



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:34 AM UTC

PDB ID : 1B9H / pdb_00001b9h
Title : CRYSTAL STRUCTURE OF 3-AMINO-5-HYDROXYBENZOIC ACID
(AHBA) SYNTHASE
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Deposited on : 1999-02-11
Resolution : 2.00 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

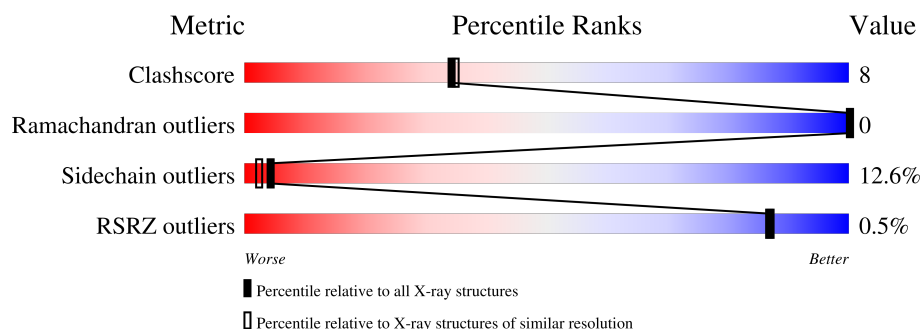
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	388	64% 27% 6% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3171 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.

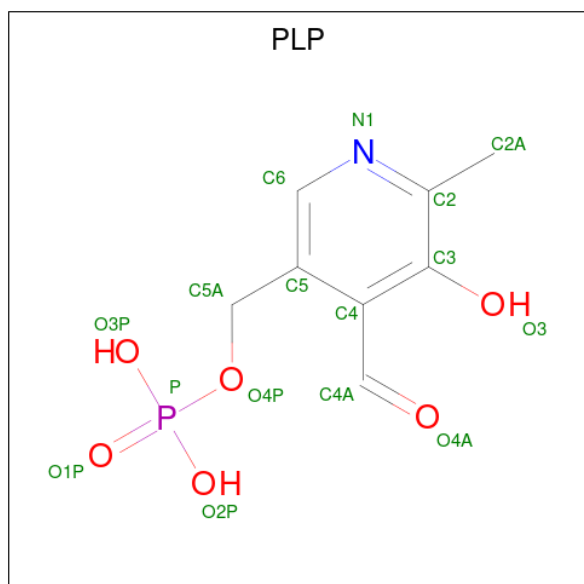
- Molecule 1 is a protein called PROTEIN (3-AMINO-5-HYDROXYBENZOIC ACID SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	2940	1839	539	549	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	ALA	GLY	REMARK 999	UNP O52552
A	262	ARG	PRO	REMARK 999	UNP O52552

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

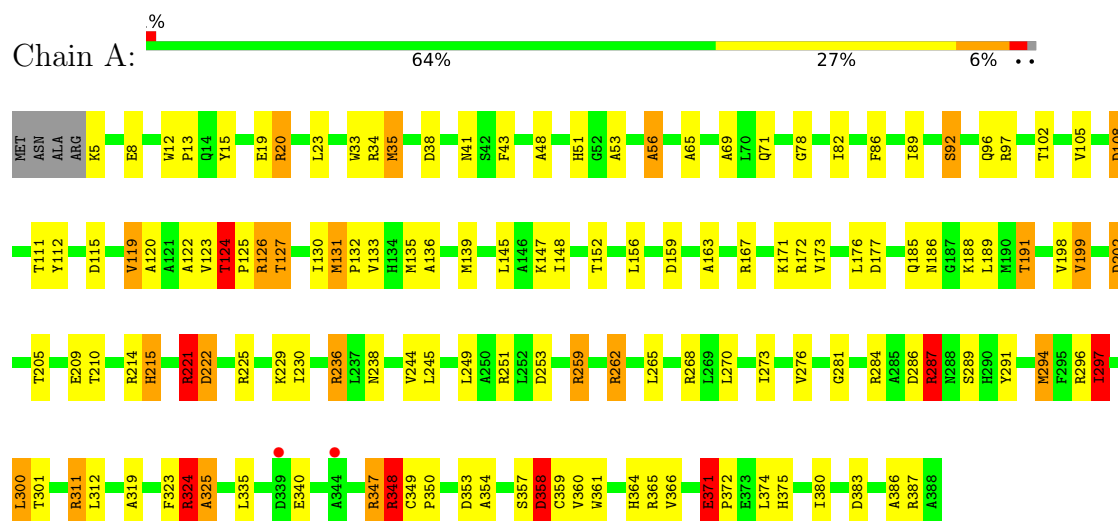
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	216	Total 216	O 216	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: PROTEIN (3-AMINO-5-HYDROXYBENZOIC ACID SYNTHASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.70Å 89.70Å 127.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (10.00-2.00) 97.5 (10.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	3.80	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.252 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 58.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3171	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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	0.99	4/3005 (0.1%)	2.05	100/4083 (2.4%)

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	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	358	ASP	CA-CB	5.92	1.62	1.53
1	A	185	GLN	CD-OE1	5.37	1.33	1.23
1	A	177	ASP	N-CA	5.24	1.52	1.46
1	A	365	ARG	CD-NE	-5.08	1.39	1.46

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ARG	CD-NE-CZ	15.39	145.94	124.40
1	A	259	ARG	NE-CZ-NH2	-12.09	108.32	119.20
1	A	371	GLU	CA-C-O	11.35	129.07	118.63
1	A	176	LEU	CA-C-O	-10.31	109.44	120.89
1	A	365	ARG	NH1-CZ-NH2	9.39	131.50	119.30
1	A	215	HIS	CA-CB-CG	9.03	122.83	113.80
1	A	221	ARG	CD-NE-CZ	8.97	136.96	124.40
1	A	202	ASP	CA-CB-CG	-8.90	103.70	112.60
1	A	347	ARG	CD-NE-CZ	8.82	136.75	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ASP	N-CA-CB	-8.80	98.40	111.43
1	A	51	HIS	CA-CB-CG	-8.46	105.34	113.80
1	A	311	ARG	CB-CG-CD	8.25	130.28	111.30
1	A	358	ASP	CB-CA-C	-8.17	93.25	109.67
1	A	311	ARG	NE-CZ-NH2	-8.07	111.94	119.20
1	A	34	ARG	CD-NE-CZ	7.97	135.56	124.40
1	A	38	ASP	CA-CB-CG	-7.92	104.69	112.60
1	A	358	ASP	N-CA-C	7.81	123.14	112.90
1	A	371	GLU	O-C-N	-7.77	113.16	120.55
1	A	324	ARG	N-CA-CB	-7.59	98.70	110.85
1	A	259	ARG	NE-CZ-NH1	7.49	128.99	121.50
1	A	176	LEU	CA-C-N	-7.38	110.78	123.25
1	A	176	LEU	C-N-CA	-7.38	110.78	123.25
1	A	365	ARG	NE-CZ-NH2	-7.33	112.61	119.20
1	A	69	ALA	CA-C-O	-7.26	113.20	120.82
1	A	286	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	41	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	A	20	ARG	CD-NE-CZ	-7.07	114.50	124.40
1	A	41	ASN	CA-C-N	7.03	129.58	120.44
1	A	41	ASN	C-N-CA	7.03	129.58	120.44
1	A	97	ARG	NE-CZ-NH2	6.78	125.31	119.20
1	A	124	THR	N-CA-CB	-6.73	102.80	111.35
1	A	176	LEU	N-CA-C	-6.66	99.71	109.63
1	A	287	ARG	NE-CZ-NH1	6.57	128.07	121.50
1	A	380	ILE	CA-C-O	6.42	127.63	120.95
1	A	251	ARG	CA-C-O	-6.28	111.99	119.15
1	A	41	ASN	CA-CB-CG	6.26	118.86	112.60
1	A	325	ALA	CA-C-O	-6.15	114.80	120.95
1	A	287	ARG	CD-NE-CZ	6.14	133.00	124.40
1	A	163	ALA	N-CA-C	6.10	120.02	111.30
1	A	8	GLU	CB-CG-CD	-6.08	102.26	112.60
1	A	148	ILE	CA-C-O	6.05	127.24	120.95
1	A	348	ARG	CD-NE-CZ	5.98	132.77	124.40
1	A	253	ASP	N-CA-C	5.98	118.56	111.33
1	A	225	ARG	CD-NE-CZ	5.95	132.73	124.40
1	A	273	ILE	N-CA-CB	5.94	117.19	110.72
1	A	251	ARG	NE-CZ-NH2	-5.85	113.94	119.20
1	A	71	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	A	210	THR	CA-CB-OG1	-5.75	100.98	109.60
1	A	294	MET	N-CA-C	5.72	119.14	109.76
1	A	323	PHE	CA-C-O	5.72	128.68	120.51
1	A	324	ARG	CG-CD-NE	-5.71	99.44	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	SER	CA-C-O	-5.71	112.86	119.14
1	A	236	ARG	CD-NE-CZ	-5.71	116.41	124.40
1	A	120	ALA	O-C-N	-5.68	116.10	122.12
1	A	122	ALA	CA-C-O	5.65	125.91	119.18
1	A	65	ALA	CA-C-O	-5.65	114.56	120.55
1	A	268	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	A	365	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	A	78	GLY	CA-C-O	-5.58	112.82	119.01
1	A	108	ASP	O-C-N	-5.56	115.97	122.81
1	A	375	HIS	N-CA-CB	5.56	118.13	110.07
1	A	199	VAL	N-CA-CB	-5.52	101.79	111.39
1	A	205	THR	CA-C-O	-5.48	114.74	120.55
1	A	357	SER	CA-C-N	5.48	131.60	121.52
1	A	357	SER	C-N-CA	5.48	131.60	121.52
1	A	319	ALA	CA-C-N	5.47	131.07	122.21
1	A	319	ALA	C-N-CA	5.47	131.07	122.21
1	A	281	GLY	CA-C-O	5.46	128.40	122.33
1	A	86	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	324	ARG	CB-CA-C	5.44	119.33	109.37
1	A	43	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	386	ALA	N-CA-C	-5.42	105.53	111.82
1	A	188	LYS	CA-C-N	5.39	128.51	120.31
1	A	188	LYS	C-N-CA	5.39	128.51	120.31
1	A	262	ARG	CD-NE-CZ	-5.38	116.86	124.40
1	A	15	TYR	CA-C-O	-5.35	115.71	121.38
1	A	131	MET	O-C-N	-5.29	116.54	121.36
1	A	387	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	131	MET	N-CA-C	5.26	118.73	108.21
1	A	375	HIS	O-C-N	5.26	127.77	122.09
1	A	296	ARG	CD-NE-CZ	5.24	131.73	124.40
1	A	284	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	A	325	ALA	CB-CA-C	5.19	116.92	109.71
1	A	265	LEU	O-C-N	-5.16	116.66	122.03
1	A	297	ILE	CA-CB-CG1	5.14	119.14	110.40
1	A	56	ALA	O-C-N	-5.13	117.19	123.30
1	A	53	ALA	CA-C-O	-5.13	115.67	121.72
1	A	221	ARG	CA-C-N	-5.12	114.59	123.25
1	A	221	ARG	C-N-CA	-5.12	114.59	123.25
1	A	276	VAL	N-CA-C	5.12	115.46	107.99
1	A	19	GLU	N-CA-CB	5.11	117.42	110.01
1	A	89	ILE	O-C-N	-5.10	116.75	121.90
1	A	198	VAL	N-CA-CB	5.09	118.17	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	LYS	CB-CG-CD	5.09	123.00	111.30
1	A	191	THR	N-CA-C	5.09	116.80	109.07
1	A	198	VAL	CA-C-N	-5.08	116.05	123.06
1	A	198	VAL	C-N-CA	-5.08	116.05	123.06
1	A	238	ASN	O-C-N	5.02	128.56	122.94
1	A	359	CYS	N-CA-C	5.02	117.80	109.46
1	A	251	ARG	CD-NE-CZ	5.02	131.42	124.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	THR	Mainchain
1	A	244	VAL	Mainchain
1	A	297	ILE	Mainchain
1	A	301	THR	Mainchain
1	A	312	LEU	Mainchain
1	A	358	ASP	Mainchain

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	2940	0	2859	44	0
2	A	15	0	6	0	0
3	A	216	0	0	3	0
All	All	3171	0	2865	44	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 8.

All (44) 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:124:THR:HG22	1:A:126:ARG:H	1.25	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:MET:HG3	1:A:294:MET:HE1	1.46	0.96
1:A:136:ALA:HB2	1:A:294:MET:HE2	1.61	0.82
1:A:136:ALA:CB	1:A:294:MET:HE2	2.17	0.74
1:A:92:SER:HB3	1:A:102:THR:HG21	1.71	0.71
1:A:133:VAL:HG22	1:A:159:ASP:HB3	1.75	0.68
1:A:135:MET:CG	1:A:294:MET:HE1	2.24	0.66
1:A:236:ARG:NH1	3:A:601:HOH:O	2.24	0.60
1:A:124:THR:HG23	1:A:125:PRO:HD2	1.85	0.59
1:A:262:ARG:HB3	1:A:374:LEU:HD11	1.86	0.58
1:A:291:TYR:O	1:A:364:HIS:HB3	2.04	0.57
1:A:297:ILE:HB	1:A:300:LEU:HD22	1.85	0.57
1:A:189:LEU:HD22	1:A:259:ARG:NH2	2.20	0.57
1:A:348:ARG:HG3	1:A:348:ARG:HH11	1.70	0.57
1:A:135:MET:HG3	1:A:294:MET:CE	2.29	0.55
1:A:371:GLU:HB2	1:A:372:PRO:HD3	1.90	0.53
1:A:96:GLN:NE2	3:A:430:HOH:O	2.41	0.52
1:A:167:ARG:HB2	1:A:287:ARG:HB3	1.90	0.52
1:A:349:CYS:N	1:A:350:PRO:CD	2.74	0.51
1:A:12:TRP:CG	1:A:13:PRO:HA	2.48	0.49
1:A:82:ILE:HD12	1:A:127:THR:HG21	1.93	0.49
1:A:33:TRP:CE2	1:A:35:MET:HB2	2.48	0.49
1:A:262:ARG:HB3	1:A:374:LEU:CD1	2.43	0.47
1:A:221:ARG:NH1	1:A:222:ASP:OD2	2.48	0.46
1:A:48:ALA:HB2	1:A:56:ALA:HB2	1.97	0.46
1:A:324:ARG:O	1:A:325:ALA:C	2.58	0.46
1:A:214:ARG:HG2	1:A:230:ILE:HD12	1.98	0.45
1:A:136:ALA:HB3	1:A:294:MET:HE2	1.99	0.44
1:A:119:VAL:O	1:A:123:VAL:HG23	2.17	0.44
1:A:360:VAL:HG12	1:A:361:TRP:N	2.33	0.44
1:A:48:ALA:HB2	1:A:56:ALA:CB	2.48	0.43
1:A:324:ARG:HD2	3:A:491:HOH:O	2.19	0.43
1:A:123:VAL:HG11	1:A:152:THR:HG21	2.01	0.43
1:A:371:GLU:N	1:A:372:PRO:HD2	2.34	0.43
1:A:20:ARG:HH11	1:A:20:ARG:HD2	1.55	0.42
1:A:124:THR:HG22	1:A:126:ARG:N	2.10	0.42
1:A:131:MET:HA	1:A:132:PRO:HD2	1.96	0.41
1:A:115:ASP:O	1:A:119:VAL:HG12	2.21	0.41
1:A:371:GLU:O	1:A:372:PRO:C	2.64	0.41
1:A:172:ARG:O	1:A:173:VAL:C	2.62	0.41
1:A:354:ALA:O	1:A:358:ASP:HB2	2.20	0.41
1:A:108:ASP:HB3	1:A:111:THR:OG1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASN:HA	1:A:191:THR:OG1	2.21	0.40
1:A:130:ILE:HB	1:A:156:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/388 (98%)	371 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	293/296 (99%)	256 (87%)	37 (13%)	4	2

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	23	LEU
1	A	35	MET
1	A	92	SER

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Mol	Chain	Res	Type
1	A	105	VAL
1	A	112	TYR
1	A	119	VAL
1	A	124	THR
1	A	126	ARG
1	A	127	THR
1	A	139	MET
1	A	145	LEU
1	A	147	LYS
1	A	171	LYS
1	A	199	VAL
1	A	202	ASP
1	A	209	GLU
1	A	215	HIS
1	A	221	ARG
1	A	222	ASP
1	A	229	LYS
1	A	245	LEU
1	A	249	LEU
1	A	270	LEU
1	A	287	ARG
1	A	289	SER
1	A	300	LEU
1	A	311	ARG
1	A	324	ARG
1	A	335	LEU
1	A	340	GLU
1	A	347	ARG
1	A	348	ARG
1	A	353	ASP
1	A	366	VAL
1	A	371	GLU
1	A	383	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	96	GLN
1	A	186	ASN
1	A	364	HIS

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 oligosaccharides 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
2	PLP	A	389	1	15,15,16	1.96	7 (46%)	21,22,23	2.30	5 (23%)

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	A	389	1	-	3/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	389	PLP	C3-C2	-3.36	1.37	1.41
2	A	389	PLP	C2A-C2	3.03	1.55	1.50
2	A	389	PLP	C2-N1	2.89	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	389	PLP	C3-C4	2.74	1.45	1.40
2	A	389	PLP	O4P-C5A	-2.40	1.36	1.44
2	A	389	PLP	O3-C3	-2.24	1.31	1.36
2	A	389	PLP	P-O3P	-2.09	1.47	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	PLP	O4P-C5A-C5	6.08	120.76	109.36
2	A	389	PLP	C5A-C5-C6	-3.94	112.94	119.36
2	A	389	PLP	C2A-C2-C3	3.91	125.37	120.80
2	A	389	PLP	C6-C5-C4	3.27	120.78	118.10
2	A	389	PLP	C3-C4-C5	-2.52	115.56	118.59

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	389	PLP	C4-C5-C5A-O4P
2	A	389	PLP	C6-C5-C5A-O4P
2	A	389	PLP	C5A-O4P-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

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	384/388 (98%)	-0.52	2 (0%) 87 87	18, 32, 52, 84	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	ASP	2.5
1	A	344	ALA	2.1

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(Å ²)	Q<0.9
2	PLP	A	389	15/16	0.98	0.04	18,23,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.