N-CA-C	6.91	118.50	110.97
1	B	300	MET	N-CA-C	6.85	120.86	112.23
1	A	60	ILE	O-C-N	6.74	128.90	121.90
1	A	216	ASN	N-CA-CB	-6.64	101.15	111.65
1	B	266	ARG	N-CA-C	6.61	118.65	110.91
1	B	122	PHE	N-CA-C	6.54	122.34	113.97
1	B	376	GLU	N-CA-C	6.50	121.50	113.50
1	A	278	GLU	CA-CB-CG	6.49	127.08	114.10
1	A	122	PHE	N-CA-C	6.48	122.27	113.97
1	A	143	HIS	N-CA-CB	6.35	119.45	110.12
1	A	91	ASN	CB-CA-C	6.29	121.56	110.37
1	A	300	MET	N-CA-C	6.22	119.35	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	PRO	N-CA-C	6.15	118.20	110.70
1	A	8	HIS	CA-CB-CG	-6.11	107.69	113.80
1	B	126	SER	N-CA-CB	-6.10	102.29	111.56
1	B	17	ILE	O-C-N	6.09	128.03	121.94
1	B	375	LYS	N-CA-C	6.09	117.59	111.07
1	A	121	ARG	N-CA-C	6.05	117.68	111.14
1	B	210	SER	CB-CA-C	6.05	120.38	110.88
1	B	67	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	6	TRP	N-CA-C	6.00	119.91	112.59
1	A	252	LEU	N-CA-CB	-5.97	100.32	111.13
1	A	333	MET	N-CA-CB	5.96	118.98	110.16
1	B	297	ASN	CB-CA-C	5.90	118.01	110.22
1	A	383	LYS	N-CA-C	5.90	119.95	112.87
1	A	71	LEU	N-CA-C	-5.90	102.45	110.36
1	B	146	ILE	N-CA-CB	5.82	116.97	110.51
1	B	195	PRO	N-CA-C	5.82	127.23	112.10
1	A	297	ASN	CB-CA-C	5.78	117.78	109.92
1	A	15	ASP	CB-CA-C	5.71	117.61	109.38
1	A	51	ASN	OD1-CG-ND2	5.70	128.30	122.60
1	B	30	SER	N-CA-C	-5.64	105.89	112.89
1	A	17	ILE	N-CA-CB	5.63	117.14	110.55
1	B	24	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	221	PHE	CA-CB-CG	5.62	119.42	113.80
1	B	33	MET	CB-CA-C	5.61	120.78	109.38
1	A	388	SER	N-CA-CB	5.58	119.58	110.37
1	A	216	ASN	OD1-CG-ND2	5.58	128.18	122.60
1	A	351	GLN	N-CA-CB	5.57	118.80	110.22
1	B	251	VAL	N-CA-CB	5.56	123.42	111.91
1	B	30	SER	CA-C-N	5.54	128.73	120.31
1	B	30	SER	C-N-CA	5.54	128.73	120.31
1	A	196	THR	N-CA-C	5.53	119.20	112.23
1	B	71	LEU	N-CA-C	-5.52	102.96	110.36
1	B	137	LYS	N-CA-CB	5.47	119.36	110.05
1	A	199	ASP	O-C-N	5.47	126.87	121.57
1	B	252	LEU	N-CA-CB	-5.45	101.26	111.13
1	B	101	VAL	N-CA-CB	5.44	120.04	111.99
1	B	216	ASN	N-CA-CB	-5.44	103.05	111.65
1	B	106	ILE	O-C-N	5.42	126.51	121.96
1	B	90	GLU	N-CA-C	5.41	117.87	111.33
1	A	251	VAL	CB-CA-C	5.39	119.13	110.82
1	B	251	VAL	N-CA-C	-5.38	100.56	108.85
1	A	18	LEU	CB-CA-C	5.37	119.70	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	THR	CA-CB-OG1	-5.33	101.61	109.60
1	A	6	TRP	N-CA-C	5.32	119.08	112.59
1	B	144	THR	O-C-N	5.30	124.57	120.38
1	B	130	ASP	N-CA-C	5.28	118.22	109.46
1	A	46	LYS	O-C-N	5.24	125.92	121.20
1	A	213	LYS	CA-C-N	5.22	127.27	120.28
1	A	213	LYS	C-N-CA	5.22	127.27	120.28
1	B	107	SER	CA-C-N	5.22	125.74	120.00
1	B	107	SER	C-N-CA	5.22	125.74	120.00
1	B	213	LYS	CA-C-N	5.21	127.22	120.44
1	B	213	LYS	C-N-CA	5.21	127.22	120.44
1	B	324	LYS	CA-C-N	5.21	125.77	119.98
1	B	324	LYS	C-N-CA	5.21	125.77	119.98
1	A	348	HIS	N-CA-C	5.21	117.25	110.43
1	B	184	SER	N-CA-C	-5.19	103.06	110.59
1	A	225	TYR	CA-C-O	-5.18	114.42	120.53
1	B	87	ALA	CA-C-N	5.17	127.63	120.29
1	B	87	ALA	C-N-CA	5.17	127.63	120.29
1	A	294	MET	N-CA-CB	5.16	118.19	110.19
1	B	171	THR	CA-CB-OG1	-5.16	101.86	109.60
1	B	89	GLY	CA-C-N	5.16	127.44	120.38
1	B	89	GLY	C-N-CA	5.16	127.44	120.38
1	B	44	ASN	CA-CB-CG	5.12	117.72	112.60
1	B	121	ARG	N-CA-C	5.12	116.67	111.14
1	A	320	LEU	CB-CA-C	5.09	119.24	110.79
1	A	282	ARG	N-CA-CB	5.08	117.44	110.07
1	B	225	TYR	N-CA-C	5.07	118.56	111.56
1	A	137	LYS	CB-CA-C	-5.06	104.55	110.17
1	A	182	GLU	N-CA-CB	5.04	117.44	109.83
1	B	201	ARG	N-CA-C	-5.04	103.75	110.55
1	B	205	TRP	CA-CB-CG	5.03	123.15	113.60
1	B	316	ARG	NE-CZ-NH2	5.02	123.72	119.20

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	3161	0	3151	46	1
1	B	3161	0	3151	55	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	12	2
All	All	7022	0	6314	97	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 8.

All (97) 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
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: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:A:333:MET:HE3	3:A:671:HOH:O	1.89	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:278:GLU:CD	1:A:282:ARG:HE	2.15	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:A:18:LEU:C	1:A:18:LEU:HD23	2.33	0.53
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
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: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:B:294:MET:HE3	3:B:420:HOH:O	2.13	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:137:LYS:NZ	3:B:720:HOH:O	2.44	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:67:ASP:C	1:A:67:ASP:OD1	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:262:LEU:O	1:B:263:TYR:C	2.60	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
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:B:27:ASP:OD1	1:B:28:THR:N	2.53	0.41
1:B:406:GLN:CD	1:B:410:LYS:HE3	2.44	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:377:PHE:O	1:B:399:TYR:OH	2.24	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

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	399/401 (100%)	389 (98%)	9 (2%)	1 (0%)	36	29
1	B	399/401 (100%)	385 (96%)	13 (3%)	1 (0%)	36	29
All	All	798/802 (100%)	774 (97%)	22 (3%)	2 (0%)	36	29

All (2) Ramachandran outliers are listed below:

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

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	335/335 (100%)	315 (94%)	20 (6%)	17	9
1	B	335/335 (100%)	314 (94%)	21 (6%)	16	8
All	All	670/670 (100%)	629 (94%)	41 (6%)	17	9

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	59	MET
1	A	90	GLU
1	A	101	VAL

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Mol	Chain	Res	Type
1	A	107	SER
1	A	124	LYS
1	A	125	PHE
1	A	195	PRO
1	A	214	LYS
1	A	215	ARG
1	A	259	ASN
1	A	278	GLU
1	A	281	LYS
1	A	292	ARG
1	A	314	GLU
1	A	339	SER
1	A	343	LYS
1	A	359	MET
1	A	362	PHE
1	A	366	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	125	PHE
1	B	138	PRO
1	B	164	LYS
1	B	195	PRO
1	B	202	GLN
1	B	210	SER
1	B	296	SER
1	B	339	SER
1	B	362	PHE
1	B	366	LYS
1	B	368	GLU
1	B	383	LYS
1	B	395	SER
1	B	410	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS

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Mol	Chain	Res	Type
1	A	44	ASN
1	A	246	GLN
1	A	259	ASN
1	A	297	ASN
1	A	336	GLN
1	A	340	ASN
1	A	351	GLN
1	B	91	ASN
1	B	154	GLN
1	B	202	GLN
1	B	204	GLN
1	B	216	ASN
1	B	226	GLN
1	B	286	GLN
1	B	297	ASN
1	B	340	ASN
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 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	1.70	4 (26%)	21,22,23	2.39	10 (47%)
2	PLP	A	411	1	15,15,16	1.71	3 (20%)	21,22,23	2.37	9 (42%)

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	-3.47	1.44	1.51
2	B	411	PLP	C4A-C4	-3.23	1.45	1.51
2	A	411	PLP	C5-C4	3.13	1.44	1.40
2	B	411	PLP	C5-C4	3.08	1.44	1.40
2	B	411	PLP	C3-C2	2.58	1.43	1.41
2	A	411	PLP	C3-C2	2.31	1.43	1.41
2	B	411	PLP	P-O2P	-2.11	1.47	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PLP	C2A-C2-C3	5.85	127.64	120.80
2	B	411	PLP	C2A-C2-C3	4.62	126.20	120.80
2	B	411	PLP	C6-C5-C4	4.34	121.65	118.10
2	A	411	PLP	C6-C5-C4	3.76	121.18	118.10
2	B	411	PLP	O3-C3-C4	3.73	127.85	118.10
2	A	411	PLP	O3-C3-C4	3.60	127.51	118.10
2	B	411	PLP	O4P-C5A-C5	3.53	115.97	109.36
2	B	411	PLP	C5A-C5-C4	-3.28	116.16	122.64
2	A	411	PLP	C3-C2-N1	-3.22	116.90	120.96
2	A	411	PLP	C6-N1-C2	3.01	124.66	119.20
2	A	411	PLP	C5-C6-N1	-2.89	119.13	123.83
2	B	411	PLP	O3-C3-C2	-2.76	111.86	117.58
2	B	411	PLP	C5-C6-N1	-2.73	119.39	123.83
2	A	411	PLP	C5A-C5-C4	-2.63	117.44	122.64
2	A	411	PLP	O3-C3-C2	-2.62	112.15	117.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PLP	O4P-C5A-C5	2.59	114.21	109.36
2	B	411	PLP	C3-C2-N1	-2.55	117.74	120.96
2	B	411	PLP	C4A-C4-C5	2.44	123.45	120.94
2	B	411	PLP	C6-N1-C2	2.41	123.57	119.20

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

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.