



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:01 PM GMT

PDB ID : 1MLZ
Title : Crystal Structure of 7,8-DiaminopelargonicAcid Synthase in complex with the trans-isomer of amiclennomycin.
Authors : Sandmark, J.; Mann, S.; Marquet, A.; Schneider, G.
Deposited on : 2002-09-02
Resolution : 2.15 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

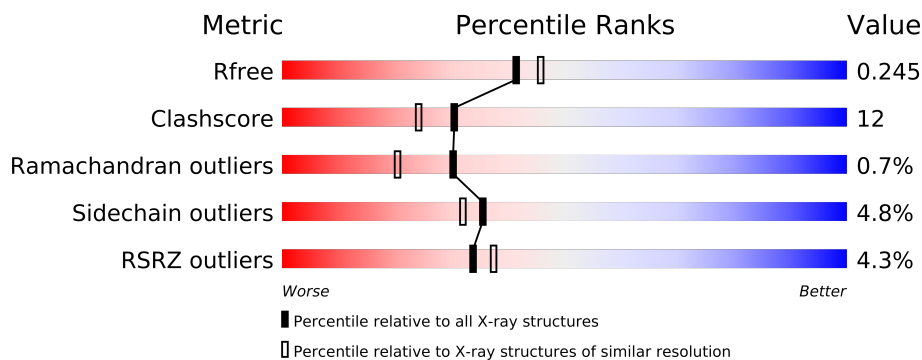
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.15 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}	66092	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	429	
1	B	429	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	TZA	A	431	-	X
3	NA	B	502	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7013 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

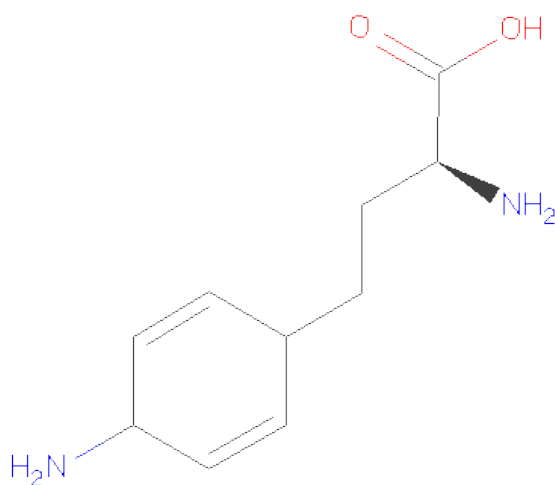
- Molecule 1 is a protein called 7,8-diamino-pelargonicacid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	102	1	0
			3299	2093	576	598	32			
1	B	428	Total	C	N	O	S	96	5	0
			3330	2121	578	599	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	LEU	TRP	SEE REMARK 999	UNP P12995
B	14	LEU	TRP	SEE REMARK 999	UNP P12995

- Molecule 2 is TRANS-AMICLENOMYCIN (three-letter code: TZA) (formula: C₁₀H₁₆N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	10	2	2		

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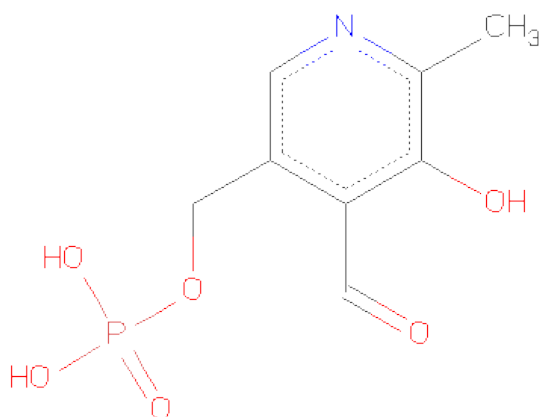
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	10	2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 5 is water.

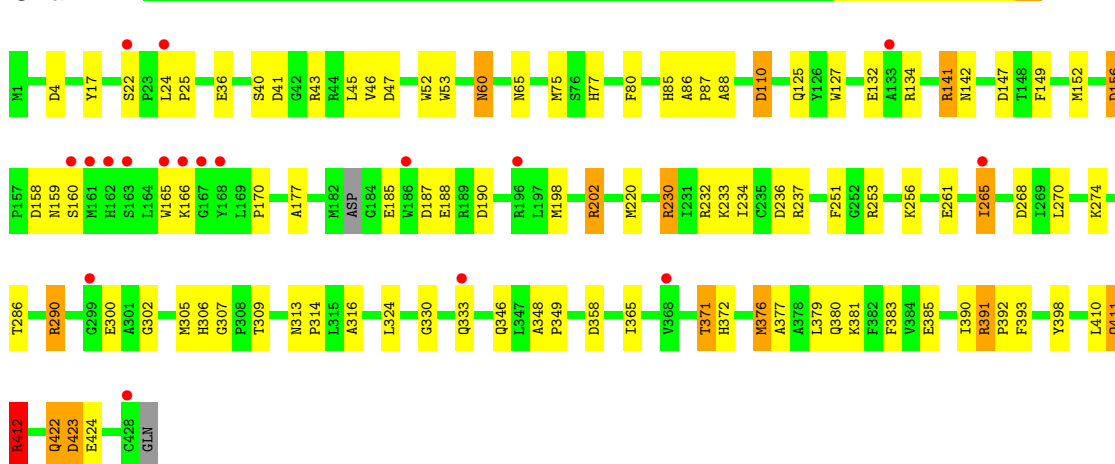
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	165	Total	O	0	0
			165	165		
5	B	159	Total	O	0	0
			159	159		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

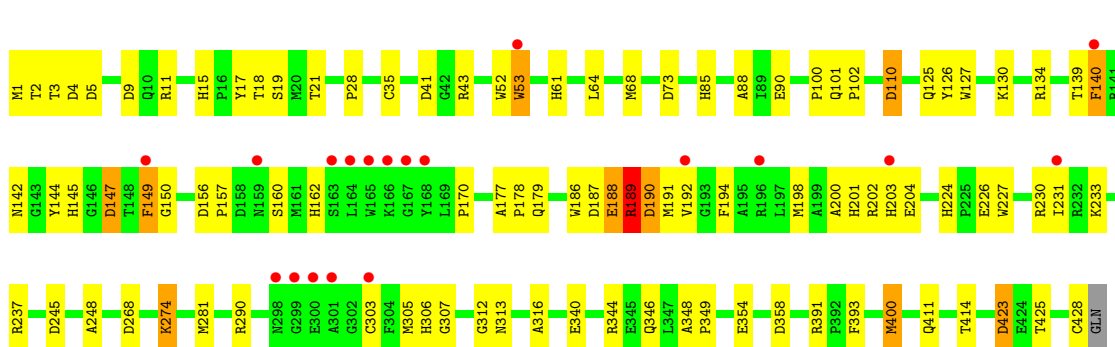
- Molecule 1: 7,8-diamino-pelargonicacid aminotransferase

Chain A:



- Molecule 1: 7,8-diamino-pelargonicacid aminotransferase

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.03Å 55.96Å 116.00Å 90.00° 109.65° 90.00°	Depositor
Resolution (Å)	22.36 – 2.15 19.92 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.5 (22.36-2.15) 98.5 (19.92-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.205 , 0.240 0.211 , 0.245	Depositor DCC
R_{free} test set	2107 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 41727 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7013	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.29 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.2364e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TZA, NA, 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	0.75	6/3380 (0.2%)	1.08	20/4586 (0.4%)
1	B	0.99	13/3432 (0.4%)	0.98	21/4658 (0.5%)
All	All	0.88	19/6812 (0.3%)	1.03	41/9244 (0.4%)

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	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53[A]	TRP	CG-CD1	25.09	1.71	1.36
1	B	53[B]	TRP	CG-CD1	25.09	1.71	1.36
1	A	385	GLU	CG-CD	13.91	1.72	1.51
1	B	90	GLU	CG-CD	10.75	1.68	1.51
1	A	423	ASP	C-N	7.25	1.50	1.34
1	B	189	ARG	CG-CD	-6.80	1.34	1.51
1	B	53[A]	TRP	CA-CB	-6.54	1.39	1.53
1	B	53[B]	TRP	CA-CB	-6.54	1.39	1.53
1	A	300	GLU	CG-CD	6.32	1.61	1.51
1	B	53[A]	TRP	CE3-CZ3	6.15	1.49	1.38
1	B	53[B]	TRP	CE3-CZ3	6.15	1.49	1.38
1	A	22	SER	C-N	-5.78	1.23	1.34
1	B	53[A]	TRP	CG-CD2	5.75	1.53	1.43
1	B	53[B]	TRP	CG-CD2	5.75	1.53	1.43
1	B	428	CYS	CA-CB	-5.63	1.41	1.53
1	B	53[A]	TRP	CD2-CE3	5.61	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53[B]	TRP	CD2-CE3	5.61	1.48	1.40
1	A	412	ARG	CB-CG	-5.19	1.38	1.52
1	A	141	ARG	CG-CD	-5.03	1.39	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ASP	O-C-N	-28.26	77.49	122.70
1	A	422	GLN	O-C-N	21.57	157.22	122.70
1	B	53[A]	TRP	CD1-CG-CD2	17.27	120.11	106.30
1	B	53[B]	TRP	CD1-CG-CD2	17.27	120.11	106.30
1	A	422	GLN	CA-C-N	-15.50	83.11	117.20
1	A	110	ASP	CB-CG-OD1	10.31	127.58	118.30
1	A	190	ASP	CB-CG-OD2	7.72	125.24	118.30
1	B	110	ASP	CB-CG-OD1	7.48	125.03	118.30
1	B	423	ASP	CB-CG-OD1	7.46	125.01	118.30
1	A	190	ASP	CB-CG-OD1	-7.25	111.78	118.30
1	B	53[A]	TRP	CB-CG-CD2	-7.17	117.28	126.60
1	B	53[B]	TRP	CB-CG-CD2	-7.17	117.28	126.60
1	B	53[A]	TRP	CE3-CZ3-CH2	-7.14	113.35	121.20
1	B	53[B]	TRP	CE3-CZ3-CH2	-7.14	113.35	121.20
1	A	268	ASP	CB-CG-OD2	7.04	124.64	118.30
1	B	140[A]	PHE	CB-CA-C	-6.86	96.68	110.40
1	B	140[B]	PHE	CB-CA-C	-6.86	96.68	110.40
1	A	358	ASP	CB-CG-OD2	6.85	124.47	118.30
1	B	4	ASP	CB-CG-OD2	6.76	124.38	118.30
1	B	358	ASP	CB-CG-OD2	6.60	124.24	118.30
1	B	268	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	423	ASP	C-N-CA	6.48	137.89	121.70
1	A	190	ASP	CA-CB-CG	6.33	127.32	113.40
1	B	147	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	156	ASP	CB-CG-OD1	5.89	123.61	118.30
1	A	158	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	53[A]	TRP	CG-CD2-CE3	-5.75	128.72	133.90
1	B	53[B]	TRP	CG-CD2-CE3	-5.75	128.72	133.90
1	B	73	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	412	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	187	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	4	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	156	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	233	LYS	CB-CG-CD	5.37	125.55	111.60
1	A	141	ARG	CB-CG-CD	5.28	125.32	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	423	ASP	CA-C-N	5.26	128.77	117.20
1	B	9	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	236	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	290	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	47	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	422	GLN	Peptide
1	A	423	ASP	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3299	0	3263	63	2
1	B	3330	0	3278	93	1
2	A	14	0	11	2	0
2	B	14	0	13	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	0	6	1	0
4	B	15	0	6	8	0
5	A	165	0	0	1	2
5	B	159	0	0	4	1
All	All	7013	0	6577	153	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (153) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:188:GLU:OE2	1:A:230:ARG:NH2	1.81	1.13
1:B:53[A]:TRP:CE2	1:B:400:MET:HE1	1.84	1.13
1:B:53[A]:TRP:CD2	1:B:400:MET:CE	2.41	1.04
1:B:274:LYS:HZ3	4:B:530:PLP:C4A	1.76	0.98
1:B:423:ASP:OD1	1:B:425:THR:OG1	1.85	0.94
1:B:53[A]:TRP:CD2	1:B:400:MET:HE2	2.04	0.93
1:B:53[A]:TRP:CE2	1:B:400:MET:CE	2.50	0.93
1:B:274:LYS:NZ	4:B:530:PLP:C4A	2.32	0.92
1:A:17:TYR:HE1	1:B:305:MET:HE3	1.39	0.88
1:B:224:HIS:CE1	1:B:226:GLU:HB2	2.09	0.87
2:B:531:TZA:NH	4:B:530:PLP:C4A	2.39	0.86
1:A:188:GLU:CD	1:A:230:ARG:HH22	1.83	0.82
1:B:17:TYR:OH	1:B:147:ASP:OD1	1.97	0.81
1:A:41:ASP:OD2	1:A:43:ARG:NH1	2.13	0.79
1:A:188:GLU:CD	1:A:230:ARG:NH2	2.36	0.78
1:A:17:TYR:CE1	1:B:305:MET:HE3	2.18	0.78
1:A:125:GLN:HE22	1:A:305:MET:H	1.30	0.78
1:A:41:ASP:OD1	1:A:43:ARG:HD3	1.84	0.77
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.52	0.74
1:B:140[B]:PHE:CZ	1:B:231:ILE:HD11	2.23	0.73
1:A:41:ASP:OD2	1:A:43:ARG:CD	2.39	0.71
1:B:189:ARG:O	1:B:192:VAL:HG13	1.93	0.69
1:A:53:TRP:CD1	1:A:53:TRP:N	2.61	0.69
1:B:53[A]:TRP:CZ2	1:B:400:MET:HE1	2.30	0.66
1:B:191:MET:O	1:B:191:MET:HG3	1.96	0.65
1:A:41:ASP:OD2	1:A:43:ARG:HD3	1.96	0.65
4:B:530:PLP:O3P	5:B:4128:HOH:O	2.13	0.64
1:B:140[B]:PHE:HE2	1:B:194:PHE:CE2	2.16	0.63
1:B:226:GLU:OE2	1:B:230:ARG:NH1	2.32	0.63
1:B:179:GLN:HB2	1:B:190:ASP:OD2	1.99	0.62
1:A:41:ASP:CG	1:A:43:ARG:HD3	2.20	0.62
1:B:85:HIS:CE1	1:B:88:ALA:HB2	2.35	0.62
1:A:147:ASP:HB3	1:B:306:HIS:CE1	2.34	0.61
1:B:140[B]:PHE:CE2	1:B:194:PHE:CD2	2.88	0.61
1:B:140[B]:PHE:CE2	1:B:194:PHE:CE2	2.89	0.61
1:B:144:TYR:HE2	2:B:531:TZA:HNH2	1.49	0.60
1:B:1:MET:SD	1:B:28:PRO:HB3	2.44	0.58
1:B:391[B]:ARG:CG	1:B:391[B]:ARG:HH11	2.17	0.57
1:B:157:PRO:HA	1:B:162:HIS:CG	2.40	0.57
1:B:125:GLN:HE22	1:B:305:MET:H	1.51	0.57
1:A:391:ARG:CG	1:A:391:ARG:HH11	2.17	0.56
1:B:274:LYS:HZ1	4:B:530:PLP:C4A	2.16	0.56
1:B:186:TRP:HE1	1:B:188:GLU:HG2	1.71	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:101:GLN:N	1:B:102:PRO:HD2	2.22	0.55
1:B:391[B]:ARG:HG3	1:B:391[B]:ARG:HH11	1.72	0.55
2:B:531:TZA:HNH1	4:B:530:PLP:C4A	2.19	0.55
1:A:41:ASP:OD2	1:A:43:ARG:HD2	2.07	0.55
1:B:53[A]:TRP:CZ3	1:B:248:ALA:HB1	2.42	0.54
1:A:330:GLY:HA2	1:A:333:GLN:OE1	2.08	0.54
1:A:330:GLY:O	1:A:333:GLN:OE1	2.25	0.54
1:B:274:LYS:HZ3	4:B:530:PLP:C4	2.19	0.54
1:B:52:TRP:C	1:B:53[B]:TRP:CG	2.81	0.54
1:A:330:GLY:CA	1:A:333:GLN:OE1	2.55	0.53
1:B:178:PRO:HB3	1:B:227:TRP:NE1	2.24	0.53
1:A:220:MET:HE2	1:A:398:TYR:CD2	2.44	0.53
1:A:141:ARG:O	1:A:142:ASN:HB2	2.09	0.53
1:B:340:GLU:O	1:B:344:ARG:HG3	2.09	0.53
1:B:53[B]:TRP:CH2	2:B:531:TZA:HE22	2.44	0.52
1:B:1:MET:SD	1:B:28:PRO:CB	2.98	0.52
1:B:140[B]:PHE:HE2	1:B:194:PHE:HE2	1.55	0.52
1:A:24:LEU:HB3	1:A:25:PRO:HD2	1.92	0.52
1:B:100:PRO:C	1:B:102:PRO:HD2	2.31	0.51
1:A:149:PHE:HD2	1:B:150:GLY:HA3	1.76	0.51
1:B:201:HIS:ND1	1:B:204:GLU:OE2	2.44	0.51
1:A:152:MET:HE3	1:A:165:TRP:NE1	2.26	0.50
1:A:306:HIS:CE1	1:B:147:ASP:HB2	2.47	0.50
1:B:140[B]:PHE:HZ	1:B:231:ILE:HD11	1.71	0.50
1:B:53[A]:TRP:CD2	1:B:400:MET:SD	3.05	0.50
1:B:53[A]:TRP:CE3	1:B:400:MET:HE2	2.47	0.50
1:B:224:HIS:ND1	1:B:226:GLU:HB2	2.26	0.50
1:B:41:ASP:OD2	1:B:43:ARG:NH2	2.45	0.49
1:B:224:HIS:ND1	1:B:226:GLU:CB	2.75	0.49
1:B:144:TYR:CE2	2:B:531:TZA:HE11	2.47	0.49
1:A:309:THR:OG1	1:B:274:LYS:NZ	2.41	0.49
1:A:77:HIS:HA	1:A:314:PRO:HD2	1.94	0.49
1:A:376:MET:O	1:A:380:GLN:HB2	2.12	0.49
1:A:85:HIS:HE1	5:A:1006:HOH:O	1.96	0.48
1:A:251:PHE:CE1	1:A:324:LEU:HD21	2.48	0.48
1:B:41:ASP:OD2	1:B:43:ARG:NE	2.47	0.47
1:A:313:ASN:ND2	1:A:316:ALA:H	2.11	0.47
1:B:348:ALA:N	1:B:349:PRO:CD	2.78	0.47
1:B:15:HIS:HB2	1:B:18:THR:HG21	1.96	0.47
1:A:379:LEU:HD23	1:A:392:PRO:HG2	1.96	0.47
1:B:140[B]:PHE:CZ	1:B:194:PHE:CD2	3.03	0.47
1:A:127:TRP:CD2	1:A:134:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:3:THR:HG23	5:B:3019:HOH:O	2.15	0.47
1:B:126:TYR:O	1:B:130:LYS:HG3	2.14	0.47
1:A:348:ALA:N	1:A:349:PRO:CD	2.78	0.47
1:A:232:ARG:HG2	1:A:265:ILE:HG13	1.96	0.47
2:B:531:TZA:NH	4:B:530:PLP:C4	2.79	0.46
1:A:379:LEU:HG	1:A:383:PHE:CE2	2.49	0.46
1:B:53[A]:TRP:CG	1:B:400:MET:SD	3.09	0.46
1:B:346:GLN:HE22	1:B:411:GLN:HA	1.80	0.46
1:B:224:HIS:HE1	1:B:226:GLU:HB2	1.74	0.45
1:A:371:THR:HB	1:A:372:HIS:ND1	2.32	0.45
1:B:145:HIS:HE1	5:B:2017:HOH:O	1.99	0.45
1:B:149[A]:PHE:CZ	1:B:170:PRO:HD3	2.51	0.45
1:B:224:HIS:CE1	1:B:226:GLU:CB	2.93	0.45
1:B:179:GLN:HG2	5:B:4050:HOH:O	2.17	0.45
1:B:142:ASN:HD22	1:B:177:ALA:HB2	1.81	0.45
2:A:431:TZA:NH	4:A:430:PLP:O3	2.50	0.45
1:A:346:GLN:NE2	1:A:411:GLN:HG3	2.32	0.45
1:B:68:MET:SD	1:B:281:MET:CE	3.05	0.44
1:A:152:MET:CE	1:A:165:TRP:NE1	2.80	0.44
1:A:85:HIS:HD2	1:A:88:ALA:H	1.66	0.44
1:B:101:GLN:N	1:B:102:PRO:CD	2.81	0.44
1:B:393:PHE:CG	2:B:531:TZA:HCA	2.53	0.43
1:A:198:MET:O	1:A:202:ARG:HB3	2.18	0.43
1:B:190:ASP:OD1	1:B:227:TRP:HZ2	2.02	0.43
1:B:178:PRO:HB3	1:B:227:TRP:CD1	2.53	0.43
1:B:157:PRO:HA	1:B:162:HIS:ND1	2.32	0.43
1:A:302:GLY:O	1:B:19:SER:HB2	2.19	0.43
1:B:313:ASN:ND2	1:B:316:ALA:H	2.16	0.43
1:A:46:VAL:HG23	1:A:412:ARG:NH1	2.34	0.43
1:A:24:LEU:HD13	1:A:377:ALA:HB2	2.01	0.42
1:A:52:TRP:C	1:A:53:TRP:CG	2.93	0.42
1:B:400:MET:HB3	1:B:400:MET:HE3	1.84	0.42
1:A:188:GLU:OE1	1:A:230:ARG:NH2	2.46	0.42
1:A:391:ARG:HD3	2:A:431:TZA:O2	2.19	0.42
1:B:139:THR:C	1:B:140[B]:PHE:HD2	2.23	0.42
1:A:393:PHE:HE1	1:A:398:TYR:CE1	2.38	0.42
1:A:234:ILE:HG12	1:A:237:ARG:NH2	2.35	0.42
1:B:2:THR:O	1:B:5:ASP:HB2	2.18	0.42
1:A:156:ASP:HB3	1:A:159:ASN:HB2	2.01	0.42
1:B:61:HIS:HB3	1:B:64:LEU:HG	2.01	0.41
1:A:253:ARG:HG3	1:A:365:ILE:HD11	2.02	0.41
1:A:270:LEU:O	1:A:286:THR:HA	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:53[A]:TRP:CE2	1:B:400:MET:SD	3.13	0.41
1:B:145:HIS:HD2	1:B:245:ASP:OD2	2.03	0.41
1:A:390:ILE:HG22	1:A:392:PRO:HD3	2.02	0.41
1:B:186:TRP:CE3	1:B:226:GLU:HB3	2.55	0.41
1:A:60:ASN:OD1	1:A:65:ASN:ND2	2.46	0.41
1:A:86:ALA:HB3	1:A:87:PRO:HD3	2.03	0.41
1:B:190:ASP:OD1	1:B:227:TRP:CZ2	2.73	0.41
1:A:142:ASN:HD22	1:A:177:ALA:HB2	1.85	0.41
1:B:346:GLN:NE2	1:B:414:THR:OG1	2.53	0.41
1:B:127:TRP:CD2	1:B:134:ARG:HD2	2.56	0.41
1:A:36:GLU:HA	1:A:45:LEU:O	2.21	0.41
1:B:15:HIS:HB2	1:B:18:THR:CG2	2.51	0.40
1:B:312:GLY:O	1:B:313:ASN:C	2.59	0.40
1:A:234:ILE:HG12	1:A:237:ARG:HH21	1.86	0.40
1:A:17:TYR:CE1	1:B:305:MET:CE	2.99	0.40
1:A:220:MET:HE1	1:A:365:ILE:HG23	2.04	0.40
1:A:348:ALA:HB3	1:A:349:PRO:HD3	2.04	0.40
1:B:198:MET:O	1:B:202:ARG:N	2.55	0.40
1:B:200:ALA:HB3	1:B:201:HIS:HD2	1.85	0.40
1:A:256:LYS:HD3	1:A:261:GLU:HB3	2.03	0.40
1:A:17:TYR:OH	1:A:147:ASP:OD1	2.39	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:381:LYS:NZ	5:A:3018:HOH:O[2_656]	0.62	1.58
1:B:21:THR:O	1:B:21:THR:O[2_655]	1.48	0.72
5:B:4038:HOH:O	5:B:4038:HOH:O[2_655]	1.83	0.37
1:A:381:LYS:CE	5:A:3018:HOH:O[2_656]	2.08	0.12

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	424/429 (99%)	406 (96%)	14 (3%)	4 (1%)	25	15
1	B	431/429 (100%)	412 (96%)	17 (4%)	2 (0%)	38	31
All	All	855/858 (100%)	818 (96%)	31 (4%)	6 (1%)	30	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	GLU
1	A	274	LYS
1	B	274	LYS
1	A	75	MET
1	A	307	GLY
1	B	307	GLY

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	344/345 (100%)	324 (94%)	20 (6%)	28	23
1	B	348/345 (101%)	334 (96%)	14 (4%)	42	41
All	All	692/690 (100%)	658 (95%)	34 (5%)	35	31

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	60	ASN
1	A	80	PHE
1	A	110	ASP
1	A	132	GLU
1	A	160	SER
1	A	166	LYS
1	A	170	PRO
1	A	185	GLU
1	A	202	ARG
1	A	230	ARG

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Mol	Chain	Res	Type
1	A	233	LYS
1	A	265	ILE
1	A	290	ARG
1	A	371	THR
1	A	376	MET
1	A	391	ARG
1	A	410	LEU
1	A	411	GLN
1	A	412	ARG
1	B	11	ARG
1	B	35	CYS
1	B	110	ASP
1	B	149[A]	PHE
1	B	149[B]	PHE
1	B	160	SER
1	B	188	GLU
1	B	189	ARG
1	B	190	ASP
1	B	237	ARG
1	B	290	ARG
1	B	303	CYS
1	B	354	GLU
1	B	400	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	125	GLN
1	A	135	GLN
1	A	142	ASN
1	A	313	ASN
1	A	335	GLN
1	B	125	GLN
1	B	142	ASN
1	B	145	HIS
1	B	262	HIS
1	B	313	ASN
1	B	335	GLN
1	B	342	GLN
1	B	346	GLN
1	B	422	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	PLP	A	430	2	14,15,16	3.96	4 (28%)	20,22,23	1.54	4 (20%)
2	TZA	A	431	4	14,14,14	6.12	5 (35%)	18,18,18	2.24	7 (38%)
4	PLP	B	530	-	14,15,16	3.83	4 (28%)	20,22,23	1.34	2 (10%)
2	TZA	B	531	-	14,14,14	6.03	5 (35%)	18,18,18	2.08	7 (38%)

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	PLP	A	430	2	-	0/6/6/8	0/1/1/1
2	TZA	A	431	4	-	0/9/19/19	0/1/1/1
4	PLP	B	530	-	-	0/6/6/8	0/1/1/1
2	TZA	B	531	-	-	0/9/19/19	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	431	TZA	CG-CD1	-16.25	1.39	1.51
2	B	531	TZA	CG-CD1	-15.89	1.39	1.51
2	A	431	TZA	CG-CD2	-15.13	1.40	1.51
2	B	531	TZA	CG-CD2	-14.37	1.40	1.51
4	A	430	PLP	C3-C2	12.73	1.49	1.40
4	B	530	PLP	C3-C2	11.69	1.49	1.40
4	B	530	PLP	C4-C5	5.84	1.49	1.39
4	A	430	PLP	C4-C5	5.39	1.48	1.39
2	B	531	TZA	CX-CG	-5.30	1.46	1.54
4	B	530	PLP	O3-C3	-4.72	1.25	1.37
4	A	430	PLP	O3-C3	-3.89	1.27	1.37
4	B	530	PLP	C4-C3	2.78	1.47	1.40
4	A	430	PLP	C4-C3	2.72	1.47	1.40
2	A	431	TZA	CX-CG	-2.69	1.50	1.54
2	A	431	TZA	O2-C	-2.61	1.21	1.30
2	B	531	TZA	O2-C	-2.30	1.22	1.30
2	B	531	TZA	CD2-CE2	2.27	1.40	1.33
2	A	431	TZA	CD2-CE2	2.20	1.40	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	431	TZA	CX-CG-CD2	5.67	125.56	111.79
2	B	531	TZA	CX-CG-CD2	4.69	123.18	111.79
2	A	431	TZA	CE1-CZ-NH	4.16	123.28	110.90
4	B	530	PLP	C3-C4-C5	-3.48	114.71	121.29
4	A	430	PLP	O3P-P-O2P	3.31	120.52	107.61
2	B	531	TZA	CD1-CG-CD2	3.15	120.67	110.78
4	A	430	PLP	C4-C3-C2	-3.02	116.21	119.67
2	B	531	TZA	CE1-CZ-NH	2.95	119.68	110.90
2	B	531	TZA	CE2-CZ-NH	2.90	119.52	110.90
2	B	531	TZA	CB-CA-N	-2.75	103.42	110.14
2	A	431	TZA	O2-C-O	-2.73	117.90	124.07
4	A	430	PLP	C3-C4-C5	-2.67	116.24	121.29
2	A	431	TZA	O2-C-CA	2.54	122.59	116.88
2	A	431	TZA	CD1-CG-CD2	2.45	118.46	110.78
2	B	531	TZA	O2-C-O	-2.26	118.96	124.07
2	A	431	TZA	CE2-CZ-NH	2.21	117.48	110.90
4	B	530	PLP	O2P-P-O4P	2.20	112.72	106.65
2	A	431	TZA	C-CA-N	-2.17	105.77	109.36
4	A	430	PLP	O3-C3-C2	2.17	121.47	117.61
2	B	531	TZA	CE1-CZ-CE2	2.13	120.80	110.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	423/429 (98%)	0.24	18 (4%) 34 37	20, 33, 54, 70	20 (4%)
1	B	425/429 (99%)	0.26	19 (4%) 32 36	18, 34, 56, 62	22 (5%)
All	All	848/858 (98%)	0.25	37 (4%) 34 36	18, 33, 55, 70	42 (4%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	ALA	6.5
1	A	166	LYS	4.7
1	A	162	HIS	4.7
1	A	163	SER	4.3
1	B	53[A]	TRP	3.6
1	A	299	GLY	3.6
1	B	163	SER	3.5
1	B	166	LYS	3.4
1	B	299	GLY	3.4
1	B	159	ASN	3.4
1	B	167	GLY	3.4
1	B	300	GLU	3.0
1	A	165	TRP	2.9
1	A	333	GLN	2.9
1	B	140[A]	PHE	2.9
1	A	168	TYR	2.9
1	B	164	LEU	2.8
1	B	192	VAL	2.8
1	B	149[A]	PHE	2.8
1	B	168	TYR	2.8
1	A	428	CYS	2.7
1	B	231	ILE	2.6
1	B	196	ARG	2.6
1	A	160	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	298	ASN	2.4
1	A	167	GLY	2.4
1	A	24	LEU	2.3
1	B	303	CYS	2.3
1	A	161	MET	2.2
1	A	265	ILE	2.2
1	A	133	ALA	2.2
1	A	368	VAL	2.2
1	A	22	SER	2.2
1	B	165	TRP	2.1
1	A	196	ARG	2.1
1	A	186	TRP	2.1
1	B	203[A]	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NA	B	502	1/1	0.28	5.44	21,21,21,21	0
2	TZA	A	431	14/14	0.19	2.16	34,43,48,49	0
2	TZA	B	531	14/14	0.24	1.56	59,60,63,64	0
3	NA	A	501	1/1	0.14	0.69	20,20,20,20	0
4	PLP	A	430	15/16	0.09	-0.15	22,24,29,30	0
4	PLP	B	530	15/16	0.08	-0.64	22,25,27,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.