

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6F5V
Title	:	Crystal structure of the prephenate aminotransferase from Arabidopsis
		thaliana
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Deposited on	:	2017-12-03
$\operatorname{Resolution}$:	1.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695(1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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 <=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	А	475	75% 10%	16%
1	В	475	79% 6%	15%
1	С	475	73% 10%	16%
1	D	475	^{6%} 76% 9%	15%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13808 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 Bifunctional aspartate aminotransferase and glutamate/aspar tate-prephenate aminotransferase.

Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace	
1	Δ	401	Total	С	Ν	0	\mathbf{S}	0	91	0	
	А	401	3146	2024	516	597	9	0	21	0	
1	В	403	Total	С	Ν	Ο	S	0	15	0	
	D	405	3119	2003	511	594	11	0	10		
1	C	200	Total	С	Ν	0	S	0	16	0	
		099	3112	2001	509	592	10	0	10	U	
1	П	40.3	Total	С	Ν	0	S	0	0	0	
		403	3098	1985	514	588	11	0	0		

• Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf		
9	Λ	1	Total	С	Ν	0	Р	0	Ο	
	Л	I	15	8	1	5	1	0	0	
0	9 D	1	Total	С	Ν	Ο	Р	0	0	
	D	L	15	8	1	5	1	0	0	



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Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf		
2	C	1	Total	С	Ν	Ο	Р	0	0	
		L	15	8	1	5	1	0		
0	п	1	Total	С	Ν	Ο	Р	0	0	
	D	L	15	8	1	5	1	0	0	

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Na 1 1	0	0
3	А	1	Total Na 1 1	0	0

• Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total C O 13 6 7	0	0
4	С	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0

• Molecule 5 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	342	Total O 342 342	0	0
5	В	365	Total O 365 365	0	0
5	С	279	Total O 279 279	0	0
5	D	246	Total O 246 246	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

 \bullet Molecule 1: Bifunctional as partate aminotransferase and glutamate/as partate-prephenate aminotransferase



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Chai	n B: <mark>'</mark>								7	79%									(6%		15%)		
MET ALA SER GLN	SER SER VAL	VAL VAL ILE	SER SER	ALA ALA ALA	ARG GLY	GLU SER	PHE PRO	ASP SER		LIE 11E	GLY SER	VAL ARG	GLN	G LN PRO	ARG		E E E	LYS CYS LYS	SER	ASN MET	SER SER	ARG	C YS ALA MET	ALA	PRO ASN
ALA GLU THR	SER SER	S26	V29	S50	P67	A121	L126	A131	1140	K176	E184	R187	N196	L207	L244	L284	<mark>5290</mark>	T313 V314		D326	V329	K339	E342 P343	0344	L349 F350
1352 1399	R423 ALA THR	VAL SER VAL																							
• Mo amin	olecul otran	e 1: .sfer 5%	B ase	ifu	ncti	ona	al a	asp	art	ate	e a	mi	no	tra	nsf	era	se	ano	d g	lut	an	nat	e/a	asp	oart





 \bullet Molecule 1: Bifunctional as partate aminotransferase and glutamate/as partate-prephenate aminotransferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	58.47Å 73.24 Å 103.32 Å	Deperitor
a, b, c, α , β , γ	92.49° 87.22° 111.05°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	23.70 - 1.70	Depositor
Resolution (A)	48.93 - 1.67	EDS
% Data completeness	96.0 (23.70-1.70)	Depositor
(in resolution range)	94.7(48.93 - 1.67)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	$2.26 (at 1.67 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
D D	0.172 , 0.201	Depositor
Π, Π_{free}	0.170 , 0.198	DCC
R_{free} test set	8785 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	20.4	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , 53.1	EDS
L-test for $twinning^2$	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.015 for -h,h+k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13808	wwPDB-VP
Average B, all atoms $(Å^2)$	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: NA, CIT, 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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.34	0/3265	0.54	0/4429	
1	В	0.34	0/3223	0.53	0/4375	
1	С	0.29	0/3219	0.49	0/4368	
1	D	0.29	0/3181	0.49	0/4316	
All	All	0.32	0/12888	0.51	0/17488	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3146	0	3256	34	0
1	В	3119	0	3205	21	0
1	С	3112	0	3203	36	0
1	D	3098	0	3176	31	0
2	А	15	0	6	2	0
2	В	15	0	6	2	0
2	С	15	0	6	1	0
2	D	15	0	6	2	0
3	А	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	1	0	0	0	0
4	В	13	0	5	0	0
4	С	13	0	5	0	0
4	D	13	0	5	0	0
5	А	342	0	0	6	0
5	В	365	0	0	4	0
5	С	279	0	0	5	0
5	D	246	0	0	0	0
All	All	13808	0	12879	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 4.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:C:340:ILE:HG12	1:C:351[B]:ILE:HD12	1.61	0.83
1:C:131:ALA:HA	1:D:29:VAL:HG21	1.73	0.70
1:C:151:GLU:OE1	1:C:154[A]:ARG:NH1	2.24	0.70
1:D:46:THR:O	1:D:50:SER:N	2.24	0.69
1:A:29[A]:VAL:HG21	1:B:131:ALA:HA	1.74	0.69
1:C:207:LEU:HB3	1:C:244:LEU:HD11	1.74	0.69
1:A:131:ALA:HA	1:B:29[B]:VAL:HG11	1.75	0.68
1:A:284[B]:LEU:HD21	1:B:29[B]:VAL:HG12	1.75	0.68
1:D:207:LEU:HB3	1:D:244:LEU:HD11	1.76	0.67
1:A:29[A]:VAL:HG22	1:B:284[A]:LEU:HD21	1.77	0.66
1:B:339:LYS:HB2	1:B:352:ASP:HB3	1.76	0.66
1:C:349:LEU:HB3	1:C:351[B]:ILE:HD11	1.79	0.65
1:B:344[B]:GLN:NE2	5:B:603:HOH:O	2.31	0.64
1:A:154[A]:ARG:NH2	5:A:601:HOH:O	2.30	0.63
1:C:344:GLN:NE2	5:C:601:HOH:O	2.30	0.62
1:A:121:ALA:HB3	2:A:501:PLP:H5A1	1.81	0.62
1:D:47:LEU:HA	1:D:50:SER:HB3	1.81	0.62
1:C:24:SER:O	1:D:187:ARG:NH2	2.32	0.61
1:C:154[A]:ARG:NH2	5:C:609:HOH:O	2.34	0.59
1:A:283:LYS:NZ	5:A:605:HOH:O	2.36	0.58
1:A:314:VAL:HA	1:A:317:MET:HE2	1.85	0.58
1:B:121:ALA:HB3	2:B:501:PLP:H5A1	1.86	0.57
1:C:29[B]:VAL:HG11	1:D:131:ALA:HA	1.86	0.57
1:C:29[A]:VAL:HG21	1:D:131:ALA:HA	1.87	0.56
1:C:284[B]:LEU:HD21	1:D:29:VAL:HG22	1.88	0.55



6F5V

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:283:LYS:NZ	5:A:606:HOH:O	2.39	0.55
1:C:39:VAL:HG13	1:C:40:ILE:HD12	1.88	0.55
1:D:121:ALA:HB3	2:D:501:PLP:H5A1	1.89	0.55
1:A:140[B]:ILE:HD11	5:A:608:HOH:O	2.06	0.54
1:B:140[B]:ILE:HD11	5:B:615:HOH:O	2.07	0.54
1:A:339:LYS:HB2	1:A:352:ASP:HB3	1.89	0.53
1:B:351:ILE:HD12	1:B:399:ILE:HD12	1.89	0.53
1:C:339:LYS:HB2	1:C:352:ASP:HB3	1.91	0.52
1:A:331[A]:SER:HB3	1:A:412:VAL:HG11	1.90	0.52
1:C:217:HIS:O	1:C:250:ARG:NH2	2.42	0.52
1:A:24:SER:O	1:B:187:ARG:NH2	2.43	0.52
1:D:331:SER:HB3	1:D:412:VAL:HG11	1.92	0.52
1:B:26:SER:OG	1:B:29[B]:VAL:HG13	2.11	0.51
1:D:255:ASN:HB3	1:D:270:TYR:CZ	2.45	0.51
1:C:417:LYS:HE2	1:C:417:LYS:HA	1.92	0.51
1:B:349:LEU:HD13	1:B:351:ILE:HD11	1.93	0.51
1:A:210:ILE:O	1:A:214[B]:ILE:HG12	2.10	0.51
1:C:55:ILE:HG21	1:C:411:ALA:HB2	1.93	0.51
1:B:207:LEU:HB3	1:B:244:LEU:HD11	1.92	0.50
1:D:179:GLU:HA	1:D:182:LEU:HD12	1.93	0.50
1:A:288:VAL:HA	1:B:126:LEU:HD22	1.93	0.50
1:A:207:LEU:HB3	1:A:244:LEU:HD11	1.93	0.50
1:B:326:ASP:HA	5:B:614:HOH:O	2.11	0.50
1:C:56:ARG:NH2	5:C:614:HOH:O	2.39	0.50
1:A:230:HIS:CE1	1:A:309:ALA:HA	2.46	0.49
1:A:385:MET:SD	1:A:399:ILE:HG12	2.52	0.49
1:D:339:LYS:HB2	1:D:352:ASP:HB3	1.94	0.49
1:D:210:ILE:O	1:D:214:ILE:HG12	2.12	0.49
1:B:314:VAL:HA	1:B:317:MET:HE2	1.93	0.49
5:C:602:HOH:O	1:D:23:MET:HE2	2.13	0.49
1:A:331[B]:SER:HB2	1:A:412:VAL:HG11	1.94	0.49
1:C:29[A]:VAL:HG11	1:D:280:ALA:HB1	1.94	0.49
1:D:48:VAL:HG21	1:D:56:ARG:HH21	1.77	0.49
1:C:121:ALA:HB3	2:C:501:PLP:H5A1	1.94	0.49
1:A:217:HIS:O	1:A:250:ARG:NH2	2.44	0.49
1:A:140[B]:ILE:HD13	1:A:161:VAL:HB	1.96	0.48
1:C:170[B]:ASN:OD1	1:C:341:SER:OG	2.32	0.48
1:C:252:LEU:HB3	1:C:271:LEU:HD11	1.95	0.48
1:A:196:ASN:HB3	2:A:501:PLP:H2A1	1.96	0.47
1:A:28:ARG:NH1	1:A:157:ASP:OD2	2.47	0.47
1:D:196:ASN:HB3	2:D:501:PLP:H2A1	1.97	0.47



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:D:211:ALA:HA	1:D:247:MET:HE2	1.96	0.47
1:C:280:ALA:HB1	1:D:29:VAL:HG11	1.96	0.47
1:C:356:TYR:HD2	1:C:422:LEU:HB2	1.80	0.46
1:C:29[B]:VAL:HG12	1:D:284[B]:LEU:HD21	1.97	0.46
1:A:343:PRO:HG3	1:A:349:LEU:CD2	2.46	0.46
1:C:288:VAL:HA	1:D:126:LEU:HD22	1.96	0.46
1:C:150:THR:O	1:C:154[B]:ARG:HG3	2.16	0.45
1:C:62:PRO:HB3	1:C:321:TYR:OH	2.17	0.45
1:B:196:ASN:HB3	2:B:501:PLP:H2A1	1.97	0.45
1:A:127:GLN:HG2	1:A:284[A]:LEU:HD23	2.00	0.44
1:C:387:PRO:HA	1:C:397:ILE:HD13	2.00	0.43
1:C:163:ILE:HG12	1:C:181:LYS:HE3	2.00	0.43
1:D:416:ARG:O	1:D:420:GLU:HG3	2.18	0.43
1:A:131:ALA:HA	1:B:29[A]:VAL:HG21	1.99	0.43
1:A:55:ILE:HG21	1:A:411:ALA:HB2	2.00	0.43
1:C:130:LEU:HD23	1:C:156:ALA:HB2	1.99	0.43
1:A:416:ARG:O	1:A:420[A]:GLU:HG3	2.18	0.43
1:A:255:ASN:HB3	1:A:270:TYR:CZ	2.54	0.43
1:B:176:LYS:NZ	5:B:613:HOH:O	2.41	0.43
1:A:327:PHE:CZ	1:A:409:GLN:HG2	2.54	0.43
1:D:163:ILE:HG12	1:D:181:LYS:HD2	2.01	0.42
1:D:182:LEU:HD13	1:D:217:HIS:CE1	2.53	0.42
1:C:230:HIS:CE1	1:C:309:ALA:HA	2.54	0.42
1:C:37:THR:HG23	5:C:759:HOH:O	2.18	0.42
1:B:329:VAL:HG11	1:B:342:GLU:OE1	2.19	0.42
1:D:328:LEU:HB3	1:D:349:LEU:HD11	2.02	0.42
1:A:130:LEU:HD12	1:A:284[A]:LEU:HD21	2.01	0.41
1:C:126:LEU:HD22	1:D:288:VAL:HA	2.02	0.41
1:A:137:ASP:HA	1:A:185[B]:LYS:HE3	2.03	0.41
1:A:403[B]:THR:HG23	5:A:751:HOH:O	2.19	0.41
1:D:57:LEU:HD13	1:D:399:ILE:HG23	2.02	0.41
1:D:130:LEU:HD23	1:D:156:ALA:HB2	2.03	0.41
1:C:32:LEU:HD11	1:D:284[B]:LEU:HD23	2.03	0.40
1:A:181:LYS:HE2	5:A:620:HOH:O	2.21	0.40
1:B:67:PRO:HB3	1:B:313:THR:HG21	2.03	0.40
1:C:126:LEU:HD13	1:C:152:GLN:HG2	2.04	0.40
1:D:179:GLU:HG3	1:D:213:ILE:HD13	2.04	0.40

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	420/475~(88%)	412 (98%)	8 (2%)	0	100	100
1	В	416/475~(88%)	406~(98%)	9~(2%)	1 (0%)	47	30
1	С	413/475~(87%)	406~(98%)	7 (2%)	0	100	100
1	D	409/475~(86%)	402 (98%)	7(2%)	0	100	100
All	All	1658/1900 (87%)	1626~(98%)	31~(2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	50	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	346/390~(89%)	344~(99%)	2(1%)	86	80
1	В	342/390~(88%)	341~(100%)	1 (0%)	92	89
1	С	341/390~(87%)	336~(98%)	5 (2%)	65	51
1	D	337/390~(86%)	335~(99%)	2(1%)	86	80
All	All	1366/1560~(88%)	1356~(99%)	10 (1%)	84	77

All (10) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	35	SER
1	А	50	SER
1	В	290	SER
1	С	47	LEU
1	С	316	GLU
1	С	406[A]	ASP
1	С	406[B]	ASP
1	С	417	LYS
1	D	157	ASP
1	D	247	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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).

Mal	Mol Tuno Chain Ros		Ros Link		Bond lengths			Bond angles		
	туре	Chain	Chann Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	С	502	-	3,12,12	1.19	0	$3,\!17,\!17$	1.62	1 (33%)



Mol Tyr	Tune	Chain	\mathbf{Res}	Res	Rog Link	Bo	Bond lengths			Bond angles				
	туре	Chain			ries	nes	nes	nes	nes		Counts	RMSZ	# Z > 2	Counts
2	PLP	D	501	1	15, 15, 16	1.79	2 (13%)	$20,\!22,\!23$	1.74	2 (10%)				
2	PLP	А	501	1	15, 15, 16	1.69	1 (6%)	20,22,23	1.70	4 (20%)				
4	CIT	В	503	-	3,12,12	1.27	0	$3,\!17,\!17$	2.08	2 (66%)				
2	PLP	С	501	1	15,15,16	1.77	2 (13%)	$20,\!22,\!23$	1.67	4 (20%)				
2	PLP	В	501	1	15, 15, 16	1.84	2 (13%)	$20,\!22,\!23$	1.72	4 (20%)				
4	CIT	D	502	-	3,12,12	1.27	0	$3,\!17,\!17$	2.62	2 (66%)				

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
4	CIT	С	502	-	-	1/6/16/16	-
2	PLP	D	501	1	-	5/6/6/8	0/1/1/1
2	PLP	А	501	1	-	5/6/6/8	0/1/1/1
4	CIT	В	503	-	-	1/6/16/16	-
2	PLP	С	501	1	-	3/6/6/8	0/1/1/1
2	PLP	В	501	1	-	5/6/6/8	0/1/1/1
4	CIT	D	502	-	-	4/6/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	501	PLP	O3-C3	-5.70	1.23	1.37
2	D	501	PLP	O3-C3	-5.67	1.23	1.37
2	В	501	PLP	O3-C3	-5.67	1.23	1.37
2	А	501	PLP	O3-C3	-5.42	1.24	1.37
2	D	501	PLP	C2-N1	2.42	1.38	1.33
2	В	501	PLP	C2-N1	2.37	1.38	1.33
2	С	501	PLP	C2-N1	2.36	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	D	501	PLP	O4P-C5A-C5	6.24	121.25	109.35
2	В	501	PLP	O4P-C5A-C5	4.51	117.95	109.35
2	А	501	PLP	O4P-C5A-C5	4.37	117.67	109.35
2	С	501	PLP	O4P-C5A-C5	4.09	117.15	109.35



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	501	PLP	C6-C5-C4	3.93	121.25	118.16
4	D	502	CIT	C3-C2-C1	-3.80	108.90	114.98
2	В	501	PLP	C6-C5-C4	3.78	121.14	118.16
2	С	501	PLP	C6-C5-C4	3.06	120.56	118.16
4	В	503	CIT	C4-C3-C2	2.80	116.81	109.33
2	С	501	PLP	C4A-C4-C5	-2.69	118.17	120.94
4	С	502	CIT	C4-C3-C2	2.68	116.49	109.33
2	D	501	PLP	C6-C5-C4	2.61	120.22	118.16
2	С	501	PLP	C5-C6-N1	-2.54	119.58	123.82
2	А	501	PLP	O3P-P-O2P	2.53	117.30	107.64
2	В	501	PLP	O2P-P-O4P	-2.50	100.08	106.73
2	В	501	PLP	C5-C6-N1	-2.32	119.96	123.82
2	А	501	PLP	C5-C6-N1	-2.31	119.97	123.82
4	В	503	CIT	C3-C2-C1	-2.25	111.38	114.98
4	D	502	CIT	C4-C3-C2	2.18	115.15	109.33

There are no chirality outliers.

Mol	Chain	\mathbf{Res}	Type	Atoms
2	С	501	PLP	C5A-O4P-P-O1P
2	С	501	PLP	C5A-O4P-P-O2P
2	С	501	PLP	C5A-O4P-P-O3P
2	D	501	PLP	C4-C5-C5A-O4P
2	D	501	PLP	C5A-O4P-P-O1P
2	D	501	PLP	C5A-O4P-P-O2P
2	D	501	PLP	C5A-O4P-P-O3P
2	А	501	PLP	C4-C5-C5A-O4P
2	А	501	PLP	C5A-O4P-P-O1P
2	А	501	PLP	C5A-O4P-P-O2P
2	А	501	PLP	C5A-O4P-P-O3P
2	В	501	PLP	C4-C5-C5A-O4P
2	В	501	PLP	C6-C5-C5A-O4P
2	В	501	PLP	C5A-O4P-P-O2P
2	В	501	PLP	C5A-O4P-P-O3P
4	D	502	CIT	C1-C2-C3-C6
4	D	502	CIT	C1-C2-C3-C4
2	D	501	PLP	C6-C5-C5A-O4P
2	A	501	PLP	C6-C5-C5A-O4P
4	С	502	CIT	O7-C3-C4-C5
4	D	502	CIT	C1-C2-C3-O7
4	D	502	CIT	O7-C3-C4-C5

All (24) torsion outliers are listed below:



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Mol	Chain	Res	Type	Atoms
4	В	503	CIT	O7-C3-C4-C5
2	В	501	PLP	C5A-O4P-P-O1P

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	PLP	2	0
2	А	501	PLP	2	0
2	С	501	PLP	1	0
2	В	501	PLP	2	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, 95^{th} 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	А	401/475~(84%)	0.01	11 (2%) 54	58	10, 22, 47, 65	0
1	В	403/475~(84%)	-0.15	2 (0%) 91	92	14, 24, 42, 73	0
1	С	399/475~(84%)	0.34	23 (5%) 23	25	16, 33, 59, 72	0
1	D	403/475~(84%)	0.21	28 (6%) 16	19	20, 34, 56, 66	0
All	All	1606/1900 (84%)	0.10	64 (3%) 38	42	10, 28, 55, 73	0

All (64) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	50	SER	7.7
1	А	51	GLY	7.4
1	А	48	VAL	6.7
1	А	50	SER	6.3
1	А	52	VAL	5.6
1	С	52	VAL	5.5
1	А	424	ALA	4.9
1	С	51	GLY	4.9
1	В	51	GLY	4.6
1	D	51	GLY	4.6
1	А	49	GLN	4.2
1	С	358	GLY	4.2
1	D	184	GLU	4.0
1	D	216	LYS	4.0
1	D	46	THR	3.9
1	D	244	LEU	3.8
1	С	47	LEU	3.8
1	A	53	PRO	3.6
1	D	179	GLU	3.3
1	С	416	ARG	3.2
1	С	421	PRO	3.1



Mol	Chain	Res	Type	RSRZ
1	D	243	SER	3.1
1	D	245	PRO	3.0
1	D	215	ALA	3.0
1	D	214	ILE	3.0
1	D	217	HIS	2.9
1	D	212	ARG	2.8
1	С	339	LYS	2.8
1	С	126	LEU	2.8
1	D	218	PRO	2.8
1	А	45	ALA	2.8
1	D	176	LYS	2.7
1	С	357	TYR	2.6
1	С	168	SER	2.6
1	D	205	SER	2.5
1	D	219	ARG	2.5
1	D	182	LEU	2.5
1	С	407	VAL	2.4
1	D	337	GLY	2.4
1	С	49	GLN	2.3
1	D	48	VAL	2.3
1	D	361	ALA	2.3
1	D	334	ASP	2.3
1	D	20	SER	2.3
1	В	184	GLU	2.2
1	С	48	VAL	2.2
1	С	46	THR	2.2
1	D	250	ARG	2.2
1	D	246	ASP	2.2
1	А	423	ARG	2.2
1	С	355	ALA	2.2
1	A	24	SER	2.2
1	С	354	SER	2.1
1	С	409[A]	GLN	2.1
1	D	210	ILE	2.1
1	C	30	GLN	2.1
1	C	284[A]	LEU	2.1
1	C	376	TYR	2.1
1	D	220	LEU	2.1
1	A	284[A]	LEU	2.0
1	C	125	LEU	2.0
1	C	419	LEU	2.0
1	D	167	ILE	2.0



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Mol	Chain	\mathbf{Res}	Type	RSRZ
1	D	241	PHE	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 carbohydrates 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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	CIT	С	502	13/13	0.85	0.14	$27,\!43,\!49,\!53$	13
4	CIT	D	502	13/13	0.87	0.13	$26,\!48,\!58,\!58$	13
3	NA	В	502	1/1	0.88	0.18	$50,\!50,\!50,\!50$	0
4	CIT	В	503	13/13	0.89	0.12	20,28,43,44	13
3	NA	А	502	1/1	0.90	0.20	$57,\!57,\!57,\!57$	0
2	PLP	D	501	15/16	0.96	0.09	$23,\!27,\!37,\!40$	0
2	PLP	С	501	15/16	0.97	0.11	21,26,33,36	0
2	PLP	В	501	15/16	0.98	0.09	13,17,25,33	0
2	PLP	А	501	15/16	0.98	0.11	12,15,22,27	0

6.5 Other polymers (i)

There are no such residues in this entry.

