



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 06:40 AM EDT

PDB ID : 9NNS / pdb_00009nns
Title : Flavín-dependent N5-ornithine monooxygenase EtcB
Authors : Li, Y.; Liu, X.; Smith, J.
Deposited on : 2025-03-06
Resolution : 3.00 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

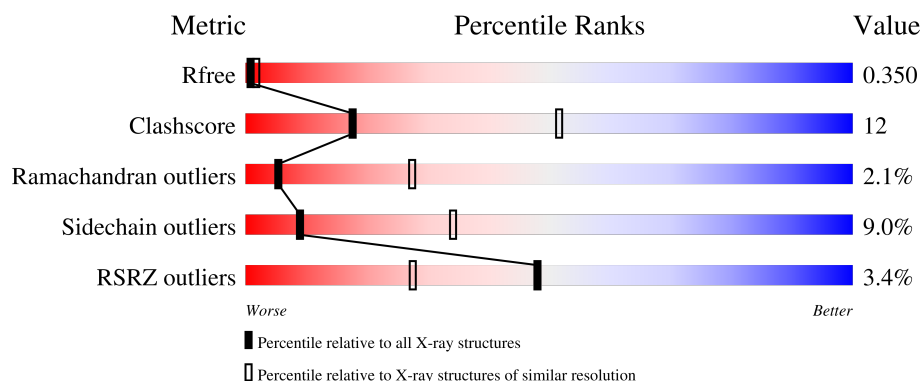
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	460	
1	B	460	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5591 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 L-lysine N6-monooxygenase MbtG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2915	1818	526	566	5			
1	B	351	Total	C	N	O	S	0	0	0
			2611	1627	471	508	5			

There are 40 discrepancies between the modelled and reference sequences:

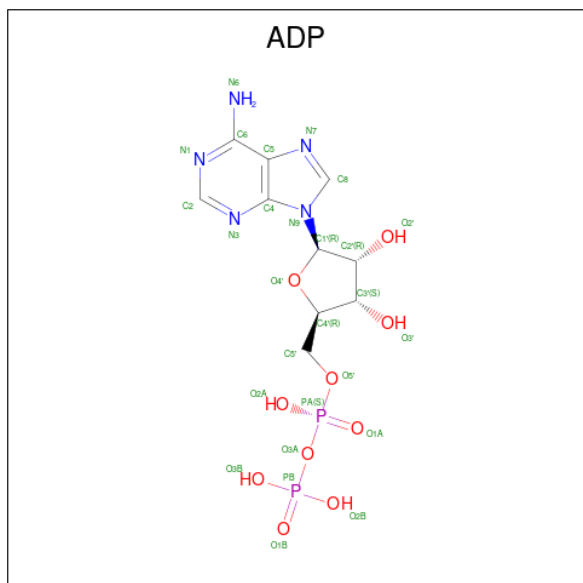
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A4FE36
A	-17	GLY	-	expression tag	UNP A4FE36
A	-16	SER	-	expression tag	UNP A4FE36
A	-15	SER	-	expression tag	UNP A4FE36
A	-14	HIS	-	expression tag	UNP A4FE36
A	-13	HIS	-	expression tag	UNP A4FE36
A	-12	HIS	-	expression tag	UNP A4FE36
A	-11	HIS	-	expression tag	UNP A4FE36
A	-10	HIS	-	expression tag	UNP A4FE36
A	-9	HIS	-	expression tag	UNP A4FE36
A	-8	SER	-	expression tag	UNP A4FE36
A	-7	SER	-	expression tag	UNP A4FE36
A	-6	GLY	-	expression tag	UNP A4FE36
A	-5	LEU	-	expression tag	UNP A4FE36
A	-4	VAL	-	expression tag	UNP A4FE36
A	-3	PRO	-	expression tag	UNP A4FE36
A	-2	ARG	-	expression tag	UNP A4FE36
A	-1	GLY	-	expression tag	UNP A4FE36
A	0	SER	-	expression tag	UNP A4FE36
A	1	HIS	-	expression tag	UNP A4FE36
B	-18	MET	-	initiating methionine	UNP A4FE36
B	-17	GLY	-	expression tag	UNP A4FE36
B	-16	SER	-	expression tag	UNP A4FE36
B	-15	SER	-	expression tag	UNP A4FE36
B	-14	HIS	-	expression tag	UNP A4FE36

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP A4FE36
B	-12	HIS	-	expression tag	UNP A4FE36
B	-11	HIS	-	expression tag	UNP A4FE36
B	-10	HIS	-	expression tag	UNP A4FE36
B	-9	HIS	-	expression tag	UNP A4FE36
B	-8	SER	-	expression tag	UNP A4FE36
B	-7	SER	-	expression tag	UNP A4FE36
B	-6	GLY	-	expression tag	UNP A4FE36
B	-5	LEU	-	expression tag	UNP A4FE36
B	-4	VAL	-	expression tag	UNP A4FE36
B	-3	PRO	-	expression tag	UNP A4FE36
B	-2	ARG	-	expression tag	UNP A4FE36
B	-1	GLY	-	expression tag	UNP A4FE36
B	0	SER	-	expression tag	UNP A4FE36
B	1	HIS	-	expression tag	UNP A4FE36

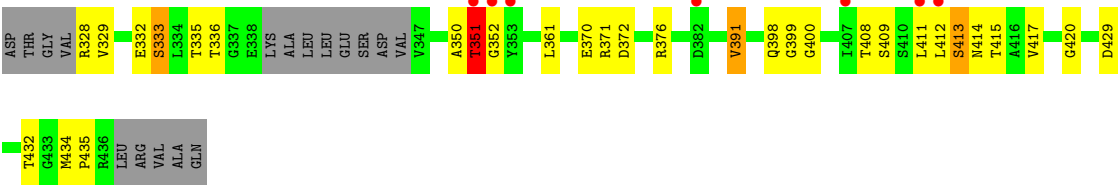
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total 7	O 7	0	0
3	B	4	Total 4	O 4	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	76.72Å 83.31Å 150.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.65 – 3.00 41.65 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.65-3.00) 99.6 (41.65-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.05 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.253 , 0.350 0.253 , 0.350	Depositor DCC
R_{free} test set	1101 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	91.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 85.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5591	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ADP

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	0.42	0/2967	0.68	0/4025
1	B	0.41	0/2653	0.68	0/3599
All	All	0.42	0/5620	0.68	0/7624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2915	0	2751	73	0
1	B	2611	0	2457	67	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
3	A	7	0	0	0	0
3	B	4	0	0	2	0
All	All	5591	0	5232	134	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 12.

All (134) 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:355:PRO:HB3	1:A:400:GLY:HA3	1.53	0.90
1:B:432:THR:HG22	1:B:434:MET:H	1.46	0.80
1:A:398:GLN:HG2	1:A:418:ARG:HE	1.48	0.78
1:B:50:LYS:HD2	1:B:57:ARG:HD3	1.66	0.78
1:A:301:GLU:HB3	1:A:307:GLU:HA	1.69	0.75
1:B:51:PRO:HD2	1:B:57:ARG:HH12	1.53	0.74
1:A:12:ASP:HA	1:A:165:ARG:HH11	1.53	0.73
1:A:322:GLU:HA	1:A:327:VAL:HA	1.71	0.72
1:B:213:ALA:H	1:B:350:ALA:HB3	1.54	0.72
1:B:12:ASP:HA	1:B:165:ARG:HH11	1.53	0.71
1:A:359:THR:HG22	1:A:377:TYR:OH	1.91	0.70
1:B:221:VAL:HG13	1:B:311:VAL:HG11	1.73	0.69
1:A:13:LEU:HD22	1:A:44:ALA:HB1	1.77	0.65
1:B:210:VAL:HG12	1:B:211:VAL:H	1.62	0.64
1:A:357:ASP:OD1	1:A:359:THR:HG23	1.98	0.63
1:A:212:GLY:HA3	1:A:217:ALA:HB2	1.82	0.62
1:A:355:PRO:CB	1:A:400:GLY:HA3	2.25	0.61
1:B:8:ASN:HB2	1:B:163:PRO:HD2	1.82	0.61
1:B:10:VAL:HA	1:B:163:PRO:HB2	1.81	0.61
1:A:71:LEU:HD13	1:B:100:ILE:HG12	1.84	0.59
1:B:145:VAL:HB	1:B:391:VAL:HG13	1.85	0.59
1:A:309:LEU:HD23	1:A:310:ARG:H	1.69	0.58
1:A:288:LEU:HA	1:A:291:ILE:HD12	1.86	0.58
1:A:49:SER:O	1:A:130:GLY:HA2	2.03	0.57
1:A:77:GLN:HG2	1:B:100:ILE:HD12	1.85	0.57
1:A:354:ARG:HA	1:A:404:THR:HG22	1.87	0.57
1:A:95:ARG:CZ	1:A:95:ARG:HB3	2.35	0.57
1:B:302:LYS:O	1:B:303:VAL:HB	2.04	0.57
1:A:66:MET:HG3	1:A:107:PRO:O	2.05	0.56
1:A:320:VAL:HA	1:A:329:VAL:HA	1.86	0.56
1:A:138:PRO:HB3	1:A:365:LEU:HD21	1.87	0.56
1:B:116:PHE:HZ	1:B:411:LEU:HD11	1.70	0.56
1:A:220:VAL:O	1:A:224:LEU:HG	2.07	0.55
1:A:228:PHE:HB3	1:A:229:GLN:OE1	2.06	0.55
1:A:60:LEU:HD13	1:A:113:HIS:CE1	2.43	0.54
1:B:136:VAL:HG13	1:B:148:PHE:HB3	1.90	0.53
1:A:36:VAL:HG23	1:A:41:GLN:NE2	2.24	0.53
1:A:73:ASP:OD2	1:A:85:SER:HA	2.09	0.53
1:A:190:ASN:OD1	1:A:350:ALA:HA	2.10	0.52
1:B:66:MET:O	1:B:106:PHE:HB3	2.10	0.52
1:A:101:ASN:O	1:A:103:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLU:CD	1:A:78:ARG:HH22	2.18	0.52
1:B:55:TRP:HD1	2:B:501:ADP:O2A	1.93	0.52
1:A:161:THR:HG22	1:A:163:PRO:HD3	1.91	0.52
1:B:250:PHE:HA	3:B:603:HOH:O	2.10	0.52
1:A:103:LYS:HD2	1:B:252:ASN:ND2	2.26	0.51
1:A:292:ASN:O	1:A:296:ARG:HB2	2.10	0.51
1:A:303:VAL:HG12	1:A:304:LEU:HD23	1.91	0.51
1:A:292:ASN:HA	1:A:295:TYR:CD1	2.45	0.51
1:B:78:ARG:HD2	1:B:420:GLY:HA3	1.92	0.51
1:B:293:ASP:O	1:B:297:ARG:HG2	2.11	0.50
1:B:55:TRP:HH2	1:B:408:THR:HA	1.76	0.50
1:B:287:ASP:O	1:B:291:ILE:HG12	2.12	0.50
1:B:14:VAL:O	1:B:167:VAL:HA	2.11	0.49
1:B:414:ASN:ND2	1:B:417:VAL:HB	2.27	0.49
1:B:153:ARG:HD3	1:B:157:GLY:HA2	1.92	0.49
1:B:69:SER:HB2	1:B:105:LEU:HB3	1.95	0.49
1:A:326:GLY:HA3	1:A:344:SER:O	2.13	0.49
1:B:225:HIS:HE1	1:B:297:ARG:HB3	1.78	0.48
1:A:13:LEU:HD12	1:A:426:ILE:HD12	1.95	0.48
1:B:189:HIS:CG	1:B:190:ASN:H	2.32	0.48
1:B:212:GLY:HA3	3:B:601:HOH:O	2.14	0.48
1:B:170:ALA:HA	1:B:399:GLY:HA3	1.95	0.48
1:A:13:LEU:HD22	1:A:44:ALA:CB	2.43	0.47
1:A:288:LEU:HD23	1:A:291:ILE:HD12	1.96	0.47
1:A:224:LEU:O	1:A:229:GLN:HB2	2.13	0.47
1:A:73:ASP:OD1	1:A:76:THR:HB	2.15	0.47
1:A:331:VAL:O	1:A:339:LYS:HA	2.15	0.47
1:B:222:ALA:HA	1:B:294:LEU:HD11	1.98	0.46
1:B:286:VAL:HB	1:B:291:ILE:HD11	1.96	0.46
1:A:55:TRP:CG	1:A:56:HIS:H	2.33	0.46
1:A:396:TYR:O	1:A:397:LEU:HD23	2.15	0.46
1:B:12:ASP:HA	1:B:165:ARG:NH1	2.25	0.46
1:A:407:ILE:O	1:A:411:LEU:HD13	2.16	0.46
1:A:70:PHE:HE2	1:A:87:LEU:HD11	1.80	0.46
1:B:414:ASN:CG	1:B:417:VAL:HB	2.41	0.46
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.71	0.45
1:A:96:LEU:HD22	1:B:80:PRO:HG3	1.97	0.45
1:B:213:ALA:N	1:B:350:ALA:HB3	2.29	0.45
1:B:140:VAL:HA	1:B:144:VAL:O	2.15	0.45
1:B:361:LEU:HA	1:B:361:LEU:HD23	1.74	0.45
1:A:208:PHE:CE2	1:A:224:LEU:HD22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG23	1:A:41:GLN:HE21	1.81	0.45
1:B:101:ASN:O	1:B:103:LYS:HG3	2.16	0.45
1:B:351:THR:HB	1:B:352:GLY:H	1.46	0.45
1:B:21:SER:HB3	1:B:398:GLN:HG3	1.99	0.44
1:B:55:TRP:CH2	1:B:408:THR:HA	2.51	0.44
1:B:328:ARG:NH1	1:B:328:ARG:HA	2.32	0.44
1:A:222:ALA:O	1:A:225:HIS:HB2	2.18	0.44
1:B:79:ASN:ND2	1:B:82:SER:HB2	2.33	0.44
1:B:307:GLU:C	1:B:309:LEU:H	2.26	0.43
1:B:72:LYS:HE3	1:B:412:LEU:HD23	2.00	0.43
1:A:355:PRO:HB3	1:A:400:GLY:CA	2.35	0.43
1:A:60:LEU:HD13	1:A:113:HIS:HE1	1.83	0.43
1:B:182:THR:HG22	1:B:183:SER:H	1.84	0.43
1:A:362:LEU:HB2	1:A:366:ALA:HB2	2.00	0.43
1:A:77:GLN:HE21	1:A:77:GLN:HB3	1.51	0.43
1:A:383:TYR:O	1:A:396:TYR:HA	2.19	0.43
1:B:49:SER:O	1:B:130:GLY:HA2	2.19	0.43
1:B:59:MET:HE2	1:B:59:MET:HB3	1.94	0.43
1:A:176:ASN:ND2	1:A:178:PRO:HG3	2.34	0.42
1:B:332:GLU:HG2	1:B:333:SER:H	1.84	0.42
1:B:73:ASP:HB2	1:B:115:TYR:CE2	2.54	0.42
1:A:10:VAL:HA	1:A:163:PRO:HB2	2.01	0.42
1:A:71:LEU:HB3	1:B:100:ILE:CD1	2.50	0.42
1:A:71:LEU:HB3	1:B:100:ILE:HD13	2.02	0.42
1:A:215:GLN:OE1	1:A:287:ASP:HB2	2.19	0.42
1:B:55:TRP:CH2	1:B:408:THR:HG22	2.55	0.42
1:A:60:LEU:HD11	1:A:110:VAL:HG12	2.02	0.42
1:B:370:GLU:C	1:B:371:ARG:HG3	2.45	0.41
1:B:432:THR:HG22	1:B:434:MET:N	2.26	0.41
1:A:89:TYR:CD2	1:A:115:TYR:HB2	2.54	0.41
1:A:217:ALA:HB2	1:A:350:ALA:HB3	2.03	0.41
1:A:144:VAL:HA	1:A:390:ALA:O	2.21	0.41
1:A:292:ASN:HA	1:A:295:TYR:HD1	1.84	0.41
1:A:301:GLU:CD	1:A:308:ARG:H	2.27	0.41
1:B:69:SER:HA	1:B:105:LEU:O	2.21	0.41
1:B:372:ASP:OD1	1:B:376:ARG:HB2	2.21	0.41
1:A:90:LEU:HD22	1:A:95:ARG:HB2	2.02	0.41
1:A:145:VAL:HB	1:A:391:VAL:HG13	2.02	0.41
1:B:175:PRO:HB3	1:B:189:HIS:CD2	2.56	0.41
1:B:411:LEU:C	1:B:413:SER:N	2.79	0.41
1:A:361:LEU:HA	1:A:361:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:HA	1:B:166:ASN:O	2.21	0.41
1:A:21:SER:HA	1:A:415:THR:HG23	2.02	0.41
1:B:189:HIS:CG	1:B:190:ASN:N	2.89	0.41
1:B:217:ALA:O	1:B:221:VAL:HG23	2.21	0.41
1:B:225:HIS:CE1	1:B:297:ARG:HB3	2.56	0.41
1:A:208:PHE:CD2	1:A:224:LEU:HD13	2.55	0.40
1:A:308:ARG:N	1:A:308:ARG:HD2	2.36	0.40
1:B:71:LEU:HA	1:B:71:LEU:HD23	1.86	0.40
1:A:400:GLY:O	1:A:401:THR:C	2.64	0.40
1:A:294:LEU:HA	1:A:294:LEU:HD23	1.69	0.40
1:B:414:ASN:O	1:B:415:THR:C	2.62	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	366/460 (80%)	325 (89%)	35 (10%)	6 (2%)	7	34
1	B	333/460 (72%)	288 (86%)	36 (11%)	9 (3%)	4	22
All	All	699/920 (76%)	613 (88%)	71 (10%)	15 (2%)	5	27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	TRP
1	A	225	HIS
1	A	401	THR
1	B	178	PRO
1	B	413	SER
1	B	305	GLY
1	B	400	GLY

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Mol	Chain	Res	Type
1	A	228	PHE
1	B	351	THR
1	B	251	ALA
1	B	336	THR
1	B	435	PRO
1	A	179	GLU
1	A	413	SER
1	B	183	SER

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	301/386 (78%)	277 (92%)	24 (8%)	11	38
1	B	266/386 (69%)	239 (90%)	27 (10%)	7	29
All	All	567/772 (73%)	516 (91%)	51 (9%)	9	34

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	13	LEU
1	A	61	ILE
1	A	76	THR
1	A	95	ARG
1	A	112	PHE
1	A	117	GLU
1	A	126	SER
1	A	137	GLU
1	A	161	THR
1	A	185	ASP
1	A	190	ASN
1	A	209	VAL
1	A	228	PHE
1	A	285	VAL

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Mol	Chain	Res	Type
1	A	308	ARG
1	A	309	LEU
1	A	314	THR
1	A	331	VAL
1	A	351	THR
1	A	391	VAL
1	A	402	GLU
1	A	403	HIS
1	A	432	THR
1	B	13	LEU
1	B	20	PRO
1	B	76	THR
1	B	112	PHE
1	B	123	LEU
1	B	140	VAL
1	B	144	VAL
1	B	154	THR
1	B	160	MET
1	B	182	THR
1	B	193	LEU
1	B	209	VAL
1	B	211	VAL
1	B	234	SER
1	B	252	ASN
1	B	294	LEU
1	B	295	TYR
1	B	302	LYS
1	B	312	LEU
1	B	313	ASN
1	B	329	VAL
1	B	333	SER
1	B	335	THR
1	B	351	THR
1	B	391	VAL
1	B	409	SER
1	B	429	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	B	91	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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	ADP	B	501	-	28,29,29	1.55	5 (17%)	43,45,45	1.91	13 (30%)
2	ADP	A	501	-	28,29,29	1.69	4 (14%)	43,45,45	1.97	14 (32%)

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	ADP	B	501	-	-	3/16/32/32	0/3/3/3
2	ADP	A	501	-	-	2/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ADP	C5-C4	5.23	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ADP	C5-C4	4.95	1.47	1.39
2	A	501	ADP	PA-O3A	4.03	1.63	1.59
2	B	501	ADP	PA-O3A	3.28	1.63	1.59
2	A	501	ADP	C5-C6	3.02	1.49	1.41
2	B	501	ADP	C5-C6	2.77	1.48	1.41
2	A	501	ADP	C8-N7	2.66	1.36	1.31
2	B	501	ADP	C8-N7	2.37	1.36	1.31
2	B	501	ADP	C5-N7	-2.19	1.35	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	ADP	C5-C4-N3	-5.33	119.38	126.72
2	A	501	ADP	C5-C4-N3	-5.29	119.43	126.72
2	B	501	ADP	N3-C4-N9	4.45	134.74	127.17
2	A	501	ADP	N3-C4-N9	4.41	134.67	127.17
2	A	501	ADP	N3-C2-N1	-3.87	122.72	128.58
2	A	501	ADP	C2-N3-C4	3.66	120.78	111.83
2	B	501	ADP	N3-C2-N1	-3.59	123.15	128.58
2	B	501	ADP	C2-N3-C4	3.55	120.50	111.83
2	B	501	ADP	C4-C5-N7	-3.31	106.80	110.58
2	A	501	ADP	C4-C5-N7	-3.30	106.81	110.58
2	A	501	ADP	C4-N9-C8	3.23	109.13	105.74
2	B	501	ADP	O3B-PB-O3A	-3.20	93.91	104.64
2	B	501	ADP	C4-N9-C8	3.03	108.92	105.74
2	A	501	ADP	C2-N1-C6	2.63	123.05	118.73
2	B	501	ADP	C5-N7-C8	2.58	107.51	103.45
2	A	501	ADP	C5-N7-C8	2.42	107.26	103.45
2	B	501	ADP	C2-N1-C6	2.35	122.59	118.73
2	A	501	ADP	O2B-PB-O3A	2.32	112.42	104.64
2	A	501	ADP	C2'-C3'-C4'	2.29	107.03	102.61
2	A	501	ADP	O3A-PB-O1B	-2.28	99.03	111.04
2	B	501	ADP	O3B-PB-O2B	2.26	116.29	107.80
2	B	501	ADP	C6-C5-N7	2.20	136.33	132.09
2	A	501	ADP	N6-C6-N1	2.17	123.21	118.38
2	B	501	ADP	N9-C8-N7	-2.14	110.90	113.94
2	A	501	ADP	N9-C8-N7	-2.14	110.90	113.94
2	A	501	ADP	C2'-C1'-N9	2.12	118.57	113.30
2	B	501	ADP	O3B-PB-O1B	2.10	119.03	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

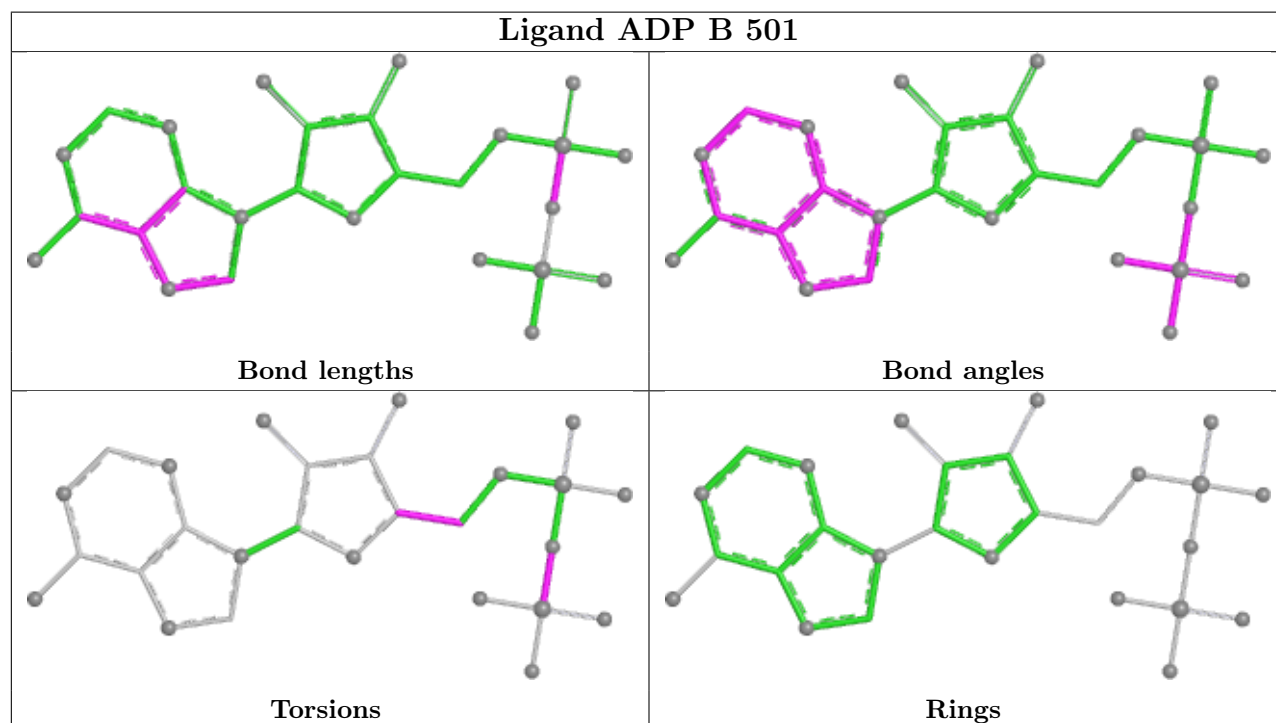
Mol	Chain	Res	Type	Atoms
2	B	501	ADP	PA-O3A-PB-O2B
2	B	501	ADP	PA-O3A-PB-O3B
2	A	501	ADP	PB-O3A-PA-O5'
2	A	501	ADP	PB-O3A-PA-O2A
2	B	501	ADP	O4'-C4'-C5'-O5'

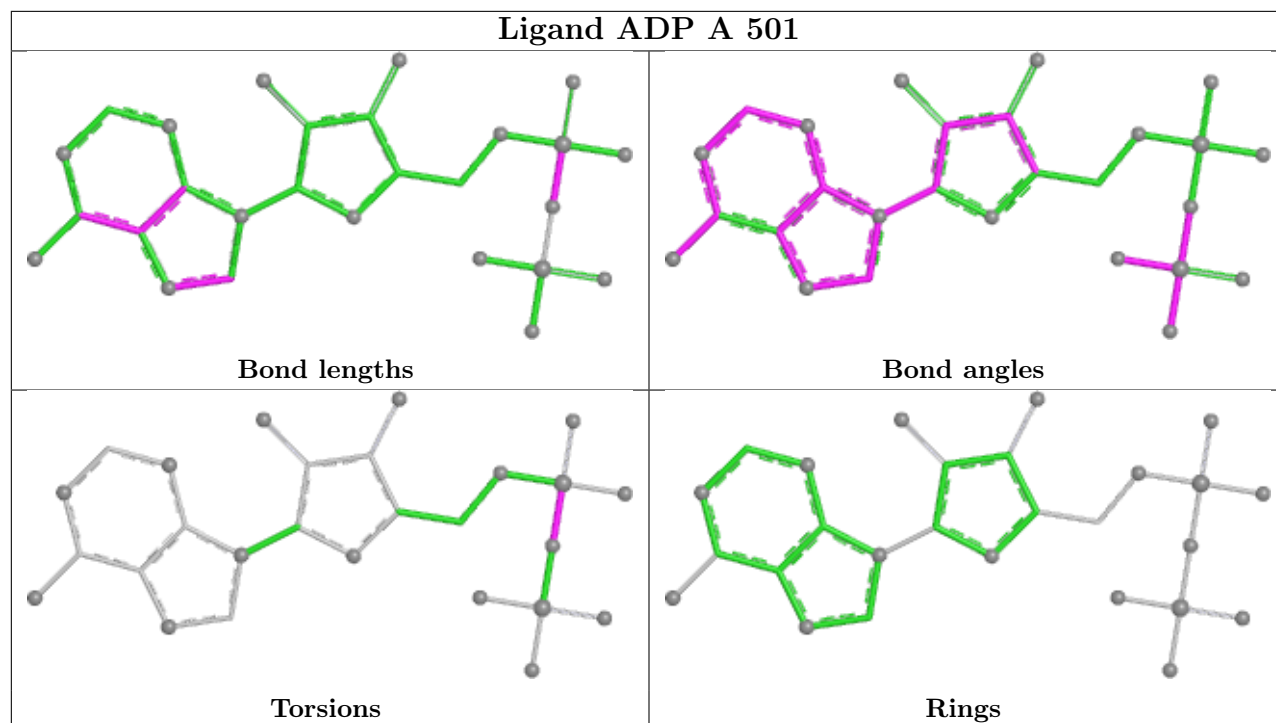
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	ADP	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

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	382/460 (83%)	0.09	8 (2%) 63 40	47, 95, 174, 192	0
1	B	351/460 (76%)	0.23	17 (4%) 35 19	49, 101, 161, 172	0
All	All	733/920 (79%)	0.16	25 (3%) 48 27	47, 98, 165, 192	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	353	TYR	5.5
1	B	252	ASN	3.3
1	B	313	ASN	3.2
1	B	236	VAL	3.0
1	A	353	TYR	3.0
1	B	412	LEU	3.0
1	B	407	ILE	2.9
1	B	237	PHE	2.7
1	A	55	TRP	2.7
1	A	212	GLY	2.7
1	B	351	THR	2.7
1	B	312	LEU	2.6
1	A	188	TRP	2.5
1	B	211	VAL	2.4
1	A	348	VAL	2.4
1	B	162	TYR	2.4
1	B	352	GLY	2.4
1	A	187	VAL	2.3
1	B	210	VAL	2.2
1	A	349	TYR	2.2
1	B	47	LEU	2.1
1	B	246	ASP	2.1
1	A	351	THR	2.0
1	B	411	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	382	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

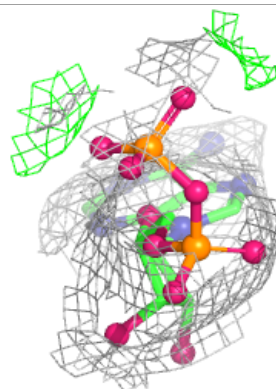
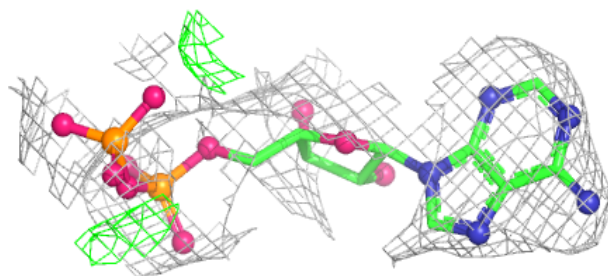
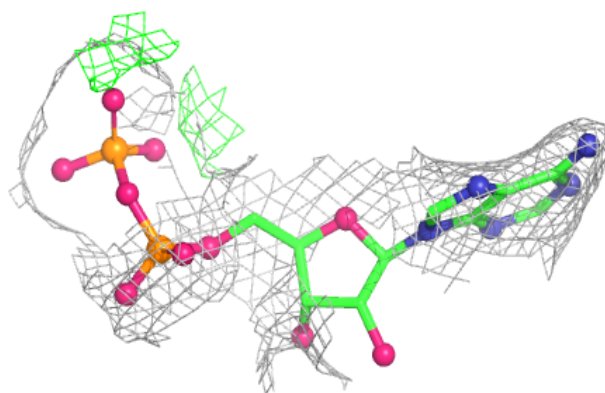
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ADP	A	501	27/27	0.81	0.10	64,86,103,107	0
2	ADP	B	501	27/27	0.89	0.09	66,85,96,97	27

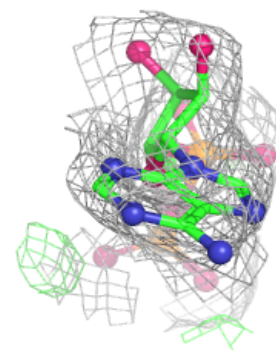
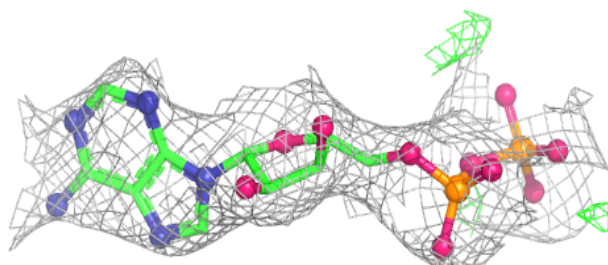
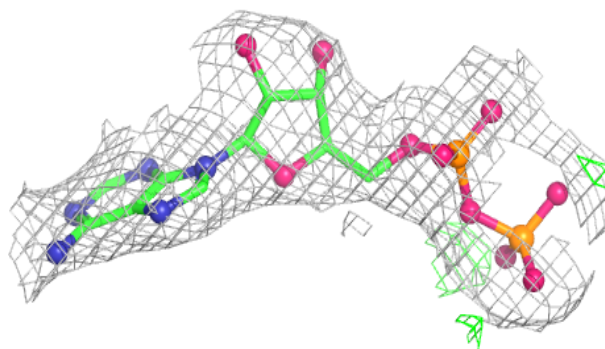
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP B 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.