



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:35 AM UTC

PDB ID : 1AIA / pdb_00001aia
Title : STRUCTURAL BASIS FOR THE CATALYTIC ACTIVITY OF ASPARTATE AMINOTRANSFERASE K258H LACKING THE PYRIDOXAL-5'-PHOSPHATE BINDING LYSINE RESIDUE
Authors : Jaeger, J.; Jansonius, J.N.
Deposited on : 1994-05-10
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

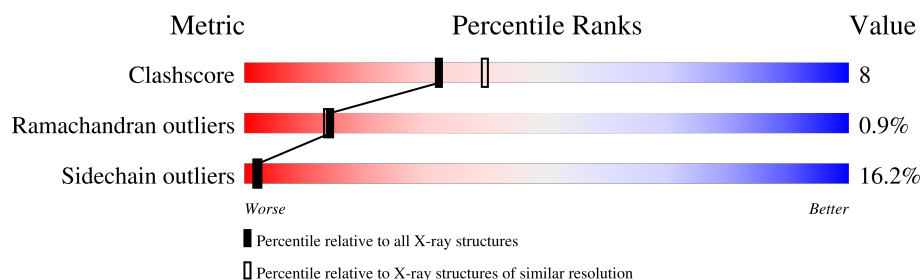
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	 62% 26% 10% •
1	B	396	 65% 27% 7% •

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.

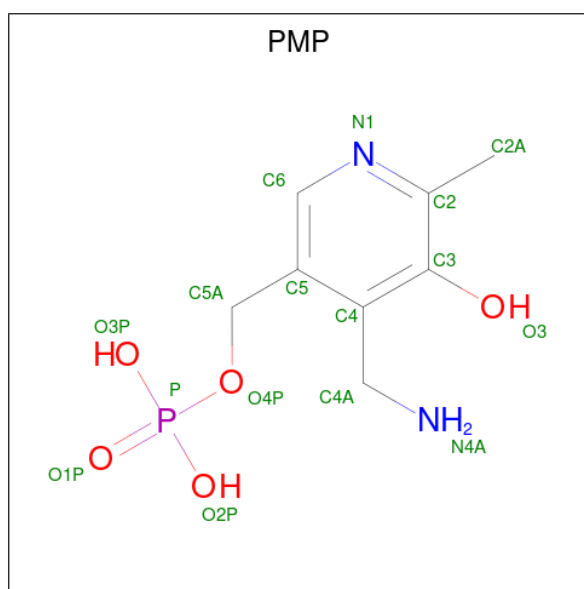
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total 3070	C 1936	N 537	O 584	S 13	0	0	0
1	B	396	Total 3070	C 1936	N 537	O 584	S 13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	HIS	LYS	engineered mutation	UNP P00509
B	258	HIS	LYS	engineered mutation	UNP P00509

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: $\text{C}_8\text{H}_{13}\text{N}_2\text{O}_5\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

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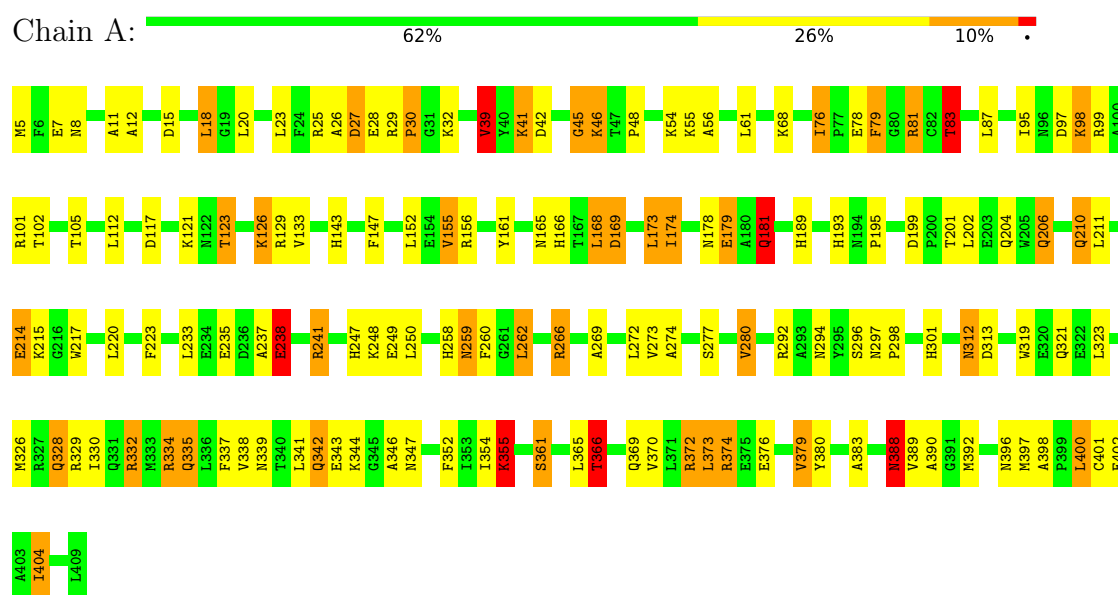
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

3 Residue-property plots

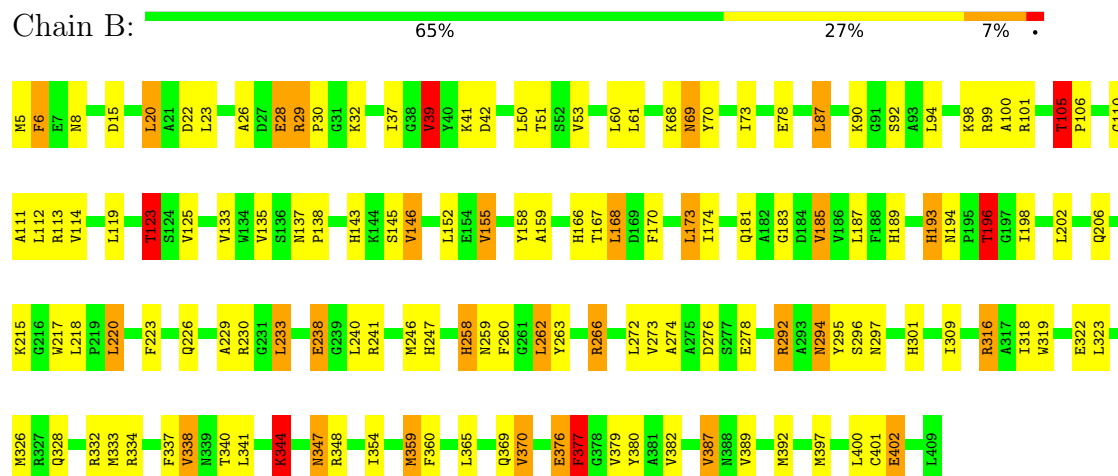
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	86.90Å 79.80Å 89.90Å 90.00° 118.90° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6172	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: PMP

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	1.09	10/3132 (0.3%)	1.97	101/4244 (2.4%)
1	B	1.08	13/3132 (0.4%)	1.85	69/4244 (1.6%)
All	All	1.08	23/6264 (0.4%)	1.91	170/8488 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	155	VAL	CA-CB	7.98	1.64	1.54
1	B	143	HIS	CD2-NE2	-7.63	1.29	1.37
1	B	258	HIS	CD2-NE2	-7.21	1.29	1.37
1	A	143	HIS	CD2-NE2	-6.78	1.30	1.37
1	B	185	VAL	CA-CB	6.75	1.62	1.54
1	B	166	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	258	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	193	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	155	VAL	CA-CB	6.49	1.62	1.54
1	B	146	VAL	CA-CB	6.42	1.63	1.54
1	B	301	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	301	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	166	HIS	CD2-NE2	-6.04	1.31	1.37
1	B	193	HIS	CD2-NE2	-6.00	1.31	1.37
1	B	189	HIS	CD2-NE2	-5.92	1.31	1.37
1	B	247	HIS	CD2-NE2	-5.86	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	ILE	CA-CB	5.86	1.62	1.54
1	B	217	TRP	CG-CD2	-5.78	1.33	1.43
1	A	193	HIS	CG-ND1	-5.41	1.32	1.38
1	A	247	HIS	CD2-NE2	-5.32	1.31	1.37
1	B	166	HIS	CG-ND1	-5.06	1.32	1.38
1	A	166	HIS	CG-ND1	-5.02	1.32	1.38
1	B	370	VAL	CA-CB	5.02	1.61	1.54

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASN	CA-CB-CG	9.42	122.02	112.60
1	A	280	VAL	CB-CA-C	-9.41	97.58	112.16
1	B	377	PHE	O-C-N	9.40	135.09	122.59
1	B	196	THR	N-CA-CB	-9.18	96.52	110.20
1	A	347	ASN	CA-CB-CG	8.99	121.59	112.60
1	B	39	VAL	N-CA-CB	-8.98	97.35	112.44
1	A	41	LYS	CB-CG-CD	-8.73	91.21	111.30
1	A	266	ARG	NE-CZ-NH2	-8.71	111.36	119.20
1	A	129	ARG	CB-CG-CD	-8.68	91.34	111.30
1	A	366	THR	N-CA-CB	-8.58	97.41	110.45
1	A	259	ASN	CA-CB-CG	8.54	121.14	112.60
1	A	388	ASN	OD1-CG-ND2	-8.51	114.09	122.60
1	B	105	THR	O-C-N	-8.40	116.33	121.71
1	A	366	THR	CA-CB-OG1	-8.25	97.23	109.60
1	A	11	ALA	N-CA-C	8.22	128.31	110.80
1	B	229	ALA	O-C-N	-8.19	113.69	123.27
1	B	105	THR	N-CA-CB	-8.13	96.55	111.18
1	A	169	ASP	CA-C-O	8.10	130.46	121.39
1	B	301	HIS	CB-CG-CD2	-8.07	120.70	131.20
1	A	39	VAL	N-CA-CB	-7.99	96.97	111.92
1	A	313	ASP	N-CA-C	7.85	121.79	111.75
1	B	266	ARG	NE-CZ-NH2	-7.83	112.15	119.20
1	A	347	ASN	N-CA-CB	-7.76	97.88	110.14
1	A	328	GLN	CA-CB-CG	-7.73	98.64	114.10
1	B	42	ASP	CA-CB-CG	7.72	120.32	112.60
1	B	194	ASN	CA-CB-CG	7.65	120.25	112.60
1	B	377	PHE	N-CA-C	7.59	126.97	110.80
1	A	301	HIS	CB-CG-CD2	-7.54	121.40	131.20
1	A	396	ASN	CA-CB-CG	7.53	120.13	112.60
1	B	123	THR	N-CA-CB	-7.52	99.11	111.66
1	A	388	ASN	CB-CG-ND2	7.51	127.67	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ASN	OD1-CG-ND2	-7.49	115.11	122.60
1	B	387	VAL	N-CA-CB	-7.41	98.49	111.39
1	B	68	LYS	CA-CB-CG	-7.35	99.41	114.10
1	A	374	ARG	CB-CA-C	-7.34	99.36	110.88
1	A	366	THR	CA-CB-CG2	7.32	122.94	110.50
1	B	316	ARG	CG-CD-NE	-7.25	96.04	112.00
1	A	8	ASN	N-CA-CB	-7.20	99.33	111.20
1	B	258	HIS	CB-CG-CD2	-7.18	121.86	131.20
1	A	41	LYS	N-CA-CB	-7.15	98.33	111.13
1	A	379	VAL	N-CA-C	7.12	119.08	108.54
1	A	238	GLU	CA-CB-CG	7.12	128.33	114.10
1	B	294	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	B	301	HIS	N-CA-C	7.06	118.62	111.07
1	A	27	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	179	GLU	N-CA-C	-7.00	95.90	110.80
1	A	81	ARG	CA-CB-CG	6.90	127.90	114.10
1	A	280	VAL	N-CA-CB	6.90	122.45	110.65
1	A	346	ALA	CA-C-O	6.84	128.57	120.70
1	A	258	HIS	CB-CG-CD2	-6.81	122.35	131.20
1	B	319	TRP	CG-CD2-CE3	6.80	140.70	133.90
1	A	342	GLN	CB-CG-CD	6.77	124.10	112.60
1	B	238	GLU	CA-CB-CG	6.76	127.62	114.10
1	B	229	ALA	CA-C-O	-6.71	113.12	120.24
1	A	123	THR	N-CA-CB	-6.70	100.47	111.66
1	B	105	THR	CB-CA-C	6.70	120.77	109.32
1	B	359	MET	N-CA-C	6.70	119.59	111.82
1	A	42	ASP	CA-CB-CG	6.57	119.17	112.60
1	B	28	GLU	CA-C-O	6.54	129.87	120.51
1	A	355	LYS	CA-CB-CG	6.54	127.17	114.10
1	A	329	ARG	NE-CZ-NH2	-6.52	113.33	119.20
1	A	342	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	A	346	ALA	CA-C-N	6.44	129.78	120.38
1	A	346	ALA	C-N-CA	6.44	129.78	120.38
1	B	39	VAL	CB-CA-C	6.42	120.30	110.55
1	A	169	ASP	CA-CB-CG	6.39	118.99	112.60
1	B	379	VAL	N-CA-CB	-6.38	103.58	110.53
1	A	301	HIS	CB-CG-ND1	6.33	132.20	122.70
1	B	301	HIS	CB-CG-ND1	6.28	132.12	122.70
1	A	7	GLU	N-CA-C	6.26	118.90	111.33
1	A	181	GLN	N-CA-C	6.25	124.12	110.80
1	A	199	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	373	LEU	CA-C-O	-6.24	114.27	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	HIS	CA-CB-CG	-6.22	107.58	113.80
1	B	217	TRP	CA-CB-CG	6.14	125.26	113.60
1	B	22	ASP	CA-CB-CG	-6.12	106.48	112.60
1	A	319	TRP	CG-CD2-CE3	6.07	139.97	133.90
1	A	143	HIS	CB-CG-CD2	-6.04	123.34	131.20
1	A	339	ASN	CA-CB-CG	-6.04	106.56	112.60
1	A	76	ILE	CA-C-N	6.02	125.50	119.24
1	A	76	ILE	C-N-CA	6.02	125.50	119.24
1	B	53	VAL	CA-C-O	-6.02	114.37	121.05
1	A	178	ASN	CA-CB-CG	-6.02	106.58	112.60
1	A	312	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	A	83	THR	N-CA-C	-5.98	105.47	112.89
1	A	334	ARG	CA-C-O	-5.96	114.57	120.70
1	A	174	ILE	CB-CG1-CD1	-5.95	101.30	113.80
1	A	32	LYS	N-CA-C	5.93	118.60	110.24
1	A	335	GLN	OE1-CD-NE2	-5.92	116.69	122.60
1	B	15	ASP	CA-C-N	5.91	125.61	119.05
1	B	15	ASP	C-N-CA	5.91	125.61	119.05
1	A	147	PHE	CA-CB-CG	-5.87	107.93	113.80
1	B	145	SER	CA-C-O	-5.86	114.34	120.55
1	B	259	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	165	ASN	N-CA-C	5.84	120.53	113.17
1	B	387	VAL	CB-CA-C	5.84	119.32	110.62
1	B	166	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	B	8	ASN	CB-CG-ND2	5.79	125.08	116.40
1	A	189	HIS	CB-CG-CD2	-5.79	123.68	131.20
1	B	276	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	97	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	328	GLN	CA-CB-CG	-5.72	102.66	114.10
1	B	70	TYR	N-CA-C	5.71	118.75	110.42
1	A	39	VAL	CB-CA-C	5.70	120.91	110.71
1	A	343	GLU	N-CA-C	5.67	117.47	111.28
1	A	79	PHE	N-CA-C	-5.67	105.01	111.07
1	B	143	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	A	214	GLU	CB-CG-CD	5.63	122.17	112.60
1	B	347	ASN	CA-CB-CG	5.60	118.20	112.60
1	A	126	LYS	N-CA-CB	-5.60	103.59	110.98
1	A	266	ARG	NE-CZ-NH1	5.60	127.10	121.50
1	B	258	HIS	CA-CB-CG	-5.59	108.21	113.80
1	A	332	ARG	CA-CB-CG	5.58	125.27	114.10
1	A	389	VAL	N-CA-CB	-5.57	101.12	110.65
1	A	383	ALA	N-CA-C	5.56	118.87	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	A	277	SER	N-CA-C	5.56	117.78	111.11
1	B	294	ASN	CB-CG-ND2	5.55	124.73	116.40
1	B	369	GLN	CA-C-O	-5.53	114.56	120.42
1	A	298	PRO	N-CA-C	5.50	117.41	110.70
1	A	334	ARG	CG-CD-NE	-5.50	99.90	112.00
1	A	29	ARG	N-CA-C	-5.46	103.19	110.07
1	B	377	PHE	CA-C-O	5.46	128.32	120.51
1	B	78	GLU	CB-CG-CD	5.41	121.79	112.60
1	A	329	ARG	CG-CD-NE	-5.38	100.16	112.00
1	B	206	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	B	113	ARG	CA-C-O	-5.37	114.72	120.42
1	A	179	GLU	CA-C-O	-5.36	112.84	120.51
1	B	226	GLN	CG-CD-NE2	5.34	124.42	116.40
1	A	366	THR	CB-CA-C	5.30	120.31	109.76
1	A	199	ASP	CA-C-N	5.30	125.59	119.92
1	A	199	ASP	C-N-CA	5.30	125.59	119.92
1	A	18	LEU	N-CA-C	5.29	117.13	111.36
1	B	233	LEU	N-CA-C	5.29	117.46	111.11
1	A	259	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	B	158	TYR	CA-CB-CG	5.29	123.42	113.90
1	B	319	TRP	CE2-CD2-CG	-5.28	100.86	107.20
1	A	210	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	217	TRP	CG-CD1-NE1	-5.26	103.37	110.20
1	B	230	ARG	N-CA-C	5.24	121.95	110.80
1	B	41	LYS	CG-CD-CE	5.23	123.32	111.30
1	A	105	THR	CA-C-O	-5.21	115.68	120.94
1	A	319	TRP	CE2-CD2-CG	-5.21	100.95	107.20
1	B	266	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	A	210	GLN	CG-CD-NE2	5.19	124.18	116.40
1	B	376	GLU	CB-CG-CD	5.15	121.35	112.60
1	A	334	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	A	8	ASN	CB-CA-C	5.14	119.35	111.02
1	A	28	GLU	CA-CB-CG	5.14	124.37	114.10
1	A	370	VAL	O-C-N	-5.13	116.89	121.87
1	B	344	LYS	N-CA-C	-5.13	107.02	113.28
1	A	45	GLY	N-CA-C	-5.13	107.98	115.72
1	A	301	HIS	N-CA-C	5.10	116.53	110.97
1	A	98	LYS	N-CA-CB	-5.09	104.25	111.84
1	B	6	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	382	VAL	CA-C-O	-5.09	115.78	121.23
1	A	247	HIS	CA-CB-CG	-5.07	108.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	GLU	CA-C-O	5.06	127.75	120.51
1	A	56	ALA	N-CA-C	-5.06	105.94	111.82
1	A	328	GLN	CG-CD-NE2	5.06	124.00	116.40
1	B	348	ARG	CA-CB-CG	5.06	124.22	114.10
1	A	319	TRP	CG-CD1-NE1	-5.04	103.64	110.20
1	B	360	PHE	N-CA-C	5.04	117.71	109.59
1	B	319	TRP	CG-CD1-NE1	-5.04	103.65	110.20
1	B	90	LYS	CA-C-O	-5.03	115.28	120.92
1	B	272	LEU	CA-C-O	-5.03	114.98	120.36
1	B	332	ARG	CB-CA-C	-5.03	102.44	110.79
1	A	161	TYR	N-CA-CB	-5.03	102.60	110.69
1	A	206	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	B	196	THR	N-CA-C	5.01	117.85	111.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	ARG	Peptide

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	3070	0	3012	57	0
1	B	3070	0	3012	49	0
2	A	16	0	10	1	0
2	B	16	0	10	1	0
All	All	6172	0	6044	98	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 8.

All (98) 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:201:THR:H	1:A:204:GLN:HE21	1.21	0.88
1:B:344:LYS:HD2	1:B:402:GLU:HA	1.57	0.83
1:A:294:ASN:HD21	1:B:294:ASN:HD21	1.25	0.82
1:B:105:THR:HG21	1:B:111:ALA:HB2	1.62	0.81
1:B:397:MET:HE3	1:B:397:MET:HA	1.67	0.75
1:A:397:MET:HE2	1:A:401:CYS:SG	2.26	0.74
1:A:5:MET:HE1	1:B:183:GLY:HA2	1.73	0.69
1:A:41:LYS:HD3	1:A:45:GLY:HA2	1.74	0.68
1:A:266:ARG:HD2	1:B:297:ASN:O	1.97	0.64
1:B:196:THR:HG23	1:B:198:ILE:HB	1.80	0.63
1:A:168:LEU:HD21	1:A:173:LEU:HD23	1.82	0.62
1:A:328:GLN:O	1:A:332:ARG:HD3	2.00	0.62
1:A:352:PHE:HA	1:A:355:LYS:HD3	1.82	0.60
1:B:193:HIS:ND1	1:B:196:THR:HB	2.17	0.60
1:A:366:THR:HG22	1:A:369:GLN:H	1.66	0.60
1:A:292:ARG:HA	1:A:296:SER:HA	1.84	0.59
1:A:41:LYS:HE3	1:A:390:ALA:O	2.02	0.59
1:A:294:ASN:HD21	1:B:294:ASN:ND2	2.00	0.58
1:A:297:ASN:O	1:B:266:ARG:HD2	2.03	0.58
1:A:117:ASP:O	1:A:121:LYS:HG2	2.04	0.58
1:A:39:VAL:HG21	1:B:69:ASN:ND2	2.19	0.57
1:B:202:LEU:HD13	1:B:238:GLU:HG2	1.86	0.57
1:A:201:THR:N	1:A:204:GLN:HE21	1.97	0.57
1:B:87:LEU:O	1:B:241:ARG:HD2	2.05	0.57
1:A:68:LYS:O	1:B:263:TYR:HB2	2.04	0.56
1:B:258:HIS:HE1	2:B:411:PMP:N4A	2.03	0.56
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.87	0.56
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.88	0.56
1:B:260:PHE:HB3	1:B:262:LEU:HD22	1.88	0.55
1:B:196:THR:HG22	1:B:198:ILE:H	1.72	0.55
1:A:330:ILE:O	1:A:334:ARG:HG3	2.07	0.54
1:B:338:VAL:HG21	1:B:354:ILE:HD11	1.88	0.54
1:A:373:LEU:HB3	1:A:379:VAL:HB	1.90	0.54
1:B:196:THR:CG2	1:B:198:ILE:HB	2.37	0.54
1:A:398:ALA:O	1:A:402:GLU:HG2	2.08	0.54
1:A:41:LYS:HD3	1:A:45:GLY:CA	2.39	0.53
1:B:167:THR:HG22	1:B:168:LEU:H	1.73	0.52
1:B:28:GLU:H	1:B:32:LYS:HZ3	1.57	0.52
1:A:237:ALA:O	1:A:241:ARG:HD3	2.10	0.52
1:A:388:ASN:HD21	1:A:390:ALA:HB3	1.74	0.52
1:B:20:LEU:HD12	1:B:380:TYR:HD2	1.76	0.51
1:A:41:LYS:NZ	1:A:45:GLY:HA2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:VAL:HG22	1:B:263:TYR:CE1	2.47	0.50
1:A:335:GLN:HE21	1:A:354:ILE:HG23	1.76	0.49
1:A:392:MET:HG2	1:A:400:LEU:HD21	1.94	0.49
1:B:397:MET:HE3	1:B:400:LEU:HD13	1.93	0.49
1:A:337:PHE:HD1	1:A:397:MET:HE1	1.78	0.49
1:A:41:LYS:HD3	1:A:45:GLY:C	2.38	0.49
1:A:397:MET:HE3	1:A:397:MET:HA	1.94	0.49
1:A:79:PHE:O	1:A:83:THR:HG23	2.13	0.48
1:A:235:GLU:O	1:A:238:GLU:HG3	2.13	0.48
1:B:159:ALA:O	1:B:173:LEU:HB2	2.14	0.48
1:B:323:LEU:HA	1:B:326:MET:HE3	1.94	0.48
1:B:292:ARG:HA	1:B:296:SER:HA	1.95	0.48
1:A:41:LYS:CD	1:A:45:GLY:HA2	2.43	0.48
1:A:388:ASN:HD22	1:A:390:ALA:H	1.62	0.48
1:A:334:ARG:NH2	1:A:361:SER:OG	2.47	0.48
1:B:258:HIS:HD2	1:B:359:MET:HE1	1.78	0.47
1:A:18:LEU:HD21	1:B:73:ILE:HD11	1.97	0.47
1:A:388:ASN:ND2	1:A:390:ALA:HB3	2.29	0.47
1:A:25:ARG:NH2	1:A:26:ALA:HB2	2.29	0.47
1:B:100:ALA:O	1:B:101:ARG:HD2	2.15	0.47
1:B:123:THR:HG22	1:B:125:VAL:H	1.80	0.46
1:B:334:ARG:HG3	1:B:389:VAL:HG11	1.98	0.46
1:B:258:HIS:CD2	1:B:359:MET:HE1	2.50	0.46
1:A:211:LEU:O	1:A:215:LYS:HB2	2.17	0.45
1:A:78:GLU:HA	1:A:81:ARG:HG3	1.99	0.44
1:B:187:LEU:HD12	1:B:220:LEU:HG	1.99	0.44
1:B:397:MET:CE	1:B:400:LEU:HD13	2.48	0.44
1:B:318:ILE:O	1:B:322:GLU:HG3	2.17	0.44
1:B:105:THR:HG21	1:B:111:ALA:CB	2.43	0.44
1:B:106:PRO:HD3	1:B:295:TYR:CZ	2.53	0.43
1:A:46:LYS:HG3	1:A:48:PRO:HG3	2.00	0.43
1:B:170:PHE:O	1:B:174:ILE:HG12	2.17	0.43
1:B:337:PHE:HB2	1:B:392:MET:HE1	2.01	0.43
1:A:323:LEU:HA	1:A:326:MET:HE3	1.99	0.43
1:A:5:MET:HE3	1:B:218:LEU:HB2	2.01	0.42
1:B:340:THR:O	1:B:344:LYS:HB2	2.20	0.42
1:A:249:GLU:HG2	1:A:274:ALA:HA	2.01	0.42
1:A:5:MET:HE2	1:A:5:MET:HB2	1.82	0.42
1:B:333:MET:HE2	1:B:392:MET:C	2.44	0.42
1:A:248:LYS:HA	1:A:248:LYS:HD3	1.90	0.41
1:A:374:ARG:HD2	1:A:380:TYR:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:O	1:A:79:PHE:HB3	2.20	0.41
2:A:411:PMP:H4A2	2:A:411:PMP:H5A1	1.76	0.41
1:A:95:ILE:HD13	1:A:95:ILE:HG21	1.88	0.41
1:A:201:THR:HG23	1:A:204:GLN:NE2	2.35	0.41
1:B:99:ARG:HD2	1:B:274:ALA:O	2.20	0.41
1:A:41:LYS:HE3	1:A:41:LYS:HB3	1.69	0.41
1:A:181:GLN:H	1:A:181:GLN:HG2	1.49	0.41
1:A:372:ARG:HD2	1:A:376:GLU:HG3	2.03	0.41
1:B:110:GLY:O	1:B:114:VAL:HG13	2.21	0.41
1:B:397:MET:HE2	1:B:401:CYS:SG	2.61	0.41
1:A:102:THR:HG23	1:A:269:ALA:HB1	2.03	0.41
1:B:39:VAL:HG22	1:B:263:TYR:CZ	2.55	0.41
1:A:99:ARG:HH11	1:A:99:ARG:HD2	1.77	0.40
1:B:137:ASN:HA	1:B:138:PRO:HA	1.83	0.40
1:B:309:ILE:O	1:B:316:ARG:HB2	2.21	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	394/396 (100%)	378 (96%)	12 (3%)	4 (1%)	12	11
1	B	394/396 (100%)	379 (96%)	12 (3%)	3 (1%)	16	16
All	All	788/792 (100%)	757 (96%)	24 (3%)	7 (1%)	14	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	181	GLN
1	B	26	ALA

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Mol	Chain	Res	Type
1	B	30	PRO
1	A	12	ALA
1	B	377	PHE
1	A	179	GLU

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	320/320 (100%)	265 (83%)	55 (17%)	2	2
1	B	320/320 (100%)	271 (85%)	49 (15%)	3	2
All	All	640/640 (100%)	536 (84%)	104 (16%)	2	2

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	23	LEU
1	A	27	ASP
1	A	30	PRO
1	A	39	VAL
1	A	46	LYS
1	A	54	LYS
1	A	55	LYS
1	A	61	LEU
1	A	83	THR
1	A	87	LEU
1	A	98	LYS
1	A	101	ARG
1	A	112	LEU
1	A	123	THR
1	A	126	LYS
1	A	133	VAL
1	A	152	LEU
1	A	155	VAL

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Mol	Chain	Res	Type
1	A	156	ARG
1	A	168	LEU
1	A	169	ASP
1	A	173	LEU
1	A	174	ILE
1	A	181	GLN
1	A	195	PRO
1	A	202	LEU
1	A	206	GLN
1	A	210	GLN
1	A	214	GLU
1	A	220	LEU
1	A	223	PHE
1	A	233	LEU
1	A	238	GLU
1	A	241	ARG
1	A	250	LEU
1	A	259	ASN
1	A	262	LEU
1	A	272	LEU
1	A	273	VAL
1	A	280	VAL
1	A	312	ASN
1	A	321	GLN
1	A	338	VAL
1	A	341	LEU
1	A	342	GLN
1	A	344	LYS
1	A	355	LYS
1	A	361	SER
1	A	365	LEU
1	A	366	THR
1	A	372	ARG
1	A	388	ASN
1	A	400	LEU
1	A	404	ILE
1	B	5	MET
1	B	6	PHE
1	B	20	LEU
1	B	23	LEU
1	B	29	ARG
1	B	37	ILE

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Mol	Chain	Res	Type
1	B	39	VAL
1	B	50	LEU
1	B	51	THR
1	B	60	LEU
1	B	61	LEU
1	B	87	LEU
1	B	92	SER
1	B	94	LEU
1	B	98	LYS
1	B	105	THR
1	B	112	LEU
1	B	119	LEU
1	B	123	THR
1	B	133	VAL
1	B	135	VAL
1	B	146	VAL
1	B	152	LEU
1	B	155	VAL
1	B	168	LEU
1	B	173	LEU
1	B	181	GLN
1	B	185	VAL
1	B	196	THR
1	B	215	LYS
1	B	220	LEU
1	B	223	PHE
1	B	233	LEU
1	B	240	LEU
1	B	246	MET
1	B	262	LEU
1	B	273	VAL
1	B	278	GLU
1	B	292	ARG
1	B	338	VAL
1	B	341	LEU
1	B	344	LYS
1	B	347	ASN
1	B	365	LEU
1	B	370	VAL
1	B	376	GLU
1	B	377	PHE
1	B	387	VAL

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Mol	Chain	Res	Type
1	B	402	GLU

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	58	GLN
1	A	166	HIS
1	A	175	ASN
1	A	189	HIS
1	A	204	GLN
1	A	210	GLN
1	A	226	GLN
1	A	259	ASN
1	A	294	ASN
1	A	312	ASN
1	A	335	GLN
1	A	339	ASN
1	A	388	ASN
1	B	58	GLN
1	B	63	ASN
1	B	69	ASN
1	B	84	GLN
1	B	258	HIS
1	B	264	ASN
1	B	335	GLN
1	B	347	ASN
1	B	357	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	PMP	A	411	-	16,16,16	2.12	3 (18%)	22,23,23	2.17	4 (18%)
2	PMP	B	411	-	16,16,16	1.75	3 (18%)	22,23,23	1.55	3 (13%)

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	PMP	A	411	-	-	3/8/8/8	0/1/1/1
2	PMP	B	411	-	-	3/8/8/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	PMP	C5-C4	-5.84	1.32	1.40
2	B	411	PMP	C5-C4	3.60	1.45	1.40
2	B	411	PMP	C3-C2	-3.35	1.37	1.41
2	A	411	PMP	C3-C2	-3.14	1.37	1.41
2	A	411	PMP	O4P-C5A	-2.72	1.34	1.44
2	B	411	PMP	C2-N1	2.55	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PMP	O4P-C5A-C5	6.97	122.43	109.36
2	B	411	PMP	O4P-C5A-C5	3.63	116.16	109.36
2	A	411	PMP	C3-C2-N1	-3.39	116.68	120.96
2	A	411	PMP	C3-C4-C5	3.07	121.52	118.73
2	B	411	PMP	C3-C2-N1	-2.59	117.69	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	PMP	C5A-C5-C6	2.31	123.13	119.36
2	A	411	PMP	C5-C6-N1	-2.11	120.39	123.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	411	PMP	C5A-O4P-P-O2P
2	A	411	PMP	C5A-O4P-P-O3P
2	B	411	PMP	C5A-O4P-P-O1P
2	B	411	PMP	C5A-O4P-P-O2P
2	A	411	PMP	C5A-O4P-P-O1P
2	B	411	PMP	C5A-O4P-P-O3P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	PMP	1	0
2	B	411	PMP	1	0

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.