



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:08 PM UTC

PDB ID : 1TAS / pdb_00001tas
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

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

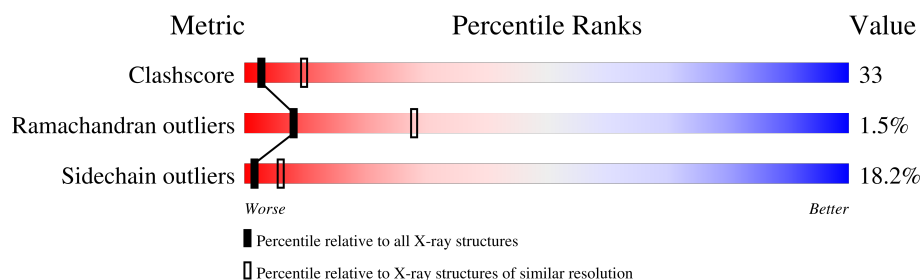
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	
1	B	401	

2 Entry composition [i](#)

There are 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.

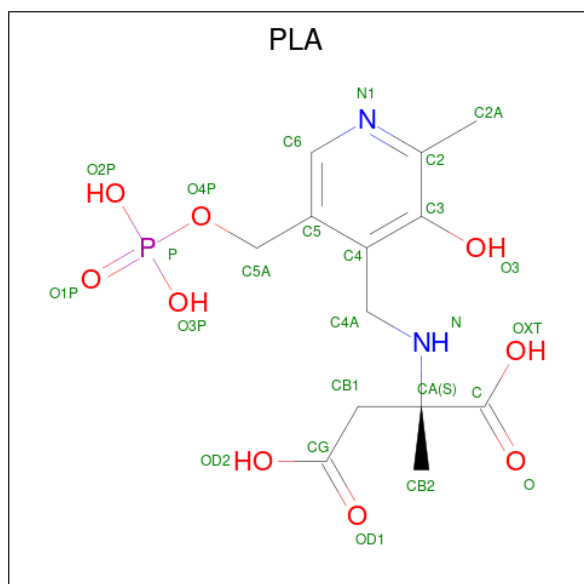
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDI N-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (CCD ID: PLA) (formula: $C_{13}H_{19}N_2O_9P$).



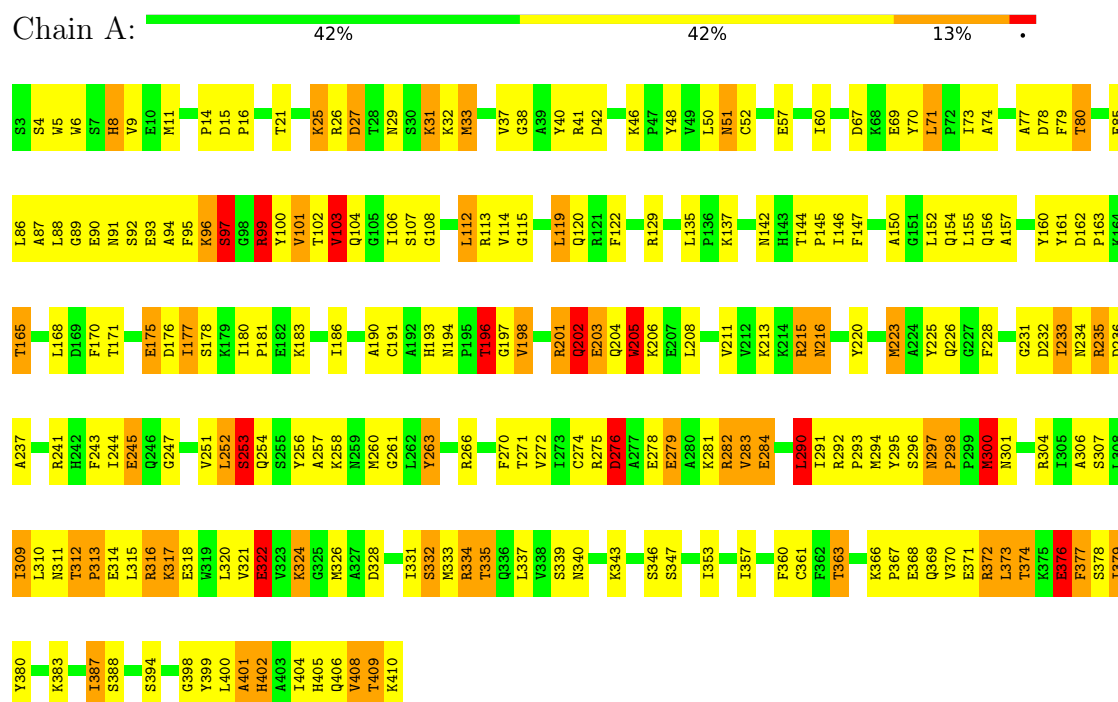
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

3 Residue-property plots

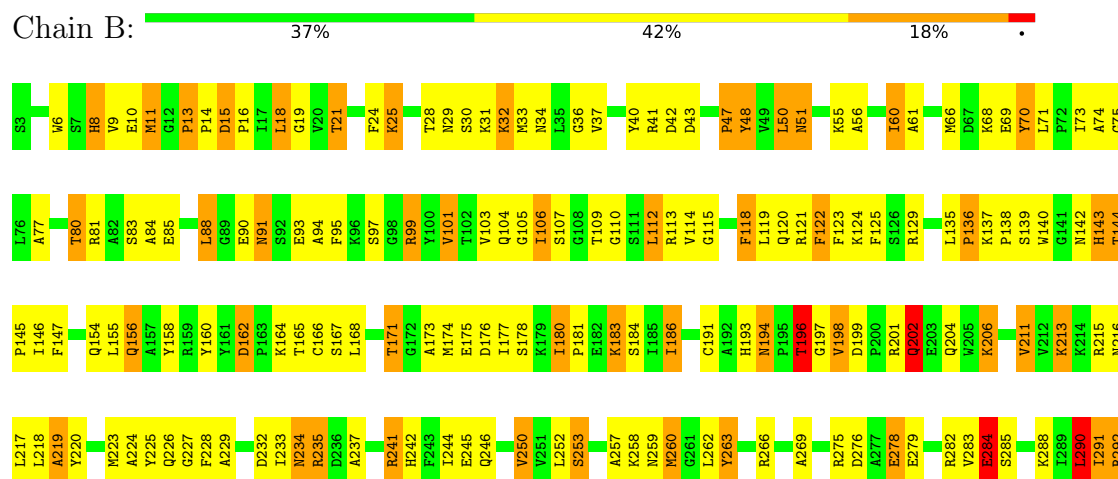
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

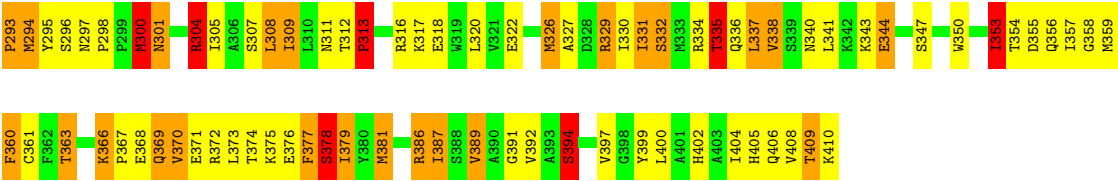
Note EDS was not executed.

• Molecule 1: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE





4 Data and refinement statistics

Xtriage (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, α , β , γ	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.	Xtriage
Total number of atoms	6372	wwPDB-VP
Average B, all atoms (Å ²)	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	1.58	20/3231 (0.6%)	1.95	79/4360 (1.8%)
1	B	1.52	15/3231 (0.5%)	1.99	94/4360 (2.2%)
All	All	1.55	35/6462 (0.5%)	1.97	173/8720 (2.0%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	GLU	CD-OE2	8.44	1.41	1.25
1	A	119	LEU	C-O	-8.03	1.14	1.24
1	B	180	ILE	CA-C	-6.59	1.47	1.53
1	A	60	ILE	CA-CB	-6.53	1.46	1.54
1	A	40	TYR	N-CA	-6.45	1.37	1.46
1	B	129	ARG	CA-C	-6.35	1.45	1.52
1	B	308	LEU	N-CA	-5.88	1.39	1.46
1	A	320	LEU	CA-C	-5.82	1.45	1.52
1	B	194	ASN	CA-C	-5.71	1.45	1.52
1	B	11	MET	N-CA	-5.59	1.39	1.46
1	B	297	ASN	N-CA	-5.57	1.40	1.46
1	A	401	ALA	CA-C	-5.53	1.45	1.52
1	A	282	ARG	CA-C	-5.52	1.46	1.52
1	A	205	TRP	N-CA	-5.48	1.39	1.46
1	B	250	VAL	CA-C	-5.39	1.48	1.52
1	A	245	GLU	C-O	-5.38	1.17	1.24
1	B	291	ILE	CA-CB	-5.34	1.47	1.54
1	B	292	ARG	C-N	-5.34	1.29	1.33
1	A	244	ILE	N-CA	-5.29	1.40	1.46
1	A	377	PHE	CA-C	-5.28	1.45	1.52
1	A	220	TYR	CA-C	-5.26	1.46	1.52
1	B	293	PRO	N-CA	-5.24	1.41	1.47
1	A	102	THR	C-N	-5.20	1.26	1.33
1	A	103	VAL	CA-CB	-5.18	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	338	VAL	N-CA	-5.14	1.40	1.46
1	A	370	VAL	CA-CB	-5.13	1.48	1.54
1	A	97	SER	N-CA	-5.12	1.39	1.46
1	A	376	GLU	CA-C	-5.12	1.45	1.52
1	A	31	LYS	CA-C	-5.11	1.46	1.52
1	B	227	GLY	C-N	-5.11	1.26	1.33
1	B	219	ALA	CA-C	-5.10	1.46	1.52
1	A	60	ILE	N-CA	-5.09	1.40	1.46
1	B	106	ILE	CA-C	-5.05	1.46	1.52
1	A	244	ILE	CA-CB	-5.04	1.48	1.54
1	B	211	VAL	CA-CB	-5.01	1.48	1.54

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	PHE	N-CA-C	11.94	125.67	111.82
1	B	125	PHE	N-CA-C	11.54	125.29	111.33
1	B	176	ASP	CA-CB-CG	-10.77	101.83	112.60
1	A	176	ASP	CA-CB-CG	-10.51	102.09	112.60
1	A	175	GLU	N-CA-CB	10.16	125.27	109.82
1	B	276	ASP	CA-CB-CG	9.91	122.51	112.60
1	B	301	ASN	N-CA-C	9.52	121.66	111.28
1	A	42	ASP	CA-CB-CG	9.40	122.00	112.60
1	B	194	ASN	CA-CB-CG	9.29	121.89	112.60
1	A	300	MET	N-CA-C	9.28	124.40	112.89
1	B	51	ASN	CA-CB-CG	-9.19	103.41	112.60
1	B	284	GLU	N-CA-CB	8.98	123.04	110.01
1	A	276	ASP	CA-CB-CG	8.98	121.58	112.60
1	A	122	PHE	N-CA-C	8.83	123.88	113.20
1	B	266	ARG	N-CA-C	8.23	120.54	110.91
1	B	363	THR	N-CA-C	8.07	122.55	112.87
1	A	225	TYR	N-CA-C	8.06	123.23	111.87
1	A	324	LYS	N-CA-CB	7.82	121.35	110.01
1	B	15	ASP	CA-C-N	7.82	128.23	119.32
1	B	15	ASP	C-N-CA	7.82	128.23	119.32
1	B	298	PRO	CB-CA-C	-7.82	101.38	110.92
1	A	231	GLY	N-CA-C	-7.80	105.07	115.21
1	A	223	MET	N-CA-C	7.72	119.43	108.54
1	A	90	GLU	N-CA-C	7.66	122.20	113.01
1	B	234	ASN	CA-CB-CG	-7.58	105.02	112.60
1	B	344	GLU	N-CA-C	-7.55	103.87	113.23
1	B	355	ASP	CA-CB-CG	7.49	120.09	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	VAL	CB-CA-C	-7.47	100.45	112.03
1	B	124	LYS	N-CA-C	7.46	120.36	111.33
1	A	196	THR	N-CA-C	7.45	119.19	111.14
1	A	233	ILE	N-CA-CB	7.34	119.96	110.57
1	A	402	HIS	CA-CB-CG	-7.32	106.48	113.80
1	A	87	ALA	N-CA-C	7.22	118.94	111.14
1	B	309	ILE	N-CA-C	7.16	117.30	110.42
1	A	363	THR	CA-CB-OG1	-7.16	98.86	109.60
1	A	281	LYS	N-CA-CB	7.14	121.35	110.28
1	A	122	PHE	CA-CB-CG	-7.12	106.68	113.80
1	B	298	PRO	N-CA-C	7.01	119.26	110.70
1	A	312	THR	CA-C-N	6.97	128.55	119.84
1	A	312	THR	C-N-CA	6.97	128.55	119.84
1	B	276	ASP	N-CA-CB	-6.94	99.95	111.20
1	A	290	LEU	N-CA-CB	-6.88	100.02	110.33
1	A	276	ASP	CB-CA-C	-6.83	95.69	111.95
1	B	13	PRO	CB-CA-C	-6.79	102.64	110.92
1	B	91	ASN	CA-CB-CG	6.78	119.38	112.60
1	A	202	GLN	N-CA-CB	-6.75	99.08	110.49
1	A	99	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	A	103	VAL	N-CA-CB	-6.61	100.61	111.45
1	B	377	PHE	CA-CB-CG	-6.57	107.23	113.80
1	A	398	GLY	O-C-N	6.48	128.41	122.18
1	A	5	TRP	CB-CA-C	-6.48	99.84	110.85
1	B	312	THR	CA-C-N	6.47	127.93	119.84
1	B	312	THR	C-N-CA	6.47	127.93	119.84
1	A	71	LEU	N-CA-C	-6.42	100.74	110.50
1	B	42	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	322	GLU	N-CA-CB	6.40	121.19	110.32
1	A	216	ASN	CA-CB-CG	6.37	118.97	112.60
1	B	162	ASP	O-C-N	6.36	128.21	121.02
1	A	334	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	B	196	THR	N-CA-C	6.22	117.94	111.03
1	B	196	THR	N-CA-CB	-6.19	101.00	109.98
1	B	288	LYS	N-CA-C	-6.18	104.09	111.69
1	A	252	LEU	N-CA-C	6.14	119.25	108.75
1	B	90	GLU	N-CA-C	6.13	118.04	111.36
1	A	360	PHE	N-CA-C	6.06	117.78	109.18
1	B	386	ARG	N-CA-C	6.05	118.15	108.41
1	B	136	PRO	CB-CA-C	-6.04	103.33	111.12
1	B	241	ARG	N-CA-C	6.03	117.94	111.36
1	B	129	ARG	CB-CA-C	-6.02	100.33	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	GLU	N-CA-C	-6.01	104.64	111.07
1	A	251	VAL	CB-CA-C	6.00	119.73	110.50
1	B	291	ILE	CB-CA-C	-5.97	104.25	112.24
1	B	344	GLU	CA-C-O	5.95	126.23	119.27
1	B	8	HIS	CA-C-N	-5.95	115.43	122.93
1	B	8	HIS	C-N-CA	-5.95	115.43	122.93
1	B	183	LYS	CB-CA-C	-5.94	103.30	111.73
1	B	297	ASN	CB-CA-C	5.92	117.98	110.76
1	B	171	THR	CA-C-N	5.88	126.46	119.94
1	B	171	THR	C-N-CA	5.88	126.46	119.94
1	A	215	ARG	CB-CA-C	-5.86	98.98	110.11
1	A	165	THR	N-CA-CB	-5.84	102.07	110.65
1	A	243	PHE	CA-CB-CG	-5.84	107.96	113.80
1	B	363	THR	CA-CB-OG1	-5.82	100.87	109.60
1	A	368	GLU	CB-CG-CD	-5.81	102.72	112.60
1	B	162	ASP	CA-C-N	5.78	125.64	119.28
1	B	162	ASP	C-N-CA	5.78	125.64	119.28
1	B	60	ILE	O-C-N	5.74	127.74	121.83
1	A	99	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	B	394	SER	N-CA-C	-5.70	104.43	111.33
1	B	6	TRP	N-CA-CB	-5.69	102.95	111.25
1	B	227	GLY	CA-C-N	-5.67	113.70	122.49
1	B	227	GLY	C-N-CA	-5.67	113.70	122.49
1	A	346	SER	N-CA-CB	5.67	118.29	109.85
1	A	60	ILE	N-CA-CB	-5.66	102.84	110.54
1	B	290	LEU	N-CA-CB	-5.64	101.79	110.20
1	A	198	VAL	N-CA-CB	-5.64	104.80	111.90
1	A	6	TRP	N-CA-CB	-5.63	101.91	110.92
1	B	21	THR	N-CA-CB	5.63	118.17	110.01
1	B	142	ASN	N-CA-C	5.63	118.96	111.75
1	A	245	GLU	N-CA-CB	5.62	118.38	110.12
1	B	180	ILE	CB-CA-C	-5.59	105.74	110.94
1	A	311	ASN	CA-CB-CG	5.57	118.17	112.60
1	B	313	PRO	N-CA-CB	-5.53	97.45	103.25
1	A	33	MET	CG-SD-CE	-5.51	88.78	100.90
1	B	202	GLN	N-CA-CB	-5.50	101.20	110.49
1	B	360	PHE	N-CA-C	5.49	117.86	109.95
1	B	47	PRO	N-CA-CB	5.48	108.12	103.35
1	B	278	GLU	O-C-N	5.48	128.01	122.09
1	A	161	TYR	CA-CB-CG	5.46	123.73	113.90
1	A	215	ARG	CD-NE-CZ	-5.46	116.76	124.40
1	A	251	VAL	CA-C-N	-5.45	112.35	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	VAL	C-N-CA	-5.45	112.35	121.94
1	A	177	ILE	N-CA-CB	5.43	116.54	110.51
1	B	329	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	B	263	TYR	CA-C-N	5.42	127.10	120.22
1	B	263	TYR	C-N-CA	5.42	127.10	120.22
1	A	377	PHE	CA-CB-CG	-5.38	108.42	113.80
1	B	61	ALA	O-C-N	5.37	127.60	122.07
1	B	143	HIS	CB-CA-C	-5.36	100.71	110.63
1	B	269	ALA	N-CA-CB	-5.36	103.20	111.46
1	A	298	PRO	CA-C-N	5.36	126.18	120.13
1	A	298	PRO	C-N-CA	5.36	126.18	120.13
1	A	86	LEU	CB-CA-C	-5.33	102.27	110.81
1	B	337	LEU	O-C-N	5.33	127.84	122.09
1	A	67	ASP	CA-CB-CG	5.30	117.91	112.60
1	A	335	THR	N-CA-C	-5.30	105.20	110.97
1	B	93	GLU	CA-C-N	5.29	129.59	121.19
1	B	93	GLU	C-N-CA	5.29	129.59	121.19
1	B	234	ASN	O-C-N	5.29	127.74	122.03
1	B	70	TYR	CA-CB-CG	5.28	123.40	113.90
1	B	311	ASN	CA-CB-CG	5.28	117.88	112.60
1	B	304	ARG	N-CA-CB	5.27	117.80	109.94
1	A	101	VAL	CB-CA-C	5.27	117.00	110.73
1	B	329	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	B	196	THR	CB-CA-C	5.24	119.08	110.95
1	B	300	MET	N-CA-C	5.24	119.77	112.90
1	A	312	THR	CB-CA-C	-5.22	105.00	110.33
1	B	276	ASP	CB-CA-C	-5.22	99.53	109.66
1	A	363	THR	CB-CA-C	-5.22	100.03	110.42
1	A	14	PRO	N-CA-C	-5.22	103.64	111.57
1	A	171	THR	CB-CA-C	5.21	118.99	110.96
1	A	70	TYR	CA-CB-CG	5.20	123.26	113.90
1	B	48	TYR	O-C-N	5.20	129.35	123.27
1	B	69	GLU	CA-C-N	5.18	128.21	120.95
1	B	69	GLU	C-N-CA	5.18	128.21	120.95
1	B	378	SER	CB-CA-C	5.17	119.23	111.89
1	B	353	ILE	CB-CA-C	5.15	118.25	111.81
1	A	96	LYS	CA-C-O	5.14	125.86	119.79
1	A	6	TRP	N-CA-C	5.14	118.86	112.59
1	A	374	THR	O-C-N	5.14	128.38	122.17
1	B	360	PHE	CA-C-O	5.14	128.66	121.73
1	A	60	ILE	CA-CB-CG1	-5.13	101.67	110.40
1	B	292	ARG	CA-C-O	5.13	123.35	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	ALA	N-CA-C	5.12	118.78	112.54
1	B	15	ASP	O-C-N	5.12	126.57	121.30
1	B	347	SER	CA-C-N	5.11	129.51	120.87
1	B	347	SER	C-N-CA	5.11	129.51	120.87
1	A	324	LYS	CB-CA-C	5.10	118.89	110.88
1	A	253	SER	CA-CB-OG	-5.10	100.90	111.10
1	A	27	ASP	N-CA-C	-5.08	101.13	109.40
1	A	254	GLN	CB-CA-C	-5.07	98.78	109.38
1	A	51	ASN	CA-CB-CG	-5.06	107.54	112.60
1	A	363	THR	N-CA-C	5.05	121.57	110.80
1	B	118	PHE	CA-CB-CG	-5.04	108.76	113.80
1	B	101	VAL	CB-CA-C	5.04	116.97	110.12
1	A	157	ALA	N-CA-C	5.03	116.84	109.24
1	B	329	ARG	N-CA-CB	5.03	117.36	110.07
1	A	251	VAL	N-CA-CB	5.02	119.68	111.44
1	A	201	ARG	N-CA-C	-5.01	101.54	109.96
1	A	309	ILE	CB-CA-C	-5.01	105.48	112.04
1	A	312	THR	O-C-N	5.01	126.14	120.83
1	B	298	PRO	CA-C-N	5.00	125.28	119.93
1	B	298	PRO	C-N-CA	5.00	125.28	119.93

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	178	0
1	B	3161	0	3154	234	0
2	A	25	0	14	6	0
2	B	25	0	14	6	0
All	All	6372	0	6336	398	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 33.

All (398) 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:260:MET:HE2	1:B:309:ILE:HD12	1.43	0.97
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:174:MET:HE1	1:B:211:VAL:HG21	1.51	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:33:MET:HE3	1:B:379:ILE:CG1	2.05	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: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:228:PHE:CZ	1:A:326:MET:HE3	2.17	0.80
1:B:260:MET:HE2	1:B:309:ILE:CD1	2.11	0.80
1:A:196:THR:CG2	1:A:198:VAL:HB	2.12	0.79
1:A:256:TYR:CD2	1:A:260:MET:HE3	2.17	0.78
1:B:292:ARG:HB3	1:B:293:PRO:HD3	1.62	0.78
1:B:300:MET:HE2	1:B:304:ARG:NH1	1.99	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:HE3	1:B:379:ILE:HG12	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HZ1	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:174:MET:HE1	1:B:211:VAL:CG2	2.21	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:33:MET:HE2	1:B:399:TYR:CD2	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
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	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:34:ASN:C	1:B:34:ASN:HD22	2.07	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: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
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:256:TYR:CE2	1:A:260:MET:HE3	2.36	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:A:290:LEU:O	1:A:294:MET:HE3	2.00	0.61
1:B:194:ASN:ND2	2:B:411:PLA:O3	2.34	0.60
1:B:33:MET:HE2	1:B:399:TYR:HD2	1.66	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:216:ASN:C	1:B:217:LEU:HD23	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:HB2	1:A:408:VAL:HG21	1.85	0.58
1:B:370:VAL:HG13	1:B:381:MET:CG	2.34	0.58
1:A:33:MET:HE2	1:A:399:TYR:HD2	1.68	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:B:335:THR:HG22	1:B:336:GLN:N	2.19	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:A:33:MET:CE	1:A:399:TYR:HD2	2.19	0.56
1:A:256:TYR:HD2	1:A:260:MET:HE3	1.69	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:A:245:GLU:C	1:A:247:GLY:H	2.12	0.56
1:A:69:GLU:CD	1:B:47:PRO:HB3	2.31	0.55
1:B:41:ARG:HH11	1:B:47:PRO:HA	1.71	0.55
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:O	1:A:106:ILE:HG22	2.08	0.54
1:B:50:LEU:HD21	1:B:326:MET:HE1	1.89	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:228:PHE:HZ	1:A:326:MET:HE3	1.72	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:HE3	1:A:379:ILE:HG12	1.91	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:291:ILE:HA	1:B:294:MET:HE3	1.92	0.52
1:B:155:LEU:C	1:B:156:GLN:HG2	2.34	0.52
1:B:334:ARG:NH1	1:B:360:PHE:O	2.37	0.52
1:A:332:SER:OG	1:A:333:MET:HE2	2.10	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:B:337:LEU:HD12	1:B:337:LEU:C	2.35	0.52
1:A:112:LEU:HD13	1:A:253:SER:CB	2.40	0.52
1:B:140:TRP:HB3	1:B:143:HIS:HD1	1.75	0.52
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: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:B:201:ARG:O	1:B:204:GLN:N	2.42	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:B:228:PHE:CE1	1:B:359:MET:HE3	2.45	0.51
1:A:93:GLU:O	1:A:97:SER:OG	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLY:HA3	1:A:270:PHE:CE1	2.46	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:11:MET:HE3	1:B:285:SER:CB	2.41	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:B:33:MET:HE2	1:B:399:TYR:CE2	2.46	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:A:33:MET:HE2	1:A:399:TYR:CD2	2.46	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:242:HIS:O	1:B:245:GLU:HG2	2.11	0.49
1:A:11:MET:HE3	1:B:285:SER:HB3	1.95	0.48
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
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:B:33:MET:HE3	1:B:379:ILE:HG13	1.93	0.48
1:B:228:PHE:CZ	1:B:359:MET:HE3	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:376:GLU:HB2	1:B:377:PHE:CD1	2.49	0.47
1:B:33:MET:CE	1:B:399:TYR:HD2	2.26	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
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: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:181:PRO:O	1:B:184:SER:OG	2.30	0.46
1:B:406:GLN:C	1:B:409:THR:H	2.23	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:27:ASP:OD2	1:A:380:TYR:OH	2.30	0.45
1:A:263:TYR:HB2	1:B:68:LYS:O	2.16	0.45
1:B:260:MET:HE1	1:B:309:ILE:HB	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:MET:HE3	1:B:309:ILE:HG21	1.98	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:203:GLU:CD	1:A:203:GLU:H	2.24	0.45
1:A:180:ILE:HA	1:A:181:PRO:HD3	1.84	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:104:GLN:CG	1:B:105:GLY:N	2.79	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:A:69:GLU:CD	1:B:41:ARG:HH12	2.26	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:A:33:MET:CE	1:A:399:TYR:CD2	3.01	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:B:373:LEU:HG	1:B:381:MET:HE1	1.99	0.44
1:A:309:ILE:HG21	1:A:309:ILE:HD13	1.66	0.44
1:B:144:THR:HB	1:B:145:PRO:CD	2.48	0.43
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:223:MET:HE3	1:A:226:GLN:OE1	2.17	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:213:LYS:NZ	1:B:246:GLN:O	2.44	0.43
1:B:336:GLN:O	1:B:340:ASN:OD1	2.37	0.43
1:B:33:MET:HE3	1:B:379:ILE:CD1	2.48	0.43
1:A:101:VAL:HG21	1:A:284:GLU:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:33:MET:CE	1:B:399:TYR:CD2	2.99	0.42
1:B:374:THR:O	1:B:378:SER:N	2.53	0.42
1:A:245:GLU:C	1:A:247:GLY:N	2.78	0.42
1:B:224:ALA:HB1	1:B:258:LYS:HZ3	1.85	0.42
1:A:196:THR:HG22	1:A:197:GLY:N	2.34	0.41
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:B:223:MET:HE3	1:B:226:GLN:CD	2.45	0.41
1:A:232:ASP:OD2	1:A:235:ARG:HB2	2.20	0.41
1:A:400:LEU:HD12	1:A:400:LEU:C	2.42	0.41
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:B:258:LYS:HZ1	2:B:411:PLA:H4A2	1.84	0.41
1:B:406:GLN:C	1:B:409:THR:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:37:VAL:CG2	1:A:38:GLY:N	2.81	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: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:A:228:PHE:CZ	1:A:326:MET:CE	2.99	0.40
1:B:41:ARG:HB2	1:B:391:GLY:HA2	2.02	0.40
1:B:120:GLN:C	1:B:120:GLN:NE2	2.79	0.40
1:B:258:LYS:NZ	2:B:411:PLA:C4A	2.78	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:228:PHE:HE2	1:B:259:ASN:HA	1.86	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/401 (100%)	354 (89%)	41 (10%)	4 (1%)	12	38
1	B	399/401 (100%)	358 (90%)	33 (8%)	8 (2%)	6	21
All	All	798/802 (100%)	712 (89%)	74 (9%)	12 (2%)	8	28

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 ⓘ

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%)	276 (82%)	59 (18%)	2	7
1	B	335/335 (100%)	272 (81%)	63 (19%)	1	5
All	All	670/670 (100%)	548 (82%)	122 (18%)	2	6

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	8	HIS
1	A	25	LYS
1	A	26	ARG

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Mol	Chain	Res	Type
1	A	46	LYS
1	A	78	ASP
1	A	80	THR
1	A	88	LEU
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	114	VAL
1	A	154	GLN
1	A	175	GLU
1	A	196	THR
1	A	203	GLU
1	A	205	TRP
1	A	213	LYS
1	A	216	ASN
1	A	235	ARG
1	A	252	LEU
1	A	253	SER
1	A	276	ASP
1	A	278	GLU
1	A	283	VAL
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
1	A	316	ARG
1	A	317	LYS
1	A	322	GLU
1	A	324	LYS
1	A	332	SER
1	A	335	THR
1	A	339	SER
1	A	343	LYS
1	A	347	SER

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Mol	Chain	Res	Type
1	A	357	ILE
1	A	371	GLU
1	A	372	ARG
1	A	373	LEU
1	A	376	GLU
1	A	379	ILE
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	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	37	VAL
1	B	71	LEU
1	B	73	ILE
1	B	80	THR
1	B	83	SER
1	B	88	LEU
1	B	91	ASN
1	B	97	SER
1	B	99	ARG
1	B	103	VAL
1	B	107	SER
1	B	112	LEU
1	B	144	THR
1	B	154	GLN
1	B	156	GLN
1	B	165	THR
1	B	167	SER
1	B	171	THR
1	B	186	ILE
1	B	196	THR
1	B	198	VAL

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Mol	Chain	Res	Type
1	B	206	LYS
1	B	213	LYS
1	B	235	ARG
1	B	244	ILE
1	B	252	LEU
1	B	253	SER
1	B	260	MET
1	B	275	ARG
1	B	278	GLU
1	B	283	VAL
1	B	284	GLU
1	B	290	LEU
1	B	294	MET
1	B	300	MET
1	B	304	ARG
1	B	307	SER
1	B	313	PRO
1	B	326	MET
1	B	331	ILE
1	B	332	SER
1	B	335	THR
1	B	343	LYS
1	B	353	ILE
1	B	366	LYS
1	B	369	GLN
1	B	370	VAL
1	B	375	LYS
1	B	378	SER
1	B	379	ILE
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 (25) 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

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Mol	Chain	Res	Type
1	A	216	ASN
1	A	234	ASN
1	A	286	GLN
1	A	297	ASN
1	A	301	ASN
1	A	340	ASN
1	A	402	HIS
1	A	405	HIS
1	B	8	HIS
1	B	34	ASN
1	B	117	ASN
1	B	120	GLN
1	B	156	GLN
1	B	216	ASN
1	B	234	ASN
1	B	246	GLN
1	B	254	GLN
1	B	286	GLN
1	B	301	ASN
1	B	349	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLA	A	411	-	25,25,25	1.77	7 (28%)	34,37,37	2.64	13 (38%)
2	PLA	B	411	-	25,25,25	1.97	5 (20%)	34,37,37	2.94	14 (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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	PLA	C5-C4	5.93	1.48	1.40
2	A	411	PLA	C4A-C4	-4.94	1.44	1.52
2	B	411	PLA	CA-N	4.41	1.53	1.47
2	B	411	PLA	C3-C4	-3.32	1.35	1.40
2	A	411	PLA	C4A-N	-2.96	1.29	1.45
2	A	411	PLA	P-O2P	-2.51	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	B	411	PLA	P-O2P	-2.27	1.46	1.54
2	B	411	PLA	C4A-N	-2.22	1.33	1.45
2	A	411	PLA	C3-C2	2.13	1.43	1.41
2	A	411	PLA	C2-N1	2.02	1.37	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	PLA	C2A-C2-C3	7.15	129.16	120.80
2	A	411	PLA	O4P-C5A-C5	7.05	122.56	109.36
2	B	411	PLA	C4A-C4-C5	7.02	127.39	119.75
2	A	411	PLA	C2A-C2-C3	5.53	127.27	120.80
2	B	411	PLA	O4P-C5A-C5	5.23	119.17	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	PLA	C5A-C5-C6	-4.70	111.70	119.36
2	A	411	PLA	CB2-CA-CB1	-4.67	104.23	110.76
2	A	411	PLA	C3-C2-N1	-4.60	115.15	120.96
2	B	411	PLA	C6-N1-C2	4.38	127.15	119.20
2	A	411	PLA	C6-N1-C2	4.14	126.71	119.20
2	B	411	PLA	C3-C2-N1	-4.09	115.80	120.96
2	B	411	PLA	C6-C5-C4	4.09	121.15	118.06
2	B	411	PLA	C5-C6-N1	-3.80	117.64	123.83
2	A	411	PLA	C5-C6-N1	-3.79	117.67	123.83
2	A	411	PLA	C6-C5-C4	3.72	120.87	118.06
2	B	411	PLA	C3-C4-C5	-3.67	115.40	118.73
2	A	411	PLA	OXT-C-CA	3.28	123.58	113.77
2	A	411	PLA	O4P-P-O1P	2.87	114.20	106.44
2	B	411	PLA	OXT-C-CA	2.74	121.98	113.77
2	B	411	PLA	C4-C4A-N	2.73	116.73	110.74
2	A	411	PLA	C4-C4A-N	2.66	116.59	110.74
2	B	411	PLA	CB2-CA-C	-2.53	102.48	108.59
2	B	411	PLA	C4A-C4-C3	-2.44	116.75	119.98
2	A	411	PLA	C4A-C4-C5	2.36	122.31	119.75
2	B	411	PLA	C5A-C5-C4	2.13	127.15	122.67
2	A	411	PLA	O-C-CA	-2.07	119.07	122.78
2	A	411	PLA	OXT-C-O	-2.04	117.33	123.86

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	OXT-C-CA-N
2	B	411	PLA	C4-C5-C5A-O4P
2	B	411	PLA	C6-C5-C5A-O4P
2	B	411	PLA	C5-C4-C4A-N
2	A	411	PLA	C3-C4-C4A-N
2	A	411	PLA	OXT-C-CA-CB2
2	B	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

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Mol	Chain	Res	Type	Atoms
2	B	411	PLA	OXT-C-CA-CB1
2	A	411	PLA	O-C-CA-N
2	B	411	PLA	O-C-CA-N
2	B	411	PLA	OXT-C-CA-N
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	A	411	PLA	C5A-O4P-P-O3P

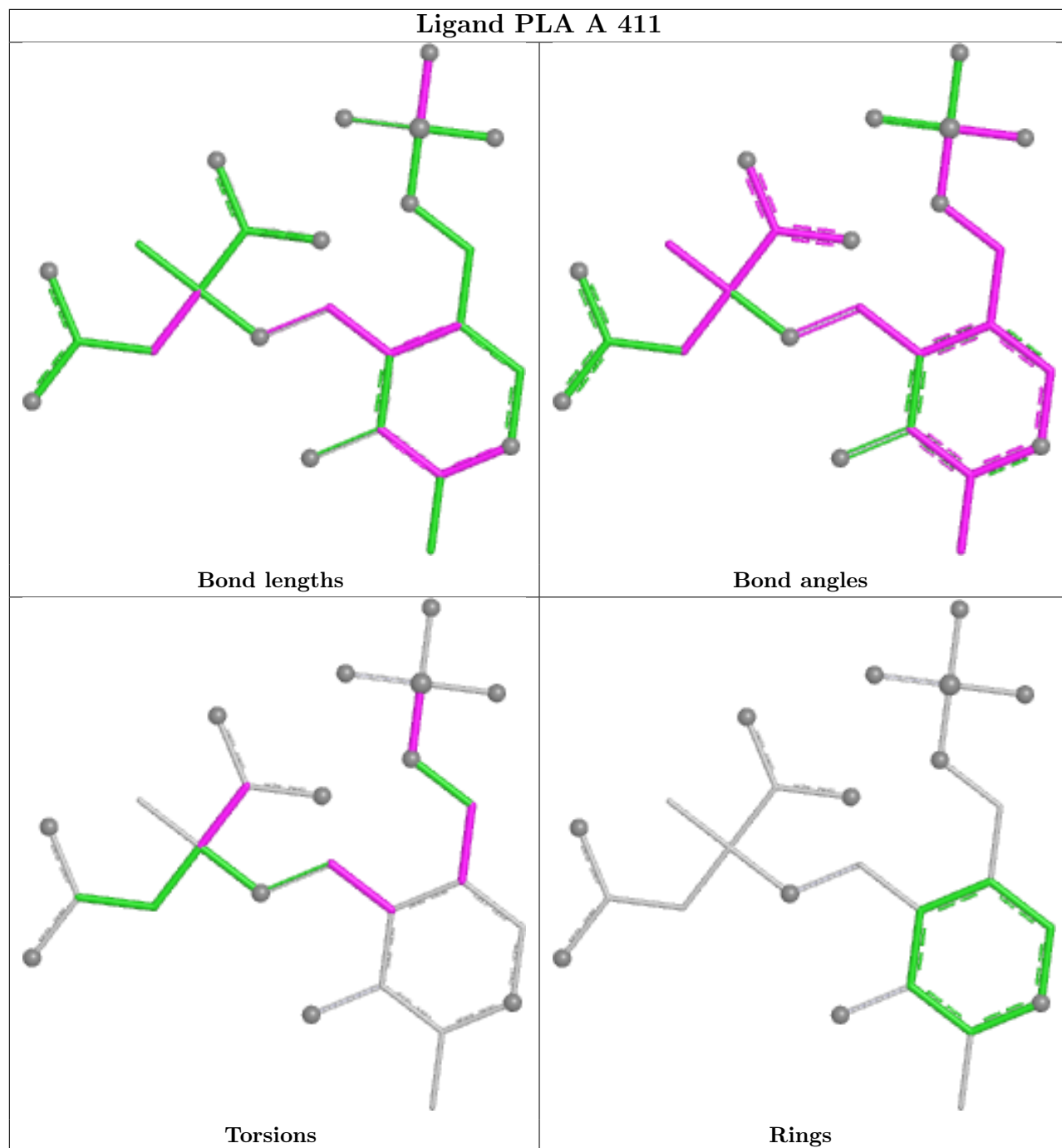
There are no ring outliers.

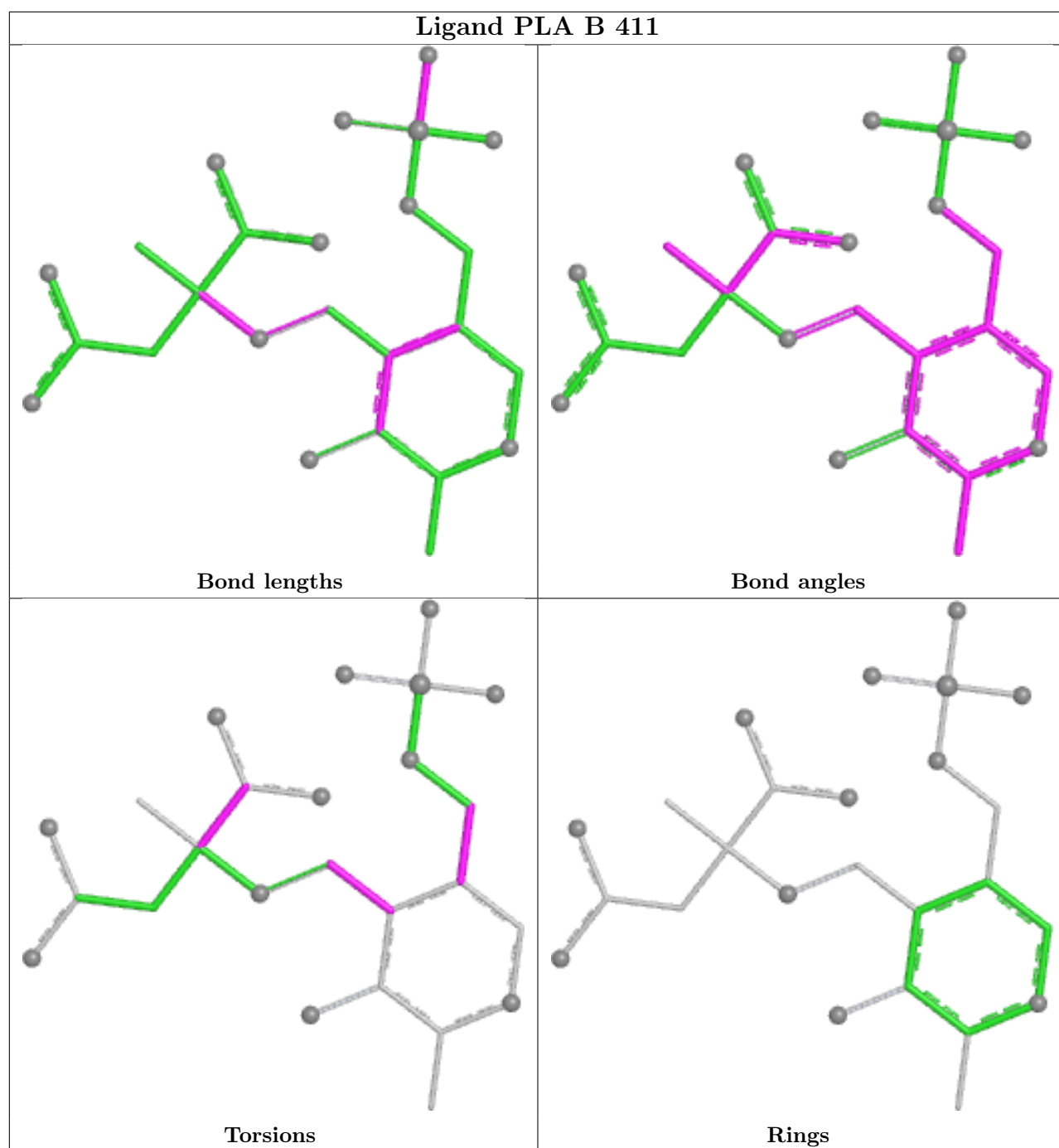
2 monomers are involved in 12 short contacts:

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

Ligand PLA A 411





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.