



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 12:51 AM EST

PDB ID : 1TAS  
Title : CRYSTALLINE MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE EXISTS IN ONLY TWO CONFORMATIONS  
Authors : Hohenester, E.; Jansonius, J.N.  
Deposited on : 1993-10-04  
Resolution : 2.80 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

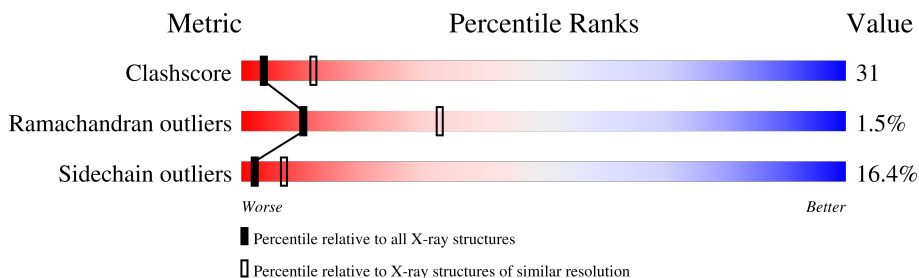
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\geq 3$ , 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	 47%                      40%                      12%                      .
1	B	401	 39%                      45%                      15%                      .

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6372 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.

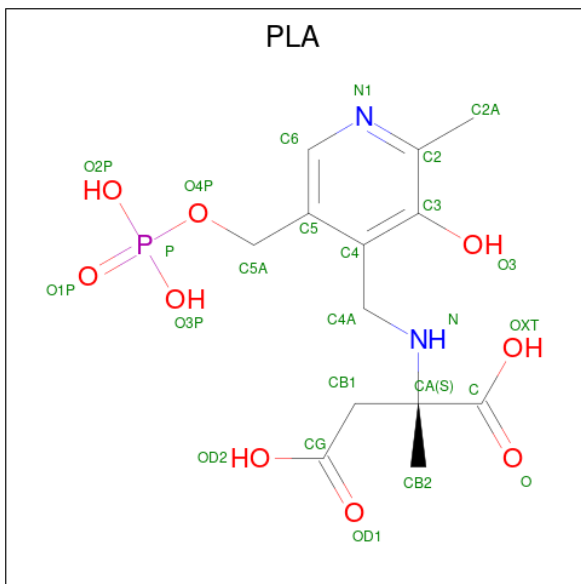
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3161	2004	558	581	18	124	0	0
1	B	401	3161	2004	558	581	18	139	0	0

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



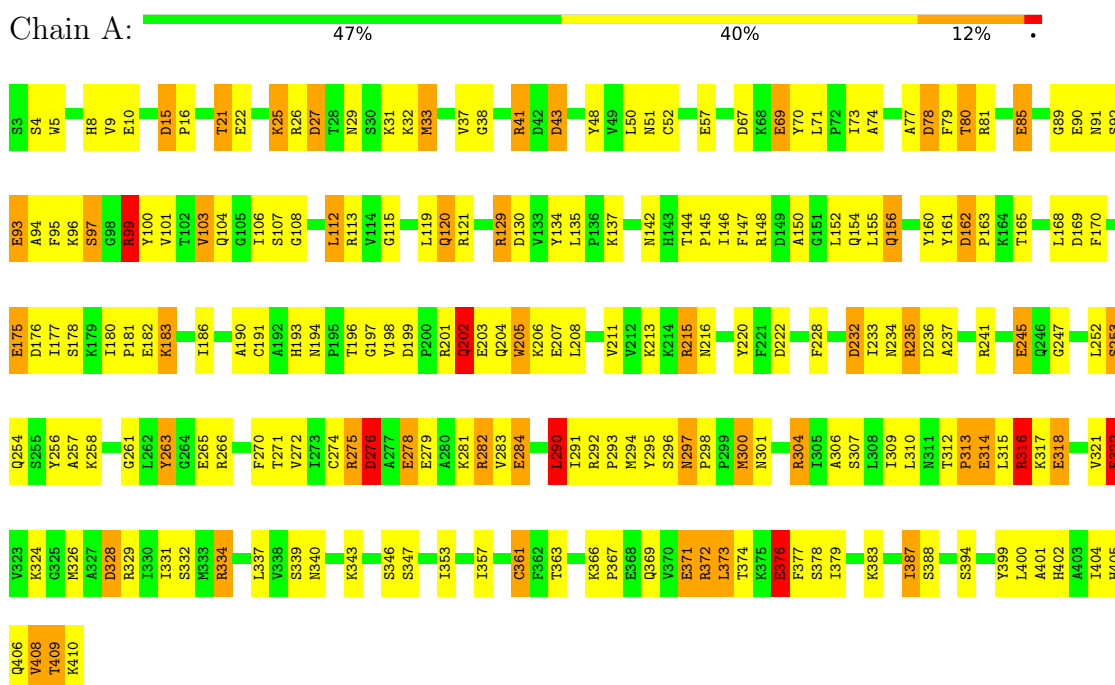
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>					<b>ZeroOcc</b>	<b>AltConf</b>
2	A	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

### 3 Residue-property plots [i](#)

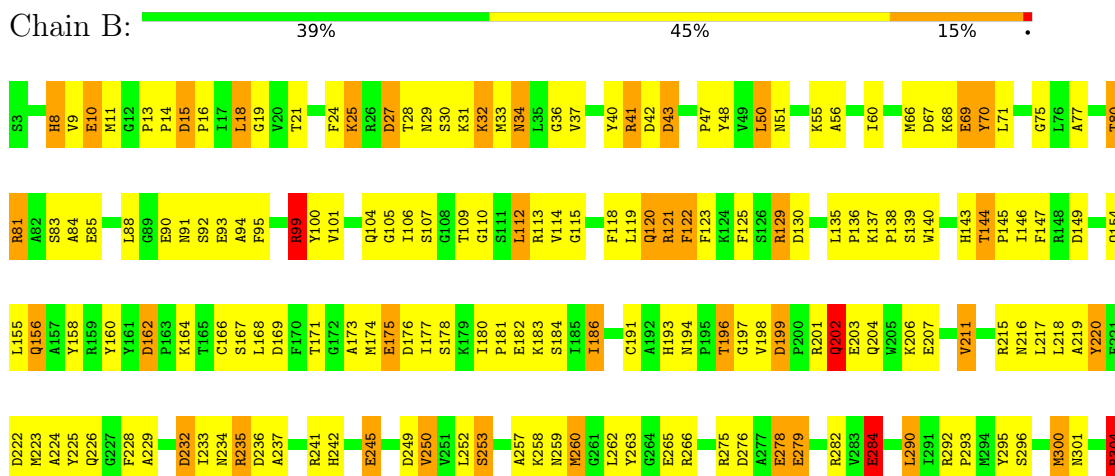
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



- Molecule 1: ASPARTATE AMINOTRANSFERASE





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.40Å 52.40Å 136.90Å 90.00° 101.50° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	1.22	17/3231 (0.5%)	1.63	56/4360 (1.3%)
1	B	1.16	19/3231 (0.6%)	1.59	57/4360 (1.3%)
All	All	1.19	36/6462 (0.6%)	1.61	113/8720 (1.3%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	GLU	CD-OE2	14.30	1.41	1.25
1	A	69	GLU	CD-OE1	8.07	1.34	1.25
1	A	376	GLU	CD-OE1	7.86	1.34	1.25
1	B	344	GLU	CD-OE1	6.96	1.33	1.25
1	B	318	GLU	CD-OE2	6.71	1.33	1.25
1	B	279	GLU	CD-OE2	6.64	1.32	1.25
1	B	93	GLU	CD-OE2	6.30	1.32	1.25
1	A	93	GLU	CD-OE2	6.17	1.32	1.25
1	A	318	GLU	CD-OE2	6.14	1.32	1.25
1	B	69	GLU	CD-OE1	5.75	1.31	1.25
1	A	85	GLU	CD-OE2	5.72	1.31	1.25
1	A	265	GLU	CD-OE2	5.69	1.31	1.25
1	A	175	GLU	CD-OE1	5.64	1.31	1.25
1	A	182	GLU	CD-OE2	5.57	1.31	1.25
1	B	10	GLU	CD-OE1	5.50	1.31	1.25
1	B	90	GLU	CD-OE1	5.45	1.31	1.25
1	B	376	GLU	CD-OE1	5.43	1.31	1.25
1	B	265	GLU	CD-OE2	5.41	1.31	1.25
1	B	314	GLU	CD-OE1	5.41	1.31	1.25
1	A	90	GLU	CD-OE1	5.38	1.31	1.25
1	B	207	GLU	CD-OE1	5.38	1.31	1.25
1	B	368	GLU	CD-OE2	5.36	1.31	1.25
1	B	182	GLU	CD-OE1	5.33	1.31	1.25
1	B	245	GLU	CD-OE1	5.31	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	GLU	CD-OE1	5.31	1.31	1.25
1	B	278	GLU	CD-OE2	5.29	1.31	1.25
1	A	371	GLU	CD-OE2	5.26	1.31	1.25
1	A	10	GLU	CD-OE1	5.26	1.31	1.25
1	A	278	GLU	CD-OE2	5.25	1.31	1.25
1	B	371	GLU	CD-OE2	5.25	1.31	1.25
1	A	314	GLU	CD-OE1	5.23	1.31	1.25
1	A	245	GLU	CD-OE1	5.21	1.31	1.25
1	B	203	GLU	CD-OE2	5.21	1.31	1.25
1	A	22	GLU	CD-OE1	5.13	1.31	1.25
1	B	322	GLU	CD-OE1	5.11	1.31	1.25
1	A	207	GLU	CD-OE1	5.05	1.31	1.25

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	ARG	NE-CZ-NH1	10.33	125.46	120.30
1	A	334	ARG	NE-CZ-NH1	-10.08	115.26	120.30
1	A	99	ARG	NE-CZ-NH2	9.70	125.15	120.30
1	A	41	ARG	NE-CZ-NH1	9.33	124.96	120.30
1	A	282	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	A	99	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	A	78	ASP	CB-CG-OD2	-8.66	110.51	118.30
1	A	27	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	B	329	ARG	NE-CZ-NH1	-8.45	116.07	120.30
1	B	222	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	A	175	GLU	N-CA-CB	8.15	125.27	110.60
1	B	67	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	A	199	ASP	CB-CG-OD1	-8.09	111.02	118.30
1	A	67	ASP	CB-CG-OD1	7.84	125.36	118.30
1	B	276	ASP	CB-CG-OD2	-7.84	111.24	118.30
1	B	355	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	B	81	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	67	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	B	222	ASP	CB-CG-OD1	7.74	125.26	118.30
1	A	162	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	B	67	ASP	CB-CG-OD1	7.59	125.13	118.30
1	B	316	ARG	NE-CZ-NH1	-7.51	116.54	120.30
1	B	232	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	43	ASP	CB-CG-OD2	-7.45	111.59	118.30
1	B	384	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	A	276	ASP	CB-CA-C	-7.35	95.69	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	A	169	ASP	CB-CG-OD2	7.30	124.87	118.30
1	B	43	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	B	329	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	A	282	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	33	MET	CG-SD-CE	-7.14	88.78	100.20
1	B	276	ASP	CB-CG-OD1	7.13	124.72	118.30
1	A	43	ASP	CB-CG-OD1	7.13	124.71	118.30
1	A	41	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	27	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	27	ASP	CB-CG-OD1	6.92	124.53	118.30
1	B	284	GLU	N-CA-CB	6.91	123.04	110.60
1	B	384	ASP	CB-CG-OD1	6.88	124.50	118.30
1	B	355	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	81	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	130	ASP	CB-CG-OD1	6.77	124.39	118.30
1	B	232	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	B	149	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	99	ARG	NE-CZ-NH1	-6.67	116.96	120.30
1	A	232	ASP	CB-CG-OD2	6.64	124.27	118.30
1	B	328	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	A	222	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	316	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	A	275	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	A	78	ASP	CB-CG-OD1	6.55	124.20	118.30
1	A	169	ASP	CB-CG-OD1	-6.54	112.42	118.30
1	A	202	GLN	N-CA-CB	-6.40	99.08	110.60
1	A	232	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	B	162	ASP	CB-CG-OD1	-6.34	112.60	118.30
1	A	222	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	B	27	ASP	CB-CG-OD2	-6.30	112.62	118.30
1	A	148	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	199	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	B	43	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	42	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	B	236	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	B	372	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	304	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	324	LYS	N-CA-CB	5.97	121.35	110.60
1	A	281	LYS	N-CA-CB	5.97	121.35	110.60
1	A	134	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	A	21	THR	CA-CB-CG2	-5.95	104.08	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	ASP	N-CA-CB	-5.91	99.95	110.60
1	A	361	CYS	CA-CB-SG	-5.89	103.40	114.00
1	A	322	GLU	N-CA-CB	5.89	121.19	110.60
1	B	266	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	B	360	PHE	CA-C-N	-5.87	104.29	117.20
1	B	149	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	15	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	B	249	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	A	254	GLN	CB-CA-C	-5.81	98.78	110.40
1	A	121	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	250	VAL	CB-CA-C	-5.76	100.45	111.40
1	B	176	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	130	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	215	ARG	CB-CA-C	-5.71	98.98	110.40
1	A	275	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	236	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	304	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	328	ASP	CB-CG-OD1	5.65	123.38	118.30
1	B	377	PHE	CB-CG-CD1	-5.63	116.86	120.80
1	A	199	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	162	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	81	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	256	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	A	161	TYR	CA-CB-CG	5.44	123.73	113.40
1	B	122	PHE	N-CA-C	5.43	125.67	111.00
1	B	276	ASP	CB-CA-C	-5.43	99.53	110.40
1	B	211	VAL	CA-CB-CG1	-5.36	102.86	110.90
1	B	125	PHE	N-CA-C	5.29	125.29	111.00
1	A	5	TRP	CB-CA-C	-5.28	99.84	110.40
1	B	15	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	B	70	TYR	CA-CB-CG	5.26	123.40	113.40
1	B	176	ASP	CA-CB-CG	-5.26	101.83	113.40
1	B	202	GLN	N-CA-CB	-5.22	101.20	110.60
1	A	346	SER	N-CA-CB	5.19	118.29	110.50
1	A	290	LEU	N-CA-CB	-5.19	100.02	110.40
1	A	70	TYR	CA-CB-CG	5.19	123.26	113.40
1	A	329	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	B	100	TYR	CB-CG-CD2	5.16	124.09	121.00
1	B	162	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	176	ASP	CA-CB-CG	-5.14	102.09	113.40
1	A	328	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	316	ARG	NE-CZ-NH2	5.12	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ARG	CB-CA-C	-5.04	100.33	110.40
1	B	169	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	A	334	ARG	NE-CZ-NH2	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	166	0
1	B	3161	0	3154	223	0
2	A	25	0	14	6	0
2	B	25	0	14	5	0
All	All	6372	0	6336	378	0

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 31.

All (378) 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:327:ALA:HA	1:B:330:ILE:HD12	1.49	0.94
1:B:196:THR:HG23	1:B:198:VAL:HG23	1.49	0.92
1:B:366:LYS:H	1:B:369:GLN:NE2	1.69	0.90
1:A:196:THR:HG22	1:A:198:VAL:H	1.39	0.88
1:B:338:VAL:HG21	1:B:354:THR:HG23	1.56	0.87
1:B:94:ALA:HA	1:B:99:ARG:HD3	1.55	0.86
1:A:170:PHE:CE1	1:A:204:GLN:HB3	2.11	0.85
1:A:168:LEU:HD13	1:A:198:VAL:HG12	1.59	0.84
1:B:177:ILE:HA	1:B:180:ILE:HD12	1.61	0.83
1:B:33:MET:HE1	1:B:399:TYR:HD2	1.42	0.82
1:A:74:ALA:HB1	1:A:103:VAL:HG22	1.62	0.82
1:A:156:GLN:HE21	1:A:156:GLN:HA	1.44	0.81
1:A:196:THR:CG2	1:A:198:VAL:HB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:HB3	1:B:293:PRO:HD3	1.62	0.78
1:B:110:GLY:O	1:B:114:VAL:HG23	1.84	0.78
1:A:147:PHE:HB2	1:A:155:LEU:HD21	1.65	0.78
1:B:137:LYS:HG3	1:B:158:TYR:O	1.83	0.77
1:A:29:ASN:OD1	1:A:31:LYS:HB2	1.85	0.76
1:A:369:GLN:HB3	1:A:408:VAL:CG1	2.15	0.76
1:B:334:ARG:O	1:B:338:VAL:HG23	1.86	0.76
1:A:69:GLU:OE2	1:B:47:PRO:HB3	1.87	0.75
1:B:405:HIS:O	1:B:409:THR:HG22	1.87	0.74
1:B:370:VAL:CG1	1:B:381:MET:HG2	2.18	0.74
1:B:199:ASP:OD2	1:B:357:ILE:HD11	1.86	0.74
1:B:258:LYS:CE	2:B:411:PLA:H4A2	2.18	0.74
1:A:237:ALA:O	1:A:241:ARG:HG3	1.88	0.73
1:B:24:PHE:HE1	1:B:32:LYS:HB2	1.53	0.73
1:B:33:MET:HE1	1:B:399:TYR:CD2	2.23	0.73
1:A:33:MET:HE1	1:A:399:TYR:HD2	1.53	0.73
1:B:258:LYS:NZ	2:B:411:PLA:H4A2	2.04	0.73
1:A:400:LEU:HD11	1:A:404:ILE:HD11	1.71	0.73
1:B:359:MET:O	1:B:389:VAL:HG12	1.89	0.73
1:A:258:LYS:NZ	2:A:411:PLA:H4A2	2.04	0.72
1:A:8:HIS:CD2	1:A:8:HIS:H	2.08	0.72
1:A:258:LYS:HE3	2:A:411:PLA:HB22	1.71	0.72
1:A:322:GLU:O	1:A:326:MET:HG3	1.90	0.72
1:A:162:ASP:OD2	1:A:165:THR:HB	1.90	0.71
1:A:196:THR:HG23	1:A:198:VAL:HB	1.72	0.71
1:A:193:HIS:ND1	1:A:196:THR:HB	2.05	0.71
1:A:92:SER:HB3	1:A:95:PHE:HB3	1.73	0.71
1:A:115:GLY:O	1:A:119:LEU:HG	1.90	0.71
1:A:258:LYS:HZ2	2:A:411:PLA:H4A2	1.55	0.70
1:B:372:ARG:HB3	1:B:408:VAL:CG2	2.21	0.70
1:A:21:THR:O	1:A:25:LYS:HG3	1.92	0.70
1:B:234:ASN:ND2	1:B:241:ARG:HH12	1.90	0.70
1:A:144:THR:HB	1:A:145:PRO:HD3	1.74	0.69
1:B:372:ARG:HB3	1:B:408:VAL:HG22	1.74	0.69
1:A:404:ILE:O	1:A:409:THR:HB	1.91	0.69
1:B:101:VAL:HG21	1:B:284:GLU:HB3	1.74	0.69
1:A:77:ALA:O	1:A:80:THR:HG22	1.92	0.69
1:A:160:TYR:CZ	1:A:168:LEU:HD11	2.28	0.68
1:B:196:THR:HG23	1:B:198:VAL:CG2	2.24	0.68
1:A:79:PHE:CE2	1:A:104:GLN:HG3	2.28	0.68
1:B:174:MET:CE	1:B:211:VAL:HG21	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ALA:HB1	1:B:357:ILE:HD13	1.76	0.68
1:B:370:VAL:HG13	1:B:381:MET:HG2	1.74	0.68
1:A:234:ASN:HD22	1:A:241:ARG:HH12	1.39	0.68
1:B:279:GLU:HG3	1:B:282:ARG:NH2	2.08	0.68
1:B:279:GLU:HG3	1:B:282:ARG:HH22	1.57	0.68
1:B:15:ASP:OD1	1:B:16:PRO:HD2	1.95	0.67
1:B:109:THR:HG23	1:B:146:ILE:HD11	1.77	0.66
1:A:366:LYS:HB3	1:A:367:PRO:HD2	1.77	0.66
1:B:15:ASP:HB3	1:B:19:GLY:H	1.60	0.66
1:B:193:HIS:ND1	1:B:196:THR:HB	2.10	0.66
1:A:93:GLU:OE1	1:A:99:ARG:NH1	2.28	0.66
1:A:293:PRO:O	1:B:113:ARG:NH1	2.29	0.66
1:B:140:TRP:HB3	1:B:143:HIS:ND1	2.11	0.66
1:B:367:PRO:O	1:B:371:GLU:HG3	1.95	0.66
1:A:156:GLN:HA	1:A:156:GLN:NE2	2.11	0.66
1:B:223:MET:HE3	1:B:226:GLN:HB2	1.77	0.65
1:B:140:TRP:HB3	1:B:143:HIS:CE1	2.32	0.64
1:B:217:LEU:HD23	1:B:217:LEU:N	2.13	0.64
1:A:196:THR:CG2	1:A:198:VAL:H	2.10	0.64
1:B:337:LEU:O	1:B:337:LEU:HD12	1.97	0.64
1:B:366:LYS:HB3	1:B:367:PRO:HD2	1.79	0.64
1:B:13:PRO:HB2	1:B:14:PRO:HD2	1.78	0.64
1:B:366:LYS:HB3	1:B:367:PRO:CD	2.28	0.64
1:B:260:MET:HE1	1:B:309:ILE:HD12	1.78	0.63
1:B:24:PHE:CE1	1:B:32:LYS:HB2	2.33	0.63
1:B:101:VAL:HG21	1:B:284:GLU:CB	2.27	0.63
1:B:260:MET:HE1	1:B:309:ILE:HB	1.81	0.63
1:B:196:THR:CG2	1:B:198:VAL:HG23	2.27	0.63
1:B:279:GLU:HA	1:B:282:ARG:NH2	2.14	0.63
1:B:366:LYS:N	1:B:369:GLN:NE2	2.45	0.62
1:B:162:ASP:O	1:B:166:CYS:N	2.33	0.62
1:B:373:LEU:HD12	1:B:379:ILE:HD13	1.81	0.62
1:B:40:TYR:CE2	1:B:326:MET:HB3	2.35	0.62
1:B:144:THR:CG2	1:B:155:LEU:HD13	2.29	0.62
1:B:144:THR:HG22	1:B:155:LEU:HD13	1.81	0.62
1:B:160:TYR:CZ	1:B:168:LEU:HD11	2.34	0.62
1:A:74:ALA:CB	1:A:103:VAL:HG22	2.30	0.62
1:A:135:LEU:HD11	1:A:155:LEU:HD22	1.82	0.62
1:B:232:ASP:HB3	1:B:235:ARG:HB3	1.82	0.62
1:A:168:LEU:CD1	1:A:198:VAL:HG12	2.30	0.62
1:A:377:PHE:HB3	1:A:399:TYR:OH	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:O	1:A:373:LEU:HD22	2.00	0.61
1:B:301:ASN:O	1:B:305:ILE:HD12	1.99	0.61
1:A:108:GLY:O	1:A:112:LEU:HB2	1.99	0.61
1:A:372:ARG:HB2	1:A:408:VAL:CG2	2.30	0.61
1:A:300:MET:O	1:A:304:ARG:HG3	2.01	0.61
1:B:219:ALA:HB3	1:B:250:VAL:HG12	1.81	0.61
1:A:129:ARG:HE	1:A:129:ARG:HA	1.64	0.61
1:B:194:ASN:ND2	2:B:411:PLA:O3	2.34	0.60
1:B:370:VAL:HG13	1:B:381:MET:SD	2.42	0.60
1:B:135:LEU:HD11	1:B:155:LEU:CD2	2.31	0.60
1:B:330:ILE:HG23	1:B:389:VAL:HG13	1.82	0.60
1:A:94:ALA:HA	1:A:99:ARG:HD3	1.84	0.59
1:B:257:ALA:HB1	1:B:263:TYR:HA	1.84	0.59
1:B:338:VAL:O	1:B:341:LEU:HB2	2.02	0.59
1:A:400:LEU:HD12	1:A:400:LEU:O	2.01	0.59
1:B:330:ILE:HG23	1:B:389:VAL:CG1	2.32	0.59
1:A:405:HIS:O	1:A:409:THR:HG22	2.02	0.59
1:A:266:ARG:HD2	1:A:266:ARG:N	2.17	0.58
1:A:372:ARG:HB2	1:A:408:VAL:HG21	1.85	0.58
1:B:34:ASN:C	1:B:34:ASN:HD22	2.07	0.58
1:B:174:MET:HE1	1:B:211:VAL:HG21	1.85	0.58
1:B:370:VAL:HG13	1:B:381:MET:CG	2.34	0.58
1:B:174:MET:HE3	1:B:211:VAL:HG21	1.85	0.58
1:B:335:THR:HG22	1:B:336:GLN:N	2.19	0.58
1:B:318:GLU:O	1:B:322:GLU:HG3	2.03	0.57
1:B:366:LYS:H	1:B:369:GLN:HE22	1.52	0.57
1:B:50:LEU:N	1:B:50:LEU:HD12	2.20	0.57
1:B:56:ALA:O	1:B:60:ILE:HG13	2.04	0.57
1:A:400:LEU:O	1:A:404:ILE:HG13	2.05	0.57
1:B:292:ARG:CB	1:B:293:PRO:HD3	2.33	0.57
1:A:400:LEU:HD12	1:A:404:ILE:HG13	1.87	0.57
1:A:142:ASN:O	1:A:146:ILE:HD12	2.03	0.56
1:A:334:ARG:HD3	1:A:353:ILE:O	2.06	0.56
1:B:115:GLY:O	1:B:119:LEU:HG	2.05	0.56
1:B:399:TYR:O	1:B:402:HIS:HB3	2.04	0.56
1:B:233:ILE:HG13	1:B:234:ASN:N	2.20	0.56
1:A:48:TYR:CE2	1:A:50:LEU:HD12	2.41	0.56
1:B:178:SER:O	1:B:215:ARG:NE	2.39	0.56
1:A:361:CYS:SG	1:A:363:THR:HG22	2.46	0.56
1:B:50:LEU:HD21	1:B:326:MET:HE1	1.88	0.56
1:B:41:ARG:HH11	1:B:47:PRO:HA	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ALA:O	1:B:88:LEU:HB2	2.07	0.55
1:B:316:ARG:O	1:B:320:LEU:HG	2.07	0.55
1:A:295:TYR:O	1:A:296:SER:HB3	2.07	0.55
1:A:361:CYS:HB3	1:A:387:ILE:HD13	1.88	0.55
1:B:216:ASN:C	1:B:217:LEU:HD23	2.27	0.55
1:B:135:LEU:HD11	1:B:155:LEU:HD22	1.89	0.55
1:B:350:TRP:O	1:B:353:ILE:HG13	2.06	0.55
1:A:201:ARG:HB2	1:A:204:GLN:OE1	2.08	0.54
1:B:94:ALA:O	1:B:99:ARG:HG3	2.07	0.54
1:B:162:ASP:OD1	1:B:164:LYS:HB2	2.07	0.54
1:B:202:GLN:O	1:B:206:LYS:HG3	2.07	0.54
1:B:237:ALA:O	1:B:241:ARG:HG3	2.08	0.54
1:B:112:LEU:HD13	1:B:253:SER:CB	2.38	0.54
1:B:260:MET:HE2	1:B:309:ILE:HG21	1.89	0.54
1:B:300:MET:O	1:B:304:ARG:HG2	2.08	0.54
1:A:8:HIS:H	1:A:8:HIS:HD2	1.54	0.54
1:A:369:GLN:HB3	1:A:408:VAL:HG13	1.86	0.54
1:B:60:ILE:HG23	1:B:66:MET:SD	2.47	0.54
1:B:121:ARG:CZ	1:B:290:LEU:HD23	2.38	0.54
1:A:106:ILE:O	1:A:106:ILE:HG22	2.08	0.54
1:A:290:LEU:O	1:A:294:MET:HE3	2.08	0.54
1:A:379:ILE:HG22	1:A:379:ILE:O	2.08	0.54
1:B:8:HIS:H	1:B:8:HIS:CD2	2.26	0.54
1:B:50:LEU:CD1	1:B:50:LEU:H	2.21	0.53
1:A:101:VAL:HG11	1:A:283:VAL:HG12	1.90	0.53
1:A:112:LEU:CD1	1:A:253:SER:HB3	2.37	0.53
1:A:51:ASN:HB2	1:A:322:GLU:OE2	2.09	0.53
1:A:361:CYS:HB3	1:A:387:ILE:CD1	2.38	0.53
1:B:121:ARG:NH1	1:B:290:LEU:HD23	2.24	0.53
1:B:329:ARG:NH2	1:B:392:VAL:O	2.39	0.53
1:A:402:HIS:CE1	1:A:406:GLN:HG3	2.44	0.52
1:A:33:MET:CE	1:A:399:TYR:HD2	2.19	0.52
1:A:190:ALA:O	1:A:191:CYS:HB3	2.09	0.52
1:A:296:SER:OG	1:A:297:ASN:ND2	2.42	0.52
1:B:51:ASN:O	1:B:55:LYS:HG3	2.08	0.52
1:A:74:ALA:HB1	1:A:103:VAL:CG2	2.37	0.52
1:A:144:THR:N	1:A:145:PRO:HD2	2.25	0.52
1:B:334:ARG:NH1	1:B:360:PHE:O	2.37	0.52
1:A:374:THR:O	1:A:378:SER:HA	2.10	0.52
1:B:260:MET:CE	1:B:309:ILE:HB	2.40	0.52
1:A:112:LEU:HD13	1:A:253:SER:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ILE:O	1:B:409:THR:HB	2.09	0.52
1:B:405:HIS:O	1:B:410:LYS:N	2.43	0.52
1:A:245:GLU:C	1:A:247:GLY:H	2.12	0.51
1:A:73:ILE:CG1	1:B:18:LEU:HD23	2.40	0.51
1:B:372:ARG:NE	1:B:408:VAL:HG22	2.26	0.51
1:A:33:MET:HE1	1:A:399:TYR:CD2	2.40	0.51
1:B:201:ARG:O	1:B:204:GLN:N	2.42	0.51
1:B:260:MET:CE	1:B:309:ILE:HD12	2.40	0.51
1:A:100:TYR:CD1	1:A:100:TYR:N	2.78	0.51
1:B:196:THR:HG22	1:B:198:VAL:H	1.75	0.51
1:A:144:THR:HG23	1:A:155:LEU:HD13	1.91	0.51
1:A:275:ARG:HB3	1:A:276:ASP:OD1	2.11	0.51
1:B:50:LEU:HD12	1:B:50:LEU:H	1.76	0.51
1:B:368:GLU:O	1:B:372:ARG:HG3	2.11	0.51
1:A:115:GLY:HA3	1:A:270:PHE:CE1	2.46	0.51
1:B:33:MET:HE3	1:B:379:ILE:HG12	1.91	0.51
1:A:33:MET:HE3	1:A:379:ILE:HG12	1.92	0.51
1:B:33:MET:HE3	1:B:379:ILE:CG1	2.40	0.51
1:B:197:GLY:HA3	1:B:356:GLN:HG2	1.93	0.51
1:B:234:ASN:HD22	1:B:241:ARG:HH12	1.54	0.51
1:A:69:GLU:CD	1:B:47:PRO:HB3	2.31	0.50
1:A:113:ARG:NH1	1:B:293:PRO:O	2.44	0.50
1:A:177:ILE:HG22	1:A:211:VAL:HG11	1.93	0.50
1:A:400:LEU:CD1	1:A:404:ILE:HD11	2.41	0.50
1:A:9:VAL:O	1:B:282:ARG:HD2	2.12	0.50
1:A:202:GLN:O	1:A:206:LYS:HG3	2.11	0.50
1:B:66:MET:HB2	1:B:304:ARG:NH2	2.27	0.50
1:B:112:LEU:HA	1:B:220:TYR:OH	2.12	0.50
1:B:8:HIS:CD2	1:B:8:HIS:N	2.79	0.50
1:B:40:TYR:CZ	1:B:326:MET:HB3	2.47	0.49
1:B:146:ILE:HG22	1:B:147:PHE:N	2.27	0.49
1:A:233:ILE:HG13	1:A:234:ASN:N	2.27	0.49
1:B:197:GLY:O	1:B:356:GLN:HA	2.12	0.49
1:B:372:ARG:HB3	1:B:408:VAL:HG21	1.92	0.49
1:A:101:VAL:O	1:A:271:THR:HA	2.13	0.49
1:A:275:ARG:HB2	1:A:279:GLU:OE1	2.13	0.49
1:B:174:MET:HE1	1:B:211:VAL:CG2	2.42	0.49
1:A:93:GLU:O	1:A:97:SER:OG	2.29	0.49
1:B:242:HIS:O	1:B:245:GLU:HG2	2.11	0.49
1:A:52:CYS:HB3	1:A:318:GLU:HG2	1.95	0.48
1:A:129:ARG:HA	1:A:129:ARG:NE	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:C	1:B:156:GLN:HG2	2.34	0.48
1:B:363:THR:CG2	1:B:387:ILE:HD13	2.43	0.48
1:A:37:VAL:HG13	1:A:37:VAL:O	2.12	0.48
1:B:224:ALA:HB1	1:B:258:LYS:NZ	2.29	0.48
1:B:331:ILE:HG22	1:B:332:SER:N	2.27	0.48
1:B:183:LYS:HA	1:B:216:ASN:O	2.13	0.48
1:A:89:GLY:O	1:A:92:SER:HB2	2.13	0.48
1:A:100:TYR:HD1	1:A:100:TYR:H	1.62	0.48
1:A:168:LEU:HD13	1:A:198:VAL:CG1	2.40	0.48
1:B:338:VAL:HG21	1:B:354:THR:CG2	2.34	0.48
1:A:292:ARG:HB3	1:A:293:PRO:HD3	1.95	0.48
1:A:137:LYS:O	1:A:160:TYR:HB3	2.13	0.48
1:A:337:LEU:CD2	1:A:353:ILE:HD13	2.43	0.48
1:B:33:MET:HE3	1:B:379:ILE:HD11	1.95	0.48
1:B:137:LYS:HA	1:B:138:PRO:HA	1.64	0.48
1:A:337:LEU:HD23	1:A:353:ILE:HD13	1.96	0.48
1:A:194:ASN:ND2	2:A:411:PLA:O3	2.46	0.47
1:A:369:GLN:HB3	1:A:408:VAL:HG11	1.92	0.47
1:B:33:MET:CE	1:B:379:ILE:HD11	2.44	0.47
1:B:361:CYS:SG	1:B:363:THR:HG22	2.53	0.47
1:B:377:PHE:CB	1:B:379:ILE:HD12	2.45	0.47
1:A:85:GLU:HB2	1:A:95:PHE:CZ	2.49	0.47
1:A:228:PHE:CZ	1:A:326:MET:HE3	2.50	0.47
1:A:366:LYS:HB3	1:A:367:PRO:CD	2.44	0.47
1:B:173:ALA:O	1:B:177:ILE:HG13	2.15	0.47
1:B:366:LYS:HB2	1:B:369:GLN:NE2	2.29	0.47
1:A:120:GLN:HG3	1:A:150:ALA:O	2.15	0.47
1:A:101:VAL:HG11	1:A:283:VAL:CG1	2.44	0.47
1:A:263:TYR:HB3	1:B:70:TYR:CD1	2.50	0.47
1:B:337:LEU:HD12	1:B:337:LEU:C	2.35	0.47
1:B:376:GLU:HB2	1:B:377:PHE:CD1	2.49	0.47
1:B:400:LEU:CD1	1:B:404:ILE:HG13	2.45	0.47
1:B:186:ILE:HG23	1:B:186:ILE:O	2.15	0.47
1:A:178:SER:O	1:A:215:ARG:HD3	2.15	0.47
1:A:377:PHE:CD1	1:A:377:PHE:N	2.83	0.47
1:B:80:THR:CG2	1:B:81:ARG:N	2.77	0.46
1:A:317:LYS:O	1:A:321:VAL:HG23	2.15	0.46
1:B:106:ILE:HG22	1:B:106:ILE:O	2.15	0.46
1:B:50:LEU:HD21	1:B:326:MET:CE	2.45	0.46
1:A:37:VAL:HG22	1:A:38:GLY:N	2.30	0.46
1:B:13:PRO:CB	1:B:14:PRO:HD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:THR:N	1:B:145:PRO:HD2	2.30	0.46
1:B:260:MET:CE	1:B:309:ILE:HG21	2.46	0.46
1:A:198:VAL:HG12	1:A:198:VAL:O	2.15	0.46
1:A:228:PHE:CZ	1:A:326:MET:CE	2.99	0.46
1:A:266:ARG:NH2	1:B:296:SER:HB3	2.31	0.46
1:A:306:ALA:O	1:A:310:LEU:HG	2.16	0.46
1:B:15:ASP:HA	1:B:16:PRO:HD2	1.38	0.46
1:A:312:THR:HB	1:A:315:LEU:HD12	1.97	0.46
1:B:313:PRO:O	1:B:317:LYS:HG3	2.16	0.46
1:A:293:PRO:HB3	1:B:145:PRO:HB2	1.97	0.45
1:A:263:TYR:HB2	1:B:68:LYS:O	2.16	0.45
1:A:73:ILE:HG13	1:B:18:LEU:HD23	1.98	0.45
1:A:205:TRP:CE3	1:A:208:LEU:HD12	2.52	0.45
1:A:270:PHE:CE2	1:A:272:VAL:CG2	2.99	0.45
1:B:50:LEU:N	1:B:50:LEU:CD1	2.79	0.45
1:B:341:LEU:HA	1:B:341:LEU:HD23	1.57	0.45
1:A:180:ILE:HA	1:A:181:PRO:HD3	1.84	0.45
1:B:104:GLN:CG	1:B:105:GLY:N	2.79	0.45
1:A:274:CYS:HB3	1:A:279:GLU:HG2	1.99	0.45
1:B:75:GLY:HA3	1:B:104:GLN:HB3	1.98	0.45
1:B:160:TYR:CZ	1:B:168:LEU:CD1	2.99	0.45
1:A:282:ARG:HD2	1:B:9:VAL:O	2.16	0.45
1:B:234:ASN:HD22	1:B:234:ASN:HA	1.45	0.45
1:A:112:LEU:HD13	1:A:253:SER:HB3	1.98	0.44
1:A:257:ALA:O	1:A:261:GLY:HA2	2.18	0.44
1:B:144:THR:HB	1:B:145:PRO:HD3	1.98	0.44
1:B:330:ILE:HG21	1:B:358:GLY:O	2.17	0.44
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.71	0.44
1:B:48:TYR:OH	1:B:322:GLU:OE1	2.32	0.44
1:B:69:GLU:O	1:B:300:MET:HE3	2.18	0.44
1:A:372:ARG:O	1:A:376:GLU:HG3	2.17	0.44
2:B:411:PLA:O3	2:B:411:PLA:N	2.50	0.44
1:A:340:ASN:HB3	1:A:401:ALA:CB	2.48	0.44
1:B:175:GLU:O	1:B:178:SER:OG	2.35	0.44
1:B:369:GLN:HE21	1:B:369:GLN:HB2	1.61	0.44
1:B:373:LEU:HD12	1:B:379:ILE:CD1	2.48	0.44
1:A:400:LEU:HD11	1:A:404:ILE:CD1	2.45	0.44
1:B:136:PRO:HG2	1:B:139:SER:HB2	1.99	0.44
1:A:309:ILE:HG21	1:A:309:ILE:HD13	1.66	0.44
1:A:37:VAL:CG2	1:A:38:GLY:N	2.81	0.43
1:B:144:THR:HB	1:B:145:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PHE:HE1	1:B:330:ILE:HD11	1.82	0.43
1:B:373:LEU:CD1	1:B:379:ILE:HD13	2.46	0.43
1:A:129:ARG:HE	1:A:129:ARG:CA	2.31	0.43
1:B:29:ASN:O	1:B:32:LYS:HG2	2.18	0.43
1:B:115:GLY:O	1:B:118:PHE:HB3	2.17	0.43
1:B:211:VAL:O	1:B:215:ARG:HG2	2.19	0.43
1:B:336:GLN:O	1:B:340:ASN:OD1	2.37	0.43
1:A:101:VAL:HG21	1:A:284:GLU:CB	2.49	0.43
1:A:328:ASP:O	1:A:331:ILE:HB	2.19	0.43
1:B:308:LEU:HA	1:B:308:LEU:HD12	1.53	0.43
1:B:377:PHE:HB3	1:B:379:ILE:HD12	1.99	0.43
1:B:397:VAL:O	1:B:397:VAL:HG22	2.19	0.43
2:A:411:PLA:O3	2:A:411:PLA:N	2.50	0.43
1:B:326:MET:O	1:B:330:ILE:HG13	2.18	0.43
1:A:27:ASP:HB3	1:A:32:LYS:HD3	2.00	0.43
1:A:162:ASP:HA	1:A:163:PRO:HD2	1.84	0.43
1:B:99:ARG:HE	1:B:99:ARG:HB2	1.57	0.43
1:B:224:ALA:HB3	1:B:225:TYR:CD2	2.54	0.43
1:B:191:CYS:O	1:B:191:CYS:SG	2.77	0.43
1:A:15:ASP:HA	1:A:16:PRO:HD3	1.71	0.42
1:B:33:MET:HE3	1:B:379:ILE:CD1	2.49	0.42
1:A:41:ARG:HA	1:A:41:ARG:HD3	1.86	0.42
1:A:292:ARG:CB	1:A:293:PRO:HD3	2.48	0.42
1:B:112:LEU:HD13	1:B:253:SER:HB3	2.01	0.42
1:B:27:ASP:O	1:B:32:LYS:NZ	2.47	0.42
1:B:181:PRO:O	1:B:184:SER:OG	2.30	0.42
1:B:340:ASN:O	1:B:344:GLU:HG2	2.19	0.42
1:B:400:LEU:O	1:B:404:ILE:HG13	2.19	0.42
1:A:93:GLU:O	1:A:96:LYS:N	2.53	0.42
1:B:33:MET:CE	1:B:399:TYR:CD2	2.99	0.42
1:B:194:ASN:OD1	1:B:386:ARG:NH1	2.52	0.42
1:B:366:LYS:HB2	1:B:369:GLN:HE22	1.84	0.42
1:A:144:THR:CB	1:A:145:PRO:HD3	2.48	0.42
1:A:196:THR:HG22	1:A:197:GLY:N	2.34	0.42
1:B:279:GLU:O	1:B:282:ARG:HB2	2.20	0.42
1:A:316:ARG:HH11	1:A:316:ARG:HD3	1.63	0.42
1:B:374:THR:O	1:B:378:SER:N	2.53	0.42
1:A:337:LEU:HD23	1:A:353:ILE:HG21	2.02	0.41
1:A:180:ILE:HG23	1:A:181:PRO:HD2	2.02	0.41
1:B:186:ILE:HG22	1:B:218:LEU:O	2.20	0.41
1:A:232:ASP:OD2	1:A:235:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:GLU:HB2	1:B:95:PHE:CE1	2.54	0.41
1:B:174:MET:O	1:B:178:SER:OG	2.29	0.41
1:A:8:HIS:CD2	1:A:8:HIS:N	2.79	0.41
1:A:8:HIS:HE1	1:B:122:PHE:O	2.03	0.41
1:A:266:ARG:HD2	1:A:266:ARG:HA	1.80	0.41
1:A:71:LEU:HD13	1:A:300:MET:CE	2.50	0.41
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.67	0.41
1:A:73:ILE:HG23	1:A:291:ILE:HG22	2.02	0.41
1:A:193:HIS:CE1	1:A:196:THR:HB	2.55	0.41
1:A:334:ARG:HD3	1:A:334:ARG:HH11	1.52	0.41
1:B:43:ASP:OD2	1:B:394:SER:HB2	2.21	0.41
1:B:406:GLN:C	1:B:409:THR:H	2.23	0.41
1:A:186:ILE:O	1:A:186:ILE:HG23	2.21	0.41
1:B:21:THR:O	1:B:24:PHE:HB3	2.20	0.41
1:A:97:SER:H	1:A:97:SER:HG	1.50	0.41
1:A:101:VAL:HG21	1:A:284:GLU:HB2	2.02	0.41
1:A:144:THR:N	1:A:145:PRO:CD	2.82	0.41
1:B:160:TYR:CE1	1:B:168:LEU:HD11	2.55	0.41
1:B:260:MET:HB3	1:B:262:LEU:HG	2.03	0.41
1:B:350:TRP:CE3	1:B:353:ILE:HD11	2.56	0.41
1:B:363:THR:CG2	1:B:387:ILE:CD1	2.98	0.41
1:A:258:LYS:HE3	2:A:411:PLA:CB2	2.46	0.41
1:B:34:ASN:ND2	1:B:36:GLY:H	2.18	0.41
1:B:99:ARG:HG3	1:B:99:ARG:H	1.28	0.41
1:A:232:ASP:O	1:A:236:ASP:HB2	2.21	0.41
1:B:224:ALA:HB1	1:B:258:LYS:HZ3	1.86	0.41
1:B:41:ARG:HB2	1:B:391:GLY:HA2	2.02	0.40
1:B:258:LYS:NZ	2:B:411:PLA:C4A	2.78	0.40
1:A:203:GLU:CD	1:A:203:GLU:H	2.24	0.40
1:A:402:HIS:HE1	1:A:406:GLN:HE21	1.68	0.40
1:B:80:THR:HG22	1:B:81:ARG:N	2.36	0.40
1:B:104:GLN:HG3	1:B:105:GLY:N	2.36	0.40
1:B:228:PHE:HE2	1:B:259:ASN:HA	1.86	0.40
1:B:33:MET:CE	1:B:379:ILE:CG1	2.99	0.40
1:B:234:ASN:HD22	1:B:241:ARG:NH1	2.18	0.40
1:B:120:GLN:HE21	1:B:120:GLN:HB3	1.69	0.40
1:B:400:LEU:HD12	1:B:404:ILE:HG13	2.02	0.40

There are no symmetry-related clashes.

## 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%)	354 (89%)	41 (10%)	4 (1%)	15	44
1	B	399/401 (100%)	358 (90%)	33 (8%)	8 (2%)	7	24
All	All	798/802 (100%)	712 (89%)	74 (9%)	12 (2%)	10	33

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	77	ALA
1	A	313	PRO
1	B	50	LEU
1	B	202	GLN
1	A	183	LYS
1	B	123	PHE
1	B	335	THR
1	A	202	GLN
1	A	263	TYR
1	B	295	TYR
1	B	25	LYS
1	B	313	PRO

### 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%)	281 (84%)	54 (16%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	335/335 (100%)	279 (83%)	56 (17%)	2	6
All	All	670/670 (100%)	560 (84%)	110 (16%)	2	7

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	25	LYS
1	A	26	ARG
1	A	43	ASP
1	A	78	ASP
1	A	80	THR
1	A	91	ASN
1	A	97	SER
1	A	99	ARG
1	A	103	VAL
1	A	107	SER
1	A	112	LEU
1	A	120	GLN
1	A	129	ARG
1	A	154	GLN
1	A	156	GLN
1	A	175	GLU
1	A	183	LYS
1	A	205	TRP
1	A	213	LYS
1	A	216	ASN
1	A	220	TYR
1	A	235	ARG
1	A	252	LEU
1	A	253	SER
1	A	276	ASP
1	A	278	GLU
1	A	284	GLU
1	A	290	LEU
1	A	297	ASN
1	A	298	PRO
1	A	300	MET
1	A	301	ASN
1	A	307	SER
1	A	313	PRO
1	A	314	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	316	ARG
1	A	322	GLU
1	A	332	SER
1	A	339	SER
1	A	343	LYS
1	A	347	SER
1	A	357	ILE
1	A	371	GLU
1	A	372	ARG
1	A	373	LEU
1	A	376	GLU
1	A	383	LYS
1	A	387	ILE
1	A	388	SER
1	A	394	SER
1	A	408	VAL
1	A	409	THR
1	A	410	LYS
1	B	8	HIS
1	B	10	GLU
1	B	11	MET
1	B	18	LEU
1	B	25	LYS
1	B	28	THR
1	B	30	SER
1	B	31	LYS
1	B	32	LYS
1	B	34	ASN
1	B	37	VAL
1	B	41	ARG
1	B	71	LEU
1	B	80	THR
1	B	83	SER
1	B	91	ASN
1	B	92	SER
1	B	99	ARG
1	B	107	SER
1	B	112	LEU
1	B	120	GLN
1	B	121	ARG
1	B	129	ARG
1	B	144	THR

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Mol	Chain	Res	Type
1	B	154	GLN
1	B	156	GLN
1	B	167	SER
1	B	171	THR
1	B	186	ILE
1	B	196	THR
1	B	202	GLN
1	B	220	TYR
1	B	235	ARG
1	B	252	LEU
1	B	253	SER
1	B	260	MET
1	B	275	ARG
1	B	278	GLU
1	B	284	GLU
1	B	290	LEU
1	B	300	MET
1	B	304	ARG
1	B	307	SER
1	B	313	PRO
1	B	326	MET
1	B	332	SER
1	B	343	LYS
1	B	362	PHE
1	B	366	LYS
1	B	369	GLN
1	B	375	LYS
1	B	381	MET
1	B	387	ILE
1	B	389	VAL
1	B	394	SER
1	B	409	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	34	ASN
1	A	120	GLN
1	A	156	GLN
1	A	216	ASN
1	A	234	ASN

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Mol	Chain	Res	Type
1	A	286	GLN
1	A	297	ASN
1	A	301	ASN
1	A	340	ASN
1	A	402	HIS
1	B	8	HIS
1	B	34	ASN
1	B	120	GLN
1	B	156	GLN
1	B	216	ASN
1	B	234	ASN
1	B	254	GLN
1	B	286	GLN
1	B	297	ASN
1	B	340	ASN
1	B	369	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 monosaccharides 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	PLA	A	411	-	25,25,25	1.83	6 (24%)	29,37,37	2.66	10 (34%)
2	PLA	B	411	-	25,25,25	1.94	5 (20%)	29,37,37	2.99	12 (41%)

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	-	-	13/23/23/23	0/1/1/1
2	PLA	B	411	-	-	10/23/23/23	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	PLA	C5-C4	5.91	1.48	1.40
2	A	411	PLA	C4A-C4	-5.63	1.44	1.51
2	B	411	PLA	CA-N	4.37	1.53	1.47
2	B	411	PLA	C3-C4	-3.18	1.35	1.40
2	A	411	PLA	C4A-N	-2.82	1.29	1.45
2	A	411	PLA	P-O2P	-2.43	1.45	1.54
2	A	411	PLA	C5-C4	2.32	1.43	1.40
2	A	411	PLA	CB1-CA	-2.31	1.52	1.55
2	A	411	PLA	C3-C2	2.27	1.43	1.40
2	B	411	PLA	P-O2P	-2.20	1.46	1.54
2	B	411	PLA	C4A-N	-2.10	1.33	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PLA	O4P-C5A-C5	6.93	122.56	109.35
2	B	411	PLA	C4A-C4-C5	6.91	127.39	119.71
2	B	411	PLA	C2A-C2-C3	6.70	129.16	120.89
2	A	411	PLA	C2A-C2-C3	5.17	127.27	120.89
2	B	411	PLA	O4P-C5A-C5	5.15	119.17	109.35
2	A	411	PLA	CB2-CA-CB1	-4.84	104.23	110.85
2	B	411	PLA	C5A-C5-C6	-4.67	111.70	119.37
2	A	411	PLA	C3-C2-N1	-4.35	115.15	120.77
2	B	411	PLA	C6-N1-C2	4.31	127.15	119.17
2	B	411	PLA	C6-C5-C4	4.29	121.15	118.12
2	A	411	PLA	C6-N1-C2	4.07	126.71	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PLA	C6-C5-C4	3.89	120.87	118.12
2	B	411	PLA	C3-C2-N1	-3.85	115.80	120.77
2	B	411	PLA	C5-C6-N1	-3.71	117.64	123.82
2	A	411	PLA	C5-C6-N1	-3.69	117.67	123.82
2	B	411	PLA	C3-C4-C5	-3.46	115.40	118.72
2	B	411	PLA	C4A-C4-C3	-3.08	116.75	120.04
2	A	411	PLA	O4P-P-O1P	2.75	114.20	106.47
2	B	411	PLA	CB2-CA-C	-2.47	102.48	108.48
2	A	411	PLA	C4A-C4-C5	2.34	122.31	119.71
2	A	411	PLA	OXT-C-O	-2.04	117.33	123.82
2	B	411	PLA	C-CA-N	2.03	112.76	107.63

There are no chirality outliers.

All (23) torsion outliers are listed below:

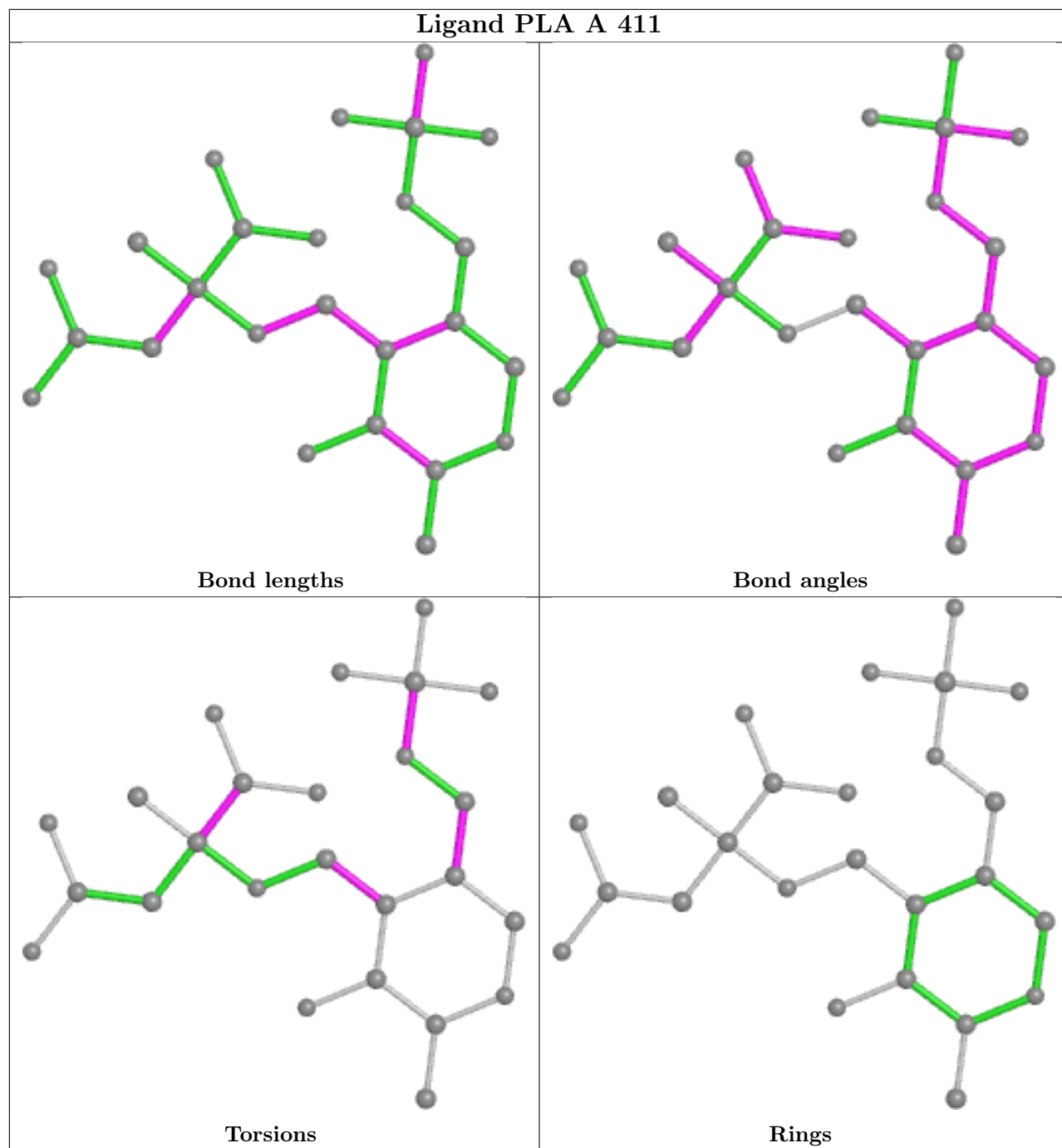
Mol	Chain	Res	Type	Atoms
2	A	411	PLA	C5-C4-C4A-N
2	A	411	PLA	C4-C5-C5A-O4P
2	A	411	PLA	C6-C5-C5A-O4P
2	A	411	PLA	C5A-O4P-P-O1P
2	A	411	PLA	C5A-O4P-P-O2P
2	A	411	PLA	O-C-CA-N
2	A	411	PLA	OXT-C-CA-N
2	B	411	PLA	C4-C5-C5A-O4P
2	B	411	PLA	C6-C5-C5A-O4P
2	B	411	PLA	O-C-CA-N
2	B	411	PLA	OXT-C-CA-N
2	B	411	PLA	C5-C4-C4A-N
2	A	411	PLA	OXT-C-CA-CB2
2	A	411	PLA	C3-C4-C4A-N
2	A	411	PLA	O-C-CA-CB1
2	A	411	PLA	OXT-C-CA-CB1
2	B	411	PLA	O-C-CA-CB1
2	B	411	PLA	OXT-C-CA-CB1
2	A	411	PLA	O-C-CA-CB2
2	B	411	PLA	O-C-CA-CB2
2	B	411	PLA	OXT-C-CA-CB2
2	B	411	PLA	C3-C4-C4A-N
2	A	411	PLA	C5A-O4P-P-O3P

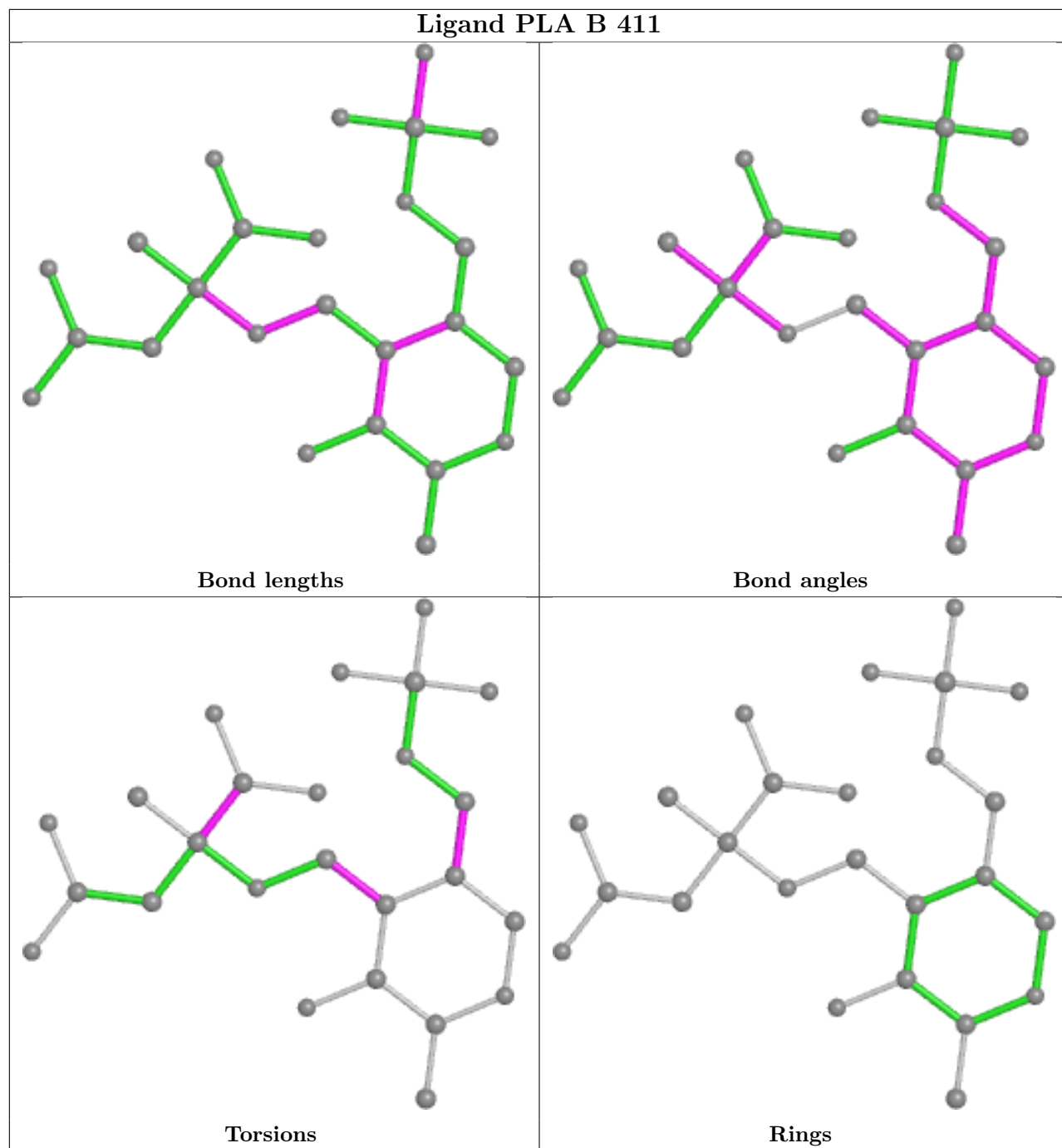
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	PLA	6	0
2	B	411	PLA	5	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.