



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:54 PM EDT

PDB ID : 3G1U / pdb_00003g1u
Title : Crystal structure of Leishmania major S-adenosylhomocysteine hydrolase
Authors : Siponen, M.I.; Welin, M.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Dahlgren, L.G.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Karlberg, T.; Kotenyova, T.; Lehtio, L.; Moche, M.; Nilsson, M.E.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Schutz, P.; Thorsell, A.G.; Tresaugues, L.; Van Den Berg, S.; Weigelt, J.; Wisniewska, M.; Schueler, H.; Structural Genomics Consortium (SGC)
Deposited on : 2009-01-30
Resolution : 2.20 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)

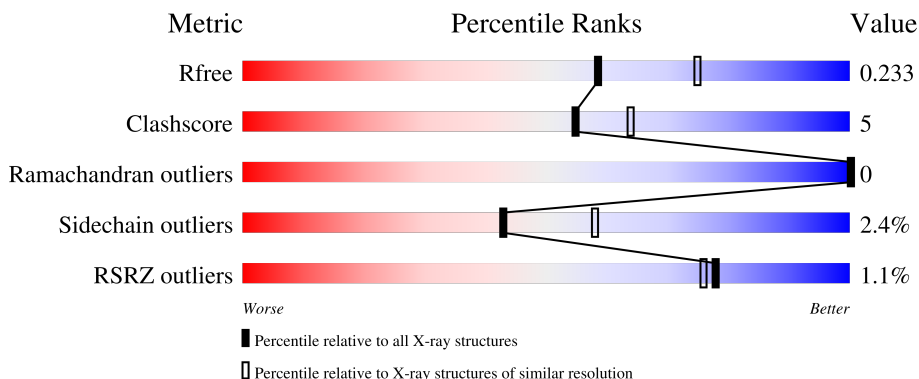
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	437	 84% 10% 6%
1	B	437	 85% 8% 6%

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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

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Mol	Chain	Length	Quality of chain
1	C	437	2% 86% 10%
1	D	437	2% 86% 10%

2 Entry composition [i](#)

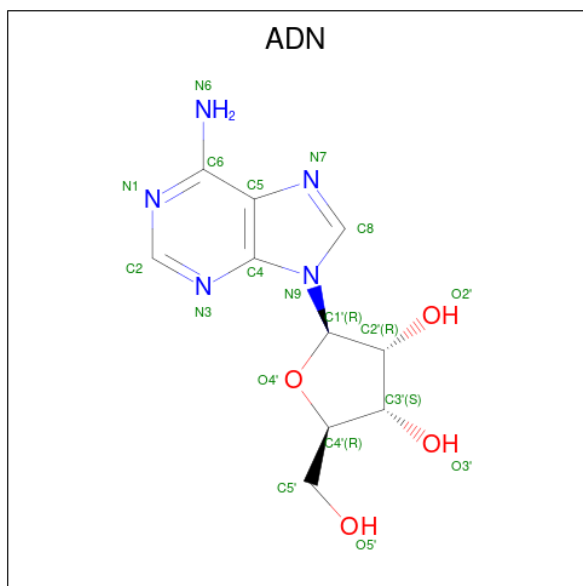
There are 4 unique types of molecules in this entry. The entry contains 13715 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	412	Total	C	N	O	S	0	0	0
			3141	1981	539	601	20			
1	B	412	Total	C	N	O	S	0	2	0
			3154	1990	545	599	20			
1	C	424	Total	C	N	O	S	0	1	0
			3249	2055	561	612	21			
1	D	418	Total	C	N	O	S	0	5	0
			3221	2031	553	617	20			

- Molecule 2 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



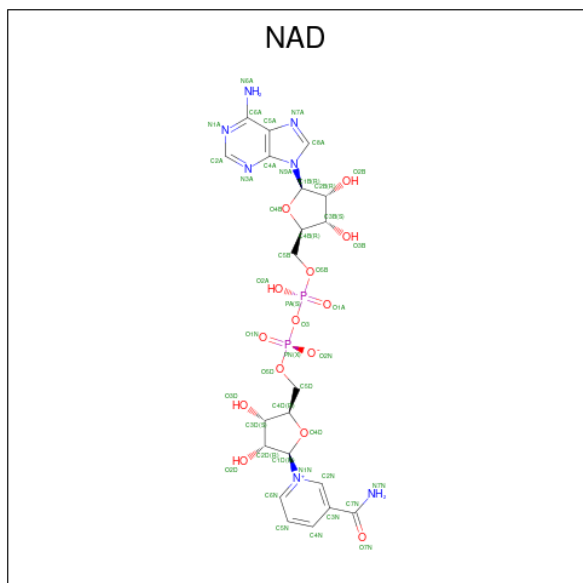
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			19	10	5	4		
2	D	1	Total	C	N	O	0	0
			19	10	5	4		

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



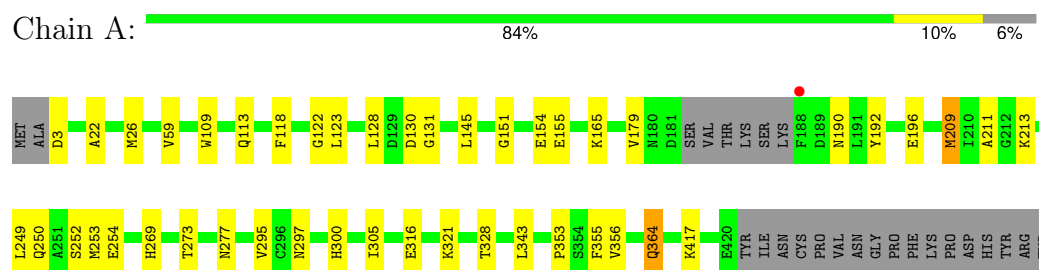
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	153	Total	O	0	0
			153	153		

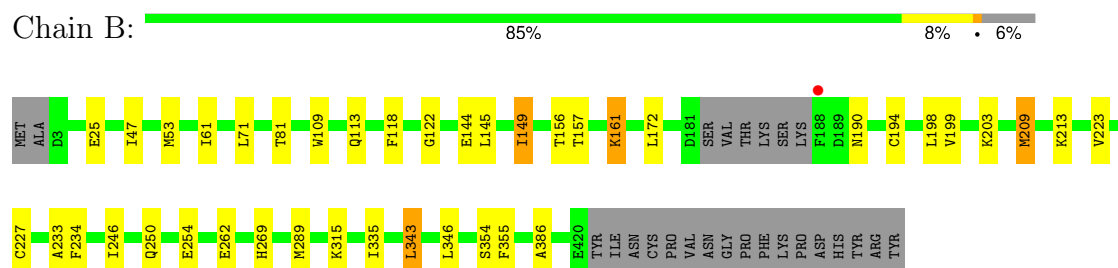
3 Residue-property plots [i](#)

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.

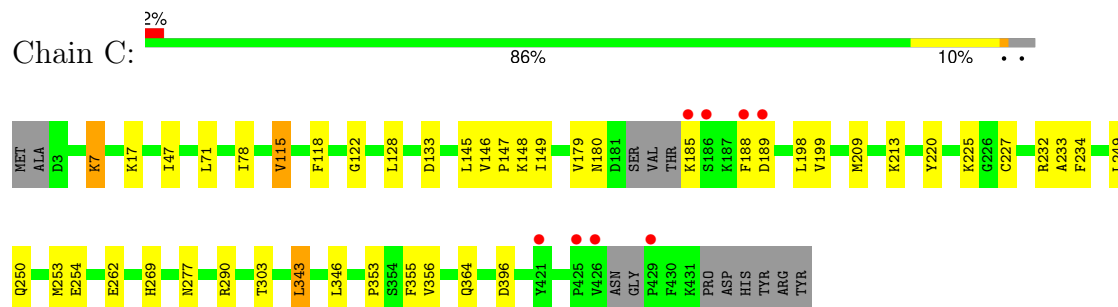
• Molecule 1: Adenosylhomocysteinase



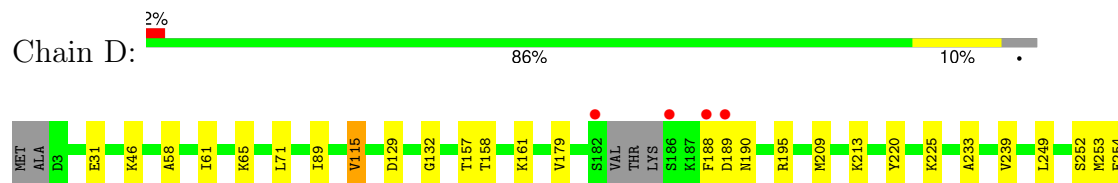
• Molecule 1: Adenosylhomocysteinase

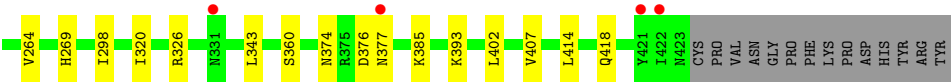


• Molecule 1: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.38Å 82.47Å 83.88Å 87.02° 71.41° 74.00°	Depositor
Resolution (Å)	22.87 – 2.20 22.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (22.87-2.20) 96.7 (22.87-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0035	Depositor
R, R_{free}	0.181 , 0.232 0.182 , 0.233	Depositor DCC
R_{free} test set	4332 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13715	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.69	0/3199	0.90	2/4336 (0.0%)
1	B	0.70	0/3218	0.88	1/4360 (0.0%)
1	C	0.67	0/3313	0.88	0/4485
1	D	0.66	0/3289	0.90	2/4454 (0.0%)
All	All	0.68	0/13019	0.89	5/17635 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	LYS	N-CA-C	-5.46	103.21	108.13
1	A	151	GLY	N-CA-C	5.27	118.19	110.38
1	D	298	ILE	CB-CA-C	5.22	115.87	110.70
1	D	393	LYS	N-CA-C	5.22	118.91	112.54
1	B	354	SER	N-CA-C	5.07	117.19	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3141	0	3106	36	0
1	B	3154	0	3133	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3249	0	3238	33	0
1	D	3221	0	3202	40	0
2	A	19	0	13	1	0
2	B	19	0	13	1	0
2	C	19	0	13	1	0
2	D	19	0	13	1	0
3	A	44	0	26	2	0
3	B	44	0	26	2	0
3	C	44	0	26	1	0
3	D	44	0	26	5	0
4	A	206	0	0	2	0
4	B	189	0	0	2	0
4	C	150	0	0	5	0
4	D	153	0	0	2	0
All	All	13715	0	12835	125	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 5.

All (125) 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:209:MET:CE	1:D:253:MET:HE1	1.66	1.24
1:A:130:ASP:HB3	1:A:155:GLU:HB3	1.21	1.17
1:B:209:MET:HE3	1:D:253:MET:HE1	1.27	1.15
1:A:22:ALA:HB1	1:A:26:MET:HE2	1.43	0.98
1:A:130:ASP:CB	1:A:155:GLU:HB3	1.94	0.95
1:B:209:MET:HE1	1:D:253:MET:HE1	1.55	0.88
1:A:130:ASP:HB3	1:A:155:GLU:CB	2.08	0.81
1:B:289:MET:HE3	1:B:335:ILE:HG12	1.66	0.78
1:A:252:SER:HB3	1:D:407:VAL:HG11	1.66	0.78
1:A:233:ALA:HB1	1:B:233:ALA:HB1	1.67	0.75
1:C:180:ASN:HA	1:C:185:LYS:HD2	1.71	0.73
1:C:233:ALA:HB1	1:D:233:ALA:HB1	1.69	0.73
1:A:26:MET:CE	1:A:59:VAL:HG21	2.20	0.71
1:B:254:GLU:HG3	4:B:582:HOH:O	1.92	0.70
1:C:355:PHE:HB3	1:D:209:MET:HE2	1.74	0.69
1:D:254:GLU:HG3	4:D:455:HOH:O	1.92	0.68
1:B:289:MET:CE	1:B:335:ILE:HG12	2.25	0.67
1:A:355:PHE:HD2	1:B:209:MET:HE2	1.58	0.67
1:B:250:GLN:O	1:B:254:GLU:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:GLU:HG2	1:D:402:LEU:HD22	1.79	0.64
1:B:213[A]:LYS:HD2	1:B:269:HIS:CG	2.33	0.63
1:D:158:THR:HG23	3:D:439:NAD:O3D	1.98	0.63
1:A:22:ALA:HB1	1:A:26:MET:CE	2.24	0.63
1:A:252:SER:CB	1:D:407:VAL:HG11	2.29	0.63
2:B:438:ADN:H3'	3:B:439:NAD:C4N	2.29	0.62
1:C:356:VAL:HB	1:D:209:MET:HE1	1.82	0.61
1:C:353:PRO:HB2	1:D:209:MET:HB2	1.85	0.58
1:A:128:LEU:HD11	1:A:364:GLN:HG3	1.86	0.58
1:A:26:MET:HE3	1:A:59:VAL:HG21	1.84	0.58
1:B:118:PHE:O	1:B:122:GLY:HA2	2.04	0.57
1:A:26:MET:HE1	1:A:59:VAL:HG21	1.86	0.57
1:B:209:MET:HE3	1:D:253:MET:CE	2.17	0.57
1:C:118:PHE:O	1:C:122:GLY:HA2	2.06	0.56
1:A:209:MET:HE2	1:A:211:ALA:HB3	1.88	0.56
1:A:417:LYS:HB2	4:A:558:HOH:O	2.06	0.55
1:D:188:PHE:O	1:D:189:ASP:C	2.49	0.55
2:C:438:ADN:H3'	3:C:439:NAD:C4N	2.38	0.54
1:A:190:ASN:CG	3:A:439:NAD:H5N	2.34	0.53
2:A:438:ADN:H3'	3:A:439:NAD:C4N	2.39	0.53
1:C:250:GLN:O	1:C:254:GLU:HG2	2.09	0.53
1:B:109:TRP:O	1:B:113:GLN:HG2	2.09	0.52
1:C:47:ILE:HB	1:C:71:LEU:HD23	1.91	0.52
1:A:130:ASP:HA	1:A:154:GLU:OE2	2.10	0.52
1:B:190:ASN:CG	3:B:439:NAD:H5N	2.35	0.52
1:A:192:TYR:HE1	1:D:254:GLU:OE2	1.93	0.52
1:D:158:THR:CG2	3:D:439:NAD:O3D	2.58	0.52
1:D:320:ILE:HD11	1:D:326:ARG:HB2	1.92	0.52
1:B:213[B]:LYS:HD2	1:B:269:HIS:CG	2.45	0.51
1:D:31:GLU:HG2	1:D:402:LEU:CD2	2.41	0.51
1:D:190:ASN:CG	3:D:439:NAD:H5N	2.35	0.51
1:A:316:GLU:HB3	1:A:328:THR:HB	1.91	0.51
1:D:254:GLU:CG	4:D:455:HOH:O	2.56	0.51
1:D:213:LYS:HD2	1:D:269:HIS:CG	2.45	0.51
1:A:26:MET:HE1	1:A:59:VAL:CG2	2.41	0.50
1:D:58:ALA:HB1	1:D:89:ILE:HD11	1.92	0.50
1:B:53:MET:HB3	1:B:81:THR:HG23	1.93	0.50
1:A:249:LEU:O	1:A:253:MET:HG2	2.11	0.49
1:C:199:VAL:HG11	1:C:234:PHE:CE2	2.47	0.49
1:A:246:ILE:O	1:A:250:GLN:HG3	2.13	0.49
1:C:198:LEU:HD22	1:C:227:CYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ILE:HG23	1:D:71:LEU:HD13	1.94	0.49
1:B:61:ILE:HG23	1:B:71:LEU:HD13	1.95	0.49
1:B:199:VAL:HG11	1:B:234:PHE:CE2	2.48	0.49
1:A:353:PRO:HB2	1:B:209:MET:HB2	1.95	0.48
1:C:213:LYS:HD2	1:C:269:HIS:CG	2.48	0.48
1:A:213:LYS:HD2	1:A:269:HIS:CG	2.48	0.48
1:C:199:VAL:HG11	1:C:234:PHE:HE2	1.79	0.48
1:A:3:ASP:N	4:A:595:HOH:O	2.47	0.48
1:C:249:LEU:O	1:C:253:MET:HG2	2.14	0.48
1:D:157:THR:HG22	1:D:161:LYS:HD2	1.96	0.48
1:B:246:ILE:HD11	1:C:396:ASP:HB3	1.95	0.48
1:C:17:LYS:NZ	4:C:525:HOH:O	2.45	0.48
1:C:290:ARG:NH1	4:C:521:HOH:O	2.47	0.47
1:D:239:VAL:HG21	1:D:264:VAL:HG11	1.96	0.47
1:B:157:THR:HG22	1:B:161:LYS:HE2	1.96	0.47
1:C:188:PHE:O	1:C:189:ASP:C	2.57	0.47
1:B:144:GLU:HB2	4:B:454:HOH:O	2.15	0.47
2:D:438:ADN:H3'	3:D:439:NAD:C4N	2.44	0.47
1:D:249:LEU:O	1:D:253:MET:HG2	2.13	0.47
1:B:145:LEU:HG	1:B:149:ILE:HD11	1.97	0.47
1:A:295:VAL:HG12	1:A:305:ILE:HD13	1.96	0.47
1:C:355:PHE:HD2	1:D:209:MET:CE	2.28	0.47
1:B:199:VAL:HG11	1:B:234:PHE:HE2	1.80	0.46
1:C:220:TYR:CZ	1:C:225:LYS:HG2	2.50	0.46
1:C:7:LYS:HD3	4:C:584:HOH:O	2.14	0.46
1:C:148:LYS:HB3	4:C:481:HOH:O	2.16	0.46
1:A:196:GLU:HB3	1:B:203:LYS:HE3	1.99	0.45
1:D:158:THR:HG23	3:D:439:NAD:C3D	2.47	0.45
1:D:414:LEU:HD22	1:D:418:GLN:HB3	1.99	0.45
1:A:123:LEU:HD22	1:A:145:LEU:HD21	1.97	0.45
1:B:289:MET:CE	1:B:335:ILE:CD1	2.94	0.45
1:A:356:VAL:HB	1:B:209:MET:HE1	1.98	0.45
1:B:25:GLU:O	1:B:355:PHE:HA	2.17	0.45
1:D:115:VAL:O	1:D:115:VAL:CG1	2.65	0.44
1:C:343:LEU:HD22	1:C:346:LEU:HD12	2.00	0.44
1:A:233:ALA:HB1	1:B:233:ALA:CB	2.42	0.43
1:A:252:SER:HB3	1:D:407:VAL:CG1	2.44	0.43
1:B:209:MET:HE1	1:D:253:MET:CE	2.36	0.43
1:C:128:LEU:HD11	1:C:364:GLN:HG3	1.99	0.43
1:C:133:ASP:HB2	4:C:486:HOH:O	2.17	0.43
1:D:220:TYR:CZ	1:D:225:LYS:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:HD22	1:B:346:LEU:HD12	2.00	0.43
1:A:109:TRP:O	1:A:113:GLN:HG2	2.19	0.43
1:B:47:ILE:HB	1:B:71:LEU:HD23	1.99	0.43
1:B:289:MET:CE	1:B:335:ILE:CG1	2.95	0.42
1:D:129:ASP:OD2	1:D:132:GLY:HA2	2.19	0.42
1:C:233:ALA:HB1	1:D:233:ALA:CB	2.45	0.42
1:B:198:LEU:HD22	1:B:227:CYS:HB3	2.01	0.42
1:B:172:LEU:O	1:B:386:ALA:HB3	2.20	0.42
1:A:118:PHE:O	1:A:122:GLY:HA2	2.20	0.42
1:C:220:TYR:CE2	1:C:225:LYS:HG2	2.55	0.42
1:A:233:ALA:CB	1:B:233:ALA:HB1	2.43	0.42
1:C:115:VAL:HG13	1:C:115:VAL:O	2.20	0.42
1:C:146:VAL:HB	1:C:147:PRO:HD3	2.01	0.42
1:C:145:LEU:HD12	1:C:148:LYS:HB2	2.03	0.41
1:D:220:TYR:CE2	1:D:225:LYS:HG2	2.55	0.41
1:A:131:GLY:HA3	1:A:300:HIS:NE2	2.35	0.41
1:A:273:THR:OG1	1:A:297:ASN:HB2	2.19	0.41
1:C:233:ALA:CB	1:D:233:ALA:HB1	2.45	0.41
1:C:355:PHE:HD2	1:D:209:MET:HE2	1.86	0.41
1:B:194:CYS:SG	1:B:223:VAL:HG13	2.61	0.41
1:C:115:VAL:O	1:C:115:VAL:CG1	2.68	0.41
1:D:374:ASN:OD1	1:D:377:ASN:ND2	2.52	0.40
1:C:232:ARG:NH2	1:C:254:GLU:O	2.33	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	408/437 (93%)	399 (98%)	9 (2%)	0	100	100
1	B	410/437 (94%)	405 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	419/437 (96%)	403 (96%)	16 (4%)	0	100	100
1	D	419/437 (96%)	405 (97%)	14 (3%)	0	100	100
All	All	1656/1748 (95%)	1612 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	332/358 (93%)	325 (98%)	7 (2%)	47	63
1	B	334/358 (93%)	327 (98%)	7 (2%)	47	63
1	C	345/358 (96%)	335 (97%)	10 (3%)	37	51
1	D	345/358 (96%)	335 (97%)	10 (3%)	37	51
All	All	1356/1432 (95%)	1322 (98%)	34 (2%)	43	56

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	LYS
1	A	179	VAL
1	A	209	MET
1	A	254	GLU
1	A	277	ASN
1	A	343	LEU
1	A	364	GLN
1	B	149	ILE
1	B	156	THR
1	B	161	LYS
1	B	209	MET
1	B	262	GLU
1	B	315	LYS
1	B	343	LEU

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Mol	Chain	Res	Type
1	C	7	LYS
1	C	78	ILE
1	C	115	VAL
1	C	149	ILE
1	C	179	VAL
1	C	209	MET
1	C	262	GLU
1	C	277	ASN
1	C	303	THR
1	C	343	LEU
1	D	65	LYS
1	D	115	VAL
1	D	179	VAL
1	D	195	ARG
1	D	252	SER
1	D	343	LEU
1	D	360[A]	SER
1	D	360[B]	SER
1	D	376	ASP
1	D	385	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	180	ASN
1	A	377	ASN
1	B	77	ASN
1	B	162	ASN
1	B	171	ASN
1	B	180	ASN
1	B	190	ASN
1	C	180	ASN
1	C	313	ASN
1	C	359	ASN
1	D	423	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	B	439	-	46,48,48	1.69	5 (10%)	64,73,73	1.64	10 (15%)
3	NAD	C	439	-	46,48,48	1.74	7 (15%)	64,73,73	1.63	9 (14%)
2	ADN	D	438	-	21,21,21	1.03	3 (14%)	31,31,31	2.10	10 (32%)
2	ADN	A	438	-	21,21,21	0.96	2 (9%)	31,31,31	2.23	10 (32%)
3	NAD	A	439	-	46,48,48	1.72	6 (13%)	64,73,73	1.68	13 (20%)
2	ADN	C	438	-	21,21,21	1.18	3 (14%)	31,31,31	2.40	11 (35%)
3	NAD	D	439	-	46,48,48	1.71	5 (10%)	64,73,73	1.70	13 (20%)
2	ADN	B	438	-	21,21,21	1.09	3 (14%)	31,31,31	2.23	11 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	B	439	-	-	8/30/62/62	0/5/5/5
3	NAD	C	439	-	-	4/30/62/62	0/5/5/5
2	ADN	D	438	-	-	0/6/22/22	0/3/3/3
2	ADN	A	438	-	-	0/6/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	439	-	-	6/30/62/62	0/5/5/5
2	ADN	C	438	-	-	1/6/22/22	0/3/3/3
3	NAD	D	439	-	-	4/30/62/62	0/5/5/5
2	ADN	B	438	-	-	0/6/22/22	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	439	NAD	O7N-C7N	8.93	1.40	1.24
3	B	439	NAD	O7N-C7N	8.60	1.40	1.24
3	A	439	NAD	O7N-C7N	8.41	1.39	1.24
3	C	439	NAD	O7N-C7N	8.29	1.39	1.24
3	C	439	NAD	C2A-N1A	3.62	1.40	1.33
2	C	438	ADN	C5-N7	-3.35	1.33	1.39
3	A	439	NAD	C2A-N1A	2.98	1.39	1.33
2	A	438	ADN	C5-N7	-2.83	1.33	1.39
3	C	439	NAD	C2A-N3A	2.77	1.38	1.33
2	D	438	ADN	C5-N7	-2.76	1.34	1.39
2	B	438	ADN	C5-N7	-2.73	1.34	1.39
3	A	439	NAD	C2A-N3A	2.70	1.38	1.33
3	B	439	NAD	C2A-N3A	2.67	1.38	1.33
3	A	439	NAD	PA-O3	2.59	1.62	1.59
3	B	439	NAD	C2A-N1A	2.58	1.38	1.33
3	D	439	NAD	C8A-N7A	2.50	1.36	1.31
3	C	439	NAD	O4D-C1D	2.48	1.44	1.40
3	D	439	NAD	C2A-N3A	2.43	1.38	1.33
2	C	438	ADN	C1'-N9	2.41	1.53	1.46
2	A	438	ADN	C4-N9	-2.38	1.32	1.37
3	D	439	NAD	C2A-N1A	2.32	1.38	1.33
3	B	439	NAD	C8A-N7A	2.29	1.36	1.31
3	A	439	NAD	C2N-N1N	2.27	1.37	1.35
3	C	439	NAD	C8A-N7A	2.21	1.35	1.31
2	C	438	ADN	C4-N9	-2.17	1.33	1.37
3	C	439	NAD	PN-O3	2.17	1.61	1.59
3	D	439	NAD	PA-O3	2.15	1.61	1.59
2	B	438	ADN	C4-N9	-2.15	1.33	1.37
2	D	438	ADN	C4-N9	-2.14	1.33	1.37
3	B	439	NAD	O4D-C1D	2.13	1.43	1.40
3	C	439	NAD	C5A-N7A	-2.11	1.35	1.39
2	B	438	ADN	C1'-N9	2.10	1.52	1.46
2	D	438	ADN	C1'-N9	2.07	1.52	1.46
3	A	439	NAD	C5A-N7A	-2.06	1.35	1.39

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	438	ADN	O4'-C1'-N9	6.39	120.37	108.09
3	D	439	NAD	N3A-C2A-N1A	-6.19	119.21	128.58
2	A	438	ADN	O4'-C1'-N9	5.79	119.21	108.09
3	A	439	NAD	N3A-C2A-N1A	-5.65	120.03	128.58
3	C	439	NAD	N3A-C2A-N1A	-5.61	120.10	128.58
3	B	439	NAD	N3A-C2A-N1A	-5.41	120.39	128.58
2	C	438	ADN	C5-C4-N3	-5.26	119.48	126.72
2	B	438	ADN	C5-C4-N3	-5.20	119.55	126.72
2	B	438	ADN	O4'-C1'-N9	5.05	117.79	108.09
2	D	438	ADN	C5-C4-N3	-4.93	119.92	126.72
2	A	438	ADN	N3-C2-N1	-4.87	121.21	128.58
2	B	438	ADN	N3-C2-N1	-4.82	121.29	128.58
3	C	439	NAD	C5A-C4A-N3A	-4.81	120.09	126.72
3	B	439	NAD	N9A-C8A-N7A	-4.69	107.28	113.94
2	A	438	ADN	C5-C4-N3	-4.65	120.31	126.72
2	C	438	ADN	C5'-C4'-C3'	-4.62	104.18	115.10
3	A	439	NAD	N9A-C8A-N7A	-4.59	107.42	113.94
2	D	438	ADN	O4'-C1'-N9	4.57	116.86	108.09
2	D	438	ADN	N3-C2-N1	-4.52	121.74	128.58
2	C	438	ADN	N3-C2-N1	-4.36	121.98	128.58
3	D	439	NAD	C5A-C4A-N3A	-4.17	120.98	126.72
3	D	439	NAD	N9A-C8A-N7A	-4.08	108.14	113.94
3	B	439	NAD	C5A-N7A-C8A	4.06	109.83	103.45
3	B	439	NAD	C5A-C4A-N3A	-4.03	121.17	126.72
3	A	439	NAD	C5A-N7A-C8A	3.95	109.66	103.45
3	A	439	NAD	C5A-C4A-N3A	-3.92	121.31	126.72
3	C	439	NAD	N9A-C8A-N7A	-3.88	108.43	113.94
3	C	439	NAD	C5A-N7A-C8A	3.79	109.41	103.45
2	B	438	ADN	C2-N3-C4	3.70	120.87	111.83
3	D	439	NAD	C2A-N3A-C4A	3.70	120.86	111.83
3	C	439	NAD	C2A-N3A-C4A	3.61	120.66	111.83
2	A	438	ADN	C2-N3-C4	3.49	120.36	111.83
3	D	439	NAD	C5A-N7A-C8A	3.48	108.92	103.45
2	C	438	ADN	C2-N3-C4	3.46	120.27	111.83
2	D	438	ADN	C2-N3-C4	3.43	120.20	111.83
3	A	439	NAD	C2A-N3A-C4A	3.38	120.10	111.83
3	B	439	NAD	C2A-N3A-C4A	3.26	119.79	111.83
3	B	439	NAD	C4A-C5A-N7A	-3.23	106.89	110.58
3	C	439	NAD	N3A-C4A-N9A	3.20	132.62	127.17
2	A	438	ADN	N3-C4-N9	3.19	132.59	127.17
2	D	438	ADN	N3-C4-N9	3.17	132.56	127.17
2	B	438	ADN	C5'-C4'-C3'	-3.16	107.64	115.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	438	ADN	N3-C4-N9	3.07	132.39	127.17
2	C	438	ADN	N3-C4-N9	2.92	132.14	127.17
2	B	438	ADN	C4-C5-N7	-2.85	107.32	110.58
3	D	439	NAD	O3D-C3D-C4D	-2.80	103.04	111.08
2	C	438	ADN	C4-C5-N7	-2.77	107.42	110.58
3	A	439	NAD	C4A-C5A-N7A	-2.76	107.42	110.58
3	C	439	NAD	C4A-C5A-N7A	-2.72	107.47	110.58
2	C	438	ADN	C4'-O4'-C1'	-2.69	103.52	109.47
3	D	439	NAD	N3A-C4A-N9A	2.65	131.67	127.17
2	A	438	ADN	C2'-C1'-N9	-2.62	106.78	113.30
3	A	439	NAD	N3A-C4A-N9A	2.61	131.61	127.17
2	A	438	ADN	N9-C8-N7	-2.59	110.26	113.94
3	B	439	NAD	O3D-C3D-C4D	-2.56	103.74	111.08
3	A	439	NAD	C4A-N9A-C8A	2.55	108.41	105.74
3	A	439	NAD	C4D-O4D-C1D	2.51	112.22	109.92
3	D	439	NAD	C4A-C5A-N7A	-2.50	107.72	110.58
2	C	438	ADN	N9-C8-N7	-2.49	110.40	113.94
2	B	438	ADN	N9-C8-N7	-2.49	110.40	113.94
2	A	438	ADN	C5'-C4'-C3'	-2.49	109.22	115.10
3	B	439	NAD	O2A-PA-O3	2.48	113.99	107.27
3	C	439	NAD	C3N-C7N-N7N	2.43	120.73	117.74
3	D	439	NAD	O2A-PA-O3	2.42	113.81	107.27
2	C	438	ADN	C5-N7-C8	2.40	107.22	103.45
2	D	438	ADN	N9-C8-N7	-2.39	110.54	113.94
2	D	438	ADN	C4-C5-N7	-2.37	107.88	110.58
2	C	438	ADN	C5-C4-N9	2.36	108.39	105.81
2	B	438	ADN	C5-N7-C8	2.36	107.15	103.45
2	D	438	ADN	C2'-C1'-N9	-2.34	107.50	113.30
3	D	439	NAD	C6N-N1N-C1D	2.31	124.26	119.73
3	A	439	NAD	O2A-PA-O3	2.31	113.50	107.27
2	D	438	ADN	C4'-O4'-C1'	-2.28	104.44	109.47
3	D	439	NAD	C2B-C3B-C4B	2.27	106.99	102.61
3	B	439	NAD	C4A-N9A-C8A	2.24	108.09	105.74
3	C	439	NAD	O3D-C3D-C4D	-2.22	104.71	111.08
3	B	439	NAD	N3A-C4A-N9A	2.20	130.91	127.17
3	D	439	NAD	C2N-N1N-C1D	-2.20	114.28	119.13
2	D	438	ADN	C5-N7-C8	2.19	106.89	103.45
3	A	439	NAD	O3D-C3D-C4D	-2.19	104.80	111.08
2	A	438	ADN	C5-N7-C8	2.18	106.87	103.45
3	A	439	NAD	C3N-C7N-N7N	2.11	120.34	117.74
3	A	439	NAD	C5A-C6A-N6A	-2.11	118.07	123.29
2	B	438	ADN	C5-C4-N9	2.06	108.06	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	438	ADN	C4'-O4'-C1'	-2.04	104.97	109.47
3	D	439	NAD	C4A-N9A-C8A	2.01	107.85	105.74
2	A	438	ADN	C4-C5-N7	-2.01	108.29	110.58

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	439	NAD	O4D-C1D-N1N-C2N
3	A	439	NAD	O4D-C1D-N1N-C6N
3	A	439	NAD	C2D-C1D-N1N-C2N
3	A	439	NAD	C2D-C1D-N1N-C6N
3	B	439	NAD	C5B-O5B-PA-O1A
3	B	439	NAD	O4D-C1D-N1N-C2N
3	B	439	NAD	O4D-C1D-N1N-C6N
3	B	439	NAD	C2D-C1D-N1N-C2N
3	B	439	NAD	C2D-C1D-N1N-C6N
3	C	439	NAD	O4D-C1D-N1N-C2N
3	C	439	NAD	O4D-C1D-N1N-C6N
3	C	439	NAD	C2D-C1D-N1N-C2N
3	C	439	NAD	C2D-C1D-N1N-C6N
3	D	439	NAD	O4D-C1D-N1N-C2N
3	D	439	NAD	O4D-C1D-N1N-C6N
3	D	439	NAD	C2D-C1D-N1N-C2N
3	D	439	NAD	C2D-C1D-N1N-C6N
3	A	439	NAD	C5B-O5B-PA-O2A
3	B	439	NAD	C5B-O5B-PA-O2A
3	A	439	NAD	O4B-C4B-C5B-O5B
3	B	439	NAD	O4B-C4B-C5B-O5B
3	B	439	NAD	C2B-C1B-N9A-C8A
2	C	438	ADN	C2'-C1'-N9-C8

There are no ring outliers.

8 monomers are involved in 10 short contacts:

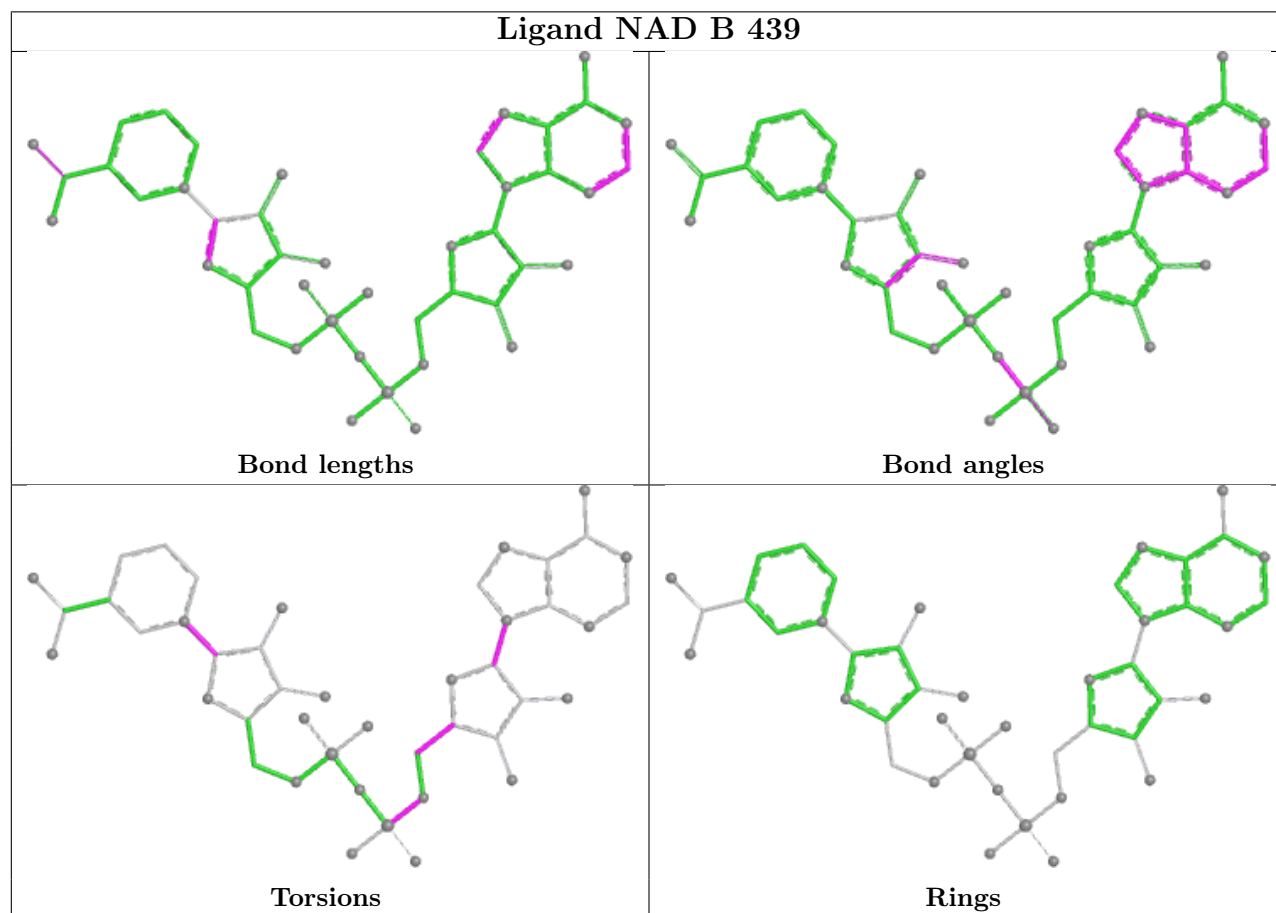
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	439	NAD	2	0
3	C	439	NAD	1	0
2	D	438	ADN	1	0
2	A	438	ADN	1	0
3	A	439	NAD	2	0

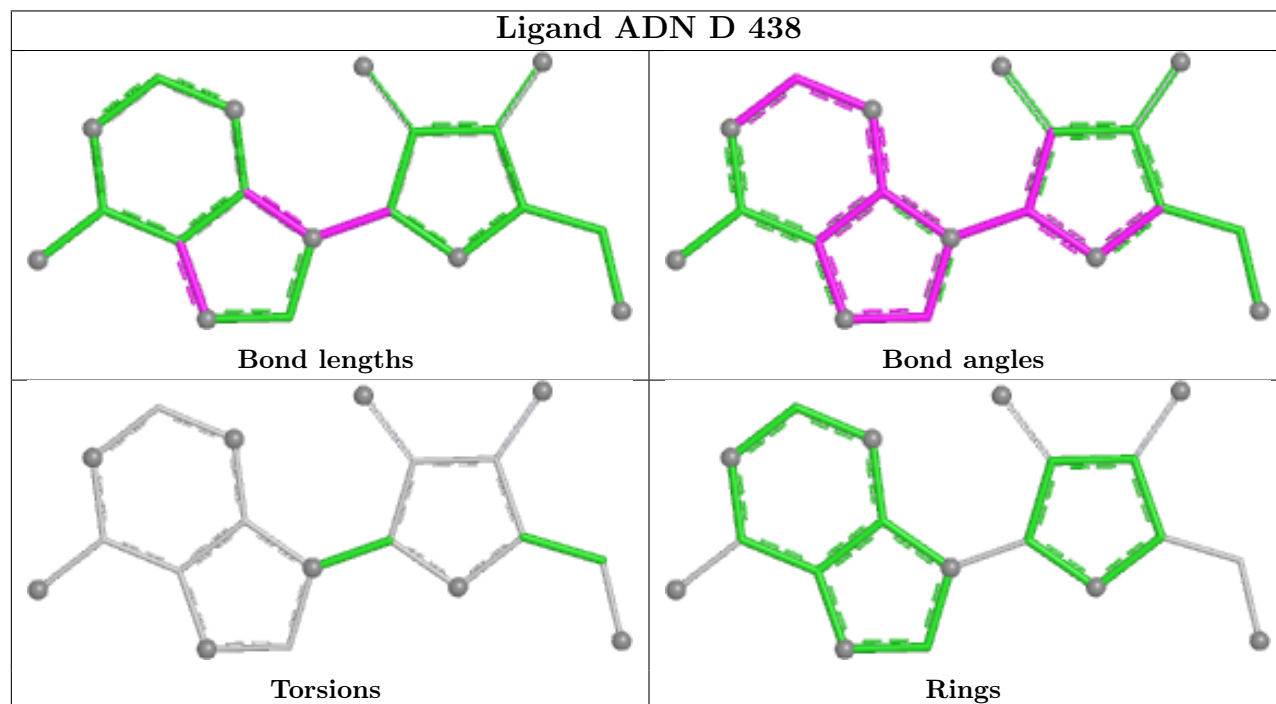
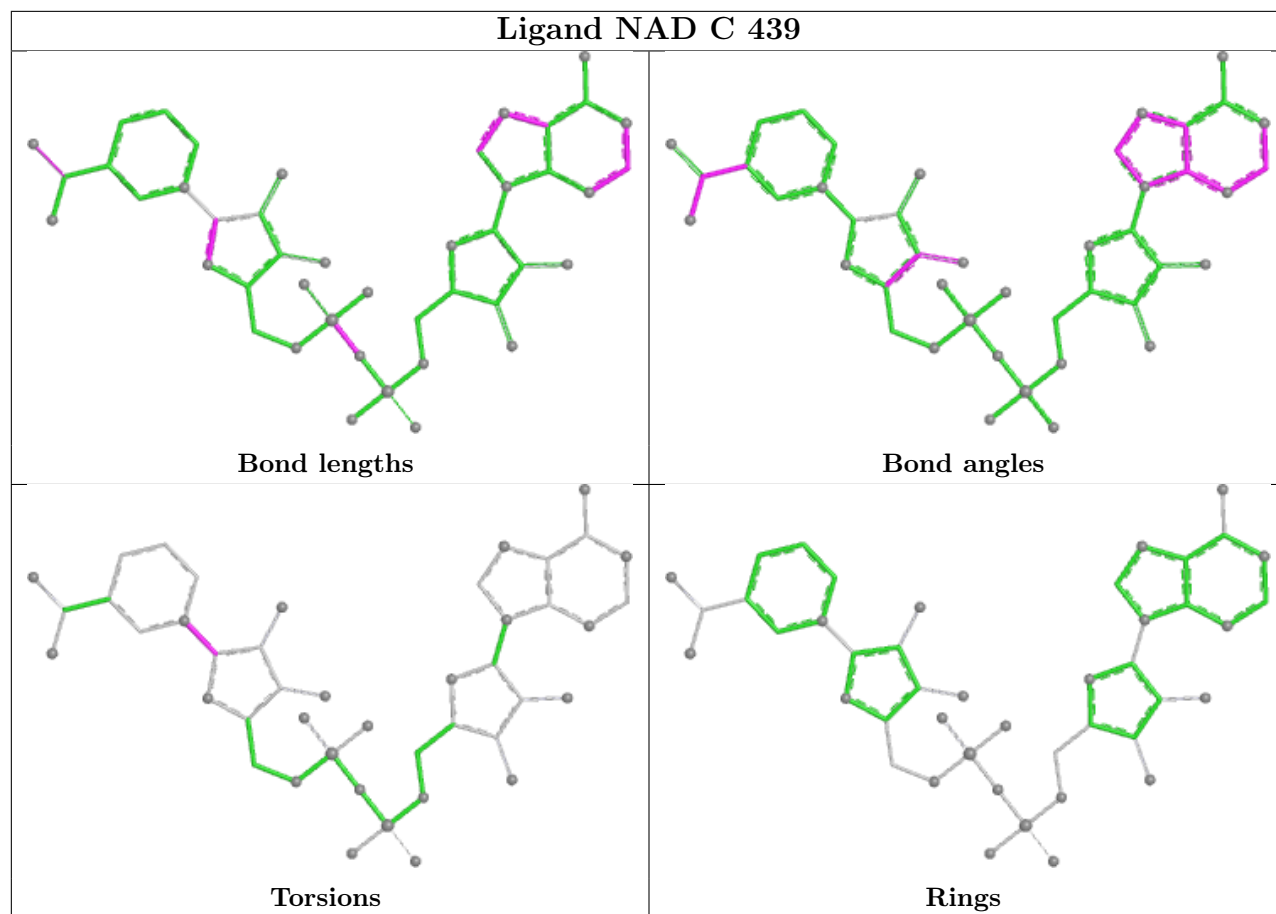
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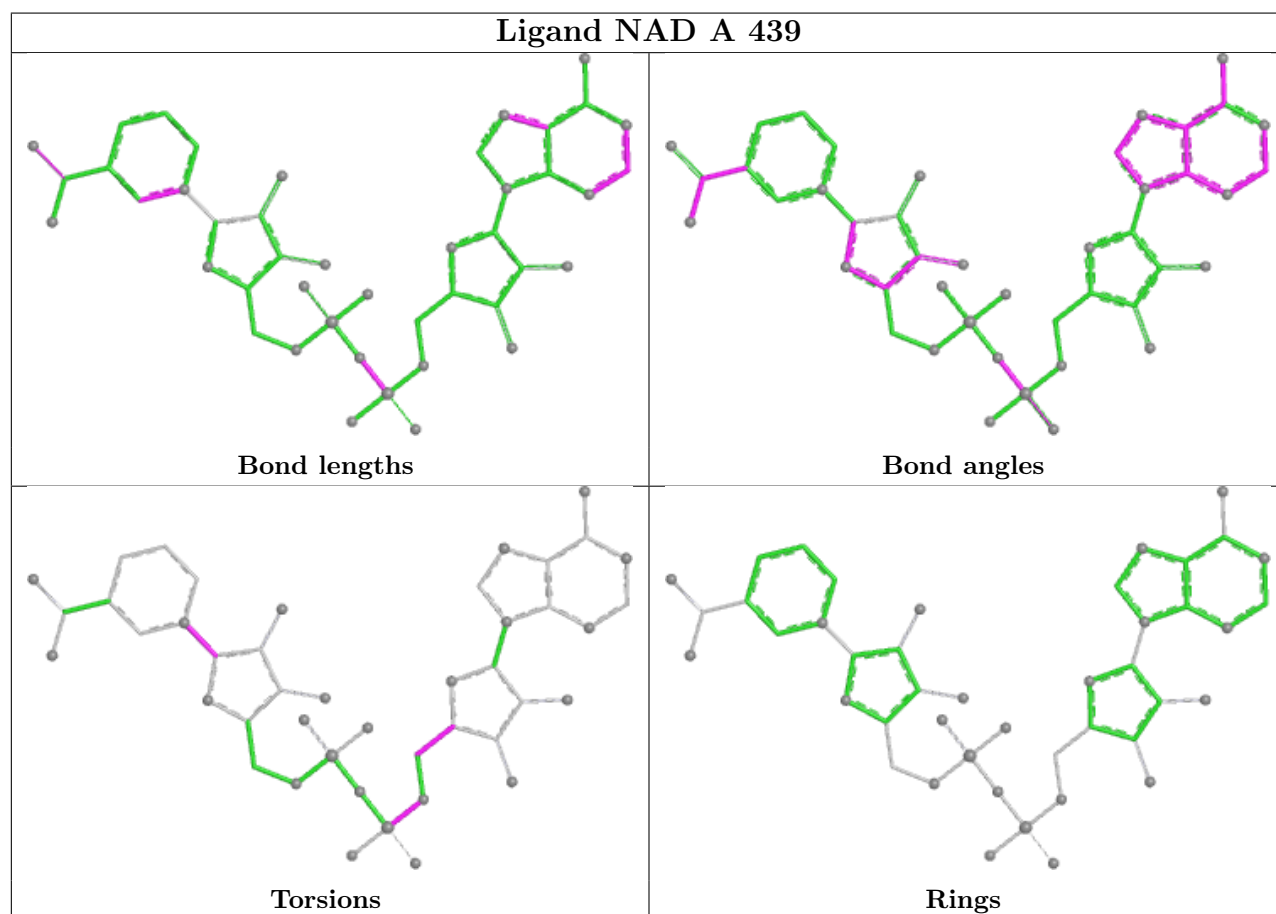
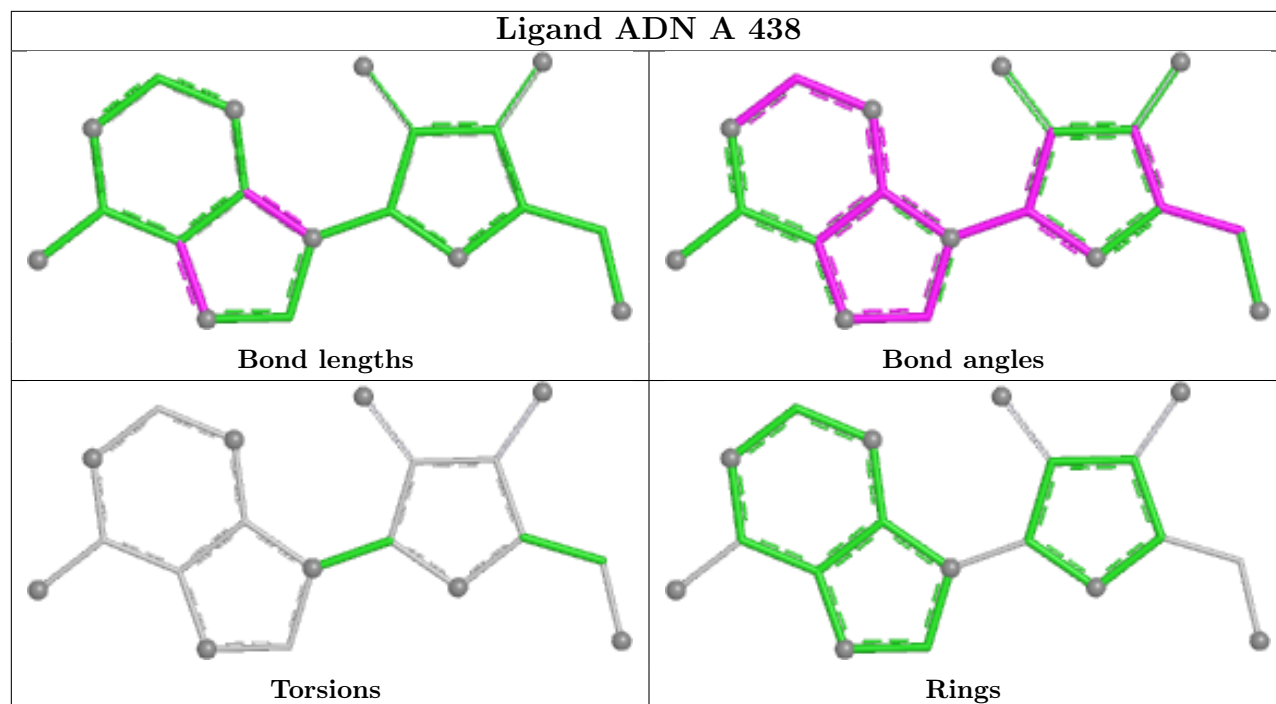
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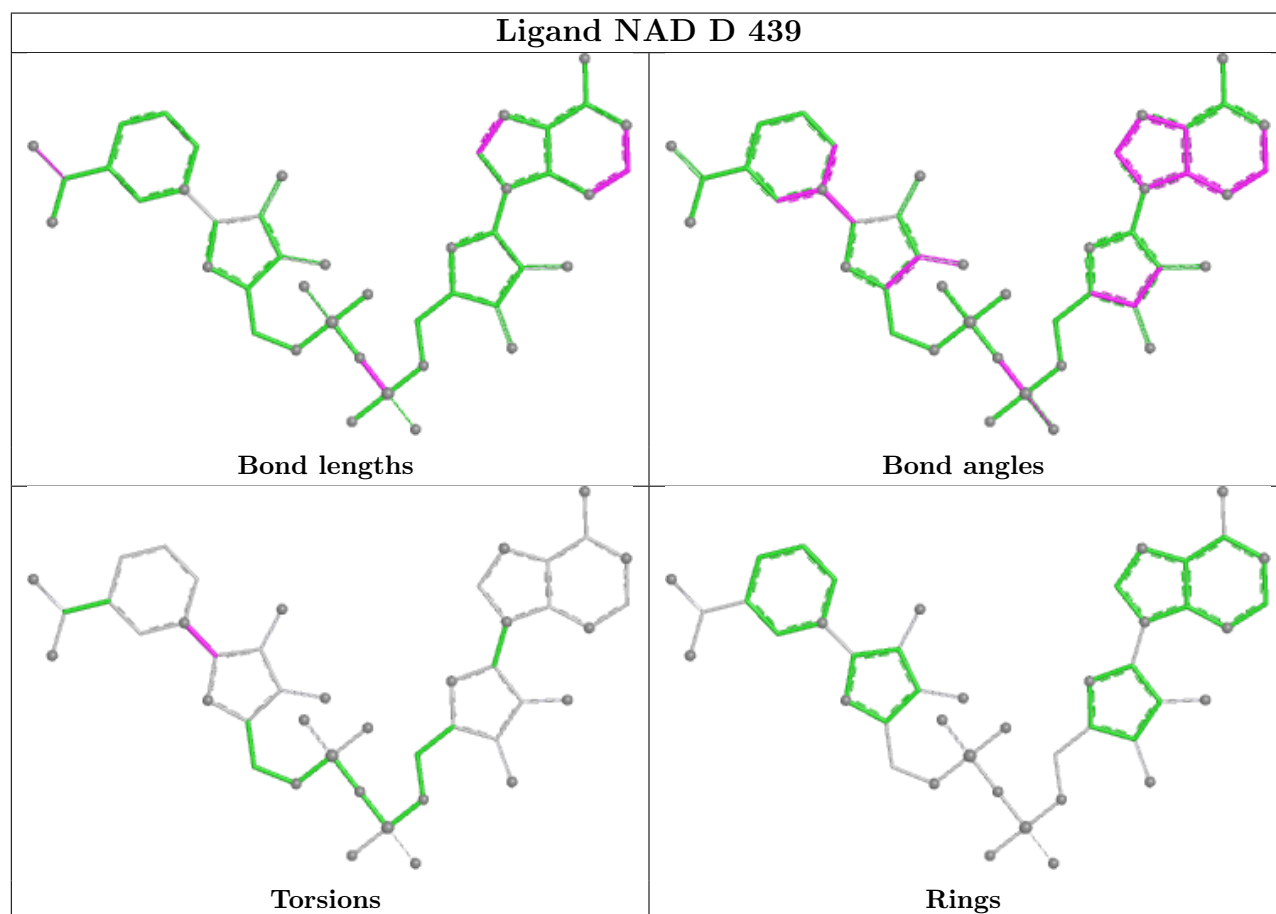
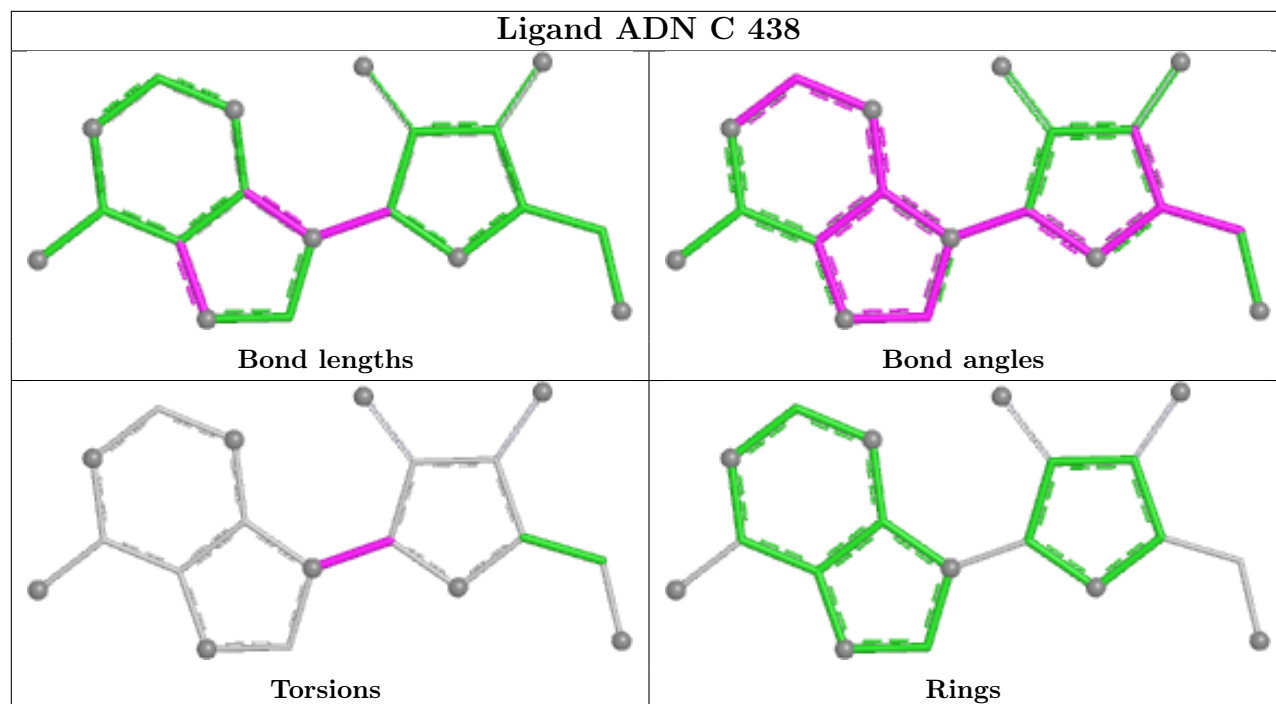
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	438	ADN	1	0
3	D	439	NAD	5	0
2	B	438	ADN	1	0

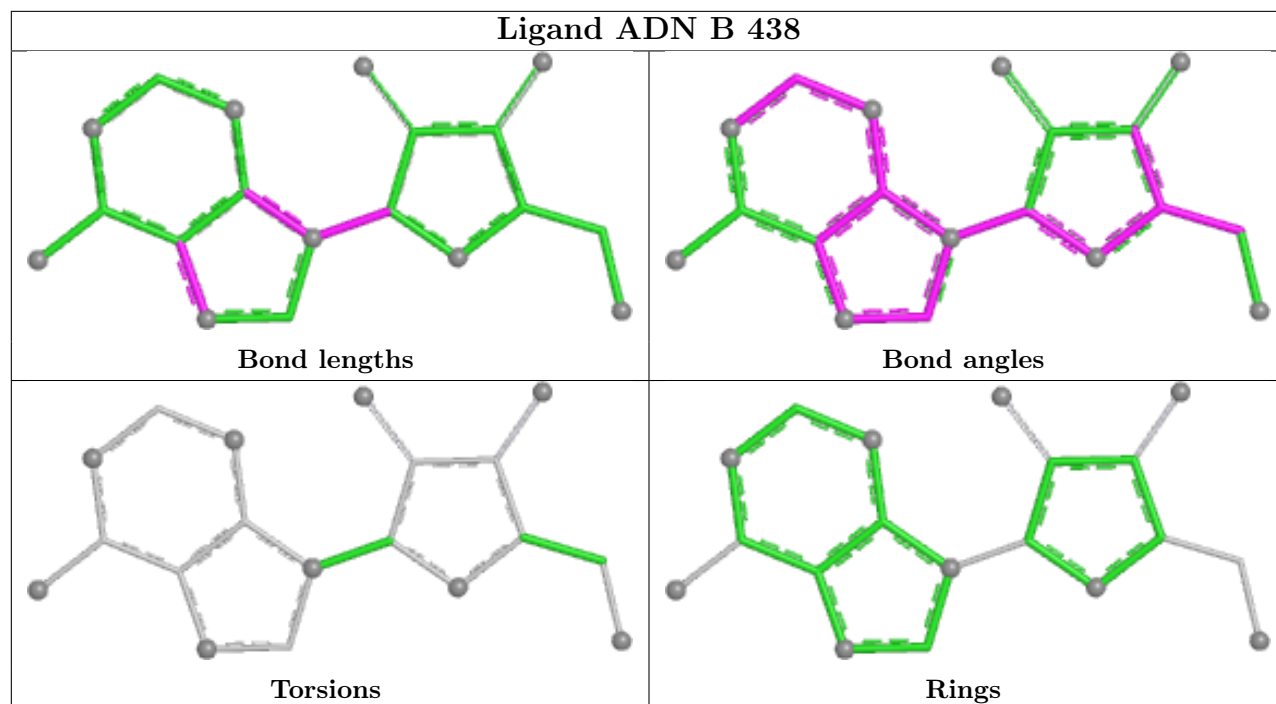
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	412/437 (94%)	-0.43	1 (0%) 91 90	15, 24, 40, 51	0
1	B	412/437 (94%)	-0.50	1 (0%) 91 90	10, 22, 38, 45	2 (0%)
1	C	424/437 (97%)	-0.28	8 (1%) 66 63	15, 26, 44, 66	1 (0%)
1	D	418/437 (95%)	-0.27	8 (1%) 66 63	9, 27, 45, 62	5 (1%)
All	All	1666/1748 (95%)	-0.37	18 (1%) 78 76	9, 25, 42, 66	8 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	421	TYR	3.8
1	D	188	PHE	3.3
1	C	189	ASP	3.2
1	C	426	VAL	3.1
1	C	425	PRO	3.1
1	D	421	TYR	3.0
1	C	185	LYS	2.9
1	D	186	SER	2.8
1	D	182	SER	2.6
1	B	188	PHE	2.6
1	C	186	SER	2.5
1	D	189	ASP	2.5
1	C	188	PHE	2.3
1	D	377	ASN	2.3
1	D	331	ASN	2.2
1	A	188	PHE	2.2
1	C	429	PRO	2.2
1	D	422	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

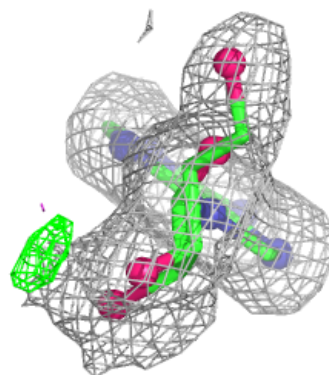
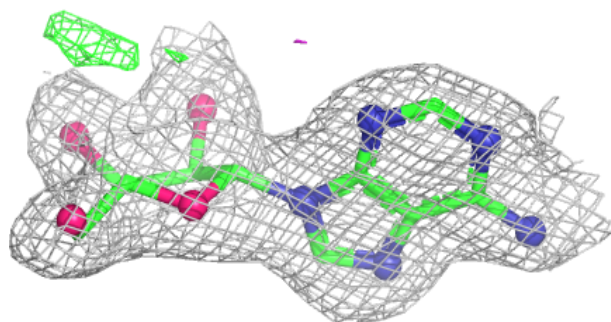
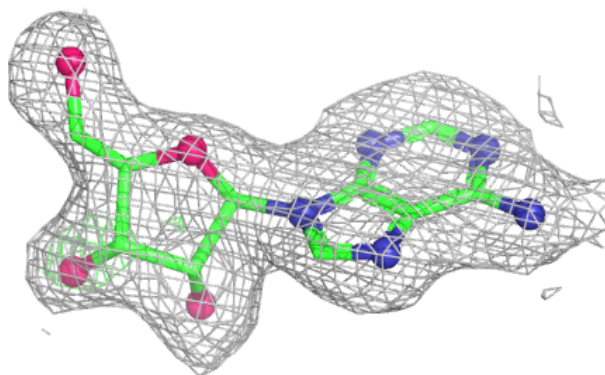
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADN	B	438	19/19	0.93	0.06	17,21,27,29	0
2	ADN	A	438	19/19	0.94	0.07	24,26,32,32	0
2	ADN	C	438	19/19	0.94	0.07	24,27,30,30	0
2	ADN	D	438	19/19	0.94	0.07	19,24,29,30	0
3	NAD	A	439	44/44	0.98	0.04	13,19,21,23	0
3	NAD	B	439	44/44	0.98	0.04	13,18,19,21	0
3	NAD	C	439	44/44	0.98	0.05	15,18,21,22	0
3	NAD	D	439	44/44	0.98	0.05	17,20,22,23	0

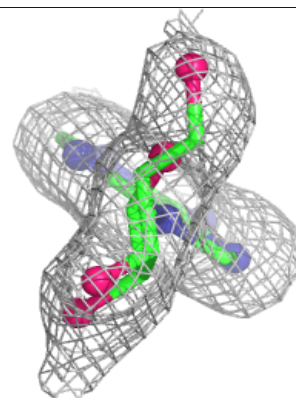
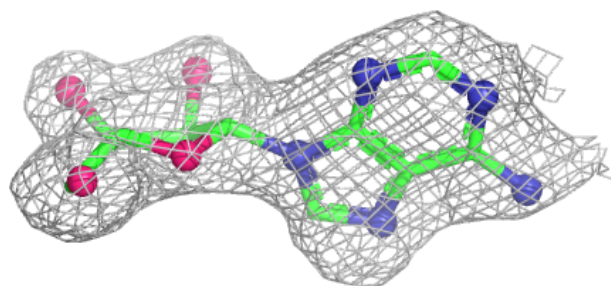
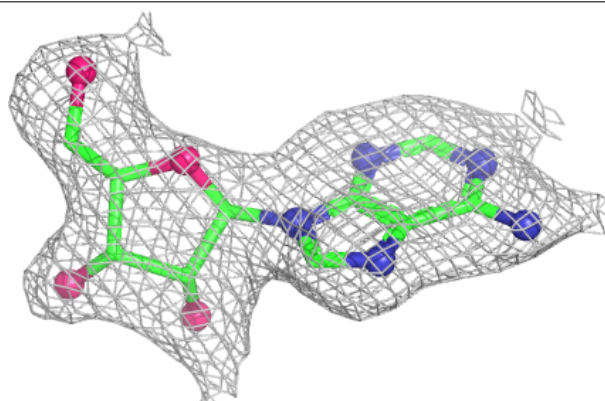
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADN B 438:

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

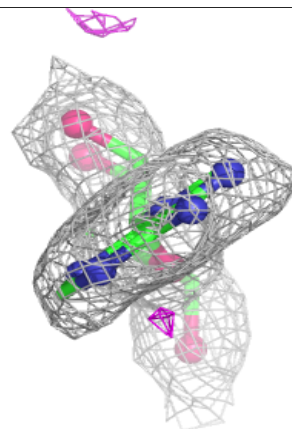
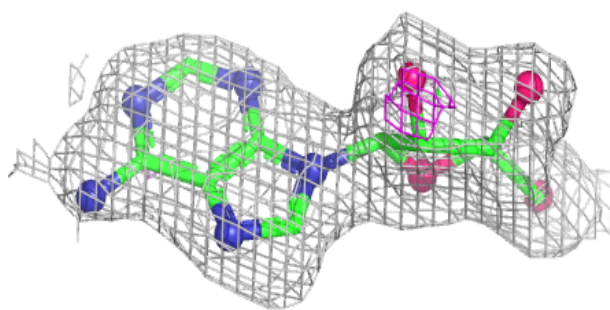
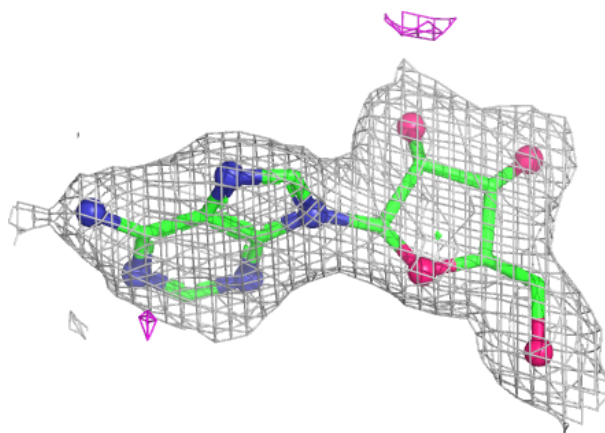
**Electron density around ADN A 438:**

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



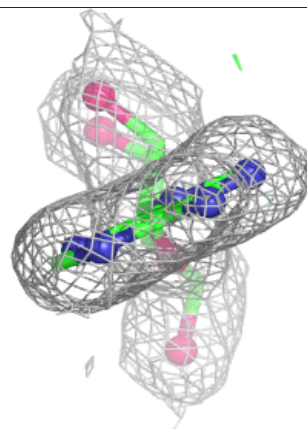
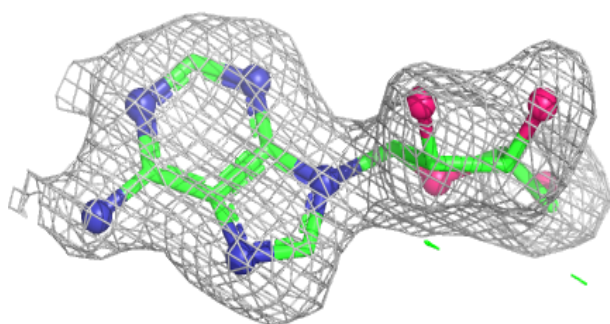
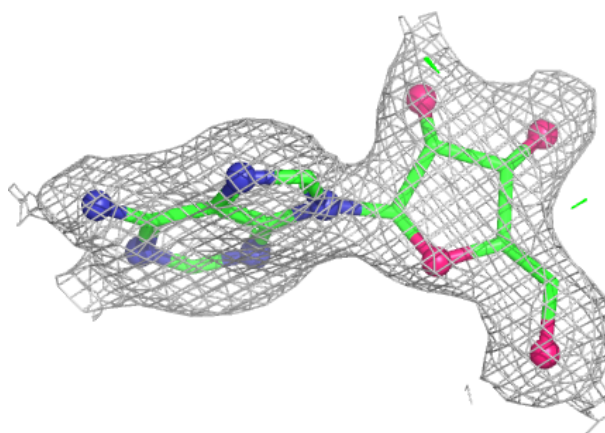
Electron density around ADN C 438:

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

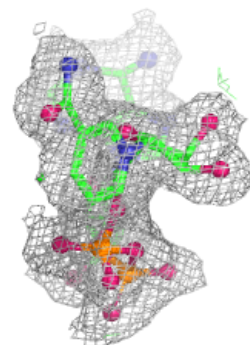
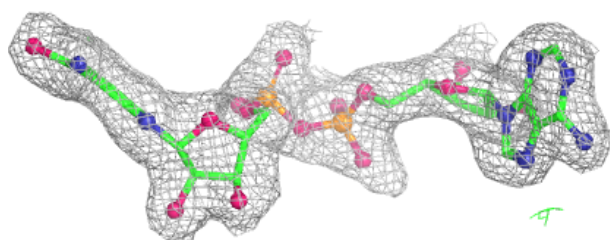
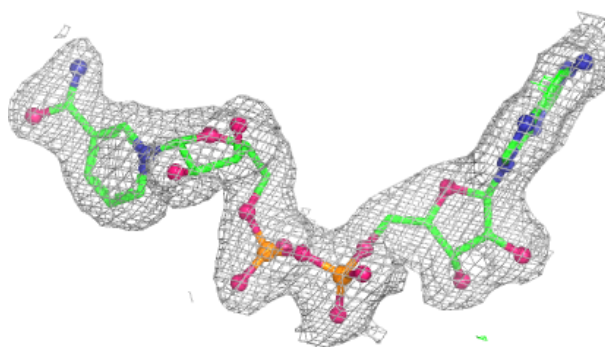


Electron density around ADN D 438:

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

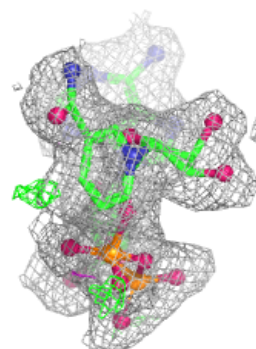
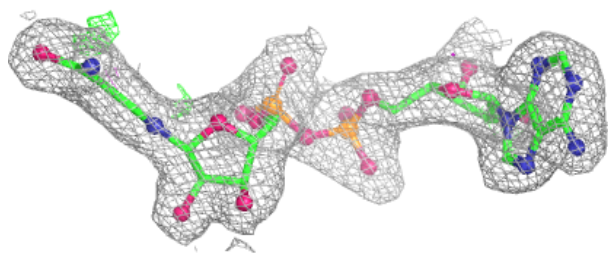
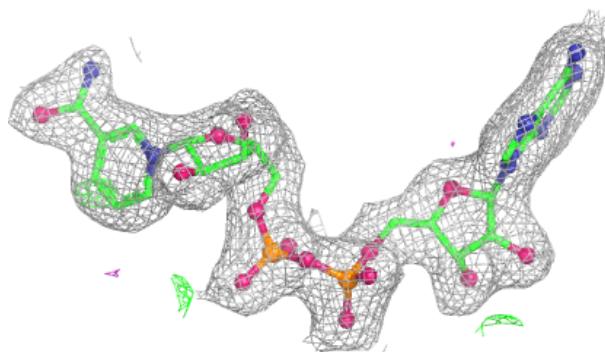
**Electron density around NAD A 439:**

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

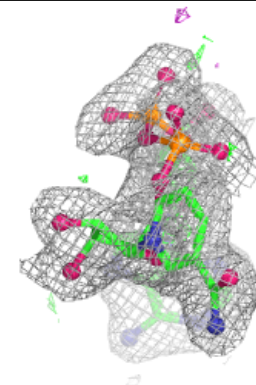
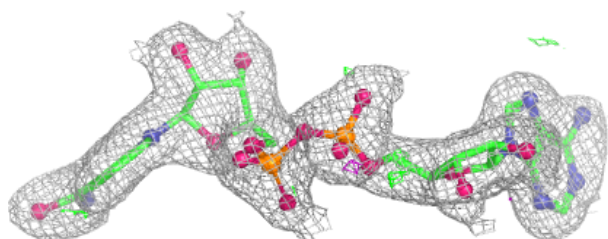
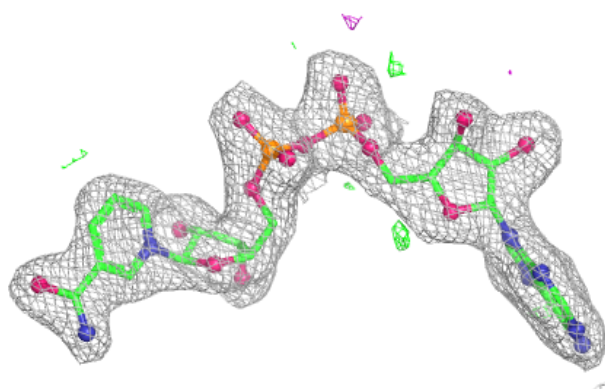


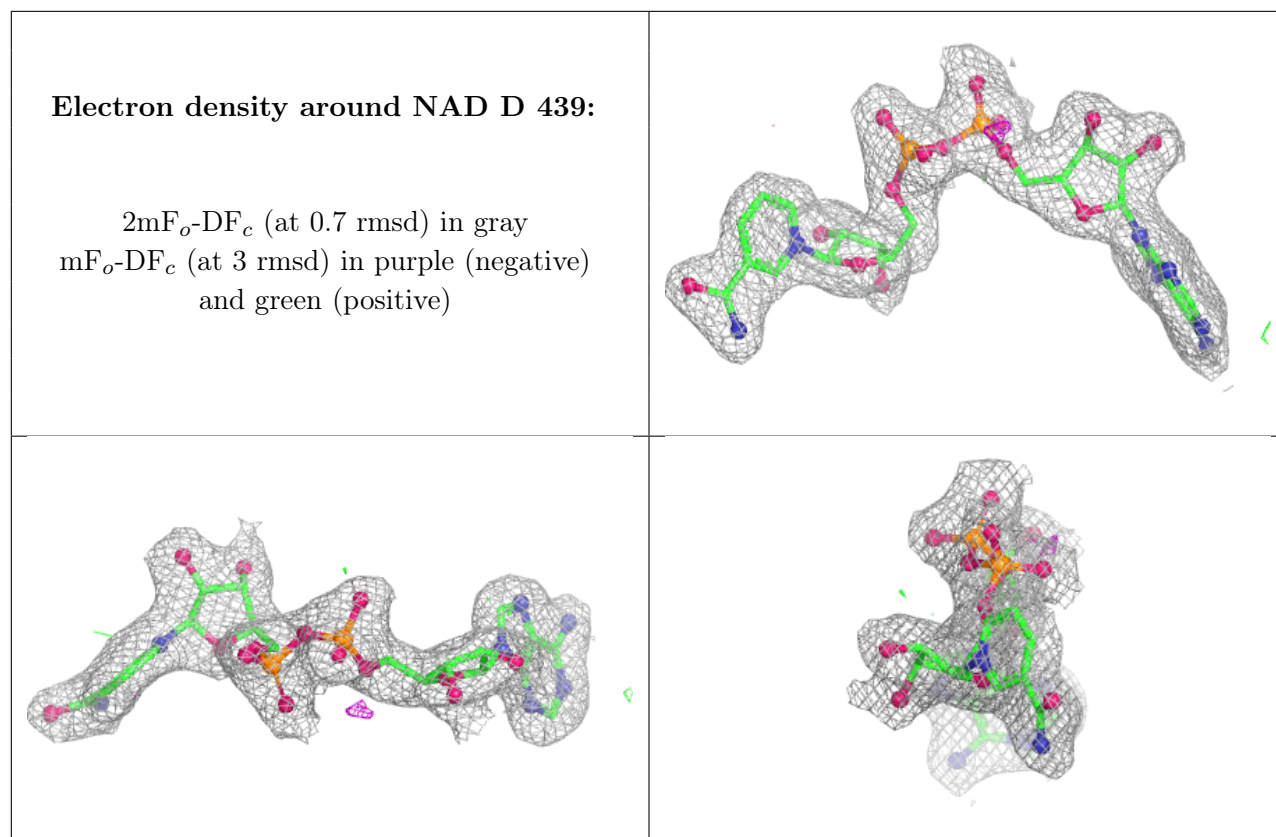
Electron density around NAD B 439:

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

**Electron density around NAD C 439:**

$2mF_o-DF_c$ (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.