



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:26 PM UTC

PDB ID : 8YTT / pdb_00008ytt
Title : Structure of cyclohexanone monooxygenase mutant from *Acinetobacter calcoaceticus*
Authors : Qiang, G.; Zheng, Y.C.; Feng, L.; Yu, H.L.
Deposited on : 2024-03-26
Resolution : 2.14 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

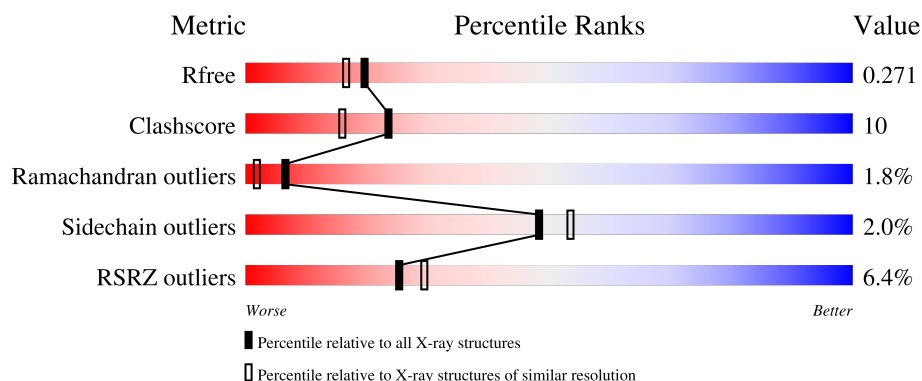
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	548	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4579 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.

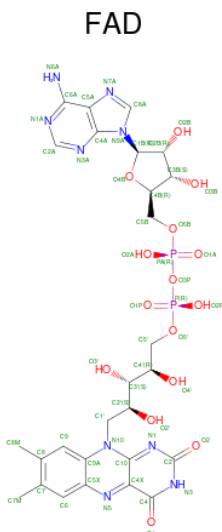
- Molecule 1 is a protein called Putative flavin-binding monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	518	4128	2629	692	788	19	0	1	0

There are 21 discrepancies between the modelled and reference sequences:

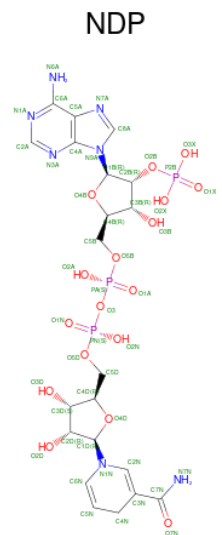
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A0A0A8XFY0
A	-4	HIS	-	expression tag	UNP A0A0A8XFY0
A	-3	HIS	-	expression tag	UNP A0A0A8XFY0
A	-2	HIS	-	expression tag	UNP A0A0A8XFY0
A	-1	HIS	-	expression tag	UNP A0A0A8XFY0
A	0	HIS	-	expression tag	UNP A0A0A8XFY0
A	1	HIS	-	expression tag	UNP A0A0A8XFY0
A	246	TYR	PHE	engineered mutation	UNP A0A0A8XFY0
A	326	CYS	LYS	engineered mutation	UNP A0A0A8XFY0
A	386	SER	ASN	engineered mutation	UNP A0A0A8XFY0
A	388	LYS	ILE	engineered mutation	UNP A0A0A8XFY0
A	390	ILE	MET	engineered mutation	UNP A0A0A8XFY0
A	426	PHE	LEU	engineered mutation	UNP A0A0A8XFY0
A	432	LEU	PHE	engineered mutation	UNP A0A0A8XFY0
A	433	ALA	THR	engineered mutation	UNP A0A0A8XFY0
A	435	SER	LEU	engineered mutation	UNP A0A0A8XFY0
A	438	ILE	SER	engineered mutation	UNP A0A0A8XFY0
A	488	LYS	GLU	engineered mutation	UNP A0A0A8XFY0
A	489	CYS	SER	engineered mutation	UNP A0A0A8XFY0
A	490	ARG	TRP	engineered mutation	UNP A0A0A8XFY0
A	505	LEU	PHE	engineered mutation	UNP A0A0A8XFY0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	350	Total 350	O 350	0	0

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.

Chain A:

6% 74% 19% 5%

MET HIS HIS HIS HIS HIS HIS THR GLN LYS W5 D6 F7 I11 I12 I13 A14 L22 K32 V33 V42 V46 M49 Q50 Y51 D57 S58 L71 R79 I82 S83 Q84 V87 V94 A95 D96 R101 I110 R111 S120 F121 W122 T126 D129 T133 A134 I138 T139 L143 L144 A145 A146 P147 M148 L149 P150 P151 I152 K153 K159 F174 R178 T187 V199 Q206 T223 K227 Y232 V258 E262 K265 K269 E273 M280 K303 E307 T321 D322 L323 V324 A325 T326 R327 P328 F338 L345 A350 I356 K357 E358 D359 C360 V361 V362 E368 R369 K370 T378 G379 F380 D381 D384 K388 K389 I390 G394 K395 D396 G397 I398 S399 I400 K401 W404 P408 N409 L412 N429 P436 P437 E440 R444 W445 I458 W459 Q460 T472 H473 T474 G475 S476 D477 T478 T482 L483 F484 A485 K488 K489 R490 ILE PHE GLY ALA ASN VAL PRO GLY LYS LYS Y501 T502 Y503 Y504 M507 R514 I517 V520 K526 L530 K531 Q532 SER VAL LYS THR ASN LEU ILE GLU SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.72Å 53.22Å 101.61Å 90.00° 96.72° 90.00°	Depositor
Resolution (Å)	34.38 – 2.14 34.38 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.38-2.14) 99.2 (34.38-2.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.211 , 0.268 0.213 , 0.271	Depositor DCC
R_{free} test set	1487 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4579	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, FAD

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	0.11	0/4219	0.32	0/5709

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 [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	4128	0	4040	84	0
2	A	53	0	31	3	0
3	A	48	0	26	1	0
4	A	350	0	0	22	0
All	All	4579	0	4097	85	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 10.

All (85) 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:150:PRO:C	1:A:152:ILE:H	1.96	0.73
1:A:488:LYS:HA	1:A:488:LYS:HE2	1.72	0.71
1:A:280:MET:HE2	1:A:328:PRO:HD2	1.73	0.69
1:A:147:PRO:HD3	1:A:380:PHE:HA	1.75	0.67
1:A:390:ILE:HG23	4:A:751:HOH:O	1.94	0.66
1:A:150:PRO:O	1:A:152:ILE:N	2.29	0.65
1:A:145:ALA:HB3	1:A:381:ASP:HB2	1.79	0.64
1:A:12:ILE:HD12	1:A:139:THR:HG22	1.81	0.62
1:A:388:LYS:NZ	4:A:709:HOH:O	2.33	0.62
1:A:159:LYS:HG3	1:A:358:GLU:HB2	1.82	0.60
1:A:488:LYS:NZ	4:A:710:HOH:O	2.33	0.60
1:A:370:LYS:HG2	4:A:974:HOH:O	2.01	0.59
1:A:520:VAL:HG23	4:A:824:HOH:O	2.01	0.59
1:A:526:LYS:NZ	4:A:712:HOH:O	2.35	0.59
1:A:401:LYS:NZ	4:A:711:HOH:O	2.34	0.58
1:A:395:LYS:O	1:A:398:ILE:HD12	2.04	0.57
1:A:206:GLN:NE2	4:A:714:HOH:O	2.37	0.57
1:A:153:LYS:NZ	4:A:708:HOH:O	2.31	0.56
1:A:178:ARG:NH2	4:A:719:HOH:O	2.40	0.53
1:A:396:ASP:HB2	1:A:398:ILE:HD11	1.90	0.53
1:A:269:LYS:O	1:A:273:GLU:HG3	2.08	0.53
1:A:49:ASN:O	1:A:84:GLN:HG3	2.10	0.51
1:A:400:ILE:HD13	4:A:1049:HOH:O	2.11	0.51
1:A:474:THR:O	1:A:478:ILE:HG13	2.09	0.51
1:A:57:ASP:N	2:A:601:FAD:O4	2.43	0.51
1:A:345:LEU:HG	4:A:779:HOH:O	2.09	0.51
1:A:490:ARG:HG2	1:A:502:THR:O	2.12	0.50
1:A:120:SER:OG	1:A:460:GLN:OE1	2.30	0.49
1:A:6:ASP:HB2	1:A:133:THR:O	2.12	0.49
1:A:174:PHE:HB3	1:A:199:VAL:HG12	1.94	0.49
1:A:11:ILE:HG12	1:A:138:ILE:HB	1.95	0.49
1:A:7:PHE:HD1	1:A:32:LYS:HD3	1.77	0.49
1:A:412:LEU:HD22	4:A:907:HOH:O	2.13	0.49
1:A:148:ASN:O	1:A:150:PRO:HD2	2.12	0.48
1:A:357:LYS:HG3	4:A:918:HOH:O	2.12	0.48
1:A:357:LYS:HB2	1:A:360:CYS:SG	2.53	0.48
1:A:71:LEU:HD21	1:A:94:VAL:HG22	1.96	0.47
1:A:530:LEU:C	1:A:531:LYS:HD2	2.39	0.47
1:A:150:PRO:C	1:A:152:ILE:N	2.63	0.47
1:A:514:ARG:HA	1:A:517:ILE:HG12	1.95	0.47
1:A:429:ASN:ND2	1:A:503:VAL:O	2.48	0.47
1:A:14:ALA:HB1	4:A:797:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HD23	4:A:1020:HOH:O	2.14	0.47
1:A:79:ARG:NH1	4:A:733:HOH:O	2.49	0.46
1:A:395:LYS:O	1:A:397:GLY:N	2.49	0.46
1:A:357:LYS:HB3	1:A:357:LYS:HE3	1.64	0.46
1:A:507:MET:HE3	1:A:507:MET:HB3	1.58	0.46
1:A:327:ARG:HB3	1:A:488:LYS:NZ	2.30	0.46
1:A:58:SER:N	2:A:601:FAD:O4	2.47	0.45
1:A:395:LYS:C	1:A:397:GLY:H	2.24	0.45
1:A:96:ASP:OD1	1:A:101:ARG:NH1	2.44	0.45
1:A:122:TRP:HB2	4:A:703:HOH:O	2.16	0.45
1:A:110:ILE:HA	1:A:126:THR:HA	1.98	0.45
1:A:490:ARG:HB3	1:A:504:TYR:H	1.82	0.45
1:A:404:TRP:NE1	1:A:409:ASN:H	2.16	0.44
1:A:445:TRP:NE1	4:A:715:HOH:O	2.50	0.44
1:A:147:PRO:HD3	1:A:380:PHE:CA	2.46	0.44
1:A:46:TRP:NE1	4:A:718:HOH:O	2.49	0.44
1:A:398:ILE:HD12	1:A:398:ILE:H	1.83	0.44
1:A:436:PRO:HB2	1:A:437:PRO:HD3	1.98	0.44
1:A:458:ILE:HD13	1:A:530:LEU:HB3	1.99	0.43
1:A:111:ARG:NH2	1:A:129:ASP:OD1	2.51	0.43
1:A:121:PHE:HB2	1:A:134:ALA:O	2.17	0.43
1:A:404:TRP:CD1	1:A:408:PRO:HA	2.52	0.43
1:A:489:CYS:SG	1:A:490:ARG:N	2.91	0.43
1:A:440:GLU:OE1	1:A:444:ARG:NH2	2.52	0.43
1:A:82:ILE:HG12	1:A:87:VAL:HG23	2.01	0.43
1:A:149:LEU:HD11	3:A:602:NDP:N6A	2.33	0.43
1:A:51:TYR:CZ	1:A:187:THR:HG23	2.53	0.42
1:A:490:ARG:HA	1:A:490:ARG:HD2	1.60	0.42
1:A:384:ASP:OD1	1:A:384:ASP:N	2.39	0.42
1:A:258:VAL:HB	1:A:262:GLU:HG2	2.02	0.42
1:A:445:TRP:HZ2	4:A:824:HOH:O	2.02	0.42
1:A:368:GLU:HB3	4:A:974:HOH:O	2.20	0.42
1:A:71:LEU:HD12	1:A:71:LEU:HA	1.91	0.41
1:A:338:PHE:CE1	1:A:345:LEU:HD13	2.55	0.41
1:A:396:ASP:HB2	1:A:398:ILE:CD1	2.49	0.41
1:A:395:LYS:C	1:A:397:GLY:N	2.78	0.41
1:A:472:THR:O	1:A:476:SER:OG	2.28	0.41
1:A:303:LYS:O	1:A:307:GLU:HG3	2.21	0.41
1:A:150:PRO:C	1:A:151:LYS:HG2	2.45	0.41
1:A:262:GLU:HA	1:A:265:LYS:HE3	2.03	0.41
1:A:152:ILE:CG2	1:A:356:ILE:HG13	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:THR:O	1:A:227:LYS:HG3	2.21	0.40
2:A:601:FAD:H9	2:A:601:FAD:H1'1	1.84	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	515/548 (94%)	488 (95%)	17 (3%)	10 (2%)	6 2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	ASP
1	A	145	ALA
1	A	150	PRO
1	A	151	LYS
1	A	321	THR
1	A	148	ASN
1	A	325	ALA
1	A	146[A]	ALA
1	A	146[B]	ALA
1	A	489	CYS

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	445/472 (94%)	436 (98%)	9 (2%)	48 53

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	42	VAL
1	A	120	SER
1	A	143	LEU
1	A	149	LEU
1	A	232	TYR
1	A	323	LEU
1	A	362	VAL
1	A	526	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	119	ASN
1	A	206	GLN
1	A	234	GLN
1	A	272	GLN
1	A	429	ASN
1	A	457	GLN
1	A	480	ASN
1	A	523	ASN

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$
3	NDP	A	602	-	51,52,52	2.45	8 (15%)	71,80,80	1.61	17 (23%)
2	FAD	A	601	-	58,58,58	0.32	0	85,89,89	0.38	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	NDP	A	602	-	-	12/34/77/77	0/5/5/5
2	FAD	A	601	-	-	8/34/50/50	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NDP	P2B-O2B	13.90	1.83	1.59
3	A	602	NDP	PA-O3	4.77	1.64	1.59
3	A	602	NDP	PN-O5D	4.25	1.76	1.59
3	A	602	NDP	O2B-C2B	-3.14	1.33	1.44
3	A	602	NDP	C5A-C4A	2.71	1.43	1.39
3	A	602	NDP	C2A-N1A	2.37	1.38	1.33
3	A	602	NDP	C4A-N3A	2.09	1.38	1.34
3	A	602	NDP	C8A-N9A	2.02	1.41	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NDP	P2B-O2B-C2B	-4.81	110.59	123.43
3	A	602	NDP	O2B-P2B-O1X	-3.58	96.58	109.33
3	A	602	NDP	O3-PA-O1A	-3.46	100.29	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NDP	O2N-PN-O3	3.03	115.47	107.27
3	A	602	NDP	PA-O5B-C5B	-2.98	104.27	121.35
3	A	602	NDP	PN-O5D-C5D	-2.89	104.79	121.35
3	A	602	NDP	O3X-P2B-O2X	2.55	117.37	107.80
3	A	602	NDP	C2A-N1A-C6A	-2.42	114.76	118.73
3	A	602	NDP	N3A-C4A-N9A	2.41	131.26	127.17
3	A	602	NDP	O2N-PN-O1N	2.33	123.28	112.44
3	A	602	NDP	O4B-C4B-C3B	2.32	109.75	105.15
3	A	602	NDP	C5A-C4A-N3A	-2.30	123.54	126.72
3	A	602	NDP	C5B-C4B-C3B	-2.29	106.96	115.21
3	A	602	NDP	O5D-PN-O1N	-2.22	100.15	108.94
3	A	602	NDP	C5D-C4D-C3D	-2.09	107.69	115.21
3	A	602	NDP	O3X-P2B-O2B	-2.07	97.80	105.85
3	A	602	NDP	O7N-C7N-C3N	2.02	124.71	120.90

There are no chirality outliers.

All (20) torsion outliers are listed below:

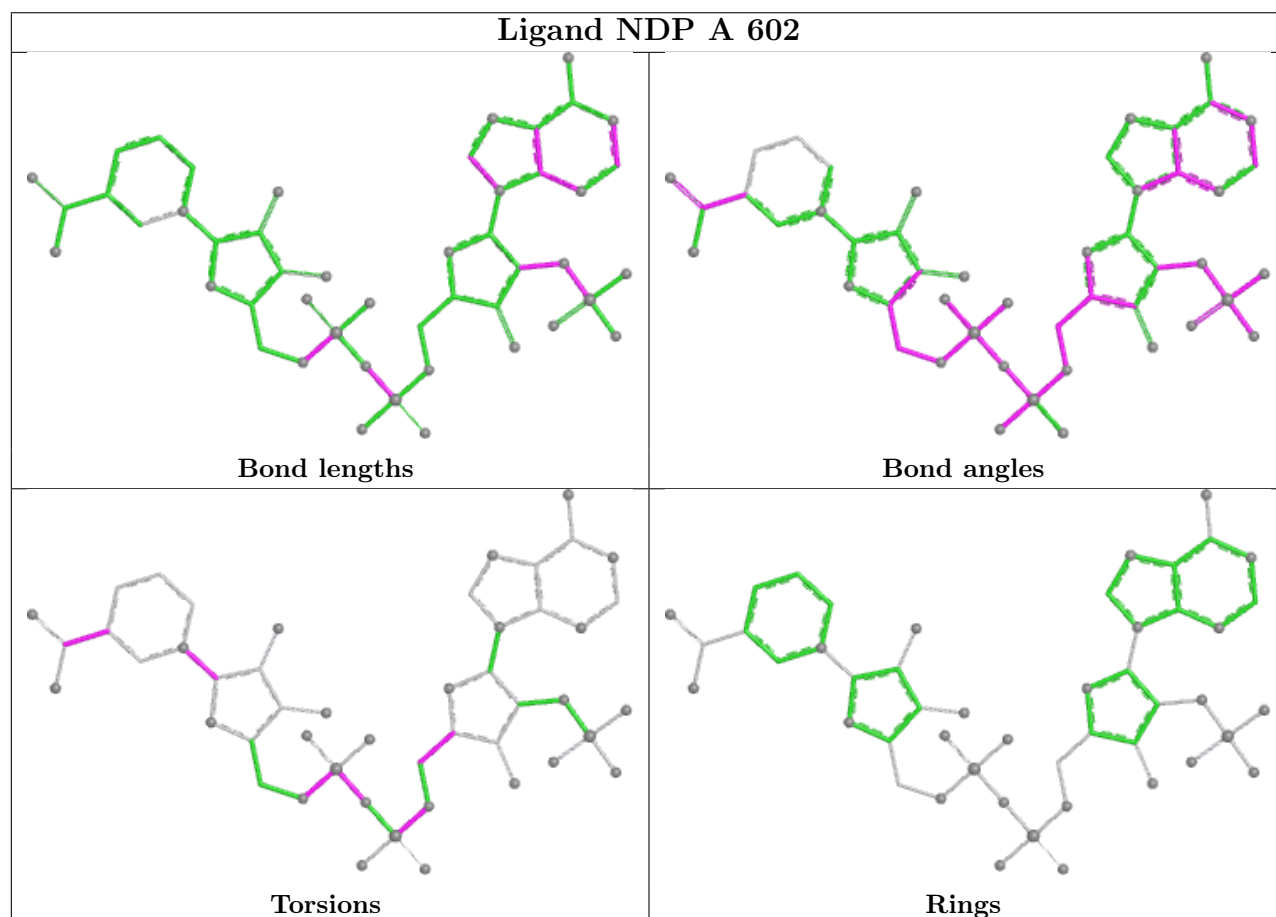
Mol	Chain	Res	Type	Atoms
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	O4'-C4'-C5'-O5'
3	A	602	NDP	C5B-O5B-PA-O1A
3	A	602	NDP	C5B-O5B-PA-O3
3	A	602	NDP	C5D-O5D-PN-O1N
3	A	602	NDP	C2N-C3N-C7N-N7N
3	A	602	NDP	O4D-C1D-N1N-C2N
3	A	602	NDP	C3B-C4B-C5B-O5B
3	A	602	NDP	O4B-C4B-C5B-O5B
3	A	602	NDP	C2N-C3N-C7N-O7N
3	A	602	NDP	C5B-O5B-PA-O2A
3	A	602	NDP	C5D-O5D-PN-O3
3	A	602	NDP	PA-O3-PN-O2N
3	A	602	NDP	C2D-C1D-N1N-C6N
2	A	601	FAD	O4B-C4B-C5B-O5B

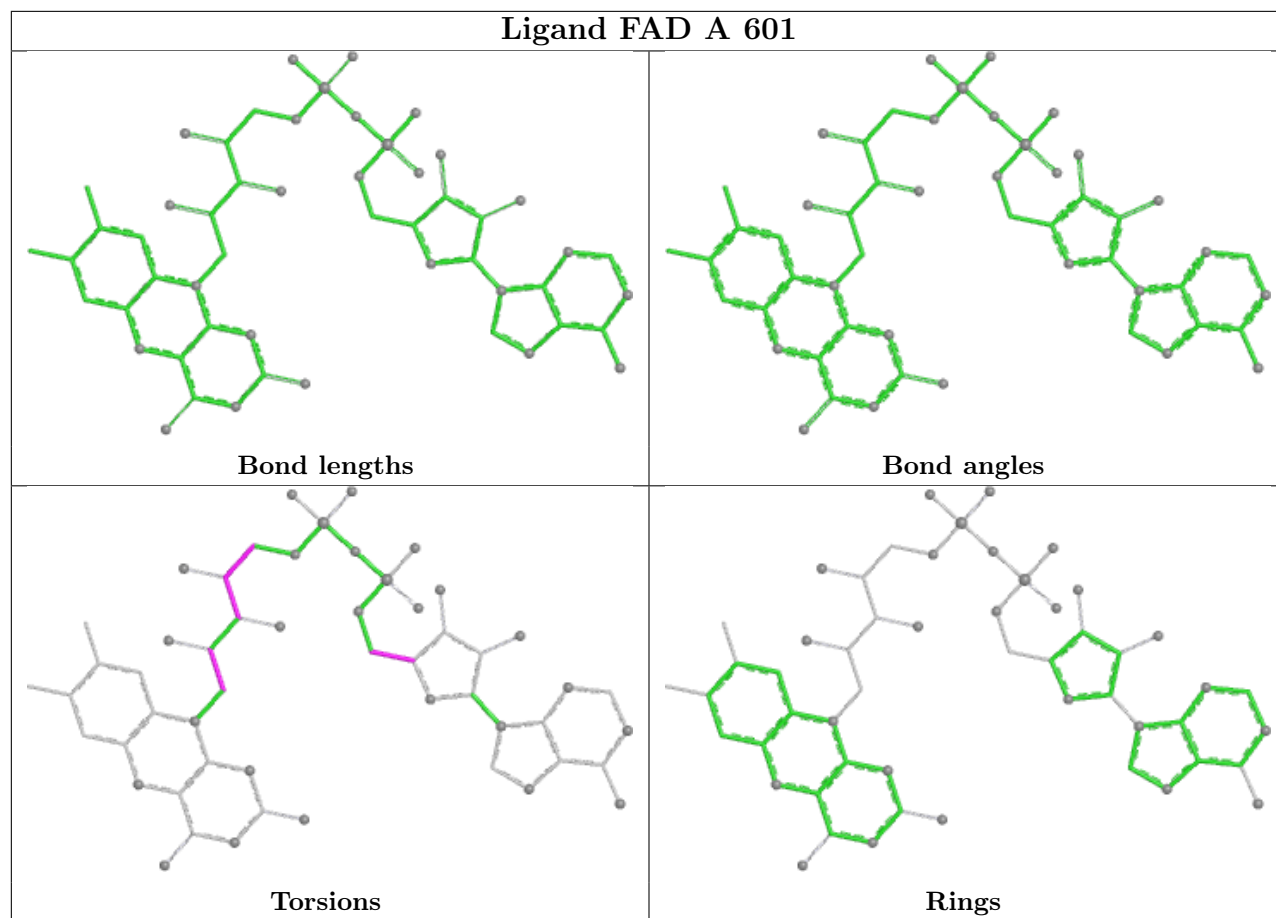
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NDP	1	0
2	A	601	FAD	3	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	518/548 (94%)	0.65	33 (6%) 25 29	34, 55, 85, 110	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	PRO	4.7
1	A	149	LEU	4.2
1	A	378	THR	3.7
1	A	326	CYS	3.6
1	A	379	GLY	3.4
1	A	324	TYR	3.3
1	A	143	LEU	3.2
1	A	150	PRO	3.0
1	A	147	PRO	3.0
1	A	323	LEU	3.0
1	A	144	LEU	2.8
1	A	152	ILE	2.8
1	A	327	ARG	2.7
1	A	394	GLY	2.6
1	A	14	ALA	2.6
1	A	321	THR	2.6
1	A	350	ALA	2.5
1	A	146[A]	ALA	2.4
1	A	380	PHE	2.4
1	A	489	CYS	2.4
1	A	145	ALA	2.4
1	A	520	VAL	2.4
1	A	504	TYR	2.4
1	A	322	ASP	2.3
1	A	49	ASN	2.3
1	A	325	ALA	2.3
1	A	530	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	110	ILE	2.2
1	A	338	PHE	2.2
1	A	484	PHE	2.1
1	A	485	ALA	2.1
1	A	5	MET	2.1
1	A	482	THR	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](#)

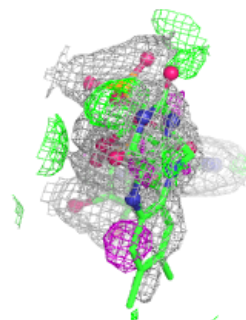
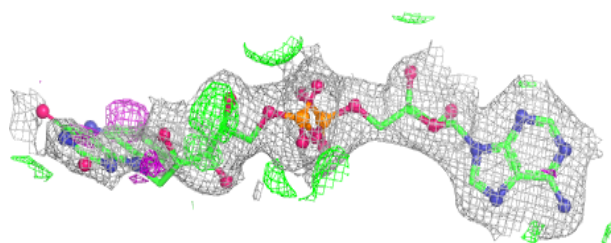
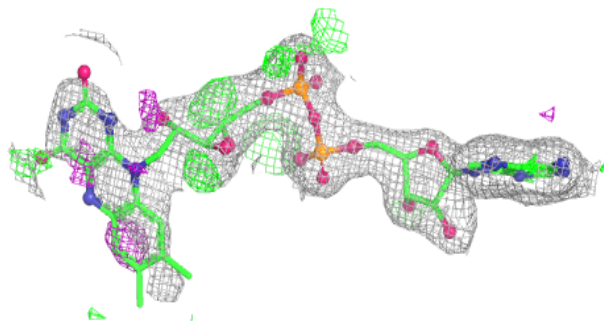
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FAD	A	601	53/53	0.91	0.13	38,53,98,101	0
3	NDP	A	602	48/48	0.92	0.10	45,59,87,89	0

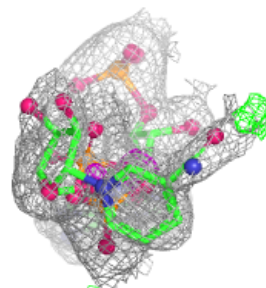
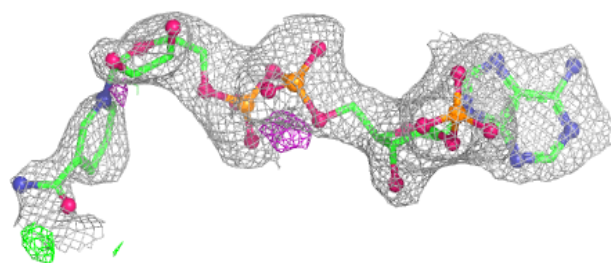
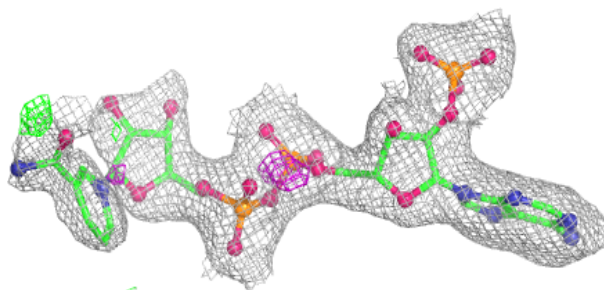
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 601:

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

**Electron density around NDP A 602:**

$2mF_o-DF_c$ (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.