



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2025 – 06:23 PM JST

PDB ID : 8Z17  
Title : Crystal structure of DiatB mutant R360A  
Authors : Peng, M.; Wu, Q.L.  
Deposited on : 2024-04-10  
Resolution : 2.43 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

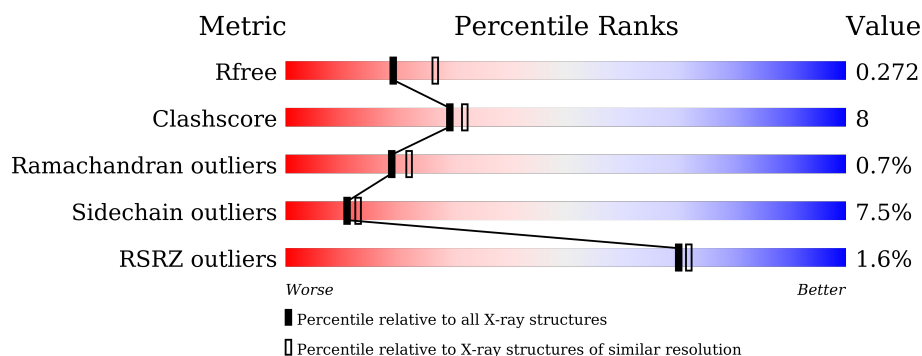
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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.



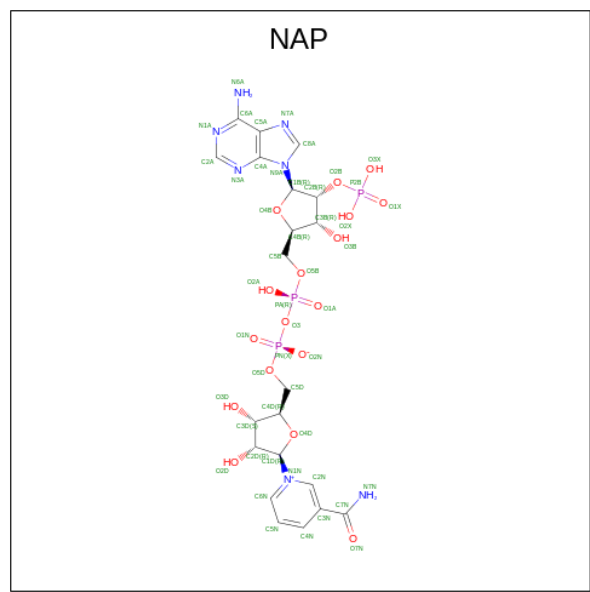
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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  $\geq 3$ , 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	432	<div> <div>2%</div> <div>72%</div> <div>23%</div> <div>...</div> </div>

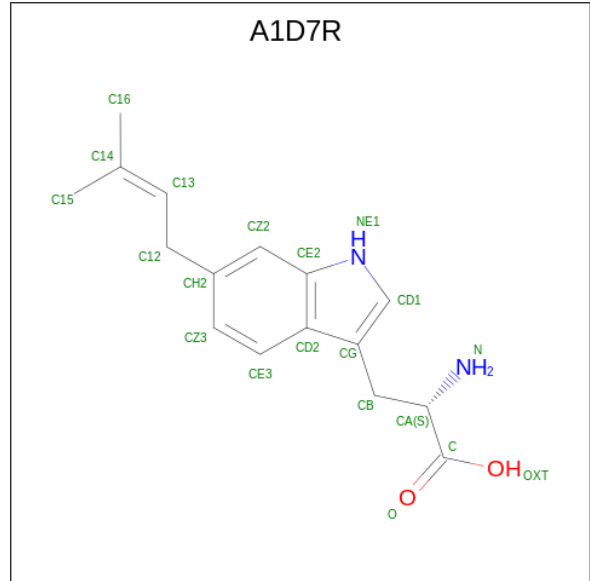


(three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 4 is (2 {S})-2-azanyl-3-[6-(3-methylbut-2-enyl)-1 {H}-indol-3-yl]propanoic acid (three-letter code: A1D7R) (formula: C<sub>16</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			20	16	2	2		

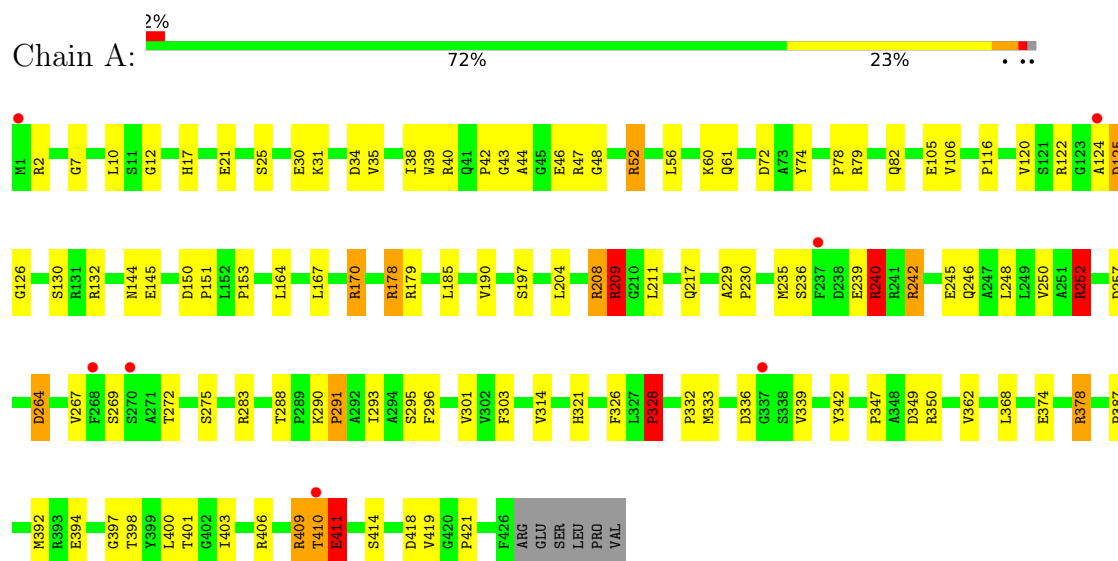
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		

### 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 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: Flavin-dependent monooxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.34Å 66.34Å 372.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.20 – 2.43 36.20 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.20-2.43) 95.3 (36.20-2.43)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, $R_{free}$	0.224 , 0.269 0.226 , 0.272	Depositor DCC
$R_{free}$ test set	17594 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3387	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FAD, A1D7R, NAP

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	0.51	0/3331	0.72	2/4540 (0.0%)

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	15

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	42	PRO	N-CA-C	-5.87	96.84	112.10
1	A	328	PRO	N-CA-CB	-5.18	96.91	102.60

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ARG	Sidechain
1	A	170	ARG	Sidechain
1	A	178	ARG	Sidechain
1	A	179	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	209	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	242	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	252	ARG	Sidechain
1	A	350	ARG	Sidechain
1	A	378	ARG	Sidechain
1	A	406	ARG	Sidechain
1	A	409	ARG	Sidechain
1	A	47	ARG	Sidechain
1	A	52	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3249	0	3182	54	0
2	A	53	0	31	4	0
3	A	48	0	25	3	0
4	A	20	0	0	0	0
5	A	17	0	0	0	0
All	All	3387	0	3238	56	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 (56) 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:30:GLU:OE1	2:A:501:FAD:H1B	1.94	0.68
1:A:10:LEU:HB3	2:A:501:FAD:H5'2	1.75	0.67
1:A:235:MET:HB3	1:A:240:ARG:HG3	1.78	0.65
1:A:204:LEU:HD13	1:A:288:THR:HB	1.80	0.64
1:A:185:LEU:HB3	1:A:211:LEU:HD12	1.79	0.63
1:A:291:PRO:HG2	1:A:303:PHE:HB3	1.81	0.63
1:A:56:LEU:HD12	1:A:78:PRO:HD2	1.83	0.59
1:A:31:LYS:HG2	1:A:105:GLU:HB2	1.85	0.59
1:A:332:PRO:HG2	1:A:347:PRO:HB3	1.84	0.59
1:A:30:GLU:HA	2:A:501:FAD:H8A	1.83	0.58
1:A:368:LEU:HD11	1:A:419:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PHE:HE2	1:A:314:VAL:HG21	1.69	0.56
1:A:400:LEU:O	1:A:403:ILE:HG13	2.06	0.56
1:A:34:ASP:OD1	1:A:35:VAL:N	2.35	0.56
1:A:387:PRO:HG2	1:A:392:MET:HG3	1.88	0.55
1:A:209:ARG:HD3	3:A:502:NAP:H8A	1.90	0.54
1:A:235:MET:HG2	1:A:239:GLU:HB3	1.88	0.54
1:A:44:ALA:HB3	1:A:46:GLU:HG3	1.91	0.53
1:A:246:GLN:O	1:A:250:VAL:HG23	2.11	0.50
1:A:293:ILE:HG23	1:A:301:VAL:HG13	1.95	0.49
1:A:74:TYR:CZ	1:A:82:GLN:HB3	2.48	0.48
1:A:264:ASP:OD1	1:A:264:ASP:N	2.47	0.48
1:A:7:GLY:O	1:A:12:GLY:HA3	2.14	0.48
1:A:120:VAL:HG22	1:A:130:SER:HB2	1.97	0.47
1:A:397:GLY:O	1:A:401:THR:HG23	2.13	0.47
1:A:116:PRO:HB2	1:A:132:ARG:NH2	2.30	0.47
1:A:418:ASP:HB3	1:A:421:PRO:HD2	1.96	0.47
1:A:394:GLU:O	1:A:398:THR:HG23	2.16	0.46
1:A:349:ASP:OD1	1:A:349:ASP:N	2.49	0.46
1:A:339:VAL:H	1:A:414:SER:HB2	1.81	0.45
1:A:150:ASP:HA	1:A:151:PRO:HA	1.80	0.45
1:A:374:GLU:OE1	1:A:378:ARG:HD2	2.17	0.45
1:A:60:LYS:HG3	1:A:61:GLN:N	2.32	0.44
1:A:38:ILE:HG13	1:A:39:TRP:N	2.33	0.44
1:A:52:ARG:NH2	1:A:79:ARG:HH22	2.15	0.44
1:A:106:VAL:H	2:A:501:FAD:H61A	1.64	0.43
1:A:43:GLY:HA2	1:A:52:ARG:HH12	1.83	0.43
1:A:35:VAL:O	1:A:40:ARG:HD2	2.19	0.43
1:A:229:ALA:HA	1:A:230:PRO:HD3	1.90	0.43
1:A:48:GLY:HA2	1:A:167:LEU:HD12	2.01	0.43
1:A:145:GLU:O	1:A:321:HIS:N	2.44	0.42
1:A:124:ALA:O	1:A:126:GLY:N	2.52	0.42
3:A:502:NAP:H6N	3:A:502:NAP:H2D	1.59	0.42
1:A:248:LEU:O	1:A:252:ARG:HG3	2.19	0.42
1:A:257:ASP:O	1:A:283:ARG:NH2	2.52	0.42
3:A:502:NAP:O2X	3:A:502:NAP:H1B	2.18	0.42
1:A:124:ALA:C	1:A:126:GLY:H	2.23	0.41
1:A:342:TYR:CG	1:A:392:MET:HG2	2.56	0.41
1:A:2:ARG:HG3	1:A:25:SER:HB3	2.03	0.41
1:A:204:LEU:HD12	1:A:290:LYS:CG	2.51	0.41
1:A:410:THR:HB	1:A:411:GLU:H	1.57	0.41
1:A:190:VAL:HG21	1:A:275:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:HA	1:A:245:GLU:HG2	2.02	0.41
1:A:326:PHE:O	1:A:328:PRO:HD3	2.20	0.40
1:A:17:HIS:O	1:A:21:GLU:HG2	2.20	0.40
1:A:153:PRO:HB2	1:A:296:PHE:CE1	2.57	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	424/432 (98%)	398 (94%)	23 (5%)	3 (1%)	19	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	GLU
1	A	125	ASP
1	A	291	PRO

### 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	333/339 (98%)	308 (92%)	25 (8%)	11	13

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	125	ASP
1	A	144	ASN
1	A	164	LEU
1	A	170	ARG
1	A	178	ARG
1	A	197	SER
1	A	208	ARG
1	A	209	ARG
1	A	217	GLN
1	A	236	SER
1	A	240	ARG
1	A	252	ARG
1	A	264	ASP
1	A	267	VAL
1	A	269	SER
1	A	272	THR
1	A	295	SER
1	A	328	PRO
1	A	333	MET
1	A	336	ASP
1	A	362	VAL
1	A	409	ARG
1	A	410	THR
1	A	411	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

3 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$
4	A1D7R	A	503	-	19,21,21	1.07	1 (5%)	23,29,29	2.04	4 (17%)
3	NAP	A	502	-	45,52,52	0.73	1 (2%)	56,80,80	0.81	2 (3%)
2	FAD	A	501	-	53,58,58	0.68	0	68,89,89	0.81	3 (4%)

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
4	A1D7R	A	503	-	-	1/12/13/13	0/2/2/2
3	NAP	A	502	-	-	12/31/67/67	0/5/5/5
2	FAD	A	501	-	-	11/30/50/50	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAP	C2N-N1N	2.56	1.38	1.35
4	A	503	A1D7R	CD1-NE1	-2.07	1.32	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	A1D7R	C12-C13-C14	-7.94	117.93	127.59
2	A	501	FAD	O4B-C1B-C2B	-2.66	103.04	106.93
4	A	503	A1D7R	C16-C14-C15	2.33	119.74	114.60
2	A	501	FAD	C5A-C6A-N6A	2.30	123.85	120.35
4	A	503	A1D7R	OXT-C-CA	2.29	121.18	113.38
3	A	502	NAP	C3D-C2D-C1D	2.25	104.37	100.98
3	A	502	NAP	C5A-C6A-N6A	2.21	123.71	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	C1B-N9A-C4A	2.15	130.42	126.64
4	A	503	A1D7R	CB-CG-CD1	2.01	130.45	127.97

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	N10-C1'-C2'-O2'
2	A	501	FAD	N10-C1'-C2'-C3'
2	A	501	FAD	C2'-C3'-C4'-O4'
2	A	501	FAD	C2'-C3'-C4'-C5'
2	A	501	FAD	O3'-C3'-C4'-O4'
2	A	501	FAD	O3'-C3'-C4'-C5'
2	A	501	FAD	C3'-C4'-C5'-O5'
2	A	501	FAD	O4'-C4'-C5'-O5'
2	A	501	FAD	C5'-O5'-P-O1P
3	A	502	NAP	C5B-O5B-PA-O2A
3	A	502	NAP	C5B-O5B-PA-O3
3	A	502	NAP	C1B-C2B-O2B-P2B
3	A	502	NAP	C5D-O5D-PN-O1N
3	A	502	NAP	O4D-C1D-N1N-C2N
3	A	502	NAP	C2D-C1D-N1N-C2N
3	A	502	NAP	C3D-C4D-C5D-O5D
3	A	502	NAP	O4D-C4D-C5D-O5D
2	A	501	FAD	PA-O3P-P-O5'
3	A	502	NAP	C4D-C5D-O5D-PN
4	A	503	A1D7R	CA-CB-CG-CD1
3	A	502	NAP	C5D-O5D-PN-O3
3	A	502	NAP	C2D-C1D-N1N-C6N
2	A	501	FAD	O4B-C4B-C5B-O5B
3	A	502	NAP	C5B-O5B-PA-O1A

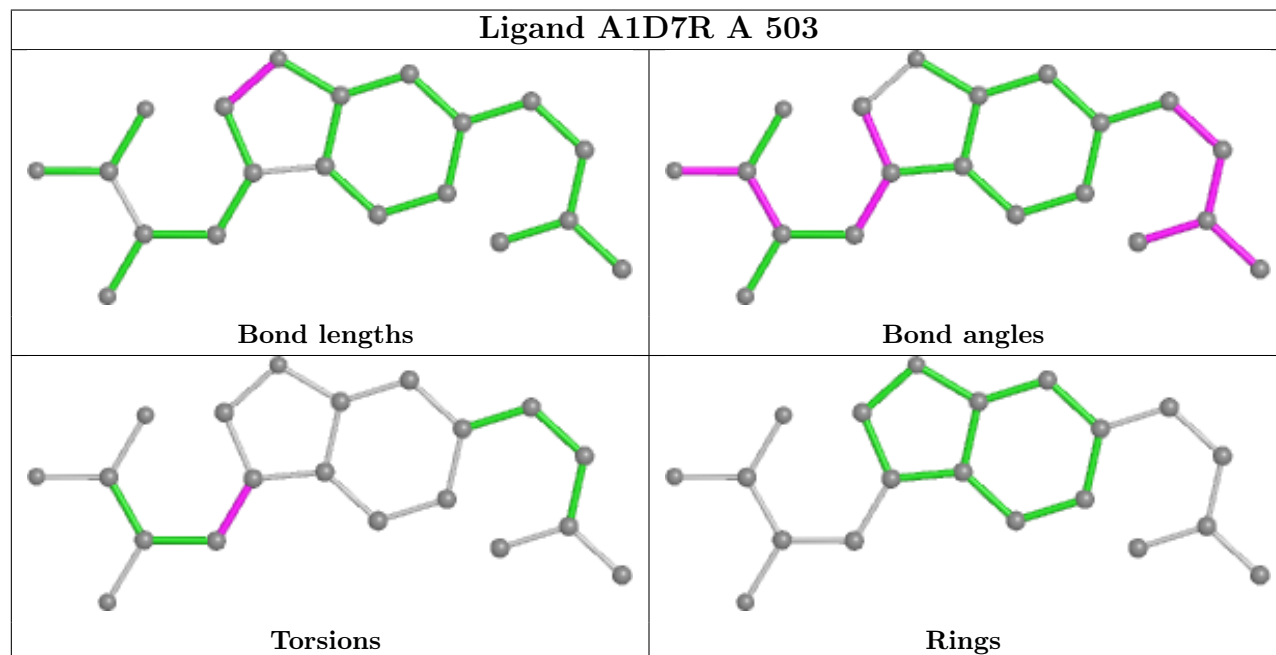
There are no ring outliers.

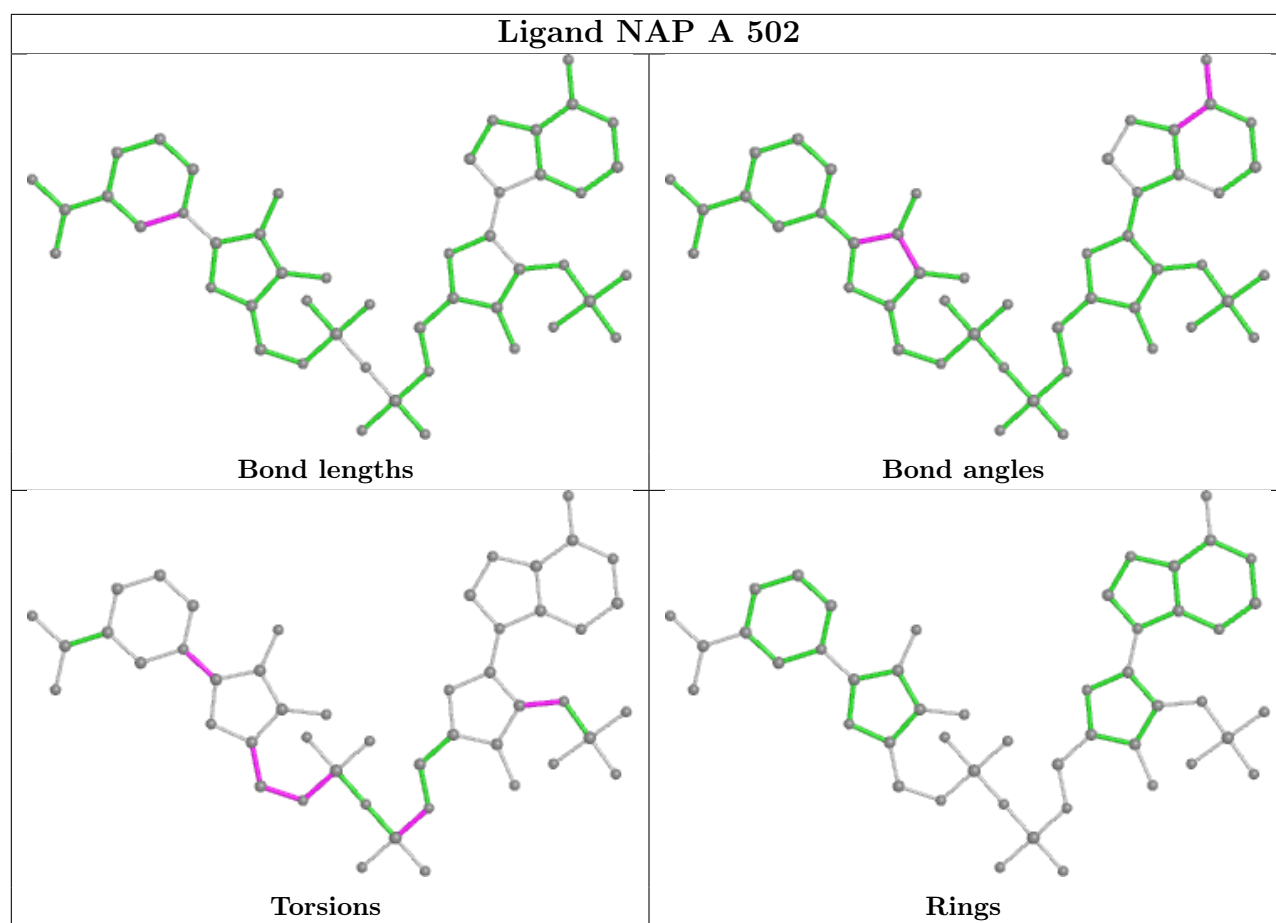
2 monomers are involved in 7 short contacts:

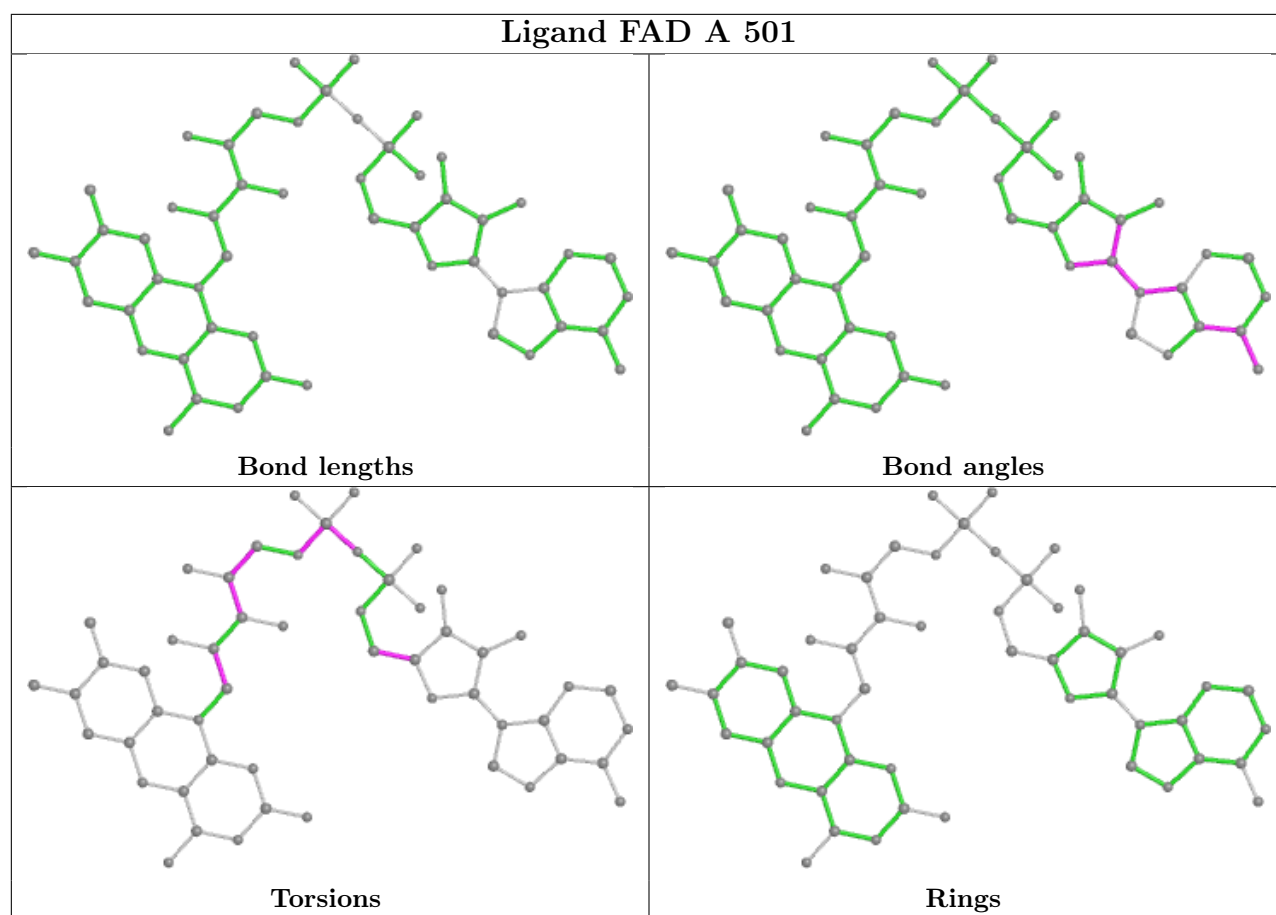
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAP	3	0
2	A	501	FAD	4	0

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	426/432 (98%)	0.07	7 (1%) 70 72	42, 59, 93, 108	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	410	THR	4.6
1	A	237	PHE	3.0
1	A	1	MET	2.6
1	A	268	PHE	2.3
1	A	270	SER	2.2
1	A	124	ALA	2.1
1	A	337	GLY	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

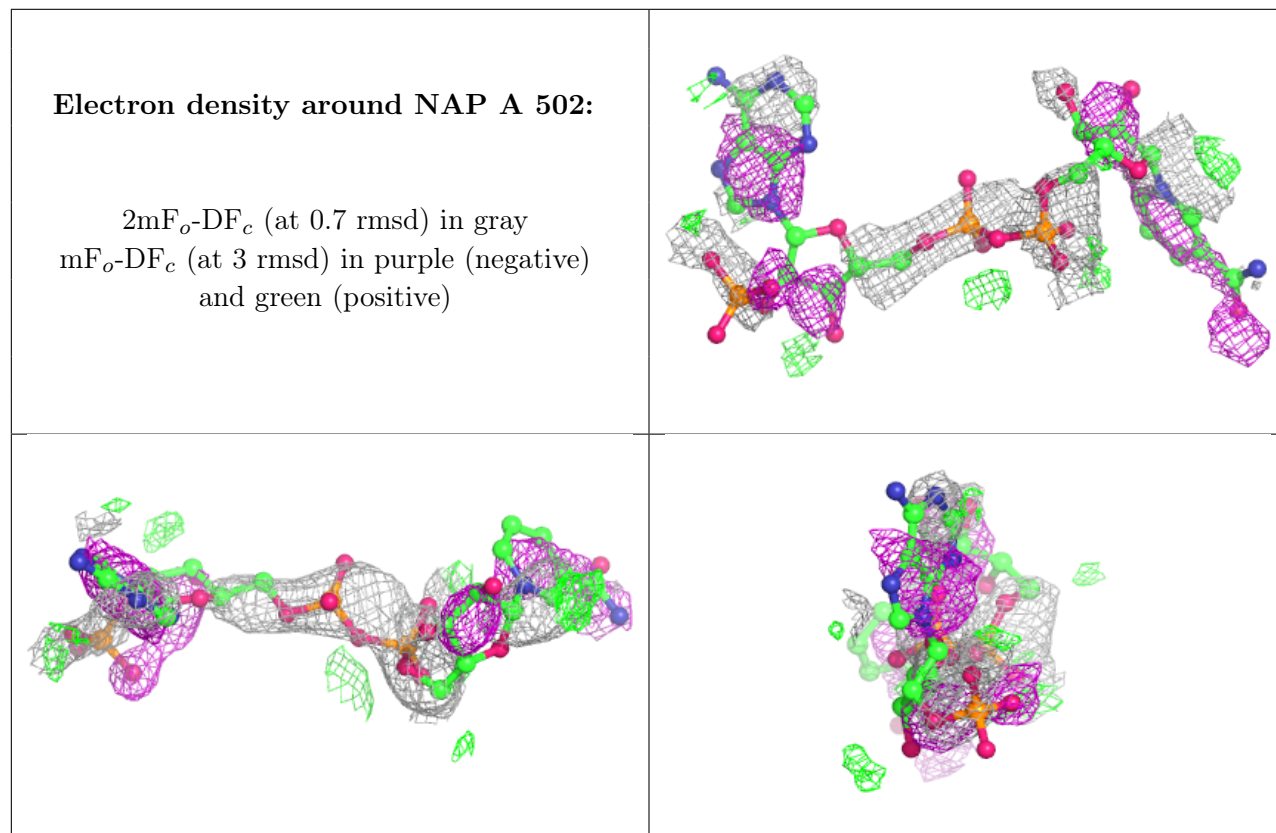
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAP	A	502	48/48	0.41	0.20	69,87,101,105	6

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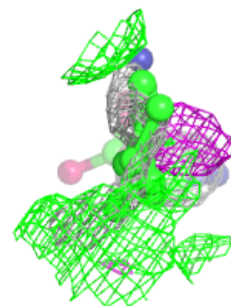
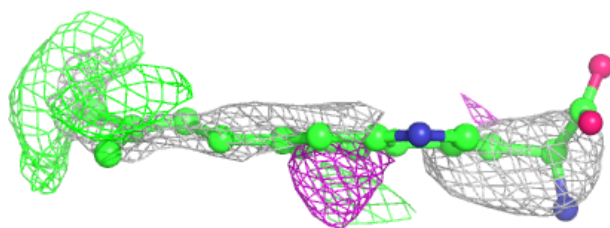
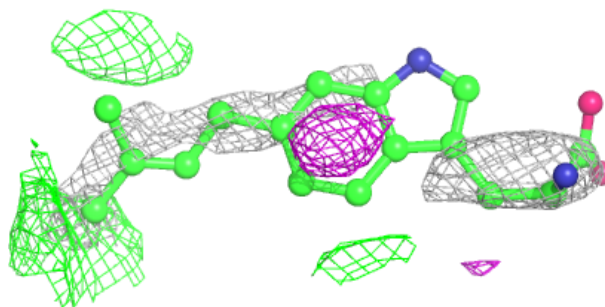
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	A1D7R	A	503	20/20	0.51	0.26	75,81,87,88	3
2	FAD	A	501	53/53	0.92	0.11	44,57,68,70	0

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.

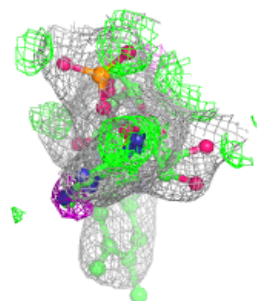
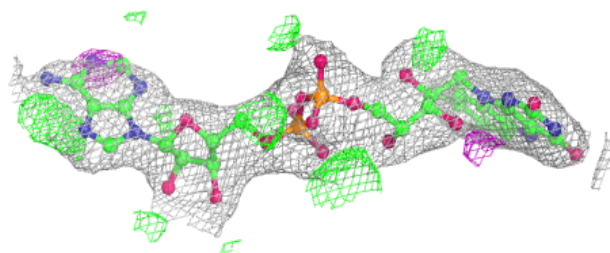
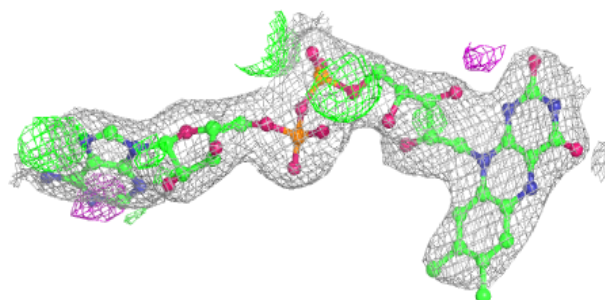


**Electron density around A1D7R A 503:**

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

**Electron density around FAD 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.