



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:30 AM UTC

PDB ID : 1B9I / pdb_00001b9i
Title : CRYSTAL STRUCTURE OF 3-AMINO-5-HYDROXYBENZOIC ACID
(AHBA) SYNTHASE
Authors : Eads, J.C.; Beeby, M.; Scapin, G.; Yu, T.-W.; Floss, H.G.
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

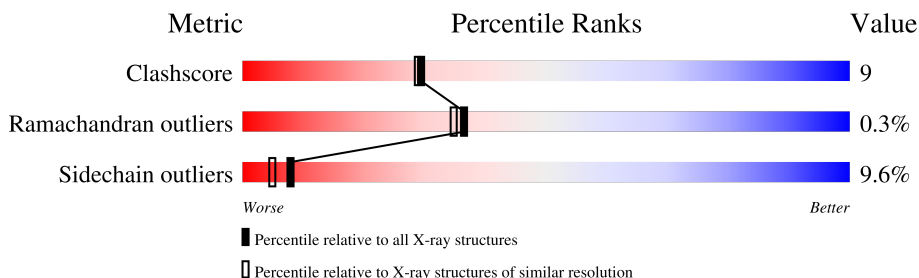
1 Overall quality at a glance

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)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	 61% 29% 7% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3157 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.

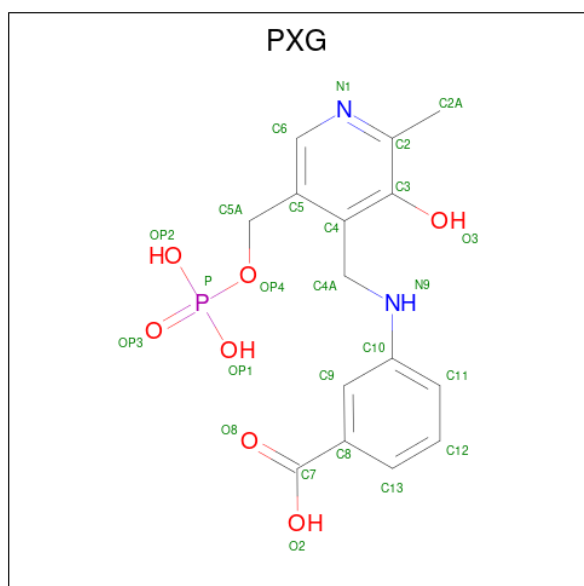
- Molecule 1 is a protein called PROTEIN (3-AMINO-5-HYDROXYBENZOIC ACID SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	2	0
			2944	1839	541	551	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	262	ARG	PRO	conflict	UNP O52552

- Molecule 2 is 3-[O-PHOSPHONOPYRIDOXYL]--AMINO-BENZOIC ACID (CCD ID: PXG) (formula: C₁₅H₁₇N₂O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	15	2	7	1		

- Molecule 3 is water.

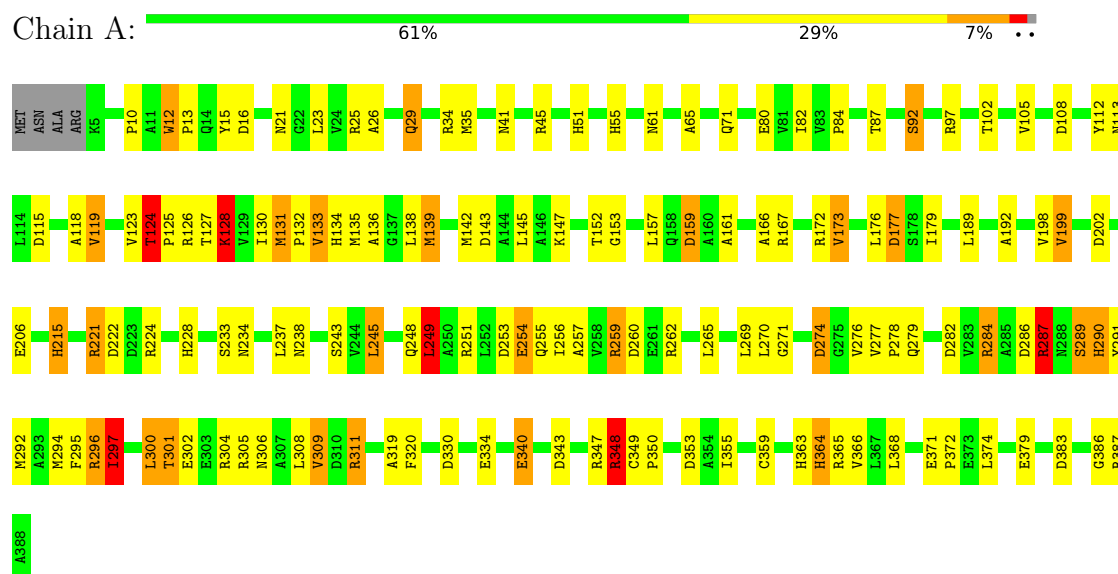
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	188	Total 188	O 188	0	0

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: PROTEIN (3-AMINO-5-HYDROXYBENZOIC ACID SYNTHASE)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.63Å 89.63Å 126.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	96.0 (20.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.222 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3157	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

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: PXG

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	1.08	1/3019 (0.0%)	2.19	119/4102 (2.9%)

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	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	MET	CA-CB	5.29	1.59	1.53

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	GLN	OE1-CD-NE2	25.33	147.93	122.60
1	A	255	GLN	OE1-CD-NE2	12.56	135.16	122.60
1	A	118	ALA	CA-C-O	-9.73	110.24	120.55
1	A	253	ASP	CA-CB-CG	-9.11	103.49	112.60
1	A	51	HIS	CA-CB-CG	-9.03	104.77	113.80
1	A	274	ASP	CA-CB-CG	8.89	121.50	112.60
1	A	286	ASP	CA-CB-CG	8.82	121.42	112.60
1	A	304	ARG	CA-C-O	-8.34	112.11	120.70
1	A	198	VAL	CA-C-O	-8.28	111.69	120.39
1	A	279	GLN	CG-CD-NE2	-8.07	104.29	116.40
1	A	363	HIS	CA-C-O	-7.95	112.44	121.19
1	A	143	ASP	CA-C-O	7.87	128.80	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	GLN	CA-C-N	7.68	130.99	120.46
1	A	255	GLN	C-N-CA	7.68	130.99	120.46
1	A	387	ARG	CD-NE-CZ	7.66	135.13	124.40
1	A	134	HIS	CA-CB-CG	-7.61	106.19	113.80
1	A	284	ARG	CD-NE-CZ	-7.49	113.91	124.40
1	A	319	ALA	CA-C-N	7.21	133.92	122.59
1	A	319	ALA	C-N-CA	7.21	133.92	122.59
1	A	248	GLN	CA-C-O	7.06	127.90	120.42
1	A	295	PHE	CA-CB-CG	6.93	120.73	113.80
1	A	304	ARG	O-C-N	6.92	129.57	122.09
1	A	348	ARG	CD-NE-CZ	6.92	134.09	124.40
1	A	84	PRO	CA-C-O	-6.91	113.02	121.31
1	A	161	ALA	O-C-N	-6.87	114.18	122.22
1	A	228	HIS	CA-CB-CG	-6.85	106.95	113.80
1	A	16	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	61	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	A	124	THR	N-CA-CB	-6.79	102.72	111.35
1	A	234	ASN	CA-C-O	-6.67	112.98	120.32
1	A	41	ASN	CA-C-N	6.66	129.09	120.44
1	A	41	ASN	C-N-CA	6.66	129.09	120.44
1	A	118	ALA	O-C-N	6.66	129.17	122.12
1	A	233	SER	CA-C-N	-6.62	113.78	123.05
1	A	233	SER	C-N-CA	-6.62	113.78	123.05
1	A	301	THR	N-CA-C	-6.59	102.30	110.41
1	A	276	VAL	N-CA-C	6.59	117.78	108.36
1	A	279	GLN	CG-CD-OE1	-6.51	107.78	120.80
1	A	334	GLU	CA-C-O	-6.50	114.00	120.82
1	A	161	ALA	CA-C-O	6.45	127.39	120.10
1	A	97	ARG	CD-NE-CZ	-6.40	115.45	124.40
1	A	274	ASP	CA-C-O	-6.35	114.05	121.16
1	A	133	VAL	CA-C-O	-6.32	113.75	120.39
1	A	251	ARG	CA-C-O	-6.32	111.66	119.18
1	A	249	LEU	CB-CA-C	-6.24	100.82	110.81
1	A	286	ASP	CA-C-N	-6.17	113.49	122.44
1	A	286	ASP	C-N-CA	-6.17	113.49	122.44
1	A	257	ALA	CA-C-O	-6.17	114.34	120.82
1	A	108	ASP	OD1-CG-OD2	6.13	137.61	122.90
1	A	173	VAL	CA-C-O	6.11	127.41	121.05
1	A	302	GLU	CA-C-O	6.09	127.42	120.90
1	A	311	ARG	NE-CZ-NH2	6.08	124.68	119.20
1	A	297	ILE	CA-CB-CG1	6.06	120.70	110.40
1	A	364	HIS	O-C-N	-6.05	114.38	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ASN	OD1-CG-ND2	6.05	128.65	122.60
1	A	45	ARG	CA-CB-CG	-6.05	102.01	114.10
1	A	271	GLY	CA-C-N	6.05	133.37	121.58
1	A	271	GLY	C-N-CA	6.05	133.37	121.58
1	A	12	TRP	O-C-N	6.02	128.20	122.06
1	A	177	ASP	CA-CB-CG	-6.01	106.59	112.60
1	A	55	HIS	CA-C-O	-5.97	114.14	121.06
1	A	243	SER	CA-C-O	-5.95	114.12	120.42
1	A	368	LEU	N-CA-C	-5.95	106.07	113.38
1	A	179	ILE	O-C-N	-5.91	116.54	122.62
1	A	302	GLU	CB-CA-C	-5.90	101.37	110.81
1	A	159	ASP	N-CA-CB	5.88	119.20	110.49
1	A	41	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	A	128	LYS	N-CA-CB	5.83	118.98	110.47
1	A	71	GLN	CA-C-O	-5.82	114.71	120.82
1	A	15	TYR	O-C-N	5.82	129.22	122.99
1	A	309	VAL	O-C-N	-5.82	116.12	121.94
1	A	21	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	237	LEU	CA-C-O	-5.81	114.23	120.92
1	A	119	VAL	N-CA-CB	5.78	119.24	110.58
1	A	254	GLU	CB-CG-CD	-5.75	102.83	112.60
1	A	113	ASN	CA-CB-CG	-5.72	106.88	112.60
1	A	259	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	A	287	ARG	O-C-N	5.66	130.50	123.14
1	A	274	ASP	N-CA-CB	5.61	118.21	109.97
1	A	15	TYR	CA-C-O	-5.60	115.32	121.31
1	A	259	ARG	CD-NE-CZ	-5.58	116.59	124.40
1	A	118	ALA	CA-C-N	-5.57	112.51	120.42
1	A	118	ALA	C-N-CA	-5.57	112.51	120.42
1	A	177	ASP	N-CA-CB	-5.57	104.08	113.15
1	A	87	THR	CA-CB-CG2	5.53	119.89	110.50
1	A	199	VAL	N-CA-CB	-5.52	101.78	111.39
1	A	256	ILE	CA-C-N	5.50	127.59	120.44
1	A	256	ILE	C-N-CA	5.50	127.59	120.44
1	A	222	ASP	CA-CB-CG	-5.47	107.13	112.60
1	A	254	GLU	CA-CB-CG	5.44	124.97	114.10
1	A	386	GLY	N-CA-C	-5.42	105.83	112.77
1	A	142	MET	CA-C-O	5.38	126.00	119.38
1	A	157	LEU	CA-C-O	-5.37	114.55	120.24
1	A	138	LEU	CA-C-O	5.36	126.31	120.58
1	A	55	HIS	O-C-N	5.35	129.47	123.27
1	A	29	GLN	N-CA-C	-5.35	106.02	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	ASN	CA-C-O	5.31	126.18	120.55
1	A	215	HIS	CA-CB-CG	5.30	119.10	113.80
1	A	224	ARG	CD-NE-CZ	5.29	131.81	124.40
1	A	290	HIS	O-C-N	5.29	128.65	122.67
1	A	131	MET	N-CA-C	5.28	120.07	108.66
1	A	26	ALA	N-CA-CB	5.25	117.68	110.07
1	A	282	ASP	N-CA-CB	5.23	118.94	110.32
1	A	80	GLU	CG-CD-OE2	-5.18	106.48	118.40
1	A	309	VAL	CA-C-O	5.18	126.66	121.27
1	A	296	ARG	O-C-N	-5.18	117.18	123.03
1	A	254	GLU	N-CA-CB	-5.17	102.27	110.28
1	A	305	ARG	CD-NE-CZ	5.16	131.62	124.40
1	A	130	ILE	CA-C-O	-5.15	114.99	120.39
1	A	34	ARG	CG-CD-NE	-5.13	100.71	112.00
1	A	84	PRO	O-C-N	5.12	129.24	123.10
1	A	199	VAL	CB-CA-C	5.11	118.24	110.62
1	A	289	SER	N-CA-C	5.10	118.76	112.54
1	A	115	ASP	CA-C-O	5.10	123.09	119.32
1	A	330	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	198	VAL	N-CA-CB	5.08	118.42	111.41
1	A	153	GLY	CA-C-N	-5.06	119.16	122.60
1	A	153	GLY	C-N-CA	-5.06	119.16	122.60
1	A	65	ALA	CA-C-O	-5.05	115.20	120.55

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	LEU	Mainchain
1	A	260	ASP	Mainchain
1	A	287	ARG	Mainchain
1	A	297	ILE	Mainchain
1	A	301	THR	Mainchain
1	A	320	PHE	Mainchain
1	A	359	CYS	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	2944	0	2853	49	0
2	A	25	0	14	1	0
3	A	188	0	0	2	0
All	All	3157	0	2867	50	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 9.

All (50) 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:135:MET:HG3	1:A:294:MET:HE1	1.51	0.91
1:A:124:THR:HG22	1:A:126:ARG:H	1.41	0.84
1:A:167:ARG:CZ	1:A:287:ARG:HH21	1.99	0.73
1:A:348:ARG:HG3	1:A:348:ARG:HH11	1.54	0.72
1:A:192:ALA:HB2	1:A:245:LEU:HD13	1.74	0.67
1:A:92:SER:HB3	1:A:102:THR:HG21	1.76	0.67
1:A:124:THR:HG23	1:A:125:PRO:HD2	1.77	0.66
1:A:296:ARG:HD2	1:A:355:ILE:HG12	1.83	0.61
1:A:135:MET:CG	1:A:294:MET:HE1	2.29	0.60
1:A:136:ALA:CB	1:A:294:MET:HE2	2.32	0.60
1:A:167:ARG:NH1	1:A:287:ARG:HH21	2.03	0.57
1:A:136:ALA:HB3	1:A:294:MET:HE2	1.86	0.55
1:A:124:THR:CG2	1:A:126:ARG:HG3	2.37	0.54
1:A:348:ARG:HG3	1:A:348:ARG:NH1	2.20	0.51
1:A:262:ARG:HB3	1:A:374:LEU:HD11	1.93	0.51
1:A:12:TRP:CG	1:A:13:PRO:HA	2.45	0.51
1:A:82:ILE:HD12	1:A:127:THR:HG21	1.93	0.51
1:A:291:TYR:O	1:A:364:HIS:HB3	2.11	0.51
1:A:124:THR:CG2	1:A:126:ARG:H	2.19	0.50
1:A:128:LYS:HE2	3:A:435:HOH:O	2.11	0.50
1:A:92:SER:CB	1:A:102:THR:HG21	2.40	0.50
1:A:128:LYS:HE3	3:A:478:HOH:O	2.11	0.50
1:A:135:MET:HG3	1:A:294:MET:CE	2.34	0.49
1:A:35:MET:SD	1:A:221:ARG:HD3	2.53	0.49
1:A:139:MET:HE2	1:A:166:ALA:HB3	1.94	0.49
1:A:124:THR:HG22	1:A:126:ARG:N	2.19	0.47
1:A:172:ARG:O	1:A:173:VAL:C	2.57	0.47
1:A:297:ILE:HB	1:A:300:LEU:HD22	1.96	0.47
2:A:389:PXG:O3	2:A:389:PXG:N9	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:CD1	1:A:289:SER:HB3	2.46	0.46
1:A:265:LEU:O	1:A:269:LEU:HG	2.16	0.45
1:A:133:VAL:HG22	1:A:159:ASP:HB3	1.98	0.45
1:A:10:PRO:HD2	1:A:365:ARG:O	2.17	0.45
1:A:176:LEU:O	1:A:177:ASP:CB	2.64	0.44
1:A:291:TYR:CD2	1:A:292:MET:HG3	2.52	0.44
1:A:25:ARG:O	1:A:29:GLN:HG3	2.17	0.44
1:A:289:SER:O	1:A:290:HIS:HB2	2.19	0.43
1:A:349:CYS:N	1:A:350:PRO:CD	2.82	0.43
1:A:167:ARG:CZ	1:A:287:ARG:NH2	2.75	0.42
1:A:131:MET:HA	1:A:132:PRO:HD2	1.91	0.42
1:A:124:THR:HG23	1:A:125:PRO:CD	2.48	0.42
1:A:308:LEU:O	1:A:309:VAL:C	2.60	0.42
1:A:343:ASP:O	1:A:347:ARG:HG3	2.19	0.42
1:A:277:VAL:HA	1:A:278:PRO:HD2	1.86	0.41
1:A:189:LEU:HD22	1:A:259:ARG:NH1	2.35	0.41
1:A:371:GLU:N	1:A:372:PRO:HD2	2.36	0.41
1:A:262:ARG:HD2	1:A:374:LEU:HD11	2.03	0.41
1:A:123:VAL:HG11	1:A:152:THR:HG21	2.02	0.41
1:A:340:GLU:OE2	1:A:348:ARG:NE	2.53	0.41
1:A:284:ARG:H	1:A:284:ARG:HG3	1.66	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	384/388 (99%)	372 (97%)	11 (3%)	1 (0%)	36	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	GLU

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	294/296 (99%)	266 (90%)	28 (10%)	8 5

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	92	SER
1	A	105	VAL
1	A	112	TYR
1	A	119	VAL
1	A	124	THR
1	A	128	LYS
1	A	139	MET
1	A	145	LEU
1	A	147	LYS
1	A	199	VAL
1	A	202	ASP
1	A	206	GLU
1	A	215	HIS
1	A	221	ARG
1	A	245	LEU
1	A	249	LEU
1	A	254	GLU
1	A	270	LEU
1	A	274	ASP
1	A	287	ARG
1	A	300	LEU
1	A	311	ARG
1	A	348	ARG
1	A	353	ASP
1	A	366	VAL

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Mol	Chain	Res	Type
1	A	379	GLU
1	A	383	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	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 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	PXG	A	389	-	26,26,26	3.54	13 (50%)	36,37,37	2.28	13 (36%)

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	PXG	A	389	-	-	5/15/15/15	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	389	PXG	C3-C4	9.03	1.53	1.40
2	A	389	PXG	C13-C8	6.95	1.49	1.39
2	A	389	PXG	C12-C11	6.61	1.50	1.38
2	A	389	PXG	C2-N1	5.86	1.44	1.33
2	A	389	PXG	C5-C4	4.67	1.47	1.40
2	A	389	PXG	C2A-C2	4.37	1.57	1.50
2	A	389	PXG	C9-C10	3.63	1.45	1.39
2	A	389	PXG	O2-C7	3.55	1.41	1.30
2	A	389	PXG	P-OP3	-3.46	1.39	1.50
2	A	389	PXG	C6-N1	3.02	1.40	1.34
2	A	389	PXG	O3-C3	-2.57	1.31	1.36
2	A	389	PXG	C6-C5	2.37	1.42	1.37
2	A	389	PXG	C5A-C5	2.00	1.56	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	PXG	C6-C5-C4	5.95	122.56	118.06
2	A	389	PXG	OP4-C5A-C5	5.19	119.08	109.36
2	A	389	PXG	C3-C4-C5	-4.00	115.10	118.73
2	A	389	PXG	OP2-P-OP4	-3.81	96.73	106.67
2	A	389	PXG	C2A-C2-C3	3.17	124.51	120.80
2	A	389	PXG	C5-C6-N1	-2.99	118.97	123.83
2	A	389	PXG	C11-C10-N9	-2.89	114.43	120.96
2	A	389	PXG	C4A-C4-C3	2.82	123.73	119.98
2	A	389	PXG	O3-C3-C2	2.79	123.36	117.58
2	A	389	PXG	OP2-P-OP3	2.44	120.34	110.83
2	A	389	PXG	C12-C13-C8	-2.42	117.98	120.36
2	A	389	PXG	OP1-P-OP4	-2.20	100.94	106.67
2	A	389	PXG	C9-C10-N9	2.03	126.25	120.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

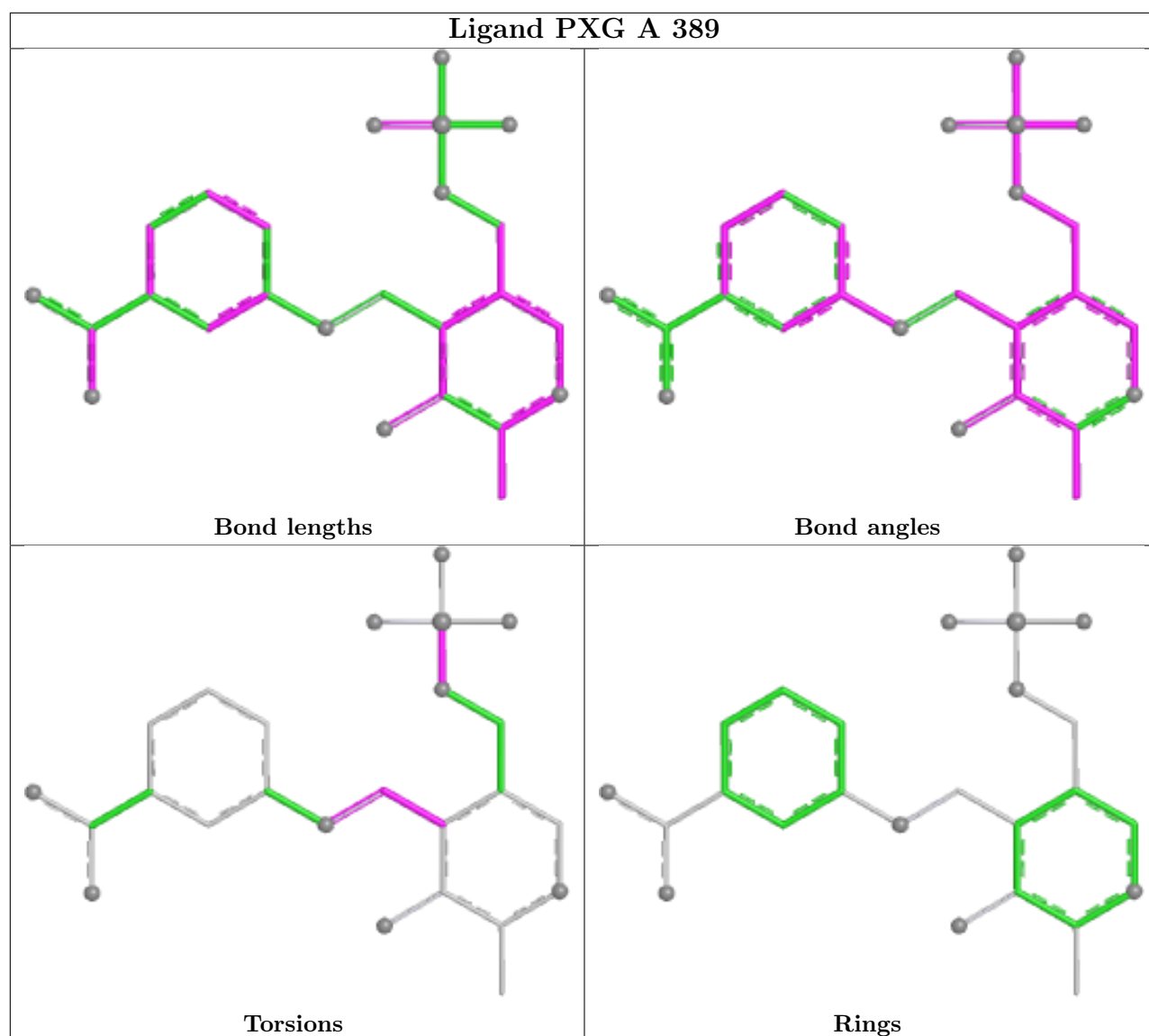
Mol	Chain	Res	Type	Atoms
2	A	389	PXG	C5A-OP4-P-OP2
2	A	389	PXG	C5-C4-C4A-N9
2	A	389	PXG	C5A-OP4-P-OP3
2	A	389	PXG	C3-C4-C4A-N9
2	A	389	PXG	C4-C4A-N9-C10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	389	PXG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.