



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:26 AM UTC

PDB ID : 1AMA / pdb_00001ama
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

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

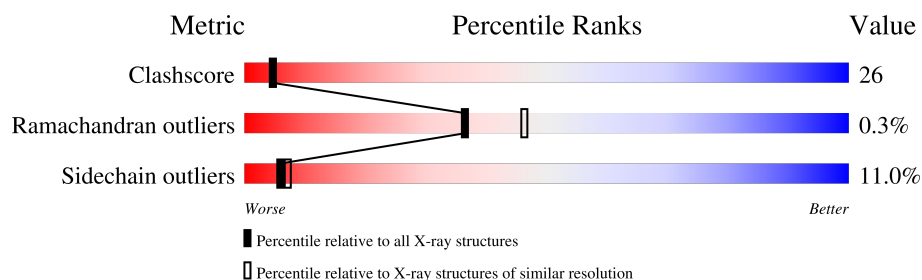
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	 44% 38% 16% .

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.

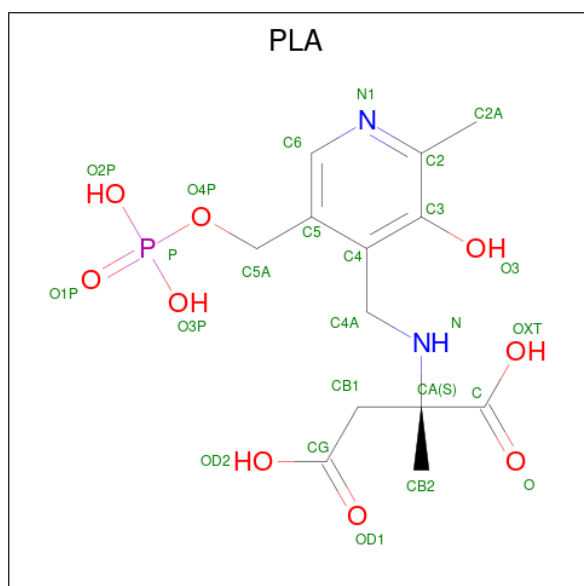
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (CCD ID: 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.

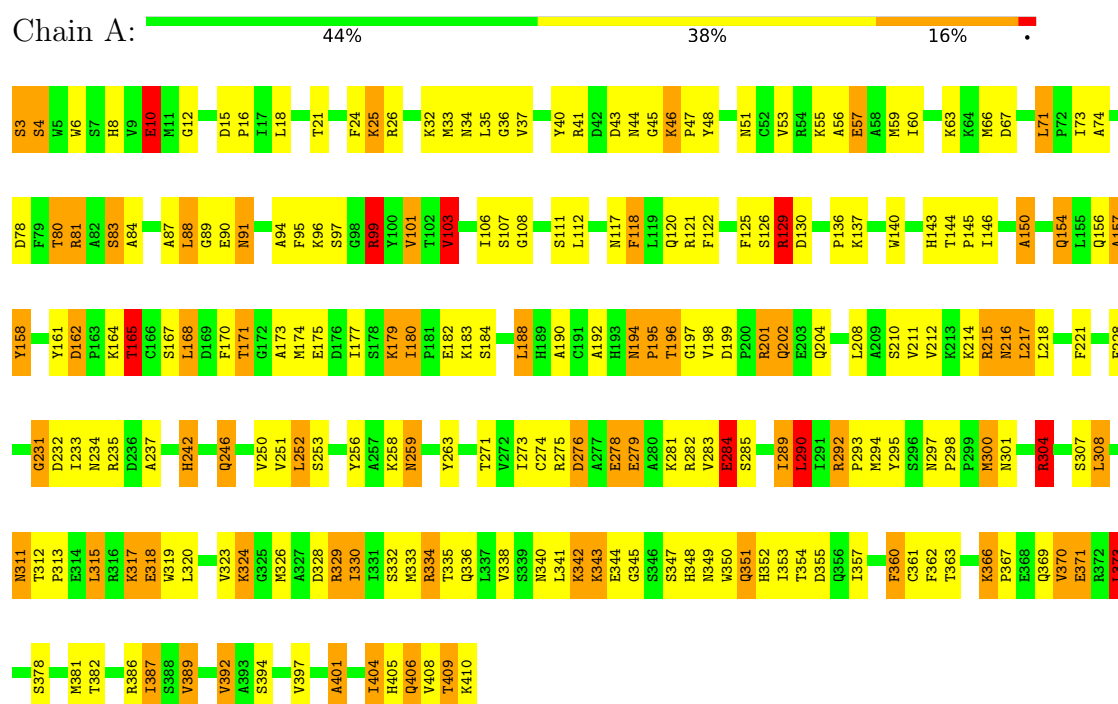
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	312	Total 312	O 312	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, 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



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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	0.92	0/3231	2.24	168/4360 (3.9%)

There are no bond length outliers.

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ASP	CA-CB-CG	15.87	128.47	112.60
1	A	275	ARG	CD-NE-CZ	12.43	141.81	124.40
1	A	165	THR	N-CA-CB	-12.30	92.04	110.61
1	A	196	THR	N-CA-C	10.97	123.32	111.36
1	A	304	ARG	CD-NE-CZ	10.92	139.69	124.40
1	A	300	MET	N-CA-C	10.14	122.42	111.36
1	A	51	ASN	OD1-CG-ND2	10.05	132.65	122.60
1	A	348	HIS	CA-CB-CG	-10.04	103.76	113.80
1	A	89	GLY	CA-C-O	-9.85	114.20	121.88
1	A	281	LYS	N-CA-CB	9.82	125.34	110.22
1	A	317	LYS	CA-CB-CG	9.35	132.79	114.10
1	A	180	ILE	O-C-N	9.09	130.95	121.14
1	A	276	ASP	N-CA-CB	-8.95	96.37	111.31
1	A	162	ASP	CA-CB-CG	-8.76	103.84	112.60
1	A	317	LYS	N-CA-CB	8.76	122.71	110.01
1	A	171	THR	CA-CB-OG1	-8.37	97.05	109.60
1	A	298	PRO	N-CA-C	8.31	120.84	110.70
1	A	87	ALA	CA-C-N	8.26	132.01	120.29
1	A	87	ALA	C-N-CA	8.26	132.01	120.29
1	A	311	ASN	CA-CB-CG	8.19	120.79	112.60
1	A	297	ASN	CB-CA-C	8.12	122.55	109.97
1	A	101	VAL	N-CA-CB	8.02	123.85	111.99
1	A	130	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	91	ASN	OD1-CG-ND2	-7.60	115.00	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	ILE	O-C-N	7.54	129.28	121.89
1	A	157	ALA	O-C-N	7.53	132.00	123.27
1	A	164	LYS	O-C-N	7.48	130.68	122.15
1	A	180	ILE	N-CA-C	-7.29	102.24	109.02
1	A	130	ASP	N-CA-C	7.24	120.06	108.41
1	A	88	LEU	CA-C-O	-7.14	112.85	120.42
1	A	304	ARG	NE-CZ-NH1	7.13	128.63	121.50
1	A	101	VAL	CA-C-O	7.01	127.19	120.25
1	A	335	THR	CA-C-N	7.00	130.35	120.28
1	A	335	THR	C-N-CA	7.00	130.35	120.28
1	A	301	ASN	CA-C-N	6.99	127.86	120.03
1	A	301	ASN	C-N-CA	6.99	127.86	120.03
1	A	84	ALA	O-C-N	6.88	129.44	122.08
1	A	315	LEU	N-CA-C	-6.87	102.90	112.45
1	A	315	LEU	CB-CA-C	6.86	123.08	110.11
1	A	88	LEU	N-CA-C	6.81	118.79	111.36
1	A	44	ASN	OD1-CG-ND2	6.80	129.40	122.60
1	A	242	HIS	CA-CB-CG	-6.74	107.06	113.80
1	A	235	ARG	CD-NE-CZ	6.73	133.82	124.40
1	A	103	VAL	N-CA-CB	-6.72	101.71	111.52
1	A	51	ASN	CA-CB-CG	-6.70	105.90	112.60
1	A	57	GLU	CB-CA-C	-6.53	99.75	110.85
1	A	275	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	A	362	PHE	CA-C-N	6.50	129.64	120.28
1	A	362	PHE	C-N-CA	6.50	129.64	120.28
1	A	78	ASP	O-C-N	6.49	128.99	122.12
1	A	202	GLN	N-CA-CB	6.48	121.44	110.49
1	A	308	LEU	CA-C-N	6.47	128.62	120.72
1	A	308	LEU	C-N-CA	6.47	128.62	120.72
1	A	251	VAL	N-CA-CB	6.41	121.96	111.44
1	A	278	GLU	N-CA-CB	6.39	119.51	110.12
1	A	363	THR	CA-C-O	-6.38	112.89	120.10
1	A	282	ARG	CD-NE-CZ	6.33	133.27	124.40
1	A	284	GLU	CA-CB-CG	6.29	126.68	114.10
1	A	251	VAL	N-CA-C	-6.28	99.10	108.46
1	A	84	ALA	N-CA-C	-6.28	103.36	111.02
1	A	136	PRO	O-C-N	6.28	130.64	122.86
1	A	370	VAL	CA-C-N	6.25	128.57	120.44
1	A	370	VAL	C-N-CA	6.25	128.57	120.44
1	A	201	ARG	CD-NE-CZ	6.25	133.15	124.40
1	A	334	ARG	CA-C-N	6.24	129.47	120.79
1	A	334	ARG	C-N-CA	6.24	129.47	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASN	CB-CA-C	6.15	123.30	110.32
1	A	81	ARG	CD-NE-CZ	6.14	133.00	124.40
1	A	217	LEU	CA-C-O	-6.04	114.15	121.28
1	A	304	ARG	NE-CZ-NH2	-6.03	113.77	119.20
1	A	318	GLU	CB-CG-CD	6.03	122.84	112.60
1	A	328	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	150	ALA	CA-C-N	6.02	130.32	122.26
1	A	150	ALA	C-N-CA	6.02	130.32	122.26
1	A	89	GLY	N-CA-C	-6.01	104.12	112.18
1	A	101	VAL	CB-CA-C	5.99	118.27	110.12
1	A	129	ARG	CA-CB-CG	5.99	126.07	114.10
1	A	117	ASN	CA-CB-CG	5.97	118.57	112.60
1	A	392	VAL	CB-CA-C	5.95	119.37	110.98
1	A	161	TYR	CA-CB-CG	5.93	124.57	113.90
1	A	184	SER	N-CA-C	-5.92	101.19	110.36
1	A	146	ILE	CB-CA-C	-5.86	104.23	112.14
1	A	397	VAL	CB-CA-C	5.86	120.05	112.14
1	A	329	ARG	CD-NE-CZ	5.84	132.58	124.40
1	A	158	TYR	CA-C-O	-5.83	113.95	120.66
1	A	161	TYR	CA-C-O	5.81	127.60	120.92
1	A	281	LYS	CA-C-O	-5.81	113.54	120.10
1	A	10	GLU	O-C-N	5.78	129.45	122.68
1	A	143	HIS	N-CA-CB	5.77	118.60	110.12
1	A	361	CYS	N-CA-C	-5.75	99.29	109.06
1	A	194	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	231	GLY	N-CA-C	-5.70	107.45	115.32
1	A	278	GLU	CA-C-O	-5.67	114.54	120.55
1	A	275	ARG	NE-CZ-NH2	-5.67	114.09	119.20
1	A	25	LYS	CA-C-N	5.67	130.18	120.72
1	A	25	LYS	C-N-CA	5.67	130.18	120.72
1	A	146	ILE	O-C-N	5.62	127.32	121.87
1	A	232	ASP	CA-CB-CG	5.58	118.19	112.60
1	A	210	SER	O-C-N	5.57	127.80	122.07
1	A	371	GLU	CA-CB-CG	5.56	125.21	114.10
1	A	250	VAL	CA-C-N	5.55	130.66	122.94
1	A	250	VAL	C-N-CA	5.55	130.66	122.94
1	A	44	ASN	N-CA-C	-5.55	105.29	113.61
1	A	273	ILE	N-CA-CB	5.54	117.32	111.00
1	A	290	LEU	CA-C-N	5.52	128.26	120.42
1	A	290	LEU	C-N-CA	5.52	128.26	120.42
1	A	345	GLY	CA-C-O	-5.50	113.16	118.98
1	A	354	THR	CA-CB-OG1	-5.49	101.36	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	LEU	CA-C-O	-5.47	114.75	120.55
1	A	80	THR	CB-CA-C	5.43	119.50	110.81
1	A	74	ALA	N-CA-C	5.41	119.73	113.18
1	A	363	THR	N-CA-C	5.41	117.93	111.71
1	A	99	ARG	CA-CB-CG	5.39	124.89	114.10
1	A	218	LEU	N-CA-CB	5.39	119.23	110.17
1	A	180	ILE	CA-C-O	-5.36	114.80	119.62
1	A	188	LEU	O-C-N	5.33	129.78	123.27
1	A	162	ASP	O-C-N	5.33	127.04	121.02
1	A	324	LYS	CB-CG-CD	-5.33	99.05	111.30
1	A	360	PHE	CA-CB-CG	5.33	119.12	113.80
1	A	129	ARG	N-CA-CB	5.30	118.70	110.80
1	A	78	ASP	OD1-CG-OD2	5.30	135.61	122.90
1	A	349	ASN	CA-C-O	-5.29	114.92	120.58
1	A	215	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	A	401	ALA	O-C-N	5.25	127.55	122.09
1	A	118	PHE	N-CA-C	-5.24	105.48	111.14
1	A	292	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	408	VAL	CA-C-N	5.23	131.36	122.36
1	A	408	VAL	C-N-CA	5.23	131.36	122.36
1	A	256	TYR	N-CA-C	-5.23	105.56	112.94
1	A	330	ILE	N-CA-C	-5.23	105.44	110.72
1	A	199	ASP	O-C-N	5.19	125.87	121.20
1	A	360	PHE	CA-C-O	5.19	127.51	121.49
1	A	140	TRP	CA-CB-CG	5.19	123.46	113.60
1	A	342	LYS	N-CA-CB	5.18	117.83	110.16
1	A	341	LEU	O-C-N	5.17	127.61	122.12
1	A	342	LYS	N-CA-C	-5.17	105.73	111.36
1	A	338	VAL	CA-C-O	5.16	126.32	120.95
1	A	202	GLN	CA-C-N	5.16	128.15	120.31
1	A	202	GLN	C-N-CA	5.16	128.15	120.31
1	A	121	ARG	CA-C-O	-5.15	115.04	120.55
1	A	363	THR	CA-CB-OG1	-5.15	101.88	109.60
1	A	216	ASN	OD1-CG-ND2	5.14	127.74	122.60
1	A	348	HIS	N-CA-C	5.12	117.47	110.55
1	A	317	LYS	O-C-N	5.12	127.34	122.07
1	A	406	GLN	CA-C-N	5.12	129.33	121.19
1	A	406	GLN	C-N-CA	5.12	129.33	121.19
1	A	12	GLY	N-CA-C	-5.11	101.91	112.34
1	A	256	TYR	O-C-N	5.11	128.37	122.19
1	A	279	GLU	CB-CG-CD	5.11	121.28	112.60
1	A	83	SER	CA-C-O	5.10	125.95	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ALA	N-CA-C	5.09	117.22	111.11
1	A	91	ASN	O-C-N	5.06	127.92	122.15
1	A	246	GLN	N-CA-C	-5.06	106.88	113.16
1	A	165	THR	CA-C-N	5.05	129.37	122.34
1	A	165	THR	C-N-CA	5.05	129.37	122.34
1	A	6	TRP	N-CA-C	5.05	118.48	112.72
1	A	48	TYR	CA-CB-CG	5.05	122.99	113.90
1	A	362	PHE	N-CA-C	-5.05	98.65	107.73
1	A	373	LEU	CA-C-N	5.04	127.30	120.44
1	A	373	LEU	C-N-CA	5.04	127.30	120.44
1	A	387	ILE	N-CA-CB	5.04	120.17	111.39
1	A	201	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	A	165	THR	CB-CA-C	-5.04	101.66	110.17
1	A	4	SER	O-C-N	5.03	128.38	122.84
1	A	122	PHE	CA-C-O	-5.02	113.53	119.05
1	A	91	ASN	CA-C-N	5.01	129.38	121.56
1	A	91	ASN	C-N-CA	5.01	129.38	121.56
1	A	292	ARG	NE-CZ-NH1	-5.00	116.50	121.50

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	163	0
2	A	25	0	14	8	0
3	A	312	0	0	37	1
All	All	3498	0	3168	164	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 (164) 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:HE1	1.31	1.10
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:CD2	1:A:381:MET:HE1	2.08	0.83
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:373:LEU:HD23	1:A:381:MET:CE	2.09	0.78
1:A:165:THR:HG22	1:A:167:SER:OG	1.84	0.77
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:290:LEU:HD13	1:A:294:MET:HE1	1.75	0.67
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:129:ARG:HE	1:A:129:ARG:CA	2.06	0.61
1:A:43:ASP:OD2	1:A:394:SER:OG	2.17	0.61
1:A:120:GLN:HG3	1:A:150:ALA:O	2.01	0.60
1:A:258:LYS:HD2	1:A:258:LYS:N	2.15	0.60
1:A:318:GLU:HB2	3:A:645:HOH:O	2.00	0.60
1:A:33:MET:HE2	1:A:35:LEU:HD21	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HD12	1:A:198:VAL:HG12	1.83	0.59
1:A:233:ILE:HG13	1:A:234:ASN:N	2.17	0.58
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:333:MET:HE2	1:A:336:GLN:NE2	2.18	0.57
1:A:8:HIS:H	1:A:8:HIS:CD2	2.23	0.57
1:A:34:ASN:C	1:A:34:ASN:HD22	2.11	0.57
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:67:ASP:C	1:A:67:ASP:OD1	2.50	0.54
1:A:333:MET:CE	1:A:336:GLN:HE22	2.22	0.52
1:A:101:VAL:O	1:A:271:THR:HA	2.09	0.52
1:A:192:ALA:HA	1:A:357:ILE:CD1	2.40	0.51
1:A:71:LEU:HD13	1:A:300:MET:HE3	1.92	0.51
1:A:340:ASN:HD22	1:A:343:LYS:HD2	1.75	0.51
1:A:290:LEU:O	1:A:294:MET:HE3	2.11	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:370:VAL:HA	1:A:381:MET:HE3	1.92	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:333:MET:HE1	1:A:336:GLN:HE22	1.75	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: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:211:VAL:HG23	3:A:573:HOH:O	2.11	0.50
1:A:258:LYS:HZ1	2:A:411:PLA:H4A2	1.76	0.49
1:A:330:ILE:O	1:A:334:ARG:HG3	2.12	0.49
1:A:194:ASN:ND2	2:A:411:PLA:O3	2.44	0.49
1:A:343:LYS:HE2	3:A:510:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:183:LYS:HD2	3:A:602:HOH:O	2.15	0.47
1:A:40:TYR:O	1:A:41:ARG:NH1	2.47	0.47
1:A:289:ILE:HG22	3:A:418:HOH:O	2.15	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:O3	2:A:411:PLA:N	2.44	0.47
1:A:34:ASN:C	1:A:34:ASN:ND2	2.73	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:CD	1:A:157:ALA:HB1	2.45	0.46
1:A:137:LYS:HG2	1:A:157:ALA:HB1	1.96	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:34:ASN:HD22	1:A:36:GLY:H	1.64	0.45
1:A:103:VAL:O	1:A:103:VAL:HG12	2.16	0.45
1:A:118:PHE:CZ	1:A:283:VAL:HG13	2.52	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:81:ARG:NH2	3:A:719:HOH:O	2.51	0.44
1:A:96:LYS:HE2	3:A:554:HOH:O	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:CE	2:A:411:PLA:HB22	2.48	0.44
1:A:208:LEU:O	1:A:212:VAL:HG23	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:340:ASN:O	1:A:344:GLU:HG2	2.17	0.43
1:A:194:ASN:HA	1:A:195:PRO:HA	1.78	0.43
1:A:279:GLU:O	1:A:283:VAL:HG23	2.18	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
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:308:LEU:O	1:A:312:THR:OG1	2.30	0.43
1:A:46:LYS:HA	1:A:47:PRO:HD3	1.91	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:HE21	1:A:156:GLN:HA	1.83	0.42
1:A:32:LYS:HA	1:A:378:SER:O	2.20	0.42
1:A:329:ARG:NH1	1:A:392:VAL:O	2.50	0.42
1:A:382:THR:OG1	1:A:386:ARG:HB3	2.20	0.42
1:A:15:ASP:HA	1:A:16:PRO:HD3	1.81	0.42
1:A:258:LYS:HZ3	2:A:411:PLA:H4A2	1.80	0.42
1:A:237:ALA:HA	3:A:509:HOH:O	2.20	0.42
1:A:330:ILE:HG23	1:A:389:VAL:CG1	2.50	0.42
1:A:182:GLU:HA	1:A:215:ARG:O	2.20	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:334:ARG:HD3	1:A:353:ILE:O	2.19	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:228:PHE:HE2	1:A:259:ASN:HA	1.86	0.40
1:A:258:LYS:HD2	1:A:258:LYS:H	1.83	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 sym-

metry 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%)	36	46

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%)	298 (89%)	37 (11%)	6	7

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	10	GLU
1	A	18	LEU

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Mol	Chain	Res	Type
1	A	37	VAL
1	A	46	LYS
1	A	71	LEU
1	A	80	THR
1	A	83	SER
1	A	99	ARG
1	A	103	VAL
1	A	107	SER
1	A	129	ARG
1	A	154	GLN
1	A	165	THR
1	A	168	LEU
1	A	179	LYS
1	A	195	PRO
1	A	196	THR
1	A	214	LYS
1	A	216	ASN
1	A	252	LEU
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	313	PRO
1	A	317	LYS
1	A	332	SER
1	A	343	LYS
1	A	347	SER
1	A	351	GLN
1	A	366	LYS
1	A	373	LEU
1	A	389	VAL
1	A	409	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	91	ASN
1	A	120	GLN
1	A	156	GLN

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Mol	Chain	Res	Type
1	A	202	GLN
1	A	216	ASN
1	A	242	HIS
1	A	246	GLN
1	A	286	GLN
1	A	297	ASN
1	A	301	ASN
1	A	336	GLN
1	A	340	ASN
1	A	351	GLN
1	A	369	GLN
1	A	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](#)

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	-	25,25,25	1.59	4 (16%)	34,37,37	2.69	12 (35%)

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	-	-	12/23/23/23	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	PLA	C4A-C4	-5.07	1.44	1.52
2	A	411	PLA	CB1-CA	-3.21	1.51	1.55
2	A	411	PLA	O3-C3	-2.36	1.31	1.36
2	A	411	PLA	C5-C4	-2.21	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	-10.64	95.88	110.76
2	A	411	PLA	C4-C4A-N	4.17	119.91	110.74
2	A	411	PLA	C6-N1-C2	3.65	125.82	119.20
2	A	411	PLA	CB2-CA-N	3.42	117.63	108.92
2	A	411	PLA	C5-C6-N1	-3.31	118.45	123.83
2	A	411	PLA	O4P-C5A-C5	3.27	115.48	109.36
2	A	411	PLA	C3-C2-N1	-3.17	116.96	120.96
2	A	411	PLA	C3-C4-C5	3.16	121.59	118.73
2	A	411	PLA	C5A-C5-C6	-2.52	115.26	119.36
2	A	411	PLA	CA-CB1-CG	2.25	117.72	113.22
2	A	411	PLA	C2A-C2-C3	2.24	123.42	120.80
2	A	411	PLA	C4A-C4-C3	-2.14	117.14	119.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	411	PLA	C5-C4-C4A-N
2	A	411	PLA	C4-C5-C5A-O4P
2	A	411	PLA	C6-C5-C5A-O4P
2	A	411	PLA	O-C-CA-N
2	A	411	PLA	OXT-C-CA-N
2	A	411	PLA	OXT-C-CA-CB2
2	A	411	PLA	O-C-CA-CB2

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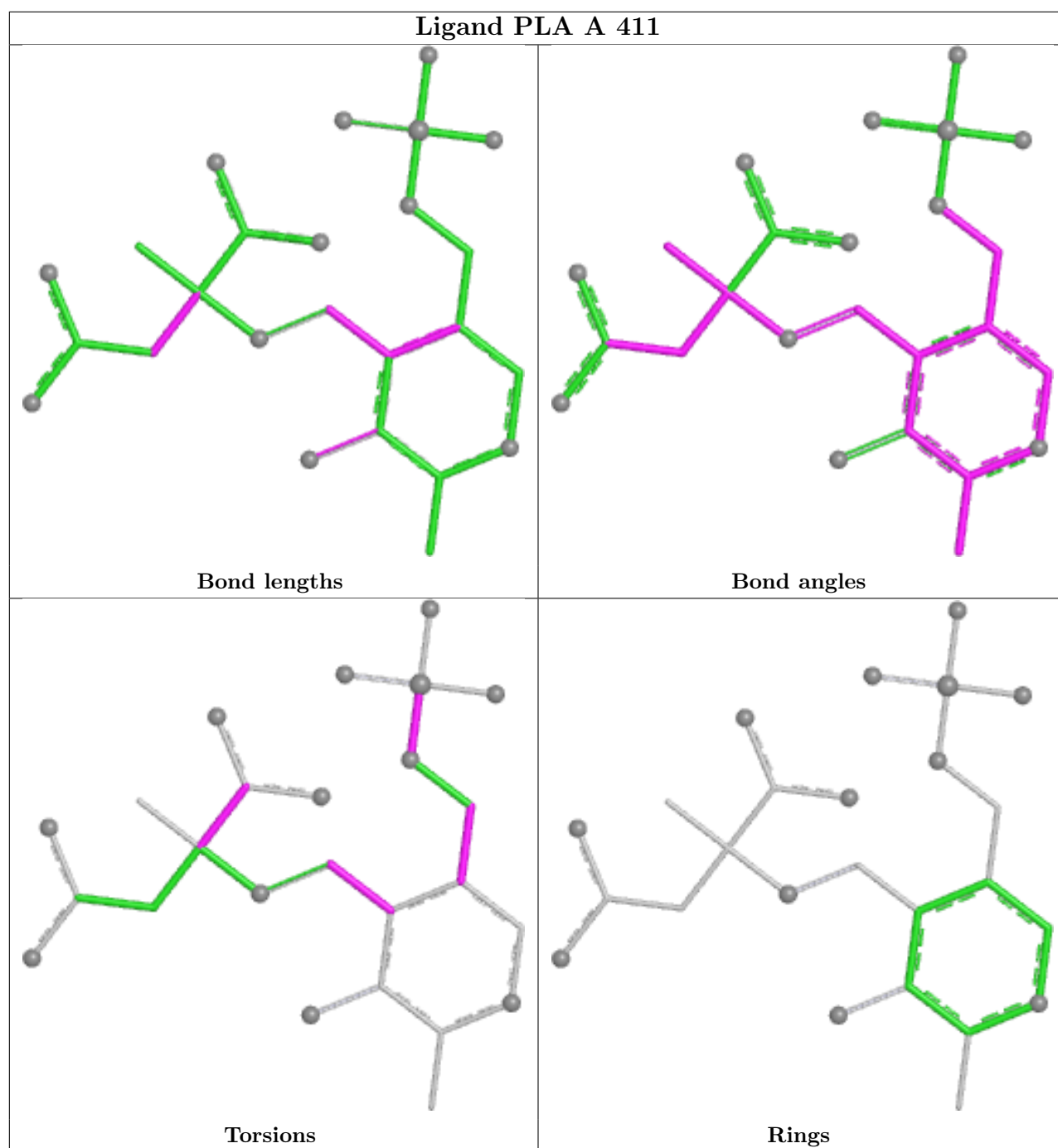
Mol	Chain	Res	Type	Atoms
2	A	411	PLA	C5A-O4P-P-O1P
2	A	411	PLA	C5A-O4P-P-O2P
2	A	411	PLA	C3-C4-C4A-N
2	A	411	PLA	O-C-CA-CB1
2	A	411	PLA	OXT-C-CA-CB1

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	PLA	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.