



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:27 AM UTC

PDB ID : 2ZJ0 / pdb_00002zj0
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

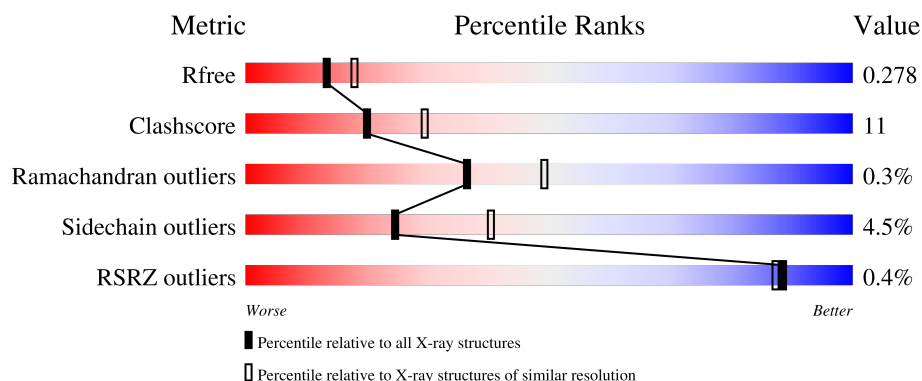
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

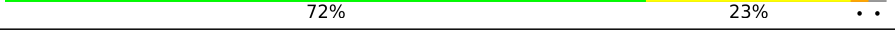
The reported resolution of this entry is 2.42 Å.

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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	495	
1	B	495	
1	C	495	
1	D	495	

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.

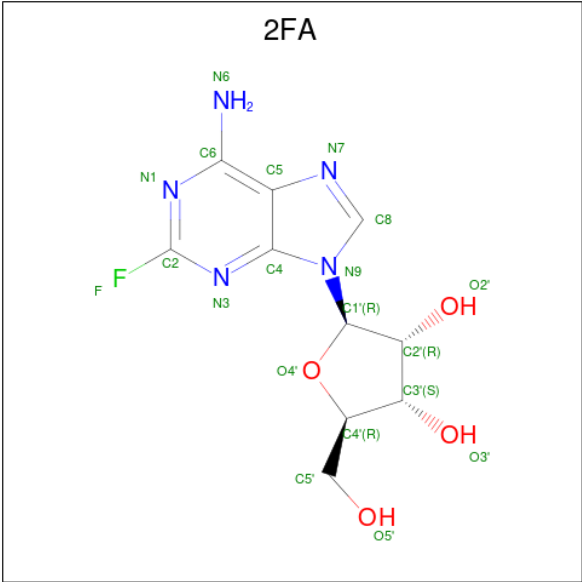
- Molecule 1 is a protein called Adenosylhomocysteinase.

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:

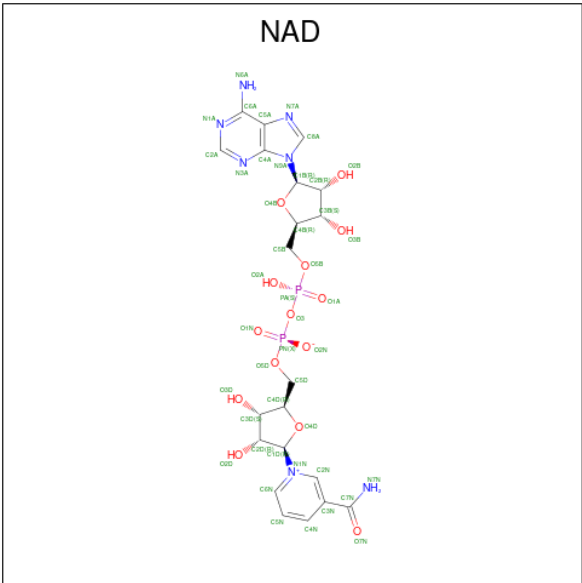
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P60176
B	1	MET	-	expression tag	UNP P60176
C	1	MET	-	expression tag	UNP P60176
D	1	MET	-	expression tag	UNP P60176

- Molecule 2 is 2-(6-AMINO-2-FLUORO-PURIN-9-YL)-5-HYDROXYMETHYL-TETRAHYDRO-FURAN-3,4-DIOL (CCD ID: 2FA) (formula: C₁₀H₁₂FN₅O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 20	C 10	F 1	N 5	O 4	0	0
2	B	1	Total 20	C 10	F 1	N 5	O 4	0	0
2	C	1	Total 20	C 10	F 1	N 5	O 4	0	0
2	D	1	Total 20	C 10	F 1	N 5	O 4	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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.

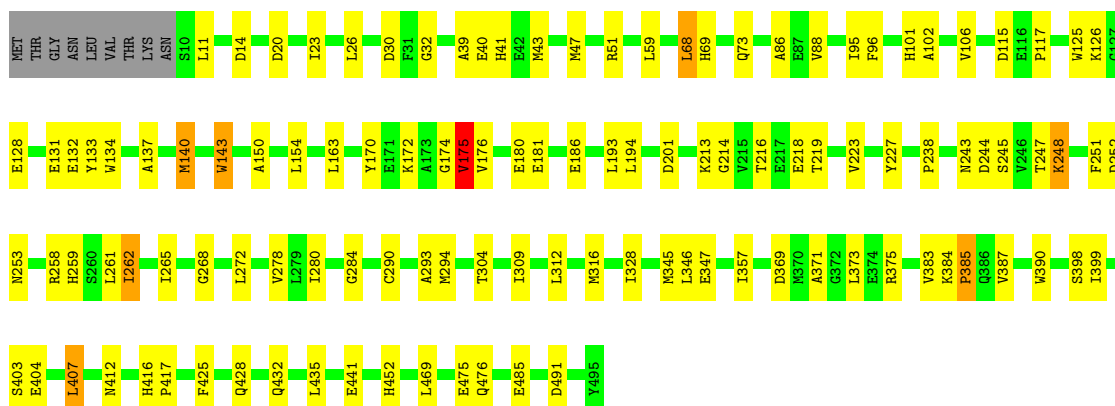
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	217	Total	O	0	0
			217	217		
4	B	182	Total	O	0	0
			182	182		
4	C	171	Total	O	0	0
			171	171		
4	D	141	Total	O	0	0
			141	141		

3 Residue-property plots [i](#)

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.

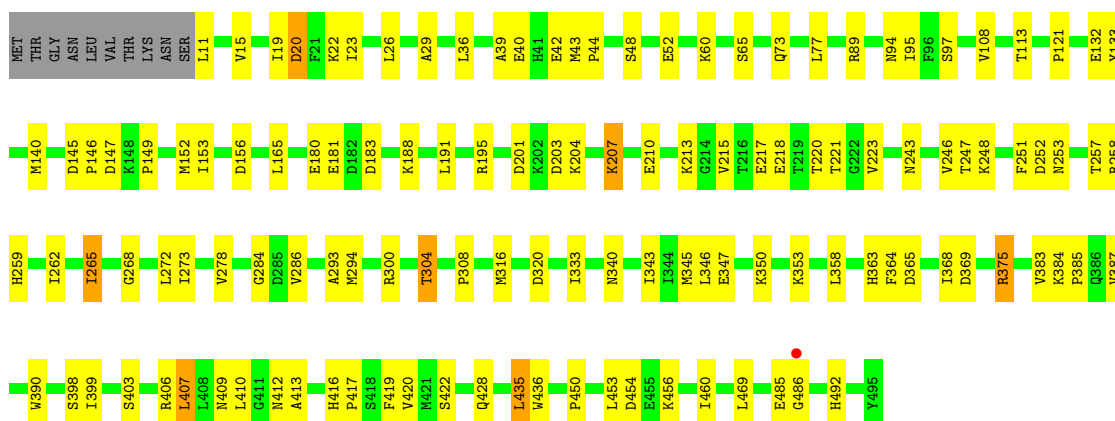
• Molecule 1: Adenosylhomocysteinase

Chain A: 



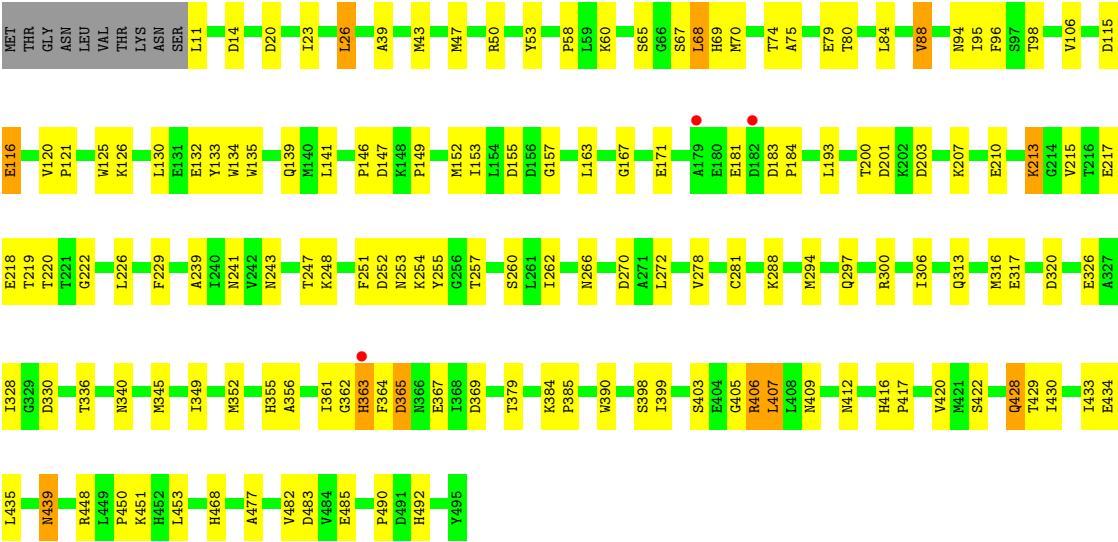
• Molecule 1: Adenosylhomocysteinase

Chain B: 

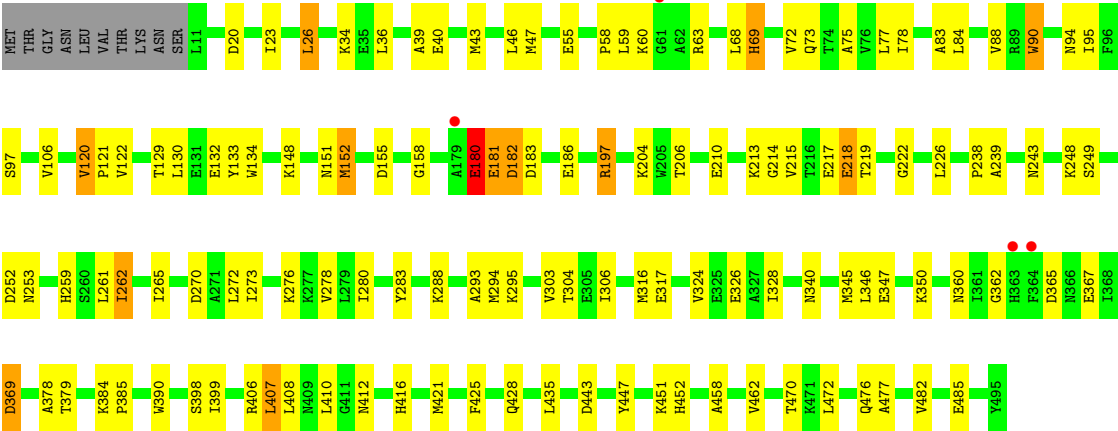


• Molecule 1: Adenosylhomocysteinase

Chain C: 



● Molecule 1: Adenosylhomocysteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.280 0.194 , 0.278	Depositor DCC
R_{free} test set	3728 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, 2FA

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	0.97	1/3829 (0.0%)	1.17	10/5193 (0.2%)
1	B	0.96	2/3824 (0.1%)	1.15	8/5186 (0.2%)
1	C	0.91	0/3824	1.09	8/5186 (0.2%)
1	D	0.90	0/3823	1.09	4/5184 (0.1%)
All	All	0.93	3/15300 (0.0%)	1.12	30/20749 (0.1%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	VAL	CA-CB	-6.27	1.51	1.55
1	B	156	ASP	N-CA	-6.19	1.39	1.46
1	B	286	VAL	CA-CB	5.42	1.60	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	365	ASP	N-CA-C	8.89	120.97	111.28
1	C	328	ILE	N-CA-C	7.45	118.22	110.62
1	A	383	VAL	N-CA-C	-7.30	104.66	111.45
1	A	328	ILE	N-CA-C	7.11	117.88	110.62
1	B	113	THR	CA-C-N	-6.90	111.88	119.19
1	B	113	THR	C-N-CA	-6.90	111.88	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	TRP	CA-C-N	6.82	127.38	119.47
1	A	143	TRP	C-N-CA	6.82	127.38	119.47
1	A	170	TYR	O-C-N	-6.72	114.32	122.11
1	C	363	HIS	N-CA-C	6.70	120.67	112.23
1	A	425	PHE	N-CA-C	6.32	118.17	111.28
1	C	439	ASN	N-CA-C	6.13	118.93	111.82
1	B	363	HIS	N-CA-C	6.12	118.92	111.82
1	C	364	PHE	CA-C-N	5.76	127.99	120.28
1	C	364	PHE	C-N-CA	5.76	127.99	120.28
1	C	229	PHE	N-CA-C	-5.70	104.32	112.13
1	D	378	ALA	N-CA-C	-5.55	102.27	110.48
1	B	165	LEU	N-CA-C	5.49	117.07	111.14
1	A	407	LEU	CB-CA-C	5.35	116.38	109.80
1	A	214	GLY	N-CA-C	5.32	118.83	110.91
1	A	219	THR	CA-C-N	5.24	127.62	120.54
1	A	219	THR	C-N-CA	5.24	127.62	120.54
1	B	265	ILE	N-CA-C	5.22	115.99	110.72
1	B	486	GLY	CA-C-N	-5.14	114.49	119.78
1	B	486	GLY	C-N-CA	-5.14	114.49	119.78
1	C	406	ARG	N-CA-C	-5.13	103.15	110.59
1	D	90	TRP	N-CA-C	5.12	117.77	109.06
1	B	365	ASP	N-CA-C	5.11	121.67	110.80
1	D	270	ASP	CB-CA-C	-5.07	104.40	111.80
1	D	120	VAL	N-CA-C	5.01	113.40	107.84

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	80	0
1	B	3748	0	3693	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3748	0	3693	98	0
1	D	3747	0	3693	92	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	2	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	344	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 11.

All (344) 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:B:43:MET:HE1	1:B:73:GLN:HA	1.33	1.10
1:A:43:MET:HE1	1:A:73:GLN:HA	1.42	1.01
1:C:483:ASP:HB3	1:C:485:GLU:OE2	1.58	1.01
1:D:43:MET:HE1	1:D:73:GLN:HA	1.43	1.00
1:C:23:ILE:HD11	1:C:26:LEU:HD13	1.47	0.94
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
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
1:C:278:VAL:HG21	1:C:294:MET:HE3	1.67	0.77
1:B:152:MET:HE2	1:B:213:LYS:HB2	1.67	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:39:ALA:HB1	1:D:43:MET:HE3	1.71	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
1:C:398:SER:C	1:C:399:ILE:HD13	2.17	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:A:137:ALA:O	1:A:140:MET:HE3	1.94	0.67
1:C:450:PRO:HD2	1:C:453:LEU:HD12	1.77	0.67
1:A:316:MET:HE1	1:D:272:LEU:HD21	1.78	0.65
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: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: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:A:40:GLU:HG2	1:A:47:MET:HE3	1.79	0.64
1:B:272:LEU:HD21	1:C:316:MET:HE1	1.80	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: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:47:MET:HE1	1:C:50:ARG:CZ	2.30	0.61
1:C:226:LEU:HD13	1:C:239:ALA:HB1	1.84	0.60
1:D:197:ARG:HA	1:D:197:ARG:NE	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:C:39:ALA:HB1	1:C:43:MET:HE2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:63:ARG:CZ	1:D:148:LYS:HB2	2.34	0.57
1:B:152:MET:CE	1:B:213:LYS:HB2	2.33	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:C:152:MET:HE3	1:C:213:LYS:HB2	1.88	0.56
1:D:252:ASP:OD1	1:D:416:HIS:HE1	1.88	0.56
1:D:384:LYS:O	1:D:385:PRO:C	2.48	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: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:A:272:LEU:HB2	1:C:417:PRO:HG2	1.88	0.55
1:C:226:LEU:HD13	1:C:239:ALA:CB	2.37	0.55
1:A:384:LYS:HB2	1:A:385:PRO:HD2	1.89	0.55
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:73:GLN:CD	1:D:73:GLN:H	2.15	0.54
1:A:125:TRP:O	1:A:128:GLU:HG3	2.06	0.54
1:D:129:THR:OG1	1:D:132:GLU:HG3	2.08	0.54
1:B:152:MET:HE3	1:B:436:TRP:HE3	1.71	0.54
1:B:316:MET:HE1	1:C:272:LEU:HD21	1.89	0.53
1:A:284:GLY:HA3	3:A:550:NAD:O5B	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HE	1:D:197:ARG:CA	2.16	0.52
1:B:262:ILE:HD12	1:B:262:ILE:C	2.35	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:A:172:LYS:C	1:A:174:GLY:N	2.67	0.52
1:C:53:TYR:CD1	1:C:58:PRO:HG3	2.45	0.52
1:C:403:SER:OG	1:C:412:ASN:ND2	2.43	0.52
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:B:180:GLU:HG2	1:B:183:ASP:CG	2.35	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:B:265:ILE:HD13	1:B:294:MET:HE1	1.93	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:252:ASP:OD1	1:B:416:HIS:HE1	1.93	0.51
1:B:409:ASN:O	1:B:413:ALA:HB3	2.11	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:A:154:LEU:C	1:A:154:LEU:HD23	2.36	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:CD2	1:C:492:HIS:H	2.30	0.50
1:D:151:ASN:O	1:D:152:MET:HG2	2.11	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:180:GLU:O	1:A:181:GLU:C	2.55	0.48
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:D:306:ILE:C	1:D:306:ILE:HD12	2.38	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:A:39:ALA:HB1	1:A:43:MET:HE3	1.94	0.47
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:172:LYS:C	1:A:174:GLY:H	2.22	0.47
1:A:243:ASN:HD21	1:A:253:ASN:HD21	1.61	0.47
1:B:147:ASP:C	1:B:149:PRO:HD3	2.39	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:32:GLY:HA3	1:A:101:HIS:O	2.14	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:15:VAL:HA	1:B:19:ILE:O	2.15	0.46
1:B:29:ALA:HB2	1:B:108:VAL:HG21	1.96	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:201:ASP:CG	1:B:204:LYS:HB2	2.39	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:72:VAL:O	1:D:75:ALA:HB3	2.14	0.46
1:A:115:ASP:C	1:A:117:PRO:HD3	2.40	0.46
1:B:36:LEU:O	1:B:40:GLU:HG3	2.15	0.46
1:A:272:LEU:HD11	1:D:316:MET:HE1	1.97	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:246:VAL:HG23	1:B:454:ASP:OD2	2.16	0.46
1:B:435:LEU:HD12	1:B:435:LEU:HA	1.78	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: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:B:398:SER:C	1:B:399:ILE:HD13	2.41	0.46
1:C:251:PHE:HA	1:C:255:TYR:CD2	2.52	0.45
1:A:174:GLY:C	1:A:175:VAL:HG12	2.41	0.45
1:B:258:ARG:HA	1:B:293:ALA:HB2	1.97	0.45
1:D:68:LEU:O	1:D:69:HIS:C	2.58	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: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
1:B:39:ALA:HB1	1:B:43:MET:CE	2.47	0.45
1:C:252:ASP:O	1:C:253:ASN:C	2.59	0.45
1:C:167:GLY:O	1:C:171:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:403:SER:O	1:A:404:GLU:C	2.61	0.44
1:D:47:MET:HE2	1:D:47:MET:N	2.32	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:A:261:LEU:HD21	1:A:294:MET:HE2	2.00	0.44
1:C:70:MET:HB3	1:C:98:THR:HG23	1.98	0.44
1:C:147:ASP:C	1:C:149:PRO:HD3	2.42	0.44
1:C:241:ASN:HB3	1:C:448:ARG:HG2	1.99	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:B:384:LYS:O	1:B:385:PRO:C	2.61	0.44
1:D:36:LEU:O	1:D:40:GLU:HG3	2.17	0.44
1:D:155:ASP:OD2	1:D:158:GLY:HA2	2.18	0.44
1:C:183:ASP:O	1:C:184:PRO:C	2.60	0.44
1:B:221:THR:HG21	1:B:364:PHE:CE2	2.53	0.44
1:B:20:ASP:OD1	1:B:20:ASP:N	2.42	0.43
1:A:265:ILE:HD13	1:A:294:MET:HE1	2.01	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:A:96:PHE:O	1:A:126:LYS:NZ	2.49	0.43
1:B:89:ARG:HG2	1:B:121:PRO:HG2	2.00	0.43
1:B:153:ILE:O	1:B:215:VAL:HA	2.18	0.43
1:C:217:GLU:CD	1:C:222:GLY:HA3	2.43	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:C:157:GLY:HA3	1:C:363:HIS:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:352:MET:HE2	1:C:356:ALA:HB3	2.01	0.43
1:B:203:ASP:O	1:B:207:LYS:HG3	2.18	0.42
1:D:252:ASP:OD1	1:D:252:ASP:C	2.61	0.42
1:C:435:LEU:HD23	1:C:435:LEU:HA	1.89	0.42
1:C:203:ASP:OD1	1:C:207:LYS:NZ	2.40	0.42
1:D:248:LYS:HD3	1:D:248:LYS:C	2.44	0.42
1:B:406:ARG:O	1:B:407:LEU:C	2.62	0.42
1:D:39:ALA:HB1	1:D:43:MET:CE	2.46	0.42
1:D:421:MET:HE2	1:D:425:PHE:CZ	2.55	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:D:451:LYS:O	1:D:452:HIS:C	2.63	0.42
1:A:131:GLU:OE1	1:A:131:GLU:N	2.48	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: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:261:LEU:HD21	1:D:294:MET:HE2	2.01	0.42
1:D:443:ASP:HB2	1:D:447:TYR:OH	2.20	0.42
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:B:257:THR:O	1:B:258:ARG:C	2.62	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:73:GLN:CD	1:A:73:GLN:H	2.28	0.41
1:A:102:ALA:O	1:A:106:VAL:HG23	2.21	0.41
1:A:469:LEU:HD11	1:B:308:PRO:HB3	2.01	0.41
1:B:52:GLU:OE1	1:B:456:LYS:NZ	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:80:THR:O	1:C:84:LEU:HG	2.21	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:D:152:MET:HE1	1:D:435:LEU:HB3	2.02	0.41
1:D:217:GLU:CD	1:D:222:GLY:HA3	2.46	0.41
1:A:68:LEU:O	1:A:69:HIS:C	2.62	0.41
1:D:130:LEU:HD21	1:D:406:ARG:NH2	2.36	0.41
1:D:152:MET:HE2	1:D:214:GLY:O	2.21	0.41
1:A:252:ASP:OD1	1:A:416:HIS:HE1	2.04	0.41
1:C:490:PRO:HB2	1:C:492:HIS:CD2	2.56	0.41
1:D:181:GLU:C	1:D:183:ASP:H	2.29	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:A:265:ILE:CD1	1:A:294:MET:HE1	2.51	0.41
1:B:383:VAL:HA	1:D:34:LYS:HD3	2.03	0.41
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.96	0.41
1:C:266:ASN:O	1:C:270:ASP:CG	2.64	0.41
1:C:435:LEU:O	1:C:439:ASN:ND2	2.48	0.41
1:D:180:GLU:HB2	1:D:181:GLU:H	1.60	0.41
1:A:252:ASP:OD1	1:A:252:ASP:C	2.63	0.41
1:A:384:LYS:O	1:A:385:PRO:C	2.62	0.40
1:C:363:HIS:CE1	2:C:500:2FA:O5'	2.74	0.40
1:C:451:LYS:HB2	1:C:451:LYS:HE2	1.80	0.40
1:D:59:LEU:O	1:D:60:LYS:C	2.64	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:B:133:TYR:CD2	1:B:133:TYR:C	2.98	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:C:193:LEU:C	1:C:193:LEU:HD23	2.46	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
1:D:265:ILE:CD1	1:D:294:MET:HE1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	43	57
1	B	483/495 (98%)	463 (96%)	20 (4%)	0	100	100
1	C	483/495 (98%)	458 (95%)	24 (5%)	1 (0%)	43	57
1	D	483/495 (98%)	457 (95%)	22 (5%)	4 (1%)	16	23
All	All	1933/1980 (98%)	1840 (95%)	87 (4%)	6 (0%)	36	49

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%)	378 (96%)	17 (4%)	26	42
1	B	395/404 (98%)	379 (96%)	16 (4%)	27	44
1	C	395/404 (98%)	376 (95%)	19 (5%)	23	38
1	D	395/404 (98%)	376 (95%)	19 (5%)	23	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1580/1616 (98%)	1509 (96%)	71 (4%)	24	40

All (71) 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
1	A	245	SER
1	A	248	LYS
1	A	262	ILE
1	A	304	THR
1	A	347	GLU
1	A	357	ILE
1	A	407	LEU
1	A	441	GLU
1	A	475	GLU
1	A	485	GLU
1	A	491	ASP
1	B	20	ASP
1	B	22	LYS
1	B	60	LYS
1	B	77	LEU
1	B	181	GLU
1	B	207	LYS
1	B	210	GLU
1	B	220	THR
1	B	273	ILE
1	B	304	THR
1	B	333	ILE
1	B	347	GLU
1	B	375	ARG
1	B	407	LEU
1	B	435	LEU
1	B	469	LEU
1	C	26	LEU
1	C	60	LYS
1	C	65	SER
1	C	68	LEU

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Mol	Chain	Res	Type
1	C	88	VAL
1	C	106	VAL
1	C	115	ASP
1	C	116	GLU
1	C	120	VAL
1	C	201	ASP
1	C	210	GLU
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	428	GLN
1	D	26	LEU
1	D	55	GLU
1	D	88	VAL
1	D	152	MET
1	D	180	GLU
1	D	181	GLU
1	D	182	ASP
1	D	197	ARG
1	D	218	GLU
1	D	219	THR
1	D	249	SER
1	D	262	ILE
1	D	295	LYS
1	D	317	GLU
1	D	326	GLU
1	D	347	GLU
1	D	365	ASP
1	D	407	LEU
1	D	485	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	243	ASN
1	A	259	HIS
1	A	310	ASN

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Mol	Chain	Res	Type
1	A	412	ASN
1	A	416	HIS
1	A	432	GLN
1	A	452	HIS
1	B	243	ASN
1	B	259	HIS
1	B	360	ASN
1	B	382	ASN
1	B	412	ASN
1	B	416	HIS
1	B	423	ASN
1	B	428	GLN
1	B	432	GLN
1	B	492	HIS
1	C	94	ASN
1	C	101	HIS
1	C	243	ASN
1	C	310	ASN
1	C	355	HIS
1	C	360	ASN
1	C	412	ASN
1	C	416	HIS
1	C	427	ASN
1	C	428	GLN
1	C	492	HIS
1	D	243	ASN
1	D	259	HIS
1	D	310	ASN
1	D	355	HIS
1	D	416	HIS
1	D	427	ASN
1	D	428	GLN
1	D	468	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
2	2FA	A	500	-	22,22,22	2.59	8 (36%)	32,33,33	2.83	14 (43%)
3	NAD	B	550	-	46,48,48	1.68	10 (21%)	64,73,73	2.40	23 (35%)
3	NAD	A	550	-	46,48,48	1.51	8 (17%)	64,73,73	2.17	22 (34%)
2	2FA	D	500	-	22,22,22	2.35	8 (36%)	32,33,33	3.06	14 (43%)
3	NAD	D	550	-	46,48,48	1.74	7 (15%)	64,73,73	1.91	18 (28%)
2	2FA	B	500	-	22,22,22	2.22	7 (31%)	32,33,33	2.63	16 (50%)
2	2FA	C	500	-	22,22,22	2.53	6 (27%)	32,33,33	2.65	11 (34%)
3	NAD	C	550	-	46,48,48	1.71	10 (21%)	64,73,73	1.96	17 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2FA	A	500	-	-	0/6/22/22	0/3/3/3
3	NAD	B	550	-	-	6/30/62/62	0/5/5/5
3	NAD	A	550	-	-	5/30/62/62	0/5/5/5
2	2FA	D	500	-	-	2/6/22/22	0/3/3/3
3	NAD	D	550	-	-	5/30/62/62	0/5/5/5
2	2FA	B	500	-	-	1/6/22/22	0/3/3/3
2	2FA	C	500	-	-	0/6/22/22	0/3/3/3
3	NAD	C	550	-	-	4/30/62/62	0/5/5/5

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	2FA	C2-N3	6.73	1.38	1.31
2	C	500	2FA	C2-N3	6.02	1.37	1.31
3	C	550	NAD	O7N-C7N	5.71	1.34	1.24
2	D	500	2FA	C2-N3	5.69	1.37	1.31
3	D	550	NAD	O4D-C1D	5.63	1.48	1.40
2	C	500	2FA	C2-N1	5.63	1.37	1.31
2	C	500	2FA	C5-C4	5.62	1.49	1.39
2	A	500	2FA	C2-N1	5.62	1.37	1.31
2	B	500	2FA	C2-N1	5.46	1.36	1.31
2	B	500	2FA	C2-N3	5.43	1.36	1.31
3	D	550	NAD	C5A-C4A	5.15	1.48	1.39
3	C	550	NAD	C5A-C4A	4.82	1.47	1.39
2	D	500	2FA	C2-N1	4.39	1.35	1.31
2	A	500	2FA	C5-C4	4.29	1.46	1.39
3	B	550	NAD	C2N-N1N	-4.23	1.30	1.35
2	D	500	2FA	C5-C4	4.12	1.46	1.39
2	C	500	2FA	C8-N7	4.04	1.39	1.31
2	D	500	2FA	C8-N7	3.87	1.39	1.31
3	D	550	NAD	C2N-N1N	-3.80	1.30	1.35
2	A	500	2FA	C6-N6	3.64	1.43	1.34
3	B	550	NAD	PN-O3	-3.56	1.55	1.59
3	D	550	NAD	C7N-N7N	-3.52	1.26	1.33
3	D	550	NAD	O7N-C7N	3.43	1.30	1.24
3	A	550	NAD	C2N-N1N	-3.40	1.31	1.35
3	B	550	NAD	O7N-C7N	3.38	1.30	1.24
3	B	550	NAD	C7N-N7N	-3.31	1.26	1.33
3	A	550	NAD	C5A-C4A	3.27	1.44	1.39
2	A	500	2FA	C5-C6	3.26	1.50	1.41
2	B	500	2FA	C5-C4	3.23	1.44	1.39
2	D	500	2FA	C6-N1	3.22	1.39	1.35
3	A	550	NAD	O7N-C7N	3.22	1.30	1.24
3	A	550	NAD	PA-O3	3.18	1.62	1.59
3	A	550	NAD	C7N-N7N	-3.15	1.27	1.33
3	B	550	NAD	C4N-C3N	-3.14	1.34	1.39
3	B	550	NAD	C5A-C4A	3.07	1.44	1.39
2	B	500	2FA	C8-N7	2.92	1.37	1.31
2	D	500	2FA	C4-N9	-2.92	1.31	1.37
2	B	500	2FA	C5-C6	2.88	1.49	1.41
3	A	550	NAD	C4A-N9A	-2.87	1.31	1.37
3	C	550	NAD	C7N-N7N	-2.74	1.27	1.33
3	C	550	NAD	C3N-C7N	2.64	1.54	1.50
3	C	550	NAD	C4A-N9A	-2.60	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	550	NAD	C2N-N1N	-2.58	1.32	1.35
3	C	550	NAD	O4D-C1D	2.58	1.44	1.40
3	C	550	NAD	C2N-C3N	2.56	1.43	1.39
2	D	500	2FA	C5-N7	-2.56	1.34	1.39
3	B	550	NAD	C4A-N9A	-2.53	1.32	1.37
3	B	550	NAD	O2B-C2B	2.52	1.49	1.43
2	B	500	2FA	C4-N9	-2.46	1.32	1.37
3	B	550	NAD	C6A-N6A	2.44	1.40	1.34
2	C	500	2FA	C4-N9	-2.43	1.32	1.37
3	A	550	NAD	C8A-N7A	2.38	1.36	1.31
2	A	500	2FA	O4'-C4'	-2.30	1.39	1.45
2	D	500	2FA	C4-N3	-2.27	1.31	1.34
3	C	550	NAD	C5A-N7A	-2.26	1.35	1.39
2	A	500	2FA	C4-N9	-2.23	1.33	1.37
2	A	500	2FA	C1'-N9	2.19	1.52	1.46
3	B	550	NAD	C2A-N3A	-2.16	1.30	1.33
3	D	550	NAD	C2A-N3A	2.15	1.37	1.33
3	A	550	NAD	O4D-C1D	2.10	1.43	1.40
3	C	550	NAD	O4B-C4B	-2.09	1.40	1.45
3	D	550	NAD	C5N-C4N	2.06	1.42	1.38
2	C	500	2FA	C5-N7	-2.04	1.35	1.39
2	B	500	2FA	C1'-N9	2.01	1.51	1.46

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	2FA	C5-C4-N3	-8.14	118.61	127.18
2	C	500	2FA	C5-C4-N3	-6.91	119.90	127.18
2	D	500	2FA	F-C2-N1	6.82	121.24	114.69
2	D	500	2FA	C5-C4-N3	-6.60	120.22	127.18
2	D	500	2FA	N6-C6-N1	6.55	125.87	117.03
2	C	500	2FA	N3-C4-N9	6.15	134.80	126.99
3	B	550	NAD	C4D-O4D-C1D	5.96	115.38	109.92
3	A	550	NAD	C5N-C4N-C3N	-5.85	114.62	120.36
3	A	550	NAD	C4A-N9A-C8A	5.82	111.84	105.74
3	C	550	NAD	C5A-C4A-N3A	-5.78	118.76	126.72
3	B	550	NAD	C4A-N9A-C8A	5.70	111.72	105.74
2	B	500	2FA	F-C2-N1	5.63	120.10	114.69
3	D	550	NAD	C5A-C4A-N3A	-5.57	119.04	126.72
2	A	500	2FA	O4'-C1'-N9	5.47	118.59	108.09
2	A	500	2FA	C4-C5-N7	-5.33	104.49	110.58
3	B	550	NAD	C5A-C4A-N3A	-5.19	119.57	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	2FA	C5-C4-N3	-5.12	121.78	127.18
2	B	500	2FA	O4'-C1'-N9	5.07	117.83	108.09
3	B	550	NAD	N3A-C2A-N1A	-5.02	120.98	128.58
2	D	500	2FA	N9-C8-N7	-4.98	106.86	113.94
3	D	550	NAD	N3A-C4A-N9A	4.91	135.53	127.17
3	B	550	NAD	N3A-C4A-N9A	4.89	135.49	127.17
3	A	550	NAD	N3A-C2A-N1A	-4.79	121.33	128.58
2	D	500	2FA	C4-C5-N7	-4.70	105.21	110.58
3	C	550	NAD	N3A-C4A-N9A	4.66	135.09	127.17
2	C	500	2FA	C4'-O4'-C1'	-4.60	99.31	109.47
2	B	500	2FA	N6-C6-N1	4.58	123.21	117.03
3	A	550	NAD	N9A-C8A-N7A	-4.52	107.52	113.94
3	B	550	NAD	N9A-C8A-N7A	-4.50	107.55	113.94
3	C	550	NAD	C4A-C5A-N7A	-4.49	105.45	110.58
2	C	500	2FA	F-C2-N3	4.47	118.98	114.69
2	A	500	2FA	N3-C4-N9	4.44	132.62	126.99
2	A	500	2FA	F-C2-N1	4.43	118.95	114.69
3	B	550	NAD	O7N-C7N-N7N	-4.41	116.24	122.62
3	D	550	NAD	C4A-N9A-C8A	4.38	110.34	105.74
3	B	550	NAD	C2A-N3A-C4A	4.38	122.52	111.83
2	C	500	2FA	N6-C6-N1	4.37	122.93	117.03
2	D	500	2FA	C4-N9-C8	4.20	110.15	105.74
2	D	500	2FA	N1-C2-N3	-4.20	124.53	130.60
2	D	500	2FA	C5-N7-C8	4.13	109.94	103.45
3	C	550	NAD	C4A-N9A-C8A	4.11	110.06	105.74
3	C	550	NAD	C5A-N7A-C8A	3.99	109.72	103.45
2	C	500	2FA	C4-N9-C8	3.98	109.92	105.74
2	D	500	2FA	N3-C4-N9	3.85	131.88	126.99
2	C	500	2FA	N1-C2-N3	-3.84	125.06	130.60
3	A	550	NAD	C3N-C7N-N7N	3.84	122.46	117.74
3	A	550	NAD	O3D-C3D-C4D	-3.83	100.09	111.08
2	B	500	2FA	C4-C5-N7	-3.79	106.25	110.58
3	C	550	NAD	N9A-C8A-N7A	-3.70	108.68	113.94
2	B	500	2FA	C4-N9-C1'	-3.61	118.18	126.63
2	A	500	2FA	C5'-C4'-C3'	3.55	123.47	115.10
3	B	550	NAD	O2B-C2B-C1B	3.49	122.11	110.10
3	D	550	NAD	C4A-C5A-N7A	-3.46	106.62	110.58
3	C	550	NAD	O7N-C7N-C3N	3.42	123.78	119.60
2	A	500	2FA	N1-C2-N3	-3.40	125.69	130.60
3	A	550	NAD	O3-PA-O1A	-3.39	100.52	110.70
3	C	550	NAD	O7N-C7N-N7N	-3.34	117.79	122.62
3	A	550	NAD	C2A-N3A-C4A	3.30	119.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	NAD	C5A-C4A-N3A	-3.29	122.19	126.72
2	B	500	2FA	C4-N9-C8	3.29	109.19	105.74
3	A	550	NAD	C2N-C3N-C4N	3.27	122.06	118.26
2	B	500	2FA	O5'-C5'-C4'	-3.24	100.29	111.33
3	D	550	NAD	C5A-N7A-C8A	3.23	108.52	103.45
3	B	550	NAD	C2B-C1B-N9A	-3.20	105.35	113.30
3	B	550	NAD	C5A-N7A-C8A	3.18	108.45	103.45
3	D	550	NAD	N9A-C8A-N7A	-3.14	109.48	113.94
3	D	550	NAD	N3A-C2A-N1A	-3.14	123.83	128.58
3	A	550	NAD	C4A-N9A-C1B	-3.09	119.41	126.63
3	A	550	NAD	C4A-C5A-N7A	-3.02	107.13	110.58
3	B	550	NAD	C3N-C7N-N7N	3.00	121.43	117.74
3	B	550	NAD	C2B-C3B-C4B	2.97	108.35	102.61
3	B	550	NAD	C6A-C5A-N7A	2.97	137.81	132.09
3	B	550	NAD	O4D-C4D-C3D	-2.96	99.27	105.15
2	D	500	2FA	C4'-O4'-C1'	-2.96	102.92	109.47
3	D	550	NAD	C2A-N3A-C4A	2.96	119.05	111.83
3	B	550	NAD	C4A-C5A-N7A	-2.95	107.21	110.58
3	D	550	NAD	O7N-C7N-N7N	-2.95	118.35	122.62
2	B	500	2FA	N3-C4-N9	2.91	130.69	126.99
3	C	550	NAD	C2B-C3B-C4B	2.89	108.20	102.61
2	B	500	2FA	N1-C2-N3	-2.88	126.44	130.60
3	A	550	NAD	N3A-C4A-N9A	2.86	132.03	127.17
3	A	550	NAD	C2B-C3B-C4B	2.85	108.12	102.61
3	A	550	NAD	C6A-C5A-N7A	2.84	137.57	132.09
3	B	550	NAD	O3-PA-O1A	-2.80	102.28	110.70
2	A	500	2FA	O5'-C5'-C4'	-2.77	101.89	111.33
2	A	500	2FA	C5-N7-C8	2.70	107.69	103.45
3	C	550	NAD	C2A-N3A-C4A	2.69	118.40	111.83
3	D	550	NAD	O2N-PN-O3	2.69	114.54	107.27
2	C	500	2FA	C3'-C2'-C1'	2.67	106.52	101.46
2	A	500	2FA	C5-C4-N9	2.64	108.69	105.81
3	C	550	NAD	C5N-C4N-C3N	-2.62	117.79	120.36
2	D	500	2FA	C4-N9-C1'	-2.62	120.51	126.63
3	B	550	NAD	C2A-N1A-C6A	2.55	122.93	118.73
2	C	500	2FA	C5-C6-N6	-2.55	116.98	123.29
3	A	550	NAD	C5A-N7A-C8A	2.54	107.44	103.45
3	C	550	NAD	O4B-C1B-N9A	2.53	112.95	108.09
3	B	550	NAD	C5N-C4N-C3N	-2.52	117.89	120.36
3	C	550	NAD	C4D-O4D-C1D	2.51	112.23	109.92
2	B	500	2FA	N9-C8-N7	-2.49	110.40	113.94
3	D	550	NAD	C5N-C4N-C3N	-2.48	117.92	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	NAD	C6N-N1N-C2N	-2.48	119.77	121.88
2	A	500	2FA	C4-N9-C1'	-2.47	120.85	126.63
3	B	550	NAD	O5B-C5B-C4B	-2.47	100.57	108.99
2	D	500	2FA	O5'-C5'-C4'	-2.44	103.02	111.33
3	B	550	NAD	C6N-N1N-C1D	2.43	124.51	119.73
2	D	500	2FA	C2-N1-C6	2.43	120.36	112.44
3	D	550	NAD	C2N-N1N-C1D	-2.43	113.77	119.13
2	B	500	2FA	C1'-N9-C8	2.43	132.48	127.09
3	D	550	NAD	O2D-C2D-C3D	2.37	119.40	111.82
2	A	500	2FA	C2-N1-C6	2.35	120.11	112.44
3	C	550	NAD	C4A-N9A-C1B	-2.32	121.22	126.63
2	B	500	2FA	C6-C5-N7	2.31	136.55	132.09
2	A	500	2FA	C6-C5-N7	2.30	136.52	132.09
3	D	550	NAD	O3-PN-O1N	-2.28	103.85	110.70
3	D	550	NAD	C5A-C6A-N6A	-2.28	117.65	123.29
3	A	550	NAD	O2B-C2B-C1B	2.26	117.90	110.10
3	A	550	NAD	O2N-PN-O1N	2.22	122.78	112.44
3	D	550	NAD	O4B-C1B-N9A	2.20	112.32	108.09
2	B	500	2FA	O3'-C3'-C2'	-2.20	104.75	111.82
2	C	500	2FA	C4-C5-N7	-2.19	108.07	110.58
2	A	500	2FA	C1'-N9-C8	2.19	131.96	127.09
3	C	550	NAD	C6A-C5A-N7A	2.18	136.30	132.09
3	A	550	NAD	C4B-O4B-C1B	-2.18	104.65	109.47
3	B	550	NAD	O7N-C7N-C3N	2.18	122.26	119.60
2	D	500	2FA	C5-C6-N6	-2.17	117.92	123.29
3	D	550	NAD	C2B-C3B-C4B	2.14	106.75	102.61
3	B	550	NAD	C2N-N1N-C1D	-2.14	114.42	119.13
3	A	550	NAD	O3-PN-O1N	-2.13	104.31	110.70
3	A	550	NAD	O7N-C7N-N7N	-2.13	119.55	122.62
2	C	500	2FA	C2-N1-C6	2.10	119.30	112.44
3	C	550	NAD	O3-PA-O1A	-2.09	104.40	110.70
3	C	550	NAD	O2A-PA-O1A	2.07	122.09	112.44
2	B	500	2FA	C5-N7-C8	2.04	106.66	103.45
3	D	550	NAD	C5D-C4D-C3D	-2.03	107.89	115.21
2	B	500	2FA	C5-C6-N6	-2.03	118.27	123.29

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	A	550	NAD	C2D-C1D-N1N-C2N
3	A	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
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	D	550	NAD	O4D-C1D-N1N-C2N
3	D	550	NAD	O4D-C1D-N1N-C6N
3	D	550	NAD	C2D-C1D-N1N-C2N
3	D	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	B	550	NAD	C2B-C1B-N9A-C8A
3	B	550	NAD	C5B-O5B-PA-O1A
3	D	550	NAD	O4B-C4B-C5B-O5B
3	A	550	NAD	C2B-C1B-N9A-C8A

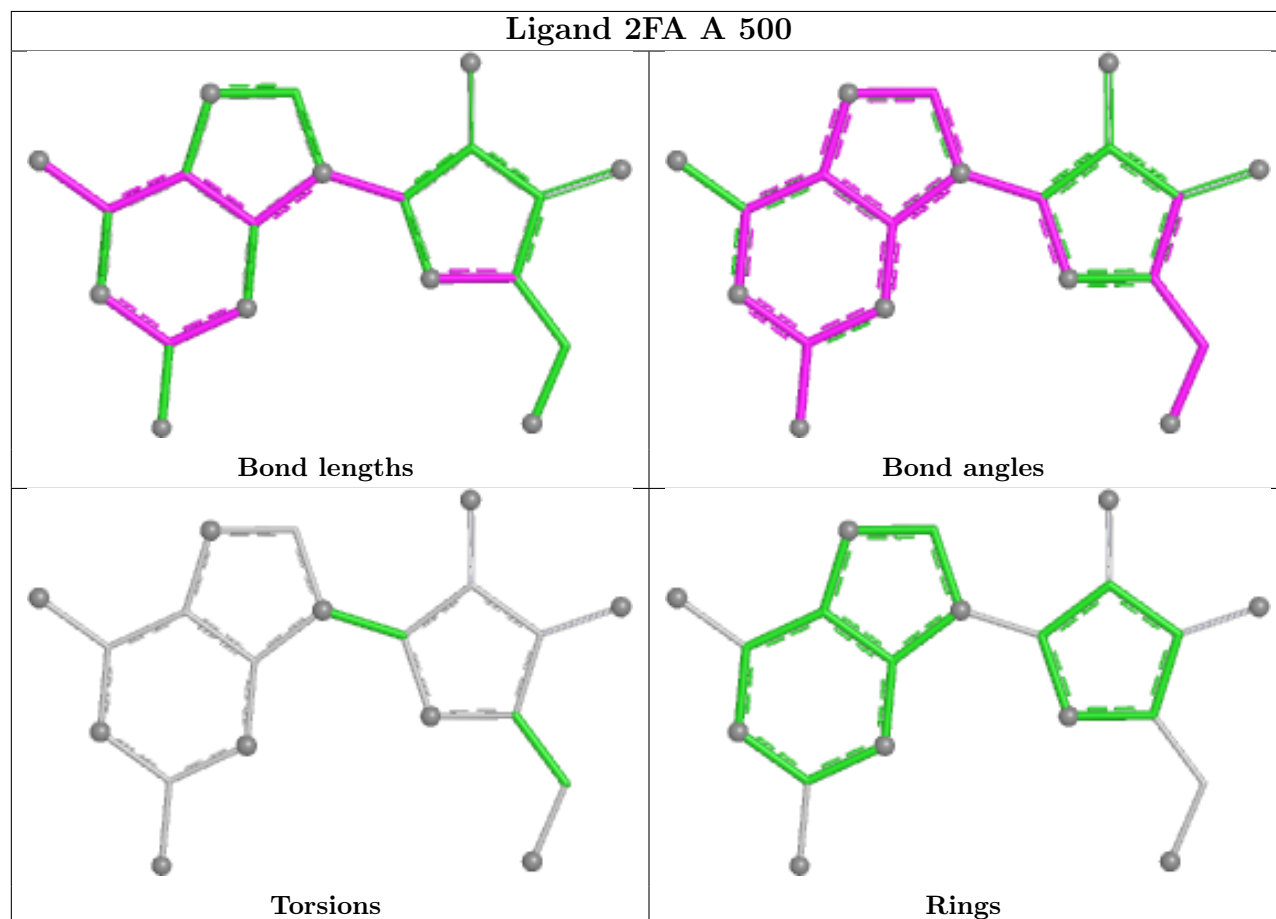
There are no ring outliers.

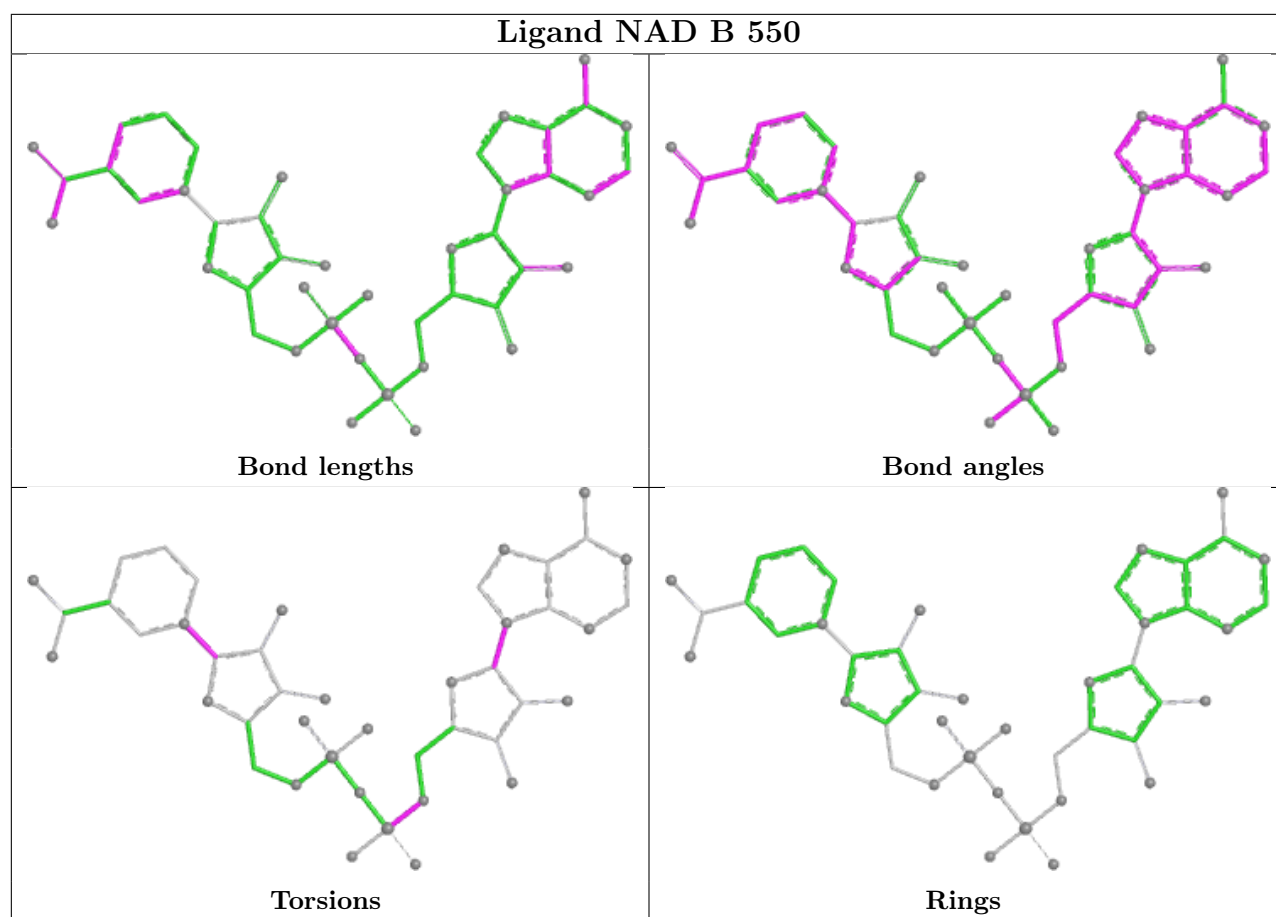
8 monomers are involved in 12 short contacts:

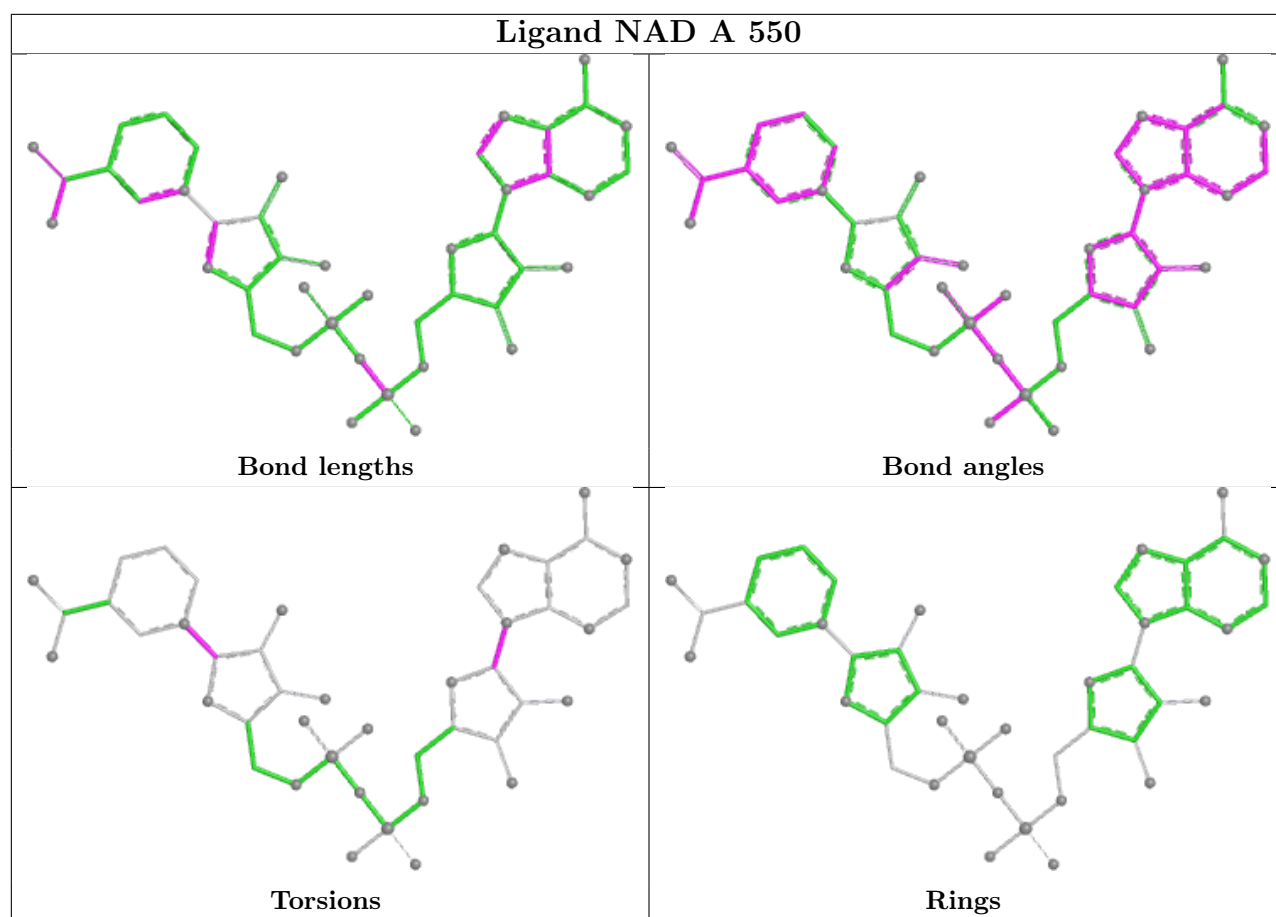
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	2FA	2	0
3	B	550	NAD	3	0
3	A	550	NAD	3	0
2	D	500	2FA	2	0
3	D	550	NAD	3	0
2	B	500	2FA	1	0
2	C	500	2FA	3	0
3	C	550	NAD	1	0

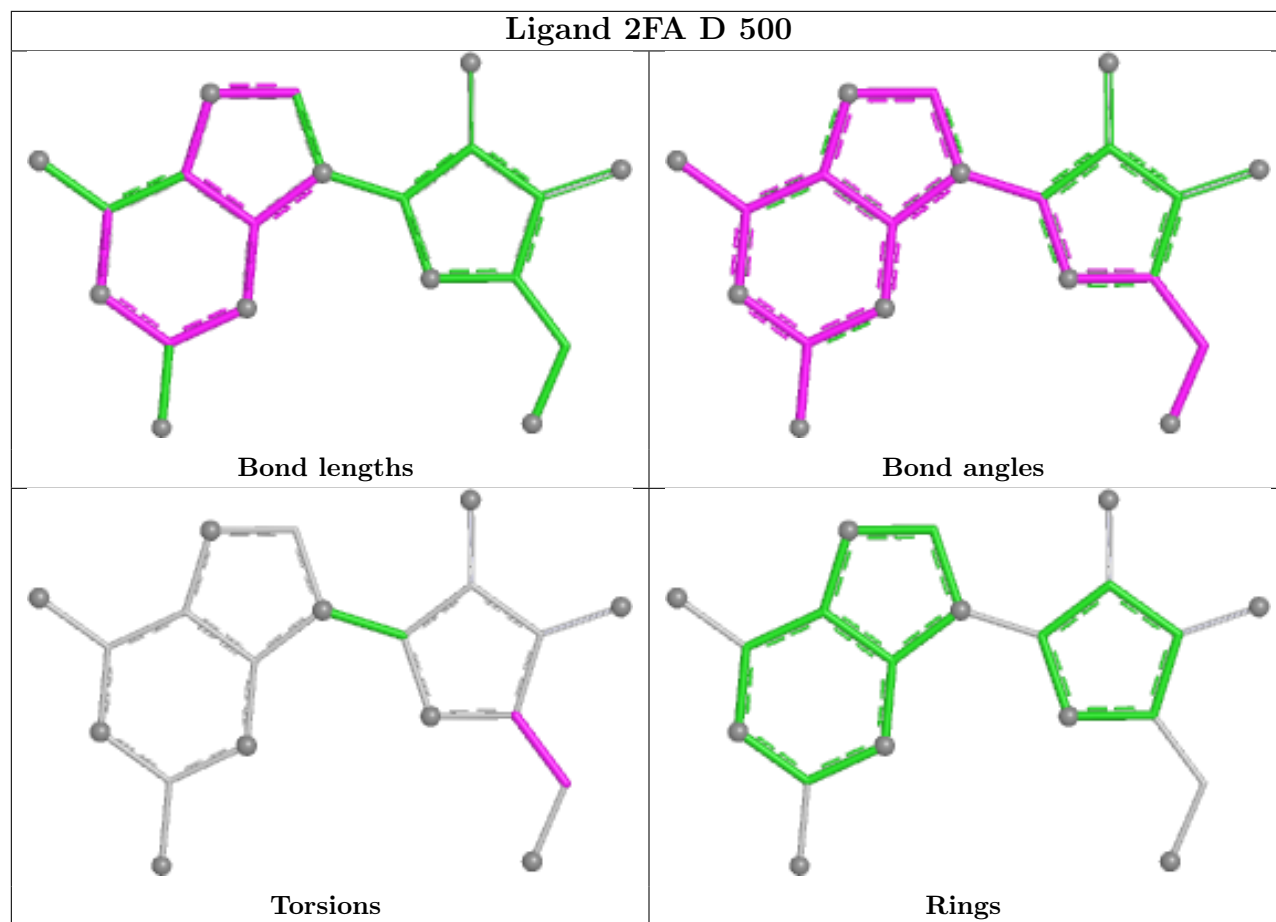
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

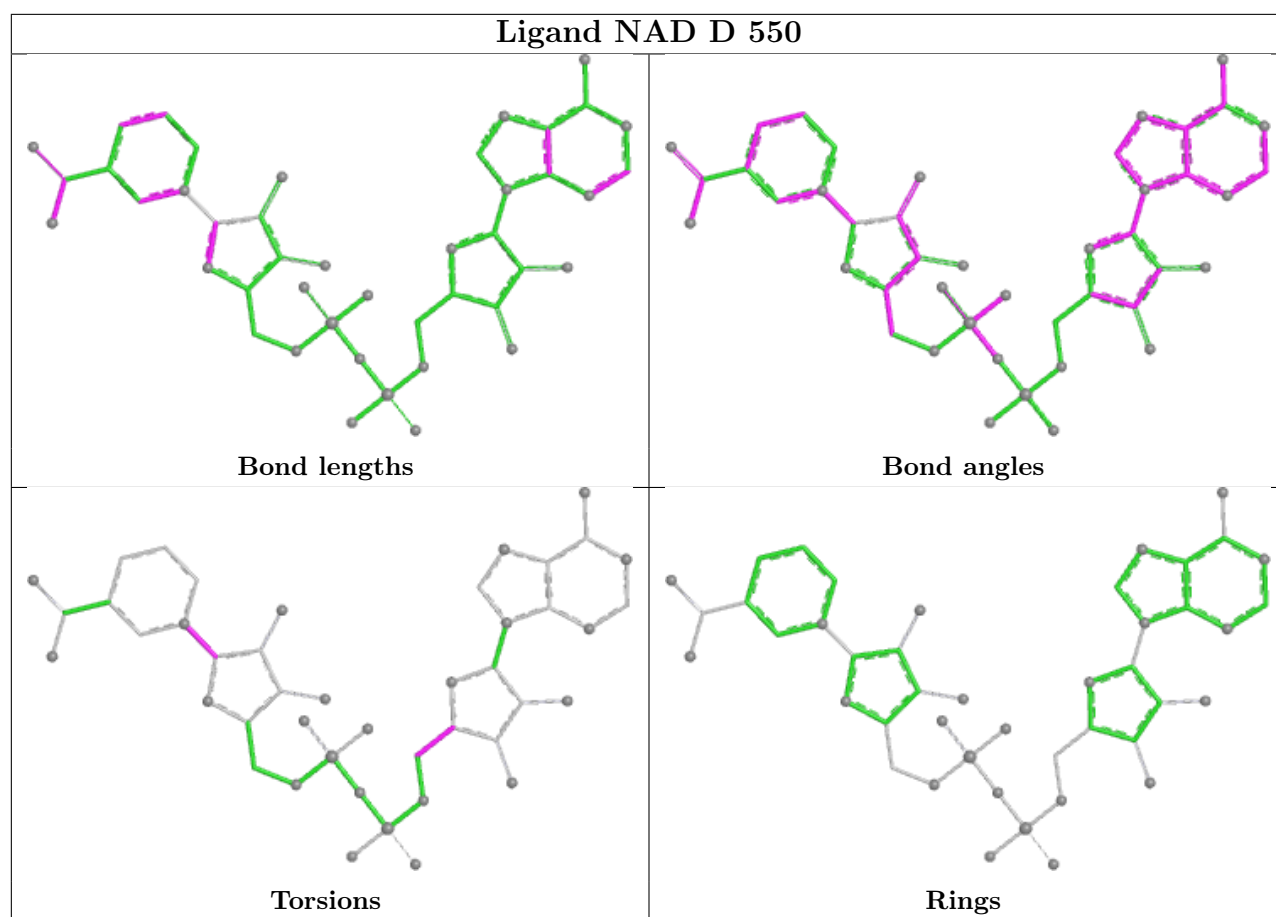
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

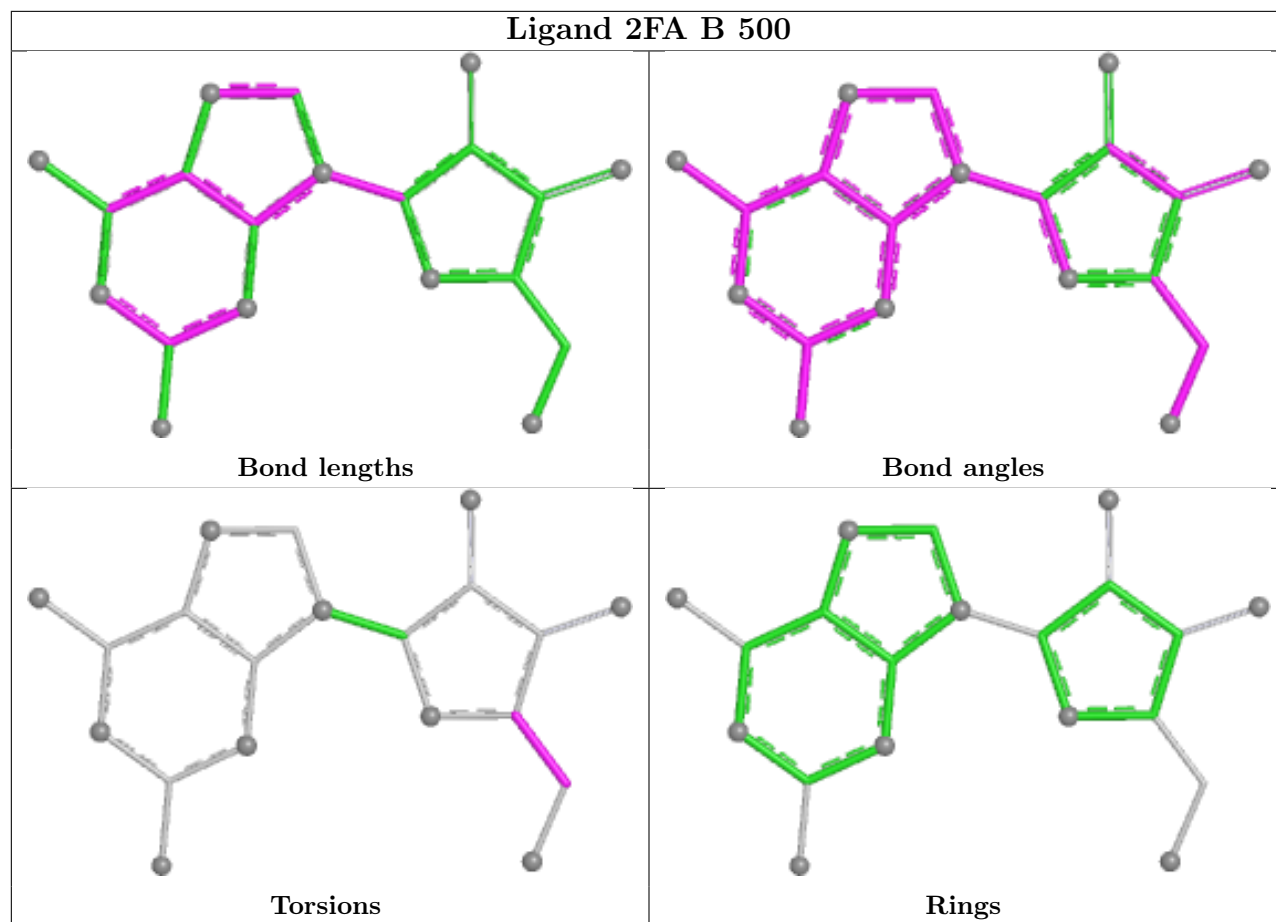


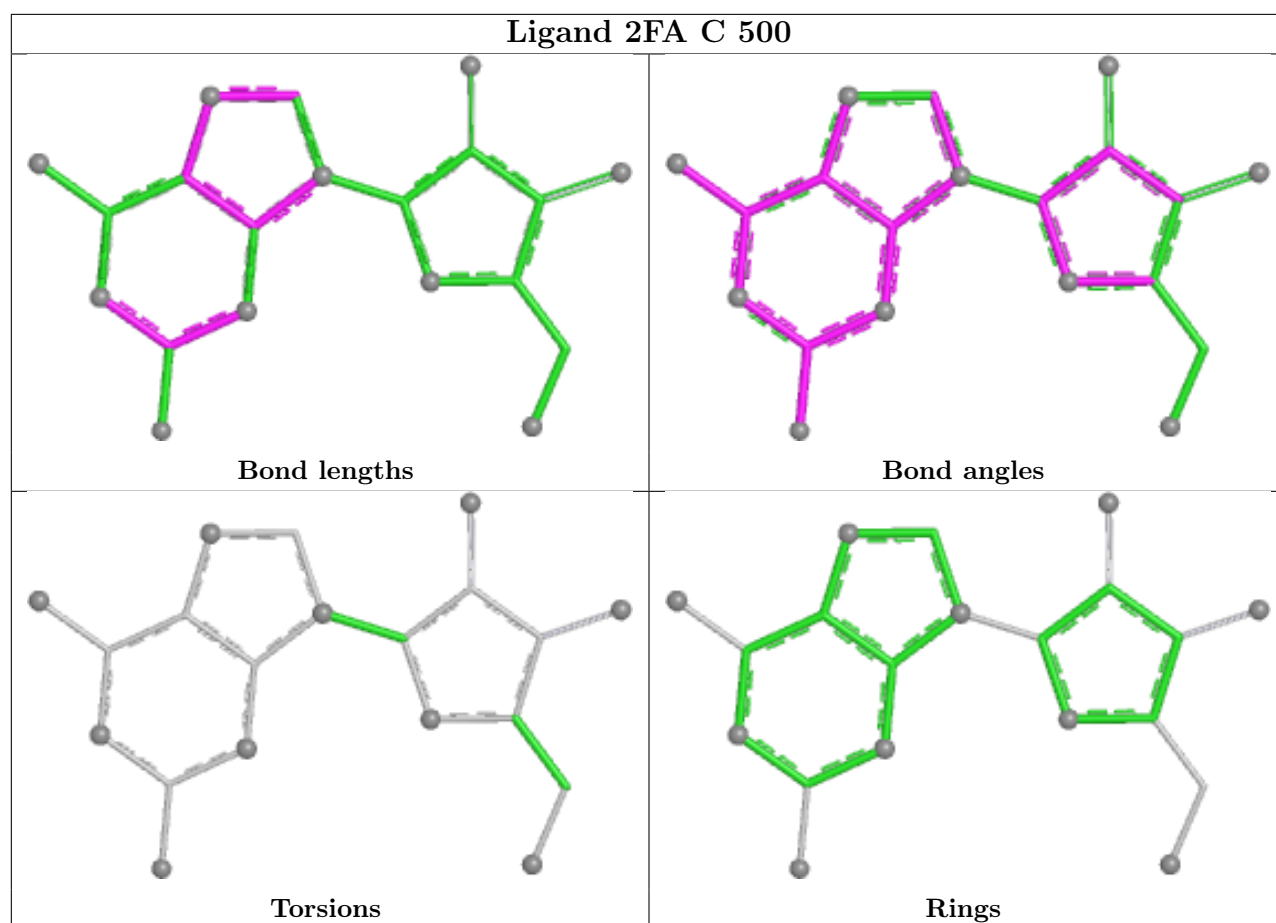


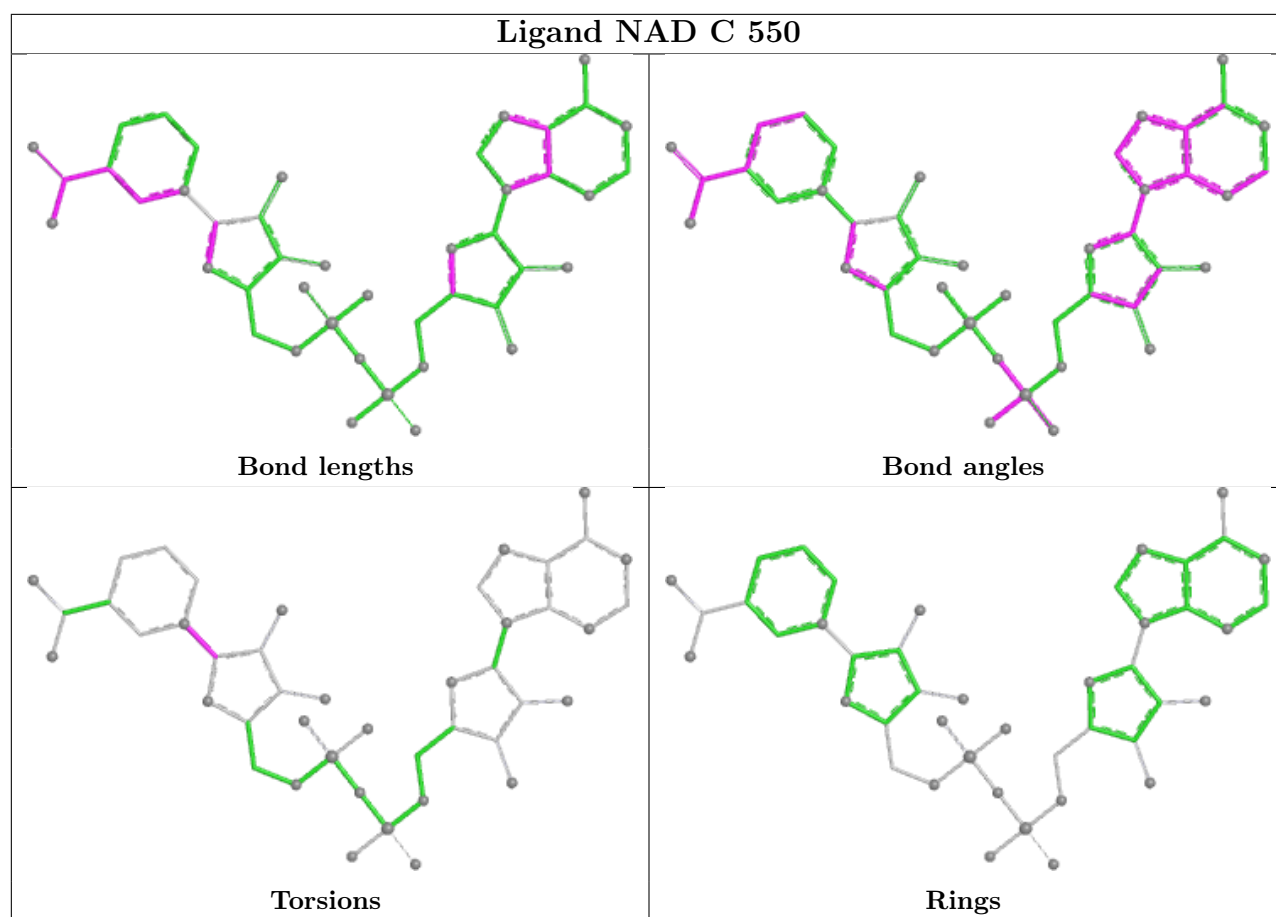












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	486/495 (98%)	-0.24	0 100 100	21, 34, 52, 70	0
1	B	485/495 (97%)	-0.30	1 (0%) 91 90	22, 34, 48, 64	0
1	C	485/495 (97%)	-0.11	3 (0%) 85 84	24, 38, 58, 89	0
1	D	485/495 (97%)	-0.11	4 (0%) 82 80	23, 38, 59, 80	0
All	All	1941/1980 (98%)	-0.19	8 (0%) 88 87	21, 36, 57, 89	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	486	GLY	2.9
1	C	179	ALA	2.8
1	D	364	PHE	2.3
1	D	363	HIS	2.3
1	C	363	HIS	2.2
1	D	179	ALA	2.1
1	D	61	GLY	2.0
1	C	182	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

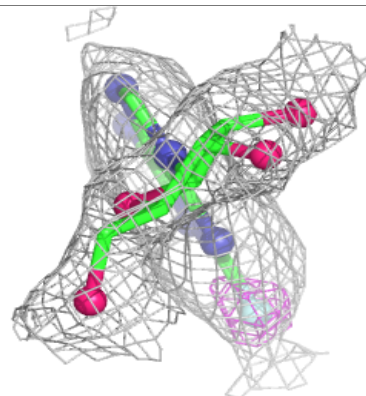
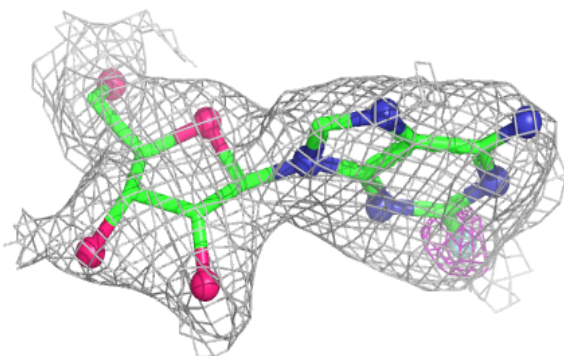
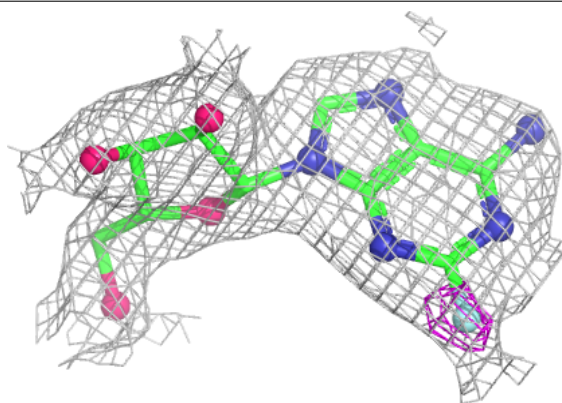
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	2FA	C	500	20/20	0.94	0.07	21,27,32,37	0
2	2FA	B	500	20/20	0.96	0.06	21,27,34,34	0
2	2FA	A	500	20/20	0.96	0.06	12,23,29,35	0
2	2FA	D	500	20/20	0.96	0.06	20,28,33,40	0
3	NAD	A	550	44/44	0.97	0.05	18,26,30,31	0
3	NAD	B	550	44/44	0.97	0.05	19,25,33,37	0
3	NAD	C	550	44/44	0.97	0.06	21,28,32,34	0
3	NAD	D	550	44/44	0.98	0.05	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.

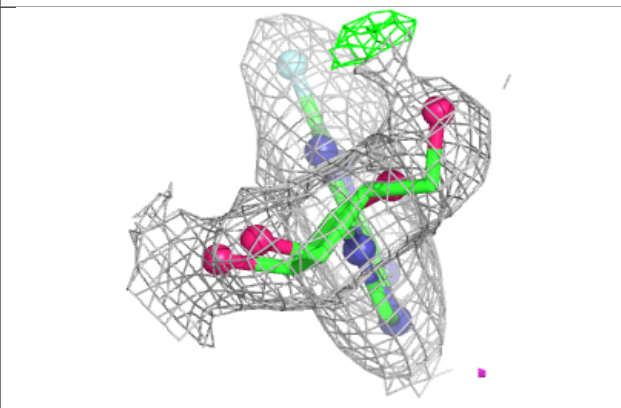
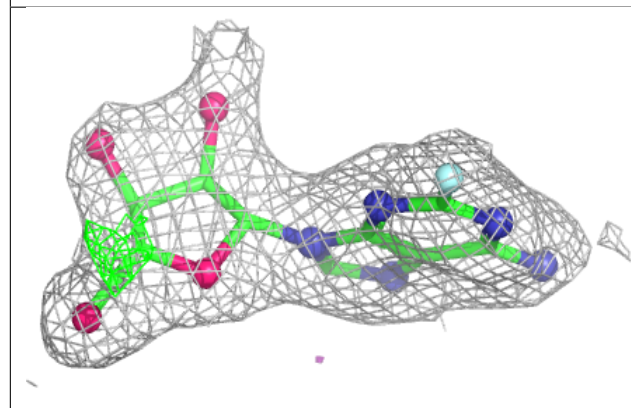
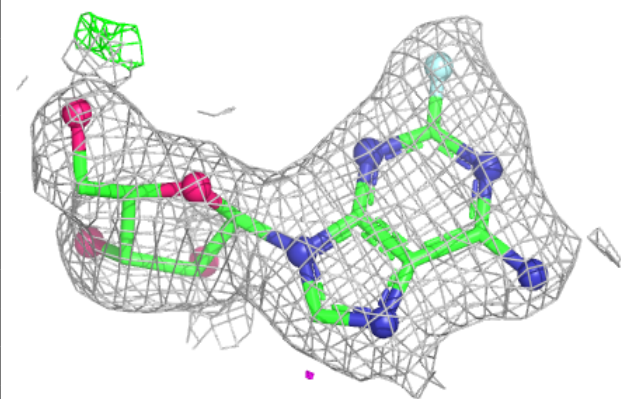
Electron density around 2FA C 500:

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

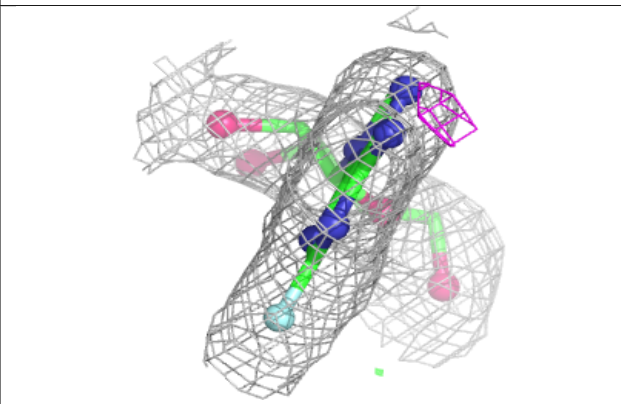
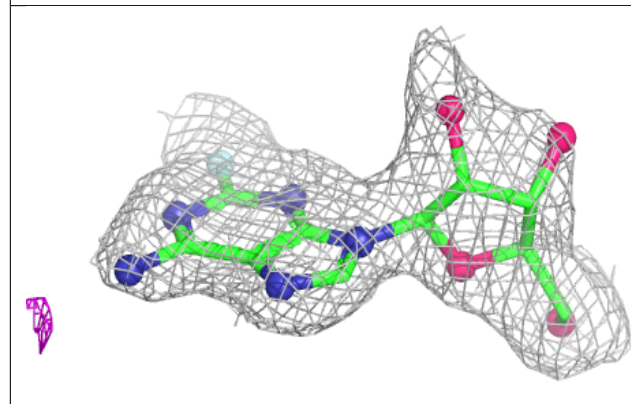
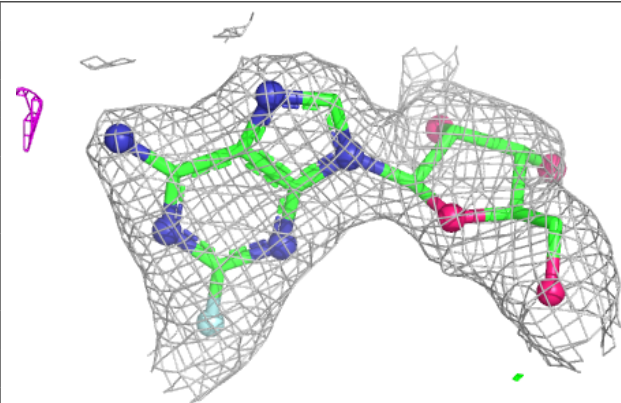


Electron density around 2FA B 500:

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

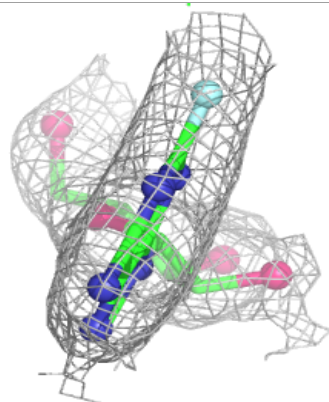
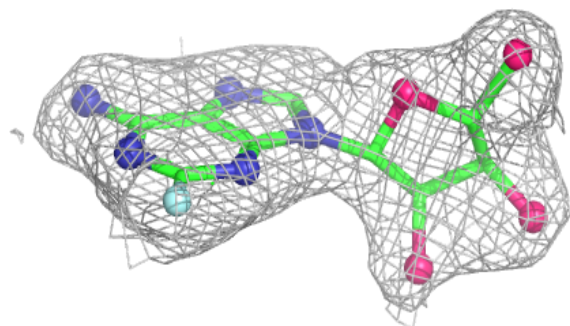
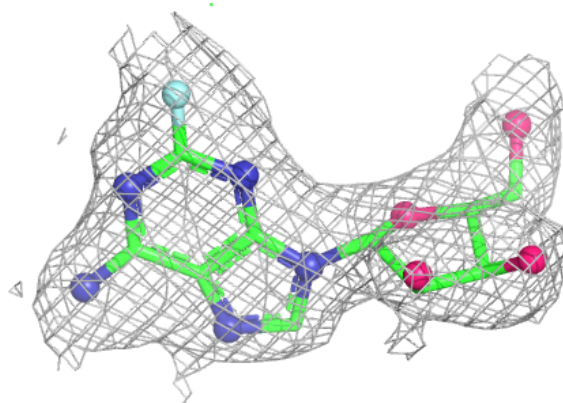
**Electron density around 2FA A 500:**

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

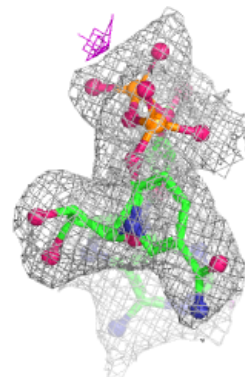
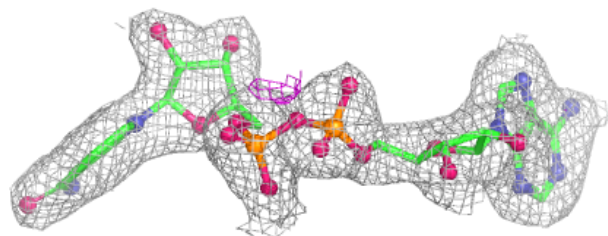
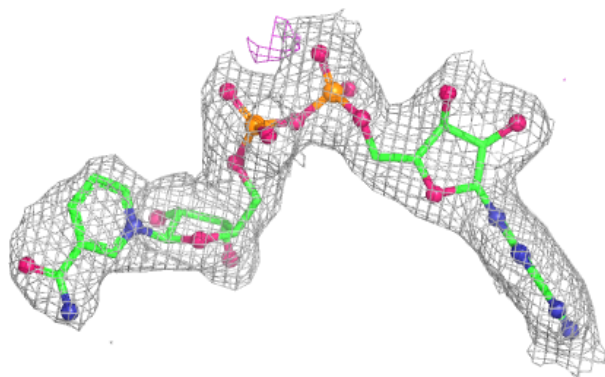


Electron density around 2FA D 500:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

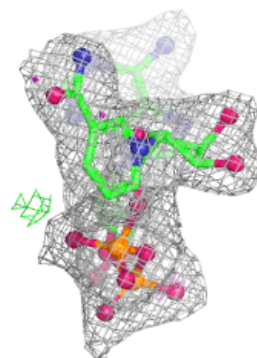
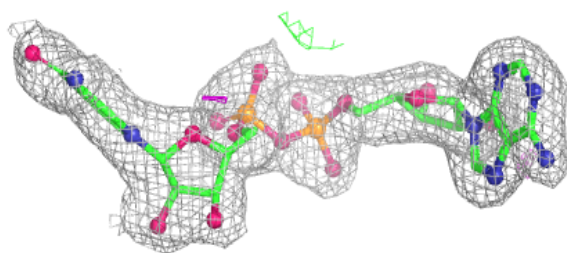
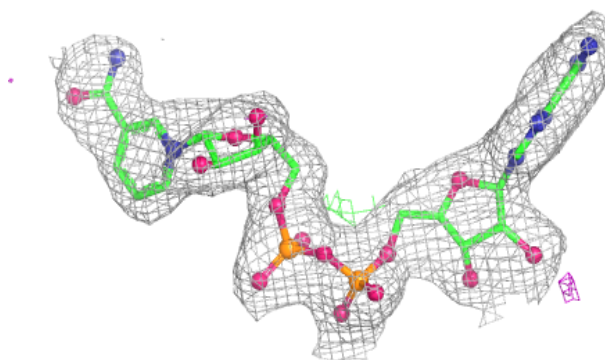
**Electron density around NAD A 550:**

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

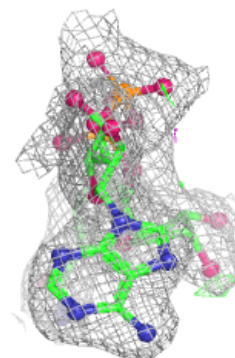
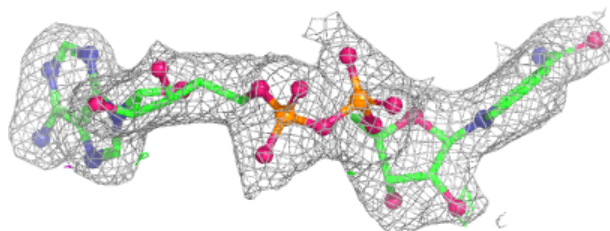
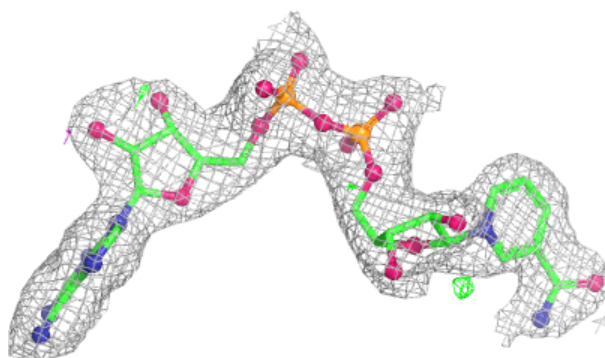


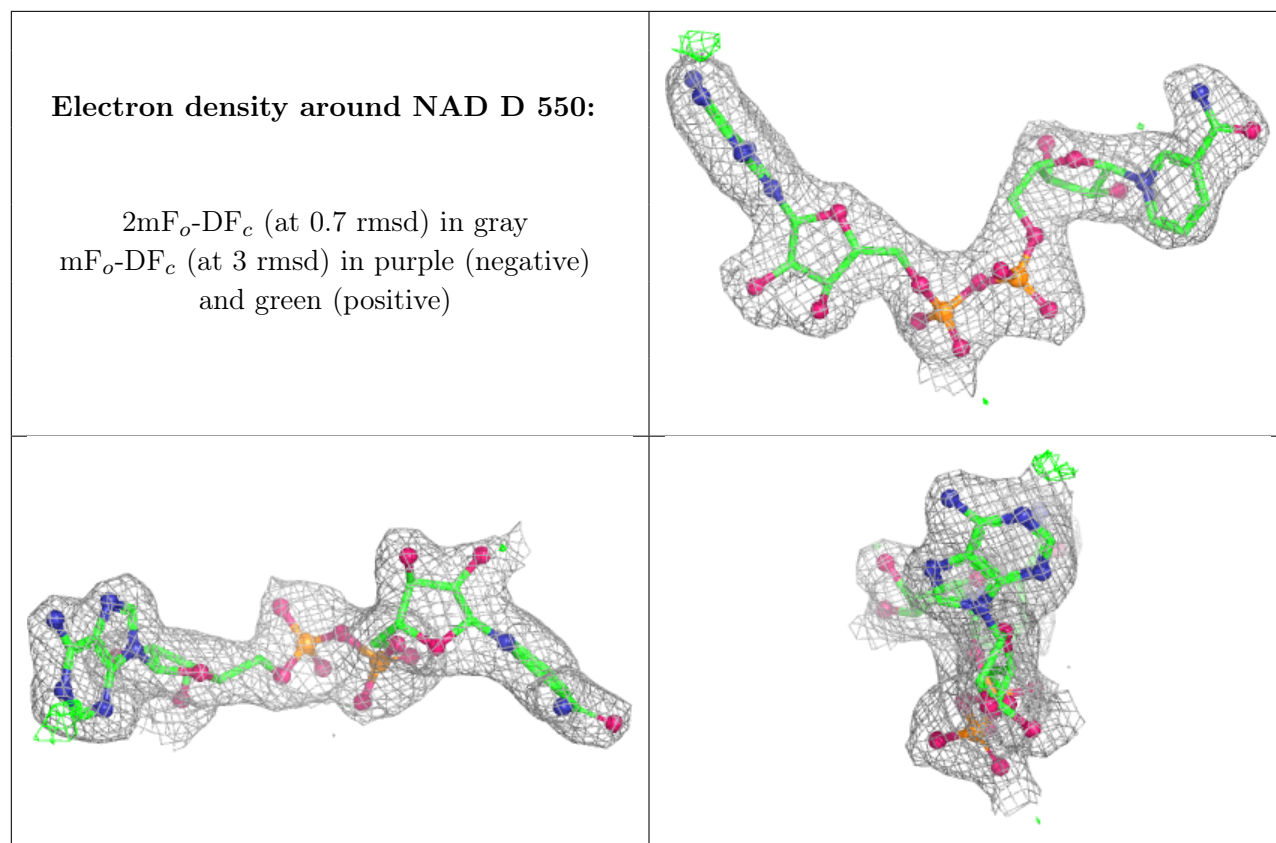
Electron density around NAD B 550:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.