



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AMA  
Title : DOMAIN CLOSURE IN MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE  
Authors : Vincent, M.G.; Genovesio-Taverne, J.-C.; Jansonius, J.N.  
Deposited on : 1992-02-05  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

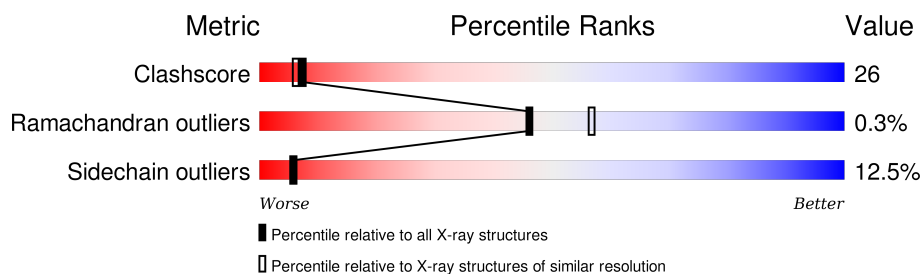
# 1 Overall quality at a glance

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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3498 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

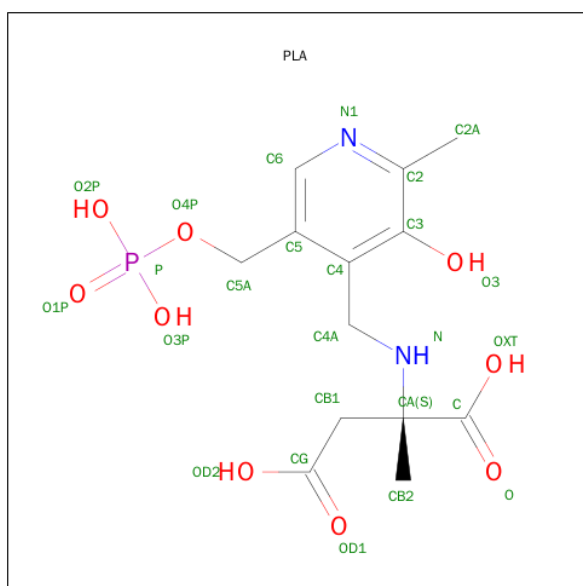
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (three-letter code: PLA) (formula:  $C_{13}H_{19}N_2O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	25	13	2	9	1	0	0

- Molecule 3 is water.

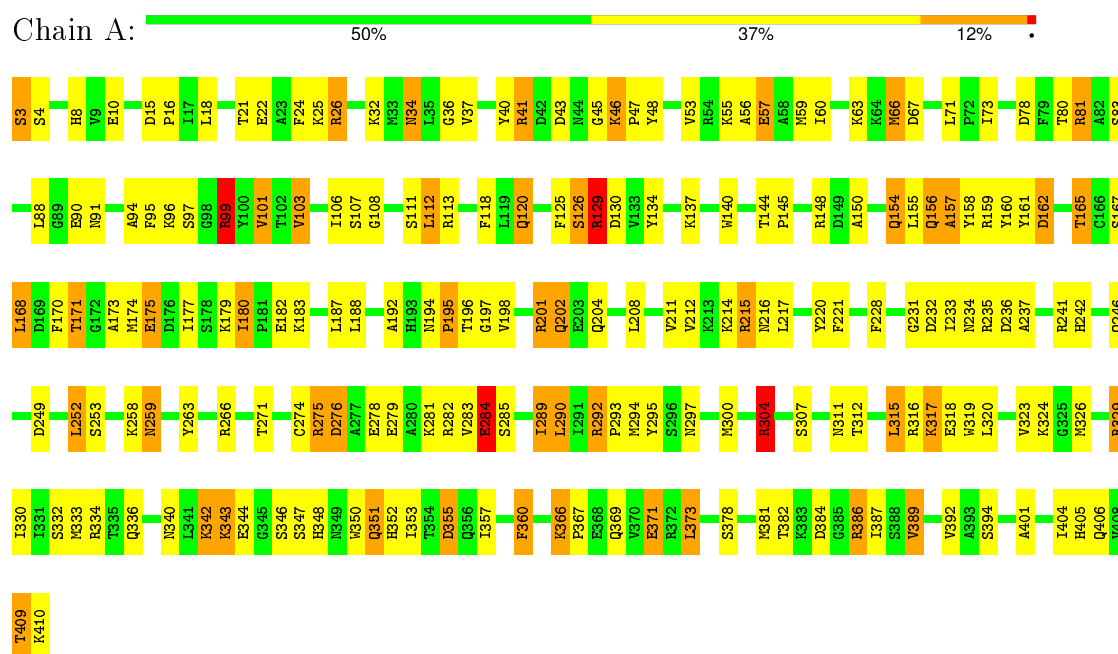
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	312	Total 312	O 312	0	0

### 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



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.70Å 91.40Å 128.50Å 90.00° 90.00° 90.00°	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, TNT	Depositor
R, $R_{free}$	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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: PLA

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	0.72	0/3231	1.82	74/4360 (1.7%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ARG	NE-CZ-NH1	16.66	128.63	120.30
1	A	275	ARG	NE-CZ-NH1	15.41	128.00	120.30
1	A	304	ARG	NE-CZ-NH2	-13.05	113.77	120.30
1	A	275	ARG	CD-NE-CZ	13.01	141.81	123.60
1	A	201	ARG	NE-CZ-NH1	12.48	126.54	120.30
1	A	275	ARG	NE-CZ-NH2	-12.41	114.09	120.30
1	A	282	ARG	NE-CZ-NH1	12.35	126.48	120.30
1	A	26	ARG	NE-CZ-NH1	12.19	126.40	120.30
1	A	276	ASP	CB-CG-OD1	12.05	129.15	118.30
1	A	304	ARG	CD-NE-CZ	11.49	139.69	123.60
1	A	329	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	A	232	ASP	CB-CG-OD1	10.17	127.45	118.30
1	A	148	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	A	235	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	A	201	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	A	165	THR	N-CA-CB	-9.61	92.04	110.30
1	A	316	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	A	329	ARG	NE-CZ-NH2	-9.51	115.54	120.30
1	A	78	ASP	CB-CG-OD1	-9.47	109.78	118.30
1	A	317	LYS	CA-CB-CG	8.81	132.79	113.40
1	A	281	LYS	N-CA-CB	8.19	125.34	110.60
1	A	130	ASP	CB-CG-OD1	7.98	125.48	118.30
1	A	276	ASP	N-CA-CB	-7.90	96.37	110.60
1	A	155	LEU	CA-CB-CG	7.69	132.99	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	A	235	ARG	CD-NE-CZ	7.30	133.82	123.60
1	A	162	ASP	CB-CG-OD1	-7.26	111.76	118.30
1	A	292	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	A	160	TYR	CB-CG-CD1	-7.22	116.67	121.00
1	A	112	LEU	CA-CB-CG	7.07	131.55	115.30
1	A	241	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	282	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	282	ARG	CD-NE-CZ	6.91	133.27	123.60
1	A	276	ASP	CA-CB-CG	6.85	128.47	113.40
1	A	201	ARG	CD-NE-CZ	6.82	133.15	123.60
1	A	315	LEU	CB-CA-C	6.78	123.08	110.20
1	A	317	LYS	N-CA-CB	6.73	122.71	110.60
1	A	81	ARG	CD-NE-CZ	6.71	133.00	123.60
1	A	78	ASP	OD1-CG-OD2	6.48	135.61	123.30
1	A	215	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	A	148	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	259	ASN	CB-CA-C	6.45	123.30	110.40
1	A	329	ARG	CD-NE-CZ	6.41	132.58	123.60
1	A	236	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	159	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	162	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	297	ASN	CB-CA-C	6.08	122.55	110.40
1	A	41	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	A	284	GLU	CA-CB-CG	6.04	126.68	113.40
1	A	202	GLN	N-CA-CB	6.02	121.44	110.60
1	A	175	GLU	OE1-CD-OE2	6.00	130.50	123.30
1	A	160	TYR	CB-CG-CD2	5.92	124.55	121.00
1	A	161	TYR	CA-CB-CG	5.88	124.57	113.40
1	A	113	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	355	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	A	157	ALA	O-C-N	5.81	132.00	122.70
1	A	348	HIS	CA-CB-CG	-5.79	103.76	113.60
1	A	129	ARG	CA-CB-CG	5.76	126.07	113.40
1	A	266	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	171	THR	CA-CB-OG1	-5.69	97.05	109.00
1	A	101	VAL	N-CA-CB	5.62	123.85	111.50
1	A	386	ARG	CD-NE-CZ	5.56	131.39	123.60
1	A	126	SER	N-CA-CB	-5.50	102.24	110.50
1	A	249	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	134	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	A	129	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	371	GLU	CA-CB-CG	5.37	125.21	113.40
1	A	57	GLU	CB-CA-C	-5.33	99.75	110.40
1	A	22	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	A	99	ARG	CA-CB-CG	5.22	124.89	113.40
1	A	180	ILE	O-C-N	5.19	130.95	121.10
1	A	140	TRP	CA-CB-CG	5.14	123.46	113.70
1	A	48	TYR	CA-CB-CG	5.05	122.99	113.40

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	3154	162	0
2	A	25	0	14	7	0
3	A	312	0	0	38	1
All	All	3498	0	3168	163	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 26.

All (163) 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:165:THR:HG21	3:A:438:HOH:O	1.34	1.22
1:A:373:LEU:HD23	1:A:381:MET:HE3	1.52	0.92
1:A:290:LEU:HD21	3:A:663:HOH:O	1.70	0.91
1:A:137:LYS:HG3	1:A:158:TYR:O	1.74	0.88
1:A:373:LEU:HD23	1:A:381:MET:CE	2.09	0.82
1:A:343:LYS:HE2	1:A:344:GLU:OE2	1.80	0.82
1:A:342:LYS:HE3	3:A:545:HOH:O	1.80	0.81
1:A:129:ARG:HA	1:A:129:ARG:HE	1.45	0.81
1:A:165:THR:HG22	1:A:167:SER:OG	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:CG2	1:A:167:SER:OG	2.33	0.75
1:A:55:LYS:O	1:A:59:MET:HG3	1.86	0.75
1:A:404:ILE:O	1:A:409:THR:HB	1.86	0.74
1:A:350:TRP:HB3	1:A:353:ILE:HD12	1.70	0.73
1:A:46:LYS:NZ	3:A:705:HOH:O	2.08	0.72
1:A:274:CYS:HB3	1:A:279:GLU:HG2	1.71	0.71
1:A:324:LYS:HD3	3:A:647:HOH:O	1.91	0.71
1:A:26:ARG:NH2	3:A:456:HOH:O	2.25	0.69
1:A:45:GLY:HA2	3:A:657:HOH:O	1.94	0.68
1:A:10:GLU:HB2	3:A:670:HOH:O	1.94	0.67
1:A:366:LYS:H	1:A:369:GLN:HE21	1.44	0.66
1:A:168:LEU:CD1	1:A:198:VAL:HG12	2.26	0.65
1:A:366:LYS:H	1:A:369:GLN:NE2	1.93	0.65
1:A:171:THR:O	1:A:175:GLU:HG3	1.97	0.64
1:A:183:LYS:HB2	3:A:602:HOH:O	1.98	0.64
1:A:258:LYS:NZ	2:A:411:PLA:H4A2	2.12	0.63
1:A:319:TRP:O	1:A:323:VAL:HG23	1.98	0.63
1:A:290:LEU:HD13	1:A:294:MET:CE	2.28	0.63
1:A:59:MET:O	1:A:63:LYS:HB2	1.98	0.62
1:A:179:LYS:HB2	1:A:179:LYS:NZ	2.15	0.62
1:A:73:ILE:HG13	3:A:550:HOH:O	1.99	0.62
1:A:97:SER:OG	1:A:99:ARG:HG3	2.00	0.61
1:A:290:LEU:HD13	1:A:294:MET:HE3	1.82	0.61
1:A:129:ARG:CA	1:A:129:ARG:HE	2.06	0.61
1:A:43:ASP:OD2	1:A:394:SER:OG	2.17	0.61
1:A:318:GLU:HB2	3:A:645:HOH:O	2.00	0.60
1:A:258:LYS:HD2	1:A:258:LYS:N	2.15	0.60
1:A:120:GLN:HG3	1:A:150:ALA:O	2.01	0.60
1:A:258:LYS:HZ1	2:A:411:PLA:H4A2	1.66	0.60
1:A:233:ILE:HG13	1:A:234:ASN:N	2.17	0.59
1:A:66:MET:HB3	3:A:486:HOH:O	2.01	0.59
1:A:4:SER:HB3	3:A:704:HOH:O	2.02	0.59
1:A:91:ASN:HA	3:A:569:HOH:O	2.01	0.59
1:A:168:LEU:HD12	1:A:198:VAL:HG12	1.83	0.59
1:A:90:GLU:O	1:A:96:LYS:HD3	2.02	0.58
1:A:94:ALA:HA	1:A:99:ARG:HD3	1.86	0.58
1:A:81:ARG:NE	3:A:719:HOH:O	2.37	0.58
1:A:333:MET:CE	1:A:336:GLN:NE2	2.67	0.58
1:A:300:MET:O	1:A:304:ARG:HG3	2.04	0.58
1:A:8:HIS:CD2	1:A:8:HIS:H	2.23	0.57
1:A:333:MET:HE1	1:A:336:GLN:HE22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLN:NE2	3:A:683:HOH:O	2.36	0.57
1:A:342:LYS:HG2	3:A:545:HOH:O	2.05	0.56
1:A:25:LYS:HB2	3:A:529:HOH:O	2.06	0.56
1:A:111:SER:HB2	1:A:253:SER:OG	2.07	0.55
1:A:21:THR:O	1:A:25:LYS:HG3	2.07	0.54
1:A:386:ARG:HD3	3:A:577:HOH:O	2.06	0.54
1:A:221:PHE:O	1:A:252:LEU:HA	2.07	0.54
1:A:34:ASN:C	1:A:34:ASN:HD22	2.11	0.52
1:A:101:VAL:O	1:A:271:THR:HA	2.09	0.52
1:A:333:MET:CE	1:A:336:GLN:HE22	2.22	0.52
1:A:192:ALA:HA	1:A:357:ILE:CD1	2.40	0.51
1:A:340:ASN:HD22	1:A:343:LYS:HD2	1.75	0.51
1:A:175:GLU:HG2	3:A:720:HOH:O	2.10	0.51
1:A:329:ARG:NH2	1:A:392:VAL:O	2.41	0.51
1:A:352:HIS:HA	1:A:355:ASP:HB2	1.92	0.51
1:A:168:LEU:HD13	1:A:198:VAL:HG12	1.93	0.51
1:A:326:MET:O	1:A:330:ILE:HG13	2.11	0.51
1:A:258:LYS:HE2	2:A:411:PLA:HB22	1.94	0.50
1:A:179:LYS:HB2	1:A:179:LYS:HZ3	1.76	0.50
1:A:202:GLN:HG2	3:A:485:HOH:O	2.10	0.50
1:A:373:LEU:CD2	1:A:381:MET:CE	2.88	0.50
1:A:300:MET:O	1:A:304:ARG:CG	2.60	0.50
1:A:91:ASN:CA	3:A:569:HOH:O	2.60	0.50
1:A:333:MET:HE2	1:A:336:GLN:NE2	2.26	0.50
1:A:211:VAL:HG23	3:A:573:HOH:O	2.11	0.50
1:A:67:ASP:OD1	1:A:67:ASP:C	2.50	0.50
1:A:333:MET:HE1	1:A:336:GLN:NE2	2.27	0.50
1:A:330:ILE:O	1:A:334:ARG:HG3	2.12	0.49
1:A:343:LYS:HE2	3:A:510:HOH:O	2.13	0.49
1:A:194:ASN:ND2	2:A:411:PLA:O3	2.44	0.49
1:A:55:LYS:NZ	3:A:658:HOH:O	2.46	0.49
1:A:360:PHE:HB3	1:A:387:ILE:O	2.13	0.48
1:A:34:ASN:ND2	1:A:36:GLY:H	2.12	0.48
1:A:88:LEU:HD23	1:A:95:PHE:HB2	1.95	0.48
1:A:197:GLY:O	1:A:357:ILE:HG13	2.14	0.47
1:A:307:SER:O	1:A:311:ASN:HB2	2.14	0.47
1:A:177:ILE:HA	1:A:180:ILE:HD12	1.96	0.47
1:A:183:LYS:HD2	3:A:602:HOH:O	2.15	0.47
1:A:24:PHE:CD2	1:A:34:ASN:HB2	2.50	0.47
1:A:173:ALA:O	1:A:177:ILE:HG13	2.14	0.47
1:A:289:ILE:HG22	3:A:418:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TYR:O	1:A:41:ARG:NH1	2.47	0.47
1:A:405:HIS:O	1:A:410:LYS:N	2.46	0.47
1:A:55:LYS:HE3	1:A:318:GLU:OE1	2.15	0.47
2:A:411:PLA:N	2:A:411:PLA:O3	2.44	0.47
1:A:137:LYS:CG	1:A:157:ALA:HB1	2.45	0.47
1:A:144:THR:HB	1:A:145:PRO:HD3	1.97	0.47
1:A:137:LYS:HG2	1:A:157:ALA:HB1	1.96	0.46
1:A:137:LYS:CD	1:A:157:ALA:HB1	2.45	0.46
1:A:192:ALA:HA	1:A:357:ILE:HD12	1.95	0.46
1:A:162:ASP:OD2	1:A:165:THR:HB	2.16	0.46
1:A:3:SER:HA	3:A:586:HOH:O	2.15	0.46
1:A:215:ARG:HB2	1:A:217:LEU:HG	1.98	0.46
1:A:56:ALA:O	1:A:60:ILE:HG13	2.15	0.46
1:A:118:PHE:CZ	1:A:283:VAL:HG13	2.52	0.45
1:A:34:ASN:HD22	1:A:36:GLY:H	1.64	0.45
1:A:103:VAL:HG12	1:A:103:VAL:O	2.16	0.45
1:A:125:PHE:O	1:A:126:SER:HB2	2.15	0.45
1:A:367:PRO:O	1:A:371:GLU:HB2	2.17	0.45
1:A:90:GLU:O	1:A:96:LYS:NZ	2.46	0.45
1:A:202:GLN:CG	3:A:485:HOH:O	2.65	0.45
1:A:137:LYS:HD2	1:A:157:ALA:HB1	1.98	0.45
1:A:81:ARG:CZ	3:A:719:HOH:O	2.65	0.45
1:A:369:GLN:O	1:A:373:LEU:HB2	2.18	0.44
1:A:96:LYS:HE2	3:A:554:HOH:O	2.16	0.44
1:A:81:ARG:NH2	3:A:719:HOH:O	2.51	0.44
1:A:103:VAL:O	1:A:103:VAL:CG1	2.66	0.44
1:A:351:GLN:O	1:A:351:GLN:HG3	2.16	0.44
1:A:373:LEU:CD2	1:A:381:MET:HE1	2.47	0.44
1:A:340:ASN:HB3	1:A:401:ALA:CB	2.47	0.44
1:A:406:GLN:HE22	1:A:410:LYS:HE2	1.83	0.44
1:A:258:LYS:HE2	2:A:411:PLA:CB2	2.47	0.44
1:A:258:LYS:CE	2:A:411:PLA:HB22	2.48	0.44
1:A:373:LEU:HD23	1:A:381:MET:HE1	1.96	0.43
1:A:208:LEU:O	1:A:212:VAL:HG23	2.17	0.43
1:A:340:ASN:O	1:A:344:GLU:HG2	2.17	0.43
1:A:91:ASN:ND2	3:A:673:HOH:O	2.51	0.43
1:A:201:ARG:O	1:A:204:GLN:HB2	2.18	0.43
1:A:279:GLU:O	1:A:283:VAL:HG23	2.18	0.43
1:A:194:ASN:HA	1:A:195:PRO:HA	1.78	0.43
1:A:320:LEU:HD22	3:A:521:HOH:O	2.18	0.43
1:A:320:LEU:O	1:A:324:LYS:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:HG2	3:A:703:HOH:O	2.18	0.43
1:A:57:GLU:O	1:A:60:ILE:HB	2.19	0.43
1:A:242:HIS:O	1:A:246:GLN:HG2	2.19	0.43
1:A:46:LYS:HA	1:A:47:PRO:HD3	1.91	0.42
1:A:71:LEU:HD13	1:A:300:MET:HE3	2.01	0.42
1:A:10:GLU:OE1	3:A:670:HOH:O	2.21	0.42
1:A:170:PHE:O	1:A:174:MET:HG2	2.19	0.42
1:A:156:GLN:HA	1:A:156:GLN:HE21	1.83	0.42
1:A:382:THR:OG1	1:A:386:ARG:HB3	2.20	0.42
1:A:34:ASN:C	1:A:34:ASN:ND2	2.73	0.42
1:A:329:ARG:NH1	1:A:392:VAL:O	2.50	0.42
1:A:32:LYS:HA	1:A:378:SER:O	2.20	0.42
1:A:15:ASP:HA	1:A:16:PRO:HD3	1.81	0.42
1:A:330:ILE:HG23	1:A:389:VAL:CG1	2.50	0.42
1:A:237:ALA:HA	3:A:509:HOH:O	2.20	0.42
1:A:182:GLU:HA	1:A:215:ARG:O	2.20	0.41
1:A:334:ARG:HD3	1:A:353:ILE:O	2.19	0.41
1:A:53:VAL:O	1:A:57:GLU:HG3	2.20	0.41
1:A:312:THR:O	1:A:315:LEU:N	2.48	0.41
1:A:312:THR:HB	1:A:315:LEU:HB2	2.03	0.41
1:A:188:LEU:HA	3:A:414:HOH:O	2.20	0.41
1:A:101:VAL:HG21	1:A:284:GLU:HB2	2.01	0.41
1:A:285:SER:O	1:A:289:ILE:HD12	2.21	0.41
1:A:292:ARG:HB3	1:A:293:PRO:HD3	2.02	0.41
1:A:231:GLY:O	1:A:324:LYS:HG3	2.21	0.41
1:A:24:PHE:CE2	1:A:34:ASN:HB2	2.56	0.40
1:A:106:ILE:HD11	1:A:295:TYR:CG	2.56	0.40
1:A:258:LYS:HD2	1:A:258:LYS:H	1.83	0.40
1:A:228:PHE:HE2	1:A:259:ASN:HA	1.86	0.40
1:A:201:ARG:O	1:A:204:GLN:N	2.54	0.40
1:A:108:GLY:O	1:A:112:LEU:HB2	2.21	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)
3:A:437:HOH:O	3:A:437:HOH:O[3_655]	1.87	0.33

## 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%)	374 (94%)	24 (6%)	1 (0%)	46 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	335/335 (100%)	293 (88%)	42 (12%)	6 6

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	18	LEU
1	A	34	ASN
1	A	37	VAL
1	A	46	LYS
1	A	66	MET
1	A	80	THR
1	A	83	SER
1	A	99	ARG
1	A	103	VAL

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Mol	Chain	Res	Type
1	A	107	SER
1	A	120	GLN
1	A	129	ARG
1	A	154	GLN
1	A	156	GLN
1	A	168	LEU
1	A	187	LEU
1	A	195	PRO
1	A	196	THR
1	A	214	LYS
1	A	216	ASN
1	A	220	TYR
1	A	252	LEU
1	A	275	ARG
1	A	276	ASP
1	A	278	GLU
1	A	284	GLU
1	A	289	ILE
1	A	290	LEU
1	A	304	ARG
1	A	317	LYS
1	A	332	SER
1	A	342	LYS
1	A	343	LYS
1	A	346	SER
1	A	347	SER
1	A	351	GLN
1	A	360	PHE
1	A	366	LYS
1	A	373	LEU
1	A	389	VAL
1	A	409	THR

Some 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	34	ASN
1	A	120	GLN
1	A	154	GLN
1	A	156	GLN
1	A	202	GLN

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Mol	Chain	Res	Type
1	A	216	ASN
1	A	242	HIS
1	A	286	GLN
1	A	336	GLN
1	A	340	ASN
1	A	369	GLN
1	A	406	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

1 ligand is 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	PLA	A	411	-	19,25,25	1.98	5 (26%)	27,37,37	2.94	12 (44%)

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	PLA	A	411	-	-	0/14/23/23	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	PLA	C4A-C4	-6.48	1.44	1.51
2	A	411	PLA	CB2-CA	-2.57	1.51	1.53
2	A	411	PLA	CB1-CA	-2.50	1.51	1.55
2	A	411	PLA	O3-C3	-2.37	1.31	1.37
2	A	411	PLA	C5-C4	-2.16	1.37	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PLA	CB2-CA-CB1	-10.94	95.88	110.94
2	A	411	PLA	C5-C6-N1	-3.12	118.45	123.86
2	A	411	PLA	C3-C2-N1	-2.64	116.96	120.61
2	A	411	PLA	C5A-C5-C6	-2.13	115.26	119.28
2	A	411	PLA	C4A-N-CA	2.11	120.92	116.69
2	A	411	PLA	C5A-C5-C4	2.39	126.49	121.89
2	A	411	PLA	O3P-P-O1P	2.39	118.28	110.58
2	A	411	PLA	C3-C4-C5	2.64	121.59	118.82
2	A	411	PLA	C4-C4A-N	2.84	119.91	111.91
2	A	411	PLA	C6-N1-C2	3.21	125.82	119.28
2	A	411	PLA	O4P-C5A-C5	3.92	115.48	108.99
2	A	411	PLA	CB2-CA-N	4.34	117.63	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	PLA	7	0

## 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.