Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 07:49 AM EDT

PDB ID	:	1MGV
Title	:	Crystal Structure of the R391A Mutant of 7,8-Diaminopelargonic Acid Synthase
Authors	:	Eliot, A.C.; Sandmark, J.; Schneider, G.; Kirsch, J.F.
Deposited on	:	2002-08-16
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

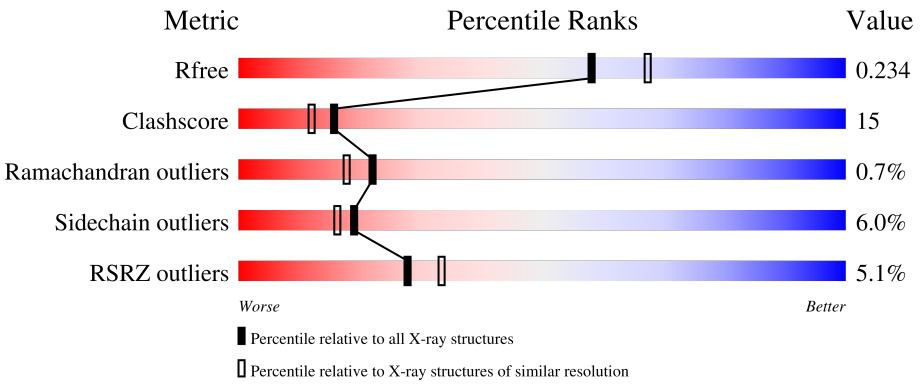
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	429	6% 71% 25% •
1	B	429	5% 76% 21% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7021 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 7,8-diamino-pelargonic acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	428	3321	2112	574	602	33	26	5	0
1	B	428	3310	2106	573	599	32	19	3	0

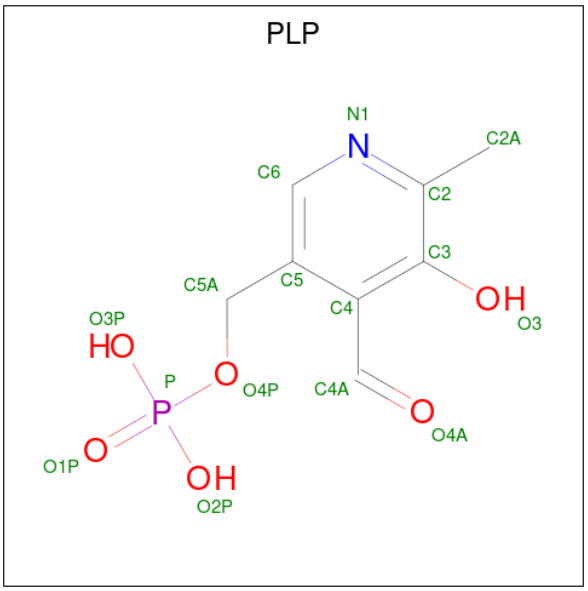
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	LEU	TRP	SEE REMARK 999	UNP P12995
A	391	ALA	ARG	engineered mutation	UNP P12995
B	14	LEU	TRP	SEE REMARK 999	UNP P12995
B	391	ALA	ARG	engineered mutation	UNP P12995

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

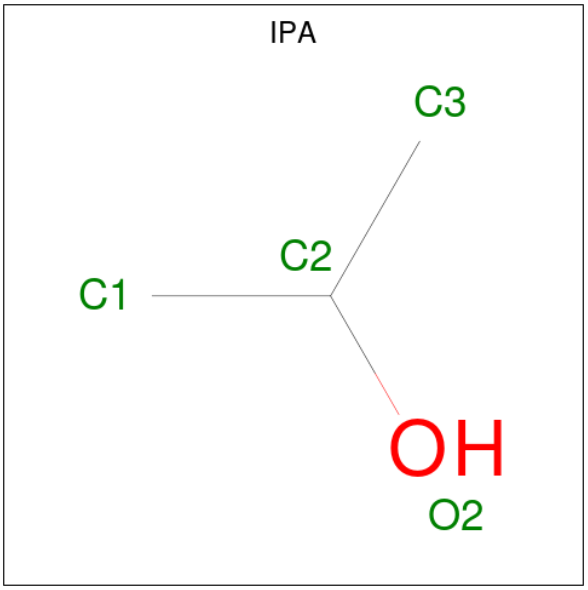
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	3	1	0	0
4	B	1	4	3	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	4	3	1	0	0
			Total	C	O		
4	B	1	4	3	1	0	0

- Molecule 5 is water.

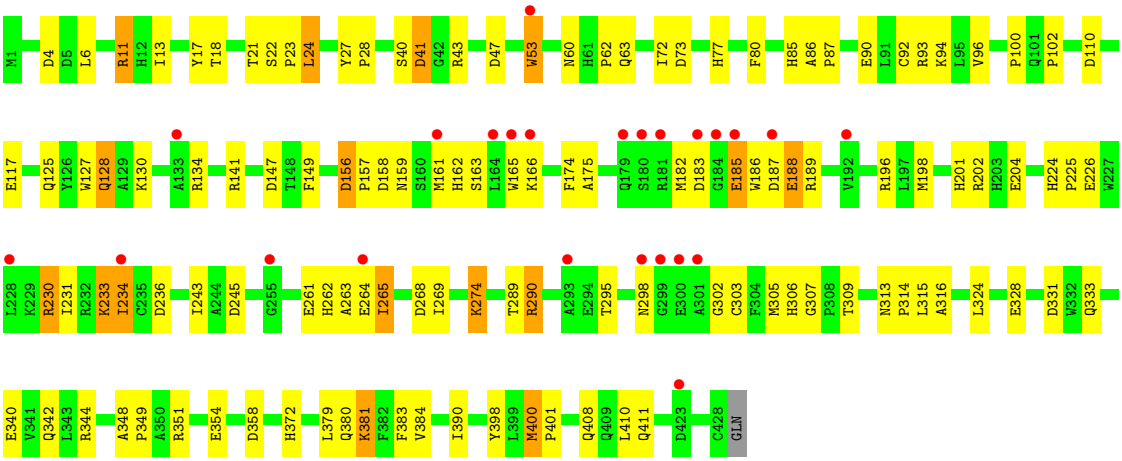
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	169	169	169	0	0
			Total	O		
5	B	173	173	173	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

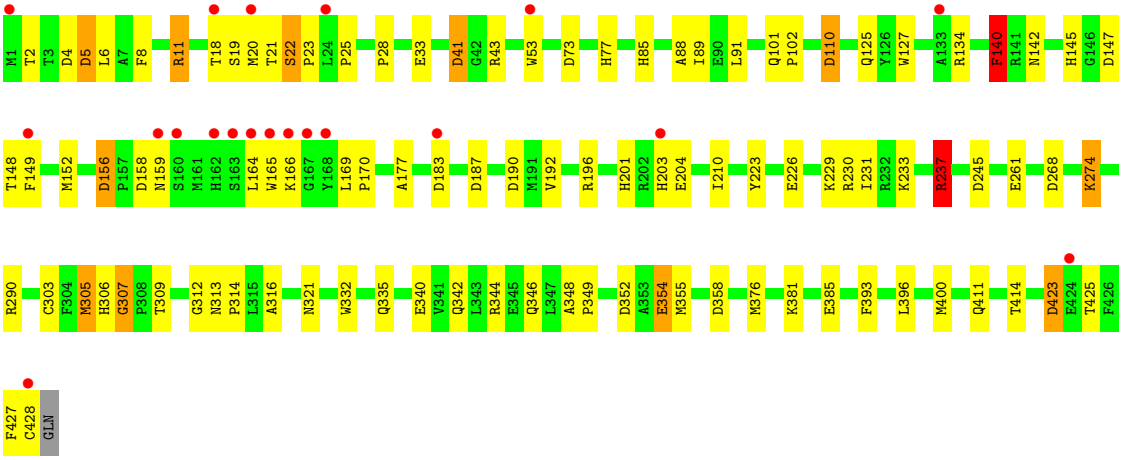
• Molecule 1: 7,8-diamino-pelargonic acid aminotransferase

Chain A:



• Molecule 1: 7,8-diamino-pelargonic acid aminotransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.88Å 55.90Å 116.24Å 90.00° 110.06° 90.00°	Depositor
Resolution (Å)	20.08 – 2.10 20.08 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.08-2.10) 99.3 (20.08-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.31 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.201 , 0.233 0.209 , 0.234	Depositor DCC
R_{free} test set	2269 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7021	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, NA, IPA

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	0.60	0/3427	0.82	12/4653 (0.3%)
1	B	0.61	2/3403 (0.1%)	0.83	15/4621 (0.3%)
All	All	0.61	2/6830 (0.0%)	0.82	27/9274 (0.3%)

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	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140[A]	PHE	CA-CB	-5.54	1.41	1.53
1	B	140[B]	PHE	CA-CB	-5.54	1.41	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	ASP	CB-CG-OD1	8.99	126.39	118.30
1	B	423	ASP	CB-CG-OD1	7.67	125.20	118.30
1	A	4	ASP	CB-CG-OD2	7.16	124.75	118.30
1	A	268	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	305	MET	CB-CG-SD	6.33	131.40	112.40
1	B	358	ASP	CB-CG-OD2	6.27	123.94	118.30
1	B	183	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	187	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	47	ASP	CB-CG-OD2	5.83	123.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	5	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	236	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	237	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	156	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	73	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	4	ASP	CB-CG-OD2	5.63	123.36	118.30
1	B	41	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	158	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	187	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	41	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	268	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	245	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	358	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	331	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	352	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	110	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	156	ASP	CB-CG-OD1	5.03	122.82	118.30
1	B	158	ASP	CB-CG-OD2	5.00	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140[A]	PHE	Sidechain
1	B	140[B]	PHE	Sidechain

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	3321	0	3279	123	3
1	B	3310	0	3257	87	3
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	6	0	0
3	B	15	0	6	1	0
4	A	4	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	12	0	24	3	0
5	A	169	0	0	11	1
5	B	173	0	0	12	0
All	All	7021	0	6580	193	5

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 15.

All (193) 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:A:53[A]:TRP:CE3	1:A:400[A]:MET:CE	1.83	1.57
1:A:53[A]:TRP:CZ3	1:A:400[A]:MET:HE1	1.49	1.45
1:A:53[A]:TRP:CE3	1:A:400[A]:MET:HE1	1.42	1.43
1:A:53[A]:TRP:CZ3	1:A:400[A]:MET:CE	2.08	1.28
1:A:128:GLN:HE21	1:B:164:LEU:HD22	1.09	1.15
1:A:53[A]:TRP:CE3	1:A:400[A]:MET:HE3	1.67	1.10
1:A:53[A]:TRP:CD2	1:A:400[A]:MET:HE1	1.89	1.08
1:A:24:LEU:H	1:A:24:LEU:CD1	1.70	1.04
1:B:190:ASP:OD1	5:B:786:HOH:O	1.79	0.97
1:A:62:PRO:O	5:A:775:HOH:O	1.85	0.94
1:B:156:ASP:HB3	1:B:159:ASN:HB2	1.48	0.94
1:A:53[A]:TRP:CH2	1:A:400[A]:MET:HE1	2.02	0.94
1:A:53[A]:TRP:CD2	1:A:400[A]:MET:CE	2.51	0.91
1:A:53[A]:TRP:CZ3	1:A:400[A]:MET:HE2	2.06	0.91
1:B:149[B]:PHE:CD1	1:B:169:LEU:HD23	2.07	0.90
1:A:125:GLN:HG2	1:A:128:GLN:NE2	1.89	0.88
1:A:128:GLN:HE21	1:B:164:LEU:CD2	1.88	0.87
1:B:226:GLU:OE2	1:B:230:ARG:NH1	2.09	0.86
1:A:24:LEU:H	1:A:24:LEU:HD13	1.38	0.86
1:A:130[B]:LYS:HE2	1:A:295:THR:CG2	2.07	0.85
1:A:128:GLN:NE2	1:B:164:LEU:HD22	1.92	0.82
1:B:149[B]:PHE:HD1	1:B:169:LEU:HD23	1.45	0.81
1:B:381:LYS:NZ	1:B:385:GLU:OE2	2.13	0.79
1:A:53[A]:TRP:HH2	1:A:398:TYR:OH	1.65	0.79
1:A:130[B]:LYS:HE2	1:A:295:THR:HG23	1.65	0.78
1:B:149[B]:PHE:HD1	1:B:169:LEU:CD2	1.96	0.78
1:A:163:SER:HA	1:A:166:LYS:HG2	1.67	0.77
1:A:24:LEU:H	1:A:24:LEU:HD12	1.48	0.77
1:A:17[B]:TYR:OH	1:A:147:ASP:OD2	2.03	0.76
1:B:142:ASN:HD22	1:B:177:ALA:HB2	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:857:HOH:O	1:B:303:CYS:SG	2.44	0.75
1:A:290:ARG:NH2	1:B:11:ARG:O	2.20	0.74
1:B:125:GLN:HE22	1:B:305:MET:H	1.36	0.74
1:A:17[A]:TYR:OH	1:A:147:ASP:OD1	2.07	0.73
1:A:21:THR:C	1:A:23:PRO:HD3	2.09	0.73
1:A:198:MET:HG2	1:A:234:ILE:HD11	1.69	0.73
1:B:149[B]:PHE:HE1	1:B:170:PRO:HD2	1.53	0.73
1:A:372:HIS:NE2	5:A:867:HOH:O	2.22	0.72
1:A:186:TRP:HE1	1:A:188:GLU:HG2	1.54	0.72
1:A:125:GLN:HE22	1:A:305:MET:H	1.37	0.72
1:A:24:LEU:HD13	1:A:24:LEU:N	2.05	0.72
1:B:423:ASP:OD1	1:B:425:THR:OG1	2.06	0.72
1:A:53[A]:TRP:HE3	1:A:400[A]:MET:HE3	1.48	0.71
1:B:376:MET:HG3	5:B:857:HOH:O	1.90	0.71
1:A:90:GLU:OE2	1:A:94:LYS:NZ	2.23	0.71
1:B:332:TRP:HA	1:B:335:GLN:HE21	1.57	0.70
1:B:145:HIS:HE1	5:B:724:HOH:O	1.73	0.70
1:B:376:MET:HE2	5:B:857:HOH:O	1.93	0.69
1:B:152:MET:SD	5:B:846:HOH:O	2.51	0.69
1:A:53[A]:TRP:CE2	1:A:400[A]:MET:HE1	2.30	0.66
1:B:149[B]:PHE:CD1	1:B:169:LEU:CD2	2.75	0.66
1:B:77:HIS:HA	1:B:314:PRO:HD2	1.78	0.65
1:B:393:PHE:CD2	5:B:836:HOH:O	2.49	0.65
1:B:101:GLN:HB3	1:B:102:PRO:HD3	1.79	0.65
1:B:348:ALA:HB3	1:B:349:PRO:HD3	1.77	0.65
1:A:130[B]:LYS:HE2	1:A:295:THR:HG21	1.79	0.64
1:B:149[B]:PHE:CE1	1:B:170:PRO:HD2	2.33	0.64
1:B:427:PHE:O	1:B:428:CYS:HB2	1.97	0.64
1:A:231:ILE:O	1:A:234:ILE:HG22	1.97	0.64
1:A:302:GLY:O	1:B:19:SER:HB2	1.97	0.64
1:A:381:LYS:HD3	5:A:807:HOH:O	1.97	0.64
1:B:261:GLU:OE2	5:B:830:HOH:O	2.15	0.63
1:A:22:SER:N	1:A:23:PRO:HD3	2.14	0.63
1:A:340:GLU:OE2	1:A:344:ARG:NH1	2.32	0.63
4:B:631:IPA:H12	4:B:632:IPA:C3	2.28	0.63
1:B:346:GLN:NE2	1:B:414:THR:OG1	2.32	0.63
1:A:372:HIS:CE1	5:A:867:HOH:O	2.52	0.63
1:B:91:LEU:HA	1:B:321:ASN:HD21	1.63	0.62
1:A:149:PHE:HB3	1:B:149[B]:PHE:CE2	2.35	0.62
1:B:149[B]:PHE:CE1	1:B:169:LEU:HD23	2.35	0.62
1:B:145:HIS:HD2	1:B:245:ASP:OD2	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:GLU:HG2	1:B:355:MET:N	2.15	0.62
1:A:381:LYS:CB	1:A:381:LYS:HZ3	2.10	0.61
1:A:163:SER:HA	1:A:166:LYS:CG	2.32	0.60
1:A:24:LEU:CD1	1:A:24:LEU:N	2.44	0.60
4:B:631:IPA:H12	4:B:632:IPA:H2	1.84	0.60
1:B:140[B]:PHE:CE1	1:B:210:ILE:HB	2.37	0.59
1:B:201:HIS:HD2	1:B:204:GLU:OE2	1.85	0.59
1:A:149:PHE:HB3	1:B:149[B]:PHE:CD2	2.37	0.59
1:B:274:LYS:NZ	3:B:700:PLP:O3	2.37	0.58
1:A:198:MET:CG	1:A:234:ILE:HD11	2.33	0.58
1:B:91:LEU:CA	1:B:321:ASN:HD21	2.17	0.57
1:A:198:MET:SD	1:A:234:ILE:HD11	2.43	0.57
1:A:41:ASP:OD2	1:A:43:ARG:NH1	2.37	0.57
1:A:17[B]:TYR:CE2	1:B:307:GLY:HA3	2.40	0.57
1:A:117:GLU:OE1	1:B:149[A]:PHE:HD2	1.88	0.57
1:A:298:ASN:O	1:A:298:ASN:OD1	2.24	0.56
1:B:423:ASP:CG	1:B:425:THR:HG1	2.08	0.56
1:A:85:HIS:HE1	5:A:759:HOH:O	1.89	0.55
1:A:102:PRO:O	1:A:289:THR:HA	2.07	0.55
1:A:348:ALA:HB3	1:A:349:PRO:HD3	1.88	0.55
1:A:53[A]:TRP:CH2	1:A:398:TYR:CE2	2.94	0.55
1:A:100:PRO:HD3	5:A:815:HOH:O	2.06	0.54
1:A:201:HIS:ND1	1:A:204:GLU:OE1	2.35	0.54
1:A:372:HIS:CD2	5:A:867:HOH:O	2.59	0.54
1:B:140[B]:PHE:HE1	1:B:223:TYR:HH	1.55	0.53
1:A:53[A]:TRP:HH2	1:A:398:TYR:CZ	2.26	0.53
1:B:142:ASN:HD22	1:B:177:ALA:CB	2.19	0.53
1:A:53[A]:TRP:CZ2	1:A:400[A]:MET:HE1	2.41	0.53
1:B:393:PHE:CE2	5:B:836:HOH:O	2.61	0.53
1:B:85:HIS:CE1	1:B:88:ALA:HB2	2.44	0.52
1:A:163:SER:CA	1:A:166:LYS:HG2	2.37	0.52
1:A:165:TRP:CH2	1:B:125:GLN:HG3	2.44	0.52
1:A:86:ALA:HB3	1:A:87:PRO:HD3	1.92	0.51
1:A:22:SER:N	1:A:23:PRO:CD	2.74	0.51
1:A:234:ILE:C	1:A:234:ILE:HD13	2.31	0.51
1:A:157:PRO:HD3	1:A:174:PHE:CE2	2.46	0.50
1:B:346:GLN:HE22	1:B:411:GLN:HA	1.76	0.50
1:A:53[A]:TRP:CH2	1:A:398:TYR:OH	2.46	0.50
1:A:125:GLN:HG2	1:A:128:GLN:HE22	1.70	0.50
1:A:231:ILE:HA	1:A:234:ILE:HG22	1.94	0.50
1:B:342:GLN:NE2	5:B:823:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASP:OD2	1:A:43:ARG:HD3	2.12	0.50
4:B:631:IPA:H12	4:B:632:IPA:C2	2.41	0.49
1:B:393:PHE:CZ	1:B:396:LEU:HD12	2.48	0.49
1:B:313:ASN:ND2	1:B:316:ALA:H	2.10	0.49
1:A:198:MET:HG2	1:A:234:ILE:CD1	2.40	0.49
1:B:376:MET:CG	5:B:857:HOH:O	2.57	0.49
1:A:231:ILE:O	1:A:234:ILE:CG2	2.61	0.49
1:A:243:ILE:HG12	1:A:269:ILE:HB	1.95	0.48
1:B:312:GLY:O	1:B:313:ASN:C	2.52	0.48
1:B:340:GLU:O	1:B:344:ARG:HG3	2.14	0.48
1:A:156:ASP:HB3	1:A:159:ASN:HB2	1.96	0.48
1:A:128:GLN:NE2	1:B:164:LEU:CD2	2.63	0.48
1:B:2:THR:O	1:B:5:ASP:HB2	2.14	0.48
1:A:53[A]:TRP:CZ3	1:A:398:TYR:HE2	2.32	0.47
1:B:148:THR:O	1:B:152:MET:HG3	2.13	0.47
1:A:77:HIS:HA	1:A:314:PRO:HD2	1.96	0.47
1:B:20:MET:O	1:B:23:PRO:HD3	2.14	0.47
1:A:24:LEU:HD13	1:A:24:LEU:O	2.15	0.47
1:A:43:ARG:HH21	1:A:384:VAL:HG12	1.80	0.47
1:A:157:PRO:HA	1:A:162:HIS:CG	2.50	0.47
1:A:43:ARG:HH21	1:A:384:VAL:CG1	2.29	0.46
1:A:263:ALA:O	1:A:265:ILE:HG23	2.15	0.46
1:A:381:LYS:HZ2	1:A:381:LYS:HG3	1.39	0.46
1:A:125:GLN:HA	1:A:128:GLN:HB3	1.97	0.46
1:A:185:GLU:OE1	1:A:186:TRP:N	2.49	0.46
1:A:261:GLU:O	1:A:263:ALA:N	2.49	0.45
1:A:313:ASN:ND2	1:A:316:ALA:H	2.14	0.45
1:B:140[B]:PHE:CZ	1:B:223:TYR:CZ	3.04	0.45
1:A:72:ILE:HG13	1:A:315:LEU:HD13	1.99	0.45
1:B:127:TRP:CD2	1:B:134:ARG:HD2	2.51	0.45
1:A:53[A]:TRP:CH2	1:A:398:TYR:CZ	3.05	0.45
1:A:93:ARG:HA	1:B:8:PHE:CZ	2.51	0.45
1:B:201:HIS:CD2	1:B:204:GLU:OE2	2.68	0.45
1:B:140[A]:PHE:CZ	1:B:231:ILE:HD11	2.52	0.45
1:A:117:GLU:OE1	1:B:149[A]:PHE:CD2	2.69	0.44
1:A:127:TRP:CD2	1:A:134:ARG:HD2	2.53	0.44
1:B:140[B]:PHE:HZ	1:B:223:TYR:HH	1.57	0.44
1:A:11:ARG:HG3	5:A:771:HOH:O	2.18	0.44
1:B:91:LEU:HA	1:B:321:ASN:ND2	2.29	0.44
1:A:379:LEU:HG	1:A:383:PHE:CE2	2.52	0.43
1:B:210:ILE:CG2	5:B:779:HOH:O	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:HIS:ND1	1:A:225:PRO:HD2	2.33	0.43
1:A:43:ARG:NH2	1:A:384:VAL:CG1	2.82	0.43
1:A:27:TYR:HA	1:A:28:PRO:HD3	1.89	0.43
1:B:6:LEU:HD21	1:B:28:PRO:HG3	2.01	0.43
1:B:145:HIS:CE1	5:B:724:HOH:O	2.58	0.43
1:A:348:ALA:N	1:A:349:PRO:CD	2.82	0.42
1:A:186:TRP:CE3	1:A:226:GLU:HB3	2.54	0.42
1:A:6:LEU:HB2	5:A:828:HOH:O	2.20	0.42
1:B:53:TRP:CZ2	1:B:400:MET:HE1	2.55	0.42
1:A:261:GLU:C	1:A:263:ALA:N	2.72	0.42
1:A:53[A]:TRP:CH2	1:A:398:TYR:HE2	2.37	0.42
1:B:41:ASP:OD1	1:B:43:ARG:HG3	2.19	0.42
1:B:53:TRP:HB2	1:B:274:LYS:HD3	2.01	0.42
1:A:306:HIS:CE1	1:B:147:ASP:HB3	2.55	0.42
1:A:147:ASP:HB3	1:B:306:HIS:CE1	2.55	0.42
1:A:18:THR:HG21	1:A:24:LEU:HD11	2.02	0.41
1:A:141:ARG:HG3	1:A:175:ALA:O	2.21	0.41
1:A:303:CYS:HB2	1:B:18:THR:C	2.41	0.41
1:A:13:ILE:HD11	1:B:89:ILE:HA	2.01	0.41
1:A:24:LEU:HD22	1:A:24:LEU:C	2.41	0.41
1:A:17[A]:TYR:OH	1:A:147:ASP:CG	2.59	0.41
1:A:92:CYS:O	1:A:96:VAL:HG23	2.19	0.41
1:A:309:THR:OG1	1:B:274:LYS:HE3	2.21	0.41
1:A:274:LYS:HE3	1:B:309:THR:OG1	2.20	0.41
1:A:342:GLN:HE21	1:A:342:GLN:HB2	1.64	0.41
1:B:149[B]:PHE:CE1	1:B:170:PRO:CD	3.03	0.41
1:A:230:ARG:HA	1:A:233[B]:LYS:HE2	2.01	0.41
1:B:140[B]:PHE:CE1	1:B:223:TYR:CZ	3.09	0.41
1:A:383:PHE:CD2	1:A:390:ILE:HB	2.56	0.40
1:A:324:LEU:O	1:A:328:GLU:HG3	2.21	0.40
1:A:411:GLN:NE2	5:A:824:HOH:O	2.55	0.40
1:A:290:ARG:NH2	1:B:11:ARG:HG3	2.36	0.40
1:B:22:SER:N	1:B:23:PRO:HD3	2.36	0.40

All (5) 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	Interatomic distance (Å)	Clash overlap (Å)
5:A:828:HOH:O	5:A:828:HOH:O[2_656]	1.66	0.54
1:A:351:ARG:O	1:A:408:GLN:NE2[4_646]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:THR:O	1:B:21:THR:O[2_655]	2.10	0.10
1:A:333:GLN:OE1	1:B:237:ARG:NH1[3_555]	2.13	0.07
1:A:333:GLN:NE2	1:B:237:ARG:NH1[3_555]	2.15	0.05

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	Percentiles	
1	A	431/429 (100%)	406 (94%)	22 (5%)	3 (1%)	22	18
1	B	429/429 (100%)	409 (95%)	17 (4%)	3 (1%)	22	18
All	All	860/858 (100%)	815 (95%)	39 (4%)	6 (1%)	22	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	LYS
1	B	274	LYS
1	A	262	HIS
1	A	307	GLY
1	B	25	PRO
1	B	307	GLY

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	Percentiles
1	A	348/344 (101%)	317 (91%)	31 (9%)	9 6
1	B	345/344 (100%)	332 (96%)	13 (4%)	33 34
All	All	693/688 (101%)	649 (94%)	44 (6%)	19 15

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	24	LEU
1	A	40	SER
1	A	53[A]	TRP
1	A	53[B]	TRP
1	A	60	ASN
1	A	63	GLN
1	A	80	PHE
1	A	110	ASP
1	A	128	GLN
1	A	161	MET
1	A	182	MET
1	A	183	ASP
1	A	185	GLU
1	A	188	GLU
1	A	189	ARG
1	A	196	ARG
1	A	202	ARG
1	A	230	ARG
1	A	233[A]	LYS
1	A	233[B]	LYS
1	A	234	ILE
1	A	264	GLU
1	A	265	ILE
1	A	290	ARG
1	A	354	GLU
1	A	380	GLN
1	A	381	LYS
1	A	400[A]	MET
1	A	400[B]	MET
1	A	410	LEU
1	B	11	ARG
1	B	22	SER
1	B	33	GLU
1	B	110	ASP

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Mol	Chain	Res	Type
1	B	165	TRP
1	B	166	LYS
1	B	192	VAL
1	B	196	ARG
1	B	229	LYS
1	B	233	LYS
1	B	237	ARG
1	B	290	ARG
1	B	354	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	125	GLN
1	A	128	GLN
1	A	135	GLN
1	A	142	ASN
1	A	298	ASN
1	A	313	ASN
1	A	335	GLN
1	B	63	GLN
1	B	125	GLN
1	B	142	ASN
1	B	145	HIS
1	B	201	HIS
1	B	262	HIS
1	B	313	ASN
1	B	321	ASN
1	B	335	GLN
1	B	342	GLN
1	B	346	GLN
1	B	380	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	PLP	B	700	1	15,15,16	1.88	1 (6%)	20,22,23	2.49	5 (25%)
4	IPA	B	630	-	3,3,3	0.56	0	3,3,3	0.29	0
4	IPA	B	632	-	3,3,3	0.55	0	3,3,3	0.24	0
3	PLP	A	700	1	15,15,16	1.95	3 (20%)	20,22,23	1.78	5 (25%)
4	IPA	B	631	-	3,3,3	0.50	0	3,3,3	0.33	0
4	IPA	A	530	-	3,3,3	0.57	0	3,3,3	0.23	0

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	B	700	1	-	3/6/6/8	0/1/1/1
3	PLP	A	700	1	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	PLP	O3-C3	-6.17	1.22	1.37
3	A	700	PLP	O3-C3	-5.47	1.24	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	PLP	C3-C2	-2.59	1.38	1.40
3	A	700	PLP	C2-N1	2.16	1.37	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	700	PLP	O4P-C5A-C5	7.37	123.39	109.35
3	A	700	PLP	O4P-C5A-C5	5.37	119.58	109.35
3	B	700	PLP	O3P-P-O4P	-5.26	92.75	106.73
3	B	700	PLP	C6-C5-C4	3.16	120.65	118.16
3	B	700	PLP	C5A-C5-C6	-2.57	115.14	119.37
3	A	700	PLP	C5-C6-N1	-2.10	120.32	123.82
3	A	700	PLP	C4A-C4-C3	-2.07	116.99	120.50
3	B	700	PLP	C3-C4-C5	-2.05	116.53	118.74
3	A	700	PLP	O3P-P-O1P	2.03	118.61	110.68
3	A	700	PLP	C2A-C2-N1	2.01	121.60	117.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	700	PLP	C4-C5-C5A-O4P
3	B	700	PLP	C6-C5-C5A-O4P
3	B	700	PLP	C5A-O4P-P-O1P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	PLP	1	0
4	B	632	IPA	3	0
4	B	631	IPA	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	428/429 (99%)	0.42	24 (5%)	24	29	20, 33, 59, 74	6 (1%)
1	B	428/429 (99%)	0.25	20 (4%)	31	37	18, 32, 50, 68	5 (1%)
All	All	856/858 (99%)	0.33	44 (5%)	28	33	18, 32, 55, 74	11 (1%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ASP	8.1
1	A	166	LYS	5.8
1	B	133	ALA	5.5
1	A	299	GLY	4.8
1	A	133	ALA	4.7
1	B	149[A]	PHE	4.4
1	A	301	ALA	4.3
1	A	298	ASN	4.1
1	B	163	SER	4.1
1	B	159	ASN	3.9
1	A	264	GLU	3.7
1	B	167	GLY	3.7
1	A	300	GLU	3.4
1	A	184	GLY	3.3
1	B	428	CYS	3.3
1	A	185	GLU	3.1
1	A	179	GLN	3.0
1	B	24	LEU	3.0
1	B	183	ASP	3.0
1	B	165	TRP	2.9
1	B	162	HIS	2.9
1	B	166	LYS	2.9
1	B	160	SER	2.8
1	A	187	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	423	ASP	2.6
1	A	164	LEU	2.6
1	B	203[A]	HIS	2.6
1	B	1	MET	2.6
1	B	164	LEU	2.5
1	A	53[A]	TRP	2.5
1	A	228	LEU	2.3
1	A	180	SER	2.3
1	A	181	ARG	2.3
1	B	168	TYR	2.3
1	B	424	GLU	2.2
1	A	293	ALA	2.2
1	A	255	GLY	2.2
1	A	192	VAL	2.1
1	A	161	MET	2.1
1	B	20	MET	2.1
1	B	53	TRP	2.1
1	A	165	TRP	2.1
1	A	234	ILE	2.0
1	B	18	THR	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 monosaccharides 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(Å^2)	Q<0.9
4	IPA	A	530	4/4	0.79	0.24	55,55,55,55	0
4	IPA	B	631	4/4	0.79	0.24	62,62,62,63	0
4	IPA	B	630	4/4	0.83	0.22	57,57,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IPA	B	632	4/4	0.88	0.25	54,54,54,54	0
2	NA	A	501	1/1	0.93	0.32	25,25,25,25	0
2	NA	B	502	1/1	0.95	0.20	13,13,13,13	0
3	PLP	A	700	15/16	0.98	0.07	22,23,29,29	0
3	PLP	B	700	15/16	0.98	0.07	16,20,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.