



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:50 AM UTC

PDB ID : 4A72 / pdb_00004a72
Title : Crystal structure of the omega transaminase from *Chromobacterium violaceum* in a mixture of apo and PLP-bound states
Authors : Logan, D.T.; Hakansson, M.; Yengo, K.; Svedendahl Humble, M.; Engelmark Cassimjee, K.; Walse, B.; Abedi, V.; Federsel, H.-J.; Berglund, P.
Deposited on : 2011-11-10
Resolution : 2.40 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

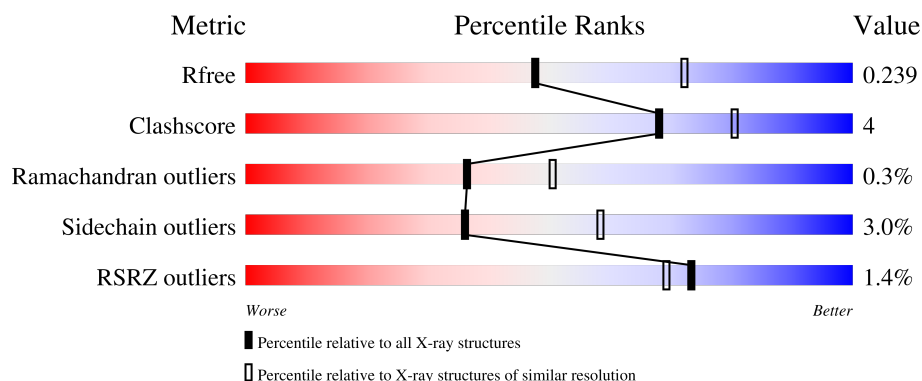
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	459	2% 85% 8% 7%
1	B	459	3% 85% 7% 7%
1	C	459	86% 11% ..
1	D	459	% 89% 9% ..

2 Entry composition [i](#)

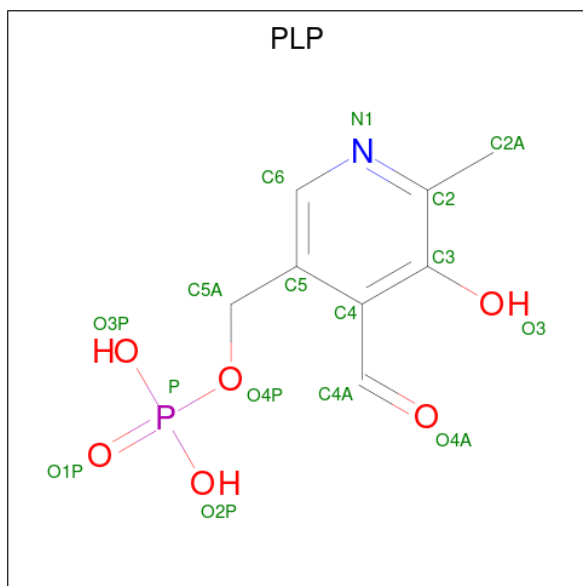
There are 3 unique types of molecules in this entry. The entry contains 14399 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OMEGA TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3370	2154	589	607	20			
1	B	426	Total	C	N	O	S	0	0	0
			3339	2134	582	602	21			
1	C	453	Total	C	N	O	S	0	0	0
			3564	2271	628	644	21			
1	D	454	Total	C	N	O	S	0	0	0
			3568	2273	629	645	21			

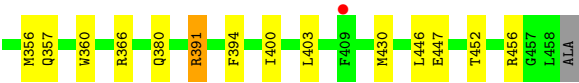
- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	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	111	Total 111	O 111	0	0
3	B	111	Total 111	O 111	0	0
3	C	188	Total 188	O 188	0	0
3	D	118	Total 118	O 118	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.35Å 62.12Å 119.24Å 105.27° 90.66° 104.43°	Depositor
Resolution (Å)	26.39 – 2.40 26.39 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (26.39-2.40) 96.3 (26.39-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.173 , 0.239 0.176 , 0.239	Depositor DCC
R_{free} test set	3141 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14399	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.75% 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	0.27	0/3457	0.65	1/4675 (0.0%)
1	B	0.28	0/3426	0.65	0/4635
1	C	0.28	0/3657	0.65	0/4949
1	D	0.31	0/3662	0.66	0/4957
All	All	0.29	0/14202	0.65	1/19216 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	LYS	CB-CA-C	-5.12	110.66	116.54

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	A	3370	0	3280	25	0
1	B	3339	0	3254	17	0
1	C	3564	0	3462	39	0
1	D	3568	0	3466	28	0
2	C	15	0	6	0	0
2	D	15	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	111	0	0	1	0
3	B	111	0	0	1	0
3	C	188	0	0	4	0
3	D	118	0	0	0	0
All	All	14399	0	13474	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 4.

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:C:172:GLN:O	1:D:129:ARG:NH1	2.07	0.88
1:C:5:ARG:NH1	1:D:98:GLU:OE2	2.17	0.78
1:C:458:LEU:C	1:C:458:LEU:HD22	2.16	0.71
1:B:89:PHE:O	1:B:322:TYR:OH	2.11	0.68
1:B:85:TYR:O	3:B:2013:HOH:O	2.10	0.68
1:B:319:GLY:O	1:B:323:SER:OG	2.09	0.65
1:C:458:LEU:C	1:C:458:LEU:CD2	2.70	0.65
1:A:85:TYR:OH	1:A:91:THR:OG1	2.16	0.61
1:A:133:ARG:NE	1:A:315:ASP:OD2	2.35	0.60
1:D:5:ARG:N	1:D:9:GLN:OE1	2.35	0.59
1:C:175:LEU:HB3	1:C:176:PRO:HA	1.85	0.59
1:C:174:ASP:N	3:C:2090:HOH:O	2.34	0.58
1:A:319:GLY:O	1:A:323:SER:OG	2.19	0.56
1:C:224:VAL:HB	1:C:257:VAL:HG22	1.85	0.56
1:D:244:GLU:OE2	1:D:247:ARG:NH1	2.38	0.56
3:C:2084:HOH:O	1:D:129:ARG:NE	2.38	0.55
1:A:56:MET:CE	1:A:424:SER:HA	2.38	0.53
1:B:35:VAL:O	1:B:47:SER:N	2.42	0.53
1:A:356:MET:HG2	1:A:380:GLN:NE2	2.24	0.53
1:B:115:PHE:CE2	1:B:319:GLY:HA3	2.44	0.52
1:D:175:LEU:HB3	1:D:176:PRO:HA	1.91	0.52
1:A:51:LYS:NZ	1:A:437:GLU:OE2	2.27	0.51
1:C:107:THR:HG23	1:C:108:PRO:HD2	1.93	0.50
1:C:284:PHE:CE1	1:C:301:PHE:CD2	3.00	0.50
1:A:132:ARG:NH1	1:A:144:LYS:O	2.45	0.49
1:A:356:MET:HB2	1:A:378:MET:HE1	1.95	0.49
1:A:132:ARG:O	1:A:144:LYS:NZ	2.46	0.48
1:B:175:LEU:HB3	1:B:176:PRO:HA	1.94	0.48
1:C:84:PHE:HA	1:C:326:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:PHE:CG	1:C:400:ILE:HG13	2.49	0.48
1:C:457:GLY:O	1:C:458:LEU:HB3	2.13	0.48
1:A:180:MET:HE3	1:A:180:MET:HA	1.95	0.48
1:A:127:MET:C	1:A:127:MET:SD	2.97	0.48
1:A:85:TYR:CE1	1:B:36:MET:HB3	2.49	0.47
1:B:143:LYS:NZ	1:B:220:VAL:O	2.46	0.47
1:C:246:GLU:O	1:C:247:ARG:CB	2.63	0.47
1:C:356:MET:HG2	1:C:380:GLN:NE2	2.30	0.47
1:C:453:LEU:O	1:C:458:LEU:HA	2.14	0.46
1:C:390:LYS:NZ	3:C:2167:HOH:O	2.43	0.46
1:C:188:TRP:CE3	1:C:192:GLY:HA3	2.50	0.46
1:A:356:MET:CB	1:A:378:MET:HE1	2.46	0.46
1:A:127:MET:HE1	1:A:224:VAL:HG21	1.98	0.45
1:B:356:MET:HG2	1:B:380:GLN:NE2	2.31	0.45
1:C:246:GLU:O	1:C:247:ARG:CG	2.64	0.45
1:D:352:ILE:HD12	1:D:430:MET:O	2.17	0.45
1:A:130:MET:HE1	1:A:300:VAL:HG11	1.98	0.45
1:C:107:THR:HG22	1:C:111:PHE:HB2	1.98	0.45
1:C:322:TYR:OH	1:D:288:LYS:HA	2.17	0.45
1:C:234:VAL:HG12	1:C:234:VAL:O	2.17	0.45
1:B:276:HIS:CE1	1:B:376:VAL:HG21	2.52	0.45
1:B:380:GLN:N	1:B:380:GLN:CD	2.75	0.45
1:D:356:MET:HG2	1:D:380:GLN:NE2	2.32	0.44
1:D:403:LEU:C	1:D:403:LEU:HD23	2.43	0.44
1:C:107:THR:CG2	1:C:111:PHE:HB2	2.47	0.44
1:D:6:THR:O	1:D:10:TRP:CD1	2.70	0.44
1:D:366:ARG:NH2	1:D:447:GLU:OE2	2.50	0.44
1:D:193:LYS:O	1:D:391:ARG:NH2	2.51	0.44
1:B:87:THR:HA	1:B:322:TYR:CE1	2.53	0.43
1:C:288:LYS:HA	1:D:322:TYR:OH	2.18	0.43
3:C:2084:HOH:O	1:D:129:ARG:NH2	2.51	0.43
1:A:283:LEU:N	1:A:283:LEU:HD23	2.33	0.43
1:D:242:TRP:N	1:D:243:PRO:CD	2.81	0.43
1:A:276:HIS:CE1	1:A:376:VAL:HG21	2.54	0.43
1:C:61:CYS:O	1:C:292:SER:HA	2.18	0.43
1:D:262:ILE:HG13	2:D:1288:PLP:O3	2.18	0.43
1:A:130:MET:CE	1:A:300:VAL:HG11	2.48	0.43
1:C:121:SER:HB3	1:C:157:THR:HG23	1.99	0.43
1:C:44:LEU:HD11	1:D:85:TYR:CE1	2.54	0.42
1:B:61:CYS:O	1:B:292:SER:HA	2.20	0.42
1:B:283:LEU:HD12	1:B:283:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:CD2	1:A:95:ALA:HB3	2.55	0.42
1:C:396:ASP:O	1:C:397:PHE:C	2.62	0.42
1:A:86:ASN:ND2	3:A:2008:HOH:O	2.47	0.42
1:C:163:LEU:HD21	1:C:224:VAL:HG11	2.01	0.42
1:D:380:GLN:CD	1:D:380:GLN:N	2.78	0.42
1:B:93:HIS:CE1	1:B:326:PRO:HB3	2.54	0.41
1:C:245:ILE:HG22	1:C:246:GLU:N	2.33	0.41
1:D:394:PHE:CG	1:D:400:ILE:HG13	2.55	0.41
1:D:452:THR:O	1:D:456:ARG:HG3	2.20	0.41
1:C:246:GLU:O	1:C:247:ARG:HG3	2.19	0.41
1:A:385:VAL:C	1:A:394:PHE:CE2	2.98	0.41
1:A:115:PHE:CE2	1:A:319:GLY:HA3	2.55	0.41
1:C:21:PRO:HB3	1:D:319:GLY:HA3	2.02	0.41
1:C:258:ALA:O	1:C:284:PHE:HA	2.21	0.41
1:B:68:ARG:HG3	1:B:70:ASP:OD1	2.20	0.41
1:C:364:PHE:CD1	1:C:446:LEU:HD12	2.55	0.41
1:A:357:GLN:NE2	1:A:357:GLN:HA	2.35	0.41
1:C:21:PRO:CB	1:D:319:GLY:HA3	2.51	0.41
1:D:143:LYS:NZ	1:D:220:VAL:O	2.53	0.41
1:D:226:GLU:O	1:D:227:PRO:C	2.63	0.41
1:B:44:LEU:HD21	1:B:66:TYR:CE2	2.55	0.41
1:C:322:TYR:CD2	1:D:296:PRO:HA	2.56	0.41
1:A:175:LEU:HB3	1:A:176:PRO:HA	2.01	0.41
1:A:163:LEU:HD13	1:A:180:MET:HE1	2.02	0.40
1:C:319:GLY:HA3	1:D:21:PRO:HB3	2.03	0.40
1:C:85:TYR:CE1	1:D:44:LEU:HD11	2.57	0.40
1:C:107:THR:CG2	1:C:108:PRO:HD2	2.51	0.40
1:C:206:ARG:NH1	1:C:244:GLU:OE2	2.54	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	423/459 (92%)	407 (96%)	16 (4%)	0	100	100
1	B	424/459 (92%)	404 (95%)	20 (5%)	0	100	100
1	C	449/459 (98%)	430 (96%)	16 (4%)	3 (1%)	18	28
1	D	452/459 (98%)	431 (95%)	18 (4%)	3 (1%)	18	28
All	All	1748/1836 (95%)	1672 (96%)	70 (4%)	6 (0%)	36	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	287	ALA
1	D	288	LYS
1	C	247	ARG
1	C	287	ALA
1	C	288	LYS
1	D	68	ARG

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	342/368 (93%)	334 (98%)	8 (2%)	44	66
1	B	340/368 (92%)	330 (97%)	10 (3%)	37	60
1	C	364/368 (99%)	348 (96%)	16 (4%)	25	43
1	D	364/368 (99%)	355 (98%)	9 (2%)	42	64
All	All	1410/1472 (96%)	1367 (97%)	43 (3%)	36	58

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	132	ARG
1	A	168	TYR
1	A	169	MET
1	A	180	MET

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Mol	Chain	Res	Type
1	A	267	ARG
1	A	283	LEU
1	A	416	ARG
1	B	76	ARG
1	B	82	LEU
1	B	143	LYS
1	B	167	LYS
1	B	172	GLN
1	B	174	ASP
1	B	283	LEU
1	B	399	GLU
1	B	446	LEU
1	B	453	LEU
1	C	23	THR
1	C	25	THR
1	C	48	GLU
1	C	68	ARG
1	C	90	LYS
1	C	146	LEU
1	C	180	MET
1	C	213	LEU
1	C	224	VAL
1	C	245	ILE
1	C	247	ARG
1	C	250	ARG
1	C	257	VAL
1	C	416	ARG
1	C	450	GLU
1	C	458	LEU
1	D	38	ARG
1	D	59	LEU
1	D	211	LYS
1	D	247	ARG
1	D	352	ILE
1	D	357	GLN
1	D	360	TRP
1	D	391	ARG
1	D	446	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	280	GLN
1	A	357	GLN
1	A	380	GLN
1	B	78	GLN
1	B	333	HIS
1	B	380	GLN
1	C	154	HIS
1	C	380	GLN
1	D	317	ASN
1	D	318	HIS
1	D	380	GLN

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	PLP	D	1288	1	15,15,16	3.01	3 (20%)	21,22,23	1.34	2 (9%)
2	PLP	C	1288	1	15,15,16	3.05	3 (20%)	21,22,23	1.36	2 (9%)

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	D	1288	1	-	0/6/6/8	0/1/1/1
2	PLP	C	1288	1	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1288	PLP	C5-C4	7.83	1.49	1.40
2	D	1288	PLP	C5-C4	7.71	1.49	1.40
2	C	1288	PLP	C3-C2	7.33	1.48	1.41
2	D	1288	PLP	C3-C2	7.25	1.48	1.41
2	C	1288	PLP	C3-C4	4.40	1.48	1.40
2	D	1288	PLP	C3-C4	4.35	1.48	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1288	PLP	C4A-C4-C5	2.86	123.88	120.94
2	C	1288	PLP	C4A-C4-C5	2.73	123.76	120.94
2	D	1288	PLP	C6-N1-C2	2.27	123.32	119.20
2	C	1288	PLP	C6-N1-C2	2.24	123.27	119.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1288	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 ⓘ

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	429/459 (93%)	-0.29	7 (1%) 70 66	14, 33, 74, 104	8 (1%)
1	B	426/459 (92%)	-0.34	13 (3%) 51 47	14, 31, 73, 124	8 (1%)
1	C	453/459 (98%)	-0.55	1 (0%) 91 89	12, 28, 55, 79	0
1	D	454/459 (98%)	-0.31	3 (0%) 84 81	14, 36, 74, 97	0
All	All	1762/1836 (95%)	-0.37	24 (1%) 73 69	12, 31, 71, 124	16 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	TYR	4.4
1	B	91	THR	3.9
1	A	168	TYR	3.4
1	B	90	LYS	3.4
1	A	15	ALA	3.1
1	B	87	THR	3.0
1	B	89	PHE	3.0
1	B	322	TYR	2.9
1	B	321	THR	2.8
1	B	88	PHE	2.6
1	A	37	THR	2.6
1	B	84	PHE	2.5
1	A	16	ALA	2.4
1	A	10	TRP	2.4
1	A	173	GLY	2.4
1	D	409	PHE	2.3
1	B	172	GLN	2.3
1	B	314	GLY	2.3
1	B	323	SER	2.3
1	A	322	TYR	2.3
1	D	351	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	86	ASN	2.1
1	D	8	SER	2.1
1	C	458	LEU	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	D	1288	15/16	0.92	0.11	29,52,68,69	0
2	PLP	C	1288	15/16	0.94	0.09	25,47,63,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.