



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:18 AM UTC

PDB ID : 3H9U / pdb_00003h9u
Title : S-adenosyl homocysteine hydrolase (SAHH) from Trypanosoma brucei
Authors : Siponen, M.I.; Schutz, P.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Karlberg, T.; Kragh Nielsen, T.; Kotenyova, T.; Kotzsch, A.; Moche, M.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Thorsell, A.G.; Tresaugues, L.; Van Den Berg, S.; Weigelt, J.; Welin, M.; Wisniewska, M.; Schueler, H.; Structural Genomics Consortium (SGC)
Deposited on : 2009-04-30
Resolution : 1.90 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)

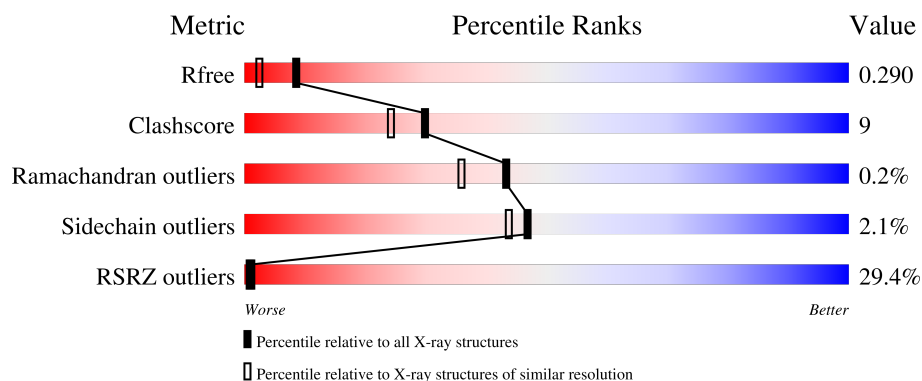
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	436	41% 80%17%..
1	B	436	61% 81%17%..

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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	436	
1	D	436	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PG4	D	1	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14413 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	430	Total	C	N	O	S	0	0	0
			3324	2098	573	628	25			
1	B	430	Total	C	N	O	S	0	0	0
			3336	2108	578	625	25			
1	C	435	Total	C	N	O	S	0	2	0
			3378	2130	584	638	26			
1	D	434	Total	C	N	O	S	0	3	0
			3381	2133	583	640	25			

There are 8 discrepancies between the modelled and reference sequences:

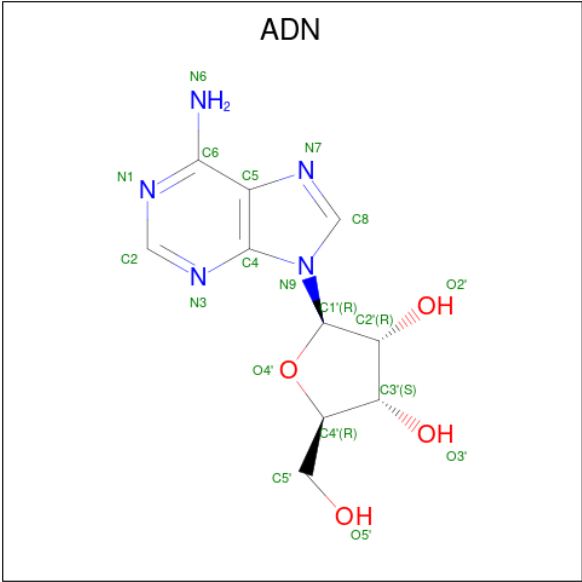
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q383X0
A	-1	MET	-	expression tag	UNP Q383X0
B	-2	SER	-	expression tag	UNP Q383X0
B	-1	MET	-	expression tag	UNP Q383X0
C	-2	SER	-	expression tag	UNP Q383X0
C	-1	MET	-	expression tag	UNP Q383X0
D	-2	SER	-	expression tag	UNP Q383X0
D	-1	MET	-	expression tag	UNP Q383X0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



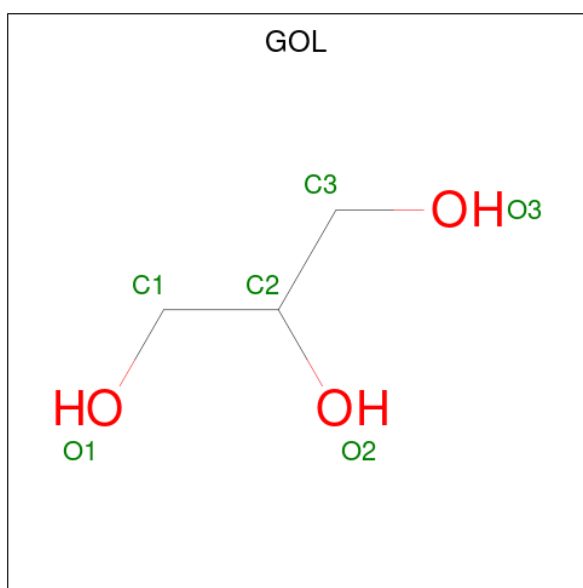
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ADENOSINE (CCD ID: ADN) (formula: C₁₀H₁₃N₅O₄).



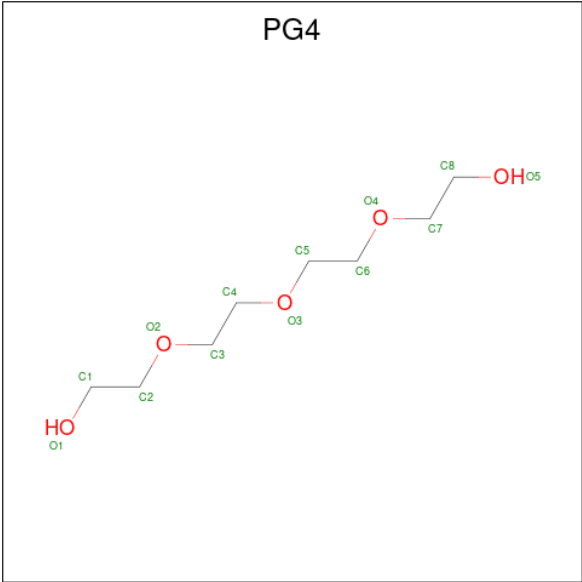
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	5	5		
3	B	1	Total	C	N	0	0
			10	5	5		
3	C	1	Total	C	N	0	0
			10	5	5		
3	D	1	Total	C	N	0	0
			10	5	5		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			13	8	5		

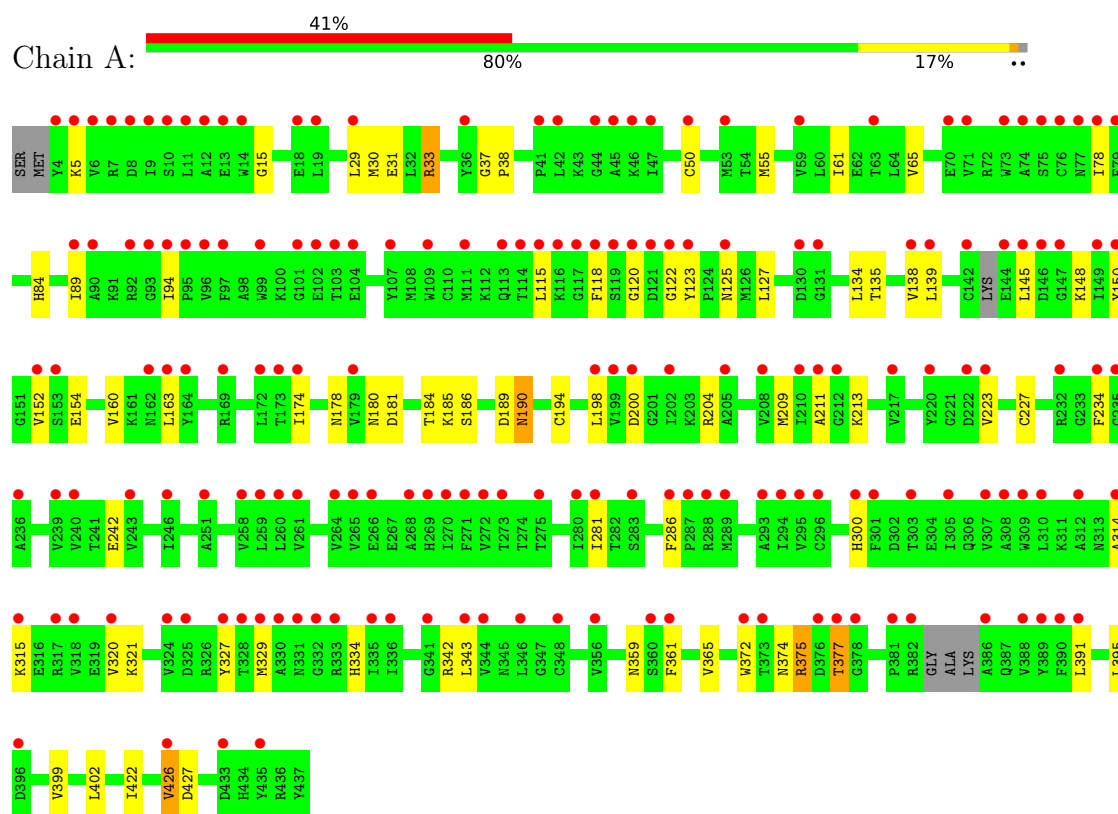
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	66	Total	O	0	0
			66	66		
6	B	70	Total	O	0	0
			70	70		
6	C	308	Total	O	0	0
			308	308		
6	D	315	Total	O	0	0
			315	315		

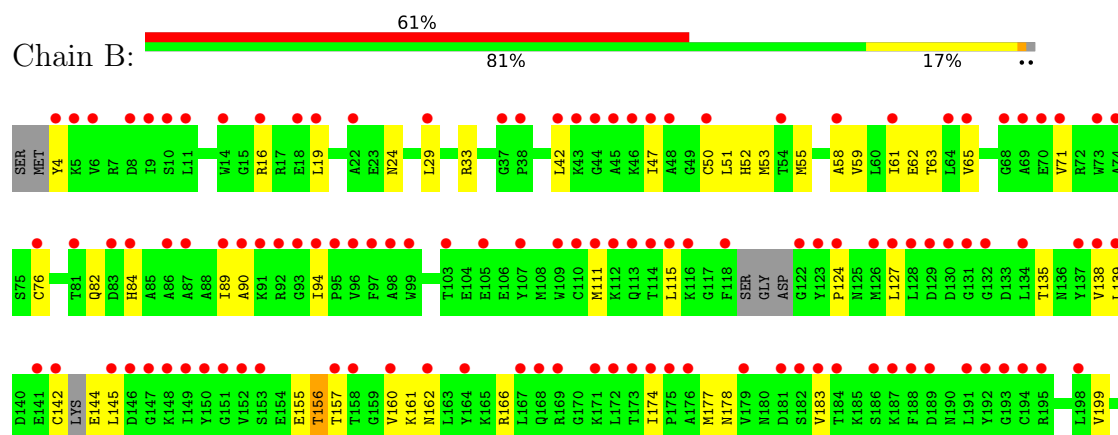
3 Residue-property plots

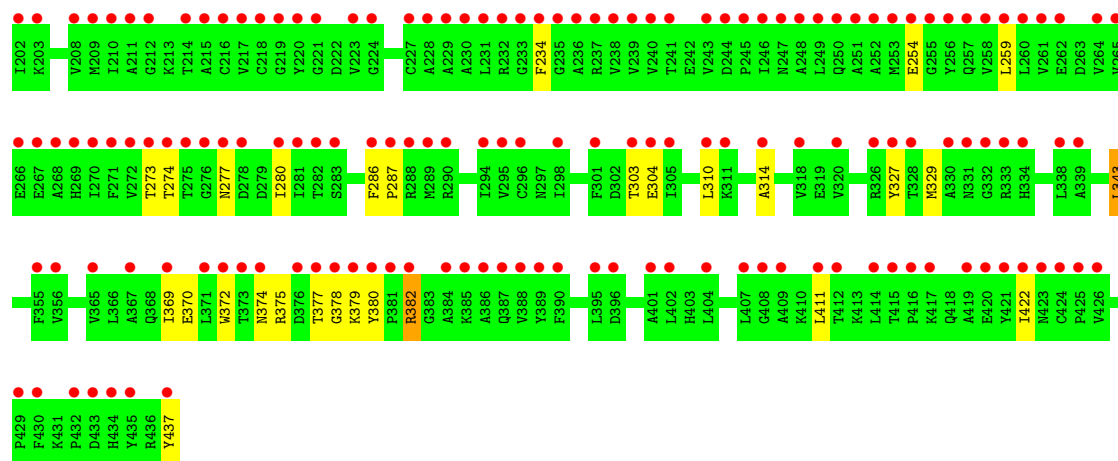
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Adenosylhomocysteinase

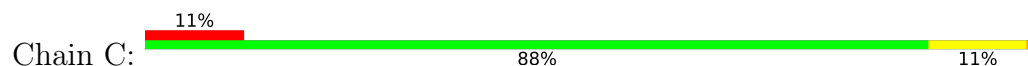


• Molecule 1: Adenosylhomocysteinase

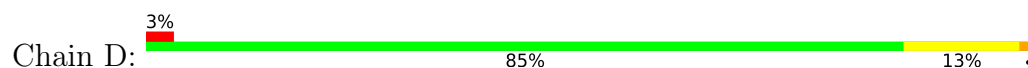




● Molecule 1: Adenosylhomocysteinase



● Molecule 1: Adenosylhomocysteinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.35Å 136.05Å 191.87Å 90.00° 99.32° 90.00°	Depositor
Resolution (Å)	45.55 – 1.90 45.55 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.55-1.90) 98.1 (45.55-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.231 (Not available) , 0.290	Depositor DCC
R_{free} test set	9087 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14413	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1036e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, ADN, PG4, GOL

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	0/3386	0.88	2/4580 (0.0%)
1	B	0.69	0/3398	0.84	2/4592 (0.0%)
1	C	1.05	1/3443 (0.0%)	1.01	4/4652 (0.1%)
1	D	1.04	2/3450 (0.1%)	0.98	1/4663 (0.0%)
All	All	0.88	3/13677 (0.0%)	0.93	9/18487 (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	C	0	1
1	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	-1	MET	C-N	16.28	1.54	1.33
1	D	-1	MET	C-N	14.69	1.52	1.33
1	D	230	ALA	CA-CB	-5.08	1.45	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-1	MET	O-C-N	-15.79	101.20	122.36
1	B	380	TYR	CA-C-N	7.89	127.95	119.90
1	B	380	TYR	C-N-CA	7.89	127.95	119.90
1	C	146	ASP	N-CA-C	7.42	120.25	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	-1	MET	O-C-N	-6.81	112.10	123.00
1	A	320	VAL	N-CA-C	-6.10	104.68	110.42
1	C	321	LYS	N-CA-C	-5.69	103.01	108.07
1	A	377	THR	N-CA-C	-5.57	107.12	114.31
1	C	-1	MET	N-CA-C	-5.09	107.62	113.88

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	-1	MET	Mainchain
1	D	-1	MET	Mainchain

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	3324	0	3286	66	0
1	B	3336	0	3321	69	0
1	C	3378	0	3358	46	0
1	D	3381	0	3359	54	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	10	0	4	0	0
3	B	10	0	4	1	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	C	6	0	8	0	0
5	D	13	0	18	7	0
6	A	66	0	0	2	0
6	B	70	0	0	1	0
6	C	308	0	0	2	0
6	D	315	0	0	6	0
All	All	14413	0	13470	231	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 9.

All (231) 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:D:281:ILE:HG22	1:D:286:PHE:HE1	1.06	1.10
1:D:299:GLY:O	1:D:343:LEU:CD1	2.05	1.05
1:D:281:ILE:HG22	1:D:286:PHE:CE1	1.97	0.99
1:C:299:GLY:O	1:C:343:LEU:CD2	2.14	0.96
1:D:299:GLY:O	1:D:343:LEU:HD11	1.66	0.95
1:B:314:ALA:HB2	1:B:329:MET:HE1	1.49	0.94
1:D:327:TYR:HB3	1:D:329:MET:HE1	1.47	0.93
1:C:327:TYR:HB3	1:C:329:MET:HE1	1.48	0.92
1:B:174:ILE:HG22	1:B:382:ARG:HH21	1.33	0.92
1:D:232:ARG:NH2	6:D:699:HOH:O	2.07	0.88
1:D:187:LYS:NZ	6:D:577:HOH:O	2.05	0.88
1:C:327:TYR:HB3	1:C:329:MET:CE	2.04	0.86
1:B:55:MET:HE1	1:B:84:HIS:CD2	2.11	0.85
1:B:273:THR:HG21	1:B:304:GLU:CB	2.06	0.85
1:B:273:THR:HG21	1:B:304:GLU:HB3	1.60	0.84
1:D:299:GLY:O	1:D:343:LEU:HD12	1.77	0.84
1:D:327:TYR:HB3	1:D:329:MET:CE	2.08	0.83
1:C:299:GLY:O	1:C:343:LEU:HD21	1.79	0.80
1:B:343:LEU:HD12	6:B:456:HOH:O	1.82	0.80
1:B:273:THR:CG2	1:B:304:GLU:OE1	2.29	0.80
1:A:395:LEU:O	1:A:399:VAL:HG23	1.82	0.80
1:C:299:GLY:O	1:C:343:LEU:HD23	1.84	0.77
1:B:55:MET:CE	1:B:84:HIS:CD2	2.68	0.76
1:A:185:LYS:NZ	1:A:190:ASN:HD21	1.85	0.75
1:B:377:THR:HG23	1:B:379:LYS:H	1.53	0.74
1:D:120:GLY:O	1:D:121:ASP:HB3	1.88	0.74
1:A:300:HIS:O	1:A:343:LEU:HD11	1.89	0.73
1:B:374:ASN:O	1:B:377:THR:CG2	2.37	0.72
1:B:314:ALA:CB	1:B:329:MET:HE1	2.19	0.71
1:A:281:ILE:HG22	1:A:286:PHE:CE1	2.27	0.70
1:D:112:LYS:NZ	1:D:137:TYR:OH	2.26	0.68
1:A:185:LYS:HZ2	1:A:190:ASN:HD21	1.41	0.68
1:C:199:VAL:HG11	1:C:234:PHE:HE2	1.59	0.67
1:A:361:PHE:O	1:A:365:VAL:HG23	1.94	0.67
1:B:286:PHE:CD1	1:B:310:LEU:HD13	2.30	0.67
1:C:327:TYR:CB	1:C:329:MET:CE	2.73	0.66
1:B:374:ASN:O	1:B:377:THR:HG21	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:GLN:HG3	6:C:657:HOH:O	1.95	0.65
1:B:47:ILE:HB	1:B:71:VAL:HG12	1.78	0.65
1:B:29:LEU:HD13	1:B:59:VAL:HG12	1.78	0.65
1:A:61:ILE:HG22	1:A:94:ILE:HD13	1.78	0.65
1:C:300:HIS:HA	1:C:343:LEU:HD21	1.78	0.64
1:D:190:ASN:HD22	1:D:190:ASN:N	1.96	0.64
1:D:300:HIS:HA	1:D:343:LEU:HD11	1.78	0.63
1:B:16:ARG:NH1	1:B:19:LEU:HD23	2.13	0.63
1:D:328:THR:C	1:D:329:MET:HE2	2.22	0.63
1:B:138:VAL:HG13	1:B:145:LEU:HD12	1.81	0.62
1:C:33:ARG:HD2	1:C:63:THR:OG1	1.99	0.62
1:B:183:VAL:HG21	1:B:437:TYR:CE2	2.34	0.62
1:A:150:TYR:CD1	1:A:375:ARG:HG2	2.35	0.62
1:A:314:ALA:HB2	1:A:329:MET:HE1	1.82	0.62
1:B:42:LEU:HD21	1:B:369:ILE:HA	1.82	0.61
1:D:185:LYS:NZ	1:D:190:ASN:HD21	1.98	0.61
1:C:327:TYR:CB	1:C:329:MET:HE1	2.28	0.61
1:C:161:LYS:HD2	1:D:422:ILE:HA	1.83	0.60
1:C:142[A]:CYS:C	1:C:144:GLU:HG2	2.27	0.60
1:C:199:VAL:HG11	1:C:234:PHE:CE2	2.36	0.60
1:C:190:ASN:N	1:C:190:ASN:HD22	2.00	0.59
1:B:374:ASN:O	1:B:377:THR:HG22	2.00	0.59
1:C:185:LYS:HZ2	1:C:190:ASN:HD21	1.49	0.59
1:A:15:GLY:HA2	1:A:55:MET:HE1	1.84	0.59
1:B:273:THR:HG21	1:B:304:GLU:HB2	1.82	0.58
1:C:183:VAL:HG21	1:C:437:TYR:CE2	2.38	0.58
1:A:242:GLU:O	1:B:411:LEU:HD12	2.02	0.58
1:A:329:MET:HA	1:A:329:MET:HE2	1.85	0.58
1:C:436:ARG:CZ	1:D:183:VAL:HG22	2.34	0.58
1:C:142[B]:CYS:C	1:C:144:GLU:OE1	2.47	0.57
1:B:53:MET:HA	1:B:53:MET:HE3	1.84	0.57
1:D:183:VAL:HG21	1:D:437:TYR:CE2	2.40	0.57
1:A:125:ASN:HA	1:A:148:LYS:O	2.03	0.57
1:B:33:ARG:HD2	1:B:63:THR:OG1	2.05	0.57
1:B:273:THR:HG22	1:B:304:GLU:OE1	2.03	0.57
1:A:300:HIS:O	1:A:343:LEU:CD1	2.53	0.56
1:C:422:ILE:HA	1:D:161:LYS:HD2	1.85	0.56
1:A:372:TRP:CZ2	1:A:375:ARG:NH1	2.73	0.56
1:C:185:LYS:NZ	1:C:190:ASN:HD21	2.03	0.56
1:C:250:GLN:O	1:C:254:GLU:HG2	2.05	0.56
1:D:372:TRP:CZ2	1:D:375:ARG:NH1	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ASN:HB3	1:A:377:THR:CG2	2.37	0.55
1:C:183:VAL:HG22	1:D:436:ARG:CZ	2.36	0.55
1:D:401:ALA:HB2	5:D:1:PG4:H22	1.87	0.55
1:B:377:THR:HG23	1:B:378:GLY:N	2.20	0.55
1:B:50:CYS:SG	1:B:111:MET:HE2	2.47	0.54
1:B:199:VAL:HG11	1:B:234:PHE:CE2	2.42	0.54
1:B:259:LEU:HD12	1:B:259:LEU:C	2.33	0.54
1:B:277:ASN:HB3	1:B:280:ILE:HD11	1.90	0.53
1:C:155:GLU:HG2	1:C:364:GLN:HE21	1.73	0.53
1:B:55:MET:CE	1:B:84:HIS:NE2	2.71	0.53
1:A:127:LEU:HB2	1:A:152:VAL:HG23	1.89	0.53
1:D:142:CYS:C	1:D:144:GLU:HA	2.33	0.53
1:A:31:GLU:HG2	1:A:402:LEU:HD22	1.90	0.53
1:A:50:CYS:HB2	1:A:134:LEU:HD22	1.91	0.52
1:C:138:VAL:HA	1:C:142[A]:CYS:SG	2.50	0.52
1:B:286:PHE:HB2	1:B:287:PRO:HD3	1.91	0.52
1:A:198:LEU:HD22	1:A:227:CYS:HB3	1.91	0.52
1:D:327:TYR:CB	1:D:329:MET:CE	2.85	0.52
1:B:377:THR:HG23	1:B:379:LYS:N	2.22	0.52
1:D:186[A]:SER:OG	1:D:222:ASP:OD2	2.27	0.52
1:D:190:ASN:HD22	1:D:190:ASN:H	1.57	0.52
1:A:135:THR:O	1:A:139:LEU:HD13	2.09	0.51
1:B:135:THR:O	1:B:139:LEU:HD13	2.10	0.51
1:A:190:ASN:N	1:A:190:ASN:HD22	2.09	0.51
1:B:382:ARG:CZ	1:B:382:ARG:HB3	2.40	0.51
5:D:1:PG4:H12	6:D:672:HOH:O	2.09	0.51
1:D:120:GLY:O	1:D:121:ASP:CB	2.56	0.51
1:A:213:LYS:HE3	6:A:746:HOH:O	2.10	0.50
1:A:374:ASN:HB3	1:A:377:THR:HG21	1.92	0.50
1:D:392:PRO:HD2	1:D:395:LEU:HD12	1.94	0.50
1:A:150:TYR:CE1	1:A:375:ARG:HG2	2.45	0.50
1:B:51:LEU:HD11	1:B:155:GLU:OE1	2.11	0.50
1:D:33:ARG:HD2	1:D:63:THR:OG1	2.10	0.50
1:B:422:ILE:HG22	1:B:422:ILE:O	2.12	0.50
1:A:211:ALA:HB2	1:A:234:PHE:O	2.12	0.50
1:B:314:ALA:CB	1:B:329:MET:CE	2.87	0.50
1:D:168:GLN:OE1	6:D:469:HOH:O	2.20	0.50
1:A:139:LEU:HD11	1:A:174:ILE:CD1	2.42	0.49
1:A:200:ASP:OD1	1:A:204:ARG:NE	2.46	0.49
1:D:249:LEU:O	1:D:253:MET:HG2	2.13	0.49
1:A:138:VAL:HG13	1:A:145:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142[B]:CYS:C	1:C:144:GLU:HG2	2.37	0.49
1:A:135:THR:HG22	1:A:139:LEU:HD22	1.95	0.49
1:B:115:LEU:HD23	1:B:124:PRO:HG3	1.95	0.49
1:C:137:TYR:CE2	1:C:142[B]:CYS:SG	3.05	0.49
1:A:327:TYR:HB3	1:A:329:MET:HE3	1.93	0.49
1:B:52:HIS:CE1	1:B:76:CYS:SG	3.05	0.49
1:B:374:ASN:HB3	1:B:377:THR:HG21	1.95	0.49
1:A:123:TYR:HB3	1:A:145:LEU:HD22	1.95	0.48
1:B:82:GLN:HB3	1:B:84:HIS:CE1	2.48	0.48
1:C:413:LYS:HE3	1:C:426:VAL:CG1	2.43	0.48
1:A:55:MET:HE2	1:A:84:HIS:CE1	2.49	0.48
1:D:118:PHE:O	1:D:122:GLY:HA2	2.14	0.48
1:B:273:THR:HG23	1:B:304:GLU:OE1	2.09	0.48
1:A:115:LEU:HD21	1:A:134:LEU:HD11	1.95	0.48
1:D:250:GLN:O	1:D:254:GLU:HG2	2.13	0.48
1:A:314:ALA:CB	1:A:329:MET:HE1	2.43	0.48
1:D:213:LYS:HD3	1:D:269:HIS:CB	2.43	0.48
1:C:65:VAL:HG11	1:C:92:ARG:NH2	2.29	0.47
1:D:401:ALA:HB1	5:D:1:PG4:H62	1.95	0.47
1:A:372:TRP:CH2	1:A:375:ARG:NH1	2.83	0.47
1:A:422:ILE:HA	1:B:161:LYS:HD2	1.95	0.47
1:B:177:MET:HE1	1:B:370:GLU:HG2	1.97	0.47
1:C:123:TYR:CD2	1:C:148:LYS:HD3	2.50	0.47
1:B:19:LEU:HD11	1:B:59:VAL:HG23	1.97	0.47
1:A:343:LEU:HD12	1:A:343:LEU:H	1.80	0.47
1:B:273:THR:CG2	1:B:304:GLU:HB3	2.38	0.47
1:D:213:LYS:HD3	1:D:269:HIS:HB3	1.96	0.47
1:D:299:GLY:C	1:D:343:LEU:HD11	2.35	0.47
1:B:156:THR:O	1:B:160:VAL:HG23	2.15	0.46
1:C:190:ASN:HD22	1:C:190:ASN:H	1.62	0.46
1:B:29:LEU:CD1	1:B:59:VAL:HG12	2.42	0.46
1:C:207:ASP:O	6:C:617:HOH:O	2.20	0.46
1:C:413:LYS:HE3	1:C:426:VAL:HG12	1.96	0.46
1:A:61:ILE:CG2	1:A:94:ILE:HD13	2.43	0.46
1:A:89:ILE:HG23	1:A:94:ILE:HB	1.97	0.46
1:A:120:GLY:C	1:A:122:GLY:N	2.72	0.46
1:A:154:GLU:HG3	1:A:160:VAL:HG23	1.96	0.46
1:C:327:TYR:O	1:C:334:HIS:HA	2.15	0.46
1:A:342:ARG:O	1:A:343:LEU:C	2.57	0.46
1:D:401:ALA:CB	5:D:1:PG4:H22	2.46	0.45
1:A:204:ARG:O	1:A:321:LYS:NZ	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:VAL:HG11	1:B:178:ASN:ND2	2.31	0.45
1:D:286:PHE:N	1:D:287:PRO:CD	2.79	0.45
1:A:327:TYR:O	1:A:334:HIS:HA	2.16	0.45
1:B:33:ARG:HG3	1:B:63:THR:HG23	1.98	0.45
1:C:139:LEU:HD23	1:C:166:ARG:HD3	1.99	0.45
1:B:138:VAL:HG13	1:B:145:LEU:CD1	2.47	0.45
1:C:65:VAL:HG11	1:C:92:ARG:HH22	1.82	0.45
1:B:58:ALA:O	1:B:62:GLU:HG3	2.17	0.45
1:B:286:PHE:CE1	1:B:310:LEU:HD13	2.52	0.45
1:A:426:VAL:HG12	1:A:427:ASP:OD1	2.17	0.44
1:B:127:LEU:HD21	1:B:138:VAL:HG21	1.99	0.44
1:C:249:LEU:O	1:C:253:MET:HG2	2.16	0.44
1:D:397:GLU:OE1	1:D:429:PRO:HA	2.17	0.44
1:A:78:ILE:HD11	1:A:342:ARG:NE	2.33	0.44
1:A:180:ASN:O	1:A:186:SER:HB3	2.18	0.44
1:C:33:ARG:HG3	1:C:63:THR:HG23	1.99	0.44
1:D:185:LYS:HZ2	1:D:190:ASN:HD21	1.63	0.44
1:A:61:ILE:O	1:A:65:VAL:HG23	2.18	0.44
1:B:329:MET:HE2	1:B:329:MET:HA	1.99	0.44
1:B:61:ILE:O	1:B:65:VAL:HG23	2.18	0.44
1:B:139:LEU:HD23	1:B:166:ARG:HH21	1.83	0.44
1:C:299:GLY:C	1:C:343:LEU:HD21	2.42	0.44
1:A:186:SER:O	1:A:190:ASN:HB2	2.18	0.44
1:A:139:LEU:HD11	1:A:174:ILE:HD11	1.99	0.44
1:B:142:CYS:C	1:B:144:GLU:HA	2.43	0.43
2:B:1:NAD:O7N	3:B:438:ADN:H8	2.18	0.43
1:C:145:LEU:HA	1:C:148:LYS:HD2	2.00	0.43
1:C:277:ASN:HD21	1:D:418:GLN:HB3	1.82	0.43
1:A:154:GLU:HB2	1:A:163:LEU:HD11	2.00	0.43
1:B:4:TYR:CD1	1:B:90:ALA:HB1	2.53	0.43
1:A:30:MET:HE1	1:A:33:ARG:NH2	2.34	0.43
1:B:89:ILE:HG23	1:B:94:ILE:HB	1.99	0.43
1:D:327:TYR:O	1:D:334:HIS:HA	2.18	0.43
1:B:377:THR:CG2	1:B:378:GLY:N	2.80	0.43
1:D:343:LEU:HD13	6:D:476:HOH:O	2.17	0.43
1:D:300:HIS:CA	1:D:343:LEU:HD11	2.45	0.43
1:C:413:LYS:NZ	1:C:427:ASP:OD1	2.41	0.43
1:A:194:CYS:SG	1:A:223:VAL:HG13	2.59	0.42
1:D:160:VAL:HG11	1:D:178:ASN:ND2	2.34	0.42
1:A:184:THR:O	1:A:359:ASN:HB3	2.20	0.42
1:A:138:VAL:HG12	1:A:139:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:ALA:HB2	1:D:329:MET:HE1	2.01	0.42
1:A:15:GLY:CA	1:A:55:MET:HE1	2.47	0.42
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.94	0.42
1:B:51:LEU:HD23	1:B:52:HIS:N	2.35	0.42
1:C:142[A]:CYS:C	1:C:144:GLU:CG	2.92	0.42
1:D:377:THR:CG2	1:D:379:LYS:H	2.33	0.42
1:B:16:ARG:CZ	1:B:19:LEU:HD23	2.50	0.42
1:B:53:MET:HE3	1:B:53:MET:CA	2.50	0.42
1:D:404:LEU:HB2	5:D:1:PG4:H71	2.01	0.42
1:D:184:THR:HA	1:D:188:PHE:CD2	2.55	0.41
1:A:329:MET:HE2	1:A:329:MET:CA	2.49	0.41
1:D:90:ALA:HB2	1:D:96:VAL:CG1	2.50	0.41
1:A:55:MET:CE	1:A:84:HIS:CD2	3.04	0.41
1:B:55:MET:O	1:B:58:ALA:HB3	2.20	0.41
1:D:404:LEU:HB2	5:D:1:PG4:C7	2.51	0.41
1:A:178:ASN:ND2	1:A:181:ASP:HB2	2.36	0.41
1:C:286:PHE:N	1:C:287:PRO:CD	2.83	0.41
5:D:1:PG4:H72	6:D:558:HOH:O	2.21	0.41
1:A:327:TYR:HB3	1:A:329:MET:CE	2.50	0.41
1:A:5:LYS:HA	6:A:583:HOH:O	2.20	0.41
1:A:118:PHE:HB2	1:A:122:GLY:O	2.21	0.41
1:D:150:TYR:HA	1:D:382:ARG:HD2	2.02	0.41
1:C:328:THR:C	1:C:329:MET:HE2	2.46	0.40
1:A:189:ASP:OD2	1:A:189:ASP:C	2.65	0.40
1:C:397:GLU:OE1	1:C:429:PRO:HA	2.22	0.40
1:B:42:LEU:HA	1:B:372:TRP:CD1	2.55	0.40
1:A:37:GLY:N	1:A:38:PRO:CD	2.85	0.40
1:B:254:GLU:HA	1:B:254:GLU:OE1	2.22	0.40
1:B:327:TYR:HB3	1:B:329:MET:HE3	2.03	0.40
1:D:180:ASN:HA	1:D:185:LYS:HD2	2.03	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	424/436 (97%)	407 (96%)	17 (4%)	0	100	100
1	B	424/436 (97%)	406 (96%)	17 (4%)	1 (0%)	43	36
1	C	432/436 (99%)	424 (98%)	7 (2%)	1 (0%)	43	36
1	D	433/436 (99%)	423 (98%)	8 (2%)	2 (0%)	24	16
All	All	1713/1744 (98%)	1660 (97%)	49 (3%)	4 (0%)	43	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	121	ASP
1	C	121	ASP
1	D	120	GLY
1	B	343	LEU

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	350/359 (98%)	343 (98%)	7 (2%)	48	46
1	B	351/359 (98%)	343 (98%)	8 (2%)	44	40
1	C	357/359 (99%)	348 (98%)	9 (2%)	42	37
1	D	357/359 (99%)	351 (98%)	6 (2%)	53	52
All	All	1415/1436 (98%)	1385 (98%)	30 (2%)	47	44

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	190	ASN
1	A	209	MET
1	A	315	LYS

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Mol	Chain	Res	Type
1	A	375	ARG
1	A	391	LEU
1	A	426	VAL
1	B	24	ASN
1	B	156	THR
1	B	157	THR
1	B	162	ASN
1	B	274	THR
1	B	303	THR
1	B	375	ARG
1	B	382	ARG
1	C	121	ASP
1	C	142[A]	CYS
1	C	142[B]	CYS
1	C	156	THR
1	C	190	ASN
1	C	209	MET
1	C	387	GLN
1	C	411	LEU
1	C	420	GLU
1	D	33	ARG
1	D	156	THR
1	D	190	ASN
1	D	209	MET
1	D	343	LEU
1	D	377	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	B	277	ASN
1	B	363	ASN
1	C	113	GLN
1	C	190	ASN
1	C	387	GLN
1	C	423	ASN
1	D	113	GLN
1	D	168	GLN
1	D	190	ASN
1	D	364	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	ADN	D	438	-	11,11,21	1.03	1 (9%)	15,15,31	2.46	6 (40%)
2	NAD	A	438	-	46,48,48	1.66	4 (8%)	64,73,73	1.58	13 (20%)
3	ADN	B	438	-	11,11,21	1.02	1 (9%)	15,15,31	2.50	6 (40%)
2	NAD	C	2	-	46,48,48	1.62	6 (13%)	64,73,73	1.75	10 (15%)
3	ADN	A	439	-	11,11,21	1.31	2 (18%)	15,15,31	2.36	5 (33%)
3	ADN	C	438	-	11,11,21	1.30	1 (9%)	15,15,31	2.41	6 (40%)
4	GOL	C	1	-	5,5,5	0.20	0	5,5,5	0.81	0
2	NAD	B	1	-	46,48,48	1.61	5 (10%)	64,73,73	1.58	11 (17%)
2	NAD	D	3	-	46,48,48	1.76	7 (15%)	64,73,73	1.82	15 (23%)
5	PG4	D	1	-	12,12,12	0.66	0	11,11,11	0.56	0

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	ADN	D	438	-	-	-	0/2/2/3
2	NAD	A	438	-	-	4/30/62/62	0/5/5/5
3	ADN	B	438	-	-	-	0/2/2/3
2	NAD	C	2	-	-	4/30/62/62	0/5/5/5
3	ADN	A	439	-	-	-	0/2/2/3
4	GOL	C	1	-	-	1/4/4/4	-
3	ADN	C	438	-	-	-	0/2/2/3
2	NAD	B	1	-	-	5/30/62/62	0/5/5/5
2	NAD	D	3	-	-	5/30/62/62	0/5/5/5
5	PG4	D	1	-	-	7/10/10/10	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	438	NAD	O7N-C7N	8.53	1.40	1.24
2	B	1	NAD	O7N-C7N	8.26	1.39	1.24
2	D	3	NAD	O7N-C7N	6.75	1.36	1.24
2	C	2	NAD	O7N-C7N	6.23	1.35	1.24
2	C	2	NAD	C2A-N1A	4.43	1.41	1.33
2	D	3	NAD	C2A-N1A	4.40	1.41	1.33
2	D	3	NAD	PA-O3	-3.80	1.55	1.59
3	A	439	ADN	C5-N7	-3.50	1.32	1.39
3	C	438	ADN	C5-N7	-3.49	1.32	1.39
2	A	438	NAD	C2A-N1A	3.19	1.39	1.33
2	D	3	NAD	C5A-C4A	3.01	1.44	1.39
2	D	3	NAD	O4D-C1D	2.90	1.44	1.40
2	B	1	NAD	C2A-N1A	2.88	1.39	1.33
2	D	3	NAD	C2N-N1N	2.70	1.38	1.35
2	B	1	NAD	C8A-N7A	2.58	1.36	1.31
3	B	438	ADN	C5-N7	-2.53	1.34	1.39
2	C	2	NAD	C2A-N3A	2.52	1.38	1.33
2	C	2	NAD	O4D-C1D	2.52	1.44	1.40
2	A	438	NAD	C2A-N3A	2.47	1.38	1.33
2	B	1	NAD	C2A-N3A	2.38	1.38	1.33
2	C	2	NAD	C5A-C4A	2.30	1.43	1.39
2	D	3	NAD	C2A-N3A	2.19	1.37	1.33
2	C	2	NAD	C8A-N7A	2.16	1.35	1.31
2	B	1	NAD	PN-O3	2.15	1.61	1.59
2	A	438	NAD	C2N-N1N	2.10	1.37	1.35
3	D	438	ADN	C5-N7	-2.07	1.35	1.39
3	A	439	ADN	C4-N9	-2.03	1.33	1.36

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAD	N3A-C2A-N1A	-5.68	119.98	128.58
2	C	2	NAD	N3A-C2A-N1A	-5.65	120.03	128.58
2	D	3	NAD	N3A-C2A-N1A	-5.20	120.70	128.58
3	C	438	ADN	C5-N7-C8	5.19	109.34	103.48
3	D	438	ADN	C5-C4-N3	-5.15	117.35	126.75
2	A	438	NAD	N3A-C2A-N1A	-4.94	121.11	128.58
3	D	438	ADN	N9-C4-N3	4.57	134.10	126.69
2	D	3	NAD	C3N-C7N-N7N	4.53	123.32	117.74
3	A	439	ADN	N3-C2-N1	-4.46	121.83	128.58
3	B	438	ADN	N3-C2-N1	-4.41	121.91	128.58
2	C	2	NAD	N9A-C8A-N7A	-4.31	107.82	113.94
3	A	439	ADN	C5-C4-N3	-4.24	119.02	126.75
2	D	3	NAD	O7N-C7N-N7N	-4.23	116.50	122.62
3	B	438	ADN	C5-N7-C8	4.21	108.23	103.48
2	A	438	NAD	N9A-C8A-N7A	-4.19	107.99	113.94
2	B	1	NAD	N9A-C8A-N7A	-4.19	107.99	113.94
2	D	3	NAD	C5A-N7A-C8A	4.15	109.97	103.45
3	C	438	ADN	C5-C4-N3	-4.06	119.35	126.75
2	D	3	NAD	N9A-C8A-N7A	-3.99	108.28	113.94
2	C	2	NAD	C3N-C7N-N7N	3.98	122.64	117.74
2	C	2	NAD	C5A-N7A-C8A	3.97	109.69	103.45
2	B	1	NAD	C5A-C4A-N3A	-3.91	121.33	126.72
3	B	438	ADN	C5-C4-N3	-3.91	119.62	126.75
3	B	438	ADN	N9-C4-N3	3.84	132.91	126.69
3	A	439	ADN	N9-C4-N3	3.74	132.75	126.69
2	C	2	NAD	C5A-C4A-N3A	-3.64	121.70	126.72
2	D	3	NAD	C4A-C5A-N7A	-3.64	106.42	110.58
3	D	438	ADN	C5-N7-C8	3.59	107.53	103.48
3	C	438	ADN	C4-C5-N7	-3.53	105.78	110.67
2	A	438	NAD	O2A-PA-O3	3.45	116.59	107.27
2	A	438	NAD	C5A-C4A-N3A	-3.39	122.05	126.72
2	A	438	NAD	C5A-N7A-C8A	3.30	108.64	103.45
2	B	1	NAD	C5A-N7A-C8A	3.24	108.54	103.45
3	A	439	ADN	C5-N7-C8	3.16	107.05	103.48
2	C	2	NAD	C4A-C5A-N7A	-3.15	106.98	110.58
2	B	1	NAD	C2A-N3A-C4A	3.09	119.38	111.83
2	C	2	NAD	O7N-C7N-N7N	-3.09	118.15	122.62
2	D	3	NAD	C4A-N9A-C8A	3.07	108.97	105.74
3	C	438	ADN	N9-C4-N3	3.07	131.67	126.69
2	C	2	NAD	C2A-N3A-C4A	3.06	119.31	111.83
3	D	438	ADN	N3-C2-N1	-2.93	124.15	128.58
2	C	2	NAD	C4A-N9A-C8A	2.91	108.79	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	438	ADN	C4-C5-N7	-2.88	106.67	110.67
2	A	438	NAD	C2A-N3A-C4A	2.85	118.79	111.83
2	D	3	NAD	C5A-C4A-N3A	-2.84	122.81	126.72
2	A	438	NAD	C4A-N9A-C8A	2.79	108.67	105.74
3	B	438	ADN	N9-C8-N7	-2.78	109.64	113.87
3	B	438	ADN	C4-C5-N7	-2.74	106.87	110.67
3	C	438	ADN	N9-C8-N7	-2.64	109.85	113.87
2	C	2	NAD	N3A-C4A-N9A	2.61	131.61	127.17
2	A	438	NAD	O7N-C7N-N7N	-2.60	118.85	122.62
2	B	1	NAD	O2A-PA-O3	2.55	114.15	107.27
2	A	438	NAD	N3A-C4A-N9A	2.53	131.46	127.17
2	B	1	NAD	N3A-C4A-N9A	2.51	131.44	127.17
2	D	3	NAD	C2A-N3A-C4A	2.49	117.91	111.83
3	C	438	ADN	C5-C4-N9	2.46	108.96	105.67
2	D	3	NAD	C4D-O4D-C1D	2.37	112.10	109.92
2	B	1	NAD	C4A-N9A-C8A	2.34	108.20	105.74
2	D	3	NAD	C2N-N1N-C1D	-2.28	114.11	119.13
3	A	439	ADN	C4-C5-N7	-2.27	107.52	110.67
2	B	1	NAD	C4A-C5A-N7A	-2.23	108.03	110.58
2	D	3	NAD	C6N-N1N-C1D	2.21	124.07	119.73
2	D	3	NAD	C2A-N1A-C6A	2.21	122.36	118.73
2	D	3	NAD	N3A-C4A-N9A	2.19	130.89	127.17
2	D	3	NAD	O2B-C2B-C3B	2.19	118.84	111.82
2	B	1	NAD	O7N-C7N-N7N	-2.11	119.57	122.62
3	D	438	ADN	C5-C4-N9	2.11	108.49	105.67
2	A	438	NAD	C3N-C7N-N7N	2.10	120.33	117.74
2	A	438	NAD	O2N-PN-O1N	2.08	122.14	112.44
2	A	438	NAD	C4A-C5A-N7A	-2.07	108.21	110.58
2	B	1	NAD	C6N-N1N-C2N	-2.05	120.13	121.88
2	A	438	NAD	C6N-N1N-C1D	2.02	123.70	119.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	438	NAD	O4D-C1D-N1N-C2N
2	A	438	NAD	O4D-C1D-N1N-C6N
2	A	438	NAD	C2D-C1D-N1N-C2N
2	A	438	NAD	C2D-C1D-N1N-C6N
2	B	1	NAD	O4D-C1D-N1N-C2N
2	B	1	NAD	O4D-C1D-N1N-C6N
2	B	1	NAD	C2D-C1D-N1N-C2N

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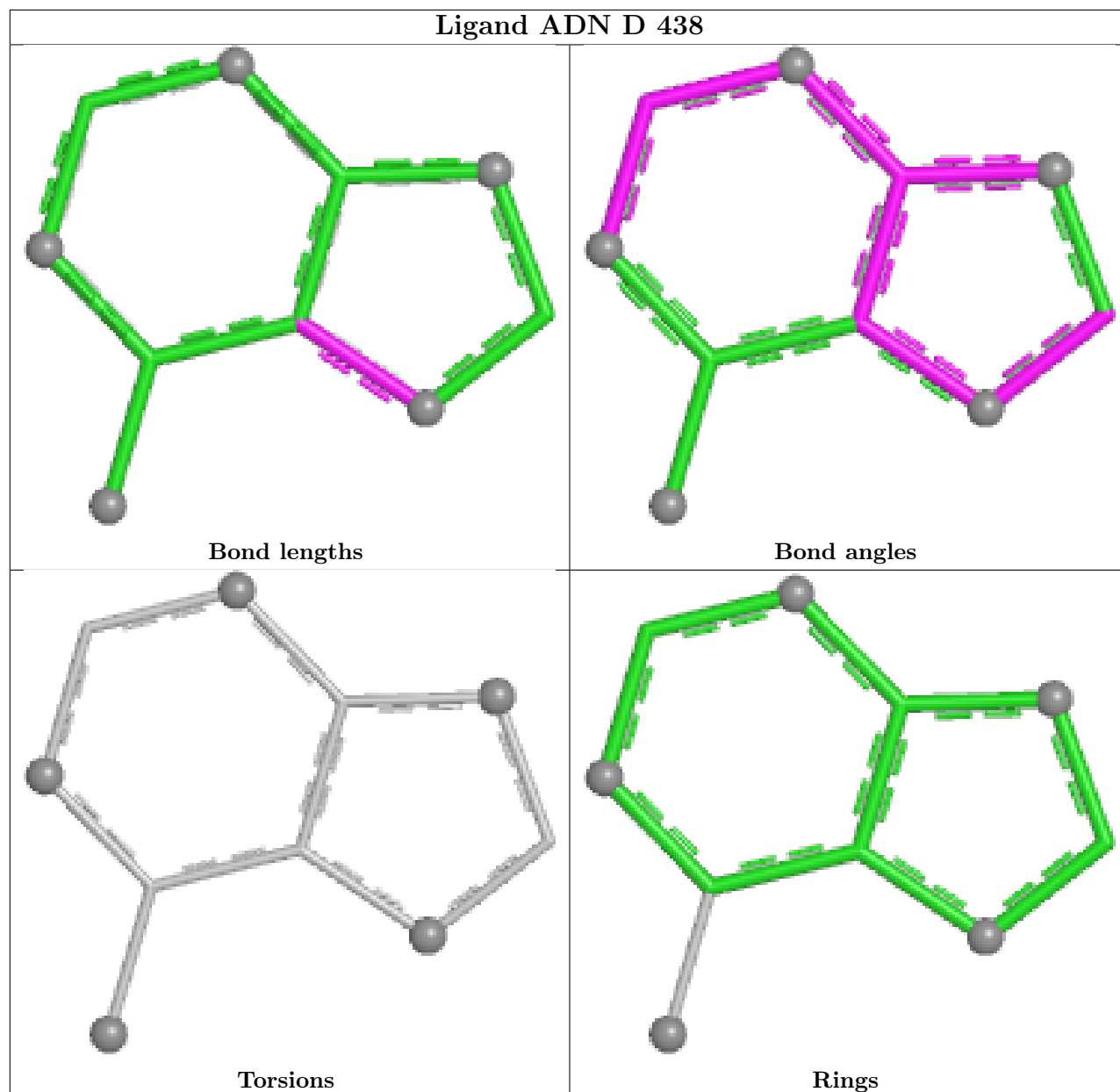
Mol	Chain	Res	Type	Atoms
2	B	1	NAD	C2D-C1D-N1N-C6N
2	C	2	NAD	O4D-C1D-N1N-C2N
2	C	2	NAD	O4D-C1D-N1N-C6N
2	C	2	NAD	C2D-C1D-N1N-C2N
2	C	2	NAD	C2D-C1D-N1N-C6N
2	D	3	NAD	O4D-C1D-N1N-C2N
2	D	3	NAD	O4D-C1D-N1N-C6N
2	D	3	NAD	C2D-C1D-N1N-C2N
2	D	3	NAD	C2D-C1D-N1N-C6N
5	D	1	PG4	O1-C1-C2-O2
5	D	1	PG4	O4-C7-C8-O5
5	D	1	PG4	C6-C5-O3-C4
5	D	1	PG4	C3-C4-O3-C5
5	D	1	PG4	C8-C7-O4-C6
4	C	1	GOL	O1-C1-C2-C3
5	D	1	PG4	C1-C2-O2-C3
2	B	1	NAD	C2B-C1B-N9A-C8A
5	D	1	PG4	O3-C5-C6-O4
2	D	3	NAD	O4B-C4B-C5B-O5B

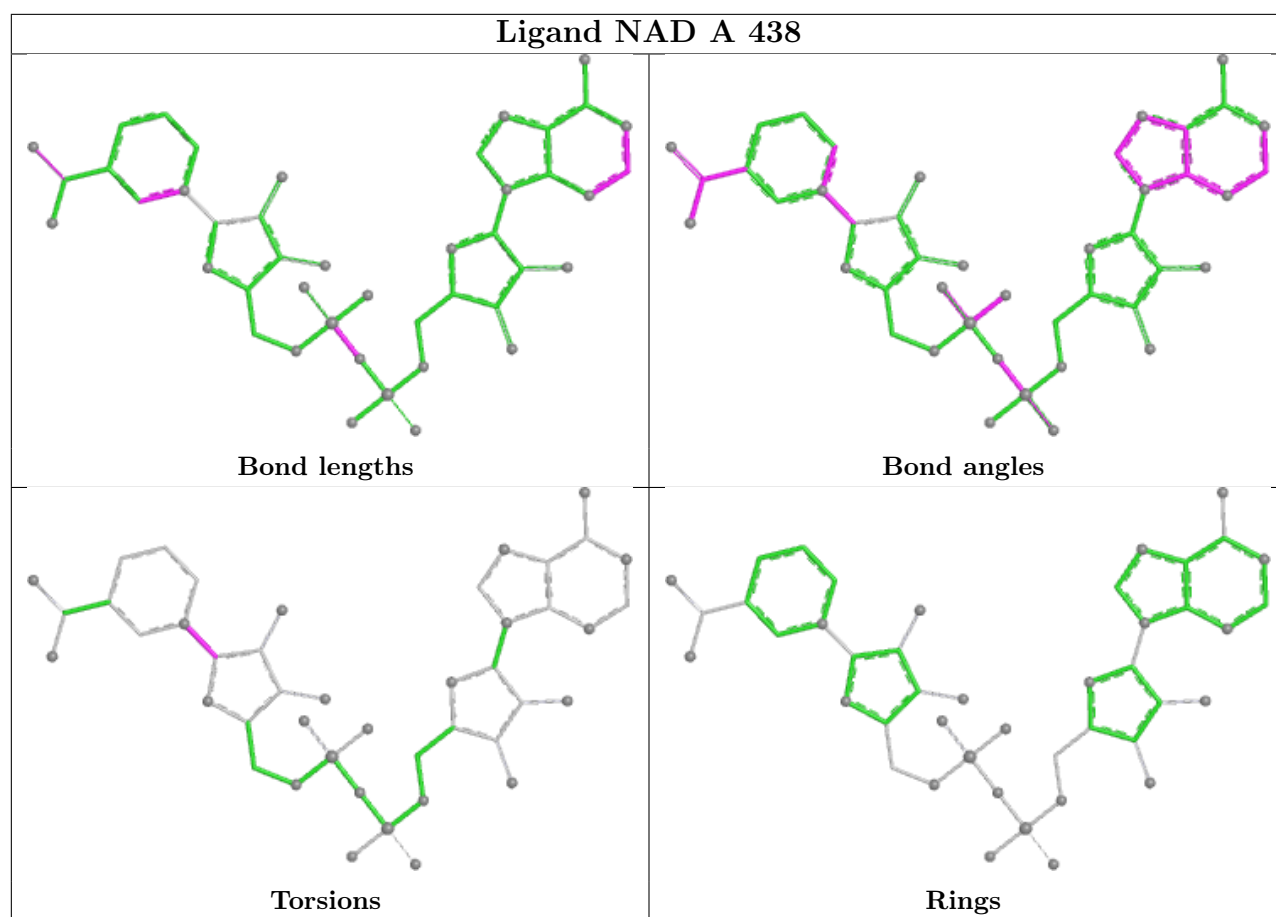
There are no ring outliers.

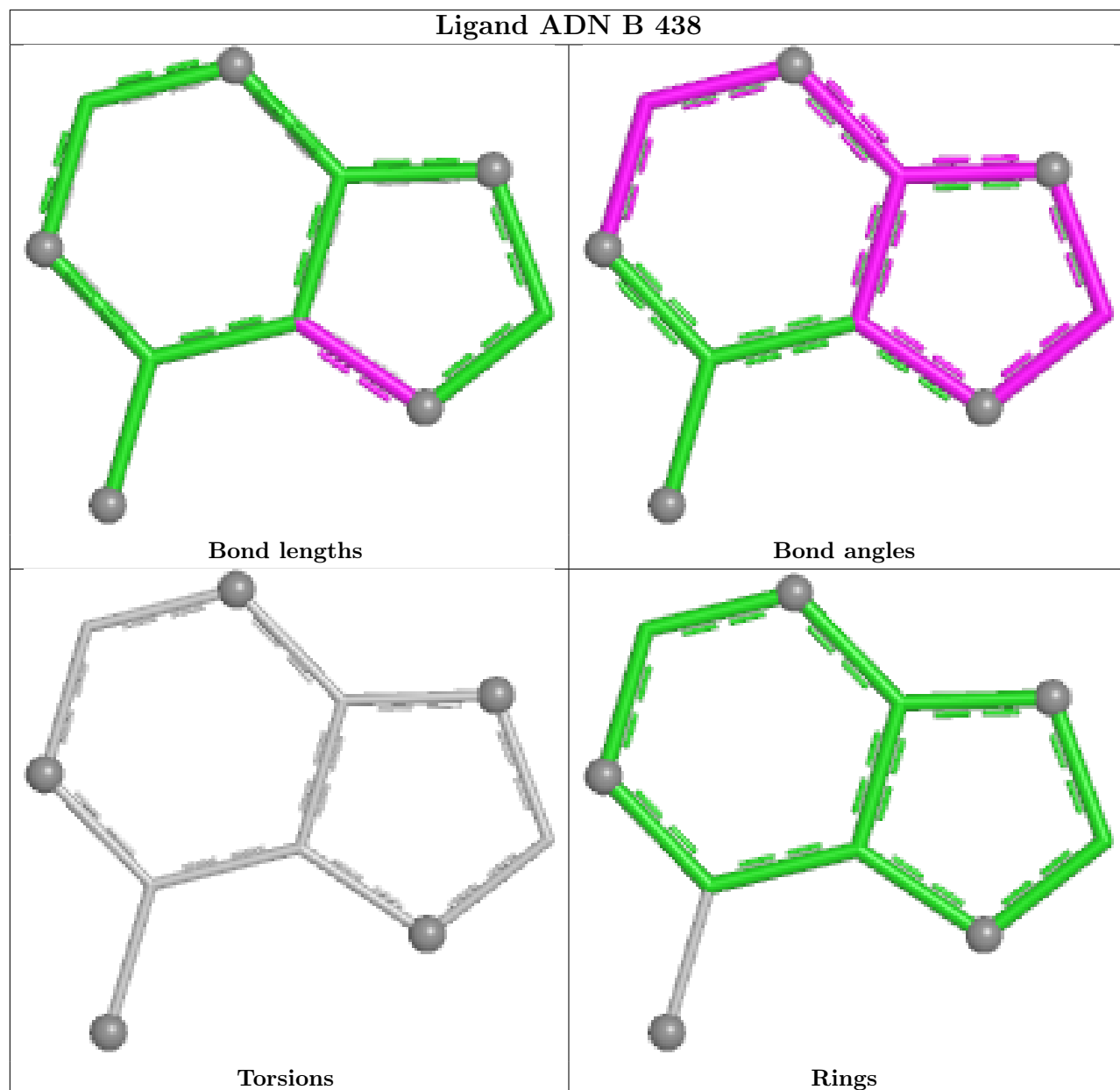
3 monomers are involved in 8 short contacts:

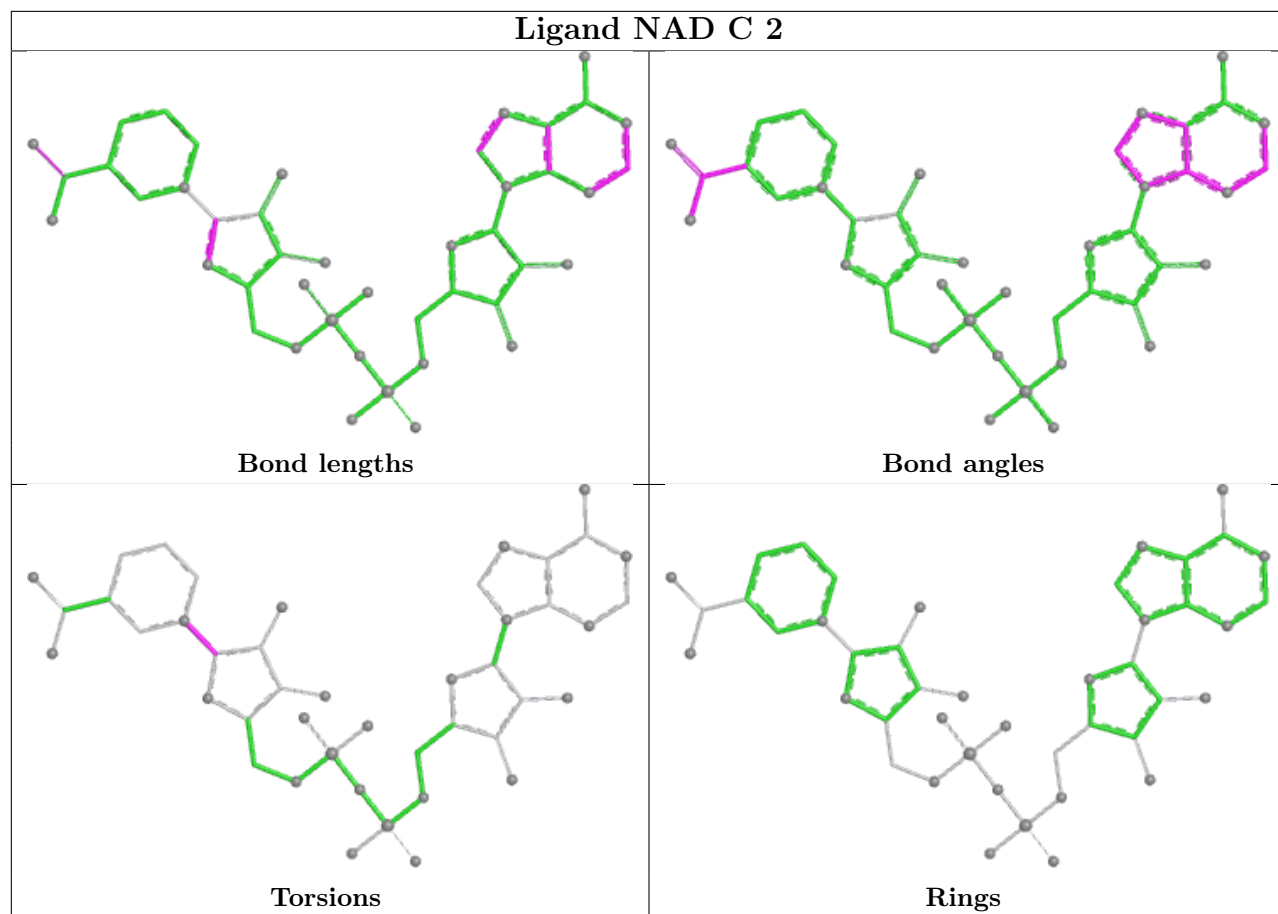
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	438	ADN	1	0
2	B	1	NAD	1	0
5	D	1	PG4	7	0

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.

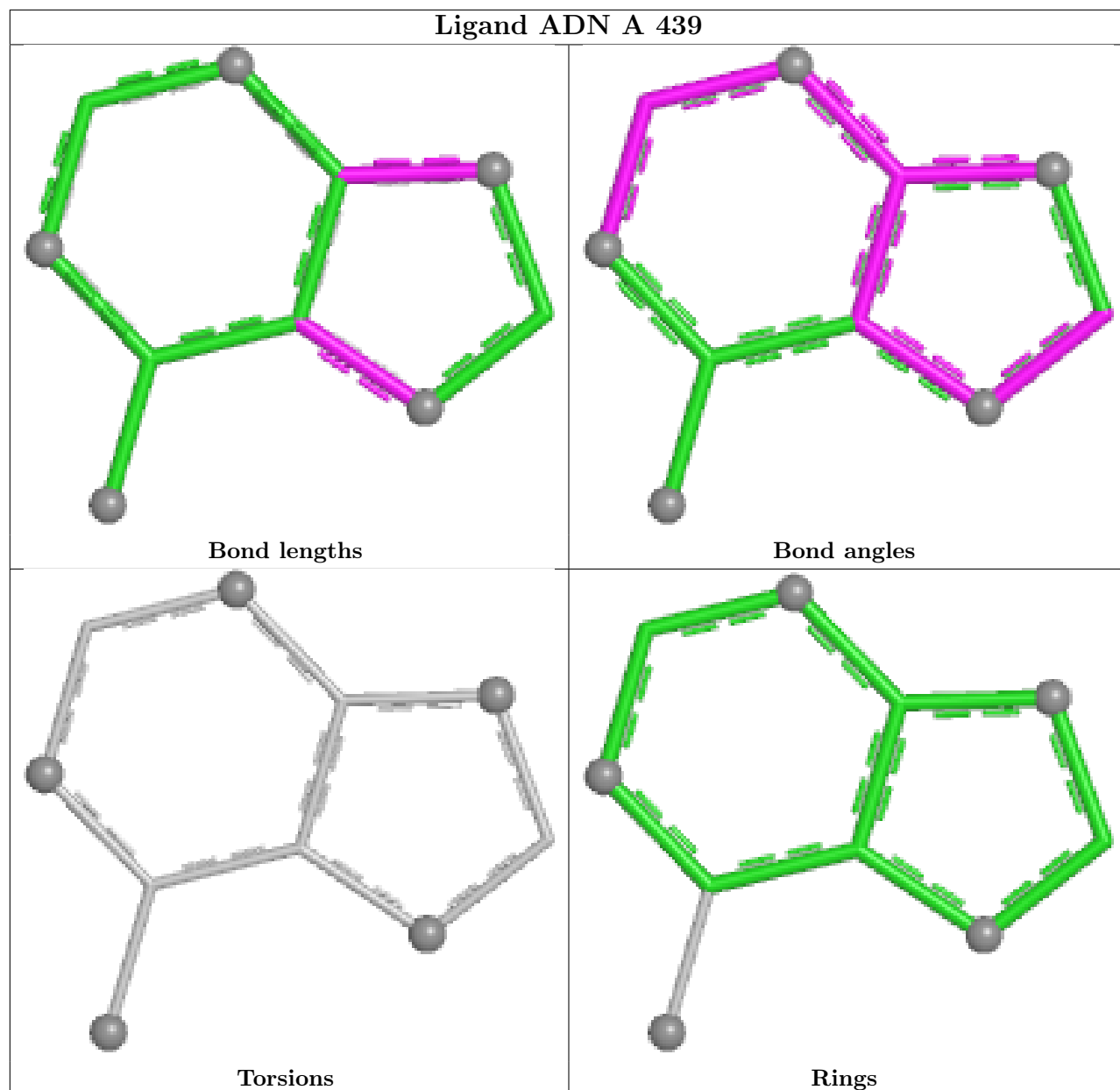


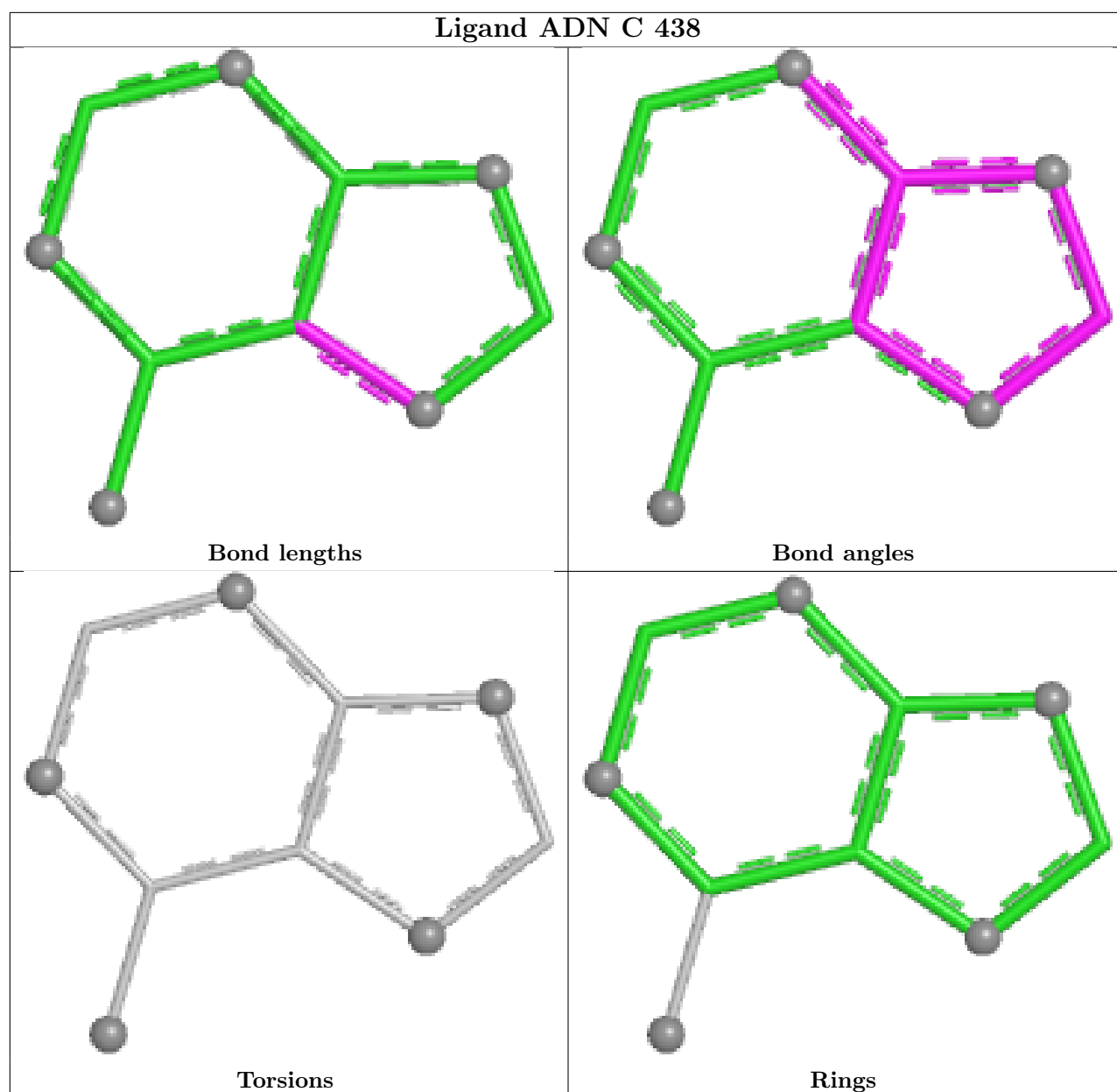


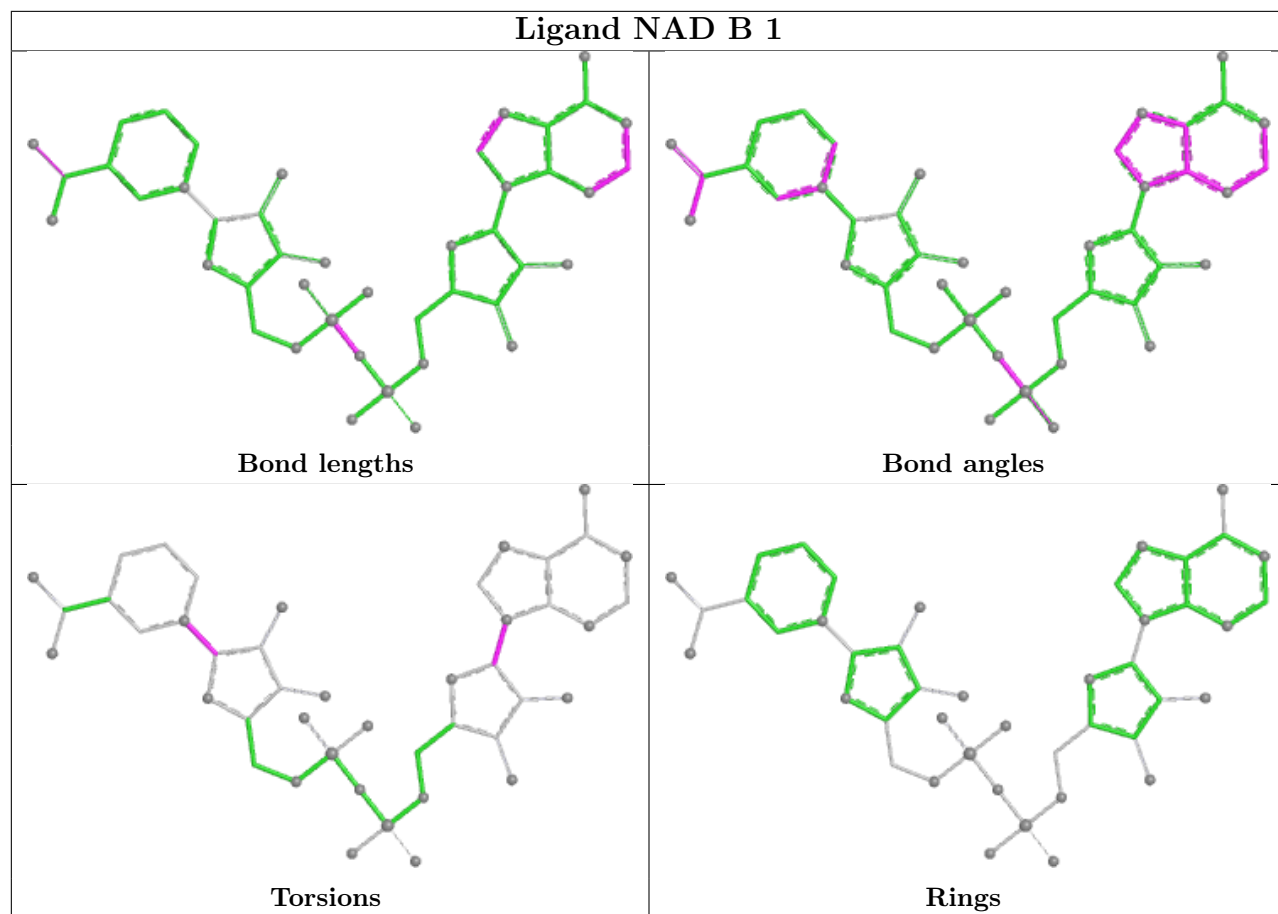


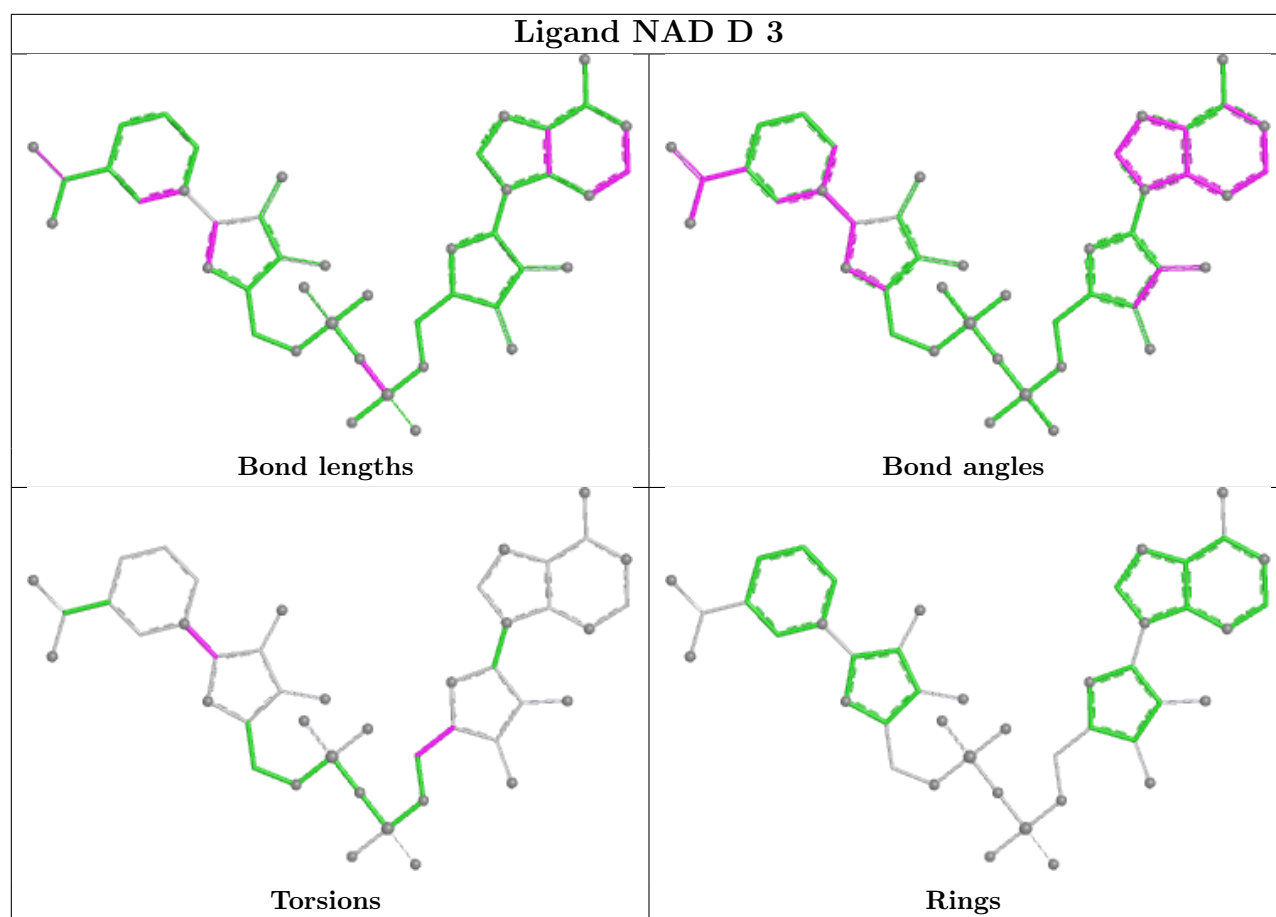


Ligand ADN A 439









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	430/436 (98%)	1.91	179 (41%) 0 0	14, 25, 34, 38	0
1	B	430/436 (98%)	2.43	268 (62%) 0 0	12, 26, 37, 41	0
1	C	435/436 (99%)	0.73	48 (11%) 10 11	2, 5, 15, 27	2 (0%)
1	D	434/436 (99%)	0.27	14 (3%) 50 54	2, 6, 14, 22	3 (0%)
All	All	1729/1744 (99%)	1.33	509 (29%) 1 1	2, 17, 33, 41	5 (0%)

All (509) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	286	PHE	6.8
1	B	286	PHE	6.7
1	C	123	TYR	6.4
1	B	421	TYR	5.9
1	A	286	PHE	5.8
1	B	211	ALA	5.8
1	B	235	GLY	5.5
1	A	94	ILE	5.2
1	B	280	ILE	5.2
1	B	212	GLY	5.1
1	B	417	LYS	5.1
1	B	258	VAL	5.1
1	B	109	TRP	5.0
1	B	90	ALA	5.0
1	B	239	VAL	5.0
1	B	146	ASP	4.9
1	A	120	GLY	4.9
1	A	146	ASP	4.8
1	B	318	VAL	4.8
1	B	8	ASP	4.8
1	B	220	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	240	VAL	4.7
1	B	264	VAL	4.7
1	B	414	LEU	4.7
1	B	167	LEU	4.6
1	B	99	TRP	4.6
1	B	37	GLY	4.6
1	B	141	GLU	4.6
1	B	11	LEU	4.6
1	B	42	LEU	4.6
1	A	150	TYR	4.5
1	A	173	THR	4.5
1	A	14	TRP	4.5
1	A	89	ILE	4.5
1	B	253	MET	4.5
1	A	261	VAL	4.4
1	D	286	PHE	4.4
1	B	259	LEU	4.3
1	B	236	ALA	4.3
1	B	251	ALA	4.3
1	B	145	LEU	4.3
1	B	430	PHE	4.3
1	B	214	THR	4.3
1	B	265	VAL	4.2
1	B	252	ALA	4.2
1	A	121	ASP	4.2
1	B	386	ALA	4.2
1	B	256	TYR	4.1
1	B	218	CYS	4.1
1	B	243	VAL	4.1
1	B	95	PRO	4.1
1	A	235	GLY	4.1
1	A	318	VAL	4.0
1	D	144	GLU	4.0
1	B	97	PHE	4.0
1	B	261	VAL	4.0
1	B	229	ALA	4.0
1	B	87	ALA	3.9
1	B	47	ILE	3.9
1	B	44	GLY	3.9
1	A	36	TYR	3.9
1	B	123	TYR	3.9
1	B	255	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	237	ARG	3.8
1	B	238	VAL	3.8
1	B	424	CYS	3.8
1	A	4	TYR	3.8
1	B	139	LEU	3.8
1	B	372	TRP	3.8
1	A	307	VAL	3.8
1	B	245	PRO	3.7
1	A	9	ILE	3.7
1	B	172	LEU	3.7
1	A	123	TYR	3.7
1	D	150	TYR	3.7
1	B	169	ARG	3.7
1	A	335	ILE	3.7
1	A	147	GLY	3.7
1	B	273	THR	3.7
1	A	162	ASN	3.7
1	A	109	TRP	3.7
1	B	191	LEU	3.6
1	B	192	TYR	3.6
1	B	380	TYR	3.6
1	B	373	THR	3.6
1	A	376	ASP	3.6
1	A	330	ALA	3.6
1	C	142[A]	CYS	3.6
1	B	174	ILE	3.6
1	B	377	THR	3.6
1	B	244	ASP	3.6
1	A	97	PHE	3.6
1	A	211	ALA	3.5
1	B	330	ALA	3.5
1	A	332	GLY	3.5
1	C	378	GLY	3.5
1	B	9	ILE	3.5
1	A	7	ARG	3.5
1	A	264	VAL	3.5
1	B	382	ARG	3.5
1	B	277	ASN	3.5
1	B	260	LEU	3.5
1	A	122	GLY	3.5
1	C	150	TYR	3.5
1	B	96	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	234	PHE	3.5
1	A	268	ALA	3.5
1	D	378	GLY	3.4
1	A	115	LEU	3.4
1	B	249	LEU	3.4
1	B	111	MET	3.4
1	A	212	GLY	3.4
1	B	384	ALA	3.4
1	B	402	LEU	3.4
1	B	275	THR	3.4
1	B	137	TYR	3.4
1	B	376	ASP	3.4
1	B	38	PRO	3.4
1	A	295	VAL	3.3
1	A	320	VAL	3.3
1	B	160	VAL	3.3
1	B	271	PHE	3.3
1	C	169	ARG	3.3
1	A	210	ILE	3.3
1	A	208	VAL	3.3
1	B	164	TYR	3.3
1	B	437	TYR	3.3
1	B	298	ILE	3.3
1	A	45	ALA	3.3
1	A	308	ALA	3.3
1	B	217	VAL	3.3
1	B	314	ALA	3.3
1	A	19	LEU	3.3
1	A	145	LEU	3.3
1	B	278	ASP	3.3
1	C	408	GLY	3.3
1	B	250	GLN	3.2
1	B	61	ILE	3.2
1	B	69	ALA	3.2
1	A	258	VAL	3.2
1	A	163	LEU	3.2
1	C	407	LEU	3.2
1	B	276	GLY	3.2
1	C	235	GLY	3.2
1	A	236	ALA	3.2
1	B	112	LYS	3.2
1	B	151	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	219	GLY	3.2
1	B	118	PHE	3.2
1	B	50	CYS	3.2
1	B	22	ALA	3.1
1	B	173	THR	3.1
1	B	209	MET	3.1
1	C	137	TYR	3.1
1	B	152	VAL	3.1
1	B	216	CYS	3.1
1	A	314	ALA	3.1
1	B	48	ALA	3.1
1	B	422	ILE	3.1
1	B	269	HIS	3.1
1	C	-2	SER	3.1
1	B	149	ILE	3.1
1	A	391	LEU	3.1
1	C	118	PHE	3.1
1	A	92	ARG	3.1
1	B	195	ARG	3.1
1	A	373	THR	3.1
1	B	412	THR	3.1
1	B	175	PRO	3.1
1	A	293	ALA	3.1
1	B	132	GLY	3.1
1	B	228	ALA	3.1
1	B	419	ALA	3.1
1	B	134	LEU	3.0
1	B	113	GLN	3.0
1	A	111	MET	3.0
1	B	92	ARG	3.0
1	B	231	LEU	3.0
1	B	179	VAL	3.0
1	B	153	SER	3.0
1	B	147	GLY	3.0
1	B	233	GLY	3.0
1	B	215	ALA	3.0
1	B	65	VAL	3.0
1	B	234	PHE	3.0
1	A	44	GLY	3.0
1	B	194	CYS	3.0
1	C	424	CYS	3.0
1	B	74	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	210	ILE	3.0
1	B	434	HIS	2.9
1	B	389	TYR	2.9
1	B	148	LYS	2.9
1	C	146	ASP	2.9
1	B	224	GLY	2.9
1	C	120	GLY	2.9
1	C	-1	MET	2.9
1	B	420	GLU	2.9
1	B	29	LEU	2.9
1	A	396	ASP	2.9
1	A	426	VAL	2.9
1	A	301	PHE	2.9
1	B	268	ALA	2.9
1	A	10	SER	2.9
1	B	270	ILE	2.9
1	C	229	ALA	2.9
1	A	333	ARG	2.9
1	A	382	ARG	2.9
1	A	119	SER	2.9
1	A	78	ILE	2.9
1	A	310	LEU	2.9
1	B	294	ILE	2.9
1	C	414	LEU	2.9
1	A	179	VAL	2.8
1	B	183	VAL	2.8
1	B	425	PRO	2.8
1	D	169	ARG	2.8
1	B	248	ALA	2.8
1	B	433	ASP	2.8
1	A	202	ILE	2.8
1	B	193	GLY	2.8
1	B	378	GLY	2.8
1	B	241	THR	2.8
1	A	265	VAL	2.8
1	B	187	LYS	2.8
1	A	325	ASP	2.8
1	A	386	ALA	2.8
1	C	252	ALA	2.8
1	A	118	PHE	2.8
1	A	142	CYS	2.8
1	A	125	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	147	GLY	2.8
1	A	11	LEU	2.8
1	B	415	THR	2.8
1	A	41	PRO	2.8
1	B	124	PRO	2.8
1	B	381	PRO	2.8
1	B	126	MET	2.8
1	C	384	ALA	2.8
1	A	13	GLU	2.8
1	A	114	THR	2.8
1	A	95	PRO	2.8
1	A	99	TRP	2.8
1	A	309	TRP	2.8
1	A	199	VAL	2.8
1	B	283	SER	2.7
1	B	188	PHE	2.7
1	C	430	PHE	2.7
1	A	93	GLY	2.7
1	B	105	GLU	2.7
1	B	267	GLU	2.7
1	B	328	THR	2.7
1	B	189	ASP	2.7
1	B	272	VAL	2.7
1	B	14	TRP	2.7
1	B	374	ASN	2.7
1	A	12	ALA	2.7
1	B	150	TYR	2.7
1	B	327	TYR	2.7
1	C	236	ALA	2.7
1	B	76	CYS	2.7
1	B	122	GLY	2.7
1	A	303	THR	2.7
1	B	303	THR	2.7
1	A	381	PRO	2.7
1	B	369	ILE	2.7
1	A	169	ARG	2.7
1	A	317	ARG	2.7
1	A	96	VAL	2.7
1	B	409	ALA	2.7
1	C	109	TRP	2.7
1	A	328	THR	2.7
1	A	139	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	198	LEU	2.7
1	B	5	LYS	2.7
1	B	68	GLY	2.6
1	C	233	GLY	2.6
1	B	232	ARG	2.6
1	B	411	LEU	2.6
1	A	53	MET	2.6
1	A	329	MET	2.6
1	D	-1	MET	2.6
1	B	110	CYS	2.6
1	A	153	SER	2.6
1	B	186	SER	2.6
1	B	247	ASN	2.6
1	A	172	LEU	2.6
1	C	411	LEU	2.6
1	A	174	ILE	2.6
1	B	257	GLN	2.6
1	A	71	VAL	2.6
1	B	138	VAL	2.6
1	A	315	LYS	2.6
1	B	81	THR	2.6
1	B	157	THR	2.6
1	B	423	ASN	2.6
1	B	390	PHE	2.6
1	A	73	TRP	2.6
1	A	47	ILE	2.6
1	A	336	ILE	2.6
1	B	89	ILE	2.6
1	A	101	GLY	2.6
1	A	5	LYS	2.6
1	A	63	THR	2.6
1	B	416	PRO	2.5
1	B	127	LEU	2.5
1	B	128	LEU	2.5
1	B	407	LEU	2.5
1	C	249	LEU	2.5
1	B	246	ILE	2.5
1	C	419	ALA	2.5
1	B	84	HIS	2.5
1	C	426	VAL	2.5
1	C	92	ARG	2.5
1	A	18	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	70	GLU	2.5
1	A	361	PHE	2.5
1	B	355	PHE	2.5
1	C	170	GLY	2.5
1	C	212	GLY	2.5
1	C	383	GLY	2.5
1	A	270	ILE	2.5
1	A	294	ILE	2.5
1	A	283	SER	2.5
1	A	217	VAL	2.5
1	B	168	GLN	2.5
1	B	429	PRO	2.5
1	A	130	ASP	2.5
1	A	107	TYR	2.5
1	A	259	LEU	2.5
1	B	115	LEU	2.5
1	B	288	ARG	2.5
1	B	202	ILE	2.5
1	A	205	ALA	2.5
1	C	409	ALA	2.5
1	C	412	THR	2.5
1	B	208	VAL	2.5
1	C	238	VAL	2.5
1	B	221	GLY	2.4
1	A	343	LEU	2.4
1	A	281	ILE	2.4
1	A	251	ALA	2.4
1	A	273	THR	2.4
1	C	214	THR	2.4
1	B	83	ASP	2.4
1	A	6	VAL	2.4
1	B	426	VAL	2.4
1	B	290	ARG	2.4
1	A	70	GLU	2.4
1	A	102	GLU	2.4
1	B	296	CYS	2.4
1	D	142	CYS	2.4
1	B	19	LEU	2.4
1	B	282	THR	2.4
1	B	45	ALA	2.4
1	B	58	ALA	2.4
1	B	230	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	251	ALA	2.4
1	A	59	VAL	2.4
1	A	223	VAL	2.4
1	A	240	VAL	2.4
1	B	73	TRP	2.4
1	A	131	GLY	2.4
1	A	378	GLY	2.4
1	B	131	GLY	2.4
1	C	255	GLY	2.4
1	A	346	LEU	2.4
1	B	301	PHE	2.4
1	A	377	THR	2.4
1	B	274	THR	2.4
1	C	246	ILE	2.4
1	A	312	ALA	2.4
1	A	287	PRO	2.4
1	B	162	ASN	2.4
1	B	289	MET	2.4
1	A	360	SER	2.4
1	B	10	SER	2.4
1	B	43	LYS	2.4
1	B	203	LYS	2.4
1	A	76	CYS	2.4
1	A	29	LEU	2.3
1	B	114	THR	2.3
1	C	415	THR	2.3
1	A	280	ILE	2.3
1	C	422	ILE	2.3
1	B	46	LYS	2.3
1	A	324	VAL	2.3
1	A	344	VAL	2.3
1	A	232	ARG	2.3
1	B	130	ASP	2.3
1	B	387	GLN	2.3
1	A	164	TYR	2.3
1	A	271	PHE	2.3
1	A	390	PHE	2.3
1	B	176	ALA	2.3
1	C	211	ALA	2.3
1	B	432	PRO	2.3
1	B	93	GLY	2.3
1	B	408	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	417	LYS	2.3
1	B	326	ARG	2.3
1	A	50	CYS	2.3
1	D	123	TYR	2.3
1	B	311	LYS	2.3
1	B	305	ILE	2.3
1	C	382	ARG	2.3
1	A	104	GLU	2.3
1	B	396	ASP	2.3
1	B	71	VAL	2.3
1	B	142	CYS	2.3
1	B	331	ASN	2.3
1	B	171	LYS	2.3
1	B	338	LEU	2.3
1	A	266	GLU	2.2
1	B	339	ALA	2.2
1	B	367	ALA	2.2
1	B	401	ALA	2.2
1	B	435	TYR	2.2
1	A	433	ASP	2.2
1	B	94	ILE	2.2
1	A	388	VAL	2.2
1	B	379	LYS	2.2
1	B	54	THR	2.2
1	A	260	LEU	2.2
1	D	170	GLY	2.2
1	A	222	ASP	2.2
1	B	86	ALA	2.2
1	B	129	ASP	2.2
1	B	181	ASP	2.2
1	A	149	ILE	2.2
1	A	305	ILE	2.2
1	B	334	HIS	2.2
1	A	138	VAL	2.2
1	C	105	GLU	2.2
1	B	395	LEU	2.2
1	A	74	ALA	2.2
1	A	116	LYS	2.2
1	A	113	GLN	2.2
1	A	239	VAL	2.2
1	A	356	VAL	2.2
1	B	365	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	275	THR	2.2
1	B	103	THR	2.2
1	B	184	THR	2.2
1	A	200	ASP	2.2
1	B	310	LEU	2.2
1	D	139	LEU	2.2
1	D	233	GLY	2.2
1	B	98	ALA	2.2
1	B	91	LYS	2.2
1	A	269	HIS	2.1
1	A	289	MET	2.1
1	A	389	TYR	2.1
1	A	372	TRP	2.1
1	C	250	GLN	2.1
1	B	158	THR	2.1
1	B	320	VAL	2.1
1	B	388	VAL	2.1
1	A	75	SER	2.1
1	B	332	GLY	2.1
1	A	348	CYS	2.1
1	B	371	LEU	2.1
1	B	116	LYS	2.1
1	A	79	PHE	2.1
1	A	246	ILE	2.1
1	B	107	TYR	2.1
1	B	281	ILE	2.1
1	B	182	SER	2.1
1	B	333	ARG	2.1
1	A	198	LEU	2.1
1	C	231	LEU	2.1
1	D	407	LEU	2.1
1	A	103	THR	2.1
1	A	144	GLU	2.1
1	B	254	GLU	2.1
1	B	266	GLU	2.1
1	B	385	LYS	2.1
1	A	117	GLY	2.1
1	A	341	GLY	2.1
1	A	243	VAL	2.1
1	B	223	VAL	2.1
1	B	287	PRO	2.1
1	B	64	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	227	CYS	2.1
1	B	16	ARG	2.1
1	C	232	ARG	2.1
1	A	46	LYS	2.0
1	B	262	GLU	2.0
1	B	304	GLU	2.0
1	A	220	TYR	2.0
1	A	327	TYR	2.0
1	B	4	TYR	2.0
1	B	6	VAL	2.0
1	B	295	VAL	2.0
1	A	42	LEU	2.0
1	A	296	CYS	2.0
1	B	404	LEU	2.0
1	A	90	ALA	2.0
1	A	8	ASP	2.0
1	A	288	ARG	2.0
1	B	18	GLU	2.0
1	D	141	GLU	2.0
1	A	300	HIS	2.0
1	A	77	ASN	2.0
1	A	331	ASN	2.0
1	A	435	TYR	2.0
1	A	152	VAL	2.0
1	A	272	VAL	2.0
1	B	356	VAL	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 [i](#)

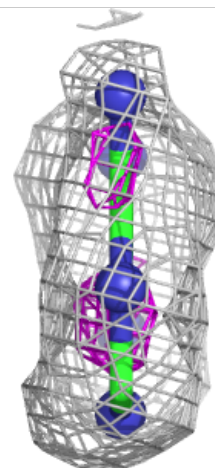
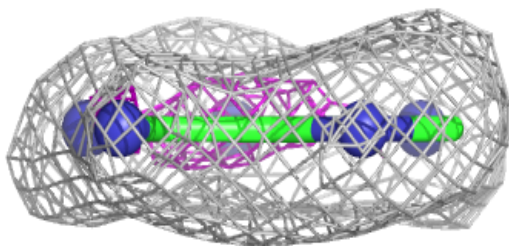
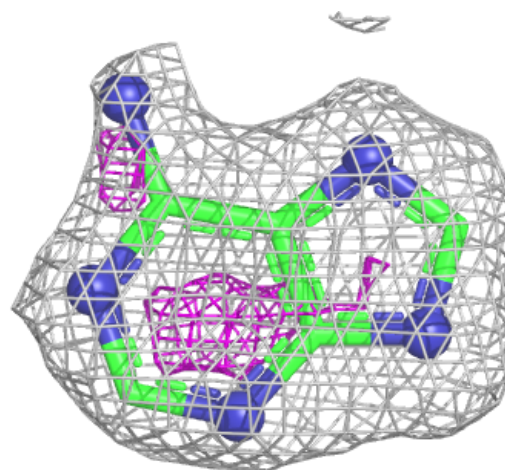
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	PG4	D	1	13/13	0.74	0.15	26,32,34,35	0
4	GOL	C	1	6/6	0.75	0.20	36,37,37,37	0
3	ADN	A	439	10/19	0.83	0.11	28,29,29,30	0
3	ADN	B	438	10/19	0.91	0.19	19,20,22,22	0
2	NAD	B	1	44/44	0.91	0.10	15,25,27,27	0
2	NAD	A	438	44/44	0.91	0.10	16,21,25,25	0
3	ADN	C	438	10/19	0.95	0.08	2,3,5,5	0
3	ADN	D	438	10/19	0.96	0.06	2,2,3,3	0
2	NAD	C	2	44/44	0.97	0.06	2,2,3,5	0
2	NAD	D	3	44/44	0.97	0.06	2,2,3,4	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.

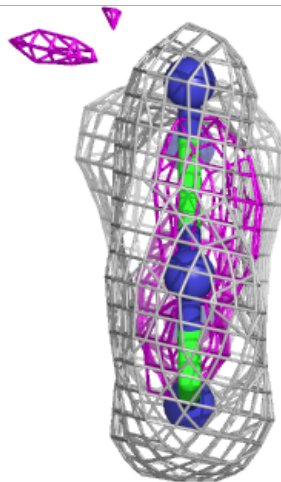
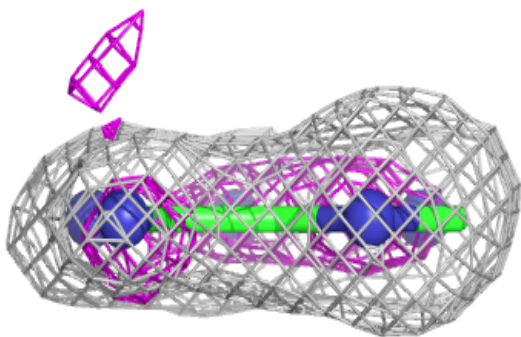
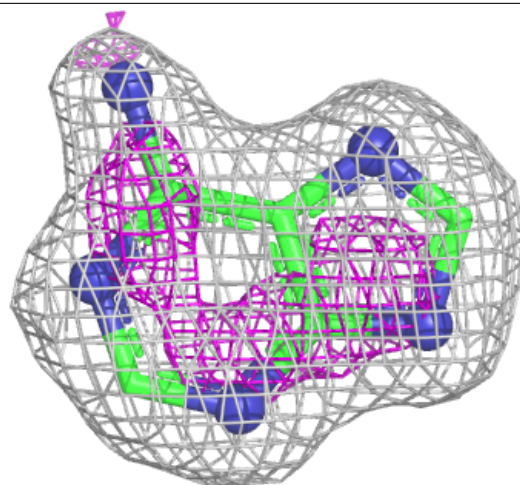
Electron density around ADN A 439:

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



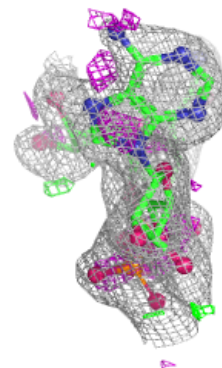
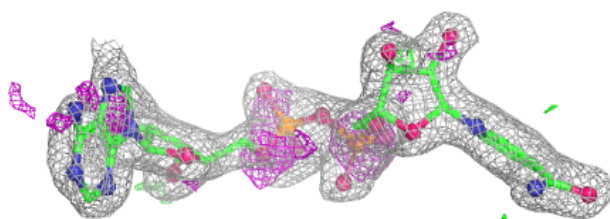
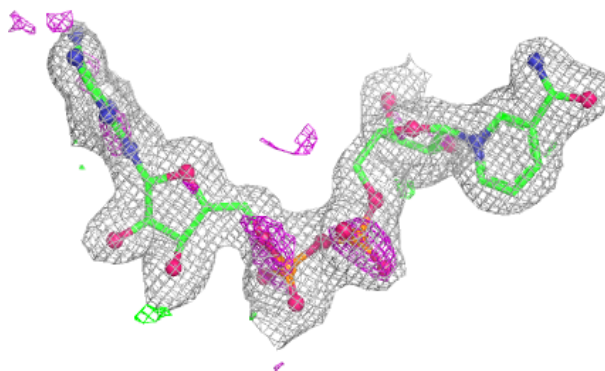
Electron density around ADN B 438:

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

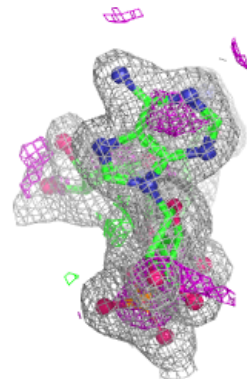
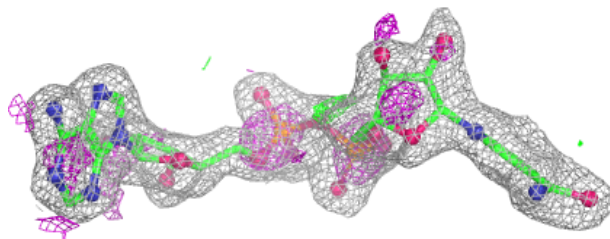
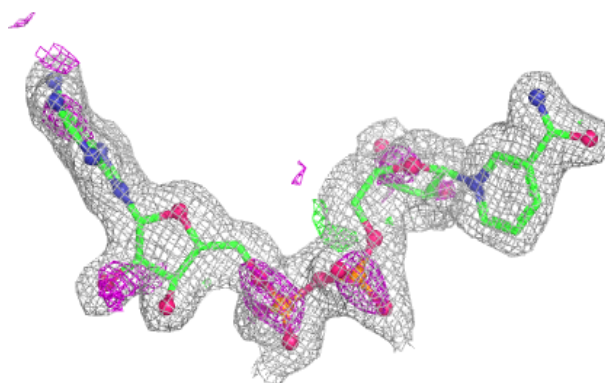


Electron density around NAD B 1:

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

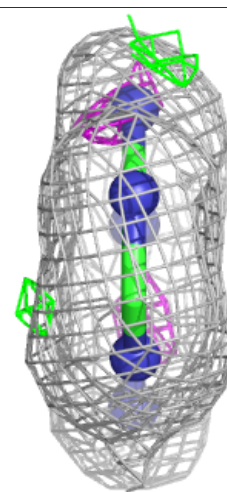
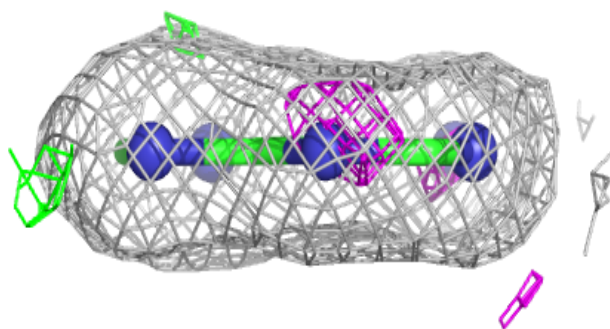
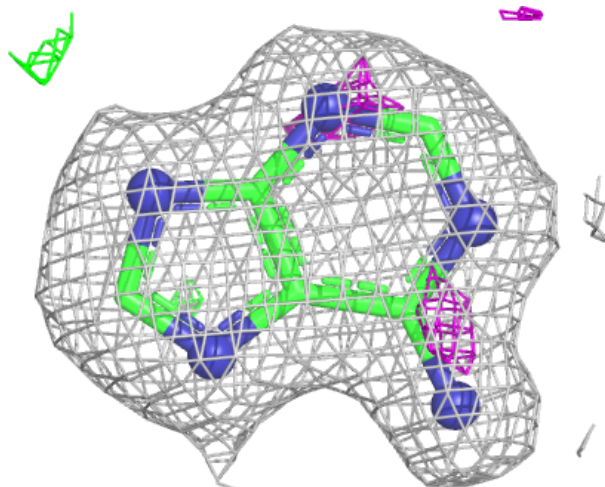
**Electron density around NAD A 438:**

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



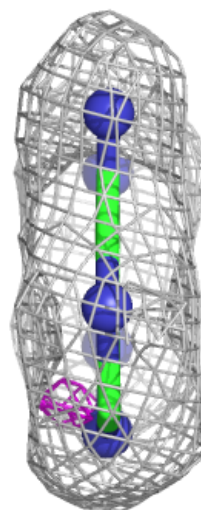
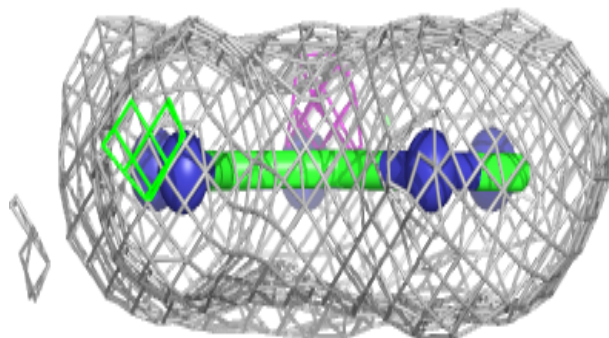
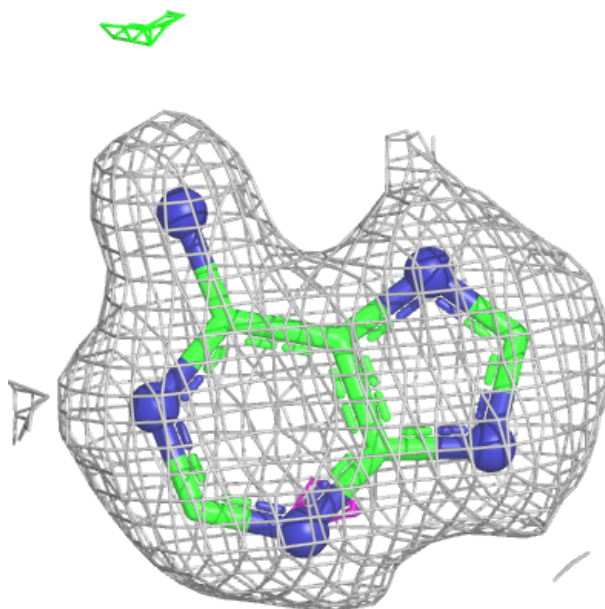
Electron density around ADN C 438:

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



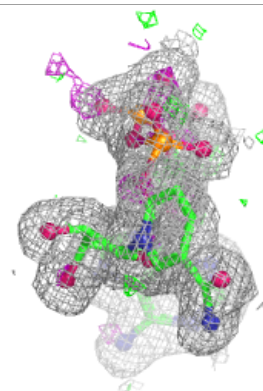
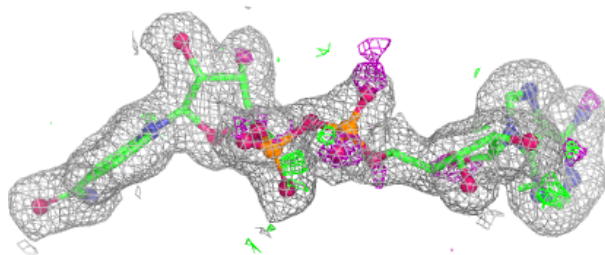
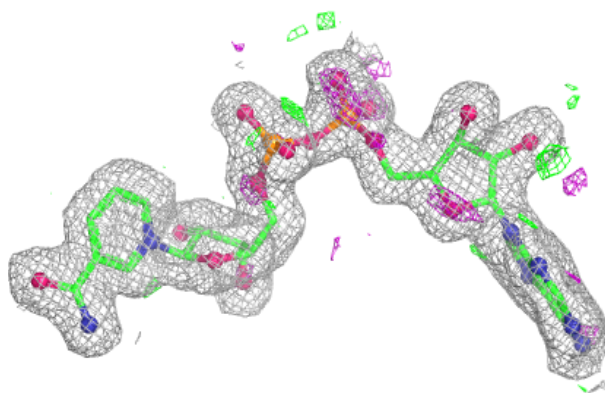
Electron density around ADN D 438:

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

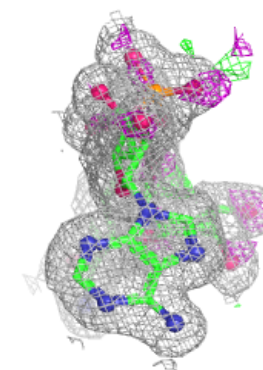
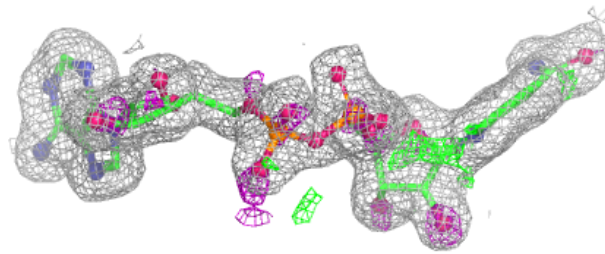
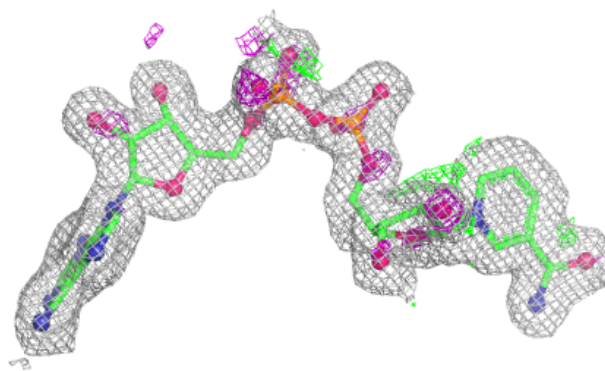


Electron density around NAD C 2:

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

**Electron density around NAD D 3:**

$2mF_o-DF_c$ (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.