



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:50 PM UTC

PDB ID : 1TAR / pdb_00001tar
Title : CRYSTALLINE MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE 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 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

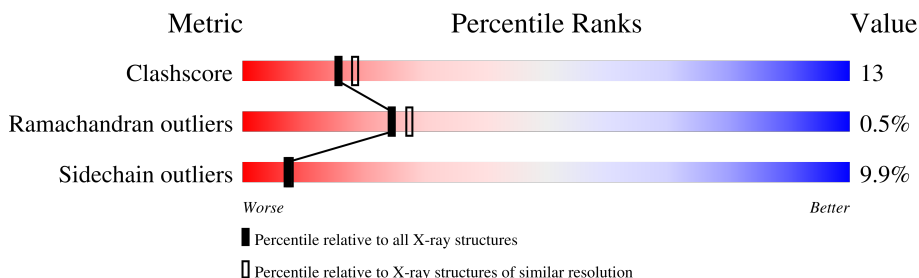
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 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 6580 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.

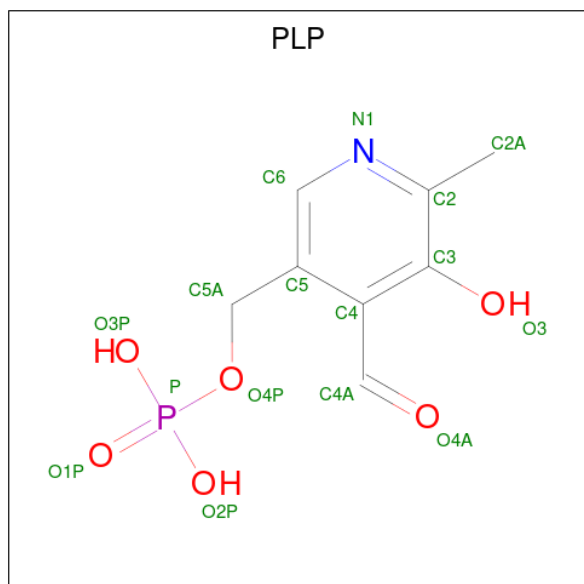
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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: $C_8H_{10}NO_6P$).



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		

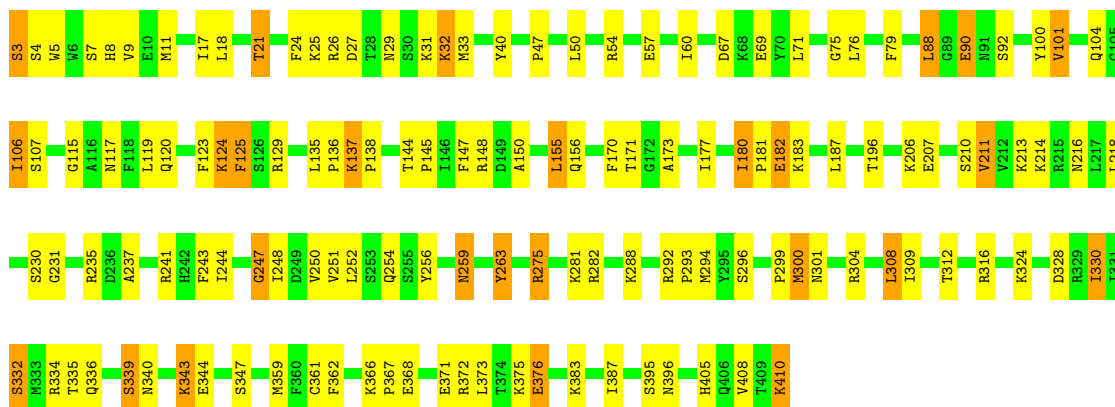
3 Residue-property plots [i](#)

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.

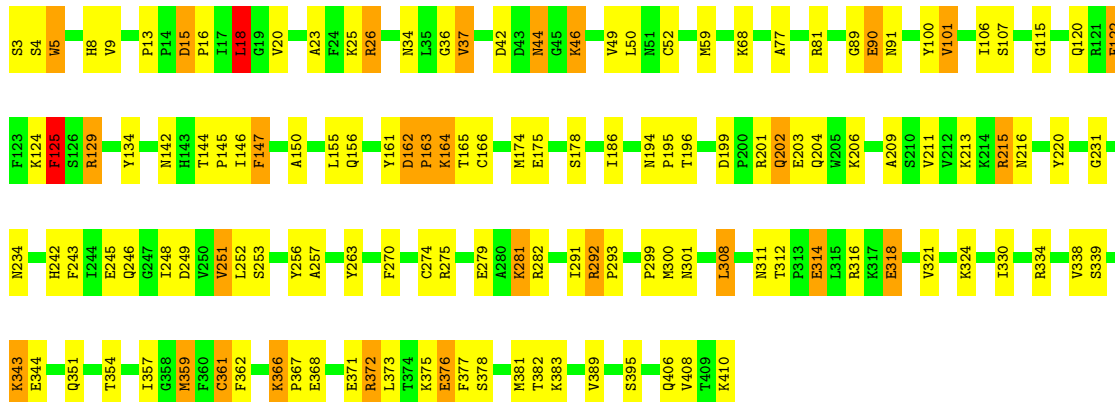
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A: 



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain B: 



4 Data and refinement statistics

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	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 ²)	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	1.11	0/3231	1.59	33/4360 (0.8%)
1	B	1.13	2/3231 (0.1%)	1.63	45/4360 (1.0%)
All	All	1.12	2/6462 (0.0%)	1.61	78/8720 (0.9%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	ARG	C-O	-5.36	1.19	1.24
1	B	256	TYR	CA-CB	5.22	1.61	1.53

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	GLU	CB-CA-C	9.41	124.48	109.61
1	A	26	ARG	O-C-N	8.50	130.87	122.03
1	B	291	ILE	N-CA-C	8.33	118.90	110.82
1	A	251	VAL	N-CA-CB	7.64	123.98	111.44
1	A	125	PHE	N-CA-C	7.56	119.60	111.36
1	A	26	ARG	CA-CB-CG	-7.40	99.30	114.10
1	B	251	VAL	N-CA-CB	7.38	123.54	111.44
1	A	101	VAL	N-CA-CB	7.36	121.21	111.64
1	B	344	GLU	N-CA-C	-7.35	104.12	113.23
1	A	206	LYS	N-CA-C	-7.33	102.07	111.02
1	A	300	MET	N-CA-C	7.09	121.17	112.23
1	A	25	LYS	N-CA-C	7.04	118.61	111.07
1	B	324	LYS	N-CA-C	-7.00	103.65	111.28
1	B	357	ILE	CA-C-N	-6.93	112.67	122.85
1	B	357	ILE	C-N-CA	-6.93	112.67	122.85
1	B	129	ARG	CB-CA-C	-6.83	98.64	110.17
1	B	234	ASN	CA-CB-CG	-6.74	105.86	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	THR	CA-C-N	6.70	131.41	120.63
1	B	382	THR	C-N-CA	6.70	131.41	120.63
1	A	359	MET	N-CA-C	6.66	119.36	111.71
1	B	13	PRO	CA-C-N	6.63	126.59	119.76
1	B	13	PRO	C-N-CA	6.63	126.59	119.76
1	B	292	ARG	NE-CZ-NH2	6.62	125.16	119.20
1	B	301	ASN	N-CA-C	6.61	119.09	111.02
1	A	88	LEU	N-CA-C	6.59	119.47	111.82
1	B	196	THR	N-CA-C	6.52	120.44	112.23
1	B	257	ALA	N-CA-C	6.49	118.36	111.28
1	B	91	ASN	CB-CA-C	6.48	120.15	111.14
1	B	163	PRO	N-CA-CB	6.47	109.47	103.46
1	B	311	ASN	N-CA-C	6.39	120.28	112.23
1	B	316	ARG	N-CA-C	-6.31	104.32	111.14
1	A	252	LEU	N-CA-C	6.22	118.75	108.99
1	B	147	PHE	CA-CB-CG	-6.17	107.63	113.80
1	B	77	ALA	N-CA-C	6.17	118.79	111.33
1	B	357	ILE	N-CA-C	6.14	116.77	108.17
1	A	21	THR	N-CA-C	6.12	118.03	111.36
1	B	91	ASN	CA-CB-CG	-6.00	106.60	112.60
1	B	231	GLY	N-CA-C	-5.97	107.16	114.92
1	B	125	PHE	CA-CB-CG	-5.95	107.85	113.80
1	B	90	GLU	N-CA-C	5.85	117.66	111.28
1	B	5	TRP	CB-CA-C	-5.79	101.17	110.79
1	A	7	SER	N-CA-C	5.76	118.33	111.71
1	A	254	GLN	CB-CG-CD	-5.73	102.86	112.60
1	B	122	PHE	N-CA-C	5.69	121.11	113.72
1	B	314	GLU	N-CA-C	5.66	118.22	111.71
1	B	202	GLN	CB-CA-C	5.63	119.82	110.81
1	A	196	THR	N-CA-C	5.60	120.23	112.45
1	A	213	LYS	N-CA-C	-5.54	104.93	110.97
1	A	21	THR	N-CA-CB	5.54	118.35	110.16
1	B	59	MET	N-CA-C	-5.53	105.15	111.07
1	A	137	LYS	CB-CA-C	-5.53	104.03	110.17
1	A	5	TRP	CB-CA-C	-5.46	100.71	110.70
1	B	162	ASP	CA-C-N	-5.45	114.14	119.64
1	B	162	ASP	C-N-CA	-5.45	114.14	119.64
1	A	180	ILE	CA-C-N	5.43	125.70	119.83
1	A	180	ILE	C-N-CA	5.43	125.70	119.83
1	B	49	VAL	N-CA-C	-5.39	99.31	107.73
1	B	199	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	32	LYS	N-CA-C	5.35	117.98	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	B	18	LEU	CA-C-N	5.34	125.91	119.98
1	B	18	LEU	C-N-CA	5.34	125.91	119.98
1	B	101	VAL	N-CA-CB	5.33	119.88	111.99
1	A	301	ASN	N-CA-C	5.29	117.47	111.02
1	A	247	GLY	CA-C-N	-5.24	116.19	122.90
1	A	247	GLY	C-N-CA	-5.24	116.19	122.90
1	A	90	GLU	N-CA-C	5.23	117.06	111.36
1	A	231	GLY	N-CA-C	-5.19	107.95	115.27
1	B	36	GLY	CA-C-N	5.17	127.51	120.63
1	B	36	GLY	C-N-CA	5.17	127.51	120.63
1	A	334	ARG	N-CA-C	-5.11	105.71	111.28
1	A	47	PRO	N-CA-CB	5.10	107.79	103.35
1	B	46	LYS	CA-C-N	5.07	125.00	119.78
1	B	46	LYS	C-N-CA	5.07	125.00	119.78
1	A	376	GLU	N-CA-C	5.07	117.93	111.69
1	A	155	LEU	N-CA-C	5.06	117.73	109.59
1	A	347	SER	N-CA-CB	-5.03	103.01	110.61
1	B	15	ASP	CB-CA-C	5.02	116.56	109.08

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	3152	92	0
1	B	3161	0	3152	88	1
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	118	0	0	9	0
3	B	110	0	0	2	0
All	All	6580	0	6316	168	1

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 13.

All (168) 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: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:B:371:GLU:HG2	1:B:375:LYS:HZ2	1.42	0.80
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
1:A:106:ILE:HD12	1:B:106:ILE:HD13	1.68	0.74
1:A:8:HIS:H	1:A:8:HIS:CD2	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:O	1:B:314:GLU:HG3	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:117:ASN:ND2	1:A:294:MET:HE3	2.09	0.66
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:HH11	1:B:275:ARG:HG2	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:HH11	1:A:275:ARG:CG	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:263:TYR:HB2	1:B:68:LYS:O	2.04	0.57
1:A:324:LYS:NZ	1:A:328:ASP:OD2	2.35	0.57
1:B:372:ARG:O	1:B:376:GLU:HG3	2.05	0.56
1:A:117:ASN:HD22	1:A:294:MET:HE3	1.71	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:18:LEU:C	1:A:18:LEU:HD23	2.31	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
1:A:29:ASN:OD1	1:A:31:LYS:HB2	2.07	0.55
1:A:368:GLU:H	1:A:368:GLU:CD	2.15	0.54
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:275:ARG:HH11	1:B:275:ARG:CG	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:334:ARG:HH12	1:B:361:CYS:HB2	1.74	0.52
1:B:406:GLN:OE1	1:B:410:LYS:HE2	2.09	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:A:123:PHE:HE1	1:B:5:TRP:CE3	2.28	0.52
1:B:23:ALA:HA	1:B:26:ARG:HD2	1.92	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:HH11	1:B:81:ARG:CG	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: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:8:HIS:CE1	1:B:124:LYS:HG2	2.47	0.50
1:A:372:ARG:HE	1:A:376:GLU:CD	2.20	0.49
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:142:ASN:O	1:B:146:ILE:HD12	2.14	0.47
1:B:164:LYS:HB2	1:B:164:LYS:HE2	1.69	0.47
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:HD12	1:B:50:LEU:N	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:HB3	1:B:81:ARG:CZ	2.46	0.46
1:B:373:LEU:HD13	1:B:381:MET:HE3	1.98	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:292:ARG:HB3	1:A:293:PRO:HD3	1.98	0.46
1:A:309:ILE:O	1:A:316:ARG:HB2	2.16	0.46
1:B:165:THR:O	1:B:166:CYS:HB2	2.16	0.46
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:A:11:MET:HE2	1:A:11:MET:HB2	1.87	0.45
1:A:148:ARG:HD3	3:A:680:HOH:O	2.17	0.45
1:B:275:ARG:CG	1:B:275:ARG:NH1	2.79	0.45
1:A:4:SER:O	1:A:4:SER:OG	2.29	0.45
1:B:81:ARG:CG	1:B:81:ARG:NH1	2.79	0.45
1:B:377:PHE:O	1:B:378:SER:HB2	2.17	0.45
1:B:359:MET:O	1:B:359:MET:HG3	2.16	0.45
1:B:34:ASN:O	1:B:37:VAL:HG23	2.17	0.45
1:B:134:TYR:CD2	1:B:156:GLN:HB2	2.52	0.45
1:B:281:LYS:HD2	1:B:281:LYS:HA	1.82	0.44
1:B:330:ILE:HG23	1:B:389:VAL:HG11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:MET:HE2	1:A:304:ARG:NH2	2.32	0.44
1:A:129:ARG:HA	1:A:129:ARG:HE	1.82	0.44
1:A:8:HIS:HE1	1:B:122:PHE:O	2.00	0.44
1:B:42:ASP:C	1:B:44:ASN:H	2.26	0.44
1:A:373:LEU:HA	1:A:373:LEU:HD23	1.76	0.44
1:B:129:ARG:HE	1:B:129:ARG:CA	2.31	0.44
1:A:88:LEU:CD2	1:A:244:ILE:HD12	2.47	0.44
1:A:405:HIS:NE2	1:A:410:LYS:CE	2.80	0.44
1:B:338:VAL:HG21	1:B:354:THR:HG23	2.00	0.44
1:B:308:LEU:O	1:B:312:THR:OG1	2.31	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:89:GLY:HA3	3:B:722:HOH:O	2.19	0.43
1:B:134:TYR:CE2	1:B:156:GLN:HB3	2.53	0.43
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:A:144:THR:HB	1:A:145:PRO:HD3	2.01	0.43
1:B:206:LYS:HG2	1:B:242:HIS:CE1	2.53	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:174:MET:HE3	1:B:174:MET:HB3	1.95	0.42
1:B:120:GLN:HG3	1:B:150:ALA:O	2.19	0.42
1:A:33:MET:HE3	1:A:396:ASN:CG	2.45	0.42
1:A:40:TYR:HE1	1:A:330:ILE:HD13	1.85	0.42
1:A:67:ASP:OD1	1:A:69:GLU:HG2	2.20	0.42
1:A:50:LEU:HD12	1:A:50:LEU:N	2.34	0.41
1:A:155:LEU:C	1:A:156:GLN:HG2	2.45	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:54:ARG:HH11	1:A:54:ARG:HD3	1.71	0.41
1:A:135:LEU:HB3	1:A:136:PRO:HD2	2.03	0.41
1:A:368:GLU:CD	1:A:368:GLU:N	2.79	0.41
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.70	0.41
1:A:100:TYR:CD1	1:A:100:TYR:C	2.99	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:PHE:CD1	1:B:125:PHE:N	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:O	1:B:186:ILE:HG23	2.22	0.40
1:B:100:TYR:CD2	1:B:100:TYR:C	2.98	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	Interatomic distance (Å)	Clash overlap (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%)	24	27
1	B	399/401 (100%)	378 (95%)	19 (5%)	2 (0%)	24	27
All	All	798/802 (100%)	759 (95%)	35 (4%)	4 (0%)	24	27

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%)	8	9
1	B	335/335 (100%)	300 (90%)	35 (10%)	7	7
All	All	670/670 (100%)	604 (90%)	66 (10%)	7	8

All (66) 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	101	VAL
1	A	106	ILE
1	A	107	SER
1	A	124	LYS
1	A	125	PHE
1	A	182	GLU
1	A	187	LEU
1	A	210	SER
1	A	211	VAL
1	A	214	LYS
1	A	250	VAL
1	A	259	ASN
1	A	275	ARG
1	A	281	LYS
1	A	288	LYS
1	A	296	SER
1	A	308	LEU
1	A	330	ILE
1	A	332	SER
1	A	335	THR
1	A	339	SER
1	A	343	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	362	PHE
1	A	366	LYS
1	A	408	VAL
1	A	410	LYS
1	B	3	SER
1	B	18	LEU
1	B	20	VAL
1	B	25	LYS
1	B	26	ARG
1	B	37	VAL
1	B	44	ASN
1	B	46	LYS
1	B	90	GLU
1	B	101	VAL
1	B	107	SER
1	B	125	PHE
1	B	164	LYS
1	B	175	GLU
1	B	202	GLN
1	B	215	ARG
1	B	216	ASN
1	B	245	GLU
1	B	281	LYS
1	B	300	MET
1	B	308	LEU
1	B	318	GLU
1	B	321	VAL
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
1	B	372	ARG
1	B	376	GLU
1	B	383	LYS
1	B	408	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	44	ASN
1	A	216	ASN
1	A	242	HIS
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	297	ASN
1	B	351	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	1.77	4 (26%)	21,22,23	2.66	7 (33%)
2	PLP	A	411	1	15,15,16	1.42	2 (13%)	21,22,23	2.81	7 (33%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	PLP	C5-C4	4.32	1.45	1.40
2	B	411	PLP	C4A-C4	-3.29	1.45	1.51
2	A	411	PLP	C5-C4	2.70	1.43	1.40
2	B	411	PLP	C2-N1	2.35	1.38	1.33
2	A	411	PLP	C4A-C4	-2.20	1.47	1.51
2	B	411	PLP	C3-C2	2.06	1.43	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PLP	C2A-C2-C3	6.56	128.47	120.80
2	B	411	PLP	C2A-C2-C3	5.55	127.29	120.80
2	A	411	PLP	O4P-C5A-C5	5.23	119.16	109.36
2	A	411	PLP	C6-C5-C4	4.92	122.13	118.10
2	B	411	PLP	C3-C2-N1	-4.64	115.11	120.96
2	B	411	PLP	O4P-C5A-C5	4.62	118.02	109.36
2	B	411	PLP	C6-N1-C2	4.48	127.32	119.20
2	B	411	PLP	C6-C5-C4	4.38	121.69	118.10
2	A	411	PLP	C3-C2-N1	-4.11	115.78	120.96
2	B	411	PLP	C5-C6-N1	-4.06	117.22	123.83
2	A	411	PLP	C6-N1-C2	3.98	126.42	119.20
2	A	411	PLP	C5-C6-N1	-3.71	117.80	123.83
2	A	411	PLP	C3-C4-C5	-2.48	115.62	118.59
2	B	411	PLP	O3-C3-C4	2.40	124.37	118.10

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

Continued on next page...

Continued from previous page...

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

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.