



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:41 PM EDT

PDB ID : 1DJU / pdb_00001dju
Title : CRYSTAL STRUCTURE OF AROMATIC AMINOTRANSFERASE FROM
PYROCOCUS HORIKOSHII OT3
Authors : Matsui, I.; Matsui, E.; Sakai, Y.; Kikuchi, H.; Kawarabayashi, H.
Deposited on : 1999-12-06
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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

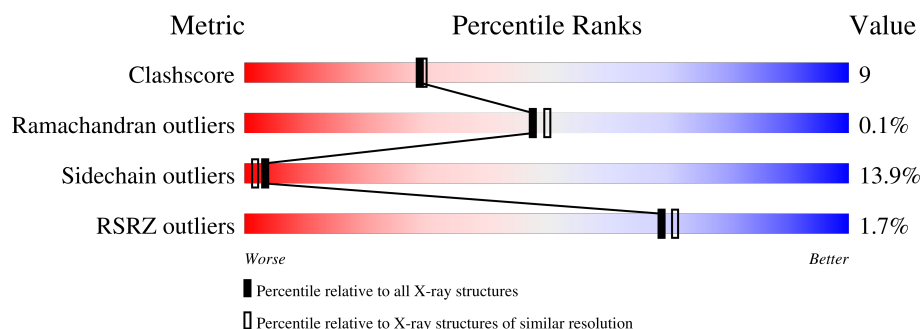
1 Overall quality at a glance

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)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	388	
1	B	388	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6182 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.

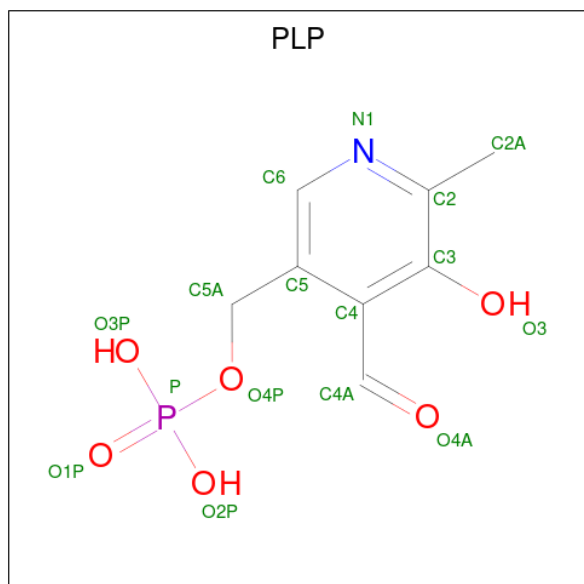
- Molecule 1 is a protein called AROMATIC AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2983	1918	498	554	13			
1	B	373	Total	C	N	O	S	0	0	0
			2969	1909	495	552	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	377	GLU	ASP	conflict	UNP O59096
B	377	GLU	ASP	conflict	UNP O59096

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

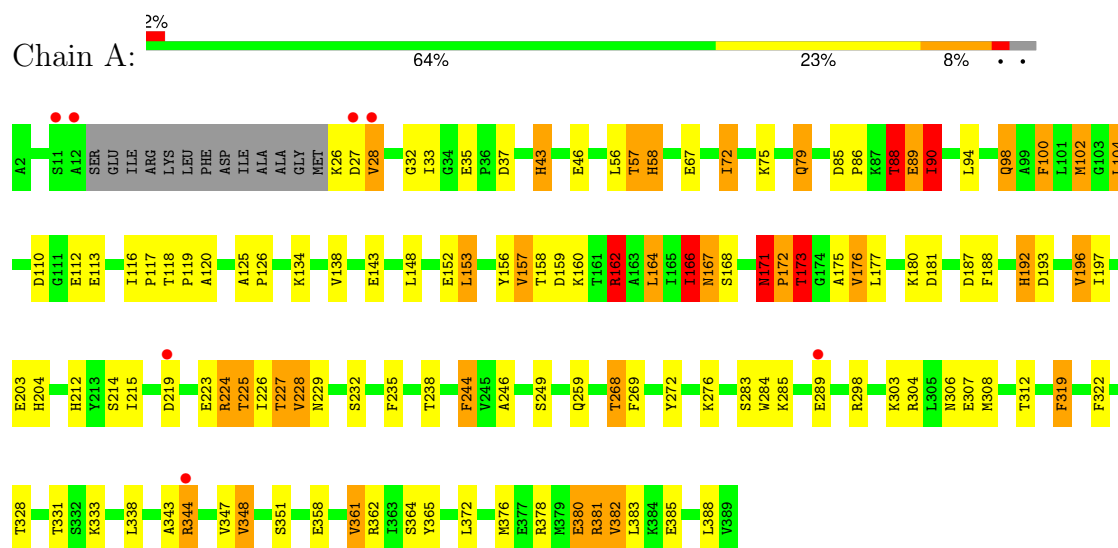
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	B	93	Total	O	0	0
			93	93		

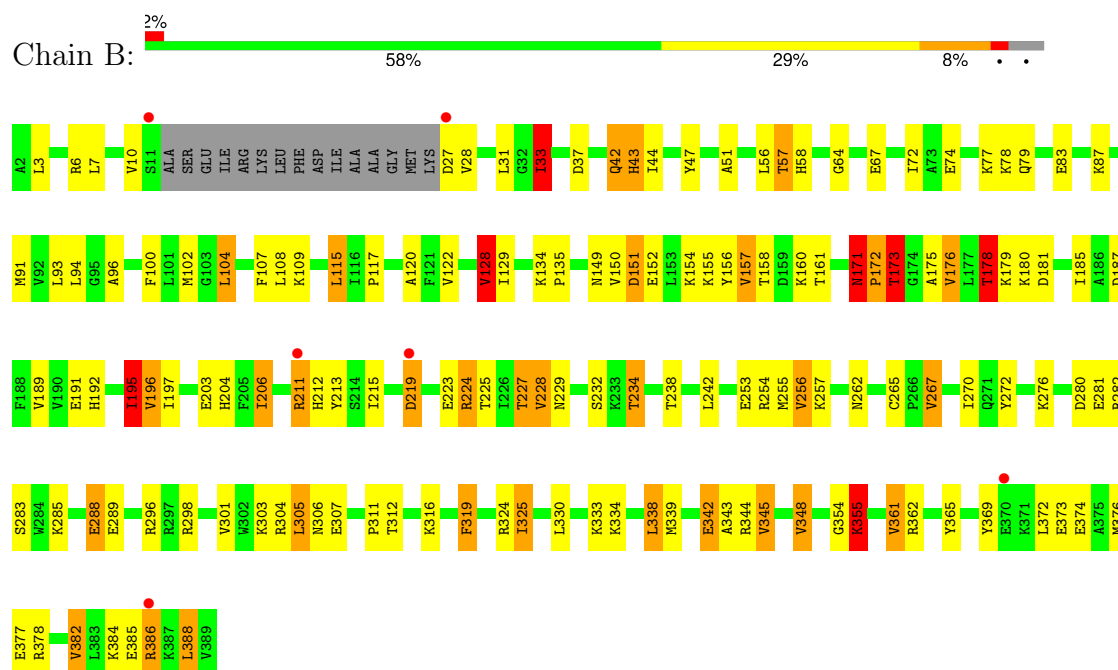
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: AROMATIC AMINOTRANSFERASE



• Molecule 1: AROMATIC AMINOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.01Å 124.87Å 128.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10 8.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.10) 88.8 (8.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.03Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.185 , 0.254 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 85.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6182	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: PLP

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	1.08	13/3043 (0.4%)	1.85	66/4105 (1.6%)
1	B	1.14	16/3029 (0.5%)	1.88	75/4087 (1.8%)
All	All	1.11	29/6072 (0.5%)	1.86	141/8192 (1.7%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	VAL	CA-CB	9.94	1.67	1.54
1	B	348	VAL	CA-CB	8.11	1.64	1.54
1	B	227	THR	CA-CB	7.75	1.65	1.53
1	B	267	VAL	CA-CB	7.62	1.63	1.54
1	A	382	VAL	CA-CB	7.53	1.64	1.54
1	A	43	HIS	CD2-NE2	-7.26	1.29	1.37
1	B	228	VAL	CA-CB	7.13	1.64	1.54
1	A	227	THR	CA-CB	7.12	1.62	1.53
1	B	204	HIS	CD2-NE2	-7.04	1.30	1.37
1	A	212	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	192	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	204	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	224	ARG	NE-CZ	6.80	1.40	1.33
1	B	212	HIS	CD2-NE2	-6.73	1.30	1.37
1	B	128	VAL	CA-CB	6.50	1.62	1.54
1	B	256	VAL	CA-CB	6.38	1.62	1.54
1	B	43	HIS	CD2-NE2	-6.26	1.30	1.37
1	B	58	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	58	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	90	ILE	CA-CB	5.80	1.64	1.55
1	B	195	ILE	CA-CB	5.65	1.62	1.54
1	A	225	THR	CA-CB	5.61	1.65	1.54
1	B	345	VAL	CA-CB	5.61	1.62	1.54
1	A	33	ILE	CA-CB	5.51	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	VAL	CA-CB	5.43	1.61	1.54
1	A	176	VAL	CA-CB	5.43	1.62	1.54
1	B	204	HIS	CG-ND1	-5.30	1.32	1.38
1	B	192	HIS	CD2-NE2	-5.27	1.32	1.37
1	A	215	ILE	CA-CB	5.17	1.62	1.54

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	ARG	CA-CB-CG	12.54	139.17	114.10
1	A	171	ASN	OD1-CG-ND2	-10.39	112.21	122.60
1	B	57	THR	N-CA-CB	-10.38	96.01	110.95
1	A	173	THR	N-CA-CB	-9.79	95.22	110.30
1	B	171	ASN	OD1-CG-ND2	-8.90	113.70	122.60
1	A	27	ASP	CA-CB-CG	8.82	121.42	112.60
1	A	110	ASP	N-CA-C	8.82	129.58	110.80
1	B	288	GLU	CB-CG-CD	8.72	127.43	112.60
1	B	173	THR	N-CA-CB	-8.50	97.21	110.30
1	B	325	ILE	CA-CB-CG1	-8.33	96.23	110.40
1	A	102	MET	CG-SD-CE	-8.21	82.84	100.90
1	A	196	VAL	CB-CA-C	-8.00	99.70	110.98
1	A	235	PHE	N-CA-C	-7.90	99.13	110.59
1	A	187	ASP	CA-CB-CG	7.87	120.47	112.60
1	A	143	GLU	CA-CB-CG	7.83	129.77	114.10
1	B	157	VAL	CB-CA-C	-7.82	102.69	111.45
1	A	159	ASP	CA-CB-CG	7.80	120.40	112.60
1	A	289	GLU	CB-CG-CD	7.77	125.81	112.60
1	A	298	ARG	CB-CG-CD	-7.75	93.47	111.30
1	A	319	PHE	CA-CB-CG	7.73	121.53	113.80
1	A	57	THR	N-CA-CB	-7.70	100.25	110.88
1	B	79	GLN	OE1-CD-NE2	-7.59	115.01	122.60
1	A	235	PHE	O-C-N	-7.57	113.83	122.68
1	B	224	ARG	N-CA-C	-7.54	103.64	112.92
1	A	27	ASP	N-CA-C	-7.51	98.55	109.59
1	B	224	ARG	CB-CG-CD	7.46	128.46	111.30
1	A	381	ARG	CA-C-O	-7.45	113.00	120.82
1	B	72	ILE	N-CA-C	-7.39	103.08	110.62
1	A	88	THR	N-CA-CB	-7.36	99.56	111.18
1	A	167	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	B	203	GLU	N-CA-C	7.21	120.98	111.75
1	B	149	ASN	N-CA-CB	-7.21	99.26	110.57
1	B	219	ASP	CA-CB-CG	7.17	119.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	PHE	CA-CB-CG	7.17	120.97	113.80
1	A	244	PHE	CA-CB-CG	7.17	120.97	113.80
1	B	42	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	B	10	VAL	O-C-N	6.95	130.21	122.98
1	B	171	ASN	N-CA-C	-6.90	97.62	109.15
1	B	180	LYS	CA-CB-CG	-6.89	100.32	114.10
1	B	178	THR	N-CA-CB	-6.82	100.34	110.17
1	A	157	VAL	CB-CA-C	-6.81	101.88	111.28
1	B	196	VAL	CB-CA-C	-6.72	100.82	110.83
1	B	204	HIS	CA-CB-CG	-6.69	107.11	113.80
1	B	151	ASP	CA-CB-CG	6.64	119.24	112.60
1	B	386	ARG	CB-CG-CD	6.64	126.56	111.30
1	B	225	THR	N-CA-C	6.55	120.18	109.24
1	B	44	ILE	N-CA-C	-6.52	103.90	111.00
1	B	195	ILE	CB-CG1-CD1	-6.51	100.13	113.80
1	B	57	THR	CB-CA-C	6.50	120.94	109.75
1	B	319	PHE	CA-CB-CG	6.46	120.26	113.80
1	A	98	GLN	OE1-CD-NE2	-6.45	116.16	122.60
1	A	79	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	B	223	GLU	CB-CG-CD	6.32	123.34	112.60
1	A	116	ILE	CA-C-N	6.32	126.65	119.83
1	A	116	ILE	C-N-CA	6.32	126.65	119.83
1	B	149	ASN	CA-CB-CG	6.32	118.92	112.60
1	B	325	ILE	CA-CB-CG2	6.30	121.21	110.50
1	A	212	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	A	58	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	A	72	ILE	N-CA-C	-6.27	104.64	110.53
1	A	226	ILE	N-CA-C	-6.20	98.81	107.80
1	A	171	ASN	CB-CG-ND2	6.18	125.67	116.40
1	B	212	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	203	GLU	N-CA-C	6.08	118.69	111.33
1	B	257	LYS	N-CA-C	-6.08	104.57	111.14
1	B	348	VAL	CA-C-N	6.01	125.95	119.76
1	B	348	VAL	C-N-CA	6.01	125.95	119.76
1	A	166	ILE	CA-CB-CG2	5.97	120.66	110.50
1	B	102	MET	CG-SD-CE	-5.96	87.79	100.90
1	A	347	VAL	O-C-N	-5.94	116.64	123.00
1	A	37	ASP	N-CA-C	-5.92	106.06	113.28
1	B	355	LYS	CA-CB-CG	-5.90	102.30	114.10
1	A	333	LYS	CA-CB-CG	5.88	125.86	114.10
1	B	298	ARG	CB-CG-CD	-5.88	97.78	111.30
1	B	192	HIS	CB-CG-CD2	-5.87	123.56	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	SER	O-C-N	-5.84	116.67	123.27
1	B	149	ASN	CB-CA-C	5.81	119.77	109.72
1	A	269	PHE	CA-CB-CG	5.78	119.58	113.80
1	A	298	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	A	43	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	A	160	LYS	N-CA-C	-5.75	105.93	113.17
1	B	191	GLU	CB-CG-CD	5.72	122.33	112.60
1	B	176	VAL	CA-C-O	5.69	126.39	120.36
1	B	33	ILE	N-CA-C	5.64	116.28	108.84
1	B	215	ILE	O-C-N	-5.62	116.20	121.87
1	B	229	ASN	O-C-N	-5.61	116.35	122.92
1	B	384	LYS	CA-CB-CG	-5.61	102.89	114.10
1	B	42	GLN	CG-CD-NE2	5.58	124.77	116.40
1	A	388	LEU	O-C-N	5.52	130.02	122.46
1	B	254	ARG	CA-CB-CG	-5.51	103.08	114.10
1	B	122	VAL	N-CA-C	5.47	120.12	113.00
1	B	79	GLN	CG-CD-NE2	5.47	124.60	116.40
1	B	361	VAL	N-CA-CB	-5.43	102.54	111.45
1	A	181	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	112	GLU	N-CA-C	5.42	118.30	110.28
1	B	354	GLY	CA-C-O	5.41	126.35	122.45
1	B	77	LYS	CA-CB-CG	-5.41	103.28	114.10
1	B	128	VAL	CA-C-O	-5.39	115.13	120.85
1	A	364	SER	O-C-N	-5.38	117.19	123.27
1	B	27	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	31	LEU	N-CA-C	-5.34	106.63	112.72
1	A	246	ALA	N-CA-C	-5.34	99.71	108.41
1	B	385	GLU	CA-C-O	-5.33	115.40	121.00
1	B	64	GLY	CA-C-O	-5.32	118.76	122.22
1	A	204	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	A	89	GLU	CA-C-N	-5.31	114.25	122.69
1	A	89	GLU	C-N-CA	-5.31	114.25	122.69
1	B	37	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	328	THR	N-CA-C	-5.30	106.89	113.19
1	A	227	THR	CB-CA-C	5.30	118.77	110.19
1	A	158	THR	N-CA-C	-5.29	101.41	108.34
1	B	67	GLU	N-CA-C	-5.28	105.52	111.28
1	A	331	THR	CA-CB-CG2	5.28	119.48	110.50
1	A	232	SER	N-CA-C	5.28	117.44	111.11
1	B	72	ILE	CA-C-O	-5.28	115.46	120.95
1	B	171	ASN	CB-CG-ND2	5.27	124.31	116.40
1	B	58	HIS	CB-CG-CD2	-5.27	124.35	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ILE	CA-CB-CG1	-5.25	101.47	110.40
1	A	162	ARG	CA-CB-CG	-5.24	103.61	114.10
1	A	143	GLU	CB-CA-C	-5.24	100.94	110.63
1	B	78	LYS	N-CA-C	5.22	116.78	111.14
1	B	388	LEU	CA-C-N	5.21	131.08	121.70
1	B	388	LEU	C-N-CA	5.21	131.08	121.70
1	A	100	PHE	CA-CB-CG	-5.21	108.59	113.80
1	B	83	GLU	CB-CG-CD	5.21	121.46	112.60
1	B	361	VAL	O-C-N	-5.19	117.29	123.05
1	A	284	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	B	265	CYS	O-C-N	-5.14	117.03	121.71
1	A	173	THR	CB-CA-C	5.10	120.79	110.38
1	A	224	ARG	CA-C-N	-5.09	114.60	122.59
1	A	224	ARG	C-N-CA	-5.09	114.60	122.59
1	B	386	ARG	CA-CB-CG	5.09	124.27	114.10
1	A	361	VAL	CA-CB-CG2	-5.08	101.76	110.40
1	B	173	THR	N-CA-C	5.06	118.60	112.23
1	B	262	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	B	43	HIS	CA-CB-CG	5.04	118.84	113.80
1	A	331	THR	CA-CB-OG1	-5.04	102.05	109.60
1	B	87	LYS	CB-CG-CD	5.03	122.88	111.30
1	B	224	ARG	NH1-CZ-NH2	-5.02	112.77	119.30
1	A	298	ARG	NE-CZ-NH1	5.01	126.51	121.50
1	A	212	HIS	CB-CG-ND1	5.01	130.21	122.70

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	2983	0	3024	49	0
1	B	2969	0	3006	56	0
2	A	15	0	6	0	0
2	B	15	0	6	1	0
3	A	107	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	93	0	0	3	0
All	All	6182	0	6042	104	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 9.

All (104) 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:MET:HE1	1:B:255:MET:HB2	1.61	0.81
1:B:173:THR:HG22	1:B:175:ALA:H	1.47	0.79
1:B:171:ASN:HD21	1:B:362:ARG:HH11	1.30	0.78
1:A:98:GLN:HE22	1:A:259:GLN:HE22	1.34	0.76
1:B:211:ARG:HD3	1:B:213:TYR:HE1	1.51	0.75
1:A:88:THR:HG22	1:A:89:GLU:HG3	1.69	0.72
1:A:348:VAL:HG13	1:A:362:ARG:HB3	1.72	0.71
1:B:158:THR:HG22	1:B:160:LYS:H	1.56	0.71
1:B:178:THR:HG22	1:B:181:ASP:H	1.57	0.68
1:B:91:MET:HE1	1:B:255:MET:CB	2.24	0.68
1:A:171:ASN:HD21	1:A:362:ARG:HH11	1.40	0.67
1:A:28:VAL:HA	1:A:344:ARG:HB3	1.78	0.65
1:B:104:LEU:HD13	1:B:197:ILE:HD11	1.76	0.65
1:B:211:ARG:HD3	1:B:213:TYR:CE1	2.30	0.63
1:B:150:VAL:HG12	1:B:154:LYS:HE2	1.83	0.59
1:A:168:SER:HB3	3:A:434:HOH:O	2.02	0.59
1:B:43:HIS:HE1	1:B:283:SER:OG	1.85	0.59
1:A:304:ARG:HH22	1:A:380:GLU:HG3	1.69	0.57
1:B:151:ASP:O	1:B:155:LYS:HD3	2.04	0.57
1:A:193:ASP:HA	1:A:224:ARG:NH2	2.20	0.57
1:B:107:PHE:CZ	1:B:195:ILE:HG12	2.41	0.56
1:A:35:GLU:HB2	1:A:238:THR:HG21	1.87	0.56
1:B:280:ASP:OD2	1:B:282:ARG:HD3	2.06	0.55
1:A:173:THR:HG22	1:A:175:ALA:H	1.73	0.54
1:B:51:ALA:HB2	1:B:272:TYR:CD2	2.41	0.54
1:A:171:ASN:HD22	1:A:172:PRO:HA	1.73	0.54
1:B:179:LYS:HB2	1:B:213:TYR:CE1	2.42	0.54
1:B:117:PRO:O	1:B:120:ALA:HB2	2.08	0.53
1:A:58:HIS:O	1:A:268:THR:HG21	2.08	0.53
1:B:171:ASN:HD21	1:B:362:ARG:NH1	2.03	0.52
1:B:6:ARG:HD3	1:B:129:ILE:O	2.11	0.51
1:B:234:THR:HG22	3:B:468:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LYS:O	1:A:307:GLU:HB2	2.11	0.51
1:A:117:PRO:O	1:A:120:ALA:HB2	2.10	0.50
1:A:372:LEU:O	1:A:376:MET:HG2	2.11	0.50
1:A:88:THR:HG23	1:A:249:SER:HB3	1.94	0.50
1:A:118:THR:HA	1:A:119:PRO:C	2.37	0.49
1:B:378:ARG:O	1:B:382:VAL:HG12	2.12	0.49
1:A:113:GLU:HA	1:A:134:LYS:O	2.13	0.49
1:B:369:TYR:O	1:B:373:GLU:HG3	2.13	0.49
1:B:386:ARG:HG3	1:B:388:LEU:HG	1.95	0.48
1:B:303:LYS:O	1:B:307:GLU:HG2	2.13	0.48
1:A:118:THR:HG22	1:A:138:VAL:O	2.12	0.48
1:B:338:LEU:HD13	1:B:339:MET:HE2	1.96	0.48
1:B:173:THR:HG21	3:B:473:HOH:O	2.13	0.47
1:B:33:ILE:H	1:B:33:ILE:HD13	1.79	0.47
1:A:164:LEU:HD13	1:A:166:ILE:HD13	1.95	0.47
1:A:229:ASN:HB3	1:A:244:PHE:CE2	2.49	0.47
1:B:206:ILE:H	1:B:206:ILE:HD13	1.80	0.47
1:B:100:PHE:O	1:B:104:LEU:HB2	2.15	0.47
1:A:32:GLY:HA2	3:A:436:HOH:O	2.15	0.47
1:A:118:THR:HG21	3:A:447:HOH:O	2.15	0.47
1:B:311:PRO:HG2	1:B:324:ARG:NH1	2.29	0.47
1:A:167:ASN:ND2	1:A:171:ASN:H	2.14	0.46
1:A:162:ARG:HD3	3:A:487:HOH:O	2.15	0.46
1:B:343:ALA:O	1:B:378:ARG:HD3	2.15	0.46
1:A:100:PHE:O	1:A:104:LEU:HB2	2.15	0.46
1:B:152:GLU:O	1:B:156:TYR:HD1	1.97	0.46
1:A:171:ASN:HD21	1:A:362:ARG:NH1	2.10	0.46
1:B:211:ARG:HD2	1:B:211:ARG:H	1.80	0.46
1:B:181:ASP:O	1:B:185:ILE:HG23	2.16	0.45
1:B:301:VAL:HG11	1:B:372:LEU:HD22	1.97	0.45
1:A:94:LEU:HD22	1:B:94:LEU:HD22	1.99	0.45
1:B:234:THR:HG21	3:B:428:HOH:O	2.16	0.45
1:A:348:VAL:CG1	1:A:362:ARG:HB3	2.44	0.45
1:A:381:ARG:HH21	1:A:385:GLU:HG2	1.82	0.45
1:A:188:PHE:O	1:A:192:HIS:HD2	2.00	0.44
1:A:85:ASP:OD1	1:A:88:THR:HB	2.17	0.44
1:B:343:ALA:HB2	1:B:382:VAL:HG11	1.99	0.44
1:A:98:GLN:CD	1:A:102:MET:HE1	2.43	0.44
1:B:232:SER:HB3	1:B:238:THR:HG22	2.00	0.44
1:B:28:VAL:HA	1:B:344:ARG:O	2.18	0.43
1:B:305:LEU:HD13	1:B:376:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LEU:O	1:B:342:GLU:HB2	2.18	0.43
1:A:28:VAL:HA	1:A:344:ARG:O	2.18	0.43
1:A:43:HIS:HE1	1:A:283:SER:OG	2.01	0.43
1:A:306:ASN:HD21	1:A:312:THR:H	1.65	0.43
1:B:171:ASN:HD22	1:B:172:PRO:HA	1.83	0.43
1:B:96:ALA:HB3	2:B:400:PLP:H5A1	2.00	0.43
1:A:193:ASP:HA	1:A:224:ARG:HH21	1.83	0.43
1:A:272:TYR:CZ	1:A:276:LYS:HE2	2.54	0.43
1:B:242:LEU:HD22	1:B:270:ILE:HG22	2.01	0.43
1:A:72:ILE:HG21	1:A:90:ILE:HD13	2.01	0.43
1:A:343:ALA:O	1:A:378:ARG:HD3	2.19	0.43
1:B:306:ASN:HD21	1:B:312:THR:H	1.66	0.43
1:A:319:PHE:HA	1:A:365:TYR:CZ	2.54	0.42
1:B:319:PHE:HA	1:B:365:TYR:CZ	2.55	0.42
1:A:85:ASP:HA	1:A:86:PRO:HD2	1.91	0.42
1:B:296:ARG:HH11	1:B:296:ARG:HD2	1.75	0.42
1:A:125:ALA:HB3	1:A:126:PRO:HD3	2.02	0.41
1:A:171:ASN:HD22	1:A:172:PRO:CA	2.34	0.41
1:B:115:LEU:HD22	1:B:161:THR:HG21	2.02	0.41
1:B:171:ASN:ND2	1:B:362:ARG:HH11	2.09	0.41
1:A:75:LYS:NZ	1:A:79:GLN:HE21	2.19	0.41
1:A:152:GLU:O	1:A:156:TYR:HD1	2.04	0.41
1:A:148:LEU:HD11	1:A:153:LEU:HD13	2.01	0.41
1:B:185:ILE:O	1:B:189:VAL:HG23	2.21	0.41
1:B:47:TYR:CD2	1:B:276:LYS:HD3	2.56	0.41
1:B:33:ILE:H	1:B:33:ILE:CD1	2.34	0.40
1:B:355:LYS:HA	1:B:355:LYS:HD3	1.66	0.40
1:A:104:LEU:HD13	1:A:197:ILE:HD11	2.02	0.40
1:A:308:MET:HB3	1:A:380:GLU:HG2	2.03	0.40
1:B:128:VAL:HG22	1:B:135:PRO:HD3	2.04	0.40
1:B:285:LYS:HE3	1:B:285:LYS:HB2	1.97	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	371/388 (96%)	358 (96%)	13 (4%)	0	100	100
1	B	369/388 (95%)	356 (96%)	12 (3%)	1 (0%)	36	36
All	All	740/776 (95%)	714 (96%)	25 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	219	ASP

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	316/326 (97%)	279 (88%)	37 (12%)	5	3
1	B	315/326 (97%)	264 (84%)	51 (16%)	2	1
All	All	631/652 (97%)	543 (86%)	88 (14%)	3	2

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	28	VAL
1	A	46	GLU
1	A	56	LEU
1	A	57	THR
1	A	67	GLU
1	A	88	THR
1	A	90	ILE
1	A	104	LEU
1	A	153	LEU
1	A	157	VAL
1	A	162	ARG

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Mol	Chain	Res	Type
1	A	164	LEU
1	A	166	ILE
1	A	171	ASN
1	A	172	PRO
1	A	173	THR
1	A	176	VAL
1	A	177	LEU
1	A	180	LYS
1	A	196	VAL
1	A	219	ASP
1	A	223	GLU
1	A	225	THR
1	A	227	THR
1	A	228	VAL
1	A	268	THR
1	A	285	LYS
1	A	338	LEU
1	A	344	ARG
1	A	348	VAL
1	A	351	SER
1	A	358	GLU
1	A	361	VAL
1	A	380	GLU
1	A	382	VAL
1	A	383	LEU
1	B	3	LEU
1	B	7	LEU
1	B	33	ILE
1	B	42	GLN
1	B	56	LEU
1	B	57	THR
1	B	74	GLU
1	B	93	LEU
1	B	104	LEU
1	B	108	LEU
1	B	109	LYS
1	B	115	LEU
1	B	128	VAL
1	B	134	LYS
1	B	157	VAL
1	B	171	ASN
1	B	172	PRO

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Mol	Chain	Res	Type
1	B	173	THR
1	B	176	VAL
1	B	178	THR
1	B	187	ASP
1	B	195	ILE
1	B	196	VAL
1	B	206	ILE
1	B	211	ARG
1	B	224	ARG
1	B	227	THR
1	B	228	VAL
1	B	234	THR
1	B	253	GLU
1	B	256	VAL
1	B	267	VAL
1	B	281	GLU
1	B	288	GLU
1	B	289	GLU
1	B	304	ARG
1	B	305	LEU
1	B	316	LYS
1	B	325	ILE
1	B	330	LEU
1	B	333	LYS
1	B	334	LYS
1	B	338	LEU
1	B	342	GLU
1	B	345	VAL
1	B	348	VAL
1	B	355	LYS
1	B	361	VAL
1	B	374	GLU
1	B	377	GLU
1	B	382	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	62	ASN
1	A	79	GLN
1	A	97	ASN

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Mol	Chain	Res	Type
1	A	98	GLN
1	A	167	ASN
1	A	171	ASN
1	A	192	HIS
1	A	204	HIS
1	A	306	ASN
1	B	43	HIS
1	B	58	HIS
1	B	79	GLN
1	B	167	ASN
1	B	171	ASN
1	B	204	HIS
1	B	306	ASN

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	B	400	1	15,15,16	1.87	2 (13%)	21,22,23	2.59	10 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	A	400	1	15,15,16	2.05	3 (20%)	21,22,23	3.16	12 (57%)

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	B	400	1	-	3/6/6/8	0/1/1/1
2	PLP	A	400	1	-	1/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	PLP	C4A-C4	-4.99	1.41	1.51
2	A	400	PLP	C4A-C4	-4.67	1.42	1.51
2	A	400	PLP	P-O4P	-3.41	1.49	1.60
2	B	400	PLP	P-O4P	-2.65	1.51	1.60
2	A	400	PLP	C2A-C2	2.30	1.54	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	PLP	C6-C5-C4	6.35	123.31	118.10
2	A	400	PLP	C6-C5-C4	6.25	123.22	118.10
2	A	400	PLP	C4A-C4-C5	5.54	126.65	120.94
2	A	400	PLP	C2A-C2-C3	5.20	126.88	120.80
2	A	400	PLP	C3-C4-C5	-5.12	112.45	118.59
2	B	400	PLP	C5A-C5-C6	-4.48	112.06	119.36
2	B	400	PLP	C5-C6-N1	-4.05	117.25	123.83
2	A	400	PLP	O4P-C5A-C5	3.93	116.72	109.36
2	A	400	PLP	C5A-C5-C6	-3.87	113.06	119.36
2	A	400	PLP	O3P-P-O4P	3.10	114.75	106.67
2	B	400	PLP	O2P-P-O4P	3.09	114.72	106.67
2	B	400	PLP	O4P-C5A-C5	3.04	115.05	109.36
2	B	400	PLP	C6-N1-C2	3.02	124.67	119.20
2	B	400	PLP	C2A-C2-C3	3.00	124.30	120.80
2	B	400	PLP	C3-C4-C5	-2.96	115.04	118.59
2	A	400	PLP	C5-C6-N1	-2.95	119.04	123.83
2	A	400	PLP	O2P-P-O4P	2.76	113.85	106.67
2	B	400	PLP	C4A-C4-C5	2.42	123.44	120.94
2	A	400	PLP	O4P-P-O1P	-2.26	100.33	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	PLP	O4P-P-O1P	2.14	112.23	106.44
2	A	400	PLP	C6-N1-C2	2.14	123.08	119.20
2	A	400	PLP	C4-C3-C2	2.00	122.88	119.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	PLP	C5A-O4P-P-O2P
2	B	400	PLP	C5A-O4P-P-O3P
2	A	400	PLP	C4-C5-C5A-O4P
2	B	400	PLP	C5A-O4P-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	375/388 (96%)	-0.40	7 (1%) 66 69	13, 23, 40, 71	0
1	B	373/388 (96%)	-0.38	6 (1%) 70 73	14, 23, 39, 61	0
All	All	748/776 (96%)	-0.39	13 (1%) 69 71	13, 23, 40, 71	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	SER	3.1
1	A	27	ASP	2.8
1	B	11	SER	2.8
1	A	344	ARG	2.7
1	A	12	ALA	2.1
1	A	289	GLU	2.1
1	B	27	ASP	2.1
1	A	28	VAL	2.1
1	B	386	ARG	2.1
1	A	219	ASP	2.1
1	B	219	ASP	2.0
1	B	370	GLU	2.0
1	B	211	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	A	400	15/16	0.95	0.07	16,22,26,26	0
2	PLP	B	400	15/16	0.97	0.06	15,18,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.