



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:24 am BST

PDB ID : 5M66  
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *Bradyrhizobium elkanii* in complex with adenosine  
Authors : Manszewski, T.; Jaskolski, M.  
Deposited on : 2016-10-24  
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

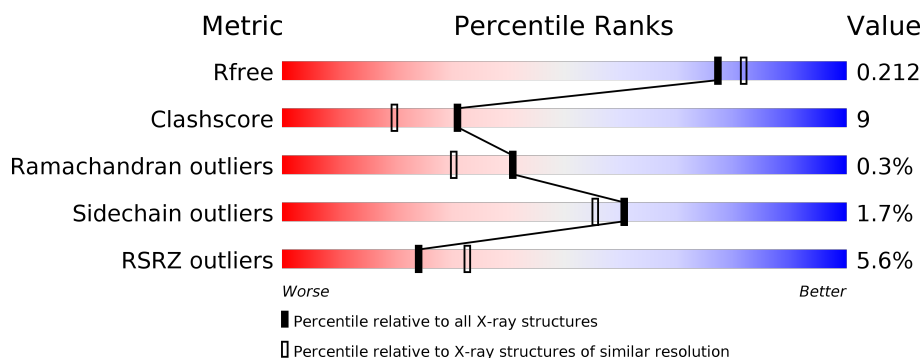
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	479	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	479	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
1	C	479	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div> </div>
1	D	479	<div> <div>13%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>..</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	B	505	-	-	X	-

## 2 Entry composition [i](#)

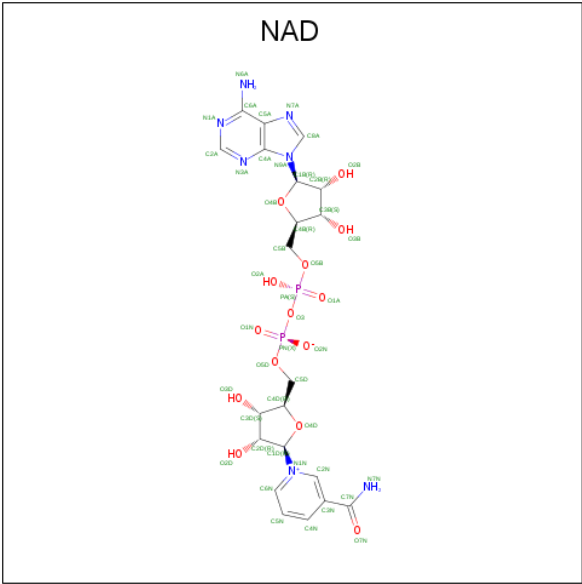
There are 6 unique types of molecules in this entry. The entry contains 15714 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	468	Total	C	N	O	S	0	4	0
			3644	2308	627	688	21			
1	B	464	Total	C	N	O	S	0	6	0
			3626	2298	626	681	21			
1	C	463	Total	C	N	O	S	0	6	0
			3615	2292	621	681	21			
1	D	468	Total	C	N	O	S	0	4	0
			3642	2306	628	687	21			

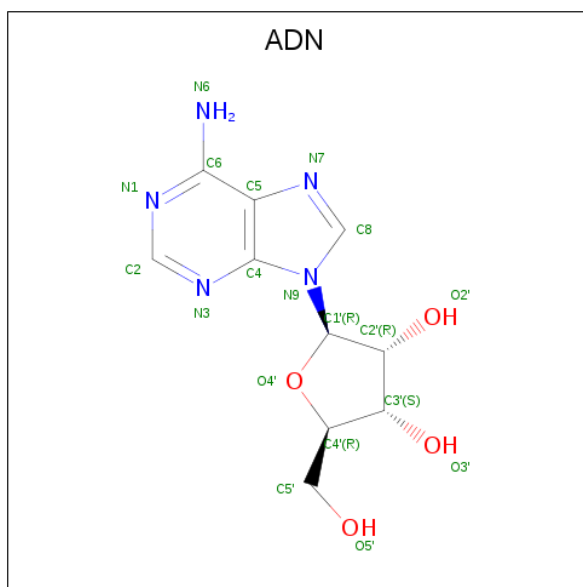
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 3 is ADENOSINE (three-letter code: ADN) (formula:  $C_{10}H_{13}N_5O_4$ ).



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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	253	Total	O	0	0
			253	253		
6	B	244	Total	O	0	0
			244	244		
6	C	217	Total	O	0	0
			217	217		

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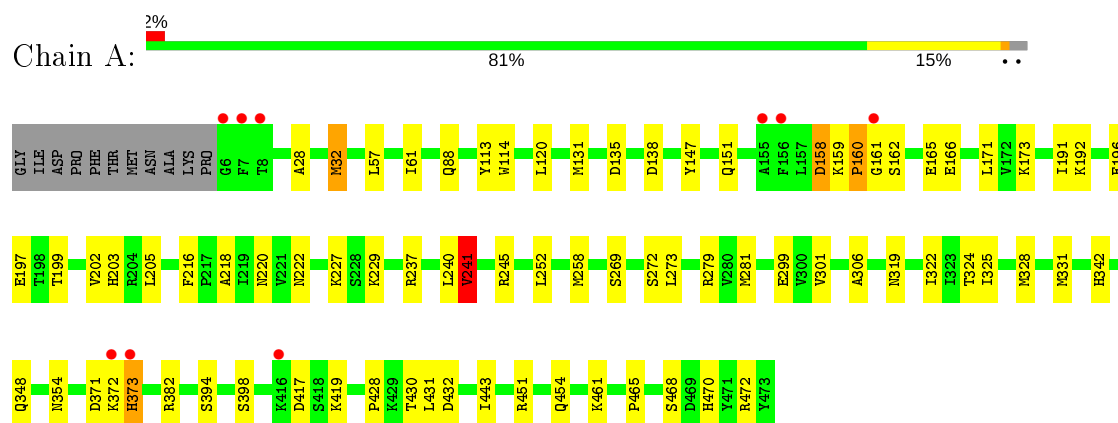
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	182	Total 182	O 182	0	0

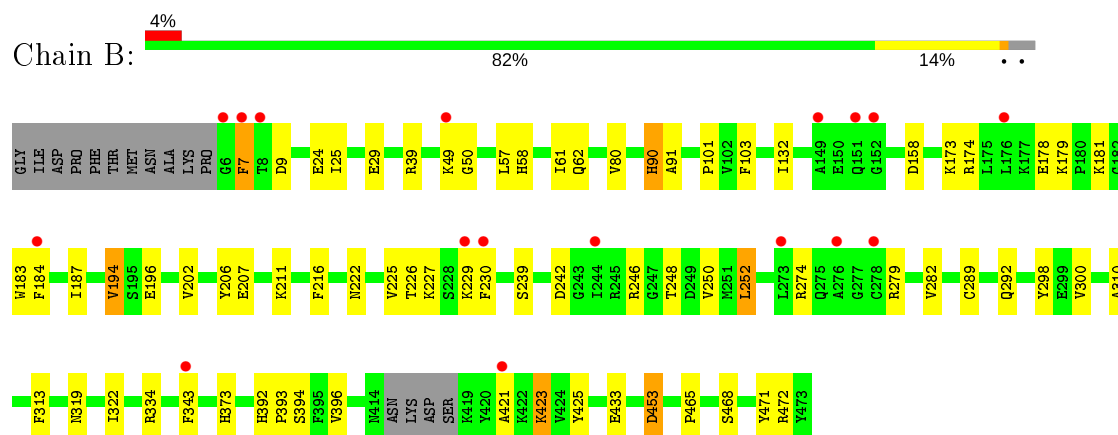
### 3 Residue-property plots [i](#)

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

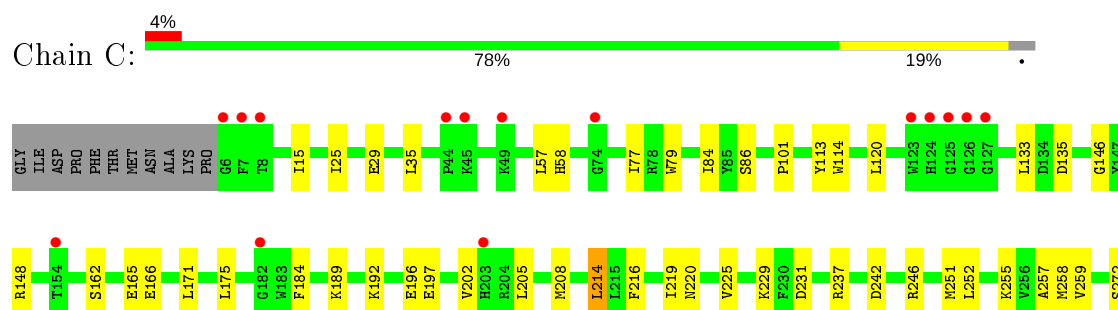
#### • Molecule 1: Adenosylhomocysteinase



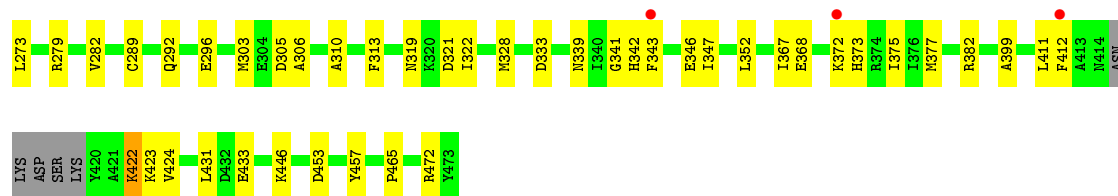
#### • Molecule 1: Adenosylhomocysteinase



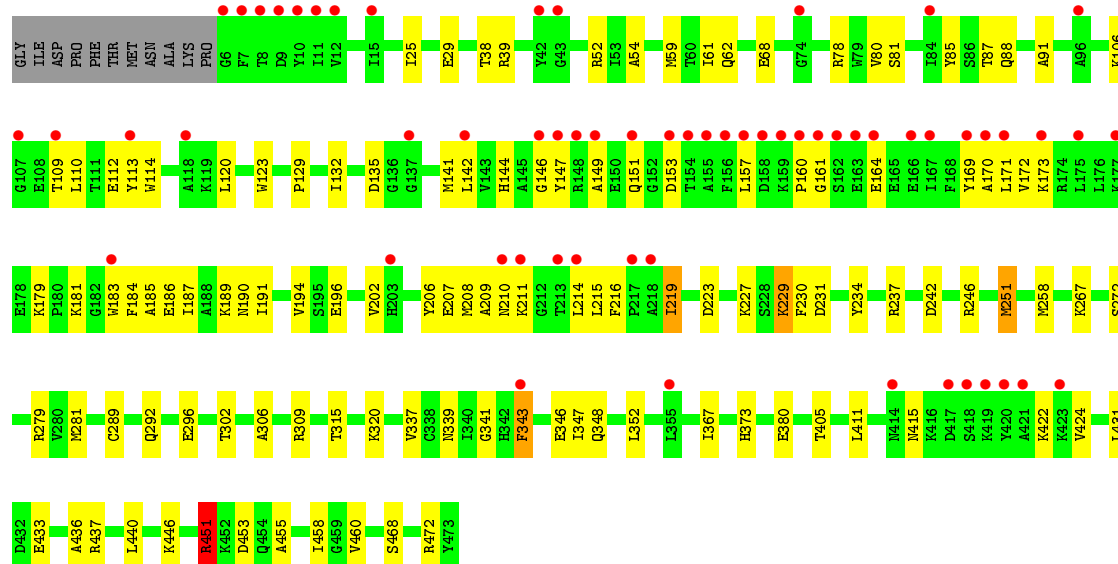
#### • Molecule 1: Adenosylhomocysteinase







● Molecule 1: Adenosylhomocysteinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.44Å 173.62Å 97.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.90 – 1.95 46.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.90-1.95) 98.9 (46.90-1.95)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.169 , 0.211 0.170 , 0.212	Depositor DCC
$R_{free}$ test set	1011 reflections (0.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 62.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15714	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.77	1/3724 (0.0%)	0.87	7/5027 (0.1%)
1	B	0.84	3/3709 (0.1%)	0.89	4/5003 (0.1%)
1	C	0.75	1/3701 (0.0%)	0.83	8/4997 (0.2%)
1	D	0.71	0/3721	0.84	8/5024 (0.2%)
All	All	0.77	5/14855 (0.0%)	0.86	27/20051 (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	A	0	1
1	D	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	VAL	CB-CG1	-9.33	1.33	1.52
1	B	298	TYR	CD2-CE2	6.53	1.49	1.39
1	C	246	ARG	CZ-NH1	6.25	1.41	1.33
1	B	194	VAL	CB-CG1	5.39	1.64	1.52
1	B	453	ASP	CB-CG	-5.07	1.41	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	451[A]	ARG	NE-CZ-NH1	-9.19	115.70	120.30
1	D	451[B]	ARG	NE-CZ-NH1	-9.19	115.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	451[A]	ARG	NE-CZ-NH2	8.91	124.75	120.30
1	D	451[B]	ARG	NE-CZ-NH2	8.91	124.75	120.30
1	C	214	LEU	CB-CA-C	-7.90	95.18	110.20
1	D	453	ASP	CB-CG-OD1	7.03	124.63	118.30
1	A	32	MET	CG-SD-CE	-6.75	89.41	100.20
1	D	453	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	C	231	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	D	219	ILE	CG1-CB-CG2	-6.14	97.88	111.40
1	A	237	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	273	LEU	CB-CG-CD2	-6.03	100.74	111.00
1	C	242	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	333	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	432	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	120	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	C	120	LEU	CB-CG-CD1	-5.64	101.41	111.00
1	B	252	LEU	CA-CB-CG	-5.55	102.54	115.30
1	A	382	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	174[A]	ARG	CA-C-O	5.43	131.50	120.10
1	B	174[B]	ARG	CA-C-O	5.43	131.50	120.10
1	C	231	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	273	LEU	CB-CG-CD1	-5.37	101.86	111.00
1	C	333	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	242	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	D	135	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	334	ARG	NE-CZ-NH2	-5.09	117.76	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	ASP	Peptide
1	D	223	ASP	Peptide
1	D	52	ARG	Sidechain

## 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	3644	0	3658	61	0
1	B	3626	0	3652	51	0
1	C	3615	0	3625	65	0
1	D	3642	0	3660	98	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	2	0
3	A	19	0	13	2	0
3	B	19	0	13	1	0
3	C	19	0	13	3	0
3	D	19	0	13	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	7	0	10	1	0
5	B	14	0	20	9	0
5	C	14	0	20	1	0
6	A	253	0	0	8	0
6	B	244	0	0	6	0
6	C	217	0	0	7	0
6	D	182	0	0	11	0
All	All	15714	0	14801	270	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 (270) 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:258:MET:HE3	1:D:306:ALA:HB2	1.41	0.99
1:A:258:MET:HE2	1:A:281:MET:HB2	1.45	0.97
1:D:451[A]:ARG:NH1	6:D:601:HOH:O	1.89	0.97
1:C:279[B]:ARG:NH1	6:C:601:HOH:O	1.96	0.97
1:A:131:MET:HE2	1:A:192:LYS:HB2	1.48	0.92
1:A:258:MET:CE	1:A:281:MET:HB2	1.98	0.91
1:A:241:VAL:HG13	6:A:734:HOH:O	1.70	0.90
1:B:393:PRO:HD2	1:D:251:MET:HE1	1.52	0.90
1:D:54:ALA:HB1	1:D:120:LEU:HG	1.56	0.88
1:A:131:MET:CE	1:A:192:LYS:HB2	2.02	0.87
1:D:258:MET:CE	1:D:306:ALA:HB2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LEU:O	1:C:422:LYS:HD3	1.80	0.81
1:A:241:VAL:HG12	1:A:272:SER:OG	1.80	0.80
1:C:305[B]:ASP:OD2	6:C:602:HOH:O	2.02	0.76
1:C:303:MET:HE3	1:C:306:ALA:HB3	1.67	0.76
1:A:28:ALA:HB1	1:A:32:MET:CE	2.16	0.75
1:A:451:ARG:H	1:A:454:GLN:HE21	1.35	0.73
1:A:203:HIS:CE1	5:B:505:PEG:H12	2.24	0.73
1:A:32:MET:HE2	1:A:394:SER:HB3	1.71	0.72
1:C:423:LYS:HG2	1:C:424:VAL:H	1.54	0.72
6:C:602:HOH:O	1:D:446:LYS:HE2	1.88	0.72
1:D:114:TRP:HB3	1:D:171:LEU:HD13	1.73	0.71
1:A:324:THR:HA	1:A:348:GLN:HG3	1.73	0.70
1:D:279[B]:ARG:NH1	6:D:604:HOH:O	2.25	0.69
2:D:501:NAD:C4N	3:D:502:ADN:H3'	2.23	0.69
1:D:279[A]:ARG:NH1	6:D:603:HOH:O	2.24	0.69
1:A:203:HIS:HE1	5:B:505:PEG:H12	1.57	0.68
1:C:229[B]:LYS:NZ	6:C:603:HOH:O	2.25	0.68
1:D:62:GLN:HE21	3:D:502:ADN:HN62	1.41	0.68
1:A:160:PRO:HG3	1:A:166:GLU:HB2	1.75	0.68
1:A:325:ILE:H	1:A:348:GLN:NE2	1.92	0.68
1:B:274:ARG:HD2	6:B:799:HOH:O	1.93	0.68
1:C:339:ASN:ND2	1:C:341:GLY:H	1.91	0.68
1:A:430:THR:HG23	1:A:465:PRO:HG3	1.76	0.67
1:B:468:SER:OG	5:B:505:PEG:H31	1.94	0.67
1:B:7:PHE:HZ	1:B:101:PRO:HG3	1.59	0.67
2:A:501:NAD:C4N	3:A:502:ADN:H3'	2.24	0.67
1:D:219:ILE:HD13	1:D:411:LEU:HG	1.79	0.65
1:D:62:GLN:NE2	3:D:502:ADN:HN62	1.95	0.65
1:A:160:PRO:HB2	1:A:165:GLU:HB3	1.79	0.64
1:B:181:LYS:HE2	1:B:181:LYS:H	1.63	0.64
1:D:189:LYS:HD2	1:D:190:ASN:OD1	1.97	0.64
1:C:303:MET:CE	1:C:306:ALA:HB3	2.27	0.63
1:B:279[A]:ARG:NH1	6:B:602:HOH:O	2.31	0.62
1:B:61:ILE:HD13	1:B:91:ALA:HB2	1.81	0.62
1:C:292:GLN:O	1:C:296:GLU:HG2	2.00	0.61
1:A:279[A]:ARG:NH1	6:A:602:HOH:O	2.25	0.61
1:D:183:TRP:CE2	1:D:187:ILE:HD11	2.34	0.61
1:A:229[A]:LYS:HE3	1:B:472:ARG:HB2	1.83	0.61
1:D:157:LEU:HD21	1:D:172:VAL:HB	1.81	0.61
2:B:501:NAD:C4N	3:B:502:ADN:H3'	2.32	0.60
1:A:258:MET:HE1	1:A:281:MET:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:TYR:OH	1:A:138:ASP:OD2	2.14	0.60
1:C:382:ARG:NH1	6:C:607:HOH:O	2.35	0.60
1:D:352:LEU:HD13	1:D:367:ILE:HD13	1.84	0.59
1:B:7:PHE:CZ	1:B:101:PRO:HG3	2.37	0.59
1:C:57:LEU:HD13	1:C:135:ASP:HB2	1.84	0.59
1:C:237:ARG:HA	1:C:272:SER:HB2	1.85	0.58
1:D:258:MET:HE2	1:D:281:MET:CE	2.34	0.58
1:C:257:ALA:HB1	1:C:273:LEU:HD13	1.85	0.58
1:C:303:MET:HA	1:C:303:MET:HE3	1.86	0.58
1:A:417:ASP:OD1	1:A:419:LYS:NZ	2.34	0.57
1:B:229[B]:LYS:HE2	6:B:618:HOH:O	2.04	0.57
1:C:258:MET:HG2	1:C:303:MET:HE1	1.85	0.57
1:D:183:TRP:CZ2	1:D:187:ILE:HD11	2.38	0.57
1:A:328:MET:HG2	1:A:331:MET:HE1	1.85	0.57
1:D:80:VAL:HG13	1:D:120:LEU:HD13	1.86	0.56
2:C:501:NAD:C4N	3:C:502:ADN:H3'	2.35	0.56
1:D:170:ALA:HA	1:D:173:LYS:HD2	1.88	0.56
1:C:114:TRP:HB3	1:C:171:LEU:HD22	1.86	0.56
1:A:328:MET:HG2	1:A:331:MET:CE	2.34	0.56
1:A:325:ILE:H	1:A:348:GLN:HE21	1.53	0.55
1:B:421:ALA:N	1:B:425:TYR:OH	2.37	0.55
1:A:451:ARG:H	1:A:454:GLN:NE2	2.04	0.55
1:B:229[B]:LYS:NZ	1:B:472:ARG:O	2.40	0.55
1:C:162:SER:O	1:C:166:GLU:HG3	2.07	0.55
1:C:58:HIS:HD2	1:C:86:SER:OG	1.90	0.54
1:D:179:LYS:HG3	1:D:183:TRP:CE3	2.43	0.54
1:B:25:ILE:O	1:B:29:GLU:HG3	2.08	0.53
5:B:505:PEG:H21	6:B:739:HOH:O	2.07	0.53
1:D:132:ILE:HG22	1:D:194:VAL:HG23	1.90	0.53
1:B:248:THR:HB	1:B:250:VAL:HG13	1.91	0.53
1:D:209:ALA:HB2	1:D:214:LEU:HD22	1.89	0.53
1:B:222:ASN:HA	1:B:227:LYS:HD2	1.90	0.53
1:B:24:GLU:OE1	1:B:90:HIS:HE1	1.91	0.53
1:B:7:PHE:CZ	1:B:9:ASP:HB3	2.44	0.53
1:D:142:LEU:HD11	1:D:171:LEU:CD2	2.38	0.53
1:C:368:GLU:OE1	1:C:372:LYS:HD2	2.08	0.53
1:A:135:ASP:OD2	1:A:197:GLU:HG2	2.09	0.52
1:A:158:ASP:OD1	1:A:173:LYS:NZ	2.43	0.52
1:A:222:ASN:HA	1:A:227:LYS:HD2	1.91	0.52
1:D:237:ARG:HA	1:D:272:SER:HB2	1.92	0.52
1:B:421:ALA:HB3	1:B:423:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:LEU:HD22	1:D:164:GLU:HG3	1.91	0.52
1:A:32:MET:HG2	1:A:398:SER:HB2	1.92	0.52
1:C:342:HIS:HB3	2:C:501:NAD:O3D	2.10	0.51
1:C:446:LYS:HE2	6:D:668:HOH:O	2.10	0.51
1:D:206:TYR:CD1	1:D:424:VAL:HG21	2.44	0.51
1:B:453:ASP:HB2	6:B:778:HOH:O	2.09	0.51
1:A:430:THR:CG2	1:A:465:PRO:HG3	2.39	0.51
1:C:135:ASP:OD2	3:C:502:ADN:H4'	2.10	0.51
1:A:205:LEU:HD13	1:A:218:ALA:HB1	1.93	0.51
1:D:85:TYR:OH	1:D:380:GLU:OE1	2.29	0.51
1:D:258:MET:HE2	1:D:281:MET:HE3	1.92	0.51
1:D:59:MET:HB3	1:D:87:THR:HG23	1.93	0.51
1:B:158:ASP:OD1	1:B:173:LYS:NZ	2.38	0.50
1:D:147:TYR:HE1	1:D:185:ALA:HB2	1.76	0.50
1:D:219:ILE:HD13	1:D:411:LEU:CG	2.41	0.50
1:D:87:THR:O	1:D:106:LYS:HB2	2.11	0.50
1:A:196:GLU:HG3	1:A:202:VAL:HG23	1.93	0.49
1:D:208:MET:HA	1:D:211:LYS:HE2	1.93	0.49
1:A:245:ARG:CZ	1:A:252:LEU:HD12	2.42	0.49
1:B:433:GLU:OE2	1:B:465:PRO:HA	2.12	0.49
1:D:132:ILE:O	1:D:194:VAL:HA	2.12	0.49
1:C:328:MET:HE1	1:C:352:LEU:HD11	1.94	0.49
1:A:61:ILE:H	1:A:88:GLN:NE2	2.09	0.49
1:D:142:LEU:HD11	1:D:171:LEU:HD21	1.95	0.49
1:A:28:ALA:HB1	1:A:32:MET:HE1	1.95	0.48
1:D:455:ALA:HB1	1:D:460:VAL:O	2.13	0.48
1:A:472:ARG:HB2	1:B:229[A]:LYS:HE3	1.93	0.48
1:C:84:ILE:HG22	1:C:113:TYR:HB2	1.95	0.48
1:B:207:GLU:O	1:B:211:LYS:HG3	2.14	0.48
1:C:202:VAL:HG11	1:C:220:ASN:ND2	2.28	0.48
1:D:451[B]:ARG:NE	6:D:602:HOH:O	2.23	0.48
1:A:241:VAL:HG23	1:A:245:ARG:HG3	1.95	0.48
1:C:189:LYS:HB3	1:C:189:LYS:HE3	1.65	0.48
1:B:471:TYR:HD1	5:B:505:PEG:C2	2.27	0.48
1:C:146:GLY:HA3	1:C:184:PHE:CD1	2.49	0.47
1:D:433:GLU:O	1:D:437:ARG:HG3	2.14	0.47
5:B:504:PEG:H31	6:B:660:HOH:O	2.13	0.47
1:A:191:ILE:O	6:A:601:HOH:O	2.20	0.47
1:D:25:ILE:O	1:D:29:GLU:HG3	2.14	0.47
1:C:446:LYS:HE2	1:D:302:THR:HG23	1.97	0.47
1:C:146:GLY:HA3	1:C:184:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:LEU:HD11	6:D:734:HOH:O	2.14	0.47
1:D:258:MET:HE1	1:D:281:MET:CB	2.45	0.47
1:D:292:GLN:O	1:D:296:GLU:HG2	2.15	0.47
1:C:319:ASN:HB3	1:C:322:ILE:HD11	1.97	0.47
1:D:267:LYS:NZ	1:D:292:GLN:HE22	2.12	0.47
1:D:196:GLU:HG3	1:D:202:VAL:HG13	1.97	0.46
1:D:279[A]:ARG:HG3	1:D:279[A]:ARG:HH11	1.80	0.46
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.69	0.46
1:C:35:LEU:HA	1:C:35:LEU:HD23	1.57	0.46
1:D:341:GLY:O	2:D:501:NAD:H1D	2.15	0.46
1:C:321:ASP:CB	1:D:451[A]:ARG:HH12	2.28	0.46
1:C:219:ILE:HD12	1:C:411:LEU:HG	1.98	0.46
1:D:146:GLY:HA3	1:D:184:PHE:CD1	2.50	0.46
1:C:135:ASP:OD2	1:C:197:GLU:HG2	2.15	0.46
1:A:158:ASP:O	1:A:159:LYS:HG3	2.15	0.46
1:B:289:CYS:HA	1:B:292:GLN:HE21	1.80	0.46
1:D:230:PHE:HA	1:D:234:TYR:CD2	2.50	0.46
1:A:319:ASN:HB3	1:A:322:ILE:HD11	1.97	0.46
1:A:114:TRP:HB3	1:A:171:LEU:HD22	1.97	0.46
1:A:57:LEU:HG	1:A:135:ASP:HB2	1.97	0.46
1:D:149:ALA:HA	1:D:153:ASP:O	2.16	0.46
1:D:183:TRP:O	1:D:186:GLU:HB3	2.15	0.46
1:C:205:LEU:HA	1:C:208:MET:HE3	1.98	0.46
1:D:227:LYS:HD3	1:D:231:ASP:HB3	1.97	0.46
1:D:339:ASN:ND2	1:D:341:GLY:H	2.14	0.46
6:A:626:HOH:O	5:B:505:PEG:H22	2.16	0.45
1:D:61:ILE:H	1:D:88:GLN:NE2	2.14	0.45
1:C:343:PHE:CD1	1:C:343:PHE:N	2.82	0.45
1:D:231:ASP:C	1:D:231:ASP:OD1	2.55	0.45
1:D:422:LYS:HB2	1:D:422:LYS:HE3	1.68	0.45
1:A:258:MET:HE3	1:A:306:ALA:CB	2.45	0.45
1:D:337:VAL:HG12	1:D:347:ILE:HD13	1.99	0.45
1:D:109:THR:HG1	1:D:112:GLU:H	1.62	0.45
1:D:81:SER:O	1:D:113:TYR:HE1	2.00	0.45
1:C:25:ILE:O	1:C:29:GLU:HG3	2.17	0.45
1:A:138:ASP:HB2	6:A:627:HOH:O	2.17	0.45
1:A:372:LYS:HA	1:A:372:LYS:HD3	1.65	0.45
1:B:239:SER:OG	1:B:392:HIS:HD2	1.99	0.44
1:D:415:ASN:ND2	6:D:610:HOH:O	2.36	0.44
1:B:319:ASN:HB3	1:B:322:ILE:HD11	1.99	0.44
1:C:165:GLU:HG2	5:C:505:PEG:H11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:THR:HG21	1:D:405:THR:HG21	1.98	0.44
1:B:181:LYS:CE	1:B:181:LYS:H	2.30	0.44
1:B:184:PHE:HA	1:B:187:ILE:HD12	2.00	0.44
1:B:62:GLN:HG3	1:B:394:SER:HA	1.99	0.44
1:D:258:MET:CE	1:D:281:MET:HB2	2.48	0.44
1:A:229[B]:LYS:NZ	6:A:603:HOH:O	2.30	0.44
1:A:135:ASP:OD2	3:A:502:ADN:H4'	2.18	0.44
1:B:202:VAL:HG13	1:B:206:TYR:CE2	2.53	0.44
1:B:393:PRO:HG2	1:D:251:MET:HE3	2.00	0.44
1:C:352:LEU:HD13	1:C:367:ILE:HD13	1.99	0.44
1:C:472:ARG:HB2	1:D:229:LYS:HE3	2.00	0.43
1:B:393:PRO:HB2	1:D:251:MET:HB2	2.00	0.43
1:D:230:PHE:O	1:D:234:TYR:N	2.51	0.43
1:C:225:VAL:HG22	1:D:472:ARG:CZ	2.49	0.43
1:C:192:LYS:HZ1	1:C:412:PHE:HE1	1.67	0.43
1:D:123:TRP:CZ3	1:D:129:PRO:HB3	2.53	0.43
1:B:421:ALA:HB3	1:B:425:TYR:OH	2.17	0.43
6:A:684:HOH:O	5:B:505:PEG:H11	2.19	0.43
1:D:207:GLU:O	1:D:211:LYS:HG3	2.18	0.43
1:D:61:ILE:HD13	1:D:91:ALA:HB2	1.99	0.43
1:B:211:LYS:HE3	1:B:211:LYS:HB3	1.85	0.43
1:A:202:VAL:HG11	1:A:220:ASN:ND2	2.33	0.43
1:A:240:LEU:HD22	1:A:269:SER:HB3	2.00	0.43
1:C:251:MET:O	1:C:255:LYS:HG3	2.19	0.43
1:D:242:ASP:O	1:D:246:ARG:HG3	2.19	0.43
1:A:354:ASN:HB2	6:A:653:HOH:O	2.18	0.43
1:B:226:THR:HA	1:B:230:PHE:CD2	2.54	0.43
1:C:259:VAL:O	1:C:282:VAL:HA	2.18	0.43
1:D:179:LYS:HA	1:D:179:LYS:HD2	1.81	0.43
1:D:210:ASN:ND2	6:D:605:HOH:O	2.26	0.43
1:C:289:CYS:HA	1:C:292:GLN:HE21	1.84	0.43
1:D:229:LYS:HD3	1:D:229:LYS:HA	1.85	0.43
1:D:258:MET:HE2	1:D:281:MET:HE2	2.01	0.42
1:D:267:LYS:HZ3	1:D:292:GLN:HE22	1.66	0.42
1:B:179:LYS:HD2	1:B:183:TRP:CE2	2.54	0.42
1:B:423:LYS:HG3	1:B:425:TYR:OH	2.19	0.42
1:B:57:LEU:HD23	1:B:58:HIS:N	2.34	0.42
1:D:114:TRP:HE1	1:D:164:GLU:HG2	1.84	0.42
1:D:309:ARG:NH2	6:D:618:HOH:O	2.49	0.42
1:B:49:LYS:HD2	1:B:50:GLY:N	2.34	0.42
1:C:310:ALA:HB3	1:C:313:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:ALA:HB3	6:C:667:HOH:O	2.20	0.42
1:B:242:ASP:O	1:B:246:ARG:HG3	2.19	0.42
1:B:393:PRO:HD2	1:D:251:MET:CE	2.37	0.42
1:C:257:ALA:CB	1:C:273:LEU:HD13	2.48	0.42
1:C:319:ASN:O	1:C:342:HIS:HE1	2.03	0.42
1:C:79:TRP:HH2	1:C:133:LEU:HD13	1.84	0.42
1:D:146:GLY:HA3	1:D:184:PHE:CE1	2.55	0.42
1:C:319:ASN:O	1:C:346:GLU:HG2	2.20	0.42
1:C:423:LYS:HG2	1:C:424:VAL:N	2.29	0.42
1:C:148:ARG:NH1	6:C:624:HOH:O	2.51	0.42
1:D:187:ILE:O	1:D:191:ILE:HG12	2.20	0.42
1:D:289:CYS:HA	1:D:292:GLN:HE21	1.85	0.42
1:A:299:GLU:HG2	1:A:301:VAL:HG13	2.02	0.42
1:C:175:LEU:HA	1:C:175:LEU:HD23	1.80	0.42
1:C:328:MET:HE3	1:C:347:ILE:CG2	2.49	0.42
1:C:431:LEU:HA	1:C:431:LEU:HD23	1.84	0.42
1:D:258:MET:HE1	1:D:281:MET:HB3	2.00	0.42
1:A:443:ILE:HD13	1:A:443:ILE:HG21	1.80	0.42
1:D:431:LEU:HD23	1:D:431:LEU:HA	1.89	0.42
1:B:132:ILE:O	1:B:194:VAL:HA	2.20	0.41
1:A:199:THR:HG22	1:A:203:HIS:CE1	2.55	0.41
1:C:58:HIS:HE1	3:C:502:ADN:O5'	2.03	0.41
1:C:457:TYR:CD1	1:D:320:LYS:HD3	2.55	0.41
1:A:428:PRO:HG3	5:A:504:PEG:H31	2.02	0.41
1:D:169:TYR:O	1:D:173:LYS:HG3	2.21	0.41
1:D:451[A]:ARG:HD3	6:D:658:HOH:O	2.19	0.41
1:A:371:ASP:OD1	1:A:373:HIS:HB3	2.21	0.41
1:A:472:ARG:CZ	1:B:225:VAL:HG22	2.51	0.41
1:B:196:GLU:HG3	1:B:202:VAL:HG23	2.02	0.41
1:B:252:LEU:HA	1:B:252:LEU:HD23	1.71	0.41
1:C:196:GLU:HG3	1:C:202:VAL:HG23	2.02	0.41
1:D:181:LYS:NZ	6:D:623:HOH:O	2.53	0.41
1:A:147:TYR:O	1:A:151:GLN:HG2	2.21	0.41
1:B:310:ALA:HB3	1:B:313:PHE:CZ	2.55	0.41
1:D:164:GLU:OE1	1:D:343:PHE:HE1	2.04	0.41
1:A:319:ASN:O	1:A:342:HIS:HE1	2.04	0.41
1:C:433:GLU:OE1	1:C:465:PRO:HA	2.20	0.41
1:D:458:ILE:HG13	1:D:460:VAL:HG22	2.03	0.41
1:B:396:VAL:HB	1:D:251:MET:SD	2.61	0.41
1:D:436:ALA:O	1:D:440:LEU:HG	2.21	0.41
1:D:78:ARG:HD3	1:D:123:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:VAL:O	1:B:300:VAL:HA	2.21	0.40
1:D:144:HIS:CD2	1:D:215:LEU:HG	2.56	0.40
1:C:328:MET:CE	1:C:377:MET:HE3	2.51	0.40
1:C:77:ILE:O	1:C:101:PRO:HD2	2.21	0.40
1:D:315:THR:HB	1:D:346:GLU:OE2	2.22	0.40
1:A:258:MET:HE3	1:A:306:ALA:HB2	2.03	0.40
1:A:431:LEU:HA	1:A:431:LEU:HD23	1.77	0.40
1:D:39:ARG:NH2	1:D:68:GLU:HB2	2.36	0.40
1:A:203:HIS:HE1	5:B:505:PEG:C1	2.30	0.40
1:B:80:VAL:HG12	1:B:103:PHE:HB2	2.04	0.40
1:C:15:ILE:HD12	1:C:15:ILE:HA	1.97	0.40
1:C:367:ILE:HD12	1:C:375:ILE:HD11	2.04	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	470/479 (98%)	449 (96%)	19 (4%)	2 (0%)	34	22
1	B	465/479 (97%)	447 (96%)	17 (4%)	1 (0%)	47	38
1	C	465/479 (97%)	450 (97%)	15 (3%)	0	100	100
1	D	470/479 (98%)	439 (93%)	28 (6%)	3 (1%)	25	14
All	All	1870/1916 (98%)	1785 (96%)	79 (4%)	6 (0%)	41	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	160	PRO
1	A	160	PRO
1	B	343	PHE

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Mol	Chain	Res	Type
1	D	348	GLN
1	A	161	GLY
1	D	161	GLY

### 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	382/387 (99%)	374 (98%)	8 (2%)	53	46
1	B	380/387 (98%)	374 (98%)	6 (2%)	62	58
1	C	379/387 (98%)	374 (99%)	5 (1%)	69	65
1	D	382/387 (99%)	372 (97%)	10 (3%)	46	36
All	All	1523/1548 (98%)	1494 (98%)	29 (2%)	60	50

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	A	216	PHE
1	A	241	VAL
1	A	373	HIS
1	A	461	LYS
1	A	468	SER
1	A	470[A]	HIS
1	A	470[B]	HIS
1	B	7	PHE
1	B	39	ARG
1	B	90	HIS
1	B	216	PHE
1	B	373	HIS
1	B	423	LYS
1	C	216	PHE
1	C	373	HIS
1	C	422	LYS
1	C	453[A]	ASP

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Mol	Chain	Res	Type
1	C	453[B]	ASP
1	D	141	MET
1	D	151	GLN
1	D	216	PHE
1	D	229	LYS
1	D	251	MET
1	D	343	PHE
1	D	373	HIS
1	D	451[A]	ARG
1	D	451[B]	ARG
1	D	468	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	88	GLN
1	A	348	GLN
1	A	454	GLN
1	B	90	HIS
1	B	292	GLN
1	B	363	GLN
1	B	392	HIS
1	B	408	GLN
1	C	58	HIS
1	C	292	GLN
1	C	339	ASN
1	D	62	GLN
1	D	88	GLN
1	D	203	HIS
1	D	292	GLN
1	D	339	ASN
1	D	462	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

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	502	-	18,21,21	1.12	2 (11%)	18,31,31	1.92	5 (27%)
2	NAD	D	501	-	42,48,48	1.89	12 (28%)	50,73,73	1.71	8 (16%)
3	ADN	B	502	-	18,21,21	1.10	3 (16%)	18,31,31	1.32	2 (11%)
5	PEG	B	505	-	6,6,6	0.42	0	5,5,5	1.70	1 (20%)
3	ADN	A	502	-	18,21,21	1.08	3 (16%)	18,31,31	1.18	1 (5%)
2	NAD	B	501	-	42,48,48	1.97	13 (30%)	50,73,73	1.47	10 (20%)
5	PEG	C	505	-	6,6,6	0.49	0	5,5,5	1.03	0
2	NAD	C	501	-	42,48,48	1.85	11 (26%)	50,73,73	1.99	11 (22%)
2	NAD	A	501	-	42,48,48	1.79	12 (28%)	50,73,73	1.37	7 (14%)
3	ADN	C	502	-	18,21,21	1.21	2 (11%)	18,31,31	1.66	2 (11%)
5	PEG	B	504	-	6,6,6	0.53	0	5,5,5	0.91	0
5	PEG	A	504	-	6,6,6	0.58	0	5,5,5	0.72	0
5	PEG	C	504	-	6,6,6	0.57	0	5,5,5	0.60	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	502	-	-	0/2/22/22	0/3/3/3
2	NAD	D	501	-	-	5/26/62/62	0/5/5/5
3	ADN	B	502	-	-	1/2/22/22	0/3/3/3
5	PEG	B	505	-	-	3/4/4/4	-
3	ADN	A	502	-	-	0/2/22/22	0/3/3/3
2	NAD	B	501	-	-	5/26/62/62	0/5/5/5
5	PEG	C	505	-	-	2/4/4/4	-
2	NAD	C	501	-	-	5/26/62/62	0/5/5/5
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
3	ADN	C	502	-	-	2/2/22/22	0/3/3/3
5	PEG	B	504	-	-	3/4/4/4	-
5	PEG	A	504	-	-	1/4/4/4	-
5	PEG	C	504	-	-	3/4/4/4	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAD	C2B-C1B	-4.47	1.47	1.53
2	A	501	NAD	C7N-N7N	4.41	1.41	1.33
2	D	501	NAD	C7N-N7N	4.41	1.41	1.33
2	B	501	NAD	C7N-N7N	4.33	1.41	1.33
2	C	501	NAD	C2B-C3B	-4.17	1.41	1.53
2	D	501	NAD	C6A-N6A	4.07	1.48	1.34
2	D	501	NAD	C2B-C3B	-4.01	1.42	1.53
2	C	501	NAD	C2N-N1N	3.96	1.39	1.35
2	B	501	NAD	C2B-C3B	-3.92	1.42	1.53
2	C	501	NAD	C5N-C4N	3.84	1.47	1.38
2	C	501	NAD	C2B-C1B	-3.80	1.48	1.53
2	D	501	NAD	C8A-N7A	3.54	1.41	1.34
2	B	501	NAD	C2N-N1N	3.53	1.39	1.35
2	D	501	NAD	C2N-N1N	3.52	1.39	1.35
2	B	501	NAD	O4B-C1B	-3.51	1.36	1.41
2	B	501	NAD	C5N-C4N	3.45	1.46	1.38
2	B	501	NAD	C4N-C3N	3.41	1.45	1.39
2	A	501	NAD	C2B-C3B	-3.29	1.44	1.53
2	B	501	NAD	C2B-C1B	-3.24	1.48	1.53
2	C	501	NAD	O4B-C4B	-3.23	1.37	1.45
2	B	501	NAD	C8A-N7A	3.23	1.40	1.34
2	D	501	NAD	C2B-C1B	-3.16	1.49	1.53
2	C	501	NAD	O4B-C1B	-3.16	1.36	1.41
2	B	501	NAD	O4B-C4B	-3.06	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAD	C5N-C4N	3.05	1.45	1.38
3	D	502	ADN	C6-N6	3.01	1.45	1.34
2	D	501	NAD	C5N-C4N	2.98	1.45	1.38
2	C	501	NAD	C6A-N6A	2.96	1.44	1.34
2	A	501	NAD	C6A-N6A	2.85	1.44	1.34
2	A	501	NAD	C4N-C3N	2.84	1.44	1.39
2	C	501	NAD	C4N-C3N	2.83	1.44	1.39
2	B	501	NAD	C2D-C1D	-2.76	1.49	1.53
3	D	502	ADN	C8-N7	2.74	1.39	1.34
3	C	502	ADN	C6-N6	2.73	1.44	1.34
2	C	501	NAD	C7N-N7N	2.72	1.38	1.33
2	D	501	NAD	O4D-C1D	2.68	1.44	1.41
2	C	501	NAD	C2A-N3A	2.42	1.36	1.32
3	A	502	ADN	C6-N6	2.42	1.42	1.34
2	A	501	NAD	C2D-C1D	-2.39	1.50	1.53
2	A	501	NAD	C8A-N7A	2.32	1.38	1.34
2	B	501	NAD	O4D-C1D	2.31	1.44	1.41
2	D	501	NAD	C2A-N3A	2.30	1.35	1.32
3	C	502	ADN	C4-N3	2.30	1.38	1.35
2	D	501	NAD	C4N-C3N	2.29	1.43	1.39
2	A	501	NAD	O4B-C1B	-2.28	1.37	1.41
2	B	501	NAD	C6N-N1N	2.24	1.40	1.35
2	A	501	NAD	C3D-C4D	-2.17	1.47	1.53
2	D	501	NAD	O3D-C3D	-2.17	1.37	1.43
3	A	502	ADN	C4-N3	2.15	1.38	1.35
3	B	502	ADN	C6-N6	2.14	1.41	1.34
3	A	502	ADN	C8-N7	2.12	1.38	1.34
2	A	501	NAD	O4B-C4B	-2.09	1.40	1.45
3	B	502	ADN	C2-N3	2.09	1.35	1.32
3	B	502	ADN	C8-N7	2.08	1.38	1.34
2	D	501	NAD	O5D-C5D	-2.07	1.36	1.44
2	A	501	NAD	O3D-C3D	-2.03	1.38	1.43
2	C	501	NAD	C2D-C1D	-2.03	1.50	1.53
2	B	501	NAD	C6A-N6A	2.01	1.41	1.34

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	N3A-C2A-N1A	-6.84	117.98	128.68
2	C	501	NAD	O7N-C7N-N7N	-5.71	114.46	122.58
2	C	501	NAD	C3N-C7N-N7N	5.50	124.35	117.75
2	D	501	NAD	N3A-C2A-N1A	-5.45	120.16	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	ADN	N3-C2-N1	-5.39	120.25	128.68
3	D	502	ADN	N3-C2-N1	-5.26	120.45	128.68
2	D	501	NAD	O7N-C7N-N7N	-4.58	116.07	122.58
2	A	501	NAD	N3A-C2A-N1A	-4.16	122.18	128.68
2	D	501	NAD	C4A-C5A-N7A	-3.93	105.30	109.40
2	B	501	NAD	N3A-C2A-N1A	-3.74	122.83	128.68
2	D	501	NAD	C3N-C7N-N7N	3.60	122.07	117.75
3	B	502	ADN	N3-C2-N1	-3.58	123.08	128.68
3	D	502	ADN	C5-C6-N6	3.52	125.70	120.35
3	A	502	ADN	N3-C2-N1	-3.50	123.21	128.68
3	D	502	ADN	C4-C5-N7	-3.42	105.83	109.40
2	B	501	NAD	PN-O3-PA	-3.21	121.81	132.83
2	C	501	NAD	PN-O3-PA	-3.19	121.86	132.83
2	B	501	NAD	O4D-C1D-C2D	-3.19	102.27	106.93
2	D	501	NAD	C1B-N9A-C4A	-3.17	121.07	126.64
3	C	502	ADN	C1'-N9-C4	-3.10	121.19	126.64
2	A	501	NAD	C5N-C4N-C3N	-3.09	116.68	120.34
2	B	501	NAD	C4A-C5A-N7A	-3.06	106.20	109.40
5	B	505	PEG	O2-C2-C1	2.99	123.19	110.07
2	C	501	NAD	O4D-C1D-C2D	-2.94	102.63	106.93
2	D	501	NAD	PN-O3-PA	-2.84	123.08	132.83
2	B	501	NAD	C6N-N1N-C2N	-2.66	119.55	121.97
2	D	501	NAD	C2A-N1A-C6A	2.65	123.29	118.75
2	C	501	NAD	C4A-C5A-N7A	-2.58	106.71	109.40
2	C	501	NAD	C5B-C4B-C3B	-2.56	105.58	115.18
2	A	501	NAD	C1B-N9A-C4A	-2.54	122.18	126.64
2	D	501	NAD	O3D-C3D-C4D	-2.50	103.81	111.05
2	C	501	NAD	C3N-C2N-N1N	2.50	122.87	120.43
2	C	501	NAD	C2A-N1A-C6A	2.48	123.00	118.75
2	B	501	NAD	C1B-N9A-C4A	-2.46	122.33	126.64
3	B	502	ADN	C1'-N9-C4	-2.45	122.33	126.64
3	D	502	ADN	C2-N1-C6	2.42	122.89	118.75
2	A	501	NAD	O2B-C2B-C3B	2.37	119.49	111.82
2	B	501	NAD	O5B-PA-O1A	2.29	118.00	109.07
2	C	501	NAD	C1B-N9A-C4A	-2.27	122.65	126.64
2	B	501	NAD	C5N-C4N-C3N	-2.26	117.67	120.34
2	B	501	NAD	O4B-C1B-C2B	-2.23	103.67	106.93
2	A	501	NAD	O5D-C5D-C4D	2.18	116.50	108.99
2	B	501	NAD	O4B-C4B-C3B	2.13	109.34	105.11
2	C	501	NAD	O2N-PN-O1N	2.10	122.61	112.24
3	D	502	ADN	C3'-C2'-C1'	2.08	104.11	100.98
2	A	501	NAD	PN-O3-PA	-2.05	125.78	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAD	C2N-C3N-C4N	2.03	120.56	118.26

There are no chirality outliers.

All (35) torsion outliers are listed below:

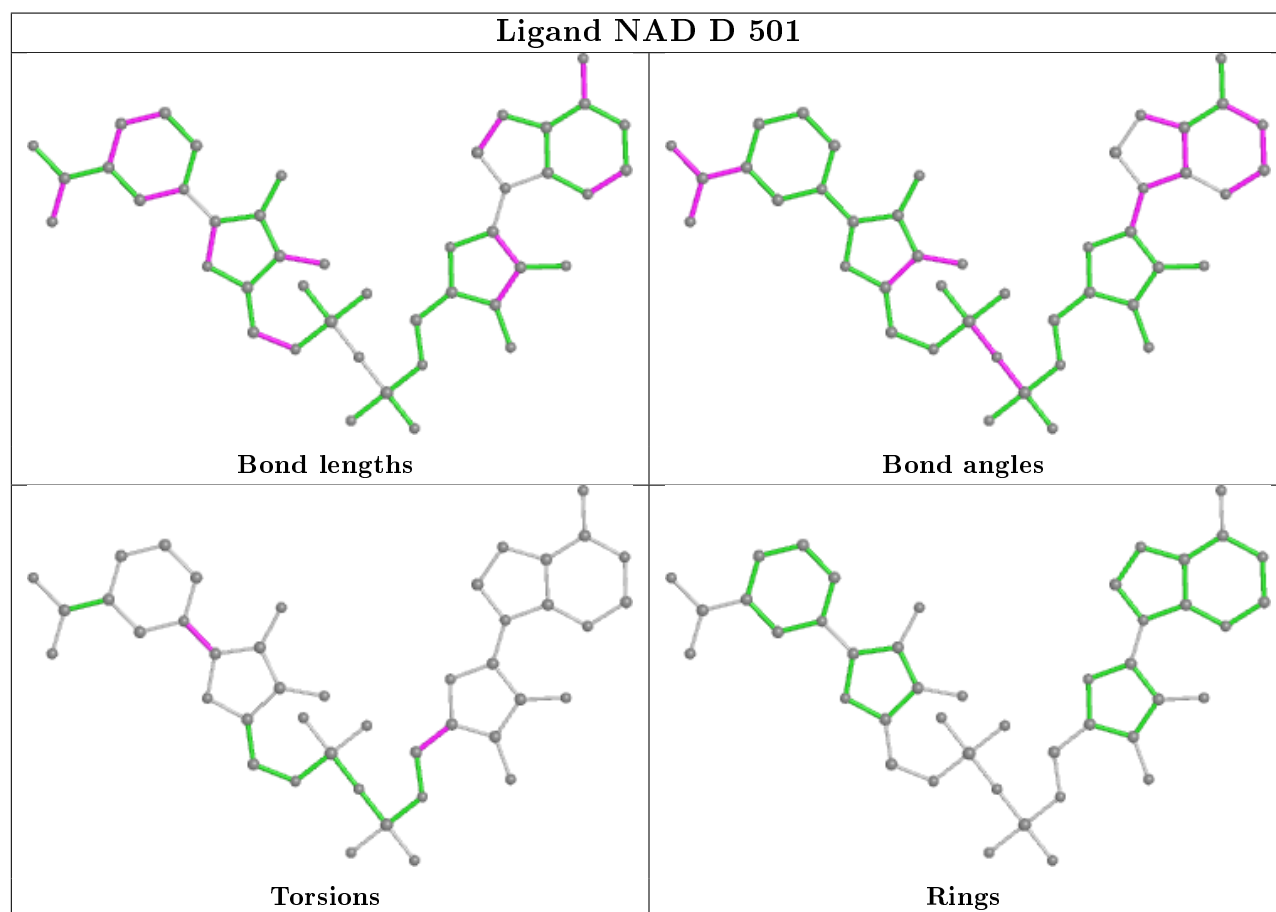
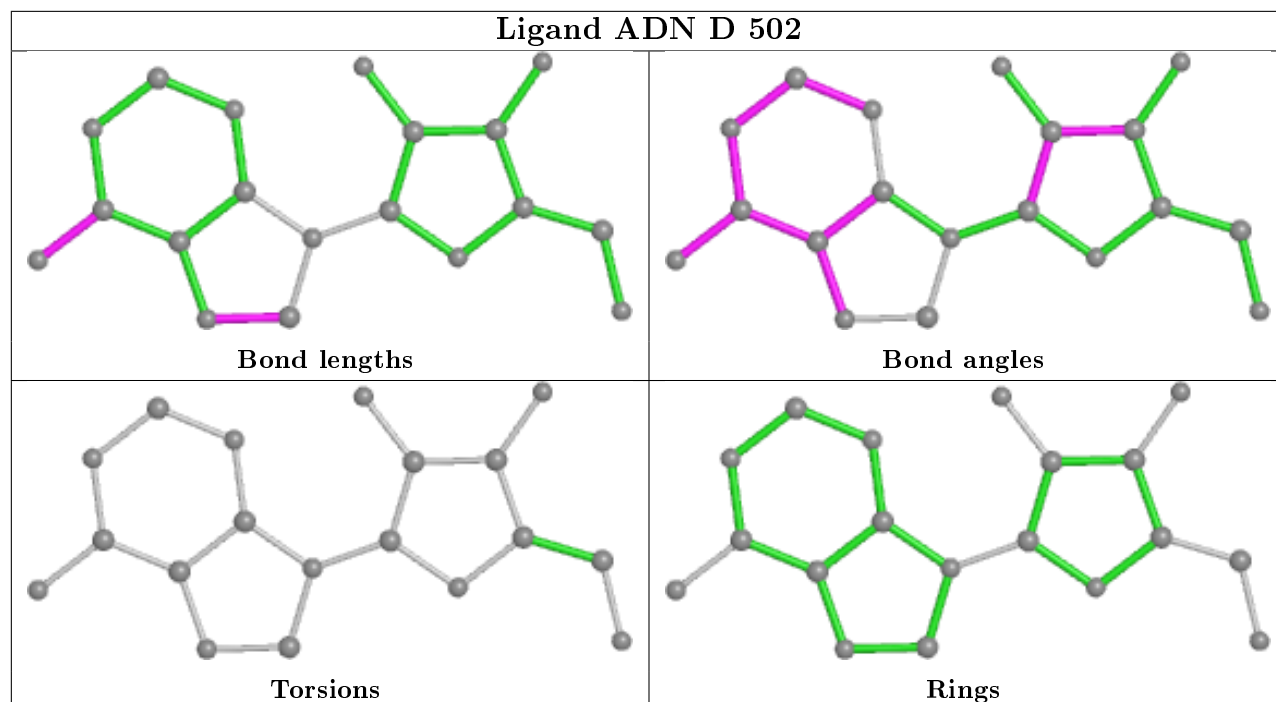
Mol	Chain	Res	Type	Atoms
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	C	501	NAD	C2D-C1D-N1N-C6N
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
5	C	505	PEG	C4-C3-O2-C2
3	C	502	ADN	C3'-C4'-C5'-O5'
3	C	502	ADN	O4'-C4'-C5'-O5'
5	B	505	PEG	O1-C1-C2-O2
5	B	504	PEG	O1-C1-C2-O2
5	C	504	PEG	O2-C3-C4-O4
5	B	504	PEG	O2-C3-C4-O4
5	A	504	PEG	O2-C3-C4-O4
3	B	502	ADN	C3'-C4'-C5'-O5'
5	C	505	PEG	C1-C2-O2-C3
5	B	505	PEG	C4-C3-O2-C2
2	B	501	NAD	O4B-C4B-C5B-O5B
5	B	505	PEG	O2-C3-C4-O4
5	C	504	PEG	C4-C3-O2-C2
5	C	504	PEG	O1-C1-C2-O2
5	B	504	PEG	C1-C2-O2-C3
2	D	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B

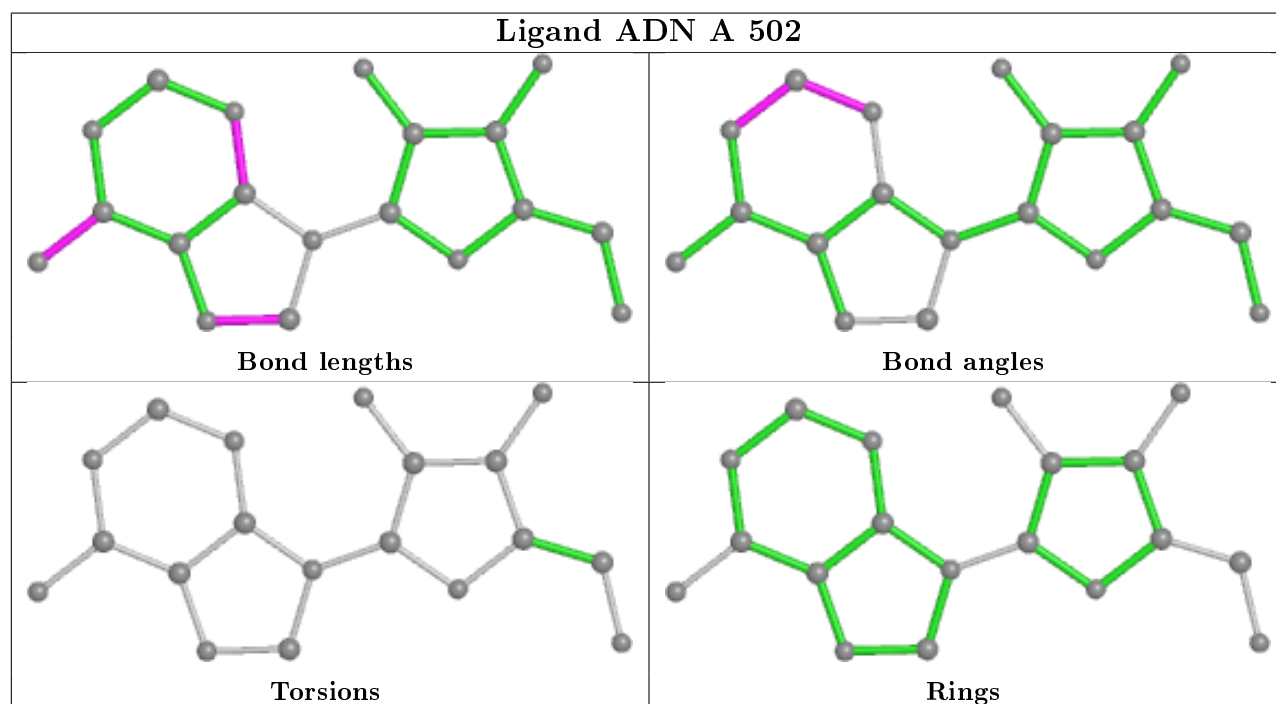
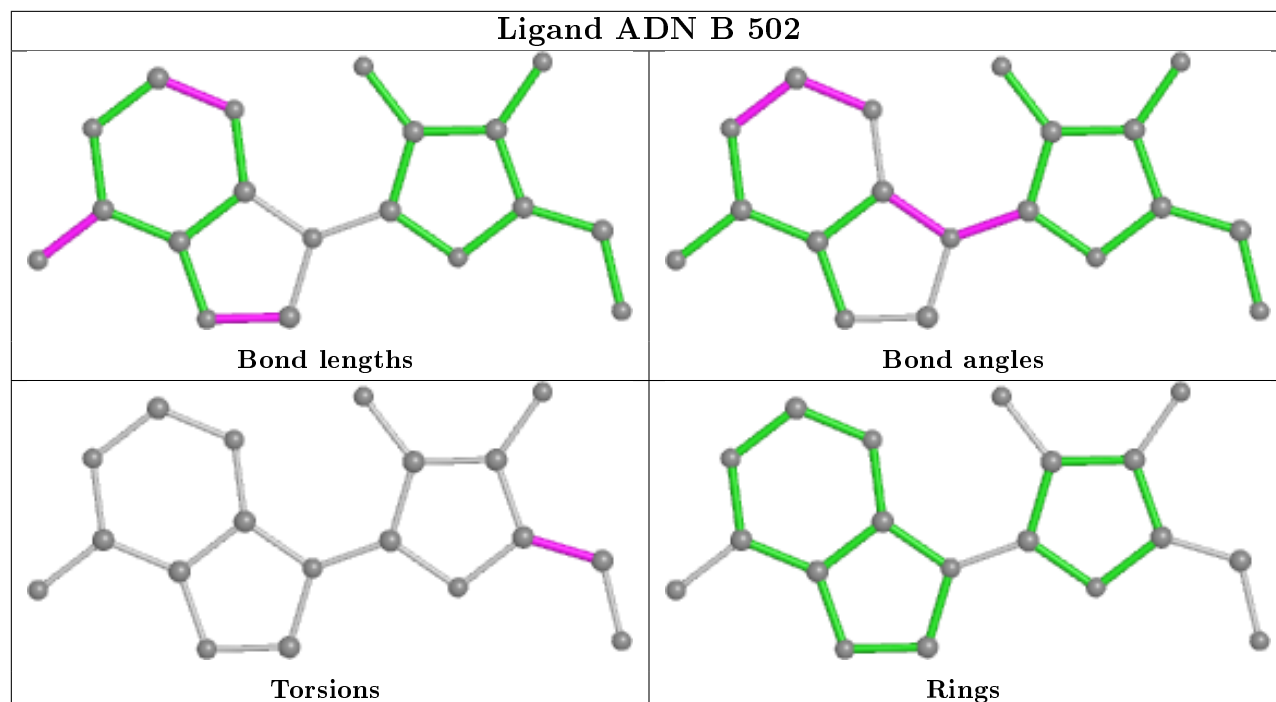
There are no ring outliers.

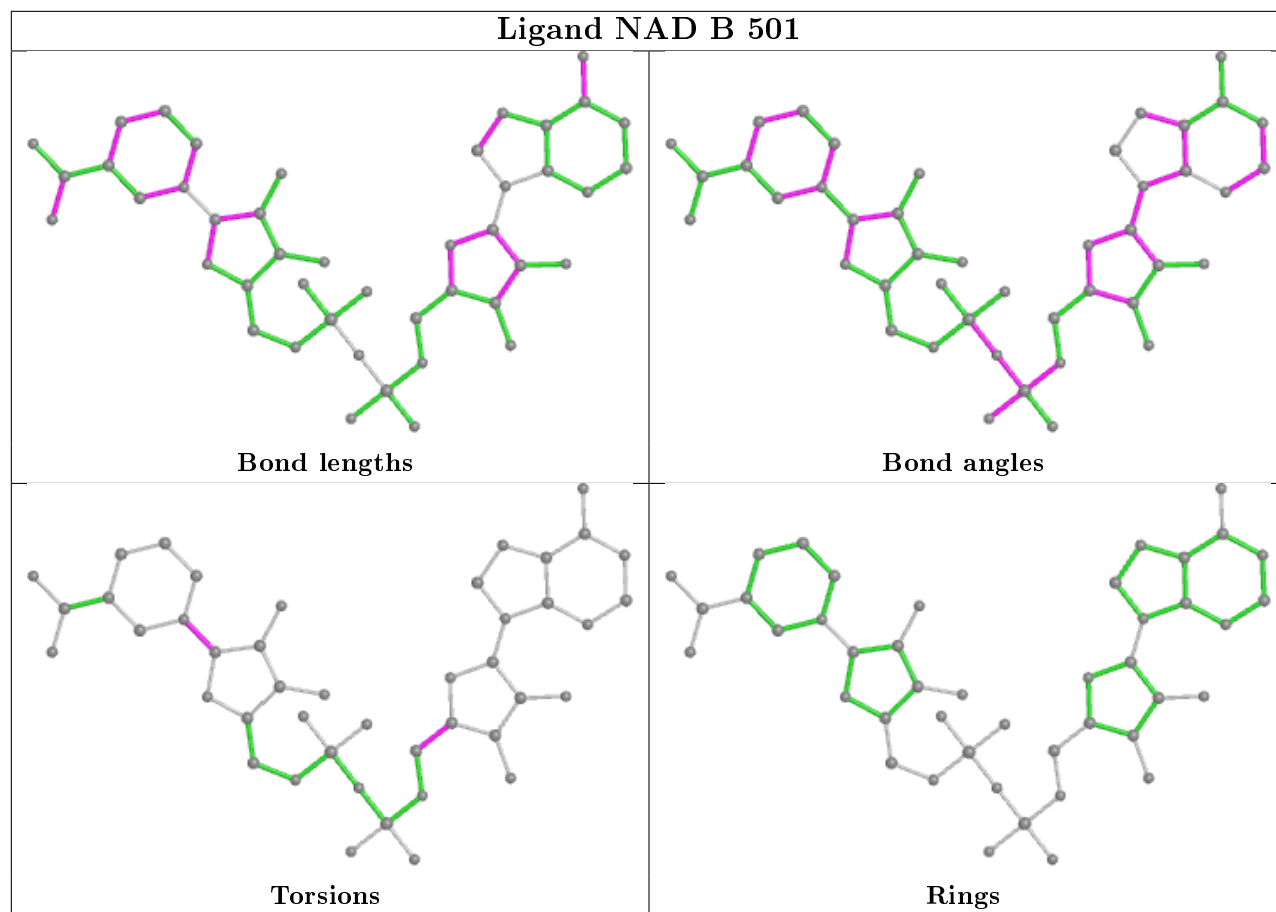
12 monomers are involved in 22 short contacts:

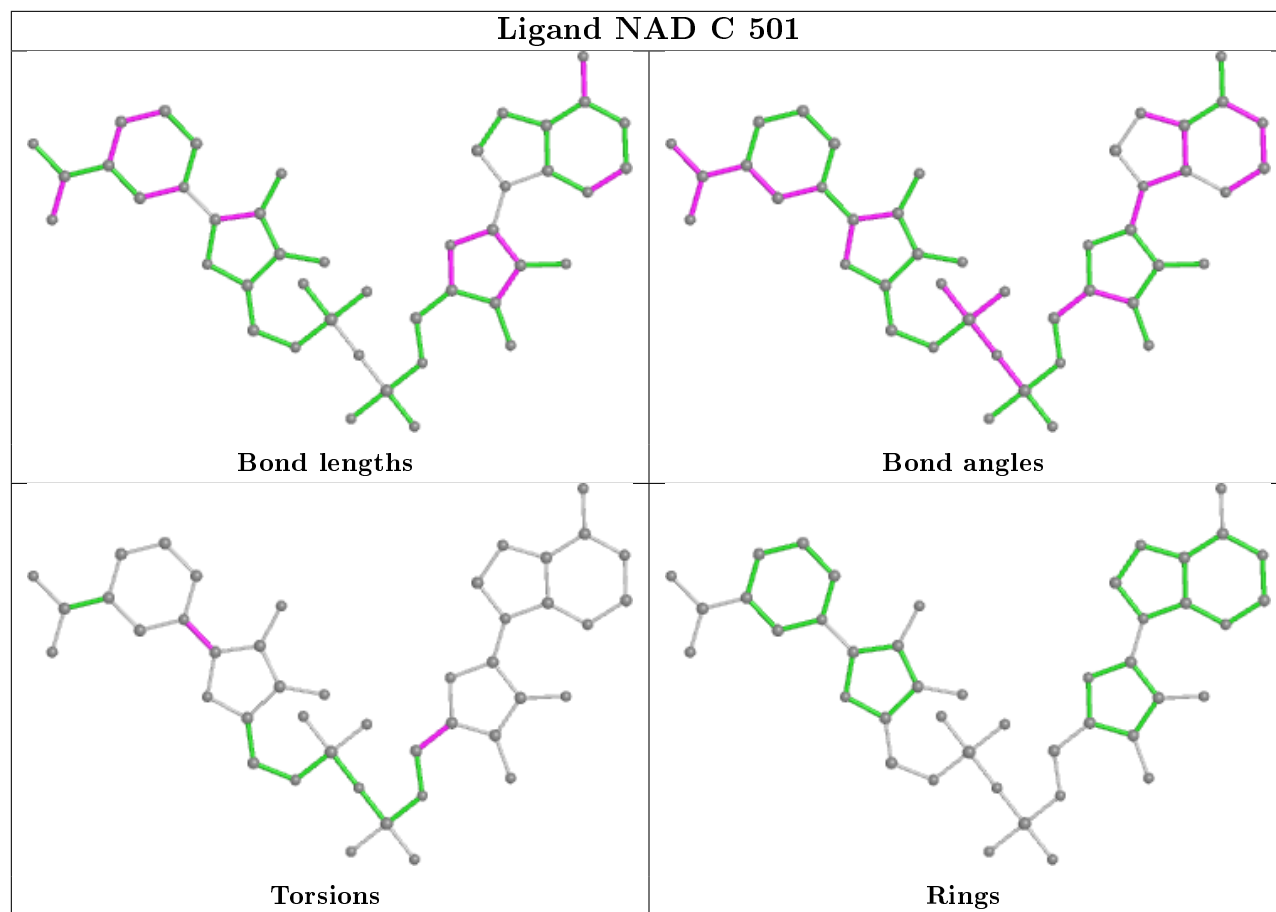
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	ADN	3	0
2	D	501	NAD	2	0
3	B	502	ADN	1	0
5	B	505	PEG	8	0
3	A	502	ADN	2	0
2	B	501	NAD	1	0
5	C	505	PEG	1	0
2	C	501	NAD	2	0
2	A	501	NAD	1	0
3	C	502	ADN	3	0
5	B	504	PEG	1	0
5	A	504	PEG	1	0

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.

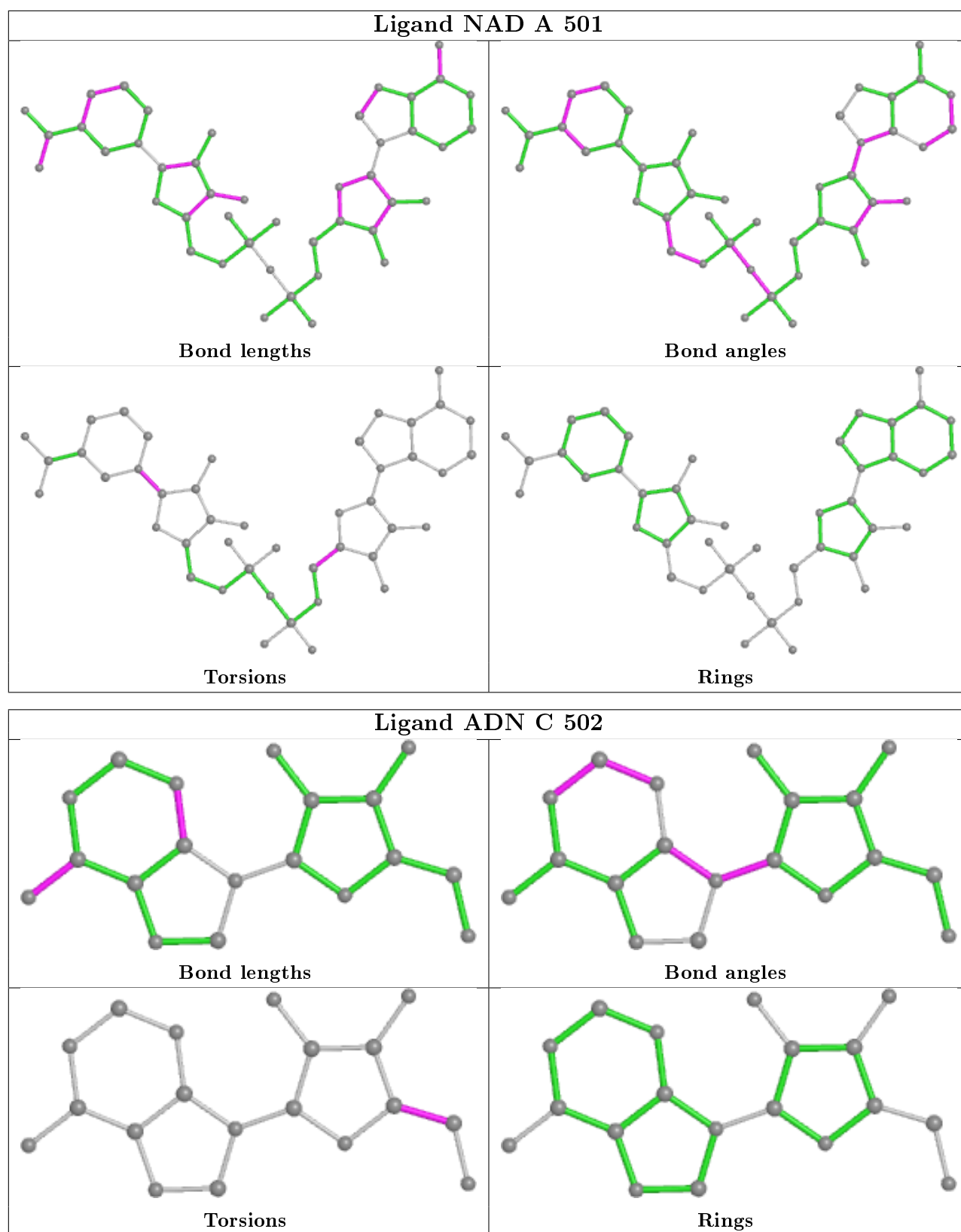












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	468/479 (97%)	-0.13	9 (1%) 66 74	16, 27, 52, 79	2 (0%)
1	B	464/479 (96%)	0.12	17 (3%) 41 51	17, 28, 52, 105	2 (0%)
1	C	463/479 (96%)	0.22	18 (3%) 39 49	17, 33, 59, 106	2 (0%)
1	D	468/479 (97%)	0.64	61 (13%) 3 5	18, 37, 88, 111	2 (0%)
All	All	1863/1916 (97%)	0.22	105 (5%) 24 33	16, 30, 66, 111	8 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	PHE	12.9
1	D	157	LEU	8.7
1	B	7	PHE	7.5
1	B	6	GLY	7.2
1	D	162	SER	7.2
1	D	155	ALA	7.0
1	C	8	THR	5.9
1	D	7	PHE	5.9
1	D	160	PRO	5.5
1	D	161	GLY	5.4
1	C	6	GLY	5.3
1	D	158	ASP	5.2
1	D	170	ALA	4.9
1	B	176	LEU	4.8
1	D	166	GLU	4.6
1	D	153	ASP	4.5
1	D	12	VAL	4.5
1	D	163	GLU	4.4
1	D	43	GLY	4.2
1	D	418	SER	4.0
1	D	169	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	417	ASP	3.8
1	D	109	THR	3.7
1	D	419	LYS	3.7
1	D	167	ILE	3.6
1	A	6	GLY	3.6
1	D	177	LYS	3.4
1	D	6	GLY	3.4
1	D	154	THR	3.4
1	D	149	ALA	3.3
1	A	156	PHE	3.3
1	D	213	THR	3.3
1	D	183	TRP	3.2
1	A	7	PHE	3.2
1	D	137	GLY	3.2
1	D	156	PHE	3.2
1	C	123	TRP	3.2
1	D	146	GLY	3.1
1	B	229[A]	LYS	3.1
1	D	11	ILE	3.1
1	A	155	ALA	3.1
1	D	15	ILE	3.0
1	C	125	GLY	3.0
1	D	210	ASN	3.0
1	D	343	PHE	2.9
1	D	10	TYR	2.9
1	C	124	HIS	2.9
1	D	171	LEU	2.9
1	C	126	GLY	2.8
1	D	74	GLY	2.8
1	D	420	TYR	2.8
1	D	414[A]	ASN	2.8
1	B	343	PHE	2.8
1	A	8	THR	2.7
1	B	273	LEU	2.6
1	D	148	ARG	2.6
1	C	343	PHE	2.6
1	B	149	ALA	2.6
1	C	203[A]	HIS	2.5
1	C	154	THR	2.5
1	D	113	TYR	2.5
1	C	44	PRO	2.5
1	D	42	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	182	GLY	2.5
1	D	8	THR	2.5
1	D	96	ALA	2.5
1	A	373	HIS	2.5
1	A	416	LYS	2.4
1	C	127	GLY	2.4
1	D	173	LYS	2.4
1	B	278	CYS	2.4
1	B	244	ILE	2.4
1	D	151	GLN	2.4
1	B	230	PHE	2.4
1	B	421	ALA	2.3
1	D	84	ILE	2.3
1	D	423	LYS	2.3
1	C	45	LYS	2.3
1	D	355	LEU	2.3
1	B	152	GLY	2.3
1	D	9	ASP	2.3
1	D	421	ALA	2.3
1	D	107	GLY	2.2
1	D	203	HIS	2.2
1	D	217	PRO	2.2
1	A	161	GLY	2.2
1	C	49	LYS	2.2
1	C	372	LYS	2.2
1	D	159	LYS	2.2
1	D	211	LYS	2.2
1	D	142	LEU	2.2
1	B	276	ALA	2.2
1	C	74	GLY	2.2
1	B	151	GLN	2.1
1	D	147	TYR	2.1
1	D	118	ALA	2.1
1	D	164	GLU	2.1
1	B	8	THR	2.1
1	A	372	LYS	2.1
1	D	218	ALA	2.1
1	C	412	PHE	2.1
1	D	214	LEU	2.1
1	D	175	LEU	2.0
1	B	184	PHE	2.0
1	B	49	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

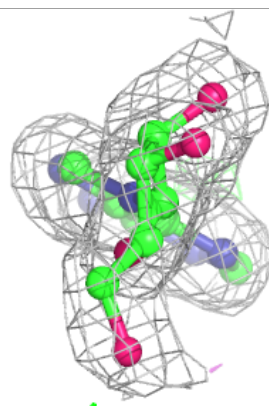
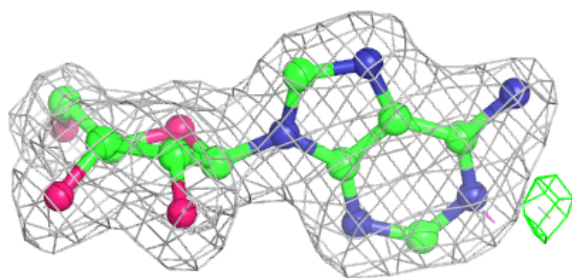
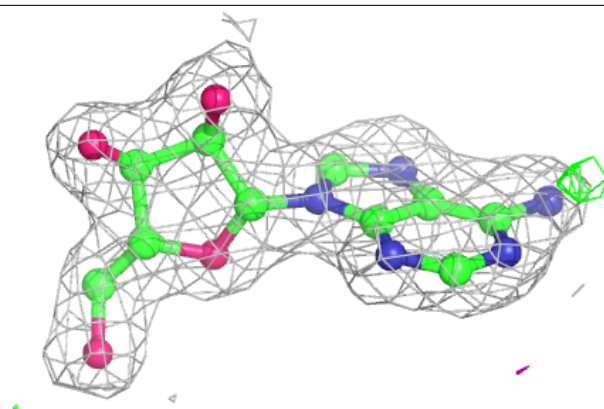
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PEG	B	505	7/7	0.72	0.30	53,57,61,62	0
5	PEG	C	505	7/7	0.78	0.16	57,65,70,72	0
5	PEG	A	504	7/7	0.82	0.19	68,70,71,72	0
5	PEG	C	504	7/7	0.89	0.13	42,50,65,75	0
5	PEG	B	504	7/7	0.91	0.14	41,49,55,58	0
3	ADN	A	502	19/19	0.96	0.09	18,24,31,32	0
2	NAD	D	501	44/44	0.96	0.09	20,31,40,45	0
3	ADN	C	502	19/19	0.96	0.11	22,27,35,37	0
3	ADN	D	502	19/19	0.97	0.08	21,30,42,42	0
3	ADN	B	502	19/19	0.97	0.12	16,22,33,34	0
4	NA	A	503	1/1	0.97	0.07	24,24,24,24	0
2	NAD	A	501	44/44	0.97	0.08	20,26,31,34	0
2	NAD	B	501	44/44	0.98	0.09	16,25,33,36	0
4	NA	D	503	1/1	0.98	0.10	34,34,34,34	0
2	NAD	C	501	44/44	0.98	0.09	16,26,38,42	0
4	NA	B	503	1/1	0.99	0.12	21,21,21,21	0
4	NA	C	503	1/1	1.00	0.07	27,27,27,27	0

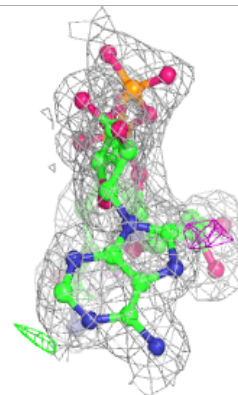
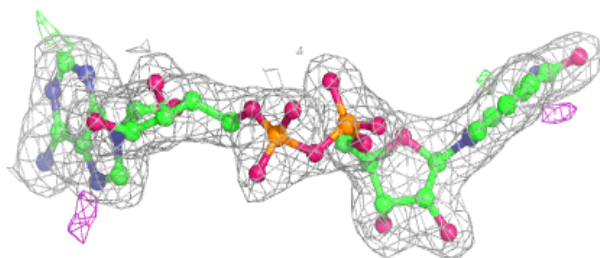
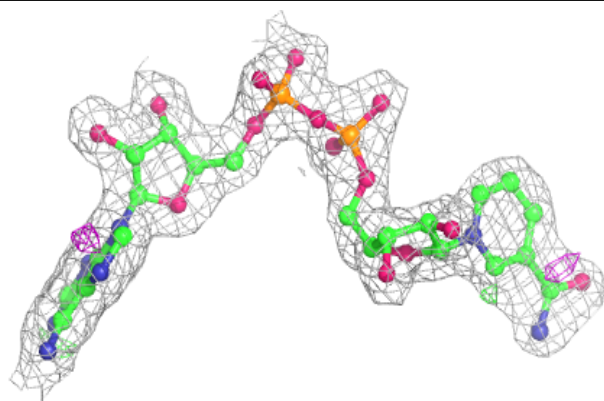
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADN A 502:**

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

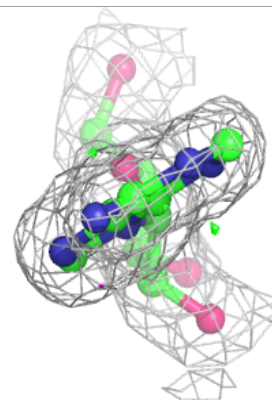
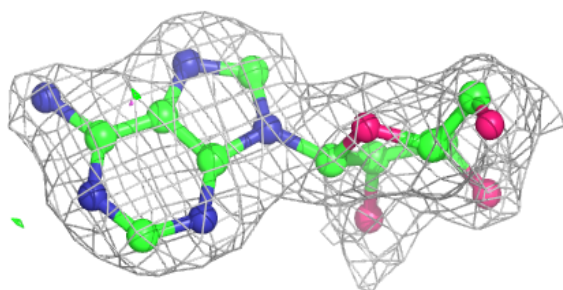
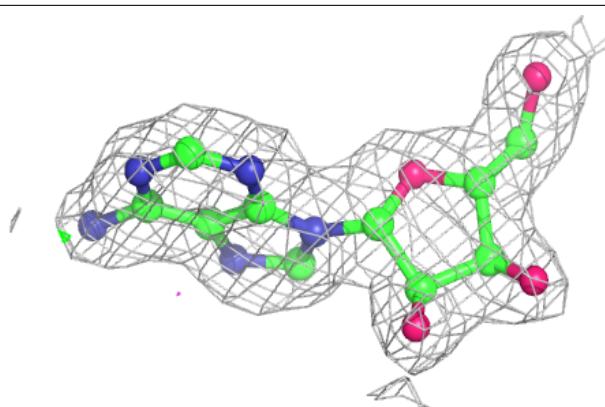
**Electron density around NAD D 501:**

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

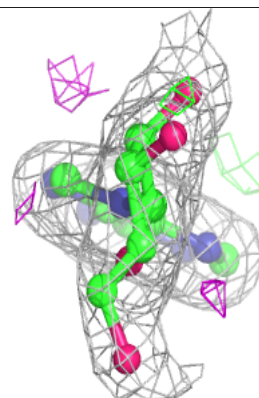
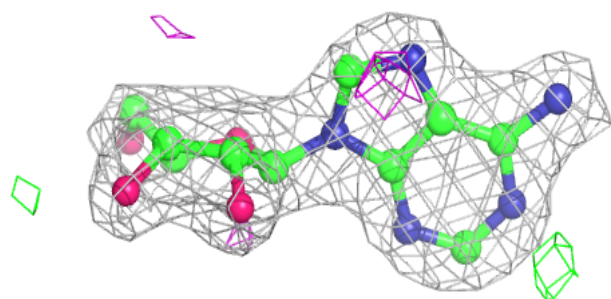
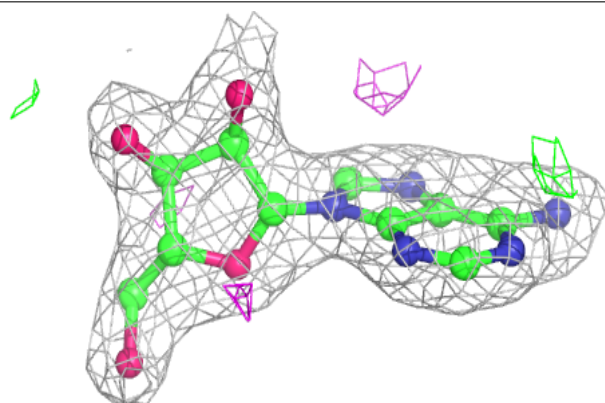


**Electron density around ADN C 502:**

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

**Electron density around ADN D 502:**

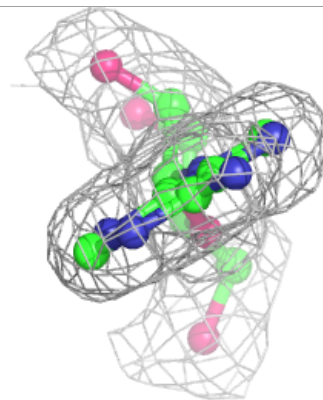
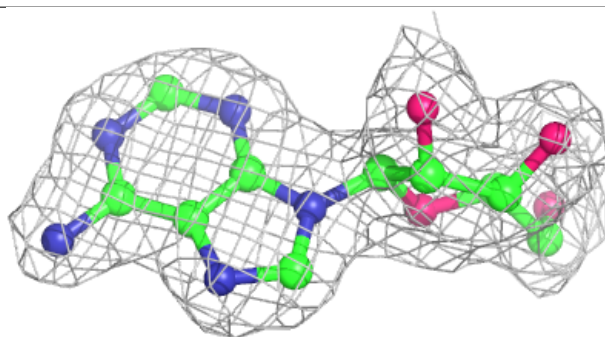
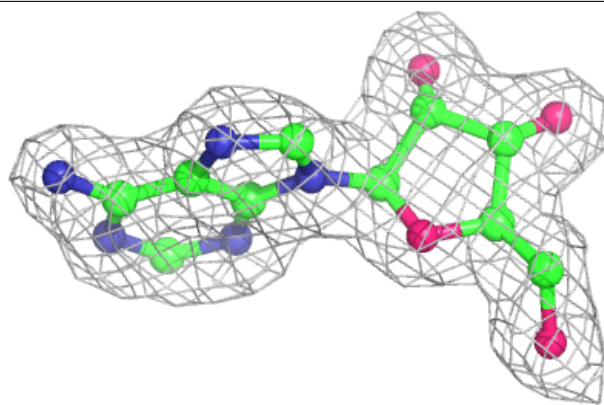
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



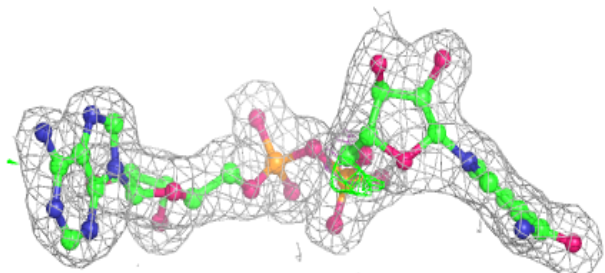
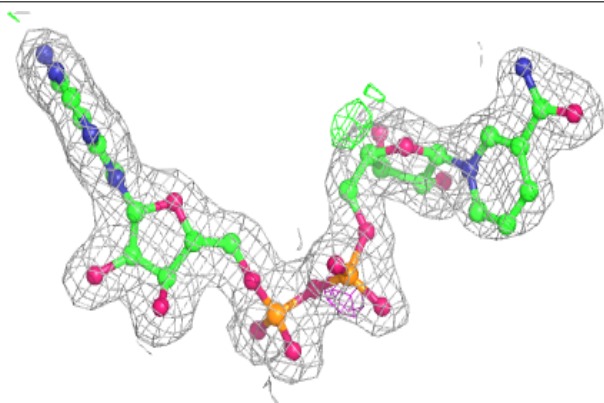


**Electron density around ADN B 502:**

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

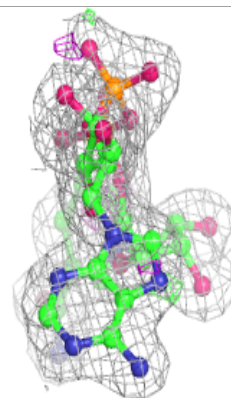
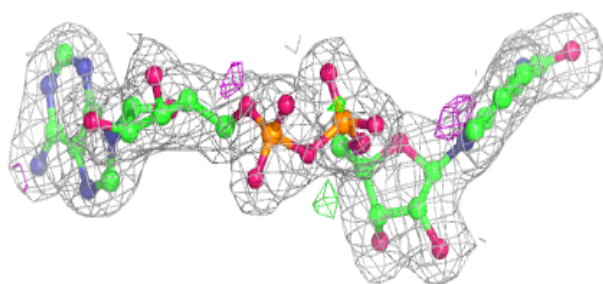
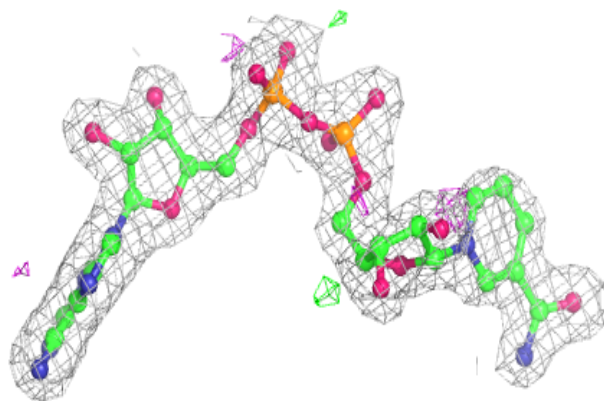
**Electron density around NAD A 501:**

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

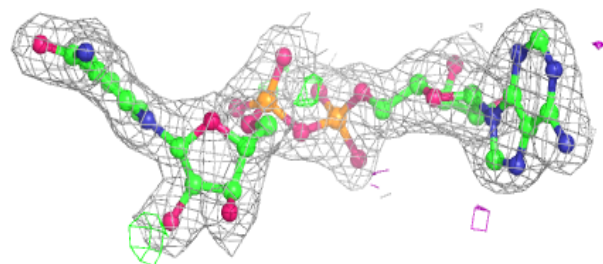
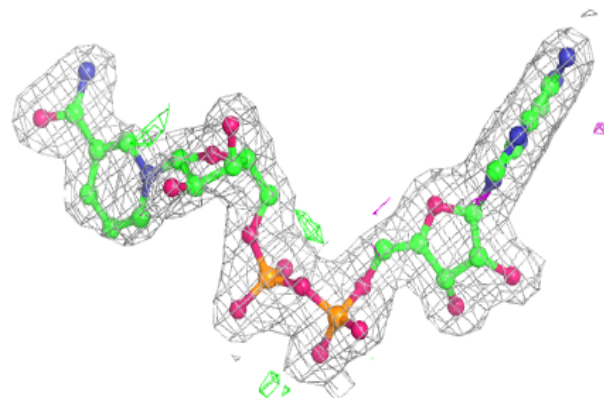


**Electron density around NAD B 501:**

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

**Electron density around NAD C 501:**

$2mF_o-DF_c$  (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.