



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:21 AM UTC

PDB ID : 1AKA / pdb_00001aka
Title : STRUCTURAL BASIS FOR THE CATALYTIC ACTIVITY OF ASPARTATE AMINOTRANSFERASE K258H LACKING ITS PYRIDOXAL-5'-PHOSPHATE-BINDING LYSINE RESIDUE
Authors : Malashkevich, V.N.; Jansonius, J.N.
Deposited on : 1994-02-28
Resolution : 2.10 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

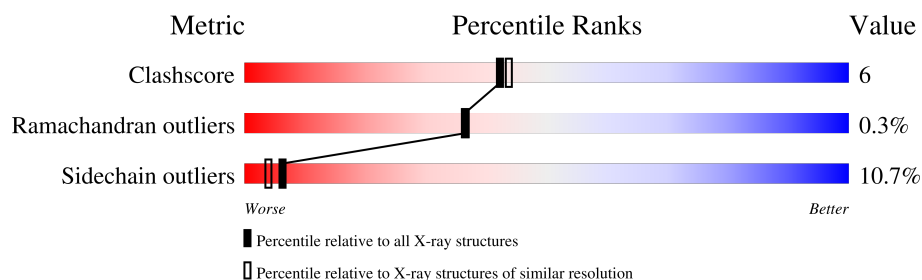
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	A	411	-	X	-	-
3	PO4	B	411	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7011 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.

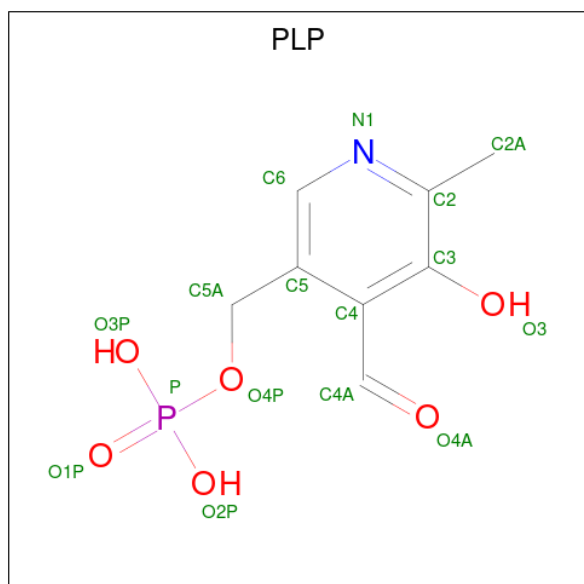
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3162	2004	559	581	18			
1	B	401	Total	C	N	O	S	0	0	0
			3162	2004	559	581	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	SER	conflict	UNP P00508
A	258	HIS	LYS	engineered mutation	UNP P00508
B	47	PRO	SER	conflict	UNP P00508
B	258	HIS	LYS	engineered mutation	UNP P00508

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

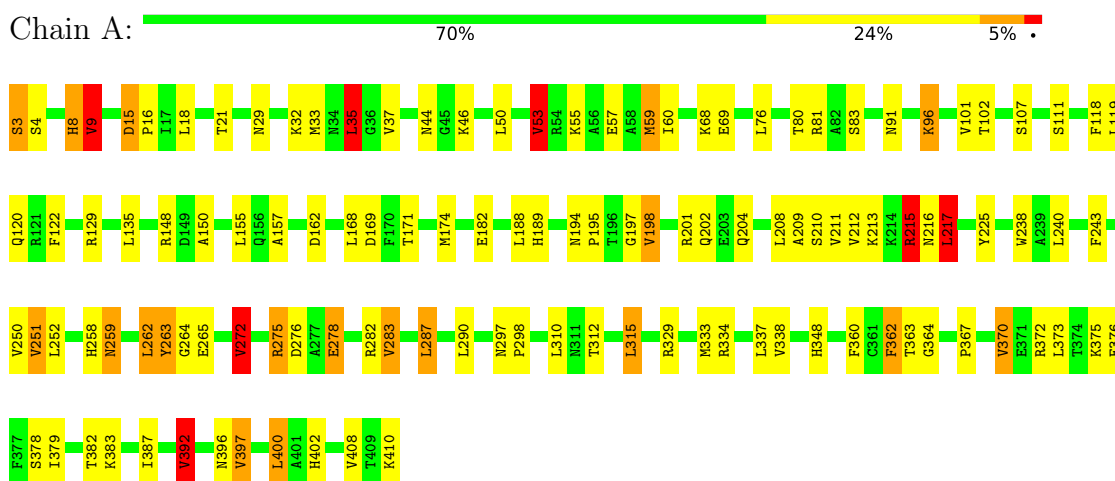
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	341	Total	O	0	0
			341	341		
4	B	325	Total	O	0	0
			325	325		

3 Residue-property plots

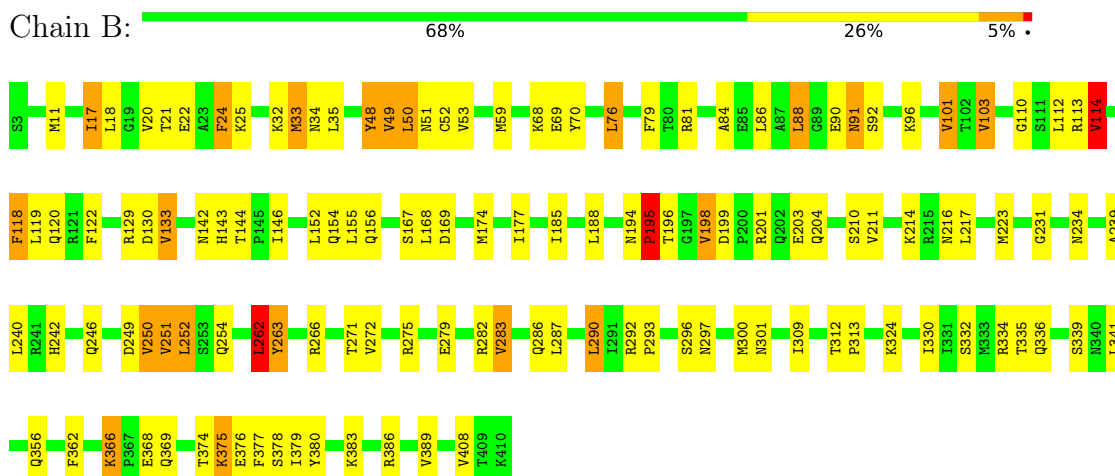
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	Depositor
Cell constants a, b, c, α , β , γ	55.87Å 58.80Å 75.81Å 85.26° 108.96° 115.57°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7011	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, PO4

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	1.02	0/3233	1.96	83/4364 (1.9%)
1	B	1.00	1/3233 (0.0%)	1.92	70/4364 (1.6%)
All	All	1.01	1/6466 (0.0%)	1.94	153/8728 (1.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	THR	CA-CB	5.23	1.61	1.53

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	VAL	N-CA-CB	-9.98	94.76	111.23
1	A	8	HIS	CA-CB-CG	-9.56	104.24	113.80
1	B	49	VAL	CB-CA-C	9.49	123.75	110.84
1	A	278	GLU	CB-CG-CD	9.45	128.66	112.60
1	A	15	ASP	CA-CB-CG	8.81	121.41	112.60
1	B	254	GLN	OE1-CD-NE2	8.80	131.40	122.60
1	B	81	ARG	CD-NE-CZ	8.55	136.37	124.40
1	A	217	LEU	N-CA-CB	-8.17	97.09	110.41
1	B	356	GLN	O-C-N	8.13	132.06	122.79
1	A	216	ASN	N-CA-CB	-7.92	99.98	111.70
1	A	189	HIS	CA-C-O	-7.72	111.78	120.43
1	B	334	ARG	CA-C-O	7.63	128.83	120.82
1	A	402	HIS	CA-CB-CG	-7.59	106.21	113.80
1	A	297	ASN	CB-CA-C	7.55	120.19	109.92
1	B	120	GLN	OE1-CD-NE2	-7.52	115.08	122.60
1	B	33	MET	CA-CB-CG	7.43	128.96	114.10
1	A	362	PHE	CA-CB-CG	7.42	121.22	113.80
1	A	392	VAL	CB-CA-C	7.30	121.28	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	GLU	N-CA-C	7.15	122.10	113.23
1	B	335	THR	CA-CB-OG1	-6.99	99.12	109.60
1	A	397	VAL	CB-CA-C	-6.98	102.71	112.14
1	A	216	ASN	OD1-CG-ND2	6.98	129.58	122.60
1	B	113	ARG	CA-C-O	-6.83	113.18	120.42
1	A	278	GLU	CA-CB-CG	6.77	127.64	114.10
1	B	122	PHE	N-CA-C	6.76	122.63	113.97
1	B	101	VAL	N-CA-CB	6.76	121.99	111.99
1	A	334	ARG	NE-CZ-NH1	6.73	128.23	121.50
1	B	301	ASN	N-CA-C	6.69	118.37	111.14
1	A	197	GLY	CA-C-O	-6.67	111.61	119.02
1	B	101	VAL	CB-CA-C	-6.67	101.05	110.12
1	B	103	VAL	N-CA-CB	-6.64	99.83	111.39
1	A	360	PHE	CA-CB-CG	-6.61	107.19	113.80
1	B	231	GLY	N-CA-C	-6.58	106.37	114.92
1	A	251	VAL	N-CA-C	-6.57	98.16	108.86
1	A	383	LYS	N-CA-C	6.53	120.70	112.87
1	B	84	ALA	CA-C-O	6.53	127.67	120.82
1	A	15	ASP	CB-CA-C	6.52	119.97	109.41
1	B	118	PHE	CA-C-O	6.52	127.46	120.55
1	A	397	VAL	N-CA-CB	6.47	119.34	110.54
1	A	298	PRO	N-CA-C	6.46	118.58	110.70
1	B	262	LEU	N-CA-CB	-6.41	101.71	110.56
1	B	198	VAL	N-CA-CB	6.41	118.31	111.00
1	A	272	VAL	CB-CA-C	6.41	120.12	110.63
1	B	59	MET	O-C-N	6.41	129.45	122.15
1	A	9	VAL	N-CA-CB	6.38	118.09	110.95
1	A	217	LEU	CA-C-O	-6.37	113.72	121.36
1	B	290	LEU	N-CA-CB	-6.33	100.77	110.20
1	A	80	THR	CA-CB-OG1	-6.33	100.11	109.60
1	A	198	VAL	N-CA-CB	6.31	118.20	111.00
1	A	348	HIS	CA-CB-CG	-6.28	107.52	113.80
1	A	96	LYS	N-CA-C	6.27	118.11	111.28
1	B	196	THR	N-CA-C	6.27	121.11	112.90
1	A	44	ASN	OD1-CG-ND2	6.26	128.86	122.60
1	B	251	VAL	CB-CA-C	6.15	119.97	110.50
1	B	300	MET	N-CA-C	6.12	120.48	112.89
1	A	210	SER	O-C-N	6.12	128.37	122.07
1	A	363	THR	N-CA-C	6.08	119.90	112.23
1	A	53	VAL	CB-CA-C	6.07	120.38	112.24
1	A	213	LYS	CA-C-O	6.04	126.92	120.70
1	A	111	SER	CA-C-O	-6.04	114.15	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	LEU	N-CA-CB	-6.00	100.36	111.52
1	B	199	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	29	ASN	OD1-CG-ND2	5.92	128.52	122.60
1	B	51	ASN	CA-CB-CG	-5.92	106.68	112.60
1	A	69	GLU	CG-CD-OE1	-5.91	104.81	118.40
1	B	252	LEU	N-CA-C	5.90	118.37	109.23
1	B	34	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	B	234	ASN	CA-CB-CG	-5.88	106.72	112.60
1	B	17	ILE	N-CA-C	-5.87	104.60	111.00
1	B	297	ASN	CB-CA-C	5.86	117.96	110.22
1	A	201	ARG	N-CA-C	-5.85	102.11	110.59
1	A	225	TYR	N-CA-C	5.84	119.62	111.56
1	A	60	ILE	O-C-N	5.83	127.78	121.94
1	A	275	ARG	O-C-N	5.80	128.76	122.15
1	A	265	GLU	CA-C-O	5.76	126.03	119.18
1	B	309	ILE	N-CA-C	5.74	115.93	110.42
1	A	57	GLU	CB-CA-C	-5.71	101.31	110.79
1	B	366	LYS	CA-C-N	5.70	125.17	119.24
1	B	366	LYS	C-N-CA	5.70	125.17	119.24
1	B	52	CYS	CA-C-O	-5.69	113.67	120.10
1	A	148	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	A	182	GLU	CA-CB-CG	5.66	125.43	114.10
1	B	69	GLU	CG-CD-OE1	-5.66	105.38	118.40
1	B	216	ASN	CA-CB-CG	-5.65	106.95	112.60
1	A	382	THR	CA-CB-OG1	-5.64	101.14	109.60
1	B	223	MET	CA-C-O	5.63	128.56	121.58
1	B	144	THR	CA-CB-OG1	-5.61	101.19	109.60
1	B	143	HIS	N-CA-CB	5.60	118.46	110.06
1	B	334	ARG	O-C-N	-5.59	116.31	122.07
1	B	24	PHE	CA-CB-CG	-5.59	108.21	113.80
1	B	234	ASN	OD1-CG-ND2	5.59	128.19	122.60
1	A	298	PRO	CB-CA-C	5.57	117.71	110.92
1	B	252	LEU	N-CA-CB	-5.55	101.21	111.53
1	A	171	THR	CB-CA-C	5.52	119.55	110.88
1	B	324	LYS	CA-C-N	5.48	126.06	119.98
1	B	324	LYS	C-N-CA	5.48	126.06	119.98
1	B	114	VAL	CA-C-N	5.47	126.02	119.94
1	B	114	VAL	C-N-CA	5.47	126.02	119.94
1	B	185	ILE	CA-C-N	-5.46	115.99	123.14
1	B	185	ILE	C-N-CA	-5.46	115.99	123.14
1	A	53	VAL	CA-CB-CG2	5.46	119.67	110.40
1	B	286	GLN	CA-C-N	5.45	128.03	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	GLN	C-N-CA	5.45	128.03	120.29
1	A	81	ARG	CA-C-O	5.45	126.54	120.82
1	A	382	THR	CA-C-N	5.43	131.09	120.99
1	A	382	THR	C-N-CA	5.43	131.09	120.99
1	B	389	VAL	O-C-N	5.41	128.23	122.06
1	A	258	HIS	CA-CB-CG	-5.39	108.41	113.80
1	A	262	LEU	N-CA-CB	-5.37	102.69	110.47
1	B	133	VAL	CB-CA-C	5.36	118.57	110.63
1	B	24	PHE	CB-CA-C	5.30	119.19	110.88
1	B	266	ARG	N-CA-C	5.29	117.10	110.91
1	B	254	GLN	CG-CD-NE2	-5.29	108.47	116.40
1	B	48	TYR	CA-C-O	-5.27	114.64	120.33
1	B	70	TYR	CA-CB-CG	5.26	123.36	113.90
1	B	195	PRO	N-CA-C	5.23	125.70	112.10
1	A	46	LYS	O-C-N	5.22	126.64	121.57
1	B	118	PHE	O-C-N	-5.22	116.59	122.12
1	A	215	ARG	N-CA-CB	5.21	118.42	110.44
1	A	35	LEU	N-CA-CB	-5.21	102.94	110.70
1	A	122	PHE	N-CA-C	5.21	120.49	113.72
1	A	259	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	367	PRO	CA-C-N	5.20	127.24	120.28
1	A	367	PRO	C-N-CA	5.20	127.24	120.28
1	A	204	GLN	OE1-CD-NE2	5.19	127.79	122.60
1	B	169	ASP	N-CA-C	-5.18	99.54	108.56
1	A	238	TRP	CA-C-O	-5.17	115.37	120.90
1	A	400	LEU	CA-C-O	5.17	126.03	120.55
1	A	278	GLU	CG-CD-OE1	5.16	130.27	118.40
1	A	57	GLU	N-CA-CB	5.15	117.69	110.12
1	A	364	GLY	N-CA-C	-5.15	108.01	115.27
1	B	239	ALA	CB-CA-C	5.13	119.31	110.79
1	A	362	PHE	N-CA-C	-5.13	100.16	108.41
1	B	156	GLN	CA-C-O	-5.12	115.78	121.51
1	A	238	TRP	O-C-N	5.12	127.41	122.09
1	A	83	SER	N-CA-CB	5.11	117.64	110.12
1	A	202	GLN	N-CA-C	5.11	117.24	111.11
1	A	329	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	A	264	GLY	N-CA-C	5.10	120.28	114.67
1	A	251	VAL	N-CA-CB	5.09	121.35	111.93
1	A	259	ASN	CB-CA-C	5.09	120.44	110.67
1	B	130	ASP	N-CA-C	5.08	118.49	109.96
1	B	330	ILE	O-C-N	5.07	126.88	121.91
1	A	213	LYS	CA-C-N	5.06	127.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	LYS	C-N-CA	5.06	127.06	120.28
1	A	392	VAL	CA-CB-CG2	5.06	119.00	110.40
1	A	400	LEU	N-CA-CB	-5.06	102.69	110.12
1	A	370	VAL	CA-C-O	-5.05	115.01	120.47
1	A	250	VAL	N-CA-CB	-5.04	102.91	111.23
1	B	156	GLN	OE1-CD-NE2	5.04	127.64	122.60
1	B	249	ASP	CA-C-O	5.03	126.15	120.92
1	A	102	THR	CA-C-N	-5.03	116.13	123.06
1	A	102	THR	C-N-CA	-5.03	116.13	123.06

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	3162	0	3148	38	0
1	B	3162	0	3148	45	0
2	A	16	0	7	1	0
3	B	5	0	0	0	0
4	A	341	0	0	2	0
4	B	325	0	0	4	0
All	All	7011	0	6303	80	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 6.

All (80) 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:91:ASN:HA	1:B:96:LYS:HE2	1.59	0.84
1:B:201:ARG:H	1:B:204:GLN:HE21	1.27	0.80
1:B:292:ARG:HB3	1:B:293:PRO:HD3	1.73	0.71
1:A:50:LEU:HB2	1:A:53:VAL:HG13	1.75	0.69
1:A:8:HIS:H	1:A:8:HIS:CD2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HA	1:A:21:THR:HG22	1.77	0.66
1:A:101:VAL:HG11	1:A:283:VAL:HG22	1.79	0.65
1:A:68:LYS:O	1:B:263:TYR:HB2	1.99	0.63
1:B:101:VAL:HG21	1:B:283:VAL:HG22	1.81	0.62
1:B:203:GLU:HB3	4:B:660:HOH:O	2.00	0.61
1:B:201:ARG:H	1:B:204:GLN:NE2	1.96	0.60
1:A:162:ASP:HB2	1:A:169:ASP:HB2	1.82	0.60
1:B:167:SER:HB2	4:B:422:HOH:O	2.02	0.60
1:A:333:MET:HB3	1:A:392:VAL:HG22	1.85	0.58
1:A:263:TYR:HB2	1:B:68:LYS:O	2.06	0.56
1:B:33:MET:HE2	1:B:35:LEU:HD21	1.87	0.56
1:A:215:ARG:HB2	1:A:217:LEU:HD13	1.88	0.55
1:B:154:GLN:NE2	4:B:636:HOH:O	2.39	0.55
1:A:251:VAL:HG12	1:A:272:VAL:HB	1.90	0.54
1:B:33:MET:HG2	1:B:379:ILE:HG12	1.89	0.54
1:B:22:GLU:HA	1:B:25:LYS:HD3	1.90	0.53
1:B:32:LYS:HA	1:B:378:SER:HB3	1.91	0.52
1:A:276:ASP:OD1	1:A:278:GLU:HB3	2.11	0.51
1:B:17:ILE:O	1:B:20:VAL:HG22	2.10	0.51
1:B:88:LEU:O	1:B:92:SER:HB2	2.10	0.51
1:A:91:ASN:HA	1:A:96:LYS:NZ	2.25	0.51
1:B:374:THR:HG23	1:B:380:TYR:CE1	2.46	0.51
1:B:377:PHE:O	1:B:378:SER:HB2	2.10	0.50
1:A:8:HIS:CD2	1:A:8:HIS:N	2.80	0.49
1:B:386:ARG:NH1	4:B:607:HOH:O	2.35	0.48
1:B:76:LEU:HB3	1:B:79:PHE:HB3	1.96	0.47
1:A:55:LYS:O	1:A:59:MET:HE3	2.13	0.47
1:A:372:ARG:HG2	1:A:408:VAL:HG12	1.97	0.47
1:A:278:GLU:CD	1:A:282:ARG:HE	2.22	0.47
1:B:48:TYR:CE2	1:B:50:LEU:HD22	2.50	0.47
1:B:262:LEU:O	1:B:263:TYR:C	2.58	0.47
1:A:15:ASP:HA	1:A:16:PRO:HD3	1.81	0.46
1:B:194:ASN:HA	1:B:195:PRO:HA	1.76	0.46
1:A:8:HIS:H	1:A:8:HIS:HD2	1.59	0.46
1:A:278:GLU:OE1	1:A:282:ARG:NH2	2.43	0.46
1:A:372:ARG:HG3	1:A:376:GLU:CD	2.41	0.46
1:A:275:ARG:HD3	4:A:557:HOH:O	2.15	0.45
1:A:3:SER:OG	1:A:4:SER:N	2.50	0.45
1:B:11:MET:HE2	1:B:11:MET:HB2	1.86	0.45
1:A:33:MET:HE3	1:A:396:ASN:CG	2.41	0.44
1:B:242:HIS:O	1:B:246:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:GLU:O	1:B:283:VAL:HG13	2.17	0.44
1:B:110:GLY:O	1:B:114:VAL:HG13	2.16	0.44
1:B:177:ILE:HG22	1:B:211:VAL:HG12	2.00	0.44
1:A:120:GLN:HG3	1:A:150:ALA:O	2.18	0.44
1:A:129:ARG:HA	1:A:129:ARG:HE	1.82	0.44
1:B:332:SER:O	1:B:336:GLN:HG3	2.18	0.44
1:B:369:GLN:HB3	1:B:408:VAL:CG1	2.48	0.43
1:A:18:LEU:HA	1:A:21:THR:CG2	2.45	0.43
1:B:101:VAL:O	1:B:271:THR:HA	2.19	0.43
1:B:142:ASN:O	1:B:146:ILE:HG13	2.18	0.43
1:A:9:VAL:O	1:B:282:ARG:HD2	2.18	0.43
1:B:375:LYS:N	1:B:375:LYS:HD2	2.32	0.43
1:A:135:LEU:O	1:A:157:ALA:HA	2.19	0.43
1:B:210:SER:O	1:B:214:LYS:HG3	2.19	0.43
1:A:209:ALA:HB2	1:A:243:PHE:CE1	2.54	0.43
1:B:312:THR:HA	1:B:313:PRO:HD3	1.82	0.42
1:A:135:LEU:HD11	1:A:155:LEU:HD22	2.01	0.42
1:A:215:ARG:HH11	1:A:215:ARG:HD2	1.67	0.42
1:B:129:ARG:HA	1:B:129:ARG:HE	1.84	0.42
1:A:194:ASN:HB3	2:A:411:PLP:H2A1	2.01	0.42
1:B:118:PHE:CD1	1:B:287:LEU:HD13	2.54	0.42
1:B:275:ARG:HH11	1:B:275:ARG:HG2	1.84	0.42
1:A:35:LEU:HD22	1:A:379:ILE:HG23	2.01	0.42
1:A:32:LYS:HA	1:A:378:SER:O	2.20	0.42
1:A:312:THR:HB	1:A:315:LEU:HB2	2.00	0.42
1:A:375:LYS:NZ	4:A:488:HOH:O	2.53	0.42
1:A:118:PHE:CD1	1:A:287:LEU:HD13	2.55	0.41
1:B:341:LEU:HD23	1:B:341:LEU:HA	1.91	0.41
1:B:275:ARG:HG2	1:B:275:ARG:NH1	2.36	0.41
1:A:174:MET:HE1	1:A:211:VAL:HG21	2.03	0.41
1:B:33:MET:CG	1:B:379:ILE:HG12	2.51	0.41
1:B:174:MET:HE1	1:B:211:VAL:HG21	2.02	0.41
1:B:21:THR:O	1:B:24:PHE:HB3	2.21	0.41
1:B:129:ARG:HA	1:B:129:ARG:NE	2.36	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%)	387 (97%)	11 (3%)	1 (0%)	36	36
1	B	399/401 (100%)	384 (96%)	14 (4%)	1 (0%)	36	36
All	All	798/802 (100%)	771 (97%)	25 (3%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR
1	B	263	TYR

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%)	299 (89%)	36 (11%)	6	4
1	B	335/335 (100%)	299 (89%)	36 (11%)	6	4
All	All	670/670 (100%)	598 (89%)	72 (11%)	6	4

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	9	VAL
1	A	35	LEU
1	A	37	VAL

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Mol	Chain	Res	Type
1	A	53	VAL
1	A	59	MET
1	A	76	LEU
1	A	107	SER
1	A	119	LEU
1	A	168	LEU
1	A	188	LEU
1	A	195	PRO
1	A	198	VAL
1	A	208	LEU
1	A	212	VAL
1	A	215	ARG
1	A	217	LEU
1	A	240	LEU
1	A	259	ASN
1	A	262	LEU
1	A	272	VAL
1	A	283	VAL
1	A	287	LEU
1	A	290	LEU
1	A	310	LEU
1	A	315	LEU
1	A	337	LEU
1	A	338	VAL
1	A	362	PHE
1	A	370	VAL
1	A	373	LEU
1	A	387	ILE
1	A	392	VAL
1	A	397	VAL
1	A	400	LEU
1	A	410	LYS
1	B	18	LEU
1	B	49	VAL
1	B	50	LEU
1	B	53	VAL
1	B	76	LEU
1	B	86	LEU
1	B	88	LEU
1	B	90	GLU
1	B	91	ASN
1	B	103	VAL

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Mol	Chain	Res	Type
1	B	112	LEU
1	B	114	VAL
1	B	119	LEU
1	B	133	VAL
1	B	152	LEU
1	B	155	LEU
1	B	168	LEU
1	B	188	LEU
1	B	195	PRO
1	B	198	VAL
1	B	217	LEU
1	B	240	LEU
1	B	250	VAL
1	B	251	VAL
1	B	252	LEU
1	B	262	LEU
1	B	272	VAL
1	B	283	VAL
1	B	290	LEU
1	B	296	SER
1	B	339	SER
1	B	362	PHE
1	B	366	LYS
1	B	368	GLU
1	B	375	LYS
1	B	383	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	44	ASN
1	A	259	ASN
1	A	297	ASN
1	A	336	GLN
1	A	348	HIS
1	B	120	GLN
1	B	154	GLN
1	B	202	GLN
1	B	204	GLN
1	B	226	GLN
1	B	297	ASN

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Mol	Chain	Res	Type
1	B	351	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	PLP	A	411	-	16,16,16	2.50	4 (25%)	20,23,23	5.20	11 (55%)
3	PO4	B	411	-	4,4,4	1.91	3 (75%)	6,6,6	1.38	1 (16%)

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	PLP	A	411	-	-	5/8/8/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	PLP	O4A-C4A	7.95	1.49	1.21
2	A	411	PLP	C3-C2	3.85	1.45	1.41
3	B	411	PO4	P-O4	2.39	1.61	1.54
2	A	411	PLP	C2A-C2	2.23	1.53	1.50
2	A	411	PLP	C2-N1	2.19	1.37	1.33
3	B	411	PO4	P-O3	-2.05	1.48	1.54
3	B	411	PO4	P-O1	-2.05	1.45	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PLP	C4-C3-C2	15.18	128.69	120.14
2	A	411	PLP	C3-C4-C5	-9.65	110.53	118.28
2	A	411	PLP	O4P-C5A-C5	7.44	123.29	109.36
2	A	411	PLP	C2A-C2-C3	7.31	129.36	120.80
2	A	411	PLP	C3-C2-N1	-6.43	112.85	120.96
2	A	411	PLP	O4A-C4A-C4	-4.11	115.05	124.80
2	A	411	PLP	O3-C3-C2	-3.96	109.36	117.58
2	A	411	PLP	C6-C5-C4	2.95	123.29	118.21
3	B	411	PO4	O2-P-O1	2.87	121.12	110.95
2	A	411	PLP	C5A-C5-C6	-2.65	115.04	119.36
2	A	411	PLP	O3P-P-O2P	2.41	116.85	107.80
2	A	411	PLP	C6-N1-C2	2.16	123.12	119.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	411	PLP	C3-C4-C4A-O4A
2	A	411	PLP	C4-C5-C5A-O4P
2	A	411	PLP	C6-C5-C5A-O4P
2	A	411	PLP	C5A-O4P-P-O2P
2	A	411	PLP	C5-C4-C4A-O4A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	PLP	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.