



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:06 pm BST

PDB ID : 2FOI  
Title : Synthesis, Biological Activity, and X-Ray Crystal Structural Analysis of Diaryl Ether Inhibitors of Malarial Enoyl ACP Reductase.  
Authors : Freundlich, J.S.; Shieh, H.; Anderson, J.W.; Kuo, M.; Yu, M.; Valderramos, J.; Karagyozev, L.; Tsai, H.; Lucumi, E.; Jacobs Jr., W.R.; Schiehser, G.A.; Jacobus, D.P.; Fidock, D.A.; Sacchettini, J.C.  
Deposited on : 2006-01-13  
Resolution : 2.50 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.

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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)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

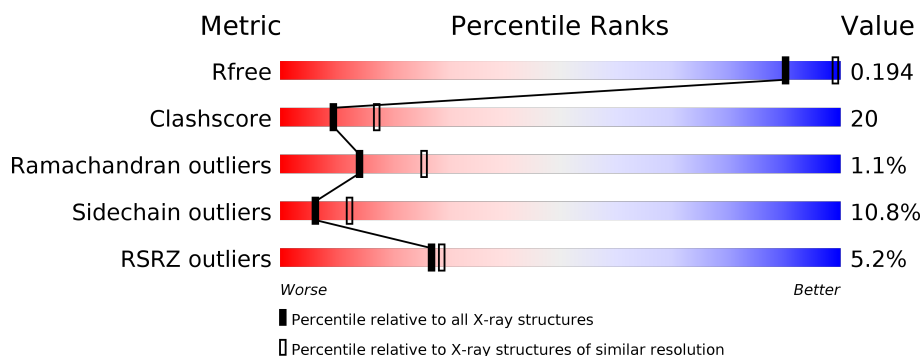
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	269	<div> <div>5%</div> <div>58% 21% 6% 15%</div> </div>
1	B	269	<div> <div>4%</div> <div>59% 23% 15%</div> </div>
2	C	60	<div> <div>5%</div> <div>77% 18% 5%</div> </div>
2	D	60	<div> <div>3%</div> <div>68% 27% 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	JPA	A	500	-	-	X	-
4	JPA	B	501	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4765 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.

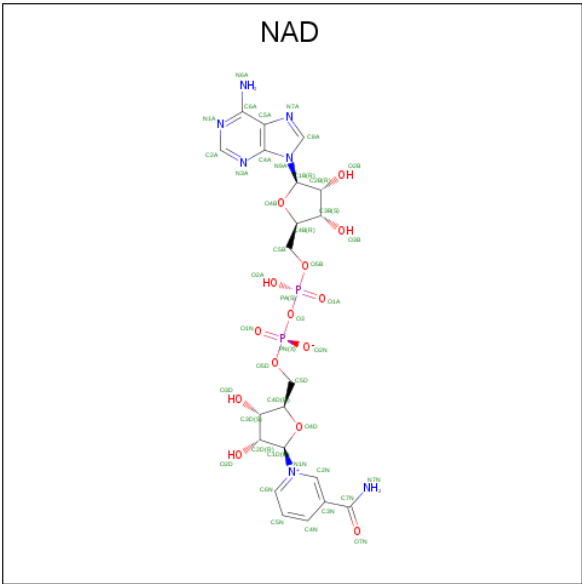
- Molecule 1 is a protein called enoyl-acyl carrier reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1148	309	339	10			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1148	309	339	10			

- Molecule 2 is a protein called enoyl-acyl carrier reductase.

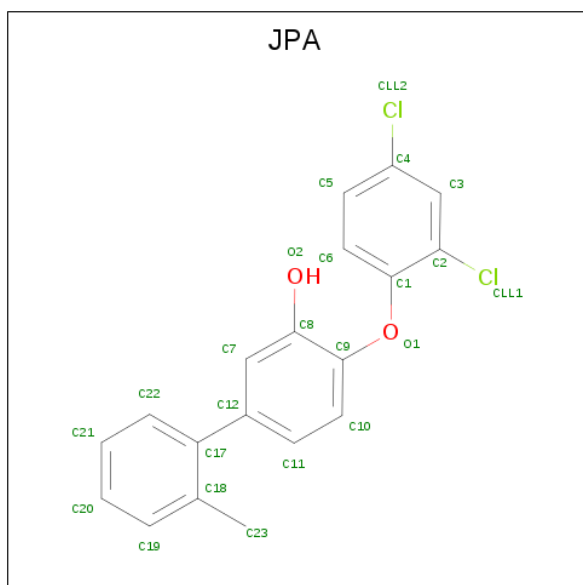
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	60	Total	C	N	O	S	0	0	0
			482	310	75	96	1			
2	D	60	Total	C	N	O	S	0	0	0
			482	310	75	96	1			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is 4-(2,4-DICHLOROPHENOXY)-2'-METHYLBIPHENYL-3-OL (three-letter code: JPA) (formula: C<sub>19</sub>H<sub>14</sub>Cl<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	O	0	0
			23	19	2	2		
4	B	1	Total	C	Cl	O	0	0
			23	19	2	2		

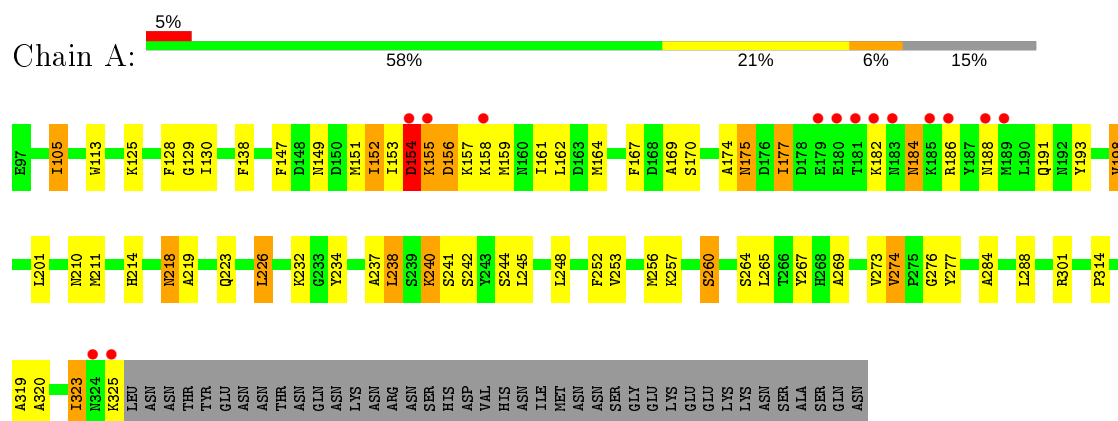
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	17	Total	O	0	0
			17	17		
5	C	12	Total	O	0	0
			12	12		
5	D	2	Total	O	0	0
			2	2		

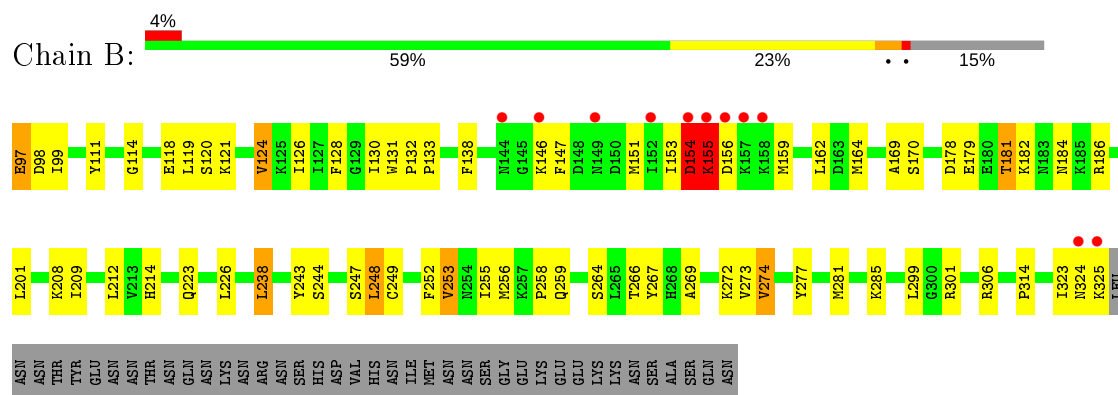
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

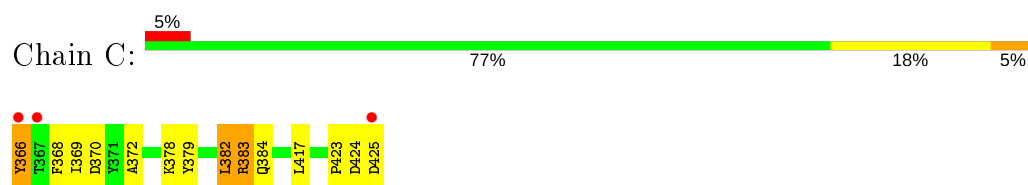
- Molecule 1: enoyl-acyl carrier reductase



- Molecule 1: enoyl-acyl carrier reductase



- Molecule 2: enoyl-acyl carrier reductase



- Molecule 2: enoyl-acyl carrier reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.86 Å 130.86 Å 82.69 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.77 – 2.50 33.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.77-2.50) 99.3 (33.77-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.24 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.193 , 0.255 0.196 , 0.194	Depositor DCC
$R_{free}$ test set	1263 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4765	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.56	0/1839	0.70	1/2477 (0.0%)
1	B	0.53	0/1839	0.69	1/2477 (0.0%)
2	C	0.60	0/491	0.65	0/664
2	D	0.55	0/491	0.77	0/664
All	All	0.55	0/4660	0.70	2/6282 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	LEU	CA-CB-CG	-7.06	99.06	115.30
1	A	238	LEU	CA-CB-CG	-6.76	99.76	115.30

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	1806	0	1824	72	0
1	B	1806	0	1824	73	0
2	C	482	0	473	27	0
2	D	482	0	473	27	0
3	A	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	2	0
4	A	23	0	14	24	0
4	B	23	0	14	24	0
5	A	24	0	0	2	0
5	B	17	0	0	0	0
5	C	12	0	0	1	0
5	D	2	0	0	0	0
All	All	4765	0	4674	184	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 20.

All (184) 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)
4:A:500:JPA:H231	2:C:368:PHE:CE2	1.54	1.42
1:B:138:PHE:HE2	1:B:164:MET:CE	1.42	1.31
4:A:500:JPA:C23	2:C:368:PHE:HE2	1.45	1.29
4:A:500:JPA:H19	2:C:368:PHE:CZ	1.81	1.14
2:D:383:ARG:HH11	2:D:383:ARG:HG2	1.12	1.14
1:B:138:PHE:CE2	1:B:164:MET:CE	2.31	1.12
4:B:501:JPA:H231	2:D:368:PHE:CE2	1.88	1.08
1:A:323:ILE:CD1	4:A:500:JPA:H233	1.85	1.07
4:B:501:JPA:C23	2:D:368:PHE:HE2	1.70	1.05
4:A:500:JPA:C23	2:C:368:PHE:CE2	2.30	1.02
1:B:314:PRO:HB3	4:B:501:JPA:H21	1.48	0.95
1:B:324:ASN:O	1:B:325:LYS:HD2	1.66	0.95
4:B:501:JPA:C23	2:D:368:PHE:CE2	2.48	0.94
1:B:314:PRO:HB3	4:B:501:JPA:C21	1.98	0.94
4:A:500:JPA:H19	2:C:368:PHE:CE2	2.03	0.93
1:B:325:LYS:HB2	2:D:368:PHE:HB2	1.52	0.92
1:A:184:ASN:ND2	1:A:186:ARG:H	1.68	0.91
1:B:138:PHE:HE2	1:B:164:MET:HE1	1.34	0.87
1:B:138:PHE:CE2	1:B:164:MET:HE1	2.03	0.87
4:A:500:JPA:C19	2:C:368:PHE:CE2	2.61	0.84
1:A:184:ASN:HD22	1:A:186:ARG:H	1.23	0.83
4:B:501:JPA:H19	2:D:368:PHE:CZ	2.13	0.83
1:B:138:PHE:HE2	1:B:164:MET:HE3	1.41	0.82
2:D:383:ARG:NH1	2:D:383:ARG:HG2	1.93	0.79
2:D:383:ARG:HH11	2:D:383:ARG:CG	1.95	0.79
1:B:277:TYR:CD1	4:B:501:JPA:H232	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:O	1:A:260:SER:HB3	1.85	0.77
1:A:105:ILE:HG22	1:A:130:ILE:CD1	2.15	0.77
1:A:218:ASN:HD22	1:A:219:ALA:H	1.33	0.76
4:A:500:JPA:C18	2:C:368:PHE:HE2	1.98	0.76
1:B:138:PHE:CE2	1:B:164:MET:HE2	2.21	0.76
1:A:314:PRO:HB3	4:A:500:JPA:C21	2.15	0.75
4:A:500:JPA:H19	2:C:368:PHE:HZ	1.52	0.75
1:B:314:PRO:CB	4:B:501:JPA:H21	2.14	0.75
1:A:323:ILE:CD1	4:A:500:JPA:C23	2.64	0.75
1:A:323:ILE:HD12	4:A:500:JPA:H233	1.69	0.75
1:B:154:ASP:O	1:B:156:ASP:N	2.20	0.75
4:B:501:JPA:H19	2:D:368:PHE:CE2	2.24	0.72
1:A:175:ASN:H	1:A:175:ASN:HD22	1.38	0.72
4:B:501:JPA:C19	2:D:368:PHE:CE2	2.72	0.72
1:A:320:ALA:HB1	2:C:369:ILE:HD13	1.74	0.70
4:B:501:JPA:C18	2:D:368:PHE:HE2	2.03	0.70
1:A:170:SER:OG	1:A:240:LYS:HE2	1.92	0.70
1:A:323:ILE:HD13	4:A:500:JPA:H233	1.74	0.69
1:B:154:ASP:N	1:B:154:ASP:OD2	2.25	0.69
4:A:500:JPA:H231	2:C:368:PHE:CZ	2.26	0.68
1:A:323:ILE:HD13	4:A:500:JPA:C23	2.22	0.68
1:B:325:LYS:O	2:D:367:THR:HA	1.94	0.68
4:B:501:JPA:H231	2:D:368:PHE:CZ	2.30	0.67
1:A:177:ILE:HG23	1:A:182:LYS:HD2	1.77	0.67
1:A:184:ASN:HD22	1:A:186:ARG:N	1.93	0.65
1:B:324:ASN:C	1:B:325:LYS:HD2	2.17	0.65
1:B:301:ARG:HH21	2:C:379:TYR:C	2.01	0.64
1:B:252:PHE:O	1:B:256:MET:HG3	1.97	0.64
1:A:314:PRO:HB3	4:A:500:JPA:H21	1.79	0.63
1:B:323:ILE:HG22	1:B:325:LYS:HD3	1.80	0.63
1:B:184:ASN:ND2	1:B:186:ARG:H	1.97	0.63
1:A:153:ILE:O	1:A:154:ASP:C	2.37	0.62
1:A:184:ASN:C	1:A:184:ASN:HD22	2.02	0.62
1:B:277:TYR:CE1	4:B:501:JPA:H232	2.34	0.62
1:A:147:PHE:O	1:A:151:MET:HG3	1.99	0.62
1:B:267:TYR:OH	4:B:501:JPA:C20	2.49	0.61
1:A:223:GLN:HB2	5:A:35:HOH:O	2.01	0.60
2:D:366:TYR:O	2:D:370:ASP:HB2	2.02	0.60
4:B:501:JPA:C19	2:D:368:PHE:HE2	2.14	0.60
1:B:111:TYR:CE1	2:D:391:ILE:HD13	2.37	0.60
1:A:177:ILE:HG23	1:A:177:ILE:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:HD22	1:A:288:LEU:HD11	1.85	0.59
1:B:119:LEU:O	1:B:124:VAL:HG13	2.03	0.59
1:A:169:ALA:HB1	1:A:244:SER:HB2	1.84	0.58
1:A:211:MET:HE1	5:C:16:HOH:O	2.03	0.58
1:A:218:ASN:HD22	1:A:219:ALA:N	2.01	0.58
2:C:366:TYR:O	2:C:370:ASP:OD2	2.21	0.57
1:B:126:ILE:HG21	1:B:128:PHE:HE1	1.69	0.57
1:A:175:ASN:N	1:A:175:ASN:HD22	2.00	0.57
1:B:249:CYS:O	1:B:253:VAL:HB	2.03	0.57
2:C:378:LYS:HD2	2:C:379:TYR:CE2	2.40	0.57
1:A:276:GLY:HA2	1:A:325:LYS:HE3	1.85	0.57
1:A:129:GLY:C	1:A:130:ILE:HD13	2.25	0.57
1:A:188:ASN:HB2	5:A:32:HOH:O	2.04	0.56
1:A:277:TYR:CD1	4:A:500:JPA:H232	2.40	0.56
1:A:156:ASP:N	1:A:156:ASP:OD2	2.39	0.56
1:B:178:ASP:OD2	1:B:181:THR:HG22	2.06	0.56
1:A:105:ILE:HD11	1:A:113:TRP:HE3	1.69	0.56
1:A:269:ALA:HB2	1:A:274:VAL:HG13	1.87	0.56
1:A:105:ILE:HG22	1:A:130:ILE:HD12	1.87	0.55
1:B:111:TYR:HE1	2:D:391:ILE:HD13	1.71	0.55
1:A:314:PRO:HA	3:A:450:NAD:O7N	2.08	0.54
1:A:128:PHE:HB3	1:A:130:ILE:HD11	1.90	0.54
1:B:126:ILE:CG2	1:B:128:PHE:CE1	2.90	0.54
1:A:159:MET:HE2	1:A:161:ILE:HD11	1.90	0.54
1:A:105:ILE:CG2	1:A:130:ILE:CD1	2.85	0.53
1:A:245:LEU:HD22	1:A:288:LEU:CD1	2.39	0.53
1:A:182:LYS:O	1:A:188:ASN:HB3	2.08	0.53
1:B:153:ILE:O	1:B:154:ASP:C	2.47	0.53
1:B:126:ILE:CG2	1:B:128:PHE:HE1	2.23	0.52
2:C:379:TYR:OH	2:C:425:ASP:HB3	2.09	0.52
1:B:147:PHE:O	1:B:151:MET:HG3	2.10	0.52
4:A:500:JPA:H20	2:C:372:ALA:HB1	1.92	0.52
1:B:301:ARG:NH2	2:C:379:TYR:C	2.63	0.52
1:A:177:ILE:CG2	1:A:177:ILE:O	2.58	0.51
1:B:97:GLU:HA	1:B:97:GLU:OE2	2.09	0.51
1:B:243:TYR:CE2	1:B:247:SER:HB2	2.46	0.51
1:A:177:ILE:HD11	1:A:193:TYR:CZ	2.46	0.51
1:B:252:PHE:CD1	1:B:255:ILE:HD11	2.46	0.51
1:A:267:TYR:OH	4:A:500:JPA:C20	2.59	0.50
1:B:258:PRO:O	1:B:259:GLN:HB2	2.11	0.50
4:A:500:JPA:C19	2:C:368:PHE:CZ	2.72	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:383:ARG:NH1	2:D:383:ARG:CG	2.63	0.50
1:B:178:ASP:OD1	1:B:181:THR:CG2	2.60	0.50
1:B:314:PRO:CA	4:B:501:JPA:H21	2.42	0.50
1:B:277:TYR:HD1	4:B:501:JPA:H232	1.76	0.49
1:A:184:ASN:ND2	1:A:184:ASN:C	2.66	0.49
1:B:126:ILE:HG21	1:B:128:PHE:CE1	2.46	0.49
1:A:210:ASN:CA	1:A:260:SER:HB2	2.43	0.49
1:A:210:ASN:HA	1:A:260:SER:HB2	1.95	0.48
3:B:451:NAD:O7N	4:B:501:JPA:H22	2.14	0.48
1:A:149:ASN:O	1:A:152:ILE:HG12	2.13	0.48
1:B:301:ARG:NH2	2:C:379:TYR:HA	2.29	0.48
4:A:500:JPA:C18	2:C:368:PHE:CE2	2.81	0.48
1:A:175:ASN:H	1:A:175:ASN:ND2	2.09	0.47
1:B:114:GLY:HA3	2:D:388:SER:OG	2.15	0.47
1:A:167:PHE:HD1	1:A:198:VAL:HG11	1.79	0.47
1:B:98:ASP:HB2	1:B:124:VAL:HB	1.96	0.47
1:B:267:TYR:CZ	4:B:501:JPA:C20	2.98	0.47
1:A:105:ILE:CG2	1:A:130:ILE:HD12	2.44	0.47
1:B:269:ALA:HA	1:B:272:LYS:O	2.14	0.47
1:B:274:VAL:CG2	1:B:277:TYR:HB2	2.45	0.47
1:A:252:PHE:O	1:A:256:MET:HG3	2.15	0.47
4:A:500:JPA:H11	2:C:369:ILE:HD13	1.97	0.47
4:B:501:JPA:H19	2:D:368:PHE:HZ	1.74	0.46
1:A:269:ALA:CB	1:A:274:VAL:HG13	2.44	0.46
1:B:118:GLU:HG3	2:D:393:SER:N	2.31	0.46
2:D:416:GLY:O	2:D:419:ILE:HG12	2.16	0.46
1:A:277:TYR:HD1	4:A:500:JPA:H232	1.80	0.46
1:B:253:VAL:HG21	1:B:299:LEU:HD22	1.98	0.46
1:A:214:HIS:O	1:A:264:SER:HA	2.16	0.46
2:D:381:PRO:HD2	2:D:415:ASN:O	2.16	0.46
1:B:277:TYR:HD1	4:B:501:JPA:C23	2.30	0.45
1:B:301:ARG:HH22	2:C:379:TYR:HA	1.80	0.45
1:B:131:TRP:CD1	1:B:132:PRO:HD2	2.51	0.45
1:B:126:ILE:HG22	1:B:128:PHE:CE1	2.52	0.45
1:B:277:TYR:CD1	4:B:501:JPA:C23	2.95	0.45
1:A:174:ALA:O	1:A:177:ILE:HG22	2.18	0.44
1:B:178:ASP:OD2	1:B:181:THR:CG2	2.66	0.44
3:B:451:NAD:H2D	4:B:501:JPA:O1	2.17	0.44
1:B:120:SER:O	1:B:121:LYS:C	2.55	0.44
1:B:301:ARG:NH2	2:C:379:TYR:O	2.51	0.44
1:B:208:LYS:HA	1:B:255:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLN:HE21	1:B:324:ASN:HB3	1.83	0.44
2:C:366:TYR:O	2:C:370:ASP:HB2	2.18	0.43
1:B:155:LYS:HE3	1:B:155:LYS:HB2	1.66	0.43
1:A:301:ARG:NH2	2:D:379:TYR:HA	2.33	0.43
1:A:301:ARG:HG3	1:A:301:ARG:NH1	2.33	0.43
1:A:320:ALA:HB1	2:C:369:ILE:CD1	2.46	0.43
1:B:214:HIS:O	1:B:264:SER:HA	2.19	0.43
1:B:266:THR:OG1	1:B:267:TYR:N	2.52	0.43
1:B:281:MET:CE	1:B:285:LYS:HE2	2.49	0.43
1:A:155:LYS:O	1:A:157:LYS:HG3	2.19	0.43
1:A:138:PHE:HE2	1:A:164:MET:HE2	1.83	0.43
1:B:274:VAL:HG22	1:B:277:TYR:HB2	2.00	0.43
1:B:212:LEU:HD21	1:B:248:LEU:HD13	2.01	0.43
1:A:325:LYS:HB2	2:C:368:PHE:HB2	2.00	0.42
1:B:306:ARG:HG2	2:C:382:LEU:HD21	2.00	0.42
1:A:301:ARG:HH21	2:D:379:TYR:HA	1.84	0.42
1:B:274:VAL:O	1:B:274:VAL:CG2	2.67	0.42
1:A:151:MET:CE	1:A:158:LYS:HE3	2.49	0.42
1:A:252:PHE:O	1:A:253:VAL:C	2.57	0.42
1:A:319:ALA:HB1	4:A:500:JPA:C2	2.49	0.42
1:B:131:TRP:CG	1:B:133:PRO:HD2	2.55	0.42
2:C:383:ARG:HA	2:C:383:ARG:HD3	1.40	0.42
1:A:301:ARG:HG3	1:A:301:ARG:HH11	1.84	0.41
1:B:281:MET:HE1	1:B:285:LYS:HE2	2.03	0.41
2:D:382:LEU:HB2	2:D:415:ASN:HB3	2.02	0.41
1:A:242:SER:OG	1:A:284:ALA:O	2.38	0.41
1:B:151:MET:HB3	1:B:159:MET:HB2	2.01	0.41
1:A:153:ILE:O	1:A:155:LYS:N	2.54	0.41
1:B:169:ALA:HB1	1:B:244:SER:HB2	2.03	0.41
1:B:277:TYR:CE2	1:B:281:MET:HB3	2.56	0.41
4:B:501:JPA:H20	2:D:372:ALA:HB1	2.03	0.40
1:B:99:ILE:HB	1:B:209:ILE:HG22	2.04	0.40
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.95	0.40
1:A:130:ILE:HD13	1:A:130:ILE:N	2.37	0.40
1:A:234:TYR:O	1:A:237:ALA:HB3	2.21	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	227/269 (84%)	213 (94%)	11 (5%)	3 (1%)	12	21
1	B	227/269 (84%)	213 (94%)	12 (5%)	2 (1%)	17	31
2	C	58/60 (97%)	52 (90%)	5 (9%)	1 (2%)	9	16
2	D	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
All	All	570/658 (87%)	531 (93%)	33 (6%)	6 (1%)	14	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	ASP
1	B	155	LYS
1	A	154	ASP
1	A	155	LYS
1	A	323	ILE
2	C	423	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	197/235 (84%)	174 (88%)	23 (12%)	5	10
1	B	197/235 (84%)	179 (91%)	18 (9%)	9	18
2	C	53/53 (100%)	47 (89%)	6 (11%)	6	11
2	D	53/53 (100%)	46 (87%)	7 (13%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	500/576 (87%)	446 (89%)	54 (11%)	6 12

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ILE
1	A	125	LYS
1	A	152	ILE
1	A	154	ASP
1	A	156	ASP
1	A	162	LEU
1	A	175	ASN
1	A	177	ILE
1	A	184	ASN
1	A	191	GLN
1	A	198	VAL
1	A	201	LEU
1	A	218	ASN
1	A	226	LEU
1	A	232	LYS
1	A	238	LEU
1	A	240	LYS
1	A	241	SER
1	A	248	LEU
1	A	260	SER
1	A	265	LEU
1	A	273	VAL
1	A	274	VAL
1	B	97	GLU
1	B	124	VAL
1	B	130	ILE
1	B	146	LYS
1	B	154	ASP
1	B	155	LYS
1	B	162	LEU
1	B	170	SER
1	B	179	GLU
1	B	181	THR
1	B	182	LYS
1	B	201	LEU
1	B	226	LEU
1	B	238	LEU

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Mol	Chain	Res	Type
1	B	248	LEU
1	B	253	VAL
1	B	273	VAL
1	B	274	VAL
2	C	366	TYR
2	C	382	LEU
2	C	383	ARG
2	C	384	GLN
2	C	417	LEU
2	C	424	ASP
2	D	366	TYR
2	D	378	LYS
2	D	382	LEU
2	D	383	ARG
2	D	384	GLN
2	D	417	LEU
2	D	424	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	175	ASN
1	A	184	ASN
1	A	191	GLN
1	A	200	ASN
1	A	203	HIS
1	A	218	ASN
1	A	228	ASN
1	A	254	ASN
1	B	184	ASN
1	B	200	ASN
1	B	223	GLN
1	B	302	ASN
2	C	384	GLN
2	D	384	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	NAD	B	451	-	42,48,48	1.20	5 (11%)	50,73,73	1.44	7 (14%)
3	NAD	A	450	-	42,48,48	1.31	4 (9%)	50,73,73	1.48	8 (16%)
4	JPA	B	501	-	25,25,25	3.46	10 (40%)	35,35,35	1.38	6 (17%)
4	JPA	A	500	-	25,25,25	3.38	11 (44%)	35,35,35	1.31	6 (17%)

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	NAD	B	451	-	-	8/26/62/62	0/5/5/5
3	NAD	A	450	-	-	5/26/62/62	0/5/5/5
4	JPA	B	501	-	-	3/8/8/8	0/3/3/3
4	JPA	A	500	-	-	4/8/8/8	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	JPA	C22-C17	-14.54	1.17	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	JPA	C22-C17	-13.74	1.18	1.40
3	A	450	NAD	O7N-C7N	5.00	1.33	1.24
4	B	501	JPA	C17-C12	-4.03	1.42	1.49
3	B	451	NAD	O7N-C7N	3.91	1.31	1.24
4	A	500	JPA	C17-C12	-3.83	1.42	1.49
4	A	500	JPA	C3-C4	3.78	1.44	1.38
3	B	451	NAD	C7N-N7N	-3.65	1.26	1.33
3	A	450	NAD	C7N-N7N	-2.87	1.27	1.33
4	B	501	JPA	C3-C4	2.84	1.43	1.38
4	A	500	JPA	C3-C2	2.83	1.43	1.38
4	B	501	JPA	C3-C2	2.78	1.43	1.38
4	B	501	JPA	C7-C12	2.73	1.44	1.39
3	B	451	NAD	C5A-C4A	2.60	1.47	1.40
4	A	500	JPA	C6-C1	2.60	1.45	1.39
4	A	500	JPA	C7-C12	2.57	1.44	1.39
3	A	450	NAD	C5A-C4A	2.55	1.47	1.40
4	B	501	JPA	C11-C12	2.44	1.44	1.39
4	A	500	JPA	C2-CLL1	2.42	1.79	1.73
4	B	501	JPA	C10-C11	2.28	1.42	1.38
3	B	451	NAD	O4D-C1D	2.27	1.44	1.41
4	B	501	JPA	C17-C18	-2.24	1.35	1.40
4	B	501	JPA	C5-C4	2.14	1.42	1.38
4	A	500	JPA	C17-C18	-2.08	1.36	1.40
3	B	451	NAD	O4B-C1B	2.08	1.44	1.41
4	A	500	JPA	C5-C4	2.07	1.42	1.38
3	A	450	NAD	O4D-C1D	2.07	1.44	1.41
4	A	500	JPA	C23-C18	2.06	1.55	1.51
4	A	500	JPA	C4-CLL2	2.04	1.78	1.74
4	B	501	JPA	C6-C5	2.02	1.42	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	450	NAD	C3N-C7N-N7N	4.35	122.97	117.75
3	B	451	NAD	N3A-C2A-N1A	-4.01	122.42	128.68
3	A	450	NAD	O7N-C7N-N7N	-3.91	117.03	122.58
3	A	450	NAD	N3A-C2A-N1A	-3.73	122.85	128.68
3	B	451	NAD	C3N-C7N-N7N	3.59	122.06	117.75
3	B	451	NAD	C4A-C5A-N7A	-3.32	105.94	109.40
4	B	501	JPA	C21-C20-C19	-3.16	115.38	120.19
3	A	450	NAD	O4D-C1D-C2D	-2.89	102.70	106.93
4	A	500	JPA	C21-C20-C19	-2.80	115.93	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	JPA	C23-C18-C19	-2.71	115.02	120.31
4	B	501	JPA	C21-C22-C17	2.60	124.72	120.33
3	A	450	NAD	C4A-C5A-N7A	-2.58	106.72	109.40
4	A	500	JPA	C3-C2-CLL1	2.47	122.47	118.49
3	B	451	NAD	PN-O3-PA	-2.42	124.53	132.83
4	A	500	JPA	C21-C22-C17	2.37	124.33	120.33
4	B	501	JPA	C20-C19-C18	-2.36	117.21	121.11
3	A	450	NAD	O4B-C1B-C2B	-2.36	103.48	106.93
3	A	450	NAD	C3N-C2N-N1N	2.32	122.70	120.43
3	B	451	NAD	C2A-N1A-C6A	2.30	122.70	118.75
3	B	451	NAD	O7N-C7N-N7N	-2.26	119.36	122.58
3	A	450	NAD	O2A-PA-O1A	2.19	123.05	112.24
4	B	501	JPA	C10-C9-C8	2.19	122.59	119.86
4	A	500	JPA	C20-C19-C18	-2.17	117.53	121.11
3	B	451	NAD	O3B-C3B-C4B	-2.06	105.11	111.05
4	A	500	JPA	C22-C17-C18	2.05	121.91	119.35
4	B	501	JPA	C10-C11-C12	-2.05	118.18	121.13
4	A	500	JPA	C11-C12-C7	2.03	121.04	118.16

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	451	NAD	C5B-O5B-PA-O1A
3	B	451	NAD	O4B-C4B-C5B-O5B
3	B	451	NAD	C5D-O5D-PN-O1N
3	B	451	NAD	C5D-O5D-PN-O2N
3	B	451	NAD	O4D-C1D-N1N-C2N
3	A	450	NAD	C5D-O5D-PN-O1N
3	A	450	NAD	C5D-O5D-PN-O2N
3	B	451	NAD	C3B-C4B-C5B-O5B
3	A	450	NAD	PN-O3-PA-O5B
4	B	501	JPA	C11-C12-C17-C18
4	A	500	JPA	C11-C12-C17-C18
4	A	500	JPA	C7-C12-C17-C18
3	A	450	NAD	O4B-C4B-C5B-O5B
4	A	500	JPA	C11-C12-C17-C22
4	B	501	JPA	C7-C12-C17-C18
4	A	500	JPA	C7-C12-C17-C22
4	B	501	JPA	C11-C12-C17-C22
3	B	451	NAD	C5D-O5D-PN-O3
3	A	450	NAD	C5D-O5D-PN-O3

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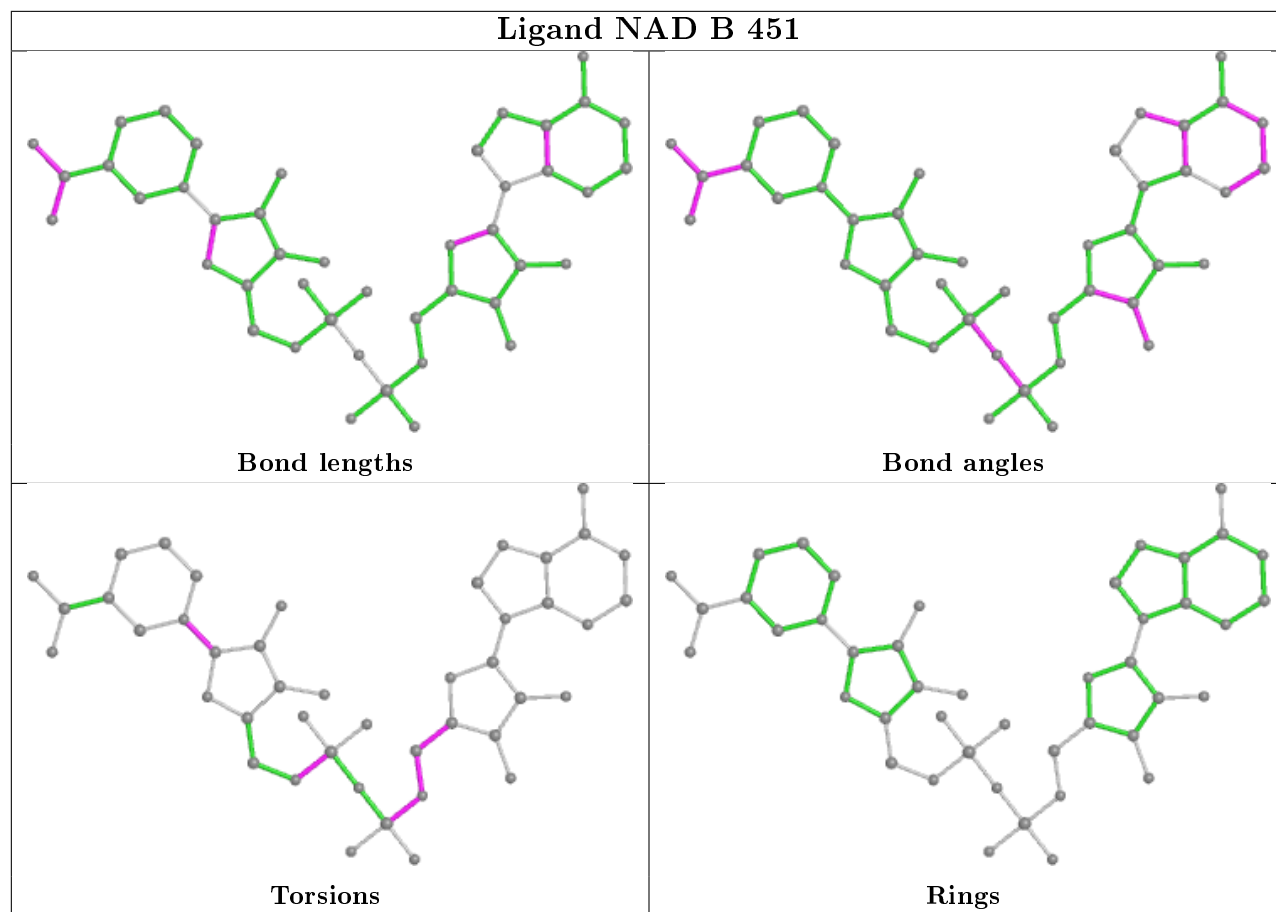
Mol	Chain	Res	Type	Atoms
3	B	451	NAD	C4B-C5B-O5B-PA

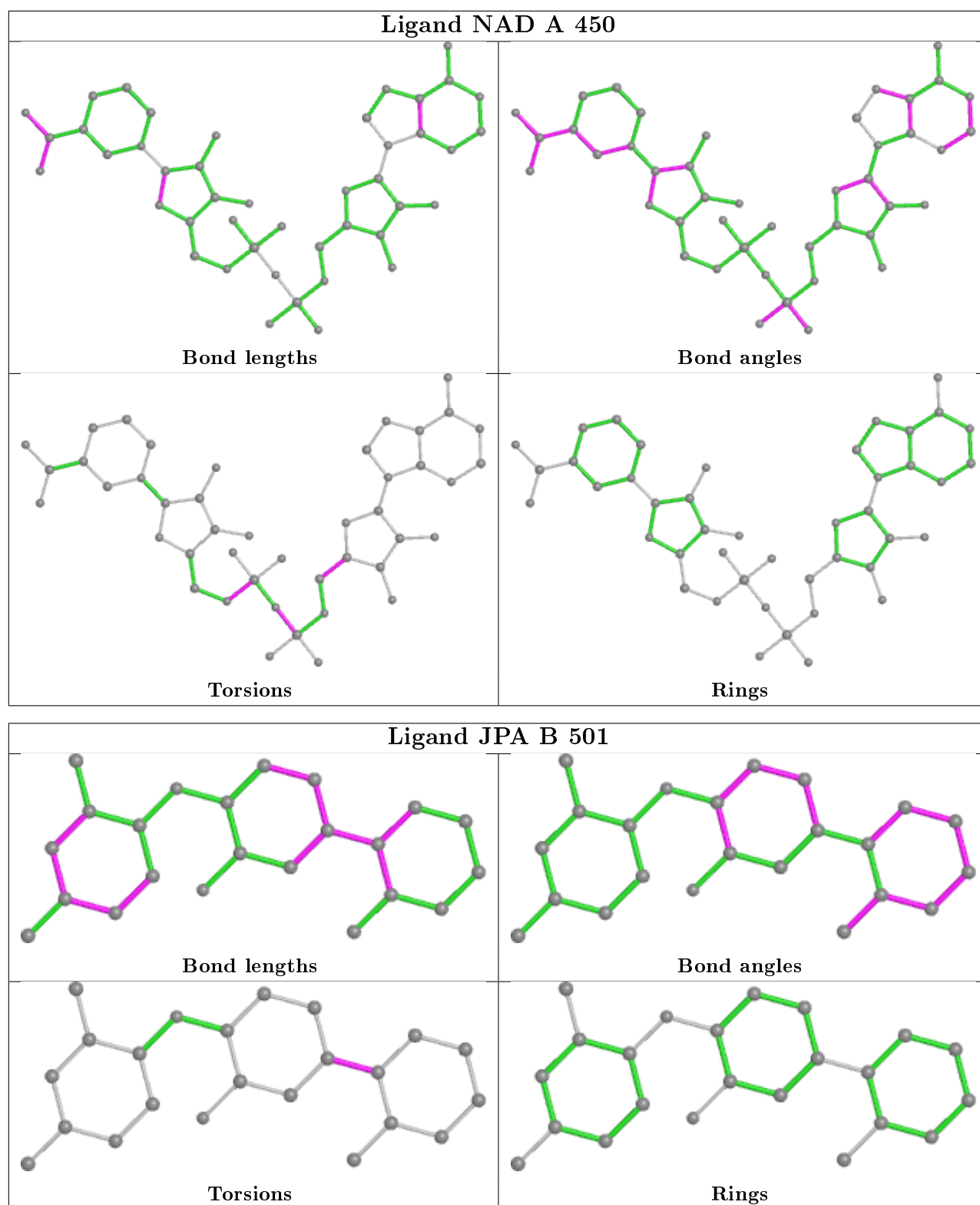
There are no ring outliers.

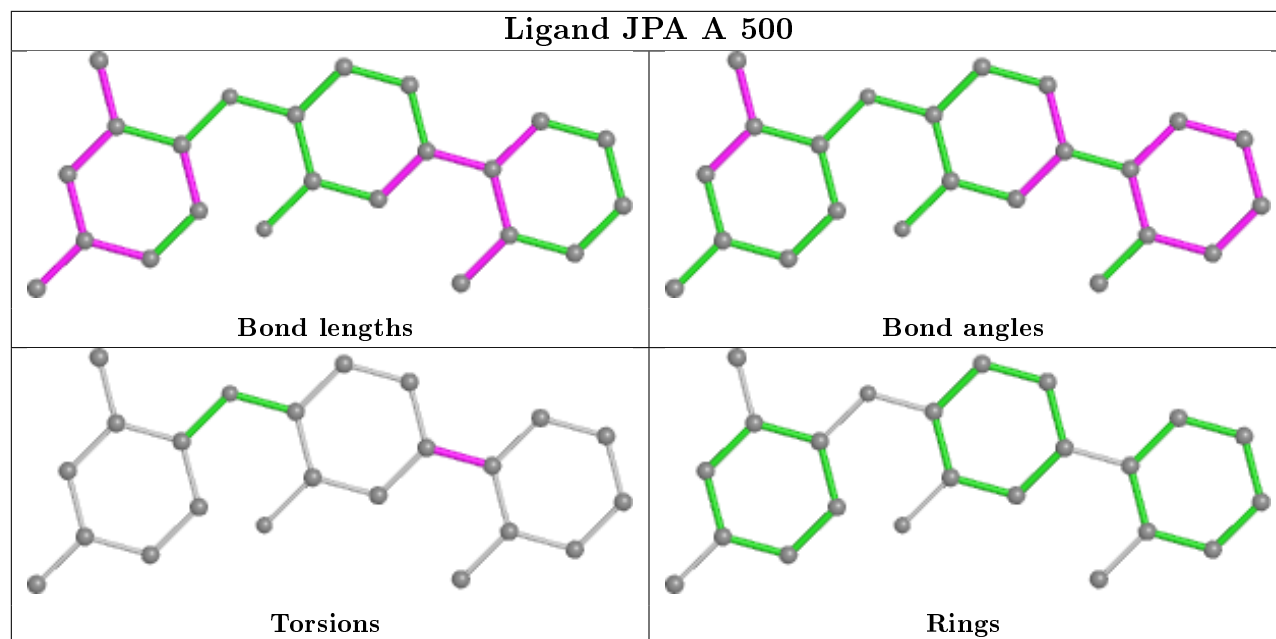
4 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	451	NAD	2	0
3	A	450	NAD	1	0
4	B	501	JPA	24	0
4	A	500	JPA	24	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, 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	229/269 (85%)	0.01	14 (6%) 21 22	16, 33, 65, 102	0
1	B	229/269 (85%)	-0.16	11 (4%) 30 32	15, 33, 64, 102	0
2	C	60/60 (100%)	0.14	3 (5%) 28 30	16, 28, 72, 90	0
2	D	60/60 (100%)	0.07	2 (3%) 46 50	17, 27, 71, 90	0
All	All	578/658 (87%)	-0.04	30 (5%) 27 29	15, 32, 65, 102	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	366	TYR	10.2
1	A	154	ASP	7.8
1	A	155	LYS	7.6
1	B	155	LYS	6.6
2	D	366	TYR	6.0
1	A	183	ASN	5.9
1	A	325	LYS	5.8
2	C	425	ASP	5.3
2	D	425	ASP	5.0
1	B	156	ASP	4.7
1	B	154	ASP	4.5
1	A	185	LYS	4.0
1	B	149	ASN	3.8
1	B	152	ILE	3.8
2	C	367	THR	3.4
1	B	325	LYS	3.2
1	A	189	MET	3.2
1	A	186	ARG	3.0
1	B	157	LYS	3.0
1	A	324	ASN	2.9
1	B	158	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	180	GLU	2.8
1	A	179	GLU	2.5
1	A	181	THR	2.5
1	A	182	LYS	2.4
1	A	188	ASN	2.3
1	B	324	ASN	2.3
1	B	146	LYS	2.2
1	A	158	LYS	2.1
1	B	144	ASN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

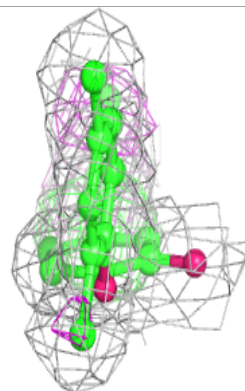
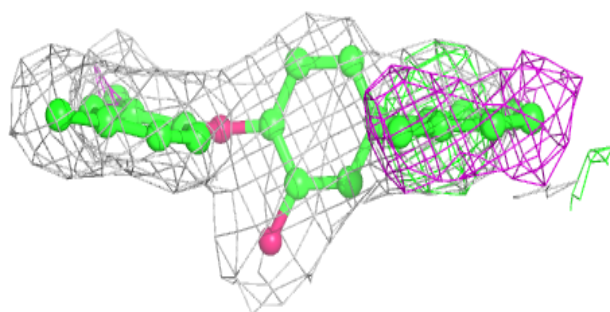
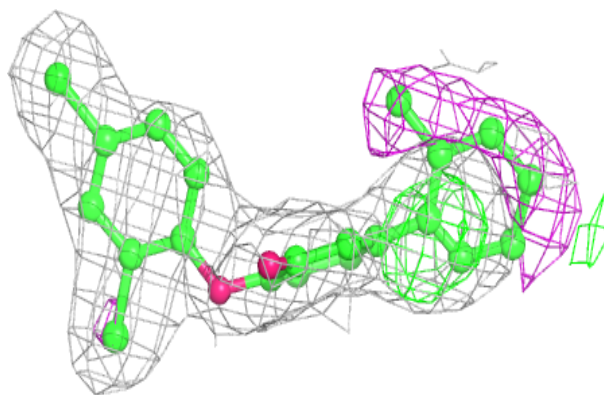
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	JPA	B	501	23/23	0.89	0.23	2,31,47,53	0
4	JPA	A	500	23/23	0.89	0.23	2,32,46,54	0
3	NAD	A	450	44/44	0.95	0.12	26,36,47,50	0
3	NAD	B	451	44/44	0.96	0.14	25,35,48,51	0

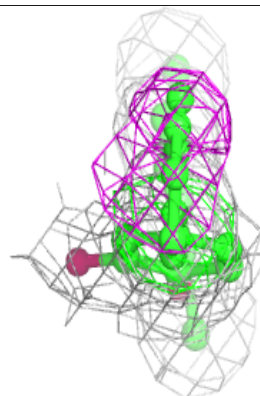
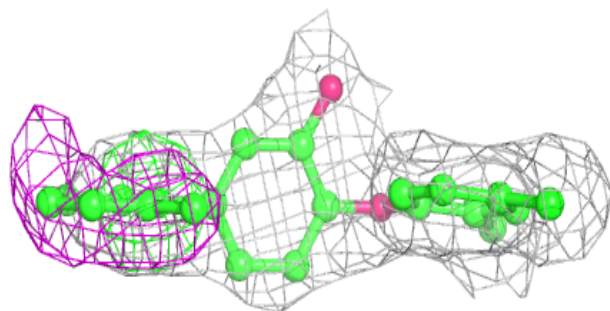
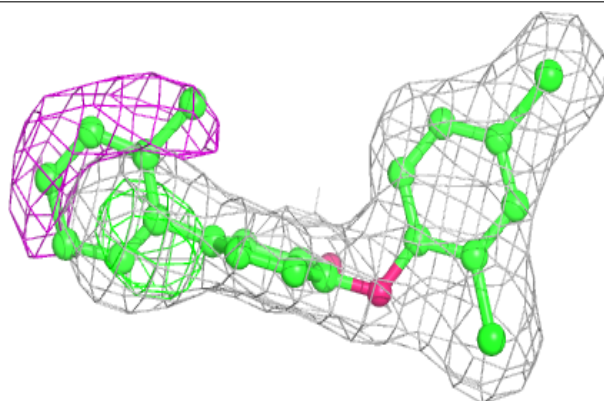
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around JPA 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)

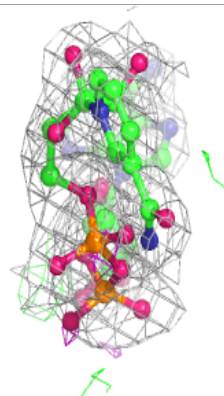
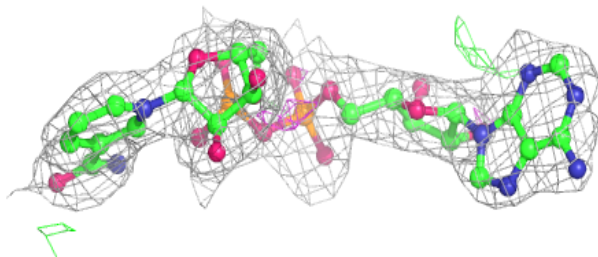
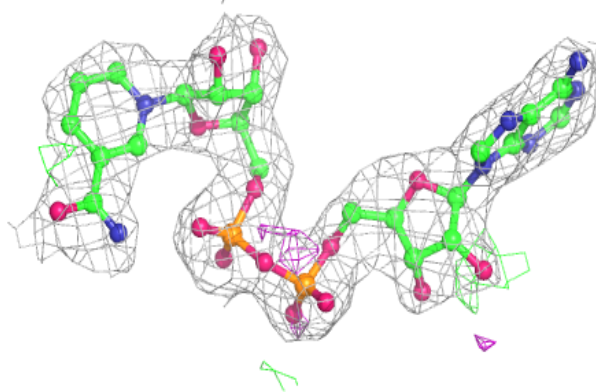
**Electron density around JPA A 500:**

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

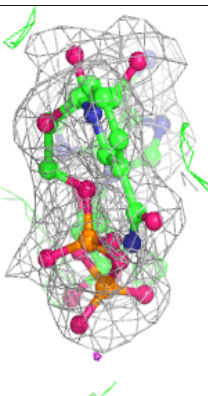
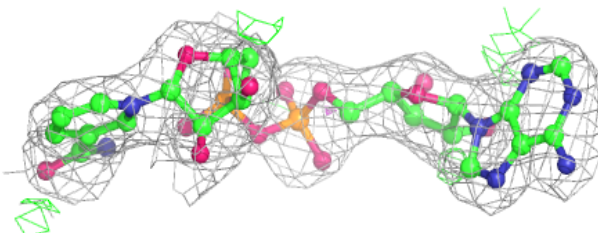
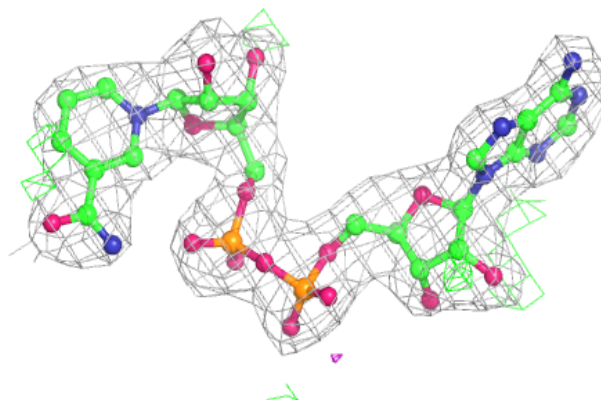


**Electron density around NAD A 450:**

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

**Electron density around NAD B 451:**

$2mF_o-DF_c$  (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.