



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:27 pm BST

PDB ID : 2ZJ0  
Title : Crystal structure of Mycobacterium tuberculosis S-Adenosyl-L-homocysteine hydrolase in ternary complex with NAD and 2-fluoroadenosine  
Authors : Reddy, M.C.M.; Gokulan, K.; Shetty, N.D.; Owen, J.L.; Ioerger, T.R.; Sacchettini, J.C.  
Deposited on : 2008-02-29  
Resolution : 2.42 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

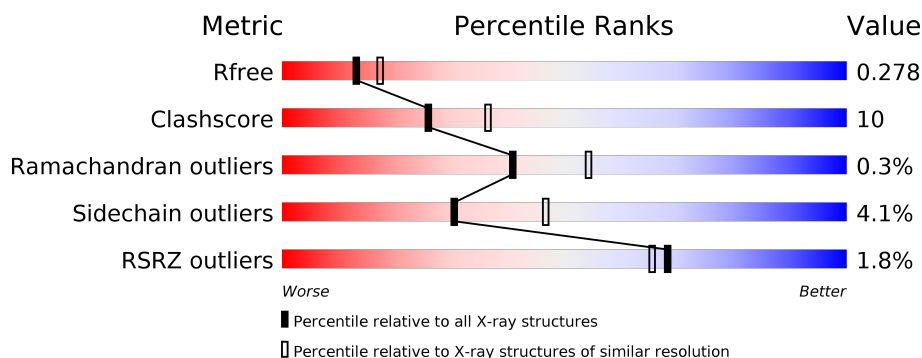
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	495	<div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	B	495	<div> <div>3%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	C	495	<div> <div>3%</div> <div>72%</div> <div>25%</div> <div>..</div> </div>
1	D	495	<div> <div>3%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15963 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.

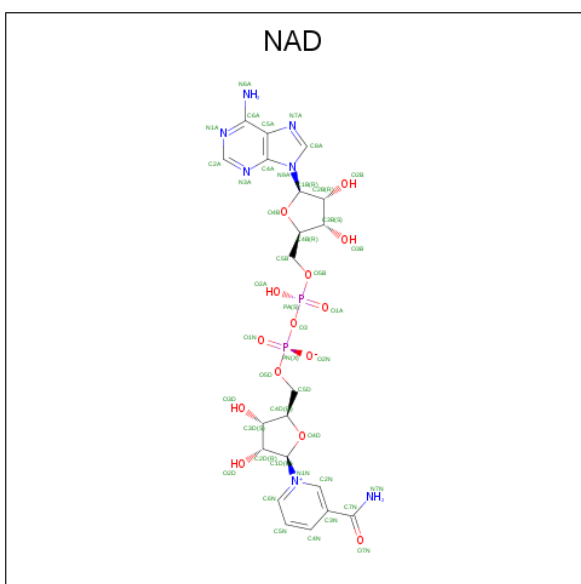
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3753	2367	644	725	17			
1	B	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	C	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	D	485	Total	C	N	O	S	0	0	0
			3747	2364	643	723	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P60176
B	1	MET	-	EXPRESSION TAG	UNP P60176
C	1	MET	-	EXPRESSION TAG	UNP P60176
D	1	MET	-	EXPRESSION TAG	UNP P60176

- Molecule 2 is 2-(6-AMINO-2-FLUORO-PURIN-9-YL)-5-HYDROXYMETHYL-TETRAHYDRO-FURAN-3,4-DIOL (three-letter code: 2FA) (formula: C<sub>10</sub>H<sub>12</sub>FN<sub>5</sub>O<sub>4</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		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

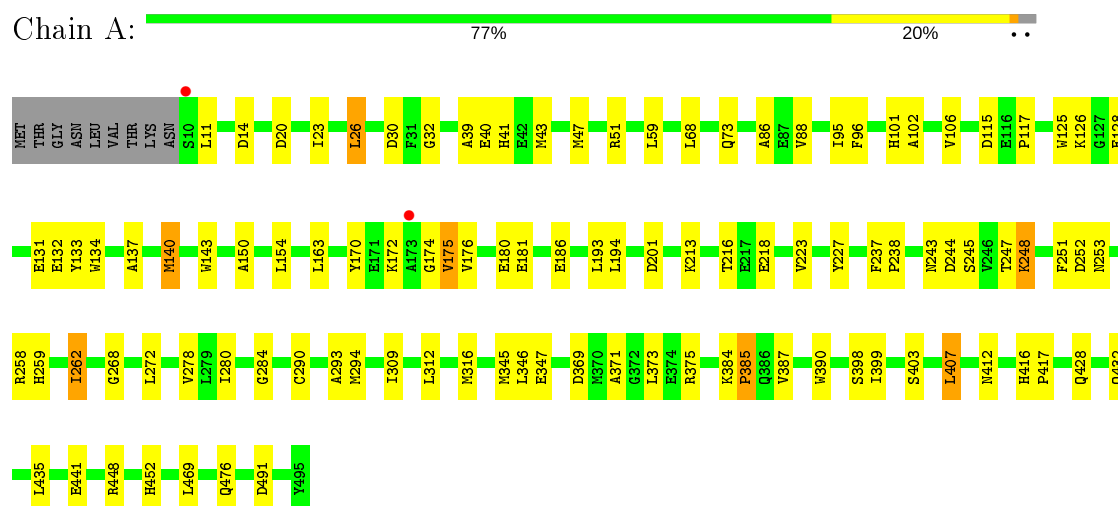
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	217	Total	O	0	0
			217	217		
4	B	182	Total	O	0	0
			182	182		
4	C	171	Total	O	0	0
			171	171		
4	D	141	Total	O	0	0
			141	141		

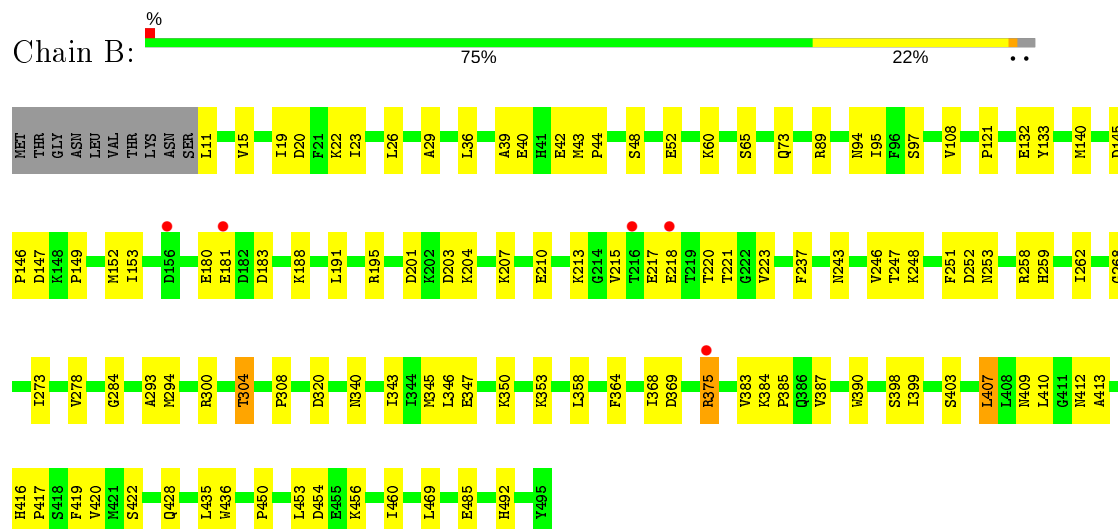
### 3 Residue-property plots

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: Adenosylhomocysteinase

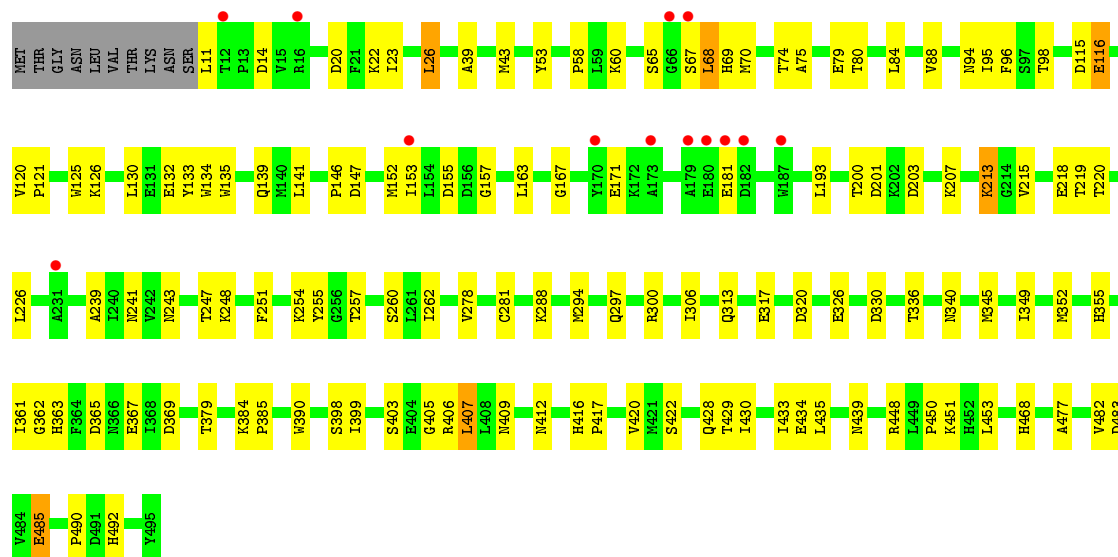


#### • Molecule 1: Adenosylhomocysteinase

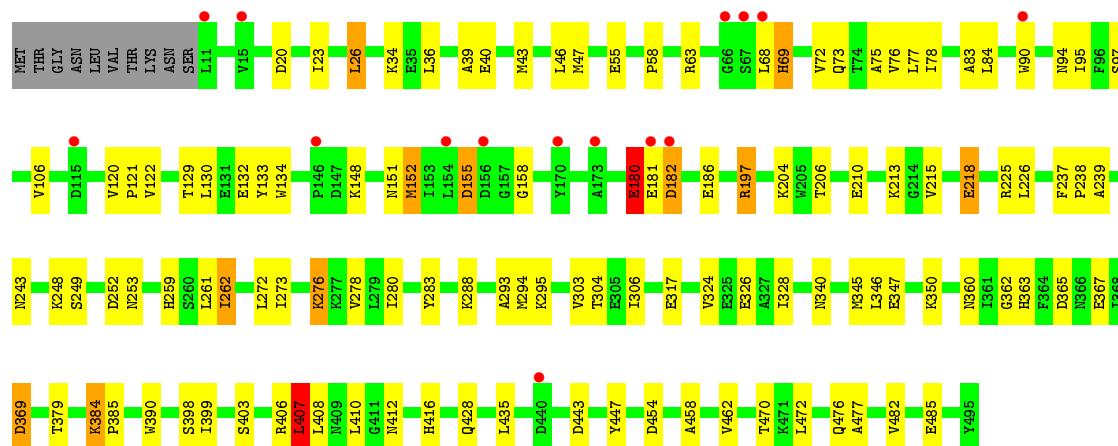
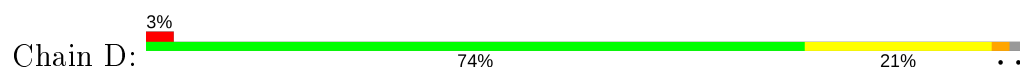


#### • Molecule 1: Adenosylhomocysteinase





● Molecule 1: Adenosylhomocysteinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.25Å 112.08Å 100.45Å 90.00° 95.15° 90.00°	Depositor
Resolution (Å)	33.15 – 2.42 33.15 – 2.42	Depositor EDS
% Data completeness (in resolution range)	91.9 (33.15-2.42) 91.9 (33.15-2.42)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.194 , 0.280 0.193 , 0.278	Depositor DCC
$R_{free}$ test set	3728 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.59% 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: 2FA, 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	0.77	0/3829	0.81	4/5193 (0.1%)
1	B	0.78	0/3824	0.82	0/5186
1	C	0.73	0/3824	0.76	0/5186
1	D	0.73	0/3823	0.77	2/5184 (0.0%)
All	All	0.75	0/15300	0.79	6/20749 (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	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	26	LEU	CA-CB-CG	7.85	133.35	115.30
1	A	407	LEU	CA-CB-CG	6.50	130.26	115.30
1	D	407	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	170	TYR	O-C-N	-5.24	114.32	122.70
1	D	155	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	448	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	485	GLU	Peptide

## 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	3753	0	3695	72	0
1	B	3748	0	3693	82	0
1	C	3748	0	3693	88	0
1	D	3747	0	3693	82	0
2	A	20	0	12	2	0
2	B	20	0	12	1	0
2	C	20	0	12	3	0
2	D	20	0	12	3	0
3	A	44	0	26	3	0
3	B	44	0	26	3	0
3	C	44	0	26	1	0
3	D	44	0	26	3	0
4	A	217	0	0	4	0
4	B	182	0	0	3	0
4	C	171	0	0	7	0
4	D	141	0	0	1	0
All	All	15963	0	14926	317	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 (317) 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:C:483:ASP:HB3	1:C:485:GLU:OE2	1.58	1.01
1:C:23:ILE:HD11	1:C:26:LEU:HD13	1.47	0.94
1:B:43:MET:HE1	1:B:73:GLN:HA	1.53	0.91
1:C:243:ASN:HA	1:C:248:LYS:HD2	1.54	0.89
1:A:371:ALA:HB1	1:A:375:ARG:HH12	1.45	0.82
1:C:398:SER:O	1:C:399:ILE:HD13	1.80	0.82
1:B:218:GLU:HG3	1:B:428:GLN:NE2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:GLU:HG3	1:C:428:GLN:NE2	1.99	0.78
1:C:39:ALA:HB1	1:C:43:MET:CE	2.14	0.78
2:D:500:2FA:H3'	3:D:550:NAD:C4N	2.14	0.76
1:C:218:GLU:CG	1:C:428:GLN:HE22	2.00	0.75
1:D:197:ARG:HE	1:D:197:ARG:HA	1.51	0.75
1:D:23:ILE:HD11	1:D:26:LEU:HD13	1.69	0.75
1:B:218:GLU:HG3	1:B:428:GLN:HE21	1.49	0.74
1:A:154:LEU:HD21	1:A:428:GLN:NE2	2.02	0.74
1:D:197:ARG:HD2	1:D:204:LYS:HD2	1.69	0.73
1:D:278:VAL:HG11	1:D:294:MET:HG3	1.71	0.71
2:B:500:2FA:H3'	3:B:550:NAD:C4N	2.22	0.70
1:B:218:GLU:O	1:B:248:LYS:HE3	1.91	0.70
1:C:23:ILE:HD11	1:C:26:LEU:CD1	2.20	0.70
2:C:500:2FA:H3'	3:C:550:NAD:C4N	2.22	0.68
1:B:300:ARG:HD2	1:C:320:ASP:OD1	1.93	0.68
1:C:450:PRO:HD2	1:C:453:LEU:HD12	1.77	0.67
1:C:23:ILE:CD1	1:C:26:LEU:HD13	2.24	0.65
1:A:268:GLY:O	1:A:387:VAL:HG21	1.97	0.65
1:C:398:SER:C	1:C:399:ILE:HD13	2.17	0.65
1:D:283:TYR:CZ	1:D:288:LYS:HG2	2.32	0.65
1:B:243:ASN:HD21	1:B:253:ASN:HD21	1.43	0.65
1:D:218:GLU:HG3	1:D:428:GLN:NE2	2.12	0.65
1:D:238:PRO:HG3	1:D:443:ASP:O	1.96	0.65
1:D:252:ASP:OD1	1:D:416:HIS:CE1	2.49	0.65
1:D:39:ALA:HB1	1:D:43:MET:HE2	1.79	0.65
1:A:175:VAL:CG2	1:A:176:VAL:N	2.59	0.64
1:B:23:ILE:HD11	1:B:26:LEU:HD13	1.79	0.64
1:D:206:THR:O	1:D:210:GLU:HG3	1.98	0.64
1:A:390:TRP:O	1:A:398:SER:HA	1.98	0.63
1:C:218:GLU:CG	1:C:428:GLN:NE2	2.61	0.63
1:D:477:ALA:HB1	1:D:482:VAL:O	1.99	0.63
1:B:278:VAL:HG11	1:B:294:MET:HG3	1.81	0.62
1:B:39:ALA:HB1	1:B:43:MET:HE3	1.81	0.62
1:B:218:GLU:CG	1:B:428:GLN:NE2	2.60	0.62
1:A:41:HIS:HD2	4:C:722:HOH:O	1.80	0.62
1:C:134:TRP:HB3	1:C:193:LEU:HD13	1.82	0.62
1:B:304:THR:OG1	3:B:550:NAD:H2A	1.99	0.62
1:B:407:LEU:HD13	1:B:410:LEU:HB2	1.82	0.61
1:C:39:ALA:HB1	1:C:43:MET:HE2	1.82	0.61
1:C:363:HIS:CE1	2:C:500:2FA:H5'	2.18	0.60
1:C:226:LEU:HD13	1:C:239:ALA:HB1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:NE	1:D:197:ARG:HA	2.15	0.60
1:A:40:GLU:HG2	1:A:47:MET:CE	2.32	0.60
1:B:11:LEU:HD11	1:B:132:GLU:HG2	1.83	0.60
1:A:309:ILE:HG21	1:B:246:VAL:HG11	1.84	0.60
1:A:216:THR:OG1	1:A:432:GLN:NE2	2.33	0.60
1:A:30:ASP:HB2	4:A:574:HOH:O	2.02	0.59
2:A:500:2FA:H3'	3:A:550:NAD:C4N	2.33	0.59
1:A:39:ALA:HB1	1:A:43:MET:HE2	1.84	0.59
1:D:304:THR:OG1	3:D:550:NAD:H2A	2.01	0.59
1:B:346:LEU:HG	1:B:350:LYS:HE2	1.85	0.58
1:B:11:LEU:CD1	1:B:132:GLU:HG2	2.33	0.58
1:D:215:VAL:O	1:D:239:ALA:HA	2.03	0.58
1:B:353:LYS:HE2	4:B:762:HOH:O	2.03	0.58
1:A:40:GLU:HG2	1:A:47:MET:HE1	1.86	0.58
1:B:152:MET:CE	1:B:213:LYS:HB2	2.33	0.58
1:D:238:PRO:HB2	1:D:435:LEU:HD21	1.86	0.58
1:A:243:ASN:HA	1:A:248:LYS:HE3	1.86	0.57
1:D:106:VAL:CG1	1:D:120:VAL:HG22	2.34	0.57
1:D:43:MET:HE1	1:D:73:GLN:HG3	1.86	0.57
1:D:63:ARG:CZ	1:D:148:LYS:HB2	2.34	0.57
1:A:39:ALA:O	1:A:43:MET:HG3	2.03	0.57
1:C:67:SER:HB3	1:C:155:ASP:OD1	2.03	0.57
1:C:200:THR:O	4:C:742:HOH:O	2.17	0.57
1:B:403:SER:OG	1:B:412:ASN:ND2	2.38	0.57
1:D:346:LEU:HG	1:D:350:LYS:NZ	2.20	0.57
1:C:116:GLU:HG3	1:C:116:GLU:O	2.05	0.56
1:C:468:HIS:HB3	4:C:865:HOH:O	2.05	0.56
1:D:252:ASP:OD1	1:D:416:HIS:HE1	1.88	0.56
1:D:43:MET:CE	1:D:73:GLN:HA	2.36	0.56
1:B:247:THR:HA	1:B:251:PHE:CD2	2.41	0.56
1:B:398:SER:O	1:B:399:ILE:HD13	2.06	0.56
1:C:365:ASP:HA	1:C:405:GLY:O	2.05	0.56
1:A:175:VAL:HG23	1:A:176:VAL:N	2.22	0.55
1:B:284:GLY:HA3	3:B:550:NAD:O5B	2.07	0.55
4:B:842:HOH:O	1:D:259:HIS:HE1	1.90	0.55
1:B:43:MET:CE	1:B:73:GLN:HA	2.30	0.55
1:B:450:PRO:HD2	1:B:453:LEU:HD12	1.89	0.55
1:A:51:ARG:NH1	4:A:686:HOH:O	2.32	0.55
1:C:226:LEU:HD13	1:C:239:ALA:CB	2.37	0.55
1:A:272:LEU:HB2	1:C:417:PRO:HG2	1.88	0.55
1:A:384:LYS:HB2	1:A:385:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:ILE:HA	1:C:352:MET:HG3	1.88	0.55
1:A:262:ILE:HD11	1:C:297:GLN:NE2	2.23	0.54
1:D:43:MET:HE3	1:D:73:GLN:HA	1.89	0.54
1:A:125:TRP:O	1:A:128:GLU:HG3	2.06	0.54
1:B:152:MET:HE2	1:B:213:LYS:HB2	1.89	0.54
1:D:129:THR:OG1	1:D:132:GLU:HG3	2.08	0.54
1:A:284:GLY:HA3	3:A:550:NAD:O5B	2.08	0.53
1:A:452:HIS:HD2	4:A:670:HOH:O	1.92	0.53
1:B:29:ALA:CB	1:B:108:VAL:HG21	2.38	0.53
1:B:252:ASP:OD1	1:B:416:HIS:CE1	2.62	0.53
1:A:43:MET:CE	1:A:73:GLN:HA	2.39	0.53
1:B:218:GLU:HB2	1:B:428:GLN:HE22	1.74	0.53
1:D:58:PRO:HD2	1:D:84:LEU:HB3	1.90	0.53
1:C:345:MET:HA	1:C:369:ASP:HB2	1.91	0.52
1:B:420:VAL:HG23	1:D:272:LEU:HD22	1.92	0.52
1:D:345:MET:HA	1:D:369:ASP:HB2	1.90	0.52
1:D:197:ARG:CA	1:D:197:ARG:HE	2.16	0.52
1:B:456:LYS:O	1:B:460:ILE:HG13	2.10	0.52
1:A:95:ILE:HG22	1:A:133:TYR:HB2	1.92	0.52
1:C:403:SER:OG	1:C:412:ASN:ND2	2.43	0.52
1:C:53:TYR:CD1	1:C:58:PRO:HG3	2.45	0.52
1:D:384:LYS:O	1:D:385:PRO:C	2.48	0.51
1:C:88:VAL:O	1:C:121:PRO:HD2	2.11	0.51
1:A:403:SER:OG	1:A:412:ASN:ND2	2.44	0.51
1:C:125:TRP:HZ2	1:C:132:GLU:OE1	1.94	0.51
1:C:218:GLU:HG3	1:C:428:GLN:HE22	1.62	0.51
1:C:74:THR:OG1	2:C:500:2FA:F	2.18	0.51
1:B:384:LYS:HB2	1:B:385:PRO:HD2	1.92	0.51
1:C:362:GLY:HA3	1:C:367:GLU:OE2	2.11	0.51
1:B:409:ASN:O	1:B:413:ALA:HB3	2.11	0.51
1:B:252:ASP:OD1	1:B:416:HIS:HE1	1.93	0.51
1:C:477:ALA:HB1	1:C:482:VAL:O	2.11	0.51
1:B:218:GLU:CB	1:B:428:GLN:HE22	2.24	0.50
1:C:260:SER:OG	1:C:416:HIS:HD2	1.93	0.50
1:C:363:HIS:HA	1:C:407:LEU:HD23	1.91	0.50
1:C:492:HIS:H	1:C:492:HIS:CD2	2.30	0.50
1:D:151:ASN:O	1:D:152:MET:HG2	2.11	0.50
1:B:152:MET:HE3	1:B:436:TRP:HA	1.93	0.50
1:A:213:LYS:O	1:A:238:PRO:HD2	2.11	0.50
1:B:340:ASN:HB3	1:B:343:ILE:HD11	1.93	0.50
1:D:78:ILE:HD11	1:D:90:TRP:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:HIS:HE1	1:C:94:ASN:HB2	1.76	0.50
1:D:261:LEU:HD12	1:D:408:LEU:HD11	1.93	0.50
1:D:73:GLN:H	1:D:73:GLN:CD	2.15	0.49
1:B:65:SER:HB3	1:B:140:MET:SD	2.52	0.49
1:A:11:LEU:CD1	1:A:132:GLU:HG2	2.42	0.49
1:A:247:THR:HA	1:A:251:PHE:CD2	2.48	0.49
1:B:191:LEU:HB3	1:B:195:ARG:NH2	2.28	0.49
1:C:14:ASP:O	1:C:20:ASP:HA	2.13	0.49
1:D:63:ARG:HD3	4:D:687:HOH:O	2.11	0.49
1:B:42:GLU:O	1:B:419:PHE:HA	2.12	0.49
1:C:399:ILE:HD11	4:C:860:HOH:O	2.13	0.49
1:C:345:MET:O	1:C:349:ILE:HG13	2.13	0.49
1:B:44:PRO:O	1:B:48:SER:HB3	2.13	0.49
1:B:390:TRP:O	1:B:398:SER:HA	2.13	0.48
1:A:272:LEU:HD13	1:C:420:VAL:HG23	1.95	0.48
1:D:398:SER:O	1:D:399:ILE:HD13	2.13	0.48
1:A:258:ARG:HA	1:A:293:ALA:HB2	1.95	0.48
1:D:46:LEU:HD13	1:D:77:LEU:HA	1.96	0.48
1:C:153:ILE:HB	1:C:215:VAL:HG23	1.94	0.48
1:A:280:ILE:HD12	1:A:290:CYS:HB3	1.95	0.48
1:D:20:ASP:O	1:D:121:PRO:HB3	2.12	0.48
1:D:362:GLY:O	1:D:407:LEU:HD12	2.14	0.48
1:A:175:VAL:HG23	1:A:176:VAL:H	1.78	0.48
1:B:183:ASP:O	1:B:188:LYS:HE2	2.14	0.48
1:C:147:ASP:HB3	4:C:709:HOH:O	2.14	0.48
1:D:384:LYS:HB2	1:D:385:PRO:HD2	1.96	0.47
1:A:476:GLN:HB3	1:B:340:ASN:HD21	1.78	0.47
1:D:458:ALA:O	1:D:462:VAL:HG23	2.15	0.47
1:C:254:LYS:HE2	1:C:288:LYS:HD2	1.95	0.47
1:D:106:VAL:HG12	1:D:120:VAL:HG22	1.97	0.47
1:A:243:ASN:HD21	1:A:253:ASN:HD21	1.61	0.47
1:C:152:MET:HE3	1:C:213:LYS:HB2	1.96	0.47
1:A:172:LYS:C	1:A:174:GLY:N	2.67	0.47
1:B:95:ILE:HG22	1:B:133:TYR:HB2	1.96	0.47
1:C:11:LEU:HD11	1:C:132:GLU:HG2	1.95	0.47
1:C:226:LEU:CD1	1:C:239:ALA:HB1	2.44	0.47
1:A:247:THR:O	1:A:251:PHE:HB2	2.15	0.47
1:B:217:GLU:HG3	1:B:223:VAL:HG23	1.96	0.47
1:A:32:GLY:HA3	1:A:101:HIS:O	2.14	0.47
1:C:340:ASN:O	1:C:367:GLU:HG2	2.15	0.47
1:D:94:ASN:HB3	1:D:97:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLU:O	1:A:248:LYS:CE	2.63	0.47
1:B:43:MET:HA	1:B:422:SER:HB2	1.97	0.47
1:D:472:LEU:HD22	1:D:476:GLN:HB3	1.97	0.47
1:A:218:GLU:O	1:A:248:LYS:HE3	2.15	0.47
1:B:268:GLY:O	1:B:387:VAL:HG21	2.15	0.47
1:C:313:GLN:O	1:C:317:GLU:HB2	2.15	0.47
1:D:83:ALA:O	1:D:84:LEU:HD23	2.15	0.47
1:B:29:ALA:HB2	1:B:108:VAL:HG21	1.96	0.46
1:B:15:VAL:HA	1:B:19:ILE:O	2.15	0.46
1:D:39:ALA:O	1:D:43:MET:HG3	2.14	0.46
1:A:59:LEU:HB3	1:A:86:ALA:HB2	1.97	0.46
1:B:262:ILE:HD12	1:B:262:ILE:C	2.35	0.46
1:B:52:GLU:OE1	1:B:456:LYS:NZ	2.45	0.46
1:C:43:MET:HG2	1:C:422:SER:HB2	1.96	0.46
1:D:106:VAL:CG1	1:D:122:VAL:HG21	2.46	0.46
1:A:243:ASN:HD22	1:A:248:LYS:NZ	2.12	0.46
1:C:306:ILE:HG22	1:D:470:THR:O	2.14	0.46
1:D:363:HIS:CE1	2:D:500:2FA:H5'	2.33	0.46
1:D:72:VAL:O	1:D:75:ALA:HB3	2.14	0.46
1:B:36:LEU:O	1:B:40:GLU:HG3	2.15	0.46
1:C:281:CYS:HB2	1:C:336:THR:HA	1.97	0.46
1:A:11:LEU:HD11	1:A:132:GLU:HG2	1.97	0.46
1:B:180:GLU:HG2	1:B:183:ASP:CG	2.35	0.46
1:B:435:LEU:HD12	1:B:435:LEU:HA	1.78	0.46
1:B:246:VAL:HG23	1:B:454:ASP:OD2	2.16	0.46
1:C:247:THR:HA	1:C:251:PHE:CD2	2.51	0.46
1:D:243:ASN:HA	1:D:248:LYS:HD2	1.98	0.46
1:A:96:PHE:O	1:A:126:LYS:NZ	2.49	0.46
1:A:134:TRP:HE1	1:A:186:GLU:HG3	1.79	0.46
1:B:345:MET:HA	1:B:369:ASP:HB2	1.98	0.46
1:C:251:PHE:HA	1:C:255:TYR:CD2	2.52	0.45
1:B:258:ARG:HA	1:B:293:ALA:HB2	1.97	0.45
1:C:125:TRP:CZ2	1:C:132:GLU:OE1	2.69	0.45
1:A:346:LEU:HD13	1:A:373:LEU:HA	1.99	0.45
1:B:248:LYS:HD3	1:B:252:ASP:HB3	1.99	0.45
1:B:320:ASP:OD1	1:C:300:ARG:HD2	2.17	0.45
1:D:36:LEU:HD21	1:D:75:ALA:HB1	1.98	0.45
1:A:154:LEU:HD23	1:A:154:LEU:C	2.36	0.45
1:B:39:ALA:O	1:B:43:MET:HG3	2.16	0.45
1:A:23:ILE:HD11	1:A:26:LEU:HD13	1.98	0.45
1:D:213:LYS:O	1:D:238:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ALA:HB1	1:B:43:MET:CE	2.47	0.45
1:C:167:GLY:O	1:C:171:GLU:HG3	2.16	0.45
1:D:95:ILE:HG22	1:D:133:TYR:HB2	1.98	0.45
2:D:500:2FA:H3'	3:D:550:NAD:C3N	2.47	0.44
1:D:360:ASN:O	1:D:407:LEU:HA	2.17	0.44
2:A:500:2FA:H3'	3:A:550:NAD:C5N	2.47	0.44
1:C:257:THR:HG23	1:C:361:ILE:HD13	1.98	0.44
1:D:106:VAL:HG11	1:D:122:VAL:HG21	1.99	0.44
1:D:218:GLU:HG3	1:D:428:GLN:HE21	1.80	0.44
1:D:340:ASN:O	1:D:367:GLU:HG2	2.17	0.44
1:D:47:MET:HE1	1:D:76:VAL:CG1	2.48	0.44
1:C:241:ASN:HB3	1:C:448:ARG:HG2	1.99	0.44
1:C:70:MET:HB3	1:C:98:THR:HG23	1.98	0.44
1:A:345:MET:HA	1:A:369:ASP:HB2	2.00	0.44
1:B:218:GLU:CG	1:B:428:GLN:HE22	2.29	0.44
1:B:259:HIS:CG	1:B:417:PRO:HG3	2.53	0.44
1:D:155:ASP:OD2	1:D:158:GLY:HA2	2.18	0.44
1:D:36:LEU:O	1:D:40:GLU:HG3	2.17	0.44
1:B:221:THR:HG21	1:B:364:PHE:CE2	2.53	0.44
1:A:180:GLU:O	1:A:181:GLU:C	2.55	0.44
1:D:306:ILE:C	1:D:306:ILE:HD12	2.38	0.44
1:B:20:ASP:N	1:B:20:ASP:OD1	2.42	0.43
1:D:384:LYS:HB2	1:D:385:PRO:CD	2.48	0.43
1:A:223:VAL:HG12	1:A:227:TYR:CE2	2.54	0.43
1:B:375:ARG:NH2	4:B:625:HOH:O	2.48	0.43
1:D:283:TYR:CE2	1:D:288:LYS:HG2	2.53	0.43
1:B:153:ILE:O	1:B:215:VAL:HA	2.18	0.43
1:B:89:ARG:HG2	1:B:121:PRO:HG2	2.00	0.43
1:C:95:ILE:HG22	1:C:133:TYR:HB2	1.99	0.43
1:C:450:PRO:CD	1:C:453:LEU:HD12	2.46	0.43
1:C:390:TRP:O	1:C:398:SER:HA	2.19	0.43
1:D:243:ASN:HD21	1:D:253:ASN:HD21	1.66	0.43
1:D:280:ILE:O	1:D:303:VAL:HA	2.19	0.43
1:D:407:LEU:HD23	1:D:410:LEU:HB2	2.01	0.43
1:B:94:ASN:HB3	1:B:97:SER:HB3	2.01	0.43
1:D:262:ILE:CG2	1:D:293:ALA:HB1	2.49	0.43
1:B:152:MET:HE1	1:B:213:LYS:HB2	1.99	0.43
1:C:157:GLY:HA3	1:C:363:HIS:NE2	2.34	0.43
1:C:429:THR:O	1:C:433:ILE:HG13	2.18	0.43
1:A:312:LEU:O	1:A:316:MET:HG2	2.18	0.43
1:A:398:SER:O	1:A:399:ILE:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:LEU:HD12	1:A:435:LEU:HA	1.82	0.43
1:C:75:ALA:O	1:C:79:GLU:HG3	2.19	0.43
1:A:40:GLU:HG2	1:A:47:MET:HE3	2.01	0.42
1:B:147:ASP:C	1:B:149:PRO:HD3	2.39	0.42
1:B:203:ASP:O	1:B:207:LYS:HG3	2.18	0.42
1:C:435:LEU:HA	1:C:435:LEU:HD23	1.89	0.42
1:C:203:ASP:OD1	1:C:207:LYS:NZ	2.40	0.42
1:C:260:SER:HB2	1:C:409:ASN:HB2	2.01	0.42
1:A:278:VAL:HG11	1:A:294:MET:HG3	2.01	0.42
1:A:131:GLU:OE1	1:A:131:GLU:N	2.48	0.42
1:A:137:ALA:O	1:A:140:MET:HE3	2.19	0.42
1:C:379:THR:O	1:C:390:TRP:HA	2.20	0.42
1:D:134:TRP:HE1	1:D:186:GLU:CG	2.33	0.42
1:D:39:ALA:HB1	1:D:43:MET:CE	2.46	0.42
1:B:145:ASP:HA	1:B:146:PRO:HD2	1.81	0.42
1:C:430:ILE:O	1:C:434:GLU:HG2	2.19	0.42
1:D:379:THR:O	1:D:390:TRP:HA	2.19	0.42
1:D:443:ASP:HB2	1:D:447:TYR:OH	2.20	0.42
1:B:201:ASP:CG	1:B:204:LYS:HB2	2.39	0.41
1:B:89:ARG:O	1:B:140:MET:HG2	2.20	0.41
1:C:135:TRP:O	1:C:139:GLN:HG2	2.20	0.41
1:D:197:ARG:NE	1:D:197:ARG:CA	2.79	0.41
1:A:163:LEU:HD12	1:A:194:LEU:HD21	2.01	0.41
1:B:358:LEU:HD11	1:B:368:ILE:HG12	2.01	0.41
1:C:141:LEU:HD12	1:C:163:LEU:HD23	2.02	0.41
1:C:146:PRO:HD2	4:C:730:HOH:O	2.20	0.41
1:C:355:HIS:HE1	4:C:846:HOH:O	2.02	0.41
1:A:102:ALA:O	1:A:106:VAL:HG23	2.21	0.41
1:A:115:ASP:C	1:A:117:PRO:HD3	2.40	0.41
1:A:172:LYS:C	1:A:174:GLY:H	2.22	0.41
1:A:469:LEU:HD11	1:B:308:PRO:HB3	2.01	0.41
1:C:278:VAL:HG21	1:C:294:MET:HE3	2.01	0.41
1:A:14:ASP:O	1:A:20:ASP:HA	2.21	0.41
1:A:452:HIS:CD2	4:A:670:HOH:O	2.70	0.41
1:B:262:ILE:CD1	1:D:262:ILE:HD11	2.50	0.41
1:D:226:LEU:HD13	1:D:239:ALA:HB1	2.02	0.41
1:D:273:ILE:O	1:D:276:LYS:HB2	2.20	0.41
1:C:130:LEU:HD21	1:C:406:ARG:HH22	1.85	0.41
1:C:384:LYS:HB2	1:C:385:PRO:CD	2.50	0.41
1:C:80:THR:O	1:C:84:LEU:HG	2.21	0.41
1:D:130:LEU:HD21	1:D:406:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASP:OD1	1:A:416:HIS:HE1	2.04	0.41
1:B:398:SER:C	1:B:399:ILE:HD13	2.41	0.41
1:C:490:PRO:HB2	1:C:492:HIS:CD2	2.56	0.41
1:A:174:GLY:C	1:A:175:VAL:HG12	2.41	0.41
1:A:259:HIS:CG	1:A:417:PRO:HG3	2.56	0.41
1:A:262:ILE:HD13	1:A:293:ALA:HB1	2.03	0.41
1:D:180:GLU:HB2	1:D:181:GLU:H	1.60	0.41
1:B:383:VAL:HA	1:D:34:LYS:HD3	2.03	0.41
1:A:43:MET:HE1	1:A:73:GLN:HG3	2.03	0.41
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.96	0.41
1:C:435:LEU:O	1:C:439:ASN:ND2	2.48	0.41
1:D:68:LEU:O	1:D:69:HIS:C	2.58	0.41
1:B:43:MET:HE2	1:B:73:GLN:HG3	2.03	0.40
1:C:451:LYS:HB2	1:C:451:LYS:HE2	1.80	0.40
1:D:324:VAL:O	1:D:328:ILE:HB	2.21	0.40
1:D:408:LEU:O	1:D:412:ASN:HB2	2.21	0.40
1:C:68:LEU:HD12	1:C:69:HIS:H	1.87	0.40
1:C:69:HIS:CE1	1:C:94:ASN:HB2	2.57	0.40
1:C:96:PHE:O	1:C:126:LYS:HG3	2.22	0.40
1:A:252:ASP:OD1	1:A:416:HIS:CE1	2.74	0.40
1:A:143:TRP:CD1	1:A:150:ALA:HB2	2.56	0.40
1:A:244:ASP:OD2	1:B:492:HIS:HE1	2.04	0.40
1:D:134:TRP:HE1	1:D:186:GLU:HG3	1.87	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	484/495 (98%)	462 (96%)	21 (4%)	1 (0%)	47 61
1	B	483/495 (98%)	463 (96%)	20 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	483/495 (98%)	458 (95%)	24 (5%)	1 (0%)	47 61
1	D	483/495 (98%)	457 (95%)	22 (5%)	4 (1%)	19 27
All	All	1933/1980 (98%)	1840 (95%)	87 (4%)	6 (0%)	41 54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	180	GLU
1	D	369	ASP
1	C	181	GLU
1	D	182	ASP
1	D	69	HIS
1	A	385	PRO

### 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	395/404 (98%)	381 (96%)	14 (4%)	36 53
1	B	395/404 (98%)	383 (97%)	12 (3%)	41 59
1	C	395/404 (98%)	378 (96%)	17 (4%)	29 44
1	D	395/404 (98%)	373 (94%)	22 (6%)	21 32
All	All	1580/1616 (98%)	1515 (96%)	65 (4%)	30 47

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LEU
1	A	88	VAL
1	A	140	MET
1	A	175	VAL
1	A	193	LEU
1	A	201	ASP

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Mol	Chain	Res	Type
1	A	237	PHE
1	A	245	SER
1	A	248	LYS
1	A	262	ILE
1	A	347	GLU
1	A	407	LEU
1	A	441	GLU
1	A	491	ASP
1	B	22	LYS
1	B	60	LYS
1	B	181	GLU
1	B	210	GLU
1	B	220	THR
1	B	237	PHE
1	B	273	ILE
1	B	304	THR
1	B	347	GLU
1	B	375	ARG
1	B	407	LEU
1	B	469	LEU
1	C	22	LYS
1	C	26	LEU
1	C	60	LYS
1	C	65	SER
1	C	68	LEU
1	C	115	ASP
1	C	116	GLU
1	C	120	VAL
1	C	201	ASP
1	C	213	LYS
1	C	219	THR
1	C	220	THR
1	C	262	ILE
1	C	326	GLU
1	C	330	ASP
1	C	407	LEU
1	C	485	GLU
1	D	26	LEU
1	D	55	GLU
1	D	152	MET
1	D	180	GLU
1	D	182	ASP

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Mol	Chain	Res	Type
1	D	197	ARG
1	D	218	GLU
1	D	225	ARG
1	D	237	PHE
1	D	249	SER
1	D	262	ILE
1	D	276	LYS
1	D	295	LYS
1	D	317	GLU
1	D	326	GLU
1	D	347	GLU
1	D	365	ASP
1	D	384	LYS
1	D	403	SER
1	D	407	LEU
1	D	454	ASP
1	D	485	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	243	ASN
1	A	310	ASN
1	A	412	ASN
1	A	416	HIS
1	A	428	GLN
1	A	432	GLN
1	A	452	HIS
1	B	57	GLN
1	B	243	ASN
1	B	259	HIS
1	B	310	ASN
1	B	412	ASN
1	B	416	HIS
1	B	428	GLN
1	B	432	GLN
1	B	492	HIS
1	C	94	ASN
1	C	243	ASN
1	C	310	ASN
1	C	355	HIS

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Mol	Chain	Res	Type
1	C	360	ASN
1	C	386	GLN
1	C	412	ASN
1	C	416	HIS
1	C	427	ASN
1	C	428	GLN
1	C	492	HIS
1	D	57	GLN
1	D	243	ASN
1	D	259	HIS
1	D	310	ASN
1	D	355	HIS
1	D	412	ASN
1	D	416	HIS
1	D	427	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	D	550	-	42,48,48	1.66	7 (16%)	50,73,73	1.52	10 (20%)
3	NAD	A	550	-	42,48,48	1.40	5 (11%)	50,73,73	1.83	13 (26%)
3	NAD	C	550	-	42,48,48	1.59	10 (23%)	50,73,73	1.61	7 (14%)
2	2FA	A	500	-	19,22,22	2.34	5 (26%)	20,33,33	2.64	8 (40%)
2	2FA	B	500	-	19,22,22	2.06	2 (10%)	20,33,33	2.51	9 (45%)
2	2FA	C	500	-	19,22,22	2.31	5 (26%)	20,33,33	2.12	7 (35%)
2	2FA	D	500	-	19,22,22	2.14	6 (31%)	20,33,33	3.06	9 (45%)
3	NAD	B	550	-	42,48,48	1.54	7 (16%)	50,73,73	2.15	16 (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
3	NAD	D	550	-	-	5/26/62/62	0/5/5/5
3	NAD	A	550	-	-	5/26/62/62	0/5/5/5
3	NAD	C	550	-	-	5/26/62/62	0/5/5/5
2	2FA	A	500	-	-	0/2/22/22	0/3/3/3
2	2FA	B	500	-	-	1/2/22/22	0/3/3/3
2	2FA	C	500	-	-	0/2/22/22	0/3/3/3
2	2FA	D	500	-	-	2/2/22/22	0/3/3/3
3	NAD	B	550	-	-	6/26/62/62	0/5/5/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	2FA	C2-N3	6.76	1.38	1.31
2	C	500	2FA	C2-N3	6.05	1.37	1.31
2	D	500	2FA	C2-N3	5.73	1.37	1.31
2	C	500	2FA	C2-N1	5.66	1.37	1.31
2	A	500	2FA	C2-N1	5.66	1.37	1.31
3	C	550	NAD	O7N-C7N	5.54	1.34	1.24
2	B	500	2FA	C2-N1	5.50	1.36	1.31
2	B	500	2FA	C2-N3	5.47	1.36	1.31
3	D	550	NAD	O4D-C1D	5.16	1.48	1.41
2	D	500	2FA	C2-N1	4.43	1.35	1.31
3	B	550	NAD	C2N-N1N	-3.79	1.30	1.35
3	A	550	NAD	O4B-C1B	3.62	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	550	NAD	O4B-C1B	3.58	1.46	1.41
3	D	550	NAD	C2A-N3A	3.51	1.37	1.32
3	D	550	NAD	C7N-N7N	-3.41	1.26	1.33
3	D	550	NAD	C2N-N1N	-3.40	1.30	1.35
3	D	550	NAD	O7N-C7N	3.32	1.30	1.24
3	B	550	NAD	O7N-C7N	3.28	1.30	1.24
3	B	550	NAD	C7N-N7N	-3.21	1.26	1.33
3	A	550	NAD	O7N-C7N	3.12	1.30	1.24
2	C	500	2FA	C5-C4	3.09	1.49	1.40
3	A	550	NAD	C7N-N7N	-3.05	1.27	1.33
3	A	550	NAD	C2N-N1N	-3.05	1.31	1.35
2	D	500	2FA	C6-N1	3.02	1.39	1.33
2	D	500	2FA	C4-N3	-2.80	1.31	1.35
3	B	550	NAD	C2D-C1D	-2.79	1.49	1.53
3	D	550	NAD	C5A-C4A	2.78	1.48	1.40
3	A	550	NAD	C4A-N3A	-2.78	1.31	1.35
3	B	550	NAD	C4N-C3N	-2.71	1.34	1.39
2	C	500	2FA	C8-N7	2.67	1.39	1.34
3	C	550	NAD	C7N-N7N	-2.65	1.27	1.33
2	C	500	2FA	O4'-C1'	2.65	1.44	1.41
3	B	550	NAD	O2B-C2B	2.64	1.49	1.43
3	C	550	NAD	C3N-C7N	2.63	1.54	1.50
3	C	550	NAD	C2N-C3N	2.61	1.43	1.39
2	A	500	2FA	C6-N6	2.60	1.43	1.34
3	C	550	NAD	C5A-C4A	2.55	1.47	1.40
3	C	550	NAD	O4B-C1B	2.53	1.44	1.41
2	D	500	2FA	C8-N7	2.49	1.39	1.34
3	C	550	NAD	C2N-N1N	-2.31	1.32	1.35
3	C	550	NAD	O4D-C1D	2.29	1.44	1.41
2	A	500	2FA	O4'-C4'	-2.29	1.39	1.45
2	A	500	2FA	C5-C4	2.19	1.46	1.40
3	C	550	NAD	C2A-N3A	2.13	1.35	1.32
3	B	550	NAD	O4B-C1B	2.11	1.44	1.41
3	C	550	NAD	O4B-C4B	-2.08	1.40	1.45
2	D	500	2FA	C5-C4	2.08	1.46	1.40

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	550	NAD	O4D-C1D-C2D	-7.48	95.99	106.93
2	D	500	2FA	C5-C6-N1	-7.40	116.15	121.01
2	D	500	2FA	F-C2-N1	6.86	121.24	114.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	2FA	F-C2-N1	5.65	120.10	114.73
2	A	500	2FA	C5-C6-N1	-5.11	117.66	121.01
3	B	550	NAD	N3A-C2A-N1A	-4.93	120.98	128.68
3	A	550	NAD	C5N-C4N-C3N	-4.84	114.62	120.34
2	B	500	2FA	C1'-N9-C4	-4.81	118.18	126.64
3	C	550	NAD	O4D-C1D-C2D	-4.76	99.98	106.93
2	A	500	2FA	C4-C5-N7	-4.71	104.49	109.40
3	A	550	NAD	N3A-C2A-N1A	-4.70	121.33	128.68
2	C	500	2FA	F-C2-N3	4.48	118.98	114.73
3	B	550	NAD	O7N-C7N-N7N	-4.46	116.24	122.58
2	A	500	2FA	F-C2-N1	4.44	118.95	114.73
2	D	500	2FA	N3-C2-N1	-4.21	124.53	130.51
3	A	550	NAD	C1B-N9A-C4A	-4.12	119.41	126.64
2	D	500	2FA	C4-C5-N7	-4.02	105.21	109.40
3	A	550	NAD	C3N-C7N-N7N	3.93	122.46	117.75
2	B	500	2FA	C5-C6-N1	-3.90	118.45	121.01
2	C	500	2FA	N3-C2-N1	-3.85	125.06	130.51
3	A	550	NAD	O3D-C3D-C4D	-3.79	100.09	111.05
3	C	550	NAD	C4A-C5A-N7A	-3.79	105.45	109.40
2	C	500	2FA	C3'-C2'-C1'	3.68	106.52	100.98
3	B	550	NAD	C3N-C2N-N1N	3.62	123.97	120.43
2	D	500	2FA	C2-N3-C4	3.59	119.39	115.03
2	D	500	2FA	C1'-N9-C4	-3.49	120.51	126.64
2	A	500	2FA	C5'-C4'-C3'	3.48	123.47	115.09
3	C	550	NAD	O7N-C7N-C3N	3.46	123.78	119.63
2	A	500	2FA	N3-C2-N1	-3.40	125.69	130.51
3	C	550	NAD	O7N-C7N-N7N	-3.37	117.79	122.58
3	A	550	NAD	C2N-C3N-C4N	3.35	122.06	118.26
2	A	500	2FA	C1'-N9-C4	-3.30	120.85	126.64
2	D	500	2FA	N6-C6-N1	3.24	125.87	117.07
2	B	500	2FA	O5'-C5'-C4'	-3.21	100.29	111.29
3	D	550	NAD	N3A-C2A-N1A	-3.10	123.83	128.68
3	B	550	NAD	PN-O3-PA	-3.10	122.20	132.83
3	C	550	NAD	C1B-N9A-C4A	-3.09	121.22	126.64
3	B	550	NAD	C3N-C7N-N7N	3.07	121.43	117.75
3	B	550	NAD	O2B-C2B-C1B	3.05	122.11	110.85
2	B	500	2FA	C4-C5-N7	-3.02	106.25	109.40
3	D	550	NAD	PN-O3-PA	-3.02	122.47	132.83
3	D	550	NAD	O7N-C7N-N7N	-2.97	118.35	122.58
3	B	550	NAD	O4D-C4D-C3D	-2.95	99.27	105.11
3	B	550	NAD	C2B-C3B-C4B	2.94	108.35	102.64
2	B	500	2FA	N3-C2-N1	-2.87	126.44	130.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	550	NAD	C2B-C3B-C4B	2.86	108.20	102.64
2	C	500	2FA	C2-N3-C4	2.83	118.48	115.03
3	A	550	NAD	C2B-C3B-C4B	2.82	108.12	102.64
2	A	500	2FA	C2-N3-C4	2.77	118.40	115.03
2	A	500	2FA	O5'-C5'-C4'	-2.74	101.89	111.29
3	B	550	NAD	C1B-N9A-C4A	-2.67	121.96	126.64
3	D	550	NAD	C4A-C5A-N7A	-2.66	106.62	109.40
2	B	500	2FA	C3'-C2'-C1'	2.61	104.91	100.98
3	A	550	NAD	O4D-C1D-C2D	-2.61	103.11	106.93
2	C	500	2FA	O4'-C1'-C2'	-2.50	103.27	106.93
3	B	550	NAD	O5B-C5B-C4B	-2.45	100.57	108.99
3	B	550	NAD	C2A-N1A-C6A	2.44	122.93	118.75
3	A	550	NAD	C6N-N1N-C2N	-2.42	119.77	121.97
2	D	500	2FA	O5'-C5'-C4'	-2.41	103.02	111.29
3	D	550	NAD	C2N-N1N-C1D	-2.41	113.77	119.14
3	D	550	NAD	O2D-C2D-C3D	2.34	119.40	111.82
3	D	550	NAD	O4D-C1D-C2D	-2.30	103.56	106.93
2	B	500	2FA	N6-C6-N1	2.26	123.21	117.07
2	C	500	2FA	C5-C6-N6	-2.22	116.98	120.35
3	B	550	NAD	O7N-C7N-C3N	2.19	122.26	119.63
2	B	500	2FA	O3'-C3'-C2'	-2.19	104.75	111.82
3	A	550	NAD	C4A-C5A-N7A	-2.17	107.13	109.40
3	C	550	NAD	C5N-C4N-C3N	-2.16	117.79	120.34
2	C	500	2FA	N6-C6-N1	2.15	122.93	117.07
2	D	500	2FA	C3'-C2'-C1'	2.15	104.21	100.98
3	A	550	NAD	O7N-C7N-N7N	-2.13	119.55	122.58
3	A	550	NAD	O2N-PN-O1N	2.13	122.78	112.24
3	B	550	NAD	C2N-N1N-C1D	-2.12	114.42	119.14
3	D	550	NAD	C2B-C3B-C4B	2.11	106.75	102.64
3	D	550	NAD	C3D-C2D-C1D	2.10	104.14	100.98
3	B	550	NAD	C4A-C5A-N7A	-2.10	107.21	109.40
3	A	550	NAD	C3B-C2B-C1B	-2.09	97.83	100.98
3	B	550	NAD	C5N-C4N-C3N	-2.08	117.89	120.34
3	D	550	NAD	C5N-C4N-C3N	-2.05	117.92	120.34

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	550	NAD	O4D-C1D-N1N-C2N
3	D	550	NAD	O4D-C1D-N1N-C6N
3	D	550	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	D	550	NAD	C2D-C1D-N1N-C6N
3	A	550	NAD	O4D-C1D-N1N-C2N
3	A	550	NAD	O4D-C1D-N1N-C6N
3	A	550	NAD	C2D-C1D-N1N-C2N
3	A	550	NAD	C2D-C1D-N1N-C6N
3	C	550	NAD	O4D-C1D-N1N-C2N
3	C	550	NAD	O4D-C1D-N1N-C6N
3	C	550	NAD	C2D-C1D-N1N-C2N
3	C	550	NAD	C2D-C1D-N1N-C6N
3	B	550	NAD	O4D-C1D-N1N-C2N
3	B	550	NAD	O4D-C1D-N1N-C6N
3	B	550	NAD	C2D-C1D-N1N-C2N
3	B	550	NAD	C2D-C1D-N1N-C6N
2	D	500	2FA	C3'-C4'-C5'-O5'
2	D	500	2FA	O4'-C4'-C5'-O5'
2	B	500	2FA	C3'-C4'-C5'-O5'
3	D	550	NAD	O4B-C4B-C5B-O5B
3	A	550	NAD	O4B-C4B-C5B-O5B
3	C	550	NAD	O4B-C4B-C5B-O5B
3	B	550	NAD	O4B-C4B-C5B-O5B
3	B	550	NAD	C5B-O5B-PA-O1A

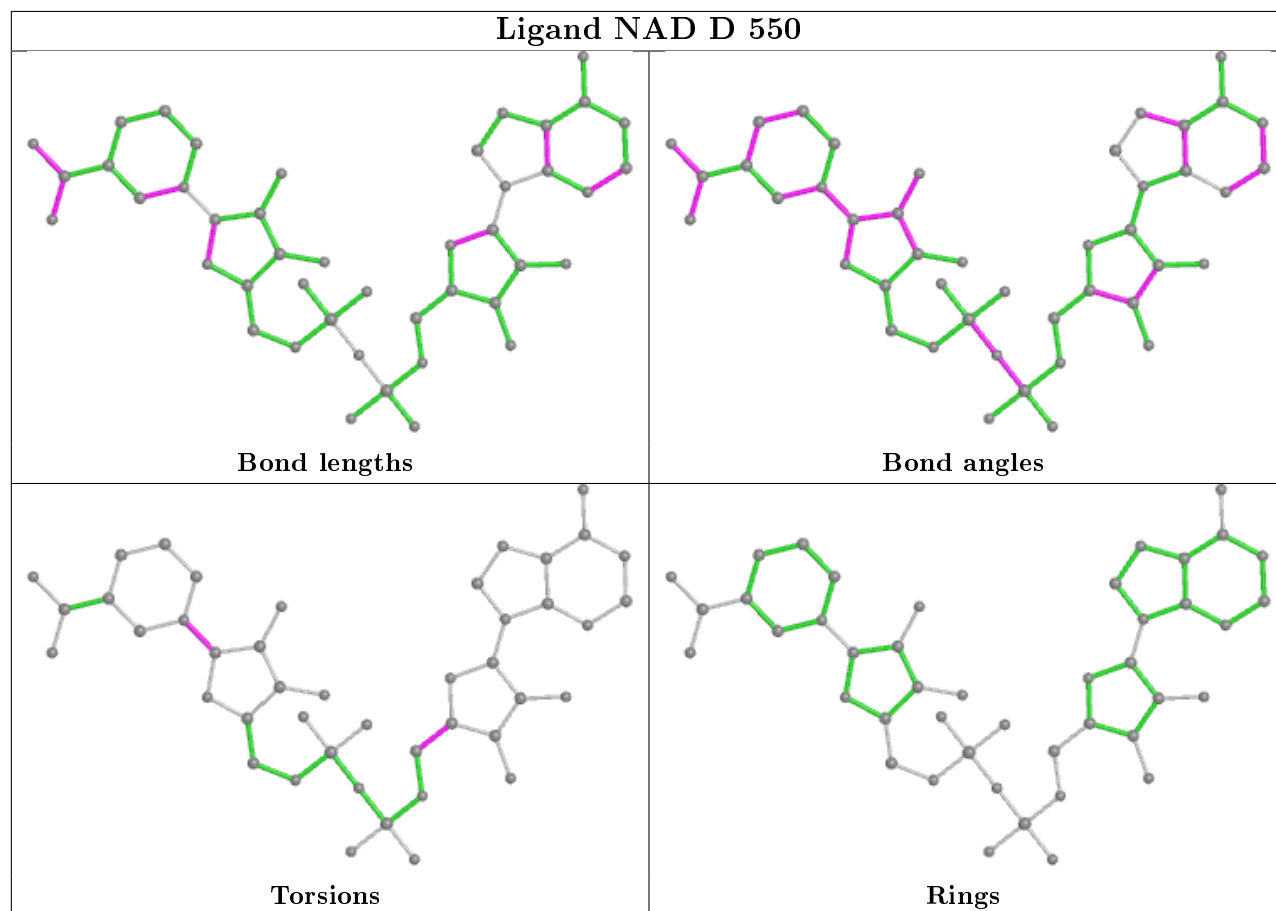
There are no ring outliers.

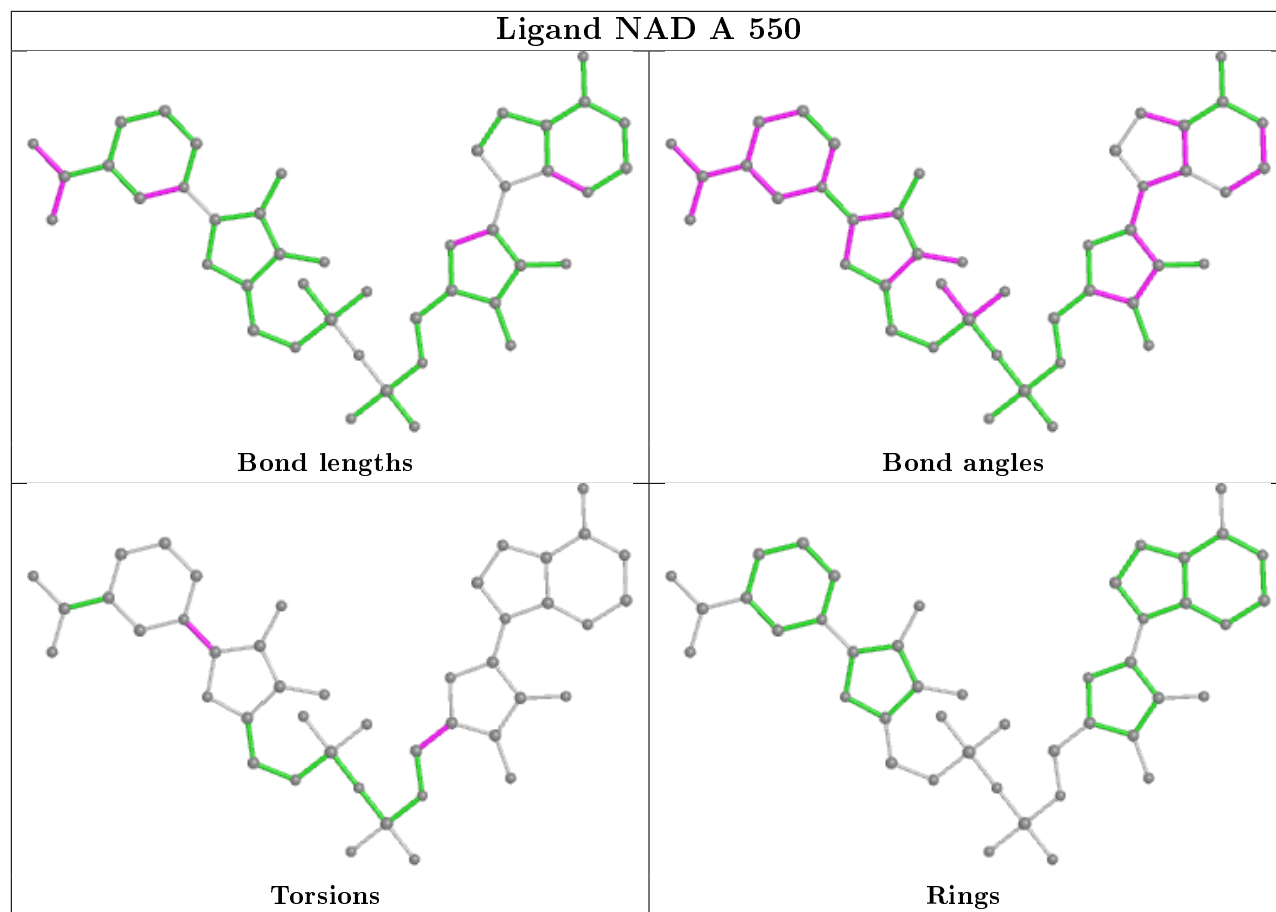
8 monomers are involved in 13 short contacts:

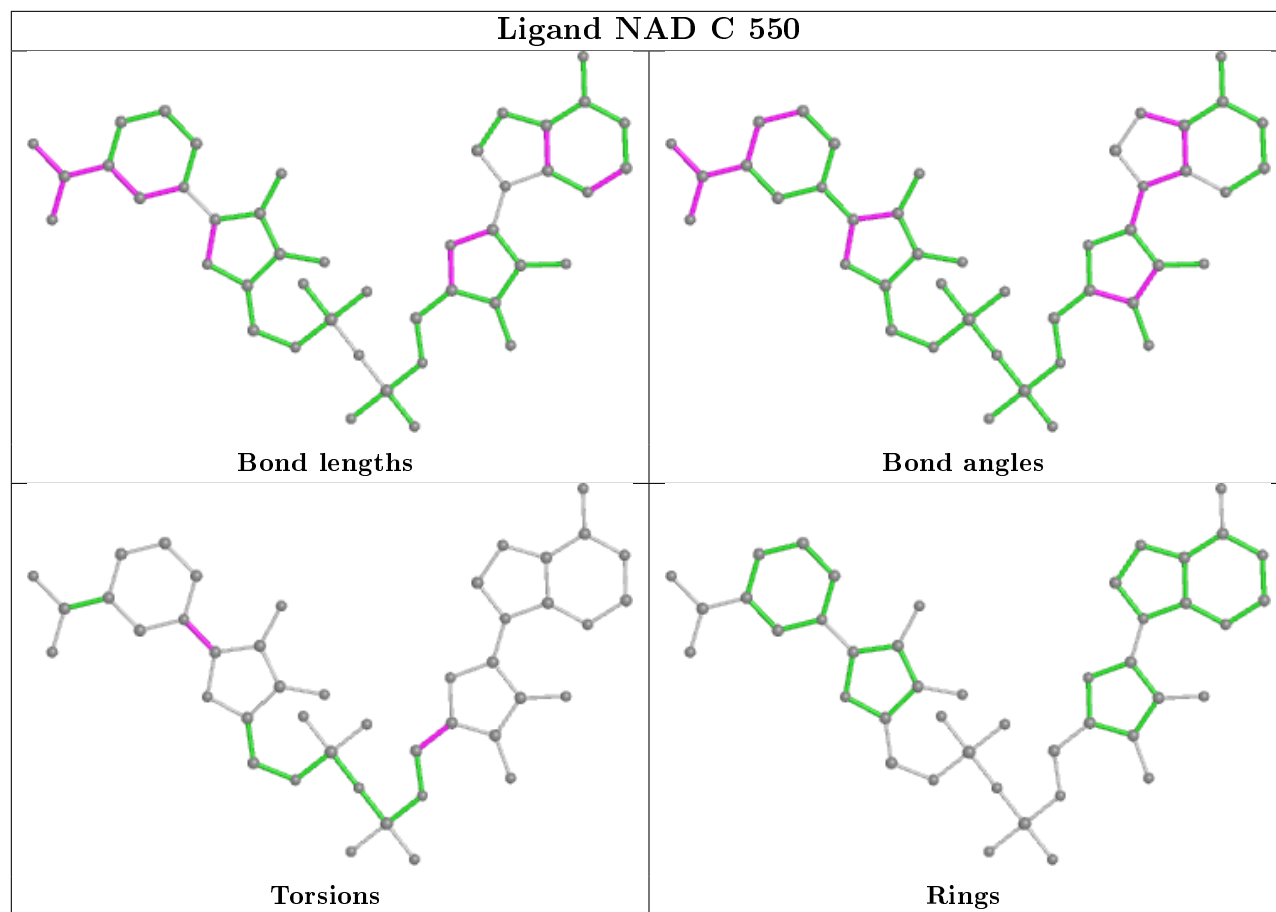
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	550	NAD	3	0
3	A	550	NAD	3	0
3	C	550	NAD	1	0
2	A	500	2FA	2	0
2	B	500	2FA	1	0
2	C	500	2FA	3	0
2	D	500	2FA	3	0
3	B	550	NAD	3	0

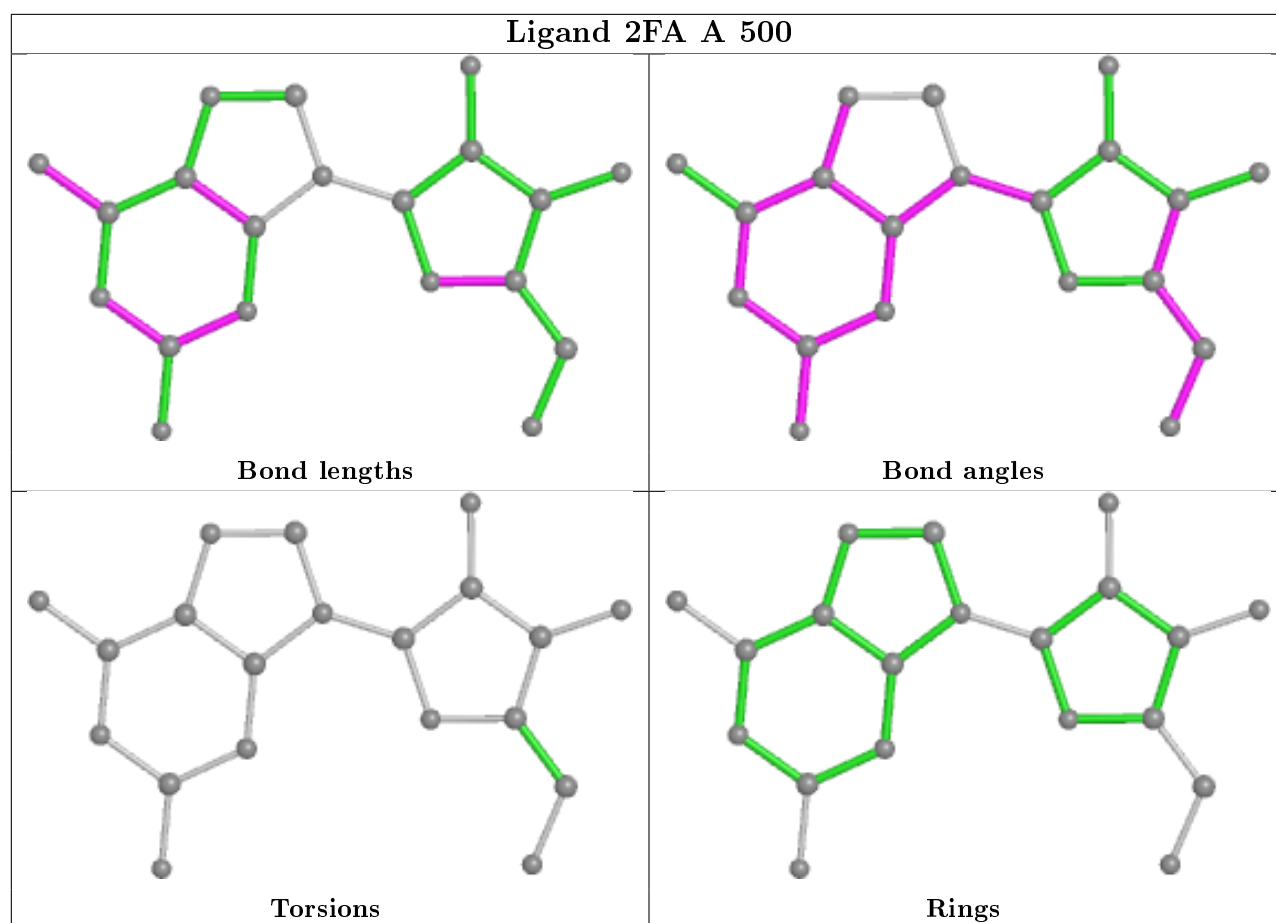
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

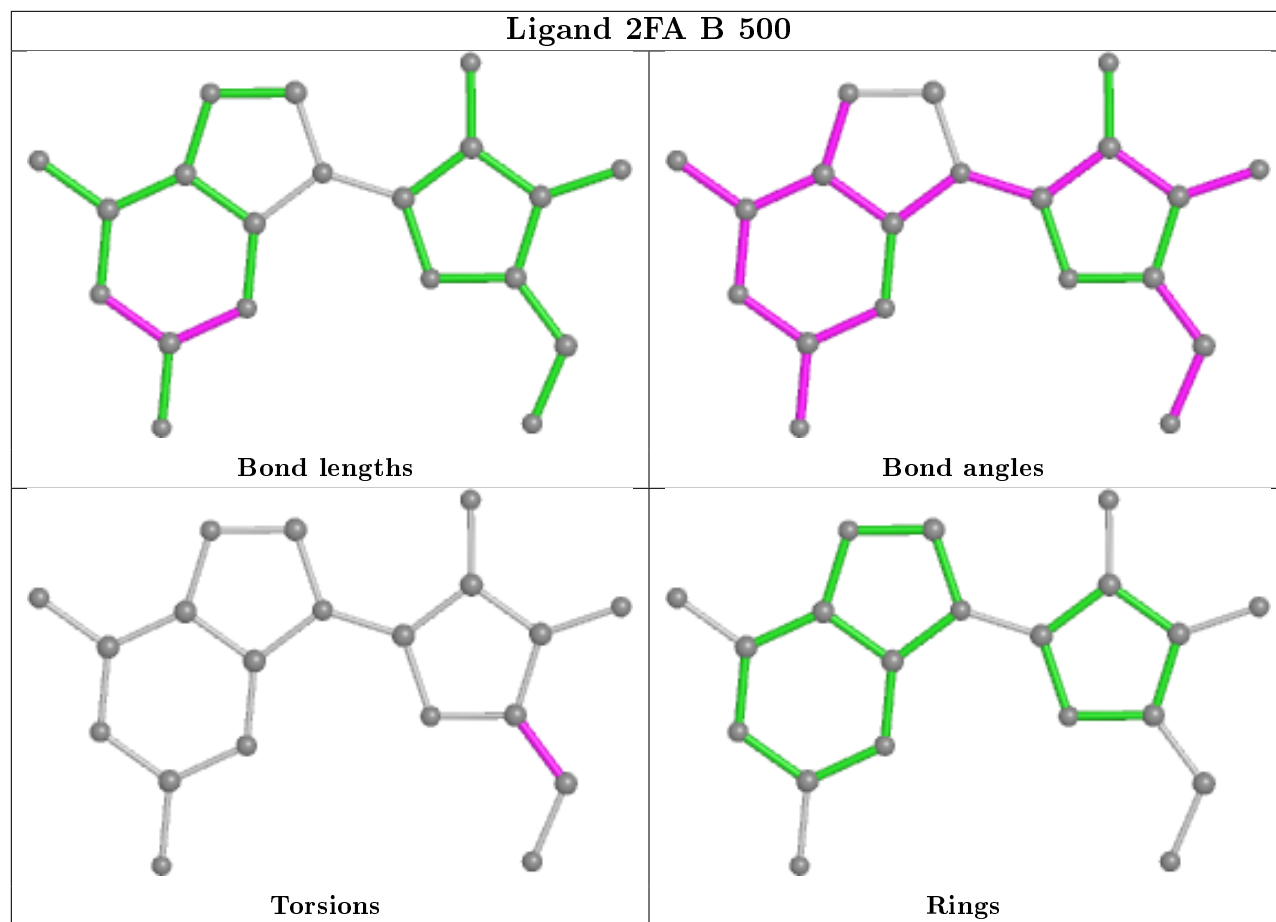
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



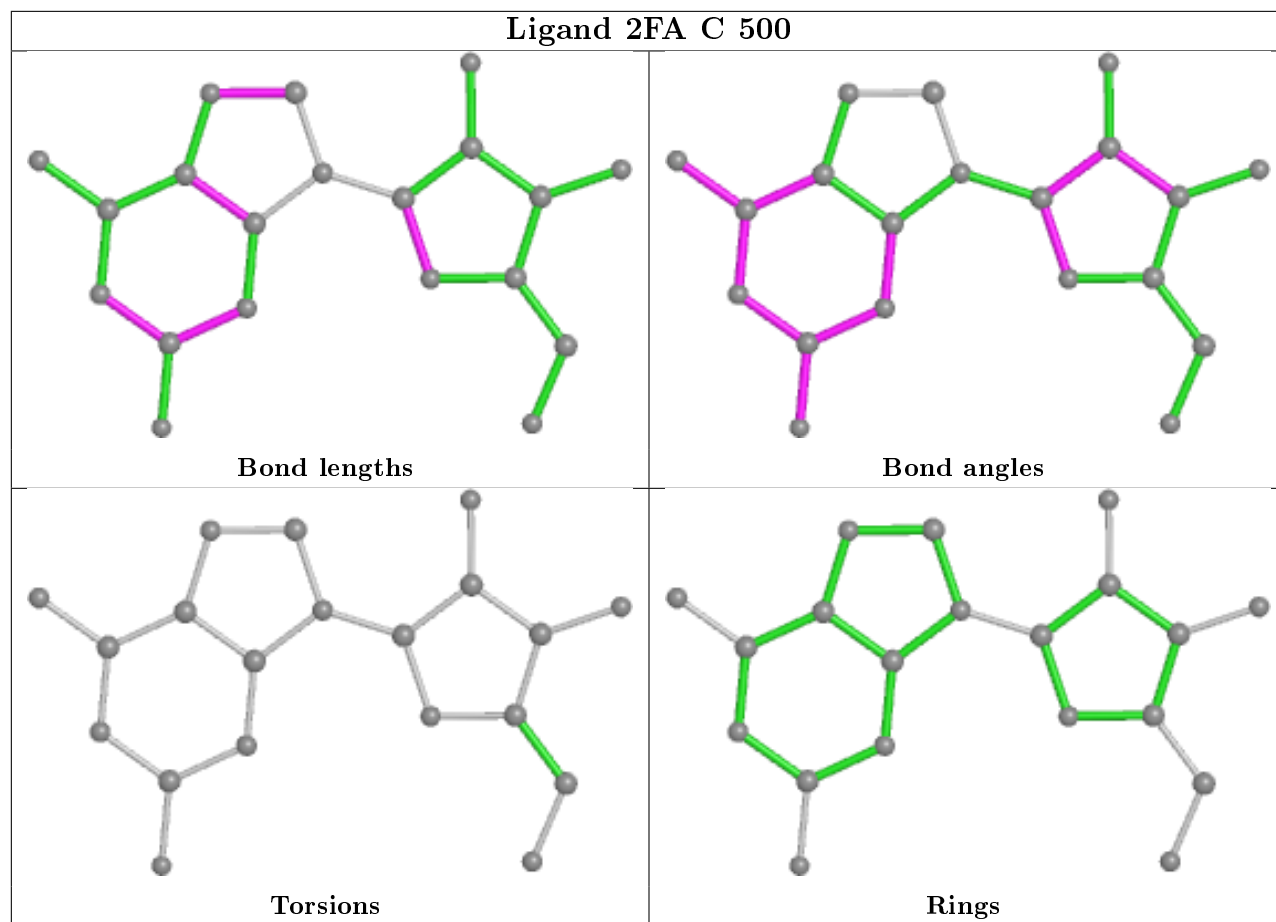


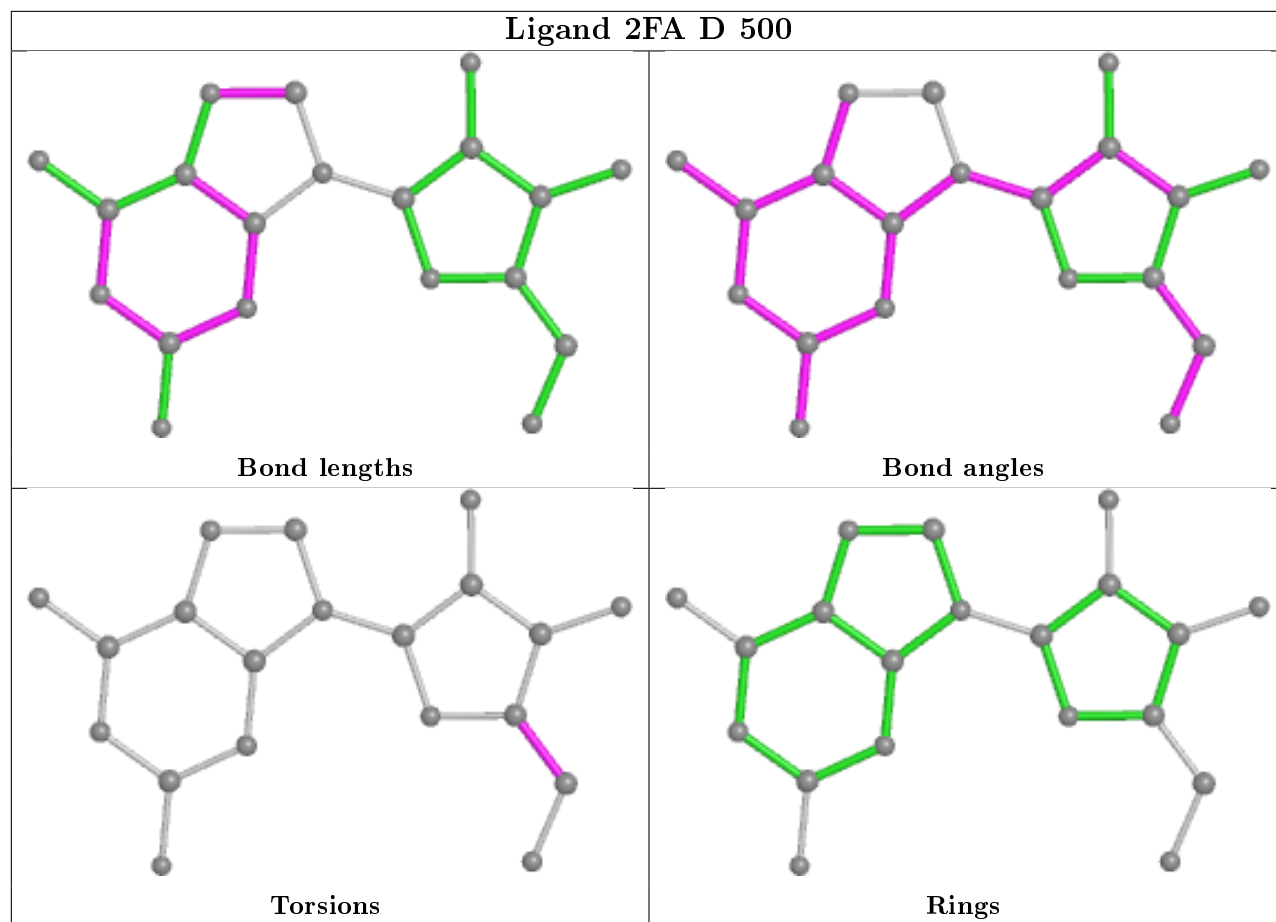


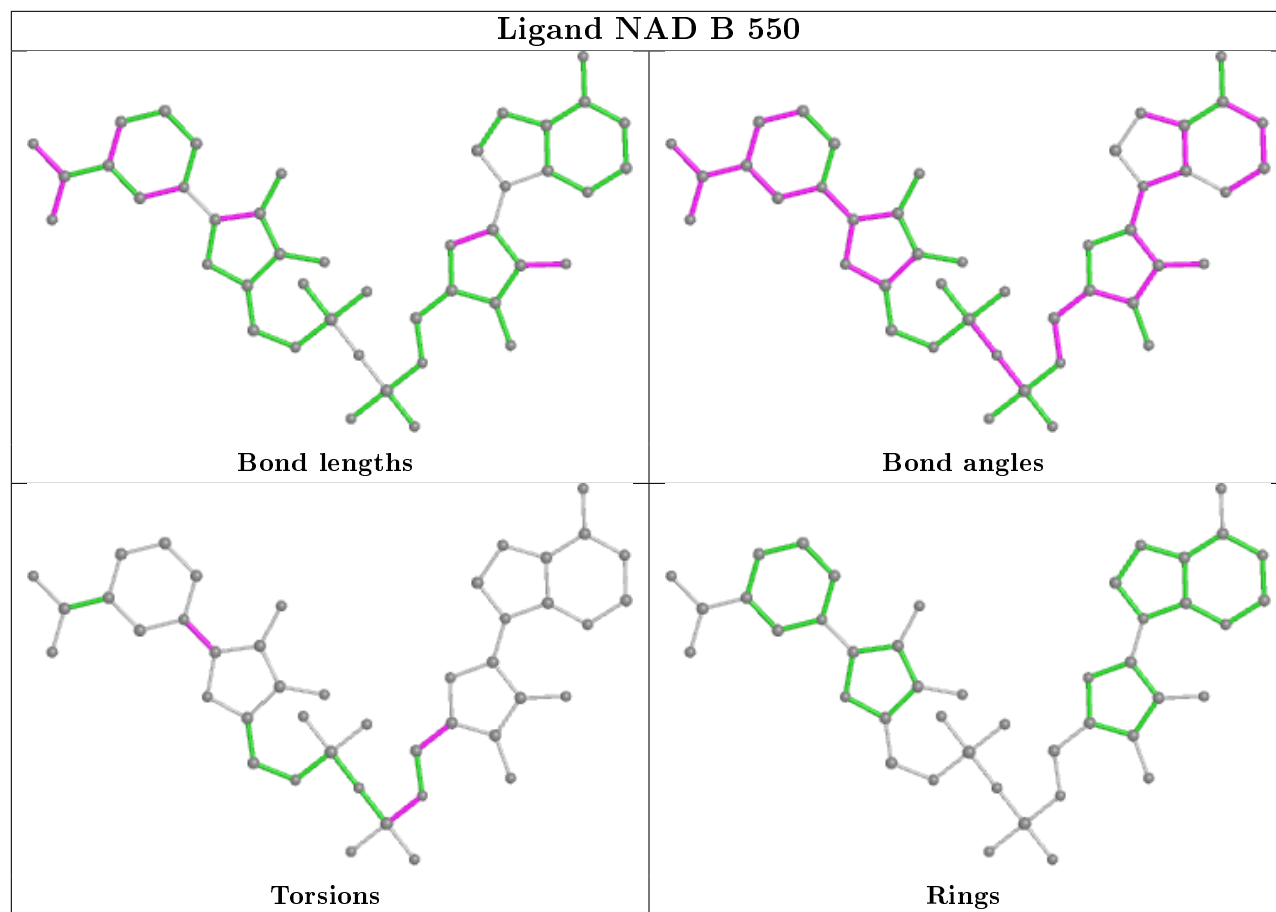












## 5.7 Other polymers [i](#)

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, 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	486/495 (98%)	-0.24	2 (0%) 92 91	21, 34, 52, 70	0
1	B	485/495 (97%)	-0.25	5 (1%) 82 80	22, 34, 48, 65	0
1	C	485/495 (97%)	-0.04	13 (2%) 54 52	24, 38, 58, 89	0
1	D	485/495 (97%)	-0.09	15 (3%) 49 46	23, 38, 59, 80	0
All	All	1941/1980 (98%)	-0.16	35 (1%) 68 65	21, 36, 57, 89	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182	ASP	5.7
1	A	10	SER	5.0
1	D	182	ASP	4.0
1	C	173	ALA	3.7
1	C	180	GLU	3.3
1	C	179	ALA	3.3
1	D	68	LEU	3.2
1	C	66	GLY	3.1
1	C	181	GLU	3.1
1	D	11	LEU	3.0
1	C	170	TYR	2.8
1	D	146	PRO	2.8
1	B	181	GLU	2.8
1	A	173	ALA	2.7
1	D	156	ASP	2.7
1	D	181	GLU	2.6
1	D	67	SER	2.6
1	D	15	VAL	2.6
1	B	218	GLU	2.5
1	C	231	ALA	2.5
1	C	153	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	66	GLY	2.4
1	D	90	TRP	2.4
1	B	216	THR	2.4
1	D	173	ALA	2.4
1	C	67	SER	2.4
1	C	12	THR	2.4
1	C	187	TRP	2.4
1	B	375	ARG	2.3
1	D	115	ASP	2.3
1	C	16	ARG	2.3
1	D	170	TYR	2.2
1	D	154	LEU	2.1
1	D	440	ASP	2.1
1	B	156	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

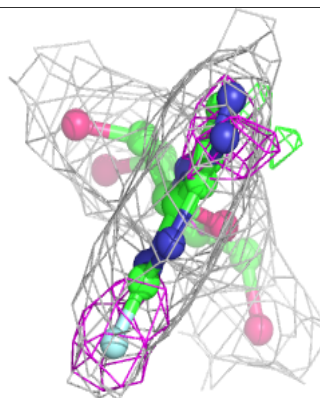
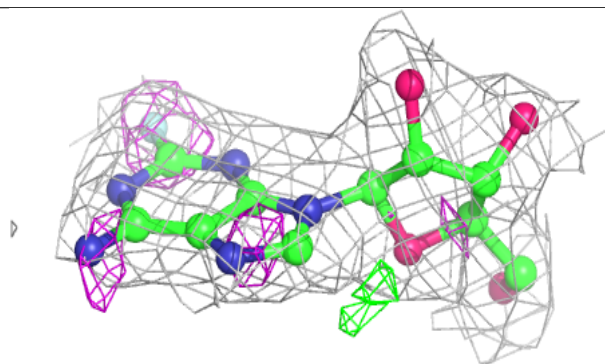
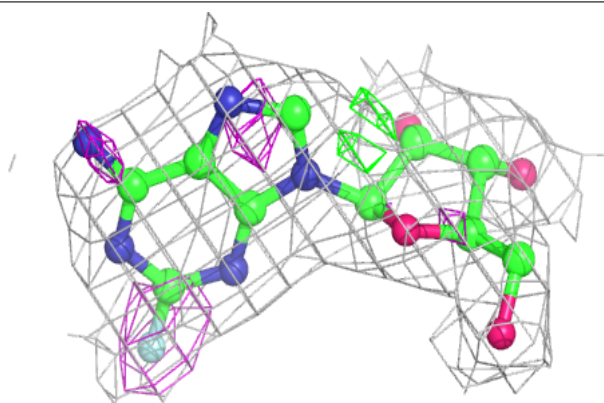
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
2	2FA	C	500	20/20	0.95	0.13	21,27,32,37	0
2	2FA	B	500	20/20	0.96	0.19	21,27,34,34	0
3	NAD	C	550	44/44	0.96	0.11	21,28,32,34	0
3	NAD	A	550	44/44	0.97	0.11	18,26,30,31	0
2	2FA	A	500	20/20	0.97	0.15	12,23,29,35	0
2	2FA	D	500	20/20	0.97	0.17	20,28,33,40	0
3	NAD	B	550	44/44	0.97	0.12	19,25,33,37	0
3	NAD	D	550	44/44	0.98	0.11	21,29,34,41	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.

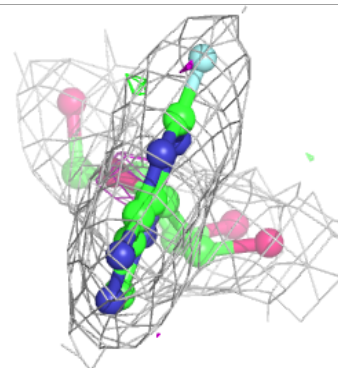
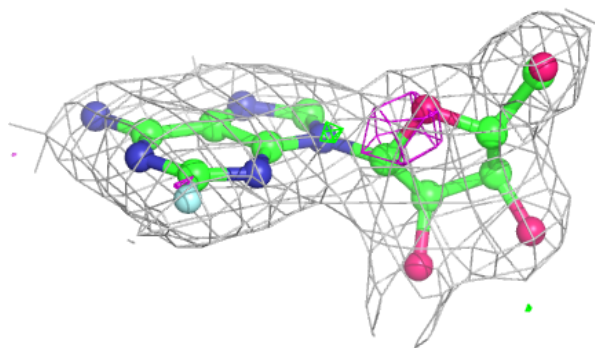
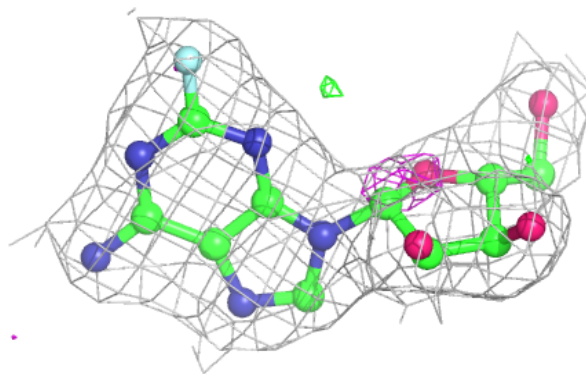
**Electron density around 2FA C 500:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

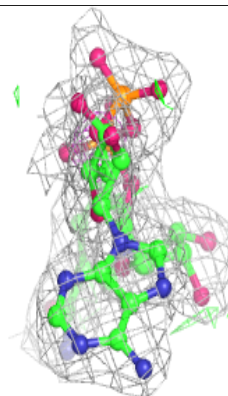
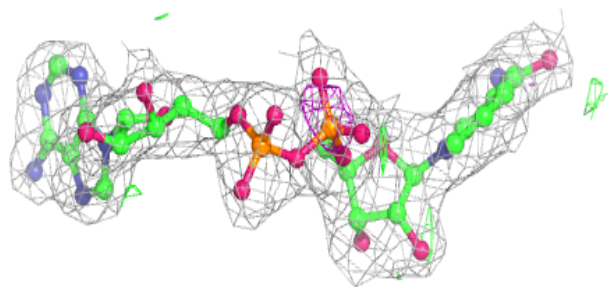
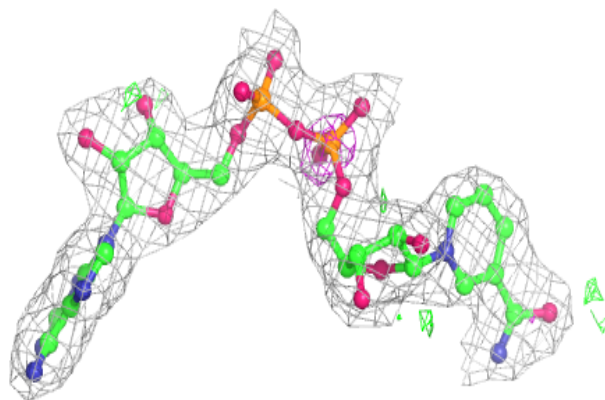


**Electron density around 2FA B 500:**

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

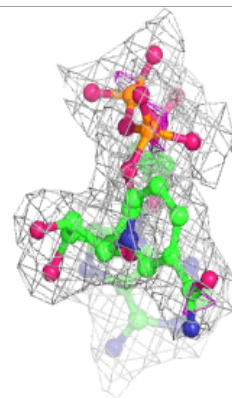
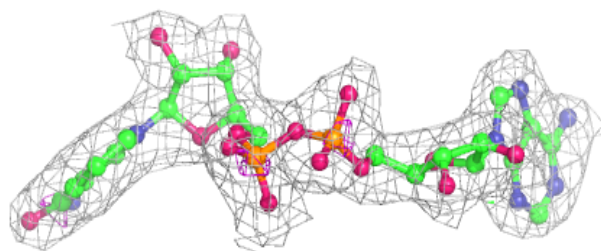
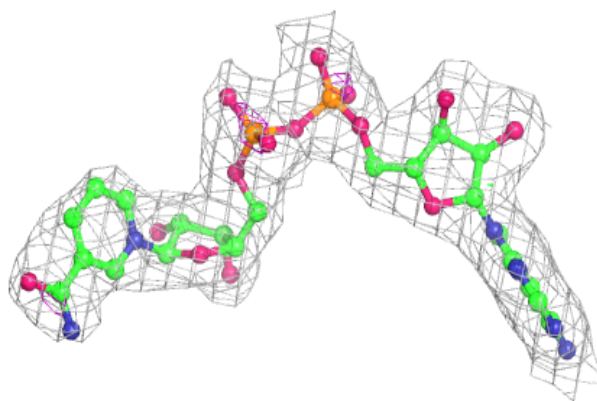
**Electron density around NAD C 550:**

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

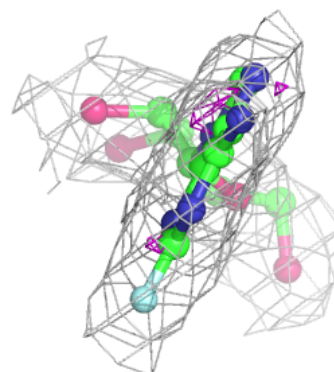
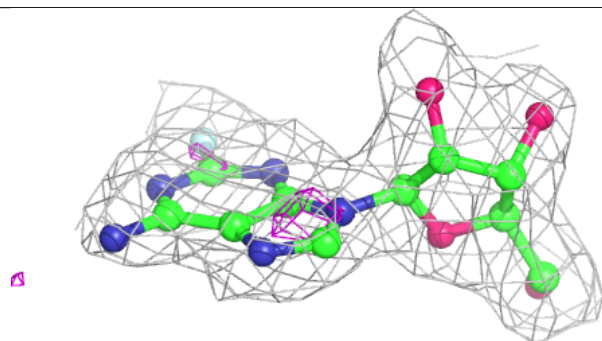
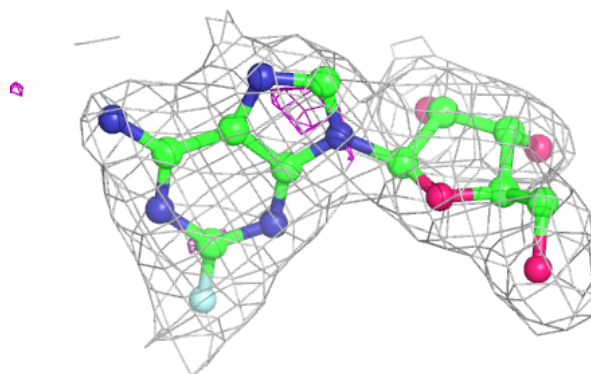


**Electron density around NAD A 550:**

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

**Electron density around 2FA A 500:**

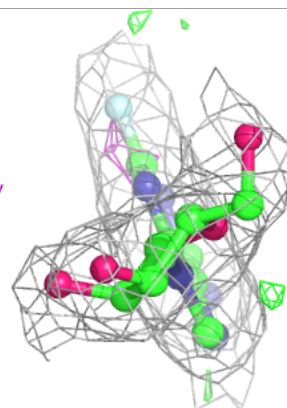
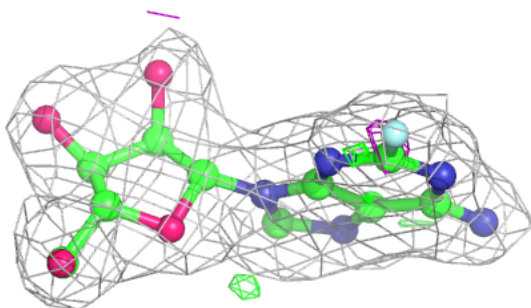
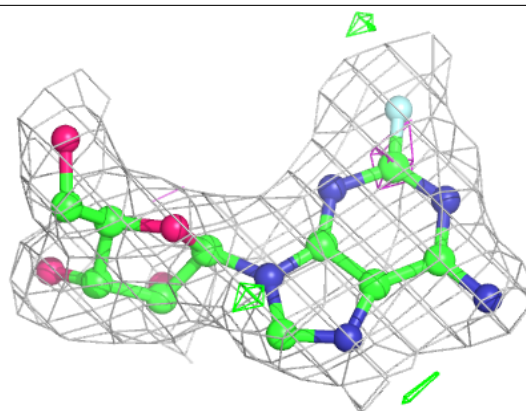
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



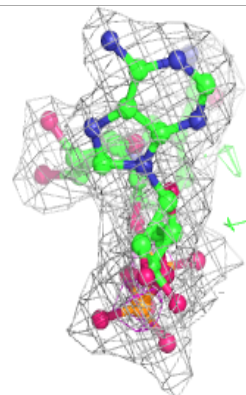
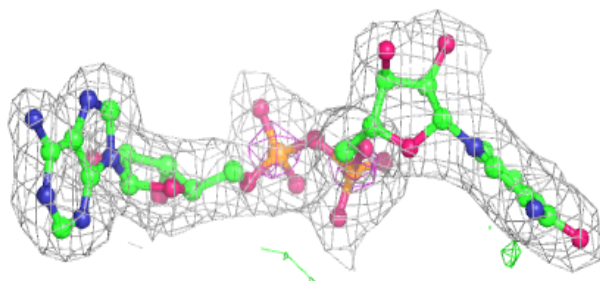
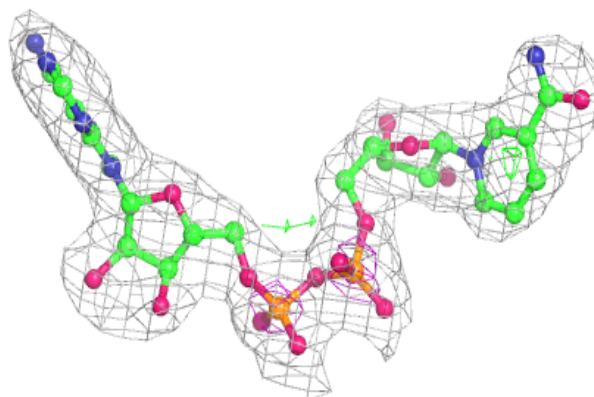


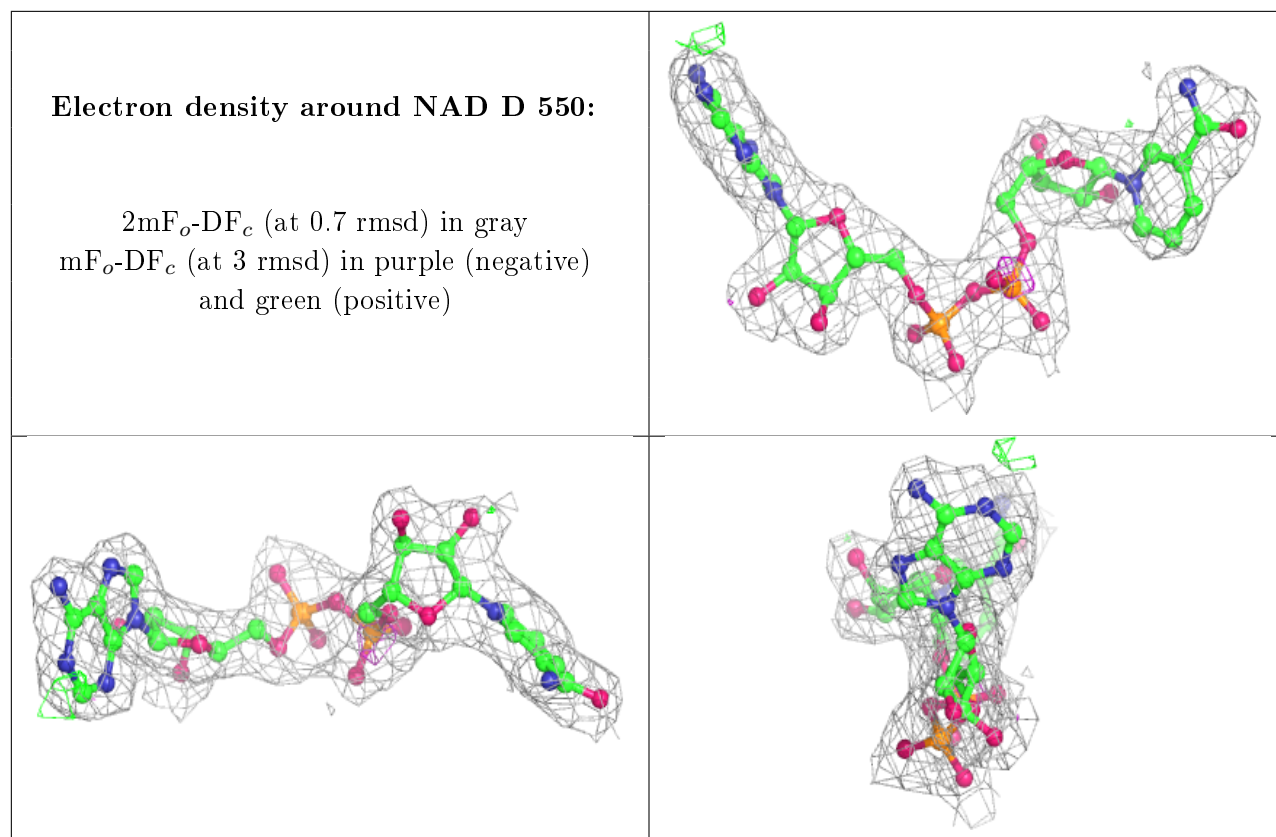
**Electron density around 2FA D 500:**

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

**Electron density around NAD B 550:**

$2mF_o-DF_c$  (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.