



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 10:23 pm BST

PDB ID : 3CE6  
Title : Crystal structure of Mycobacterium tuberculosis S-adenosyl-L-homocysteine hydrolase in ternary complex with NAD and adenosine  
Authors : Reddy, M.C.M.; Gokulan, K.; Shetty, N.D.; Owen, J.L.; Ioerger, T.R.; Sacchettini, J.C.  
Deposited on : 2008-02-28  
Resolution : 1.60 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

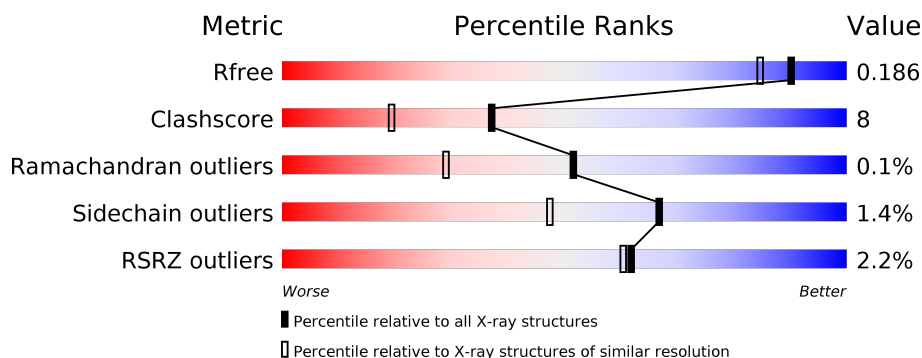
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	494	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 17%, green 81%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>81%</span> <span>17%</span> <span>..</span> </div> </div>
1	B	494	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 82%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>82%</span> <span>15%</span> <span>..</span> </div> </div>
1	C	494	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 19%, green 77%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>77%</span> <span>19%</span> <span>..</span> </div> </div>
1	D	494	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 17%, green 79%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>79%</span> <span>17%</span> <span>..</span> </div> </div>

## 2 Entry composition [i](#)

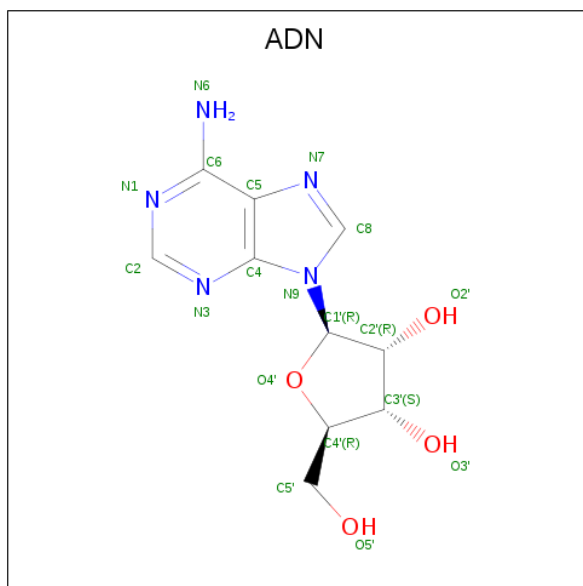
There are 4 unique types of molecules in this entry. The entry contains 16984 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3753	2367	644	725	17			
1	B	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	C	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	D	485	Total	C	N	O	S	0	0	0
			3747	2363	643	724	17			

- Molecule 2 is ADENOSINE (three-letter code: ADN) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>4</sub>).



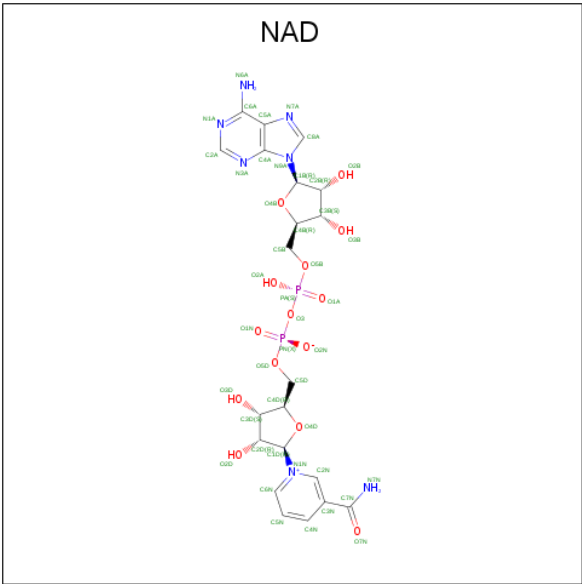
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (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>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	446	Total	O	0	0
			446	446		
4	B	465	Total	O	0	0
			465	465		
4	C	396	Total	O	0	0
			396	396		

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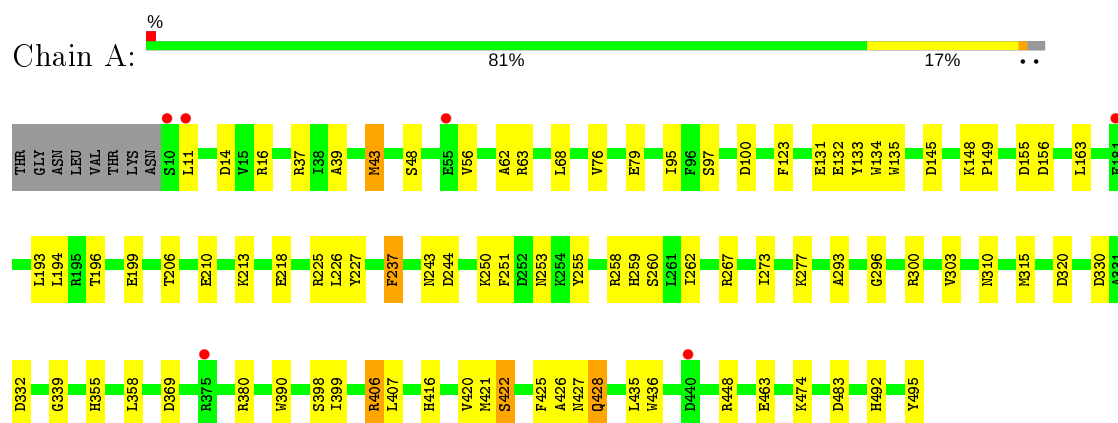
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	429	Total	O	0	0
			429	429		

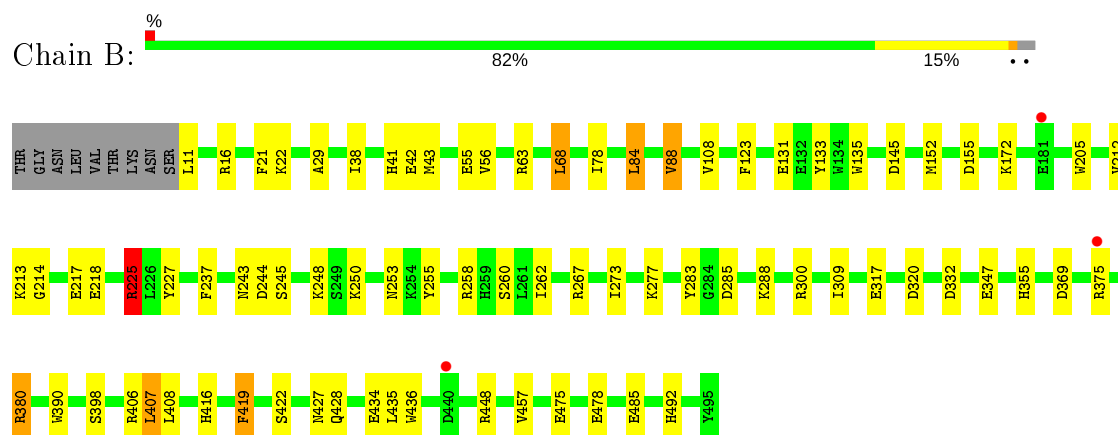
### 3 Residue-property plots [i](#)

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.

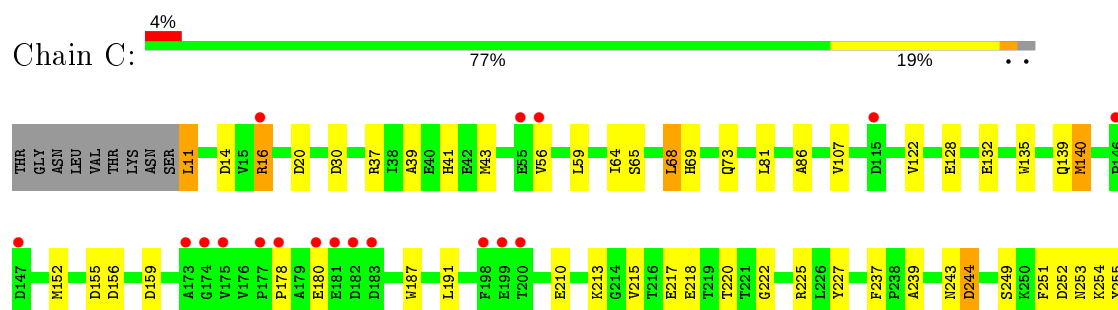
#### • Molecule 1: Adenosylhomocysteinase

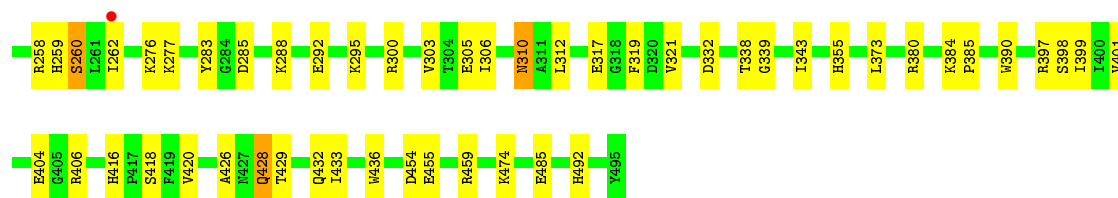


#### • Molecule 1: Adenosylhomocysteinase

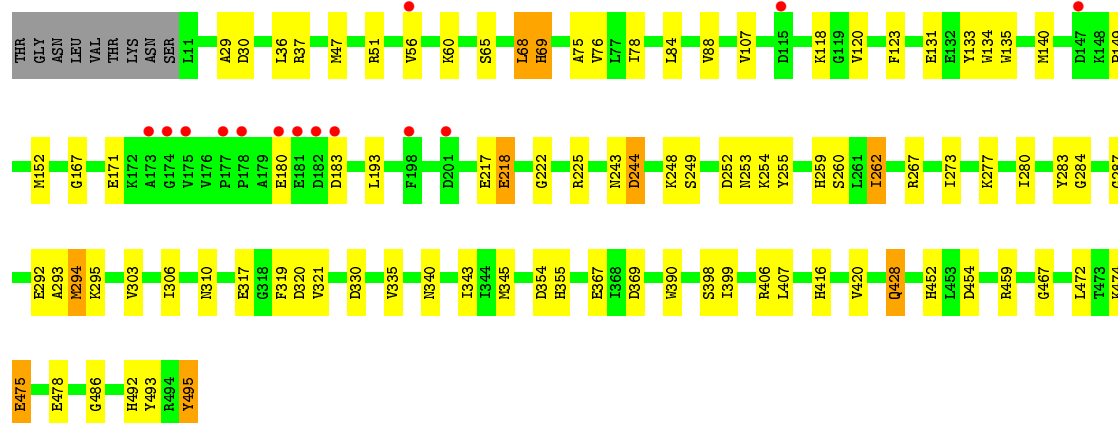
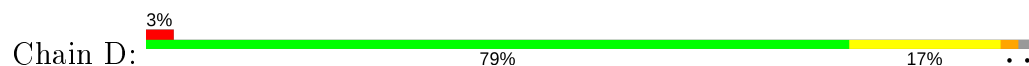


#### • Molecule 1: Adenosylhomocysteinase





• Molecule 1: Adenosylhomocysteinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.04Å 112.13Å 100.23Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 45.72 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-1.60) 94.9 (45.72-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.200 , 0.238 0.181 , 0.186	Depositor DCC
$R_{free}$ test set	16448 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.7	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.076 for h,-k,-l 0.004 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, 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	1.51	24/3829 (0.6%)	1.40	37/5193 (0.7%)
1	B	1.51	24/3824 (0.6%)	1.34	25/5186 (0.5%)
1	C	1.42	16/3824 (0.4%)	1.23	26/5186 (0.5%)
1	D	1.46	16/3822 (0.4%)	1.25	21/5182 (0.4%)
All	All	1.47	80/15299 (0.5%)	1.31	109/20747 (0.5%)

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	GLU	CG-CD	8.19	1.64	1.51
1	C	107	VAL	CB-CG1	8.08	1.69	1.52
1	D	475	GLU	CD-OE2	8.05	1.34	1.25
1	D	249	SER	CB-OG	8.04	1.52	1.42
1	D	107	VAL	CB-CG1	7.39	1.68	1.52
1	B	131	GLU	CG-CD	7.37	1.62	1.51
1	D	495	TYR	CE2-CZ	7.23	1.48	1.38
1	B	205	TRP	CE3-CZ3	7.19	1.50	1.38
1	A	131	GLU	CD-OE1	7.16	1.33	1.25
1	A	237	PHE	CE2-CZ	7.12	1.50	1.37
1	C	459	ARG	CB-CG	-6.62	1.34	1.52
1	A	483	ASP	CB-CG	6.50	1.65	1.51
1	D	459	ARG	CB-CG	-6.39	1.35	1.52
1	C	128	GLU	CG-CD	6.28	1.61	1.51
1	A	225	ARG	CZ-NH1	6.20	1.41	1.33
1	B	283	TYR	CG-CD1	6.15	1.47	1.39
1	B	131	GLU	CD-OE1	6.12	1.32	1.25
1	A	255	TYR	CD1-CE1	6.11	1.48	1.39
1	C	319	PHE	CE2-CZ	6.07	1.48	1.37
1	B	255	TYR	CE1-CZ	6.07	1.46	1.38
1	C	305	GLU	CD-OE1	6.05	1.32	1.25
1	B	225	ARG	CB-CG	-5.97	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	VAL	CB-CG1	5.92	1.65	1.52
1	D	475	GLU	CG-CD	5.92	1.60	1.51
1	B	133	TYR	CE1-CZ	5.92	1.46	1.38
1	B	212	VAL	CB-CG2	5.85	1.65	1.52
1	D	123	PHE	CD1-CE1	5.85	1.50	1.39
1	A	339	GLY	C-O	5.85	1.33	1.23
1	B	317	GLU	CD-OE2	5.84	1.32	1.25
1	A	255	TYR	CZ-OH	5.83	1.47	1.37
1	C	225	ARG	CZ-NH2	5.81	1.40	1.33
1	A	255	TYR	CE1-CZ	5.74	1.46	1.38
1	D	133	TYR	CD2-CE2	5.72	1.48	1.39
1	B	237	PHE	CE2-CZ	5.65	1.48	1.37
1	D	262	ILE	C-O	-5.59	1.12	1.23
1	D	287	GLY	N-CA	5.55	1.54	1.46
1	A	495	TYR	CE1-CZ	5.54	1.45	1.38
1	C	426	ALA	CA-CB	5.54	1.64	1.52
1	B	288	LYS	CD-CE	5.54	1.65	1.51
1	A	135	TRP	CD2-CE2	5.49	1.48	1.41
1	C	249	SER	CB-OG	5.48	1.49	1.42
1	B	21	PHE	CE1-CZ	5.47	1.47	1.37
1	B	457	VAL	CB-CG1	5.45	1.64	1.52
1	A	62	ALA	CA-CB	5.44	1.63	1.52
1	A	421	MET	C-O	5.42	1.33	1.23
1	C	260	SER	CB-OG	-5.41	1.35	1.42
1	C	222	GLY	C-O	5.41	1.32	1.23
1	A	251	PHE	CD2-CE2	5.39	1.50	1.39
1	C	135	TRP	CG-CD1	5.39	1.44	1.36
1	C	404	GLU	CG-CD	5.39	1.60	1.51
1	C	122	VAL	CB-CG1	5.37	1.64	1.52
1	C	276	LYS	CD-CE	5.37	1.64	1.51
1	C	251	PHE	CD1-CE1	5.36	1.50	1.39
1	A	303	VAL	CB-CG1	-5.35	1.41	1.52
1	B	255	TYR	CD1-CE1	5.33	1.47	1.39
1	B	217	GLU	CB-CG	5.29	1.62	1.52
1	A	48	SER	CB-OG	5.29	1.49	1.42
1	D	29	ALA	CA-CB	5.29	1.63	1.52
1	A	97	SER	CA-CB	-5.26	1.45	1.52
1	A	79	GLU	CB-CG	5.24	1.62	1.52
1	D	255	TYR	CE1-CZ	5.23	1.45	1.38
1	B	419	PHE	CE2-CZ	5.22	1.47	1.37
1	B	135	TRP	CG-CD1	5.21	1.44	1.36
1	A	426	ALA	N-CA	5.21	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	TYR	CZ-OH	5.20	1.46	1.37
1	D	218	GLU	CD-OE1	5.20	1.31	1.25
1	A	135	TRP	CG-CD1	5.19	1.44	1.36
1	B	38	ILE	CA-CB	-5.18	1.43	1.54
1	C	310	ASN	CG-OD1	5.17	1.35	1.24
1	B	347	GLU	CD-OE2	5.17	1.31	1.25
1	A	76	VAL	N-CA	5.16	1.56	1.46
1	D	222	GLY	C-O	5.16	1.31	1.23
1	D	135	TRP	CG-CD1	5.16	1.44	1.36
1	B	245	SER	CB-OG	5.14	1.49	1.42
1	B	434	GLU	CG-CD	5.12	1.59	1.51
1	A	293	ALA	CA-CB	-5.11	1.41	1.52
1	A	425	PHE	CE2-CZ	5.10	1.47	1.37
1	A	296	GLY	N-CA	5.07	1.53	1.46
1	B	309	ILE	CA-CB	-5.05	1.43	1.54
1	D	131	GLU	CG-CD	5.04	1.59	1.51

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	MET	CG-SD-CE	-24.62	60.80	100.20
1	A	406	ARG	NE-CZ-NH2	-17.21	111.69	120.30
1	A	225	ARG	NE-CZ-NH2	-14.59	113.00	120.30
1	A	406	ARG	CD-NE-CZ	14.06	143.28	123.60
1	A	406	ARG	CG-CD-NE	-13.08	84.34	111.80
1	A	300	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	C	225	ARG	NE-CZ-NH1	-12.62	113.99	120.30
1	A	406	ARG	NE-CZ-NH1	11.92	126.26	120.30
1	A	406	ARG	CB-CG-CD	10.78	139.63	111.60
1	A	225	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	B	16	ARG	NE-CZ-NH1	10.25	125.43	120.30
1	C	406	ARG	NE-CZ-NH1	-9.79	115.41	120.30
1	A	369	ASP	CB-CG-OD2	-9.25	109.98	118.30
1	B	300	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	D	406	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	C	225	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	B	448	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	A	332	ASP	CB-CG-OD2	8.21	125.69	118.30
1	A	63	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	D	454	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	B	63	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	D	294	MET	CG-SD-CE	-7.96	87.46	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ASP	CB-CG-OD1	7.77	125.30	118.30
1	A	16	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	B	332	ASP	CB-CG-OD2	7.62	125.15	118.30
1	D	217	GLU	OE1-CD-OE2	-7.59	114.19	123.30
1	C	244	ASP	CB-CG-OD2	7.55	125.10	118.30
1	C	217	GLU	OE1-CD-OE2	-7.51	114.29	123.30
1	D	320	ASP	CB-CG-OD1	7.33	124.89	118.30
1	B	63	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	C	258	ARG	NE-CZ-NH1	-7.31	116.64	120.30
1	D	267	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	B	407	LEU	CA-CB-CG	7.24	131.94	115.30
1	A	156	ASP	CB-CG-OD1	7.22	124.80	118.30
1	D	406	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	D	493	TYR	CB-CG-CD1	-7.14	116.72	121.00
1	C	81	LEU	CB-CG-CD1	-7.03	99.05	111.00
1	B	68	LEU	CB-CG-CD1	6.96	122.83	111.00
1	A	258	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	267	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	B	155	ASP	CB-CG-OD1	6.81	124.43	118.30
1	D	495	TYR	CB-CG-CD2	-6.79	116.92	121.00
1	B	406	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	B	375	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	267	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	C	406	ARG	NE-CZ-NH2	6.51	123.55	120.30
1	A	194	LEU	CB-CG-CD2	6.48	122.01	111.00
1	C	454	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	C	155	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	123	PHE	CB-CG-CD2	-6.34	116.36	120.80
1	C	319	PHE	CB-CG-CD1	-6.26	116.42	120.80
1	A	330	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	D	84	LEU	CB-CG-CD1	-6.23	100.41	111.00
1	A	63	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	D	319	PHE	CB-CG-CD1	-6.15	116.50	120.80
1	C	277	LYS	CD-CE-NZ	-6.10	97.66	111.70
1	D	84	LEU	CB-CG-CD2	6.10	121.37	111.00
1	D	345	MET	CG-SD-CE	6.10	109.95	100.20
1	A	300	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	312	LEU	CB-CG-CD2	-6.09	100.65	111.00
1	B	369	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	A	315	MET	CA-CB-CG	-6.04	103.04	113.30
1	C	305	GLU	OE1-CD-OE2	-6.04	116.06	123.30
1	C	152	MET	CG-SD-CE	-6.02	90.56	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	D	354	ASP	CB-CG-OD1	5.98	123.69	118.30
1	A	163	LEU	CB-CG-CD2	-5.94	100.90	111.00
1	A	251	PHE	CB-CG-CD2	-5.93	116.65	120.80
1	C	159	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	380	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	14	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	448	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	244	ASP	CB-CG-OD2	5.82	123.53	118.30
1	C	332	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	226	LEU	CB-CG-CD1	-5.80	101.14	111.00
1	C	285	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	A	123	PHE	CB-CG-CD2	-5.75	116.77	120.80
1	A	420	VAL	CA-CB-CG2	-5.73	102.31	110.90
1	A	320	ASP	CB-CG-OD1	5.72	123.45	118.30
1	C	262	ILE	CB-CG1-CD1	-5.66	98.06	113.90
1	D	133	TYR	CZ-CE2-CD2	-5.65	114.72	119.80
1	C	159	ASP	CB-CG-OD1	5.58	123.33	118.30
1	B	258	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	16	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	407	LEU	CB-CG-CD1	5.46	120.28	111.00
1	A	100	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	D	152	MET	CG-SD-CE	-5.42	91.53	100.20
1	D	37	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	D	225	ARG	CG-CD-NE	-5.37	100.52	111.80
1	B	133	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	C	140	MET	CG-SD-CE	5.35	108.76	100.20
1	B	406	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	448	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	373	LEU	CB-CG-CD1	5.24	119.91	111.00
1	A	255	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	A	483	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	255	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	B	300	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	145	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	C	16	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	380	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	435	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	422	SER	N-CA-CB	-5.08	102.89	110.50
1	A	43	MET	CA-CB-CG	-5.07	104.67	113.30
1	A	358	LEU	CB-CG-CD2	-5.05	102.41	111.00
1	C	155	ASP	CB-CG-OD2	-5.04	113.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	LEU	CB-CG-CD1	-5.03	102.44	111.00
1	A	37	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	D	68	LEU	CB-CG-CD2	-5.03	102.45	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3753	0	3695	38	0
1	B	3748	0	3693	42	0
1	C	3748	0	3693	76	0
1	D	3747	0	3690	76	0
2	A	19	0	13	1	0
2	B	19	0	13	1	0
2	C	19	0	13	1	0
2	D	19	0	13	1	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
3	C	44	0	26	6	0
3	D	44	0	26	2	0
4	A	446	0	0	20	0
4	B	465	0	0	25	0
4	C	396	0	0	40	0
4	D	429	0	0	44	0
All	All	16984	0	14927	234	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 8.

All (234) 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:343:ILE:HG21	4:D:1453:HOH:O	1.26	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ILE:HG12	4:C:1347:HOH:O	1.21	1.31
1:C:321:VAL:CG1	4:D:1454:HOH:O	1.74	1.29
3:C:550:NAD:C3D	4:C:1355:HOH:O	1.81	1.26
3:C:550:NAD:H3D	4:C:1355:HOH:O	1.33	1.26
1:B:78:ILE:HG23	4:B:1024:HOH:O	1.33	1.26
1:B:84:LEU:HG	4:B:1025:HOH:O	1.07	1.24
1:D:306:ILE:HG12	4:D:1447:HOH:O	1.34	1.23
1:D:317:GLU:HG2	4:D:1340:HOH:O	1.34	1.21
1:A:463:GLU:HG2	4:A:946:HOH:O	1.40	1.21
1:D:306:ILE:CD1	4:D:1447:HOH:O	1.86	1.20
1:C:37:ARG:HD3	4:C:1280:HOH:O	1.38	1.18
1:B:227:TYR:OH	4:B:1006:HOH:O	1.59	1.17
1:D:452:HIS:HB2	4:D:1468:HOH:O	1.44	1.14
1:C:39:ALA:HB1	1:C:43:MET:HE3	1.27	1.14
1:C:16:ARG:HD3	4:C:1276:HOH:O	1.51	1.10
1:C:401:VAL:HG23	4:C:1357:HOH:O	0.93	1.10
1:D:254:LYS:HD3	4:D:1448:HOH:O	1.48	1.09
1:C:474:LYS:HD2	4:C:1325:HOH:O	1.53	1.09
1:A:227:TYR:OH	4:A:976:HOH:O	1.60	1.07
1:D:306:ILE:CG1	4:D:1447:HOH:O	1.87	1.06
1:C:39:ALA:HB1	1:C:43:MET:CE	1.88	1.04
1:D:474:LYS:HD2	4:D:1384:HOH:O	1.60	1.00
1:B:262:ILE:HD13	4:B:936:HOH:O	1.64	0.97
1:C:56:VAL:HG23	4:C:1265:HOH:O	1.62	0.97
1:A:250:LYS:NZ	4:A:970:HOH:O	1.82	0.96
1:C:288:LYS:HE3	4:C:1283:HOH:O	0.75	0.92
1:D:280:ILE:HG23	4:D:1449:HOH:O	1.69	0.91
1:D:262:ILE:CD1	1:D:294:MET:HE1	2.01	0.91
1:A:56:VAL:HG23	4:A:851:HOH:O	1.72	0.88
1:D:474:LYS:CD	4:D:1384:HOH:O	2.19	0.87
1:D:262:ILE:HD11	1:D:294:MET:CE	2.04	0.87
1:B:84:LEU:CD2	4:B:1025:HOH:O	2.17	0.87
1:C:474:LYS:CD	4:C:1325:HOH:O	2.16	0.87
1:C:398:SER:O	1:C:399:ILE:HD13	1.75	0.86
1:D:262:ILE:CD1	1:D:294:MET:CE	2.55	0.84
1:C:338:THR:HG23	4:C:1354:HOH:O	1.78	0.83
1:C:306:ILE:CG1	4:C:1347:HOH:O	1.95	0.83
1:D:343:ILE:CG2	4:D:1453:HOH:O	2.00	0.82
1:D:56:VAL:HG23	4:D:1317:HOH:O	1.79	0.81
1:D:478:GLU:HG3	4:D:1421:HOH:O	1.79	0.81
1:D:467:GLY:O	4:D:1452:HOH:O	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:ILE:HD11	1:D:294:MET:HE2	1.64	0.78
1:D:149:PRO:HG3	4:D:1354:HOH:O	1.82	0.78
1:C:399:ILE:HD11	4:C:1248:HOH:O	1.83	0.78
1:C:213:LYS:HD3	1:C:436:TRP:CZ3	2.19	0.77
1:A:206:THR:O	1:A:210:GLU:HG3	1.83	0.77
1:C:339:GLY:HA3	4:C:1355:HOH:O	1.83	0.77
1:C:455:GLU:OE2	4:C:1379:HOH:O	2.03	0.77
1:A:277:LYS:HE2	4:A:881:HOH:O	1.83	0.76
1:C:306:ILE:CD1	4:C:1347:HOH:O	2.27	0.76
1:C:321:VAL:HG11	4:D:1454:HOH:O	1.52	0.75
1:D:118:LYS:HE2	4:D:1289:HOH:O	1.88	0.73
1:D:486:GLY:N	1:D:486:GLY:C	2.42	0.73
1:C:321:VAL:HG12	4:D:1454:HOH:O	1.59	0.72
3:C:550:NAD:C4D	4:C:1355:HOH:O	2.21	0.72
1:B:172:LYS:HE3	4:B:986:HOH:O	1.89	0.72
1:A:250:LYS:NZ	4:A:903:HOH:O	2.19	0.71
1:A:262:ILE:HD11	4:A:848:HOH:O	1.92	0.70
1:D:295:LYS:HE3	4:D:1235:HOH:O	1.91	0.70
1:B:262:ILE:HD11	4:B:907:HOH:O	1.91	0.70
1:D:398:SER:O	1:D:399:ILE:HD13	1.92	0.69
1:B:88:VAL:HG21	4:B:1024:HOH:O	1.92	0.69
1:C:343:ILE:HG21	4:C:1354:HOH:O	1.92	0.68
1:D:292:GLU:OE1	4:D:1464:HOH:O	2.12	0.68
1:C:401:VAL:CG2	4:C:1357:HOH:O	1.72	0.67
1:C:338:THR:CG2	4:C:1354:HOH:O	2.38	0.67
1:D:474:LYS:HE2	4:D:1433:HOH:O	1.93	0.67
1:D:399:ILE:HD11	4:D:1305:HOH:O	1.95	0.67
1:C:43:MET:HE2	1:C:73:GLN:HG3	1.76	0.67
1:C:213:LYS:HD3	1:C:436:TRP:HZ3	1.61	0.66
1:B:285:ASP:OD2	4:B:960:HOH:O	2.13	0.66
1:D:474:LYS:CE	4:D:1384:HOH:O	2.43	0.66
1:C:292:GLU:OE1	4:C:1337:HOH:O	2.14	0.65
1:C:474:LYS:HE2	4:C:1281:HOH:O	1.95	0.64
1:B:56:VAL:HG23	4:B:874:HOH:O	1.96	0.64
1:A:492:HIS:HE1	1:B:244:ASP:OD2	1.82	0.63
1:B:88:VAL:HG11	4:B:1024:HOH:O	1.97	0.63
3:C:550:NAD:C5D	4:C:1355:HOH:O	2.47	0.62
1:C:218:GLU:HG3	1:C:428:GLN:HE22	1.64	0.61
1:C:492:HIS:HE1	1:D:244:ASP:OD2	1.82	0.61
1:B:243:ASN:HD21	1:B:253:ASN:HD21	1.49	0.61
1:C:254:LYS:HD3	4:C:1167:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:PRO:HD3	4:C:1266:HOH:O	2.00	0.60
1:A:250:LYS:CE	4:A:903:HOH:O	2.50	0.60
1:D:218:GLU:HG3	1:D:428:GLN:HE22	1.67	0.60
1:C:243:ASN:HD21	1:C:253:ASN:HD21	1.49	0.59
1:C:492:HIS:HD2	4:C:1359:HOH:O	1.85	0.59
3:C:550:NAD:H52N	4:C:1355:HOH:O	2.04	0.58
1:A:244:ASP:OD2	1:B:492:HIS:HE1	1.87	0.58
1:B:285:ASP:CG	4:B:960:HOH:O	2.42	0.58
1:C:43:MET:CE	1:C:418:SER:HB3	2.34	0.58
1:B:380:ARG:NH1	4:B:1009:HOH:O	2.37	0.57
4:C:1347:HOH:O	1:D:472:LEU:HD21	2.05	0.57
1:C:310:ASN:HD22	1:C:310:ASN:H	1.52	0.56
1:D:355:HIS:HE1	4:D:1290:HOH:O	1.89	0.56
1:C:30:ASP:OD1	4:C:1351:HOH:O	2.17	0.56
1:A:11:LEU:HD11	1:A:132:GLU:HG2	1.87	0.56
1:B:485:GLU:HG2	4:B:925:HOH:O	2.06	0.56
1:C:11:LEU:HD11	1:C:132:GLU:HG2	1.88	0.55
1:A:243:ASN:HD21	1:A:253:ASN:HD21	1.52	0.55
1:C:39:ALA:HB1	1:C:43:MET:HE1	1.84	0.55
1:D:262:ILE:HD12	1:D:273:ILE:HD13	1.89	0.55
1:B:213:LYS:HD3	1:B:436:TRP:CZ3	2.42	0.55
1:C:65:SER:HB3	1:C:140:MET:SD	2.46	0.55
1:D:243:ASN:HD21	1:D:253:ASN:HD21	1.54	0.54
1:D:280:ILE:HA	4:D:1449:HOH:O	2.07	0.54
1:D:56:VAL:HG21	4:D:1381:HOH:O	2.07	0.54
1:A:463:GLU:CG	4:A:946:HOH:O	2.21	0.54
1:D:335:VAL:O	4:D:1449:HOH:O	2.18	0.54
1:C:384:LYS:HB2	1:C:385:PRO:CD	2.37	0.53
1:D:343:ILE:CG1	4:D:1453:HOH:O	2.57	0.53
1:C:474:LYS:CE	4:C:1325:HOH:O	2.51	0.53
1:D:51:ARG:HG3	4:D:1417:HOH:O	2.09	0.53
1:B:273:ILE:HD12	4:B:939:HOH:O	2.08	0.52
1:C:187:TRP:NE1	1:C:191:LEU:HD11	2.24	0.52
1:A:380:ARG:HD3	1:A:390:TRP:CZ2	2.45	0.52
2:C:500:ADN:H3'	3:C:550:NAD:C4N	2.39	0.52
1:B:78:ILE:CG2	4:B:1024:HOH:O	2.17	0.52
1:D:492:HIS:HD2	4:D:1401:HOH:O	1.91	0.52
1:C:295:LYS:HE3	4:C:1187:HOH:O	2.08	0.52
1:C:64:ILE:HD13	1:C:432:GLN:OE1	2.09	0.52
1:D:134:TRP:HB3	1:D:193:LEU:HD12	1.92	0.51
2:D:500:ADN:H3'	3:D:550:NAD:C4N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:NZ	4:A:894:HOH:O	2.34	0.50
1:D:218:GLU:HG3	1:D:428:GLN:NE2	2.27	0.50
1:D:283:TYR:OH	1:D:317:GLU:OE1	2.23	0.49
1:D:36:LEU:HD21	1:D:75:ALA:HB1	1.94	0.49
1:C:218:GLU:HG3	1:C:428:GLN:NE2	2.26	0.49
1:C:355:HIS:HE1	4:C:1178:HOH:O	1.95	0.49
1:D:343:ILE:HG13	4:D:1453:HOH:O	2.13	0.49
2:A:500:ADN:H3'	3:A:550:NAD:C4N	2.42	0.49
1:C:390:TRP:O	1:C:398:SER:HA	2.13	0.49
1:C:227:TYR:CE2	4:D:1053:HOH:O	2.65	0.48
1:D:65:SER:HB3	1:D:140:MET:SD	2.53	0.48
1:B:475:GLU:HG3	4:B:921:HOH:O	2.12	0.48
1:C:16:ARG:CD	4:C:1276:HOH:O	2.30	0.48
1:D:262:ILE:HG12	1:D:293:ALA:HB1	1.96	0.48
1:B:218:GLU:O	1:B:248:LYS:HE3	2.14	0.48
4:A:987:HOH:O	1:C:41:HIS:HD2	1.96	0.47
1:C:244:ASP:OD2	1:D:492:HIS:HE1	1.97	0.47
1:D:262:ILE:HD13	1:D:294:MET:CE	2.43	0.47
1:C:252:ASP:HA	1:C:420:VAL:CG1	2.44	0.47
1:D:167:GLY:O	1:D:171:GLU:HG3	2.14	0.47
1:C:492:HIS:CD2	4:C:1359:HOH:O	2.63	0.47
1:A:148:LYS:N	1:A:149:PRO:HD3	2.30	0.47
1:A:196:THR:O	1:A:199:GLU:HB2	2.14	0.47
1:C:288:LYS:NZ	1:D:495:TYR:OXT	2.45	0.47
1:C:485:GLU:CD	4:C:1369:HOH:O	2.53	0.47
1:D:180:GLU:O	1:D:183:ASP:HB2	2.15	0.47
1:C:384:LYS:HB2	1:C:385:PRO:HD2	1.96	0.46
1:D:306:ILE:HD13	4:D:1447:HOH:O	1.82	0.46
1:C:139:GLN:HG2	4:C:1240:HOH:O	2.14	0.46
1:C:343:ILE:HG13	4:C:1354:HOH:O	2.15	0.46
1:B:427:ASN:ND2	4:B:937:HOH:O	2.48	0.46
1:D:243:ASN:HD22	1:D:248:LYS:HZ2	1.62	0.46
1:B:355:HIS:HE1	4:D:1049:HOH:O	1.99	0.46
1:D:478:GLU:CG	4:D:1421:HOH:O	2.51	0.45
2:B:500:ADN:H3'	3:B:550:NAD:C4N	2.46	0.45
4:A:844:HOH:O	1:C:259:HIS:HE1	1.99	0.45
1:D:280:ILE:CG2	4:D:1449:HOH:O	2.45	0.45
1:D:260:SER:OG	1:D:416:HIS:HD2	2.00	0.45
1:D:47:MET:CE	1:D:76:VAL:CG1	2.95	0.45
1:A:39:ALA:O	1:A:43:MET:HG3	2.16	0.45
1:C:339:GLY:CA	4:C:1355:HOH:O	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:TYR:OH	1:C:317:GLU:OE1	2.22	0.45
1:C:215:VAL:O	1:C:239:ALA:HA	2.16	0.45
1:A:398:SER:O	1:A:399:ILE:HD13	2.16	0.44
1:A:218:GLU:HG3	1:A:428:GLN:HE22	1.82	0.44
1:B:492:HIS:H	1:B:492:HIS:CD2	2.36	0.44
4:B:903:HOH:O	1:D:259:HIS:HD2	2.00	0.44
1:A:492:HIS:HD2	4:A:758:HOH:O	1.99	0.44
1:C:227:TYR:HD2	4:D:1053:HOH:O	1.98	0.44
1:C:397:ARG:HB3	4:C:1248:HOH:O	2.17	0.44
1:A:492:HIS:CE1	1:B:244:ASP:OD2	2.68	0.44
1:B:42:GLU:O	1:B:419:PHE:HA	2.17	0.44
1:A:310:ASN:HD22	1:A:310:ASN:H	1.66	0.44
1:A:427:ASN:ND2	4:A:879:HOH:O	2.45	0.44
1:D:390:TRP:O	1:D:398:SER:HA	2.18	0.44
1:B:260:SER:OG	1:B:416:HIS:HD2	2.00	0.44
1:A:95:ILE:HG22	1:A:133:TYR:HB2	1.99	0.44
1:A:355:HIS:HE1	4:A:829:HOH:O	2.00	0.44
1:A:95:ILE:HG12	1:A:406:ARG:HD2	1.99	0.44
1:D:68:LEU:O	1:D:69:HIS:C	2.56	0.44
1:C:260:SER:OG	1:C:416:HIS:HD2	2.01	0.43
1:C:43:MET:HE3	1:C:418:SER:HB3	2.00	0.43
1:A:145:ASP:HB3	1:A:148:LYS:HB2	2.00	0.43
1:A:474:LYS:HE3	4:A:974:HOH:O	2.18	0.43
1:B:478:GLU:CD	4:B:964:HOH:O	2.56	0.43
4:C:1164:HOH:O	1:D:475:GLU:HG2	2.18	0.43
1:C:429:THR:O	1:C:433:ILE:HG13	2.19	0.43
1:A:134:TRP:HB3	1:A:193:LEU:HD13	2.00	0.43
1:A:259:HIS:HE1	4:A:820:HOH:O	2.01	0.43
1:B:43:MET:HA	1:B:422:SER:HB2	1.99	0.43
4:B:897:HOH:O	1:D:259:HIS:HE1	2.02	0.43
1:C:14:ASP:O	1:C:20:ASP:HA	2.18	0.42
1:B:320:ASP:OD1	1:C:300:ARG:HD2	2.19	0.42
1:B:29:ALA:CB	1:B:108:VAL:HG21	2.49	0.42
1:B:390:TRP:O	1:B:398:SER:HA	2.19	0.42
1:C:68:LEU:HG	1:C:156:ASP:HB2	2.01	0.42
1:D:252:ASP:HA	1:D:420:VAL:CG1	2.49	0.42
1:D:284:GLY:HA3	3:D:550:NAD:O5B	2.19	0.42
1:D:399:ILE:HD12	1:D:399:ILE:HG23	1.79	0.42
1:A:218:GLU:HG3	1:A:428:GLN:NE2	2.35	0.42
1:D:277:LYS:HE2	4:D:1249:HOH:O	2.18	0.42
1:D:310:ASN:HD22	1:D:310:ASN:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:MET:HA	1:A:422:SER:HB2	2.02	0.42
1:B:243:ASN:HD22	1:B:248:LYS:HZ1	1.68	0.42
1:A:273:ILE:HD12	4:A:906:HOH:O	2.20	0.42
1:B:84:LEU:CG	4:B:1025:HOH:O	1.85	0.42
1:D:306:ILE:HD11	4:D:1447:HOH:O	1.82	0.42
1:B:41:HIS:HD2	4:D:1245:HOH:O	2.02	0.42
1:B:277:LYS:HE3	4:B:951:HOH:O	2.20	0.41
1:A:260:SER:OG	1:A:416:HIS:HD2	2.02	0.41
1:B:492:HIS:HD2	4:B:755:HOH:O	2.02	0.41
1:D:303:VAL:O	1:D:321:VAL:HA	2.21	0.41
1:C:303:VAL:O	1:C:321:VAL:HA	2.20	0.41
1:A:213:LYS:HE2	1:A:436:TRP:CE3	2.56	0.41
4:A:987:HOH:O	1:C:41:HIS:CD2	2.73	0.41
1:D:340:ASN:O	1:D:367:GLU:HG2	2.21	0.41
1:D:248:LYS:C	1:D:248:LYS:HD3	2.41	0.41
1:B:225:ARG:NH2	4:B:780:HOH:O	2.40	0.41
1:B:11:LEU:HD22	1:B:22:LYS:HE2	2.03	0.41
1:B:408:LEU:HD12	1:B:408:LEU:C	2.42	0.41
1:D:88:VAL:CG2	1:D:120:VAL:HG21	2.51	0.41
1:D:478:GLU:CD	4:D:1309:HOH:O	2.60	0.41
1:A:463:GLU:CD	4:A:946:HOH:O	2.54	0.40
1:C:227:TYR:CD2	4:D:1053:HOH:O	2.57	0.40
1:C:310:ASN:H	1:C:310:ASN:ND2	2.18	0.40
1:C:59:LEU:HB3	1:C:86:ALA:HB2	2.03	0.40
1:D:280:ILE:CA	4:D:1449:HOH:O	2.66	0.40
1:D:218:GLU:CG	1:D:428:GLN:HE22	2.31	0.40
1:D:78:ILE:HG23	1:D:88:VAL:HG21	2.03	0.40
1:B:214:GLY:HA3	1:B:435:LEU:HD13	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	484/494 (98%)	473 (98%)	11 (2%)	0	100	100
1	B	483/494 (98%)	470 (97%)	13 (3%)	0	100	100
1	C	483/494 (98%)	471 (98%)	11 (2%)	1 (0%)	47	26
1	D	482/494 (98%)	472 (98%)	9 (2%)	1 (0%)	47	26
All	All	1932/1976 (98%)	1886 (98%)	44 (2%)	2 (0%)	51	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	69	HIS
1	C	69	HIS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/403 (98%)	391 (99%)	4 (1%)	76	61
1	B	395/403 (98%)	389 (98%)	6 (2%)	65	44
1	C	395/403 (98%)	388 (98%)	7 (2%)	59	36
1	D	395/403 (98%)	390 (99%)	5 (1%)	69	50
All	All	1580/1612 (98%)	1558 (99%)	22 (1%)	67	47

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LEU
1	A	237	PHE
1	A	407	LEU
1	A	428	GLN
1	B	55	GLU
1	B	68	LEU
1	B	225	ARG
1	B	250	LYS
1	B	407	LEU

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Mol	Chain	Res	Type
1	B	428	GLN
1	C	11	LEU
1	C	68	LEU
1	C	180	GLU
1	C	210	GLU
1	C	220	THR
1	C	237	PHE
1	C	428	GLN
1	D	30	ASP
1	D	60	LYS
1	D	330	ASP
1	D	407	LEU
1	D	428	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	243	ASN
1	A	259	HIS
1	A	310	ASN
1	A	355	HIS
1	A	412	ASN
1	A	416	HIS
1	A	427	ASN
1	A	428	GLN
1	A	432	GLN
1	A	452	HIS
1	A	492	HIS
1	B	41	HIS
1	B	57	GLN
1	B	243	ASN
1	B	259	HIS
1	B	310	ASN
1	B	355	HIS
1	B	412	ASN
1	B	416	HIS
1	B	427	ASN
1	B	428	GLN
1	B	432	GLN
1	B	492	HIS
1	C	41	HIS

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Mol	Chain	Res	Type
1	C	243	ASN
1	C	259	HIS
1	C	310	ASN
1	C	355	HIS
1	C	412	ASN
1	C	416	HIS
1	C	427	ASN
1	C	428	GLN
1	C	492	HIS
1	D	41	HIS
1	D	243	ASN
1	D	259	HIS
1	D	310	ASN
1	D	355	HIS
1	D	412	ASN
1	D	416	HIS
1	D	427	ASN
1	D	428	GLN
1	D	492	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ADN	C	500	-	18,21,21	1.01	1 (5%)	18,31,31	1.49	3 (16%)
3	NAD	B	550	-	42,48,48	1.17	4 (9%)	50,73,73	1.68	8 (16%)
3	NAD	C	550	-	42,48,48	1.09	3 (7%)	50,73,73	1.56	9 (18%)
3	NAD	A	550	-	42,48,48	1.19	3 (7%)	50,73,73	1.58	8 (16%)
2	ADN	B	500	-	18,21,21	0.89	1 (5%)	18,31,31	1.58	5 (27%)
2	ADN	D	500	-	18,21,21	0.93	1 (5%)	18,31,31	1.54	4 (22%)
3	NAD	D	550	-	42,48,48	1.19	4 (9%)	50,73,73	1.59	8 (16%)
2	ADN	A	500	-	18,21,21	1.03	2 (11%)	18,31,31	1.39	5 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADN	C	500	-	-	0/2/22/22	0/3/3/3
3	NAD	B	550	-	-	5/26/62/62	0/5/5/5
3	NAD	C	550	-	-	5/26/62/62	0/5/5/5
3	NAD	A	550	-	-	5/26/62/62	0/5/5/5
2	ADN	B	500	-	-	0/2/22/22	0/3/3/3
2	ADN	D	500	-	-	0/2/22/22	0/3/3/3
3	NAD	D	550	-	-	5/26/62/62	0/5/5/5
2	ADN	A	500	-	-	0/2/22/22	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	550	NAD	O7N-C7N	4.01	1.31	1.24
3	D	550	NAD	O7N-C7N	4.01	1.31	1.24
3	C	550	NAD	O7N-C7N	3.79	1.31	1.24
3	B	550	NAD	O7N-C7N	3.34	1.30	1.24
3	B	550	NAD	C7N-N7N	-3.01	1.27	1.33
3	B	550	NAD	O4D-C1D	2.97	1.45	1.41
2	A	500	ADN	C2-N3	2.84	1.36	1.32
2	C	500	ADN	C5-C4	2.64	1.47	1.40
3	D	550	NAD	C7N-N7N	-2.63	1.28	1.33
3	A	550	NAD	C7N-N7N	-2.62	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	550	NAD	C5A-C4A	2.55	1.47	1.40
2	A	500	ADN	C5-C4	2.30	1.47	1.40
3	D	550	NAD	C5A-C4A	2.29	1.47	1.40
3	A	550	NAD	C5A-C4A	2.28	1.47	1.40
3	B	550	NAD	C5A-C4A	2.22	1.46	1.40
2	D	500	ADN	C5-C4	2.09	1.46	1.40
2	B	500	ADN	C5-C4	2.08	1.46	1.40
3	C	550	NAD	O4D-C1D	2.07	1.44	1.41
3	D	550	NAD	C2D-C1D	-2.01	1.50	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	550	NAD	C3N-C7N-N7N	5.20	123.99	117.75
3	B	550	NAD	N3A-C2A-N1A	-4.69	121.34	128.68
3	D	550	NAD	O7N-C7N-C3N	-4.62	114.11	119.63
3	A	550	NAD	O7N-C7N-C3N	-4.60	114.13	119.63
3	C	550	NAD	C3N-C7N-N7N	4.54	123.20	117.75
3	A	550	NAD	C3N-C7N-N7N	4.54	123.20	117.75
3	D	550	NAD	C3N-C7N-N7N	4.52	123.17	117.75
3	B	550	NAD	O7N-C7N-C3N	-4.34	114.44	119.63
3	C	550	NAD	N3A-C2A-N1A	-4.13	122.22	128.68
3	A	550	NAD	N3A-C2A-N1A	-4.02	122.40	128.68
3	D	550	NAD	N3A-C2A-N1A	-4.02	122.40	128.68
2	D	500	ADN	N3-C2-N1	-3.52	123.17	128.68
3	C	550	NAD	O7N-C7N-C3N	-3.52	115.42	119.63
3	D	550	NAD	O4D-C1D-C2D	-3.50	101.80	106.93
3	A	550	NAD	O4D-C1D-C2D	-3.50	101.81	106.93
3	B	550	NAD	C5N-C4N-C3N	-3.40	116.33	120.34
3	B	550	NAD	O4D-C1D-C2D	-3.38	101.98	106.93
2	C	500	ADN	C4-C5-N7	-3.31	105.94	109.40
3	C	550	NAD	O4D-C1D-C2D	-3.28	102.13	106.93
2	B	500	ADN	N3-C2-N1	-3.14	123.78	128.68
3	C	550	NAD	C4A-C5A-N7A	-2.95	106.32	109.40
2	B	500	ADN	C4-C5-N7	-2.93	106.34	109.40
3	D	550	NAD	C4A-C5A-N7A	-2.90	106.38	109.40
3	A	550	NAD	C4A-C5A-N7A	-2.85	106.43	109.40
2	D	500	ADN	C1'-N9-C4	-2.80	121.73	126.64
2	D	500	ADN	C2-N1-C6	2.76	123.48	118.75
2	C	500	ADN	N3-C2-N1	-2.75	124.37	128.68
3	C	550	NAD	C5N-C4N-C3N	-2.73	117.11	120.34
3	D	550	NAD	C1B-N9A-C4A	-2.67	121.95	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	ADN	N6-C6-N1	2.65	124.08	118.57
3	A	550	NAD	C1B-N9A-C4A	-2.65	121.98	126.64
3	B	550	NAD	C4A-C5A-N7A	-2.62	106.67	109.40
2	C	500	ADN	C1'-N9-C4	-2.59	122.09	126.64
2	B	500	ADN	C1'-N9-C4	-2.58	122.11	126.64
3	C	550	NAD	PN-O3-PA	-2.50	124.25	132.83
2	A	500	ADN	N3-C2-N1	-2.48	124.80	128.68
3	B	550	NAD	C2N-C3N-C4N	2.44	121.02	118.26
2	B	500	ADN	N6-C6-N1	2.42	123.60	118.57
3	D	550	NAD	C2N-N1N-C1D	-2.42	113.76	119.14
3	D	550	NAD	C5N-C4N-C3N	-2.41	117.49	120.34
3	A	550	NAD	C2N-N1N-C1D	-2.41	113.77	119.14
3	A	550	NAD	C5N-C4N-C3N	-2.38	117.53	120.34
3	C	550	NAD	C2N-C3N-C4N	2.36	120.94	118.26
2	B	500	ADN	C2-N1-C6	2.35	122.77	118.75
2	A	500	ADN	C1'-N9-C4	-2.31	122.58	126.64
3	B	550	NAD	C1B-N9A-C4A	-2.31	122.58	126.64
2	A	500	ADN	C2-N1-C6	2.31	122.70	118.75
3	C	550	NAD	O4B-C1B-C2B	-2.26	103.62	106.93
2	D	500	ADN	C4-C5-N7	-2.22	107.09	109.40
2	A	500	ADN	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

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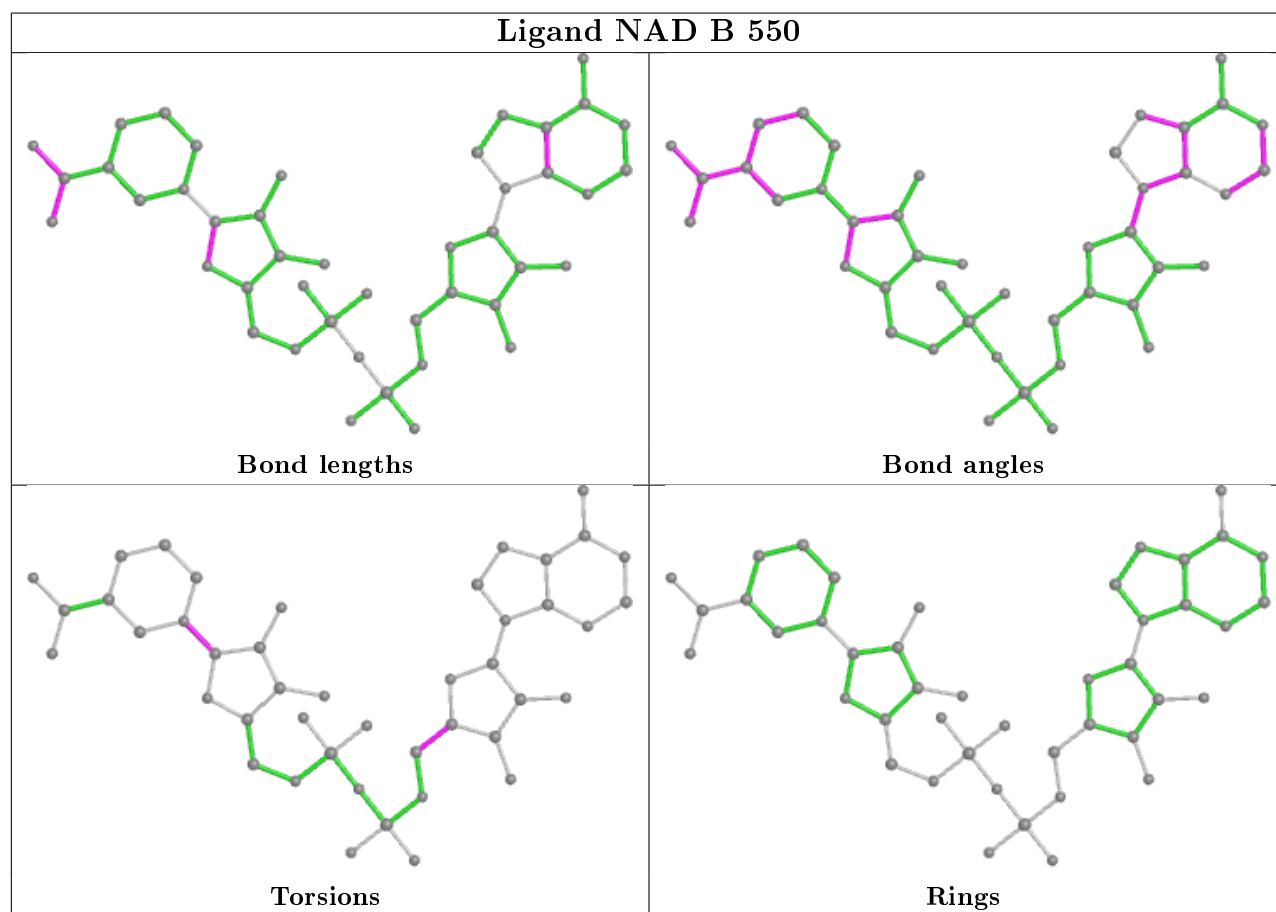
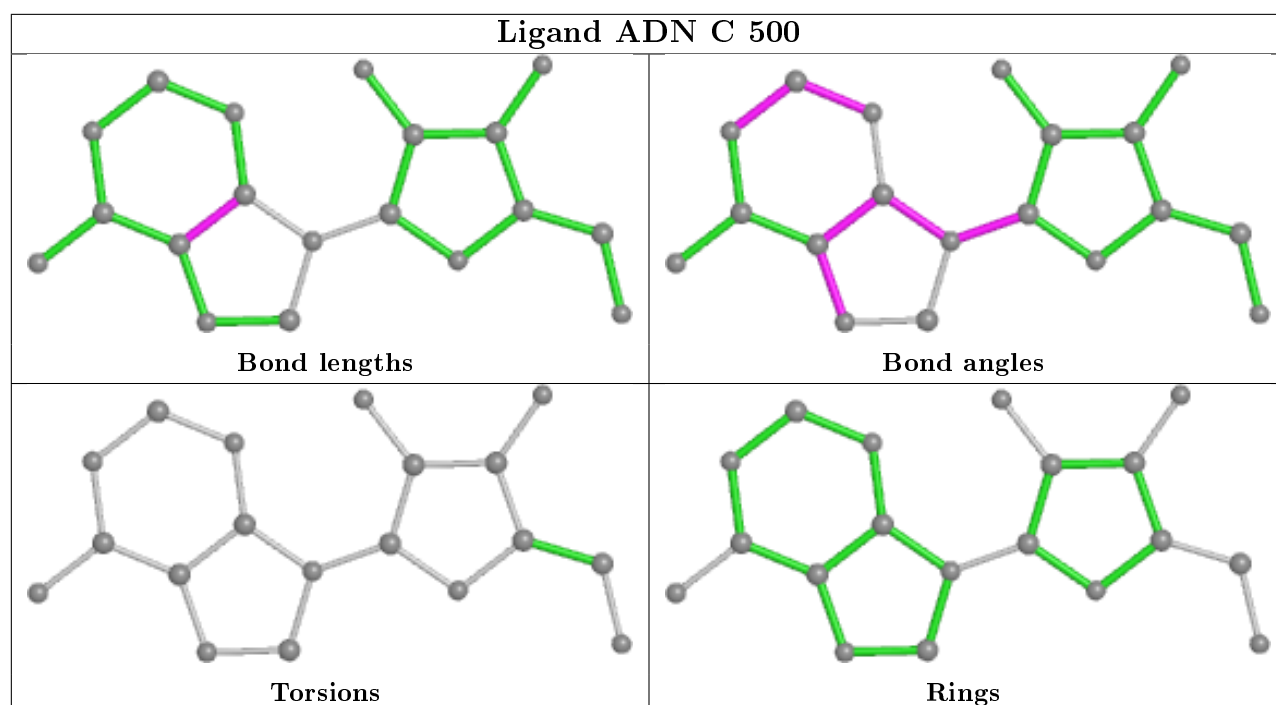
Mol	Chain	Res	Type	Atoms
3	C	550	NAD	O4B-C4B-C5B-O5B
3	B	550	NAD	O4B-C4B-C5B-O5B
3	A	550	NAD	O4B-C4B-C5B-O5B
3	D	550	NAD	O4B-C4B-C5B-O5B

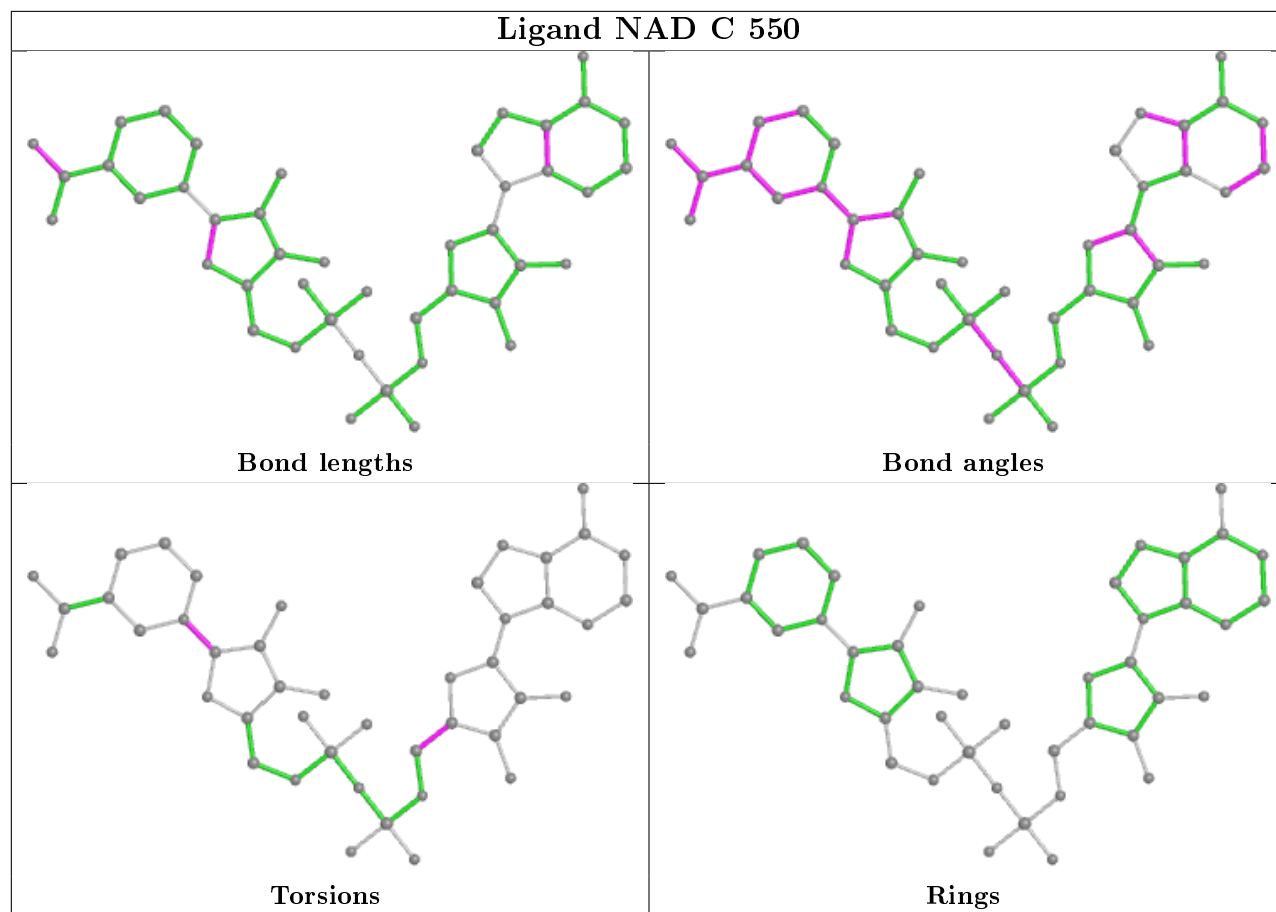
There are no ring outliers.

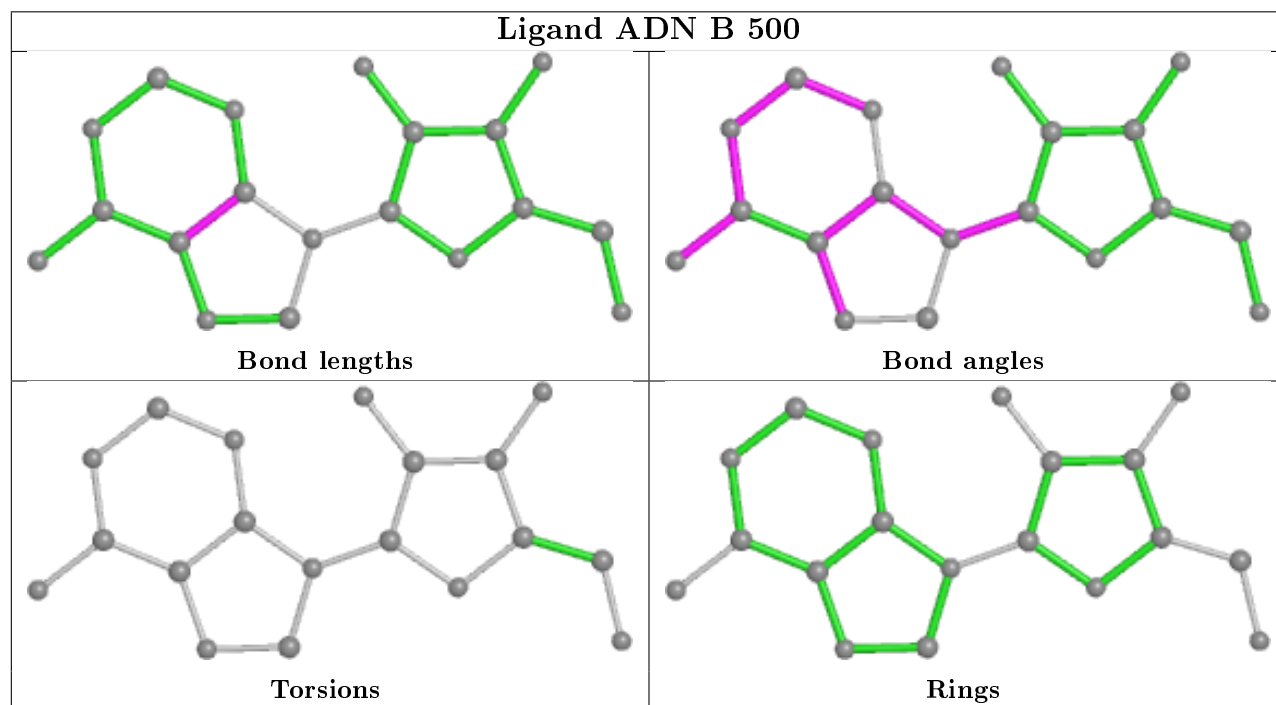
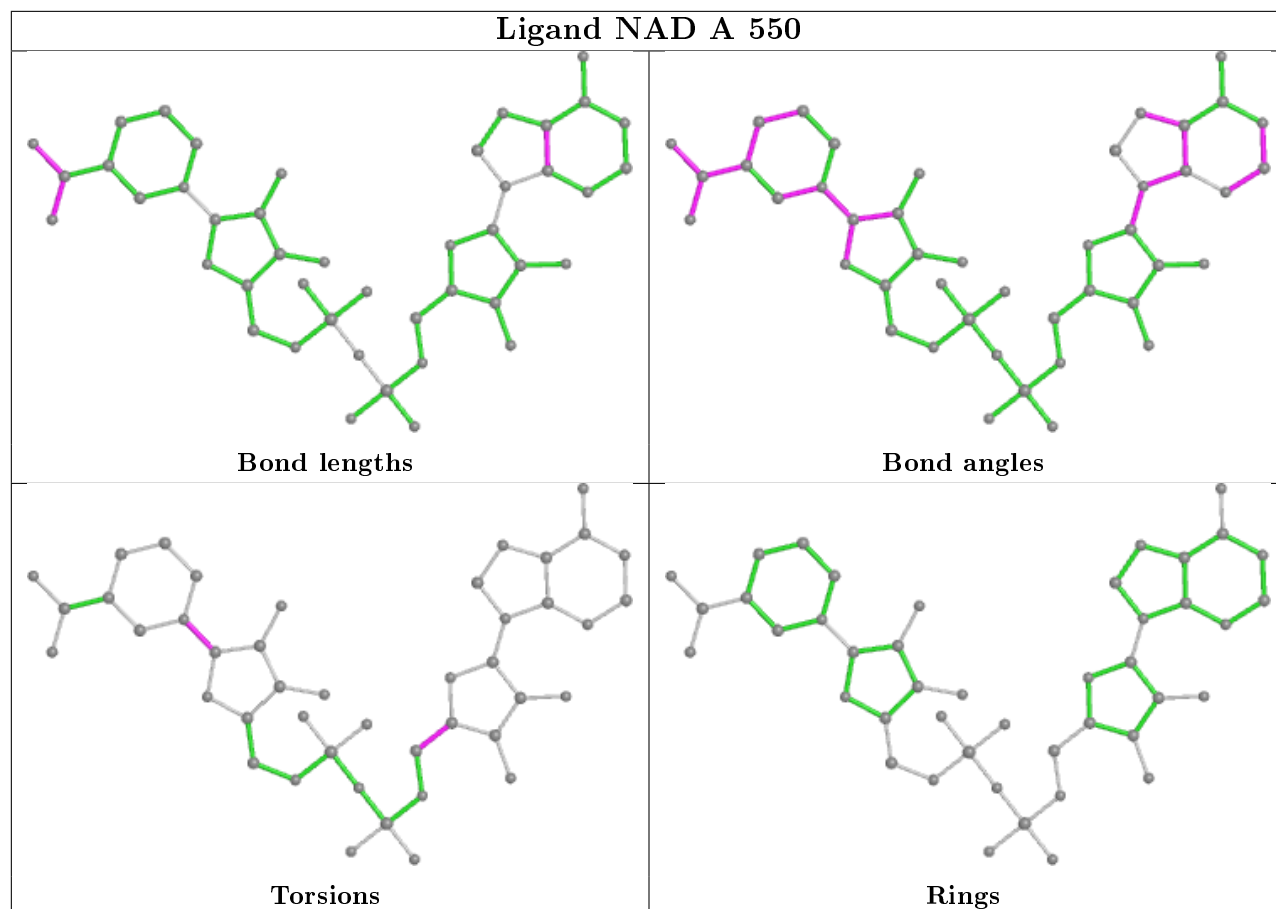
8 monomers are involved in 10 short contacts:

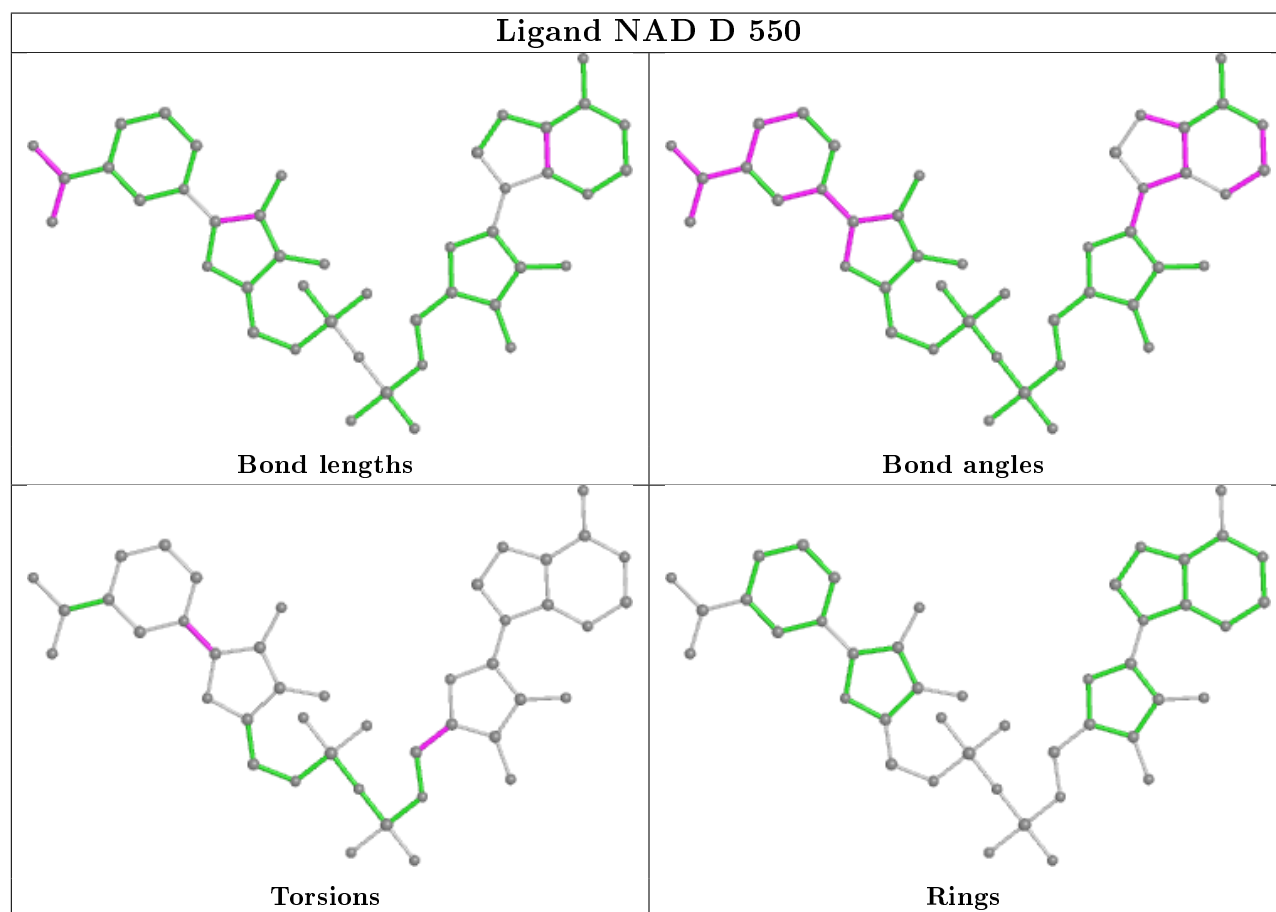
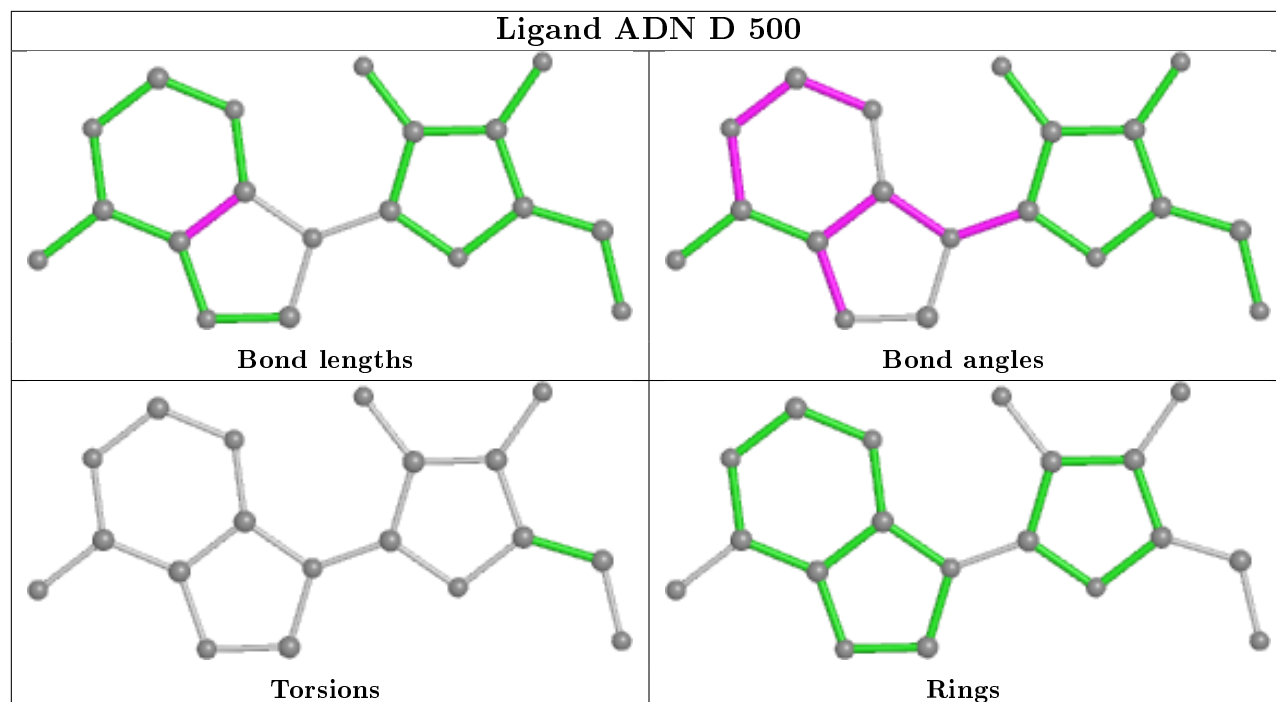
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	ADN	1	0
3	B	550	NAD	1	0
3	C	550	NAD	6	0
3	A	550	NAD	1	0
2	B	500	ADN	1	0
2	D	500	ADN	1	0
3	D	550	NAD	2	0
2	A	500	ADN	1	0

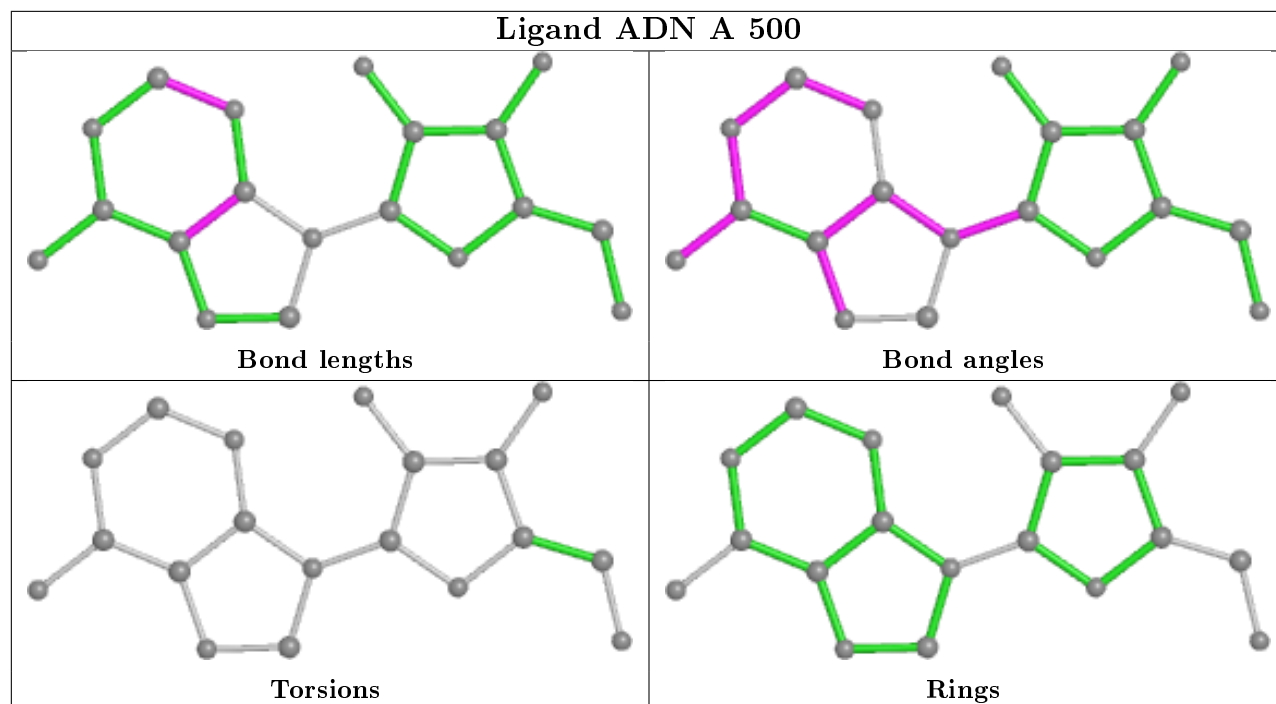
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	486/494 (98%)	-0.12	6 (1%) 79 78	8, 14, 30, 49	0
1	B	485/494 (98%)	-0.16	3 (0%) 89 89	8, 14, 28, 44	0
1	C	485/494 (98%)	0.15	19 (3%) 39 36	7, 16, 36, 88	0
1	D	485/494 (98%)	0.08	14 (2%) 51 49	8, 16, 34, 80	0
All	All	1941/1976 (98%)	-0.01	42 (2%) 62 60	7, 15, 32, 88	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182	ASP	6.0
1	D	182	ASP	5.7
1	D	181	GLU	5.7
1	C	181	GLU	5.3
1	D	180	GLU	4.7
1	D	178	PRO	4.3
1	C	180	GLU	3.8
1	A	10	SER	3.8
1	C	56	VAL	3.7
1	C	178	PRO	3.5
1	C	183	ASP	3.3
1	C	177	PRO	3.2
1	A	375	ARG	3.1
1	C	173	ALA	3.0
1	A	440	ASP	2.9
1	C	175	VAL	2.8
1	B	375	ARG	2.8
1	D	174	GLY	2.7
1	C	16	ARG	2.7
1	D	56	VAL	2.7
1	D	198	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	200	THR	2.6
1	D	175	VAL	2.6
1	C	55	GLU	2.6
1	A	55	GLU	2.5
1	A	181	GLU	2.5
1	C	147	ASP	2.5
1	A	11	LEU	2.5
1	C	146	PRO	2.5
1	C	174	GLY	2.4
1	B	181	GLU	2.3
1	C	115	ASP	2.3
1	D	177	PRO	2.2
1	C	198	PHE	2.2
1	C	199	GLU	2.2
1	C	262	ILE	2.2
1	D	183	ASP	2.2
1	B	440	ASP	2.1
1	D	173	ALA	2.1
1	D	147	ASP	2.1
1	D	115	ASP	2.0
1	D	201	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

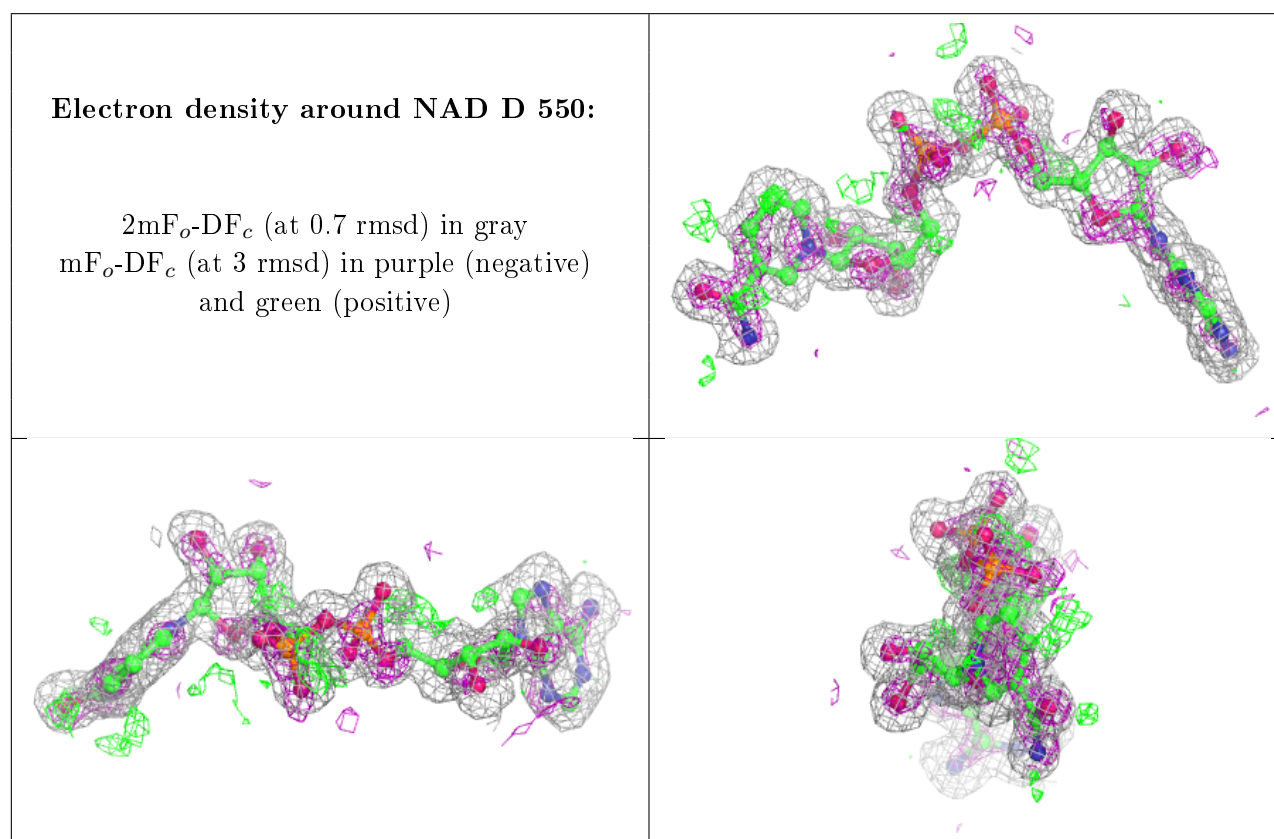
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAD	D	550	44/44	0.95	0.09	8,10,11,13	0
3	NAD	B	550	44/44	0.96	0.07	7,10,11,13	0

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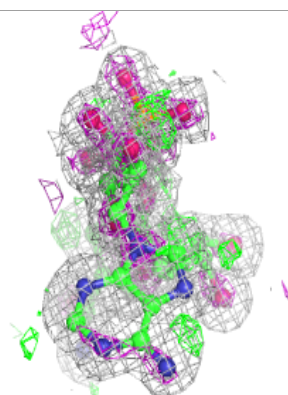
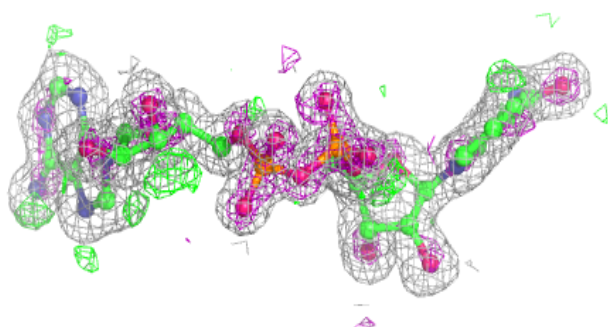
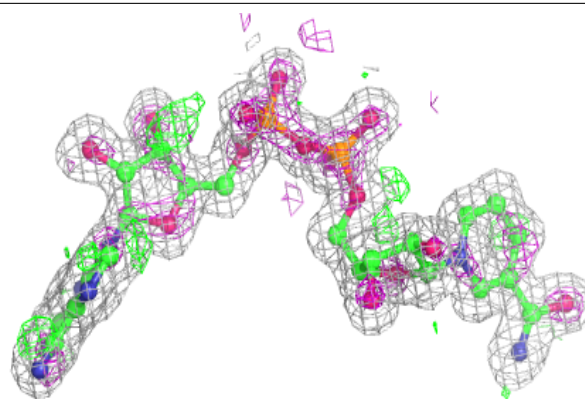
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAD	C	550	44/44	0.96	0.07	8,11,12,14	0
3	NAD	A	550	44/44	0.96	0.07	8,10,11,13	0
2	ADN	B	500	19/19	0.96	0.07	6,9,11,11	0
2	ADN	D	500	19/19	0.96	0.10	9,10,12,13	0
2	ADN	C	500	19/19	0.96	0.10	10,11,12,13	0
2	ADN	A	500	19/19	0.97	0.07	7,9,12,12	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.

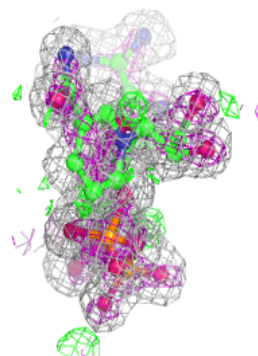
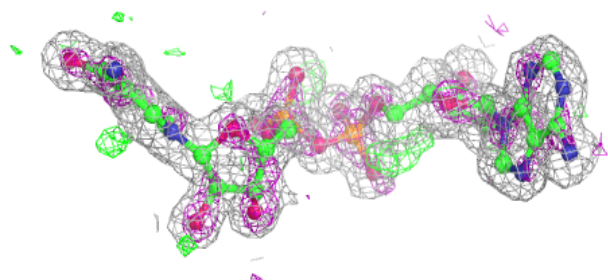
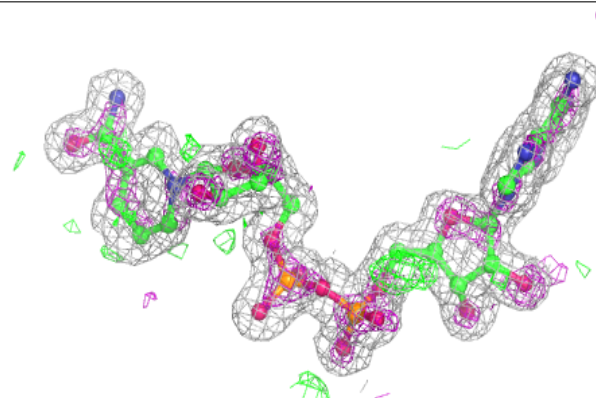


**Electron density around NAD B 550:**

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

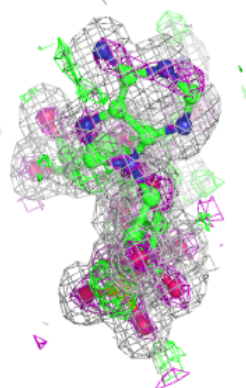
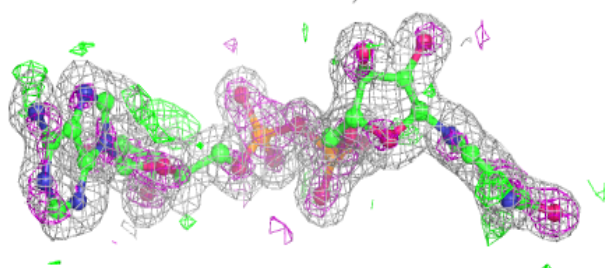
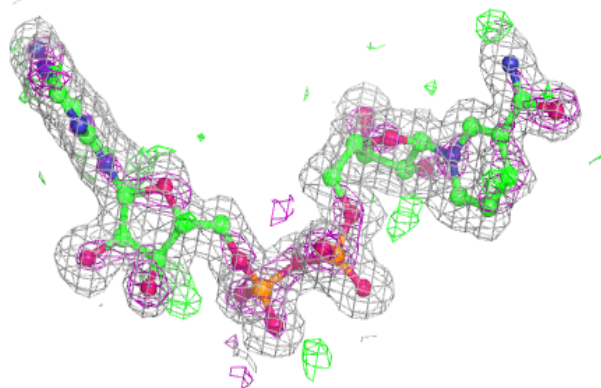
**Electron density around NAD C 550:**

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

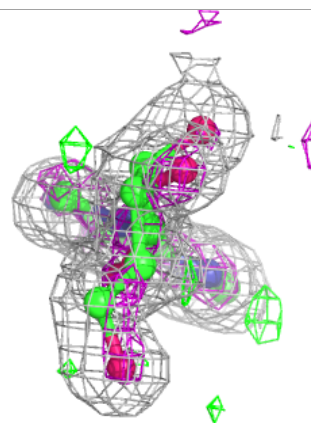
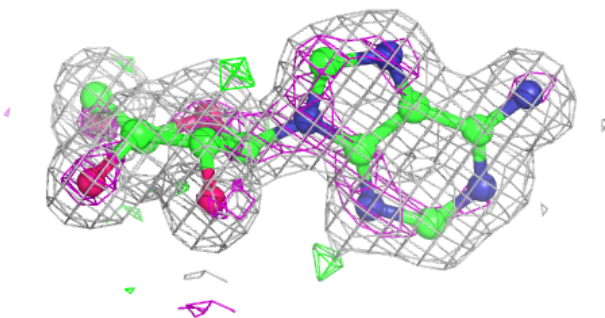
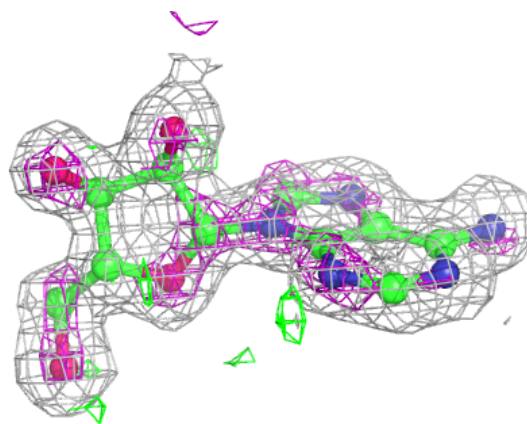


**Electron density around NAD A 550:**

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

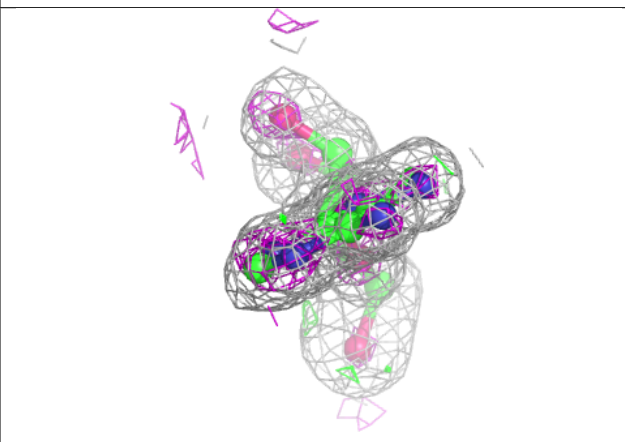
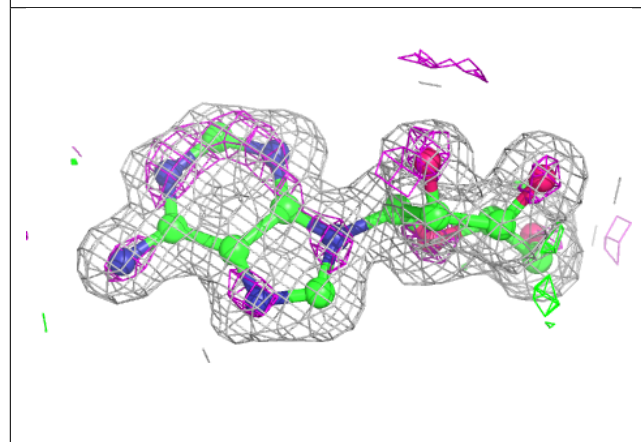
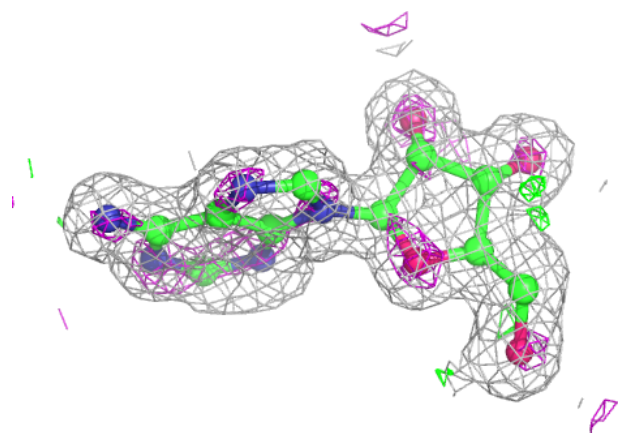
**Electron density around ADN B 500:**

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



**Electron density around ADN D 500:**

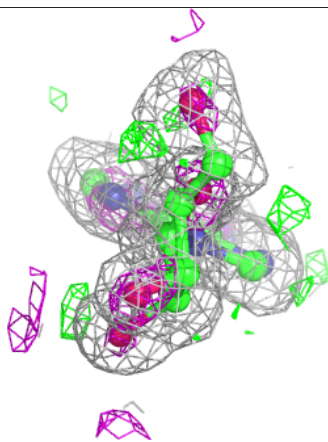
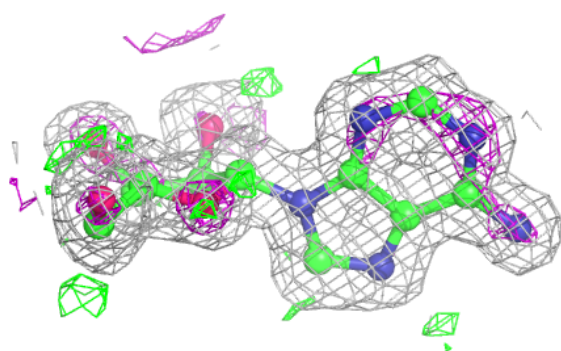
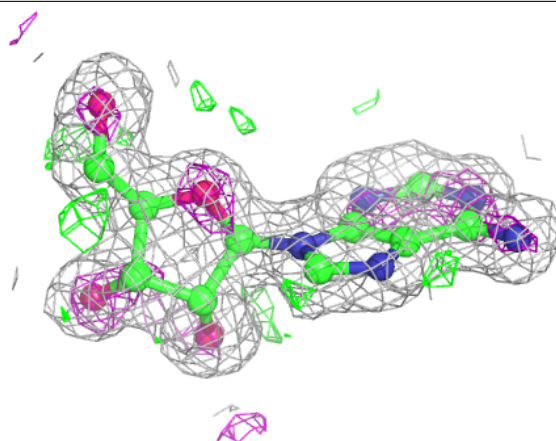
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



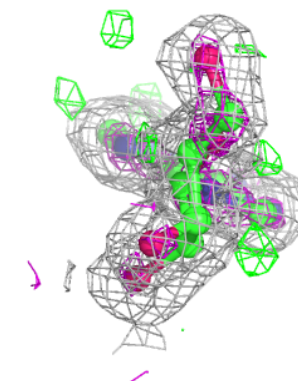
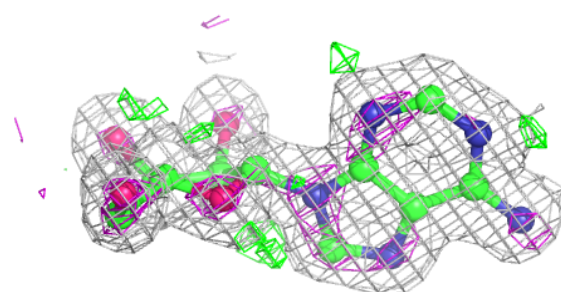
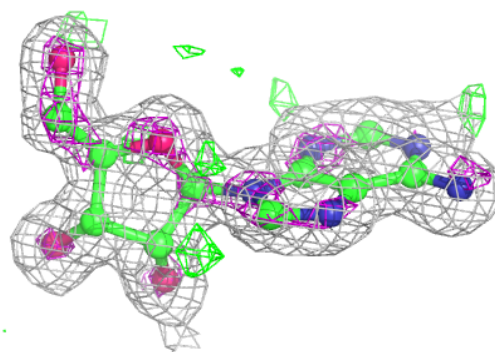


**Electron density around ADN C 500:**

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

**Electron density around ADN A 500:**

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



## 6.5 Other polymers

There are no such residues in this entry.