



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:36 AM GMT

PDB ID : 1TAR  
Title : CRYSTALLINE MITOCHONDRIAL ASPARTATE AMINOTRANS-  
FERASE EXISTS IN ONLY TWO CONFORMATIONS  
Authors : Hohenester, E.; Jansonius, J.N.  
Deposited on : 1993-10-04  
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

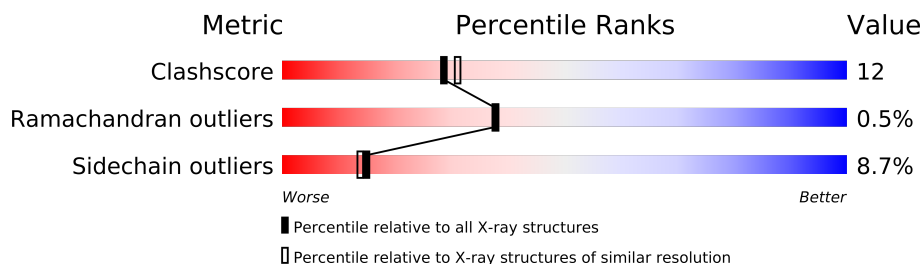
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 6580 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

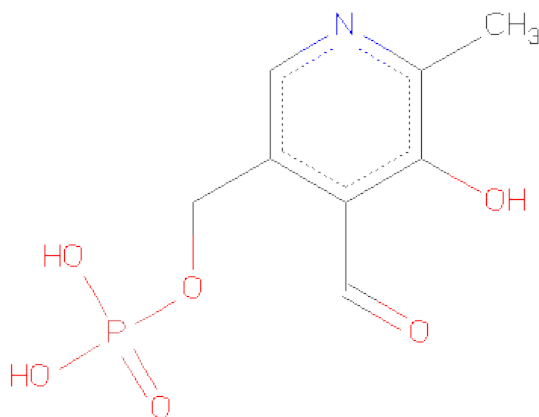
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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 (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

*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	118	Total	O	0	0
			118	118		
3	B	110	Total	O	0	0
			110	110		

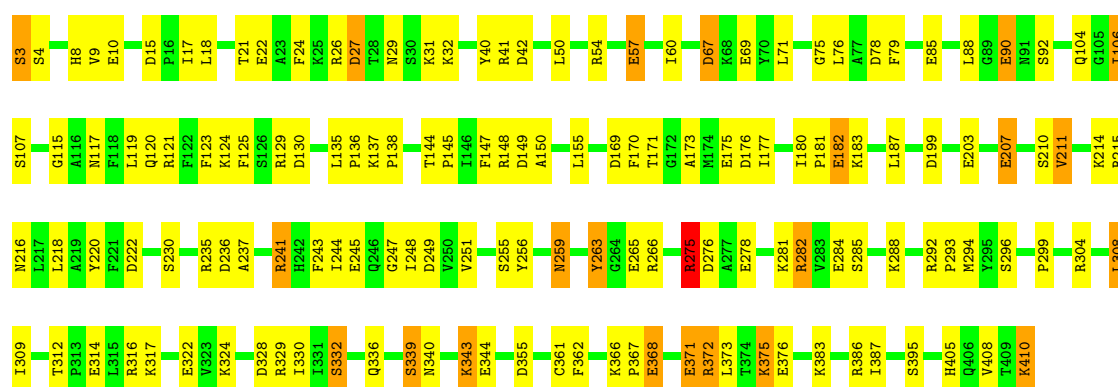
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

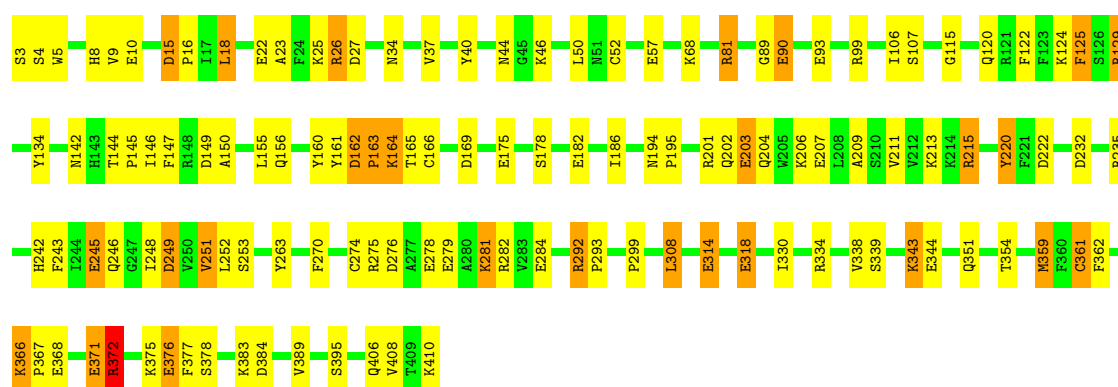
#### • Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A:



#### • Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain B:



## 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, $\alpha$ , $\beta$ , $\gamma$	57.40Å 59.40Å 65.50Å 83.10° 104.80° 83.30°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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	0.96	17/3231 (0.5%)	1.37	47/4360 (1.1%)
1	B	0.98	17/3231 (0.5%)	1.31	30/4360 (0.7%)
All	All	0.97	34/6462 (0.5%)	1.34	77/8720 (0.9%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	GLU	CD-OE1	8.31	1.34	1.25
1	A	22	GLU	CD-OE1	8.28	1.34	1.25
1	B	376	GLU	CD-OE1	8.10	1.34	1.25
1	B	284	GLU	CD-OE1	7.96	1.34	1.25
1	A	278	GLU	CD-OE2	7.83	1.34	1.25
1	B	22	GLU	CD-OE1	7.79	1.34	1.25
1	A	57	GLU	CD-OE1	7.78	1.34	1.25
1	A	182	GLU	CD-OE2	7.62	1.34	1.25
1	B	371	GLU	CD-OE2	7.58	1.33	1.25
1	B	344	GLU	CD-OE1	7.52	1.33	1.25
1	B	57	GLU	CD-OE1	7.23	1.33	1.25
1	B	10	GLU	CD-OE1	7.14	1.33	1.25
1	B	314	GLU	CD-OE1	7.06	1.33	1.25
1	A	371	GLU	CD-OE2	6.98	1.33	1.25
1	A	368	GLU	CD-OE2	6.77	1.33	1.25
1	B	90	GLU	CD-OE1	6.68	1.33	1.25
1	A	203	GLU	CD-OE1	6.64	1.32	1.25
1	A	314	GLU	CD-OE2	6.61	1.32	1.25
1	B	318	GLU	CD-OE1	6.54	1.32	1.25
1	A	10	GLU	CD-OE2	6.44	1.32	1.25
1	B	182	GLU	CD-OE2	6.41	1.32	1.25
1	A	245	GLU	CD-OE1	6.41	1.32	1.25
1	B	175	GLU	CD-OE2	6.34	1.32	1.25
1	B	245	GLU	CD-OE1	6.21	1.32	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	GLU	CD-OE2	6.18	1.32	1.25
1	B	203	GLU	CD-OE2	6.16	1.32	1.25
1	A	265	GLU	CD-OE2	6.09	1.32	1.25
1	A	90	GLU	CD-OE2	6.03	1.32	1.25
1	B	207	GLU	CD-OE2	5.85	1.32	1.25
1	A	322	GLU	CD-OE1	5.55	1.31	1.25
1	A	284	GLU	CD-OE1	5.46	1.31	1.25
1	B	278	GLU	CD-OE2	5.42	1.31	1.25
1	A	85	GLU	CD-OE2	5.34	1.31	1.25
1	A	207	GLU	CD-OE2	5.07	1.31	1.25

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ARG	NE-CZ-NH2	9.71	125.16	120.30
1	A	236	ASP	CB-CG-OD1	9.21	126.58	118.30
1	A	169	ASP	CB-CG-OD1	8.96	126.37	118.30
1	B	249	ASP	CB-CG-OD1	8.89	126.30	118.30
1	A	42	ASP	CB-CG-OD1	8.78	126.20	118.30
1	B	249	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	A	27	ASP	CB-CG-OD2	-8.64	110.53	118.30
1	A	215	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	176	ASP	CB-CG-OD1	8.54	125.99	118.30
1	A	169	ASP	CB-CG-OD2	-8.37	110.77	118.30
1	B	292	ARG	NE-CZ-NH1	-8.29	116.15	120.30
1	A	121	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	B	222	ASP	CB-CG-OD1	7.77	125.30	118.30
1	A	275	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	A	275	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	27	ASP	CB-CG-OD1	7.45	125.01	118.30
1	A	249	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	249	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	A	67	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	372	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	B	232	ASP	CB-CG-OD1	-7.29	111.74	118.30
1	A	41	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	A	236	ASP	CB-CG-OD2	-7.16	111.85	118.30
1	B	15	ASP	CB-CG-OD1	-7.16	111.85	118.30
1	A	182	GLU	CB-CA-C	7.04	124.48	110.40
1	B	276	ASP	CB-CG-OD1	-7.03	111.98	118.30
1	A	42	ASP	CB-CG-OD2	-6.99	112.00	118.30
1	A	176	ASP	CB-CG-OD2	-6.95	112.05	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ASP	CB-CG-OD2	6.84	124.46	118.30
1	B	40	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	B	372	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	B	276	ASP	CB-CG-OD2	6.77	124.39	118.30
1	B	162	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	B	384	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	222	ASP	CB-CG-OD1	6.56	124.21	118.30
1	A	26	ARG	CA-CB-CG	-6.41	99.30	113.40
1	A	276	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	27	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	241	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	355	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	15	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	B	27	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	169	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	235	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	A	276	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	129	ARG	CB-CA-C	-5.88	98.64	110.40
1	B	160	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	B	169	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	149	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	A	67	ASP	CB-CG-OD2	-5.71	113.17	118.30
1	A	329	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	251	VAL	N-CA-CB	5.67	123.98	111.50
1	A	130	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	B	162	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	129	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	215	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	149	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	B	99	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	384	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	251	VAL	N-CA-CB	5.47	123.54	111.50
1	B	15	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	329	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	241	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	78	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	282	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	266	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	A	130	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	355	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	199	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	163	PRO	N-CA-CB	5.15	109.47	103.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	A	26	ARG	O-C-N	5.11	130.87	122.70
1	A	222	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	121	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	232	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	81	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	A	386	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3161	0	3152	85	0
1	B	3161	0	3152	85	1
2	A	15	0	6	0	0
2	B	15	0	6	1	0
3	A	118	0	0	9	0
3	B	110	0	0	2	0
All	All	6580	0	6316	158	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (158) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:201:ARG:H	1:B:204:GLN:HE21	1.20	0.90
1:B:292:ARG:HB3	1:B:293:PRO:HD3	1.58	0.86
1:B:371:GLU:HG2	1:B:375:LYS:NZ	1.91	0.83
1:A:275:ARG:HG2	1:A:275:ARG:HH11	1.44	0.81
1:A:343:LYS:HB2	1:A:343:LYS:NZ	1.98	0.78
1:A:24:PHE:CE1	1:A:32:LYS:HG3	2.19	0.77
1:A:343:LYS:HE2	3:A:686:HOH:O	1.83	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:371:GLU:HG2	1:B:375:LYS:HZ2	1.49	0.74
1:A:106:ILE:HD12	1:B:106:ILE:HD13	1.68	0.74
1:A:8:HIS:CD2	1:A:8:HIS:H	2.06	0.73
1:A:371:GLU:HG3	1:A:383:LYS:NZ	2.04	0.73
1:B:147:PHE:HB2	1:B:155:LEU:HD21	1.72	0.71
1:A:332:SER:O	1:A:336:GLN:HG3	1.92	0.70
1:A:367:PRO:HD3	3:A:720:HOH:O	1.93	0.69
1:B:52:CYS:HB3	1:B:318:GLU:HG2	1.74	0.69
1:A:237:ALA:O	1:A:241:ARG:HG3	1.92	0.69
1:B:243:PHE:O	1:B:248:ILE:HB	1.93	0.68
1:B:81:ARG:HH11	1:B:81:ARG:HG2	1.59	0.68
1:B:314:GLU:HG3	1:B:314:GLU:O	1.94	0.68
1:A:71:LEU:O	3:A:688:HOH:O	2.11	0.67
1:B:201:ARG:HD2	1:B:203:GLU:OE2	1.93	0.67
1:A:3:SER:N	1:B:249:ASP:OD2	2.29	0.66
1:A:173:ALA:O	1:A:177:ILE:HG13	1.97	0.64
1:A:339:SER:O	1:A:343:LYS:NZ	2.30	0.64
1:B:275:ARG:HG2	1:B:275:ARG:HH11	1.63	0.64
1:B:201:ARG:H	1:B:204:GLN:NE2	1.96	0.63
1:B:162:ASP:OD2	1:B:164:LYS:NZ	2.29	0.63
1:A:375:LYS:HD3	1:A:375:LYS:N	2.12	0.63
1:A:207:GLU:O	1:A:211:VAL:HG12	2.00	0.62
1:B:274:CYS:HB3	1:B:279:GLU:HG2	1.81	0.61
1:A:75:GLY:HA3	1:A:104:GLN:HB3	1.83	0.60
1:A:8:HIS:H	1:A:8:HIS:HD2	1.48	0.60
1:A:76:LEU:HB3	1:A:79:PHE:HB3	1.84	0.59
1:B:201:ARG:NH1	1:B:203:GLU:OE2	2.29	0.59
1:A:120:GLN:HG3	1:A:150:ALA:O	2.02	0.59
1:A:275:ARG:CG	1:A:275:ARG:HH11	2.13	0.59
1:A:361:CYS:HB3	1:A:387:ILE:HG12	1.83	0.58
1:A:9:VAL:O	1:B:282:ARG:HD2	2.03	0.58
1:B:274:CYS:HB3	1:B:279:GLU:OE2	2.02	0.58
1:A:343:LYS:HB2	1:A:343:LYS:HZ2	1.67	0.58
1:B:242:HIS:O	1:B:246:GLN:HG2	2.05	0.57
1:A:371:GLU:HG3	1:A:383:LYS:HZ1	1.69	0.57
1:A:324:LYS:NZ	1:A:328:ASP:OD2	2.35	0.57
1:A:263:TYR:HB2	1:B:68:LYS:O	2.04	0.57
1:B:372:ARG:O	1:B:376:GLU:HG3	2.05	0.56
1:A:371:GLU:HG3	1:A:383:LYS:HZ3	1.71	0.56
1:A:171:THR:HG22	3:A:681:HOH:O	2.06	0.55
1:A:282:ARG:HD2	1:B:9:VAL:O	2.06	0.55
1:A:405:HIS:CE1	1:A:410:LYS:HE2	2.42	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:29:ASN:OD1	1:A:31:LYS:HB2	2.07	0.55
1:A:343:LYS:HB2	1:A:343:LYS:HZ3	1.72	0.54
1:A:183:LYS:HG2	1:A:216:ASN:ND2	2.22	0.54
1:B:220:TYR:CD1	1:B:251:VAL:HG23	2.43	0.54
1:A:124:LYS:HD3	1:B:8:HIS:CD2	2.43	0.53
1:B:371:GLU:HG2	1:B:375:LYS:HZ3	1.73	0.53
1:B:275:ARG:CG	1:B:275:ARG:HH11	2.20	0.53
1:A:275:ARG:HG2	1:A:275:ARG:NH1	2.20	0.53
1:B:129:ARG:HA	1:B:129:ARG:HE	1.72	0.52
1:B:406:GLN:OE1	1:B:410:LYS:HE2	2.09	0.52
1:B:334:ARG:HH12	1:B:361:CYS:HB2	1.74	0.52
1:A:144:THR:HG23	1:A:155:LEU:HD13	1.91	0.52
1:B:213:LYS:HD2	1:B:246:GLN:O	2.10	0.52
1:B:23:ALA:HA	1:B:26:ARG:HD2	1.92	0.52
1:A:123:PHE:HE1	1:B:5:TRP:CE3	2.28	0.52
1:B:144:THR:HB	1:B:145:PRO:HD3	1.92	0.51
1:A:3:SER:OG	1:A:4:SER:N	2.43	0.51
1:B:81:ARG:CG	1:B:81:ARG:HH11	2.24	0.51
1:A:395:SER:HB3	3:A:518:HOH:O	2.10	0.51
1:A:115:GLY:O	1:A:119:LEU:HG	2.10	0.51
1:B:343:LYS:O	1:B:343:LYS:HG3	2.09	0.51
1:B:211:VAL:HG23	3:B:682:HOH:O	2.11	0.50
1:A:18:LEU:C	1:A:18:LEU:HD23	2.31	0.50
1:A:183:LYS:HG2	1:A:216:ASN:HD22	1.76	0.50
1:A:123:PHE:CE1	1:B:5:TRP:CE3	2.99	0.50
1:A:368:GLU:CD	1:A:368:GLU:H	2.15	0.50
1:A:8:HIS:CE1	1:B:124:LYS:HG2	2.47	0.50
1:B:371:GLU:O	1:B:375:LYS:HD3	2.12	0.49
1:A:230:SER:HB2	1:A:235:ARG:HH11	1.76	0.49
1:B:330:ILE:HG23	1:B:389:VAL:CG1	2.43	0.49
1:A:372:ARG:NE	1:A:376:GLU:OE2	2.45	0.49
1:B:274:CYS:CB	1:B:279:GLU:HG2	2.42	0.49
1:B:115:GLY:HA2	1:B:270:PHE:CZ	2.48	0.48
1:A:57:GLU:OE2	1:B:68:LYS:NZ	2.41	0.48
1:A:340:ASN:O	1:A:344:GLU:HG2	2.12	0.48
1:A:129:ARG:HB2	3:A:717:HOH:O	2.12	0.48
1:B:292:ARG:CB	1:B:293:PRO:HD3	2.35	0.48
1:B:15:ASP:OD2	1:B:18:LEU:HB2	2.14	0.48
1:A:299:PRO:HG3	1:B:299:PRO:HG3	1.96	0.48
1:B:209:ALA:HB2	1:B:243:PHE:CE1	2.49	0.48
1:B:164:LYS:HB2	1:B:164:LYS:HE2	1.69	0.47
1:B:142:ASN:O	1:B:146:ILE:HD12	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:252:LEU:HG	1:B:253:SER:N	2.28	0.47
1:B:201:ARG:N	1:B:204:GLN:HE21	2.01	0.47
1:A:67:ASP:OD1	1:A:69:GLU:N	2.34	0.47
1:A:243:PHE:O	1:A:248:ILE:HB	2.15	0.47
1:B:50:LEU:N	1:B:50:LEU:HD12	2.30	0.47
1:A:50:LEU:H	1:A:50:LEU:HD12	1.80	0.47
1:B:366:LYS:HB3	1:B:367:PRO:HD2	1.98	0.46
1:B:81:ARG:CZ	1:B:81:ARG:HB3	2.46	0.46
1:A:244:ILE:O	1:A:247:GLY:N	2.45	0.46
1:A:256:TYR:HA	1:A:259:ASN:HD21	1.81	0.46
1:A:309:ILE:O	1:A:316:ARG:HB2	2.16	0.46
1:A:292:ARG:HB3	1:A:293:PRO:HD3	1.98	0.46
1:B:165:THR:O	1:B:166:CYS:HB2	2.16	0.46
1:B:194:ASN:HB3	2:B:411:PLP:H2A1	1.97	0.45
1:A:230:SER:CB	1:A:235:ARG:HD2	2.46	0.45
1:B:18:LEU:HA	1:B:18:LEU:HD23	1.73	0.45
1:A:405:HIS:CE1	1:A:410:LYS:CE	3.00	0.45
1:A:308:LEU:O	1:A:312:THR:HB	2.16	0.45
1:B:275:ARG:CG	1:B:275:ARG:NH1	2.79	0.45
1:A:148:ARG:HD3	3:A:680:HOH:O	2.17	0.45
1:B:377:PHE:O	1:B:378:SER:HB2	2.17	0.45
1:B:81:ARG:CG	1:B:81:ARG:NH1	2.79	0.45
1:A:4:SER:O	1:A:4:SER:OG	2.29	0.45
1:A:372:ARG:HE	1:A:376:GLU:CD	2.20	0.45
1:B:359:MET:HG3	1:B:359:MET:O	2.16	0.45
1:B:134:TYR:CD2	1:B:156:GLN:HB2	2.52	0.45
1:B:34:ASN:O	1:B:37:VAL:HG23	2.17	0.45
1:B:330:ILE:HG23	1:B:389:VAL:HG11	1.98	0.44
1:B:281:LYS:HD2	1:B:281:LYS:HA	1.82	0.44
1:A:129:ARG:HE	1:A:129:ARG:HA	1.82	0.44
1:A:8:HIS:HE1	1:B:122:PHE:O	2.00	0.44
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.76	0.44
1:B:129:ARG:CA	1:B:129:ARG:HE	2.31	0.44
1:A:405:HIS:NE2	1:A:410:LYS:CE	2.80	0.44
1:A:88:LEU:CD2	1:A:244:ILE:HD12	2.47	0.44
1:B:338:VAL:HG21	1:B:354:THR:HG23	2.00	0.44
1:A:180:ILE:HG23	1:A:181:PRO:HD2	2.00	0.43
1:B:161:TYR:O	1:B:163:PRO:HD3	2.18	0.43
1:B:164:LYS:H	1:B:164:LYS:HG3	1.55	0.43
1:B:134:TYR:CE2	1:B:156:GLN:HB3	2.53	0.43
1:B:89:GLY:HA3	3:B:722:HOH:O	2.19	0.43
1:A:117:ASN:ND2	1:A:294:MET:CE	2.82	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:THR:HB	1:B:145:PRO:CD	2.48	0.43
1:A:137:LYS:HA	1:A:138:PRO:HA	1.87	0.43
1:B:206:LYS:HG2	1:B:242:HIS:CE1	2.53	0.43
1:A:144:THR:HB	1:A:145:PRO:HD3	2.01	0.43
1:B:178:SER:O	1:B:215:ARG:NH1	2.52	0.43
1:A:147:PHE:HB2	1:A:155:LEU:HD21	2.01	0.42
1:B:178:SER:O	1:B:215:ARG:HD3	2.19	0.42
1:A:8:HIS:CD2	1:A:8:HIS:N	2.79	0.42
1:A:60:ILE:HD11	1:A:304:ARG:HB3	2.01	0.42
1:B:274:CYS:HB3	1:B:279:GLU:CG	2.49	0.42
1:B:120:GLN:HG3	1:B:150:ALA:O	2.19	0.42
1:A:67:ASP:OD1	1:A:69:GLU:HG2	2.20	0.42
1:A:40:TYR:HE1	1:A:330:ILE:HD13	1.85	0.42
1:A:50:LEU:HD12	1:A:50:LEU:N	2.34	0.41
1:A:230:SER:OG	1:A:235:ARG:HD2	2.20	0.41
1:B:15:ASP:OD1	1:B:16:PRO:HD2	2.20	0.41
1:B:194:ASN:HA	1:B:195:PRO:HA	1.85	0.41
1:B:215:ARG:HE	1:B:215:ARG:HB3	1.76	0.41
1:A:135:LEU:HB3	1:A:136:PRO:HD2	2.03	0.41
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.70	0.41
1:A:54:ARG:HH11	1:A:54:ARG:HD3	1.71	0.41
1:B:125:PHE:N	1:B:125:PHE:CD1	2.78	0.41
1:A:170:PHE:N	3:A:681:HOH:O	2.54	0.40
1:A:218:LEU:HA	3:A:524:HOH:O	2.22	0.40
1:B:186:ILE:HG23	1:B:186:ILE:O	2.22	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:B:124:LYS:NZ	1:B:395:SER:OG[1_565]	2.12	0.08

## 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%)	381 (96%)	16 (4%)	2 (0%)	38	38
1	B	399/401 (100%)	378 (95%)	19 (5%)	2 (0%)	38	38
All	All	798/802 (100%)	759 (95%)	35 (4%)	4 (0%)	38	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR
1	B	263	TYR
1	A	27	ASP
1	B	4	SER

### 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%)	304 (91%)	31 (9%)	13	12
1	B	335/335 (100%)	308 (92%)	27 (8%)	17	16
All	All	670/670 (100%)	612 (91%)	58 (9%)	15	14

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	17	ILE
1	A	21	THR
1	A	90	GLU
1	A	92	SER
1	A	106	ILE
1	A	107	SER
1	A	125	PHE
1	A	182	GLU
1	A	187	LEU
1	A	210	SER
1	A	211	VAL
1	A	214	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	220	TYR
1	A	255	SER
1	A	259	ASN
1	A	275	ARG
1	A	281	LYS
1	A	285	SER
1	A	288	LYS
1	A	296	SER
1	A	308	LEU
1	A	317	LYS
1	A	332	SER
1	A	339	SER
1	A	343	LYS
1	A	362	PHE
1	A	366	LYS
1	A	375	LYS
1	A	408	VAL
1	A	410	LYS
1	B	3	SER
1	B	18	LEU
1	B	25	LYS
1	B	26	ARG
1	B	44	ASN
1	B	46	LYS
1	B	90	GLU
1	B	107	SER
1	B	125	PHE
1	B	164	LYS
1	B	202	GLN
1	B	215	ARG
1	B	220	TYR
1	B	245	GLU
1	B	281	LYS
1	B	308	LEU
1	B	339	SER
1	B	343	LYS
1	B	351	GLN
1	B	359	MET
1	B	361	CYS
1	B	362	PHE
1	B	366	LYS
1	B	368	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	372	ARG
1	B	383	LYS
1	B	408	VAL

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

Mol	Chain	Res	Type
1	A	8	HIS
1	A	44	ASN
1	A	216	ASN
1	A	259	ASN
1	A	340	ASN
1	A	351	GLN
1	B	44	ASN
1	B	202	GLN
1	B	204	GLN
1	B	226	GLN
1	B	348	HIS
1	B	351	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	411	1	14,15,16	1.39	2 (14%)	20,22,23	2.47	7 (35%)
2	PLP	B	411	1	14,15,16	1.59	3 (21%)	20,22,23	2.33	6 (30%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	PLP	C4-C5	3.57	1.45	1.39
2	B	411	PLP	C3-C2	3.27	1.43	1.40
2	A	411	PLP	C3-C2	2.69	1.42	1.40
2	A	411	PLP	C4-C5	2.54	1.43	1.39
2	B	411	PLP	C2-N1	2.25	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PLP	C2A-C2-C3	6.13	128.47	121.02
2	B	411	PLP	C2A-C2-C3	5.16	127.29	121.02
2	A	411	PLP	O4P-C5A-C5	4.87	119.16	109.26
2	B	411	PLP	O4P-C5A-C5	4.31	118.02	109.26
2	B	411	PLP	C3-C2-N1	-4.04	115.11	120.66
2	B	411	PLP	C6-N1-C2	3.75	127.32	119.28
2	B	411	PLP	C5-C6-N1	-3.68	117.22	123.86
2	A	411	PLP	C3-C2-N1	-3.56	115.78	120.66
2	A	411	PLP	C5-C6-N1	-3.36	117.80	123.86
2	A	411	PLP	C6-N1-C2	3.33	126.42	119.28
2	A	411	PLP	C3-C4-C5	-3.00	115.62	121.29
2	A	411	PLP	C4-C3-C2	2.25	122.25	119.67
2	B	411	PLP	C3-C4-C5	-2.02	117.46	121.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.