



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:23 pm GMT

PDB ID : 5BWA  
Title : Crystal structure of ODC-PLP-AZ1 ternary complex  
Authors : Wu, D.H.  
Deposited on : 2015-06-07  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

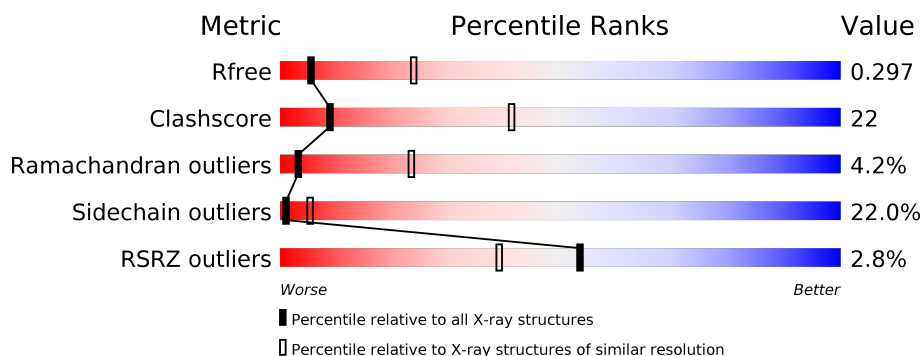
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	461	<div> <div>2%</div> <div>41%</div> <div>28%</div> <div>6%</div> <div>24%</div> </div>
2	B	160	<div> <div>4%</div> <div>28%</div> <div>35%</div> <div>11%</div> <div>24%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3751 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.

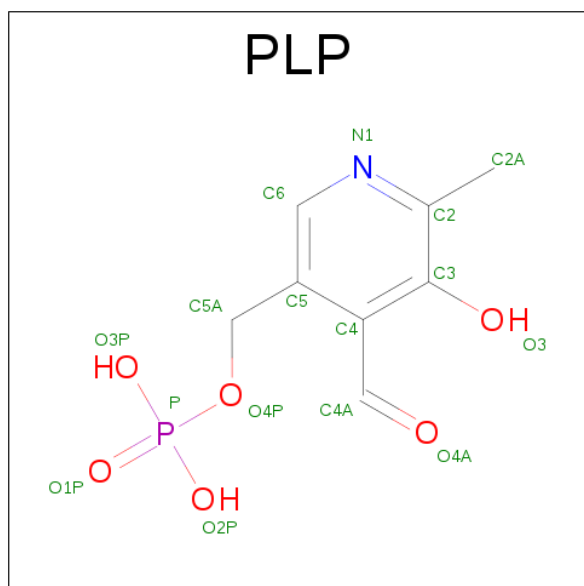
- Molecule 1 is a protein called Ornithine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	2755	1767	458	511	19	0	4	0

- Molecule 2 is a protein called Ornithine decarboxylase antizyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	121	980	625	172	180	3	0	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.15Å 74.08Å 157.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.76 – 3.20 78.54 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.4 (42.76-3.20) 93.9 (78.54-3.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.229 , 0.289 0.228 , 0.297	Depositor DCC
$R_{free}$ test set	939 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	101.7	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3751	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0.30	0/2810	0.51	1/3796 (0.0%)
2	B	0.51	0/1000	0.70	3/1348 (0.2%)
All	All	0.37	0/3810	0.57	4/5144 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	199	ARG	C-N-CD	6.05	141.11	128.40
2	B	209	PRO	CA-N-CD	-5.51	103.78	111.50
2	B	162	PHE	N-CA-C	-5.21	96.92	111.00
1	A	243	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	375	MET	Peptide
2	B	161	GLU	Peptide

## 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	2755	0	2748	105	0
2	B	980	0	958	87	0
3	A	16	0	8	1	0
All	All	3751	0	3714	168	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 22.

All (168) 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)
2:B:205:VAL:HG13	2:B:213:PHE:CE2	1.35	1.60
2:B:205:VAL:CG1	2:B:213:PHE:CE2	2.03	1.42
1:A:324:GLY:HA2	2:B:199:ARG:NH2	1.42	1.31
2:B:205:VAL:HG13	2:B:213:PHE:CD2	1.81	1.16
2:B:205:VAL:CG1	2:B:213:PHE:CD2	2.29	1.14
1:A:324:GLY:CA	2:B:199:ARG:HH21	1.61	1.11
1:A:324:GLY:CA	2:B:199:ARG:NH2	2.20	1.03
2:B:105:GLU:OE1	2:B:114:ARG:NH1	2.00	0.94
2:B:114:ARG:HH11	2:B:114:ARG:HG3	1.31	0.94
2:B:208:ARG:CG	2:B:210:ASP:OD1	2.16	0.93
1:A:166:LEU:HG	2:B:189:THR:HG22	1.51	0.93
1:A:323:TYR:HB3	2:B:199:ARG:HG2	1.51	0.92
2:B:205:VAL:HG13	2:B:213:PHE:HE2	1.15	0.90
2:B:205:VAL:HG11	2:B:213:PHE:CD2	2.02	0.89
1:A:167:SER:H	2:B:189:THR:HG21	1.36	0.89
2:B:202:HIS:ND1	2:B:203:PRO:HD2	1.89	0.87
1:A:398:ASN:O	2:B:202:HIS:CE1	2.29	0.86
2:B:208:ARG:HG3	2:B:210:ASP:OD1	1.74	0.85
2:B:208:ARG:HD3	2:B:210:ASP:OD1	1.80	0.81
1:A:323:TYR:CB	2:B:199:ARG:HG2	2.10	0.81
2:B:208:ARG:CD	2:B:210:ASP:OD1	2.33	0.77
2:B:118:VAL:HG21	2:B:159:LEU:HD13	1.66	0.75
1:A:166:LEU:CG	2:B:189:THR:HG22	2.17	0.75
1:A:292:ALA:HB3	1:A:317:TYR:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:LYS:HA	2:B:179:ASN:C	2.09	0.73
1:A:119:GLN:NE2	2:B:219:GLU:OE1	2.20	0.72
1:A:167:SER:N	2:B:189:THR:HG21	2.04	0.72
1:A:242:GLU:O	1:A:243:ASP:OD1	2.08	0.72
1:A:58:ALA:HB1	1:A:252:THR:HG21	1.72	0.71
2:B:163:ALA:HB1	2:B:167:LEU:HB2	1.72	0.70
1:A:230:TYR:O	1:A:270:ARG:N	2.26	0.68
1:A:353:SER:OG	1:A:354:SER:N	2.26	0.68
1:A:366:ILE:HG22	1:A:367:VAL:HG12	1.74	0.68
1:A:166:LEU:HG	2:B:189:THR:CG2	2.21	0.68
1:A:92:LYS:HE2	2:B:219:GLU:HB3	1.77	0.67
1:A:324:GLY:HA2	2:B:199:ARG:HH21	0.67	0.66
2:B:193:LEU:O	2:B:195:PHE:N	2.26	0.66
1:A:185:LYS:HD3	1:A:225:VAL:HG22	1.77	0.66
2:B:114:ARG:HH11	2:B:114:ARG:CG	2.08	0.65
1:A:205:PRO:HB3	1:A:254:VAL:HG21	1.77	0.65
2:B:132:THR:HG22	2:B:141:ILE:HG23	1.77	0.65
1:A:293:LYS:NZ	1:A:374:GLU:OE2	2.31	0.63
2:B:205:VAL:HG12	2:B:213:PHE:CE2	2.23	0.62
2:B:180:ARG:NH1	2:B:182:ASP:OD1	2.32	0.62
1:A:109:ILE:HG13	1:A:130:MET:HB3	1.82	0.62
1:A:355:ILE:HB	1:A:367:VAL:HG13	1.81	0.61
1:A:62:VAL:HG13	1:A:271:ILE:HG22	1.81	0.61
1:A:95:ILE:HG13	1:A:122:TYR:HE2	1.64	0.61
2:B:197:ILE:CD1	2:B:213:PHE:O	2.49	0.61
1:A:396:THR:O	1:A:398:ASN:N	2.34	0.60
1:A:112:ASN:ND2	1:A:114:CYS:O	2.35	0.60
2:B:105:GLU:HG2	2:B:115:ILE:O	2.01	0.60
1:A:398:ASN:HB3	1:A:399:GLY:HA3	1.82	0.60
1:A:95:ILE:HA	1:A:98:VAL:HG12	1.84	0.59
2:B:179:ASN:HB3	2:B:180:ARG:HA	1.84	0.59
2:B:114:ARG:HG3	2:B:114:ARG:NH1	2.10	0.59
1:A:252:THR:O	1:A:256:ASN:ND2	2.36	0.59
2:B:176:PHE:CD2	2:B:180:ARG:HD2	2.38	0.59
1:A:326:PHE:HB3	1:A:329:ILE:HD11	1.85	0.58
2:B:209:PRO:HD2	2:B:210:ASP:H	1.68	0.58
2:B:197:ILE:HD12	2:B:213:PHE:O	2.02	0.58
1:A:167:SER:H	2:B:189:THR:CG2	2.13	0.58
1:A:398:ASN:O	2:B:202:HIS:NE2	2.37	0.57
2:B:190:PHE:HA	2:B:193:LEU:HD22	1.86	0.56
2:B:205:VAL:CG1	2:B:213:PHE:CZ	2.82	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:PHE:HZ	2:B:187:LEU:HD13	1.73	0.54
1:A:75:ALA:O	1:A:79:THR:HG23	2.07	0.54
1:A:51:LYS:HG2	1:A:278:TYR:CZ	2.43	0.53
2:B:164:GLU:HB2	2:B:218:PHE:CE1	2.44	0.53
2:B:138:SER:HB3	2:B:171:HIS:HB2	1.91	0.52
2:B:202:HIS:CG	2:B:203:PRO:HD2	2.45	0.52
2:B:204:LEU:CD2	2:B:204:LEU:N	2.73	0.52
2:B:209:PRO:HD2	2:B:210:ASP:N	2.23	0.52
1:A:365:ARG:NH1	1:A:368:GLU:HB3	2.25	0.52
1:A:54:ARG:NH1	1:A:249:GLU:OE1	2.34	0.51
2:B:203:PRO:HG2	2:B:204:LEU:CD2	2.41	0.51
2:B:179:ASN:CB	2:B:180:ARG:HA	2.40	0.51
2:B:100:ARG:HH21	2:B:158:VAL:HG22	1.75	0.51
2:B:172:VAL:HG13	2:B:216:TYR:HB3	1.93	0.50
2:B:171:HIS:HB3	2:B:173:PHE:CE1	2.46	0.50
2:B:122:LEU:CD1	2:B:154:ASP:HB3	2.42	0.49
1:A:400:PHE:O	2:B:199:ARG:NH1	2.45	0.49
1:A:222:GLY:HA2	1:A:225:VAL:HG12	1.94	0.49
2:B:185:ALA:O	2:B:189:THR:HG23	2.12	0.49
1:A:401:GLN:O	1:A:402:ARG:NH1	2.46	0.48
1:A:83:THR:OG1	1:A:84:GLY:N	2.44	0.48
1:A:329:ILE:HA	1:A:334:ALA:H	1.78	0.48
2:B:177:HIS:O	2:B:180:ARG:HG3	2.12	0.48
2:B:209:PRO:CD	2:B:210:ASP:N	2.76	0.48
1:A:251:ILE:O	1:A:255:ILE:HG13	2.13	0.48
1:A:250[B]:GLU:HG3	1:A:251:ILE:HD12	1.96	0.48
1:A:75:ALA:HA	1:A:78:LYS:HG2	1.95	0.48
1:A:92:LYS:HG3	1:A:122:TYR:CD2	2.48	0.48
1:A:323:TYR:HB2	2:B:199:ARG:HG2	1.93	0.48
2:B:190:PHE:O	2:B:195:PHE:HB2	2.13	0.48
1:A:122:TYR:O	1:A:126:ASN:ND2	2.34	0.47
1:A:285:THR:HG23	1:A:384:GLU:HA	1.96	0.47
1:A:322[B]:VAL:HG22	1:A:329:ILE:HG13	1.97	0.47
1:A:324:GLY:HA3	2:B:199:ARG:NH2	2.23	0.47
1:A:375:MET:HB3	1:A:376:HIS:O	2.14	0.47
1:A:95:ILE:HG12	1:A:95:ILE:H	1.52	0.47
1:A:248:PHE:O	1:A:251:ILE:N	2.46	0.47
1:A:79:THR:O	1:A:83:THR:HG23	2.14	0.47
2:B:204:LEU:HD22	2:B:204:LEU:N	2.30	0.47
1:A:69:LYS:HB3	1:A:69:LYS:HE3	1.63	0.46
1:A:355:ILE:HG12	1:A:381:MET:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:H	1:A:21:LYS:HG2	1.41	0.46
2:B:187:LEU:HD12	2:B:214:MET:SD	2.55	0.46
1:A:39:ALA:H	1:A:319:ASN:ND2	2.13	0.46
1:A:65:PHE:HB2	1:A:273:ALA:O	2.15	0.46
2:B:133:VAL:HG13	2:B:140:TYR:HB2	1.98	0.46
1:A:42:VAL:HG12	1:A:406:TYR:HB2	1.98	0.45
1:A:25:ASP:HA	1:A:28:ILE:HG12	1.97	0.45
1:A:55:TRP:O	1:A:59:LEU:N	2.31	0.45
1:A:92:LYS:HB2	2:B:219:GLU:OE1	2.17	0.45
1:A:140:MET:O	1:A:144:ARG:HG2	2.16	0.45
1:A:20:ALA:C	1:A:22:ASP:H	2.19	0.45
1:A:288:VAL:HG21	1:A:383:PHE:HE2	1.82	0.45
2:B:204:LEU:C	2:B:205:VAL:CG2	2.85	0.45
1:A:25:ASP:OD1	1:A:25:ASP:N	2.49	0.45
1:A:116:GLN:O	1:A:120:ILE:HG12	2.16	0.45
1:A:155:ILE:HG21	1:A:218:VAL:HG21	1.98	0.45
1:A:173:THR:HG1	1:A:176:THR:HG1	1.63	0.44
2:B:153:LYS:H	2:B:153:LYS:HG3	1.44	0.44
2:B:209:PRO:CD	2:B:210:ASP:H	2.31	0.44
1:A:66:TYR:OH	1:A:71:ASN:HB3	2.18	0.44
2:B:210:ASP:N	2:B:210:ASP:OD1	2.49	0.44
1:A:52:HIS:HB2	1:A:279:TYR:HE1	1.83	0.43
1:A:261:LYS:HE3	1:A:261:LYS:HB2	1.75	0.43
2:B:144:PRO:O	2:B:180:ARG:NH2	2.49	0.43
2:B:112:LYS:HG3	2:B:113:THR:HA	2.00	0.43
1:A:151:LEU:HD22	1:A:189:ILE:HG21	2.00	0.43
1:A:329:ILE:H	1:A:329:ILE:HG12	1.40	0.43
1:A:376:HIS:CG	1:A:377:VAL:H	2.36	0.43
1:A:66:TYR:HB3	1:A:87:PHE:CD1	2.54	0.42
1:A:19:THR:HB	1:A:20:ALA:H	1.63	0.42
1:A:323:TYR:HB3	2:B:199:ARG:CG	2.35	0.42
1:A:50:LYS:HE3	1:A:50:LYS:HB2	1.69	0.42
1:A:181:LEU:HD22	1:A:222:GLY:HA2	2.00	0.42
1:A:85:THR:O	1:A:107:ARG:NH2	2.53	0.42
2:B:176:PHE:HD2	2:B:180:ARG:HD2	1.82	0.42
2:B:182:ASP:OD1	2:B:182:ASP:N	2.51	0.42
1:A:55:TRP:HE1	1:A:64:PRO:HD3	1.85	0.42
1:A:158:ASP:OD1	1:A:158:ASP:N	2.53	0.42
1:A:255:ILE:HG23	1:A:259:LEU:HD23	2.02	0.42
1:A:322[A]:VAL:HG22	1:A:364:ASP:HA	2.02	0.42
1:A:259:LEU:HA	1:A:259:LEU:HD13	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:HA	1:A:233:ASP:O	2.20	0.41
1:A:88:ASP:OD1	1:A:111:ALA:HB3	2.20	0.41
2:B:143:ILE:HA	2:B:144:PRO:HD2	1.79	0.41
1:A:167:SER:OG	2:B:189:THR:HG21	2.20	0.41
1:A:117:VAL:HG11	1:A:144:ARG:NH2	2.34	0.41
1:A:249:GLU:CD	1:A:249:GLU:H	2.24	0.41
1:A:183:ARG:HG3	1:A:187:LEU:HD22	2.02	0.41
2:B:197:ILE:HD12	2:B:198:VAL:H	1.85	0.41
2:B:122:LEU:HD11	2:B:154:ASP:HB3	2.02	0.41
1:A:123:ALA:O	1:A:128:VAL:HG13	2.21	0.41
2:B:98:ASP:OD1	2:B:101:LEU:HB2	2.21	0.41
1:A:259:LEU:HD12	1:A:271:ILE:HD13	2.03	0.41
1:A:331:TYR:HD1	2:B:187:LEU:HB3	1.85	0.41
2:B:205:VAL:HG12	2:B:213:PHE:CZ	2.54	0.41
1:A:328:CYS:O	1:A:332:ASP:N	2.52	0.40
1:A:52:HIS:O	1:A:55:TRP:HB3	2.21	0.40
1:A:112:ASN:HB3	1:A:115:LYS:HG2	2.02	0.40
1:A:274:GLU:O	3:A:600:PLP:H6	2.22	0.40
1:A:331:TYR:CD1	2:B:187:LEU:HB3	2.57	0.40
1:A:365:ARG:HD2	1:A:368:GLU:HA	2.04	0.40
2:B:96:TYR:HB3	2:B:103:VAL:CG1	2.51	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	338/461 (73%)	285 (84%)	41 (12%)	12 (4%)	4	27
2	B	115/160 (72%)	97 (84%)	11 (10%)	7 (6%)	2	13
All	All	453/621 (73%)	382 (84%)	52 (12%)	19 (4%)	3	23

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	SER
1	A	397	PHE
2	B	161	GLU
1	A	278	TYR
1	A	401	GLN
2	B	124	ASP
2	B	180	ARG
2	B	194	GLY
2	B	209	PRO
1	A	21	LYS
1	A	84	GLY
1	A	248	PHE
1	A	276	GLY
1	A	264	PRO
1	A	402	ARG
2	B	144	PRO
2	B	151	GLY
1	A	168	VAL
1	A	298	LYS

### 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	299/391 (76%)	242 (81%)	57 (19%)	2	9
2	B	105/138 (76%)	74 (70%)	31 (30%)	0	1
All	All	404/529 (76%)	316 (78%)	88 (22%)	1	6

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

Mol	Chain	Res	Type
1	A	19	THR
1	A	21	LYS
1	A	22	ASP
1	A	25	ASP

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Mol	Chain	Res	Type
1	A	27	LYS
1	A	29	ASN
1	A	50	LYS
1	A	53	LEU
1	A	56	LEU
1	A	68	VAL
1	A	69	LYS
1	A	78	LYS
1	A	92	LYS
1	A	93	THR
1	A	95	ILE
1	A	97	LEU
1	A	101	LEU
1	A	109	ILE
1	A	128	VAL
1	A	137	VAL
1	A	144	ARG
1	A	146	HIS
1	A	148	LYS
1	A	151	LEU
1	A	152	VAL
1	A	165	ARG
1	A	169	LYS
1	A	176	THR
1	A	178	ARG
1	A	187	LEU
1	A	194	VAL
1	A	198	VAL
1	A	209	VAL
1	A	213	SER
1	A	219	PHE
1	A	221	MET
1	A	252	THR
1	A	265	SER
1	A	270	ARG
1	A	285	THR
1	A	297	LEU
1	A	300	GLN
1	A	310	SER
1	A	312	GLN
1	A	329	ILE
1	A	330	LEU

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Mol	Chain	Res	Type
1	A	332	ASP
1	A	335	HIS
1	A	337	LYS
1	A	359	THR
1	A	363	LEU
1	A	367	VAL
1	A	372	LEU
1	A	391	VAL
1	A	397	PHE
1	A	400	PHE
1	A	401	GLN
2	B	94	LEU
2	B	99	ASP
2	B	100	ARG
2	B	105	GLU
2	B	114	ARG
2	B	115	ILE
2	B	116	LEU
2	B	122	LEU
2	B	123	THR
2	B	133	VAL
2	B	134	LEU
2	B	135	SER
2	B	139	LEU
2	B	152	SER
2	B	153	LYS
2	B	154	ASP
2	B	165	GLU
2	B	166	GLN
2	B	175	CYS
2	B	178	LYS
2	B	179	ASN
2	B	180	ARG
2	B	181	GLU
2	B	186	LEU
2	B	187	LEU
2	B	188	ARG
2	B	191	SER
2	B	193	LEU
2	B	197	ILE
2	B	204	LEU
2	B	210	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	256	ASN
1	A	401	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
3	PLP	A	600	-	16,16,16	1.16	1 (6%)	22,23,23	0.96	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
3	PLP	A	600	-	-	0/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	PLP	C2-N1	2.12	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	PLP	C5-C6-N1	-2.06	120.38	123.87
3	A	600	PLP	C3-C4-C4A	-2.04	116.92	119.91

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
3	A	600	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	350/461 (75%)	0.34	7 (2%) 65 50	25, 61, 102, 155	0
2	B	121/160 (75%)	0.48	6 (4%) 30 17	29, 63, 103, 164	0
All	All	471/621 (75%)	0.37	13 (2%) 53 39	25, 61, 103, 164	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	GLN	3.5
2	B	199	ARG	2.9
1	A	322[A]	VAL	2.9
2	B	212	CYS	2.6
2	B	106	GLU	2.5
1	A	146	HIS	2.3
2	B	132	THR	2.3
2	B	137	GLY	2.2
2	B	211	ALA	2.2
1	A	242	GLU	2.2
1	A	247	LYS	2.0
1	A	196	PHE	2.0
1	A	355	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PLP	A	600	16/16	0.95	0.20	-0.75	44,48,51,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.