



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:01 AM UTC

PDB ID : 6Y87 / pdb_00006y87
Title : Crystal Structure of the Homospermidine Synthase (HSS) from *Pseudomonas aeruginosa* in Complex with NAD and PUT
Authors : Helfrich, F.; Scheidig, A.J.
Deposited on : 2020-03-03
Resolution : 2.15 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

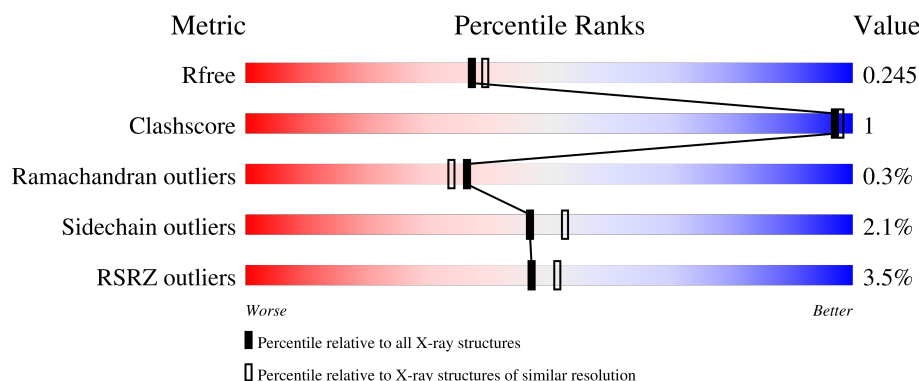
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	471	4% 94% 5%
1	B	471	3% 95% 2%
1	C	471	6% 93% 1%
1	D	471	3% 92% 2%
1	E	471	2% 94% 2%

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Mol	Chain	Length	Quality of chain
1	F	471	3% 93%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 44700 atoms, of which 21561 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 Homospermidine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	470	Total	C	H	N	O	S	0	1	0
			7307	2354	3631	614	697	11			
1	B	466	Total	C	H	N	O	S	0	0	0
			7218	2325	3587	606	690	10			
1	C	454	Total	C	H	N	O	S	0	0	0
			7055	2273	3508	593	671	10			
1	D	456	Total	C	H	N	O	S	0	0	0
			7086	2282	3525	595	674	10			
1	E	460	Total	C	H	N	O	S	0	4	0
			7208	2318	3583	608	689	10			
1	F	458	Total	C	H	N	O	S	0	0	0
			7110	2289	3535	598	678	10			

There are 12 discrepancies between the modelled and reference sequences:

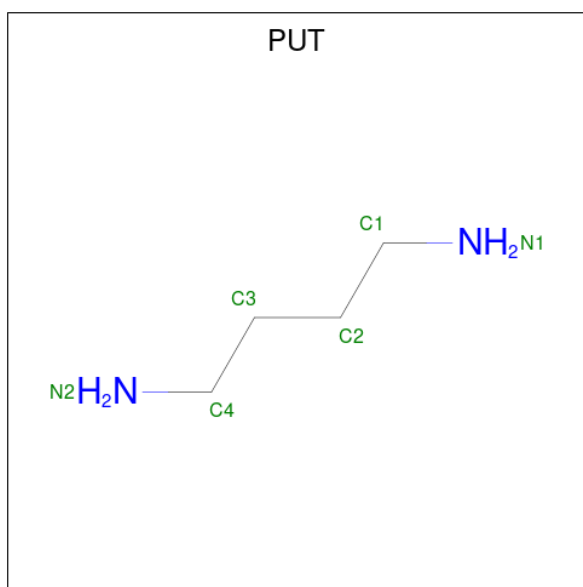
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6X2Y9
A	0	PRO	-	expression tag	UNP Q6X2Y9
B	-1	GLY	-	expression tag	UNP Q6X2Y9
B	0	PRO	-	expression tag	UNP Q6X2Y9
C	-1	GLY	-	expression tag	UNP Q6X2Y9
C	0	PRO	-	expression tag	UNP Q6X2Y9
D	-1	GLY	-	expression tag	UNP Q6X2Y9
D	0	PRO	-	expression tag	UNP Q6X2Y9
E	-1	GLY	-	expression tag	UNP Q6X2Y9
E	0	PRO	-	expression tag	UNP Q6X2Y9
F	-1	GLY	-	expression tag	UNP Q6X2Y9
F	0	PRO	-	expression tag	UNP Q6X2Y9

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	E	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	F	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂) (labeled as "Lig- and of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			18	4	12	2		
3	C	1	Total	C	H	N	0	0
			18	4	12	2		
3	E	1	Total	C	H	N	0	0
			18	4	12	2		

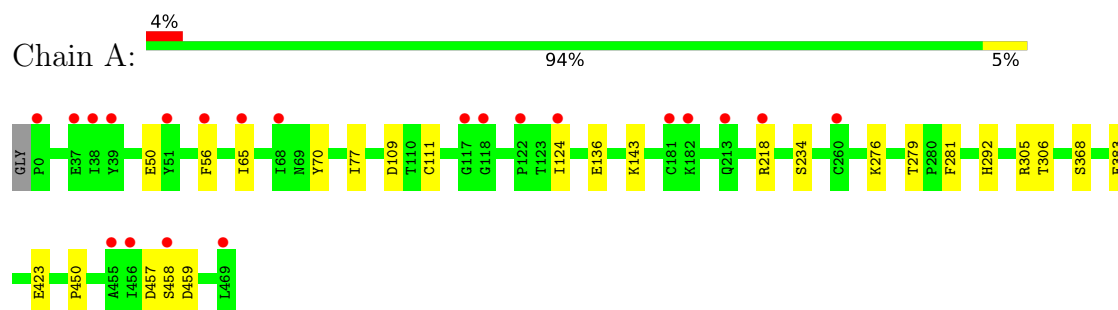
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	168	Total	O	0	0
			168	168		
4	B	191	Total	O	0	0
			191	191		
4	C	132	Total	O	0	0
			132	132		
4	D	184	Total	O	0	0
			184	184		
4	E	318	Total	O	0	0
			318	318		
4	F	249	Total	O	0	0
			249	249		

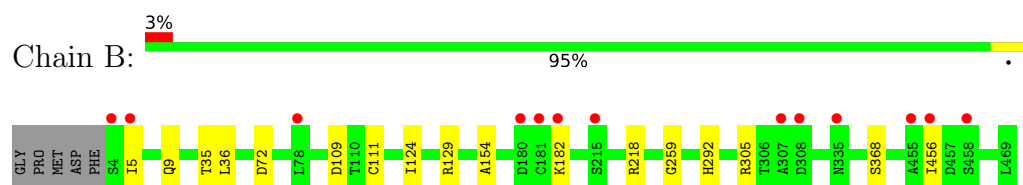
3 Residue-property plots [i](#)

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

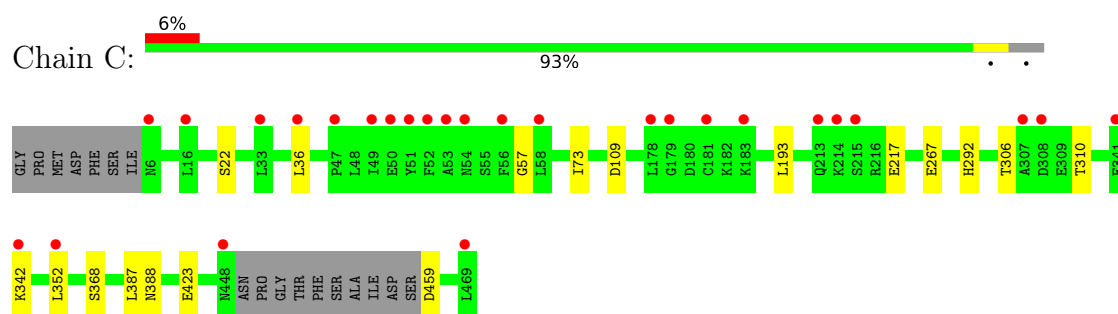
- Molecule 1: Homospermidine synthase



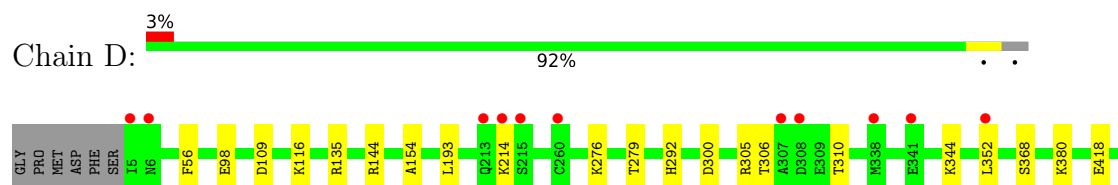
- Molecule 1: Homospermidine synthase

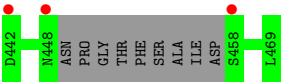


- Molecule 1: Homospermidine synthase

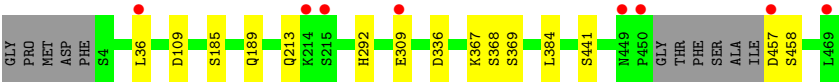


- Molecule 1: Homospermidine synthase

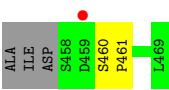
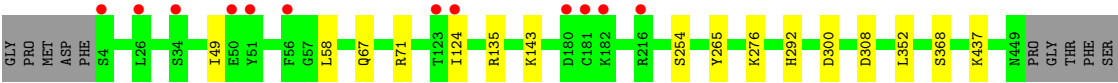
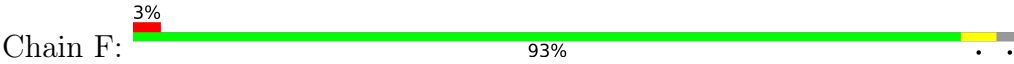




● Molecule 1: Homospermidine synthase



● Molecule 1: Homospermidine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	103.24Å 103.24Å 548.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.31 – 2.15 80.31 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.2 (80.31-2.15) 98.2 (80.31-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.203 , 0.244 0.204 , 0.245	Depositor DCC
R_{free} test set	9598 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.099 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	44700	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.10	0/3771	0.25	0/5134
1	B	0.09	0/3724	0.25	0/5072
1	C	0.09	0/3637	0.25	0/4951
1	D	0.09	0/3651	0.25	0/4970
1	E	0.10	0/3716	0.27	0/5057
1	F	0.10	0/3665	0.26	0/4989
All	All	0.10	0/22164	0.26	0/30173

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3676	3631	3631	8	0
1	B	3631	3587	3587	8	0
1	C	3547	3508	3508	6	0
1	D	3561	3525	3524	12	0
1	E	3625	3583	3579	6	0
1	F	3575	3535	3535	6	0
2	A	44	26	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	26	26	0	0
2	C	44	26	26	0	0
2	D	44	26	26	0	0
2	E	44	26	26	0	0
2	F	44	26	26	2	0
3	A	6	12	12	0	0
3	C	6	12	12	0	0
3	E	6	12	12	0	0
4	A	168	0	0	0	0
4	B	191	0	0	3	0
4	C	132	0	0	1	0
4	D	184	0	0	5	0
4	E	318	0	0	0	0
4	F	249	0	0	2	0
All	All	23139	21561	21556	40	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 1.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ARG:NH2	1:C:306:THR:O	2.21	0.72
1:B:154:ALA:O	4:B:601:HOH:O	2.08	0.70
1:C:22:SER:OG	1:C:388:ASN:OD1	2.09	0.69
1:B:124:ILE:O	1:B:129:ARG:NH1	2.25	0.69
1:C:217:GLU:N	1:C:217:GLU:OE1	2.31	0.62
1:D:344:LYS:NZ	4:D:607:HOH:O	2.31	0.62
1:E:336:ASP:OD1	1:F:276:LYS:NZ	2.32	0.61
1:B:72:ASP:OD2	4:B:602:HOH:O	2.17	0.59
1:B:259:GLY:O	1:C:310:THR:OG1	2.20	0.59
1:A:281:PHE:O	1:B:218:ARG:NH2	2.36	0.57
1:D:154:ALA:O	4:D:601:HOH:O	2.17	0.57
2:F:501:NAD:O4D	4:F:601:HOH:O	2.18	0.56
1:E:368:SER:OG	1:E:441:SER:O	2.24	0.55
1:C:423:GLU:OE1	4:C:601:HOH:O	2.18	0.55
1:A:305:ARG:NH1	1:D:310:THR:OG1	2.39	0.55
1:D:98:GLU:OE1	1:D:144:ARG:NH2	2.40	0.54
2:F:501:NAD:O2N	4:F:602:HOH:O	2.19	0.52
1:D:135:ARG:NH2	1:D:300:ASP:OD2	2.41	0.51
1:D:116:LYS:O	4:D:602:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASP:OD1	1:A:111:CYS:N	2.39	0.49
1:A:305:ARG:NH2	1:D:306:THR:O	2.48	0.47
1:D:56:PHE:O	4:D:603:HOH:O	2.20	0.47
1:D:380:LYS:NZ	4:D:614:HOH:O	2.46	0.47
1:D:418:GLU:OE1	1:D:418:GLU:N	2.47	0.46
1:C:109:ASP:OD1	1:C:109:ASP:C	2.59	0.45
1:E:457:ASP:OD1	1:E:458:SER:N	2.50	0.44
1:E:368:SER:OG	1:E:369:SER:N	2.50	0.44
1:D:109:ASP:OD1	1:D:109:ASP:C	2.61	0.44
1:F:460:SER:N	1:F:461:PRO:HD2	2.33	0.44
1:A:457:ASP:O	1:A:459:ASP:N	2.51	0.42
1:F:254:SER:HB2	1:F:265:TYR:CZ	2.54	0.42
1:E:109:ASP:OD1	1:E:109:ASP:C	2.63	0.42
1:B:109:ASP:OD1	1:B:109:ASP:C	2.63	0.42
1:A:306:THR:O	1:D:305:ARG:NH2	2.52	0.41
1:F:135:ARG:NH1	1:F:300:ASP:OD2	2.52	0.41
1:F:308:ASP:N	1:F:308:ASP:OD1	2.53	0.41
1:A:450:PRO:O	1:F:71:ARG:NH1	2.54	0.41
1:B:182:LYS:NZ	4:B:628:HOH:O	2.53	0.41
1:A:65:ILE:HG23	1:A:70:TYR:HB2	2.04	0.40
1:E:185:SER:OG	1:E:189:GLN:OE1	2.32	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	469/471 (100%)	448 (96%)	19 (4%)	2 (0%)	30	26
1	B	464/471 (98%)	443 (96%)	20 (4%)	1 (0%)	43	44
1	C	450/471 (96%)	425 (94%)	23 (5%)	2 (0%)	30	26
1	D	452/471 (96%)	429 (95%)	22 (5%)	1 (0%)	43	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	460/471 (98%)	446 (97%)	14 (3%)	0	100	100
1	F	454/471 (96%)	438 (96%)	15 (3%)	1 (0%)	43	44
All	All	2749/2826 (97%)	2629 (96%)	113 (4%)	7 (0%)	36	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	SER
1	C	57	GLY
1	A	368	SER
1	B	368	SER
1	C	368	SER
1	D	368	SER
1	F	368	SER

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	403/402 (100%)	389 (96%)	14 (4%)	32	32
1	B	398/402 (99%)	391 (98%)	7 (2%)	51	58
1	C	388/402 (96%)	379 (98%)	9 (2%)	44	49
1	D	390/402 (97%)	384 (98%)	6 (2%)	57	64
1	E	398/402 (99%)	391 (98%)	7 (2%)	51	58
1	F	392/402 (98%)	384 (98%)	8 (2%)	48	54
All	All	2369/2412 (98%)	2318 (98%)	51 (2%)	47	51

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	56	PHE
1	A	77	ILE

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Mol	Chain	Res	Type
1	A	124	ILE
1	A	136	GLU
1	A	143	LYS
1	A	218[A]	ARG
1	A	218[B]	ARG
1	A	234	SER
1	A	276	LYS
1	A	279	THR
1	A	292	HIS
1	A	383	GLU
1	A	423	GLU
1	B	5	ILE
1	B	9	GLN
1	B	35	THR
1	B	36	LEU
1	B	111	CYS
1	B	292	HIS
1	B	456	ILE
1	C	36	LEU
1	C	73	ILE
1	C	193	LEU
1	C	267	GLU
1	C	292	HIS
1	C	342	LYS
1	C	352	LEU
1	C	387	LEU
1	C	459	ASP
1	D	193	LEU
1	D	214	LYS
1	D	276	LYS
1	D	279	THR
1	D	292	HIS
1	D	352	LEU
1	E	36	LEU
1	E	213	GLN
1	E	292	HIS
1	E	309[A]	GLU
1	E	309[B]	GLU
1	E	367	LYS
1	E	384	LEU
1	F	49	ILE
1	F	58	LEU

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Mol	Chain	Res	Type
1	F	67	GLN
1	F	124	ILE
1	F	143	LYS
1	F	292	HIS
1	F	352	LEU
1	F	437	LYS

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

Mol	Chain	Res	Type
1	A	21	GLN
1	A	127	HIS
1	A	133	HIS
1	A	137	GLN
1	B	133	HIS
1	C	62	ASN
1	C	133	HIS
1	C	335	ASN
1	D	127	HIS
1	D	210	GLN
1	D	236	GLN
1	D	256	HIS
1	D	422	HIS
1	E	133	HIS
1	F	62	ASN
1	F	127	HIS
1	F	330	HIS
1	F	448	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

9 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	NAD	A	501	-	46,48,48	1.29	7 (15%)	64,73,73	1.68	10 (15%)
2	NAD	C	501	-	46,48,48	1.04	3 (6%)	64,73,73	1.80	15 (23%)
2	NAD	B	501	-	46,48,48	1.32	7 (15%)	64,73,73	1.91	14 (21%)
3	PUT	C	502	-	5,5,5	0.21	0	4,4,4	0.34	0
2	NAD	D	501	-	46,48,48	1.27	6 (13%)	64,73,73	2.04	19 (29%)
3	PUT	A	502	-	5,5,5	0.21	0	4,4,4	0.35	0
3	PUT	E	502	-	5,5,5	0.20	0	4,4,4	0.39	0
2	NAD	F	501	-	46,48,48	1.26	7 (15%)	64,73,73	1.90	17 (26%)
2	NAD	E	501	-	46,48,48	1.37	5 (10%)	64,73,73	2.10	18 (28%)

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	NAD	A	501	-	-	4/30/62/62	0/5/5/5
2	NAD	C	501	-	-	3/30/62/62	0/5/5/5
2	NAD	B	501	-	-	9/30/62/62	0/5/5/5
3	PUT	C	502	-	-	2/3/3/3	-
2	NAD	D	501	-	-	7/30/62/62	0/5/5/5
3	PUT	A	502	-	-	1/3/3/3	-
3	PUT	E	502	-	-	2/3/3/3	-
2	NAD	F	501	-	-	5/30/62/62	0/5/5/5
2	NAD	E	501	-	-	6/30/62/62	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	NAD	C5A-C4A	4.25	1.46	1.39
2	E	501	NAD	O4D-C1D	4.17	1.46	1.40
2	C	501	NAD	C5A-C4A	4.07	1.46	1.39
2	D	501	NAD	C5A-C4A	4.07	1.46	1.39
2	F	501	NAD	C5A-C4A	4.05	1.46	1.39
2	A	501	NAD	C5A-C4A	4.00	1.46	1.39
2	B	501	NAD	C5A-C4A	3.72	1.45	1.39
2	F	501	NAD	C5A-N7A	-3.24	1.33	1.39
2	A	501	NAD	O4D-C1D	3.22	1.45	1.40
2	B	501	NAD	C3N-C7N	3.17	1.55	1.50
2	B	501	NAD	C8A-N7A	3.07	1.37	1.31
2	B	501	NAD	C4A-N9A	-2.87	1.31	1.37
2	B	501	NAD	O4D-C1D	2.83	1.44	1.40
2	D	501	NAD	C7N-N7N	2.65	1.37	1.33
2	D	501	NAD	C8A-N7A	2.65	1.36	1.31
2	B	501	NAD	C5A-N7A	-2.61	1.34	1.39
2	A	501	NAD	C4A-N9A	-2.58	1.32	1.37
2	E	501	NAD	C5A-N7A	-2.58	1.34	1.39
2	A	501	NAD	C8A-N7A	2.56	1.36	1.31
2	D	501	NAD	C3N-C7N	2.56	1.54	1.50
2	F	501	NAD	C4A-N9A	-2.51	1.32	1.37
2	E	501	NAD	PN-O3	2.51	1.62	1.59
2	D	501	NAD	O4D-C1D	2.45	1.44	1.40
2	F	501	NAD	C7N-N7N	2.40	1.37	1.33
2	F	501	NAD	O4D-C1D	2.40	1.44	1.40
2	A	501	NAD	C5A-N7A	-2.24	1.35	1.39
2	C	501	NAD	O4D-C1D	2.24	1.43	1.40
2	D	501	NAD	C4A-N9A	-2.22	1.33	1.37
2	F	501	NAD	C5A-C6A	2.12	1.46	1.41
2	C	501	NAD	C5A-C6A	2.11	1.46	1.41
2	A	501	NAD	C7N-N7N	2.10	1.36	1.33
2	A	501	NAD	PA-O3	2.09	1.61	1.59
2	B	501	NAD	C7N-N7N	2.05	1.36	1.33
2	E	501	NAD	C8A-N7A	2.04	1.35	1.31
2	F	501	NAD	C8A-N7A	2.03	1.35	1.31

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	C3N-C7N-N7N	6.39	125.61	117.74
2	E	501	NAD	C5A-C4A-N3A	-5.86	118.64	126.72
2	E	501	NAD	N3A-C2A-N1A	-5.55	120.18	128.58
2	E	501	NAD	N3A-C4A-N9A	5.52	136.55	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAD	C3N-C7N-N7N	5.41	124.40	117.74
2	C	501	NAD	C5A-C4A-N3A	-5.36	119.33	126.72
2	A	501	NAD	C5A-C4A-N3A	-5.27	119.46	126.72
2	F	501	NAD	C3N-C7N-N7N	5.19	124.13	117.74
2	F	501	NAD	C5A-C4A-N3A	-5.07	119.73	126.72
2	C	501	NAD	N3A-C4A-N9A	5.05	135.75	127.17
2	D	501	NAD	C4A-N9A-C8A	4.77	110.75	105.74
2	E	501	NAD	C2A-N3A-C4A	4.64	123.16	111.83
2	B	501	NAD	C5A-C4A-N3A	-4.53	120.47	126.72
2	D	501	NAD	C5A-C4A-N3A	-4.49	120.53	126.72
2	E	501	NAD	C4A-N9A-C8A	4.46	110.42	105.74
2	B	501	NAD	O7N-C7N-C3N	-4.36	114.27	119.60
2	D	501	NAD	N3A-C4A-N9A	4.32	134.51	127.17
2	A	501	NAD	N3A-C4A-N9A	4.30	134.48	127.17
2	C	501	NAD	O4B-C1B-N9A	4.29	116.33	108.09
2	D	501	NAD	O7N-C7N-C3N	-4.21	114.45	119.60
2	F	501	NAD	N3A-C4A-N9A	4.16	134.25	127.17
2	D	501	NAD	N3A-C2A-N1A	-4.06	122.44	128.58
2	C	501	NAD	N3A-C2A-N1A	-3.79	122.84	128.58
2	E	501	NAD	C3N-C7N-N7N	3.68	122.27	117.74
2	A	501	NAD	N3A-C2A-N1A	-3.59	123.14	128.58
2	B	501	NAD	N3A-C4A-N9A	3.57	133.24	127.17
2	C	501	NAD	C2A-N3A-C4A	3.53	120.46	111.83
2	F	501	NAD	O7N-C7N-C3N	-3.52	115.29	119.60
2	F	501	NAD	N3A-C2A-N1A	-3.52	123.26	128.58
2	A	501	NAD	C2A-N3A-C4A	3.51	120.40	111.83
2	D	501	NAD	N9A-C8A-N7A	-3.50	108.97	113.94
2	E	501	NAD	N9A-C8A-N7A	-3.50	108.98	113.94
2	B	501	NAD	N3A-C2A-N1A	-3.49	123.30	128.58
2	C	501	NAD	C4A-N9A-C8A	3.47	109.39	105.74
2	F	501	NAD	C2A-N3A-C4A	3.37	120.07	111.83
2	D	501	NAD	C2A-N3A-C4A	3.30	119.89	111.83
2	A	501	NAD	C3N-C7N-N7N	3.26	121.75	117.74
2	F	501	NAD	C4A-N9A-C8A	3.23	109.12	105.74
2	E	501	NAD	C5A-N7A-C8A	3.20	108.48	103.45
2	A	501	NAD	O4B-C1B-N9A	3.18	114.21	108.09
2	B	501	NAD	C4A-N9A-C8A	3.18	109.08	105.74
2	F	501	NAD	C4A-C5A-N7A	-3.14	106.99	110.58
2	B	501	NAD	C2A-N3A-C4A	3.07	119.33	111.83
2	A	501	NAD	C4A-N9A-C8A	3.05	108.94	105.74
2	D	501	NAD	O4B-C1B-N9A	3.04	113.92	108.09
2	F	501	NAD	O2A-PA-O3	3.03	115.47	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	NAD	C6A-C5A-N7A	3.02	137.91	132.09
2	B	501	NAD	O3-PA-O1A	-3.01	101.64	110.70
2	F	501	NAD	C5A-N7A-C8A	2.98	108.13	103.45
2	F	501	NAD	N9A-C8A-N7A	-2.96	109.74	113.94
2	D	501	NAD	C4A-N9A-C1B	-2.92	119.81	126.63
2	E	501	NAD	C4A-C5A-N7A	-2.83	107.35	110.58
2	E	501	NAD	O4B-C1B-N9A	2.81	113.48	108.09
2	C	501	NAD	C3N-C7N-N7N	2.72	121.09	117.74
2	D	501	NAD	N6A-C6A-N1A	2.72	124.43	118.38
2	F	501	NAD	O2D-C2D-C3D	2.68	120.39	111.82
2	F	501	NAD	O4B-C1B-N9A	2.64	113.17	108.09
2	F	501	NAD	O2A-PA-O5B	2.62	119.46	107.57
2	E	501	NAD	O3D-C3D-C2D	2.61	120.17	111.82
2	E	501	NAD	C4B-O4B-C1B	-2.60	103.72	109.47
2	D	501	NAD	C4B-O4B-C1B	-2.58	103.76	109.47
2	B	501	NAD	N9A-C8A-N7A	-2.58	110.27	113.94
2	D	501	NAD	C5A-N7A-C8A	2.58	107.50	103.45
2	F	501	NAD	C2A-N1A-C6A	2.52	122.87	118.73
2	E	501	NAD	C2A-N1A-C6A	2.51	122.86	118.73
2	C	501	NAD	O7N-C7N-N7N	-2.47	119.05	122.62
2	C	501	NAD	C6N-N1N-C2N	-2.47	119.78	121.88
2	D	501	NAD	C4A-C5A-N7A	-2.42	107.81	110.58
2	A	501	NAD	O5D-PN-O1N	2.41	118.50	108.94
2	B	501	NAD	C4A-N9A-C1B	-2.40	121.01	126.63
2	A	501	NAD	C4A-C5A-N7A	-2.37	107.88	110.58
2	B	501	NAD	C2A-N1A-C6A	2.36	122.60	118.73
2	D	501	NAD	C5A-C6A-N6A	-2.36	117.45	123.29
2	D	501	NAD	C2A-N1A-C6A	2.35	122.60	118.73
2	C	501	NAD	O2A-PA-O1A	2.32	123.26	112.44
2	B	501	NAD	O5D-PN-O1N	2.32	118.12	108.94
2	E	501	NAD	O2B-C2B-C3B	2.30	119.20	111.82
2	D	501	NAD	O2A-PA-O3	2.30	113.50	107.27
2	E	501	NAD	O2A-PA-O1A	2.30	123.15	112.44
2	C	501	NAD	N9A-C8A-N7A	-2.30	110.68	113.94
2	D	501	NAD	O2N-PN-O5D	2.24	117.73	107.57
2	C	501	NAD	C5A-N7A-C8A	2.20	106.91	103.45
2	C	501	NAD	C4A-C5A-N7A	-2.18	108.08	110.58
2	C	501	NAD	O2B-C2B-C3B	2.18	118.80	111.82
2	F	501	NAD	O5D-PN-O1N	2.18	117.56	108.94
2	B	501	NAD	C4A-C5A-N7A	-2.13	108.15	110.58
2	B	501	NAD	O4B-C1B-N9A	2.12	112.17	108.09
2	A	501	NAD	N9A-C8A-N7A	-2.10	110.96	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAD	O2N-PN-O1N	2.10	122.20	112.44
2	E	501	NAD	O7N-C7N-N7N	-2.09	119.60	122.62
2	E	501	NAD	O4B-C4B-C5B	-2.02	102.85	109.33
2	F	501	NAD	C6A-C5A-N7A	2.02	135.99	132.09
2	C	501	NAD	O3-PA-O1A	-2.02	104.64	110.70

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C5D-O5D-PN-O3
2	B	501	NAD	C5D-O5D-PN-O1N
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	C	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C5D-O5D-PN-O2N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	E	501	NAD	O4D-C1D-N1N-C2N
2	E	501	NAD	O4D-C1D-N1N-C6N
2	E	501	NAD	C2D-C1D-N1N-C2N
2	F	501	NAD	O4D-C1D-N1N-C2N
2	F	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	C2B-C1B-N9A-C8A
3	C	502	PUT	C2-C3-C4-N2
2	C	501	NAD	C2B-C1B-N9A-C8A
2	B	501	NAD	C5D-O5D-PN-O2N
2	D	501	NAD	C5D-O5D-PN-O3
3	C	502	PUT	N1-C1-C2-C3
2	A	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	E	501	NAD	C2D-C1D-N1N-C6N
2	F	501	NAD	C2D-C1D-N1N-C2N
3	A	502	PUT	C2-C3-C4-N2
3	E	502	PUT	N1-C1-C2-C3
2	C	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4B-C1B-N9A-C8A
2	E	501	NAD	O4B-C4B-C5B-O5B

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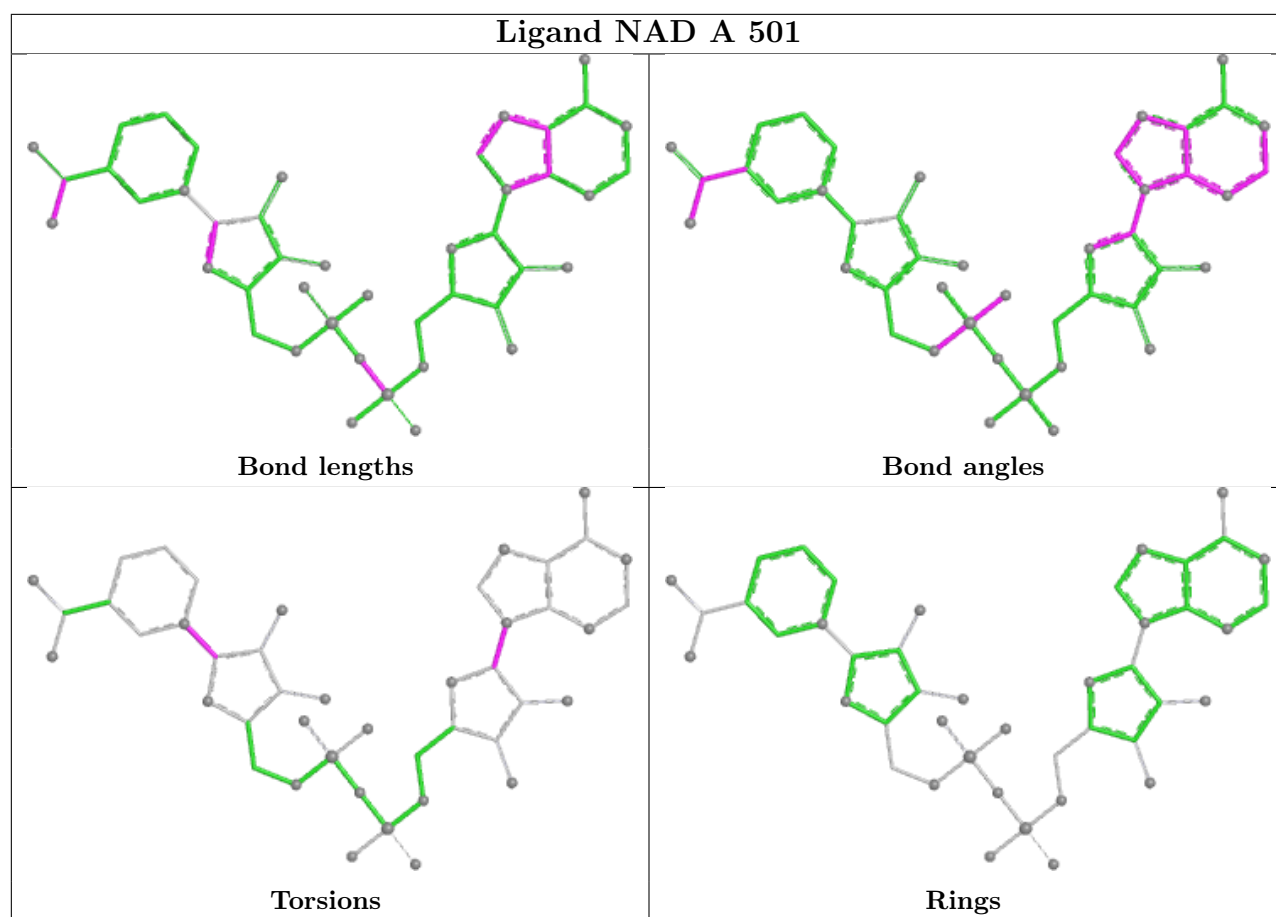
Mol	Chain	Res	Type	Atoms
2	F	501	NAD	O4B-C4B-C5B-O5B
2	E	501	NAD	C2B-C1B-N9A-C8A
2	A	501	NAD	C2B-C1B-N9A-C8A
2	D	501	NAD	C2B-C1B-N9A-C8A
2	F	501	NAD	C2B-C1B-N9A-C8A
3	E	502	PUT	C1-C2-C3-C4
2	D	501	NAD	PA-O3-PN-O1N

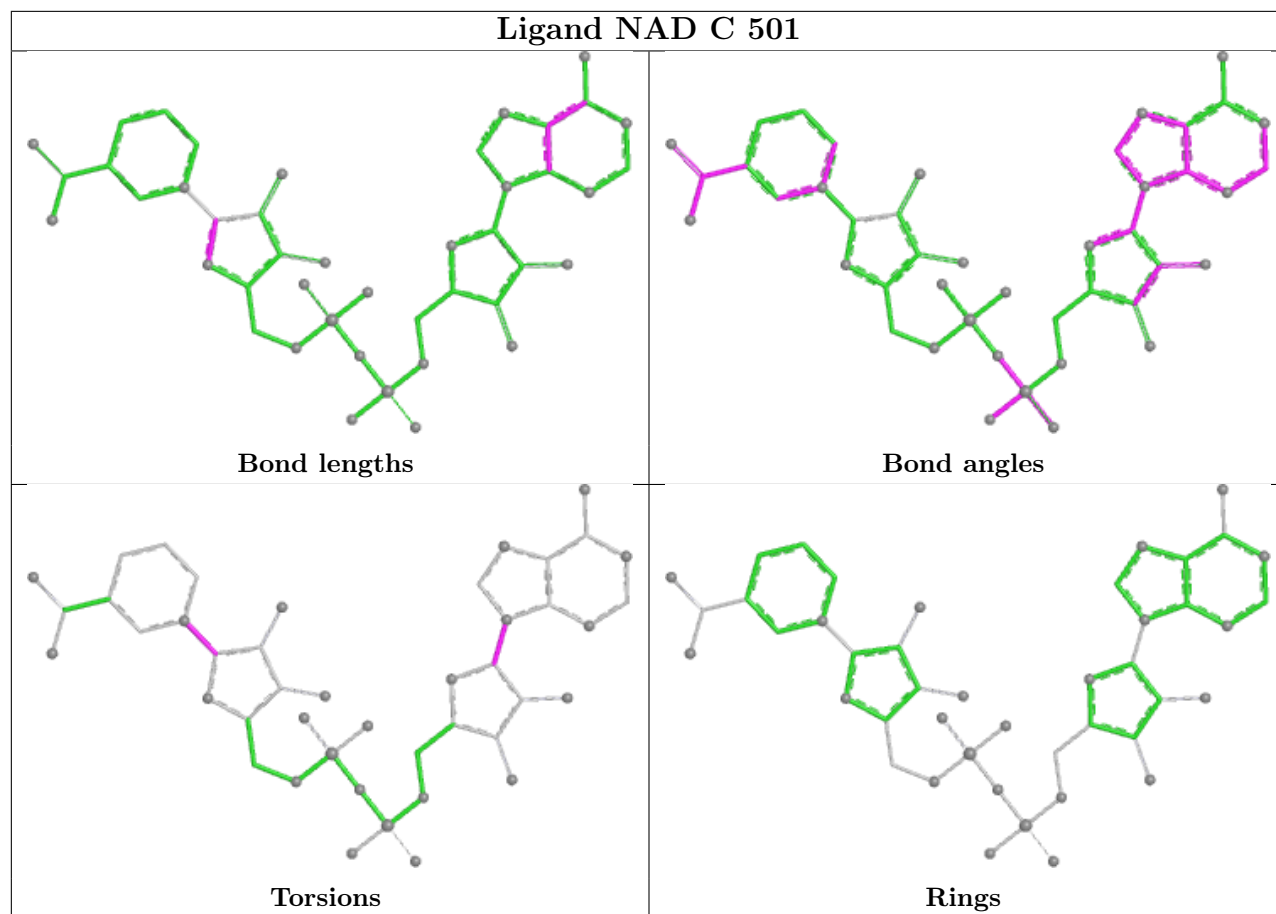
There are no ring outliers.

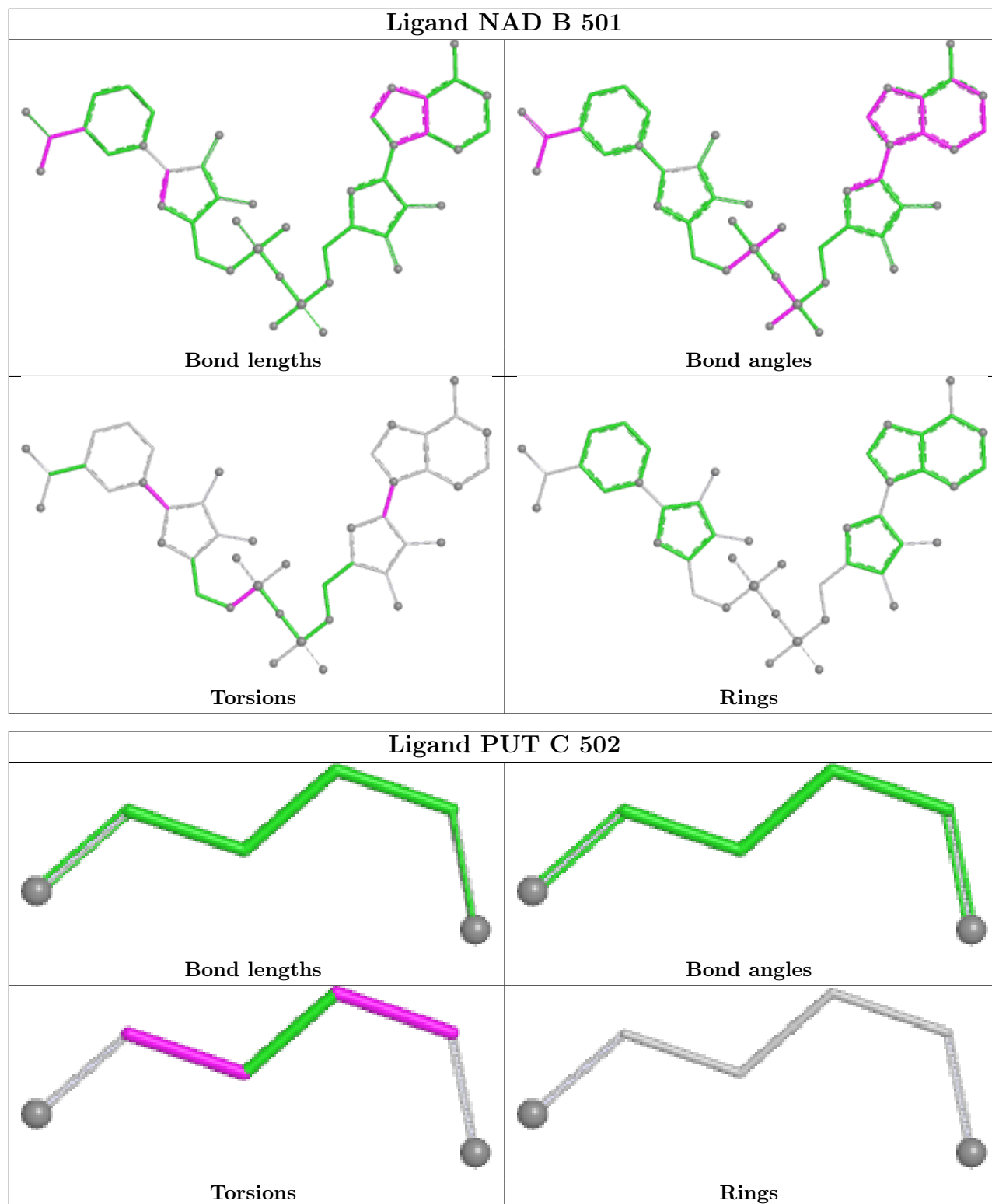
1 monomer is involved in 2 short contacts:

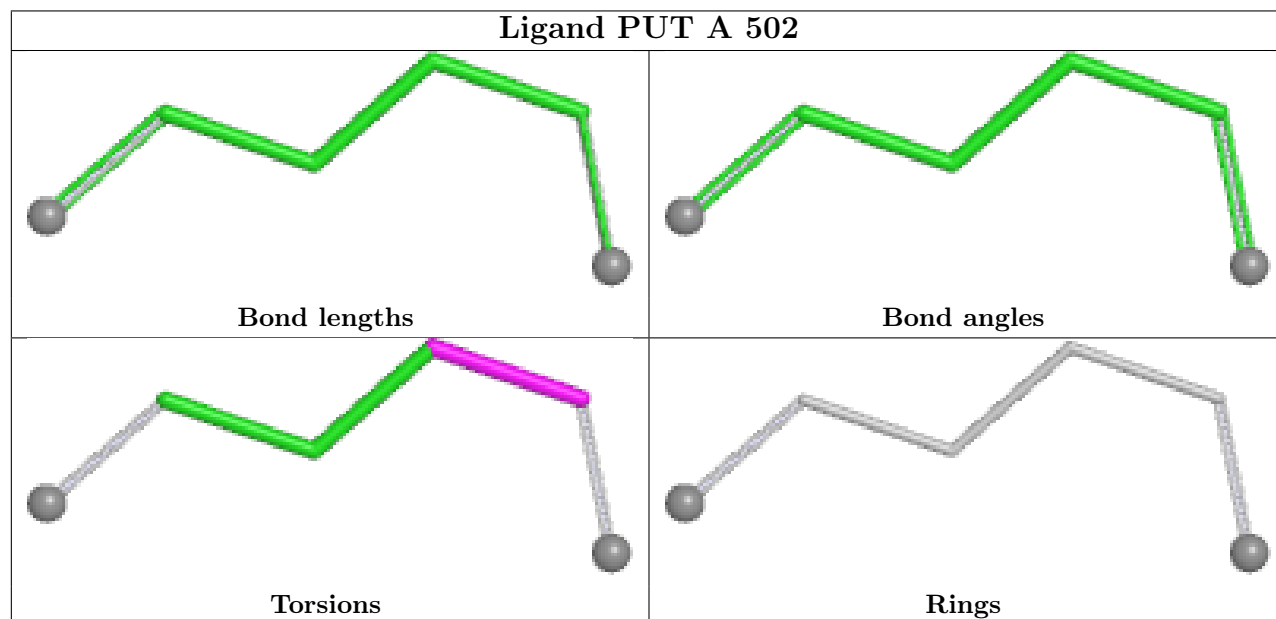
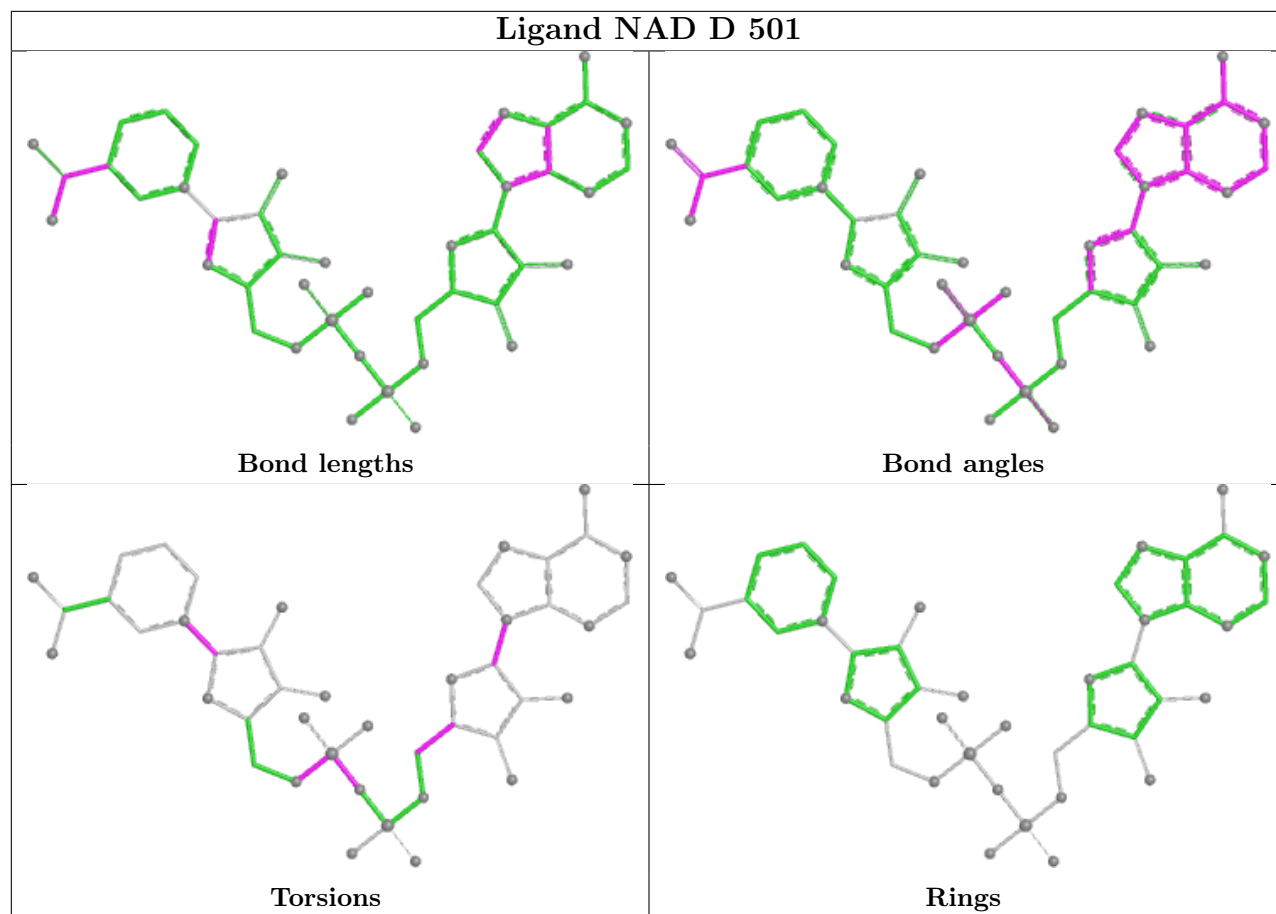
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	NAD	2	0

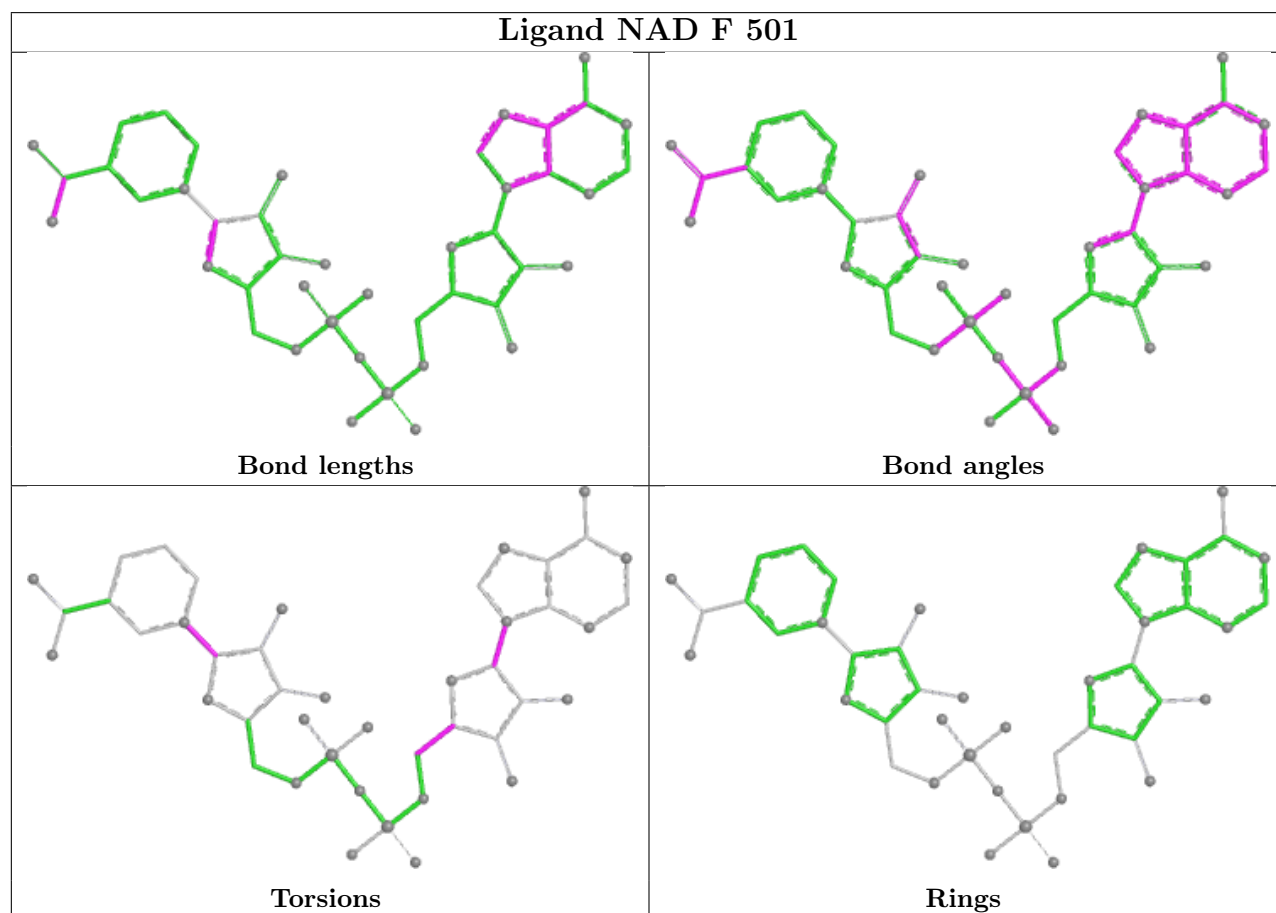
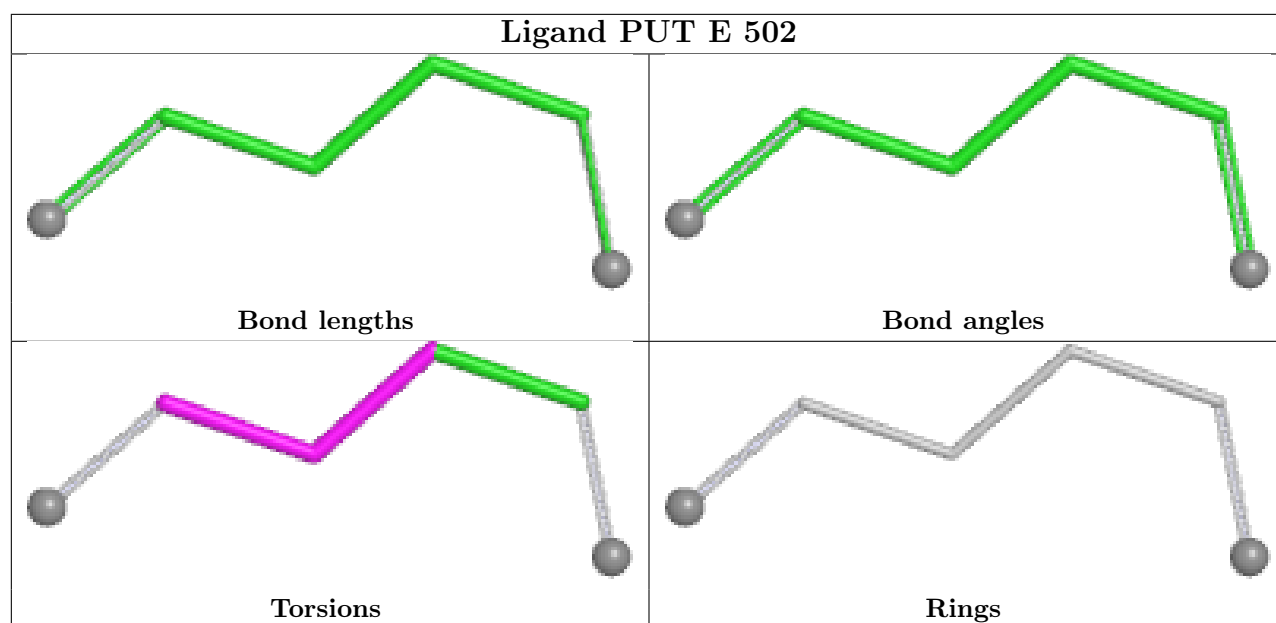
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

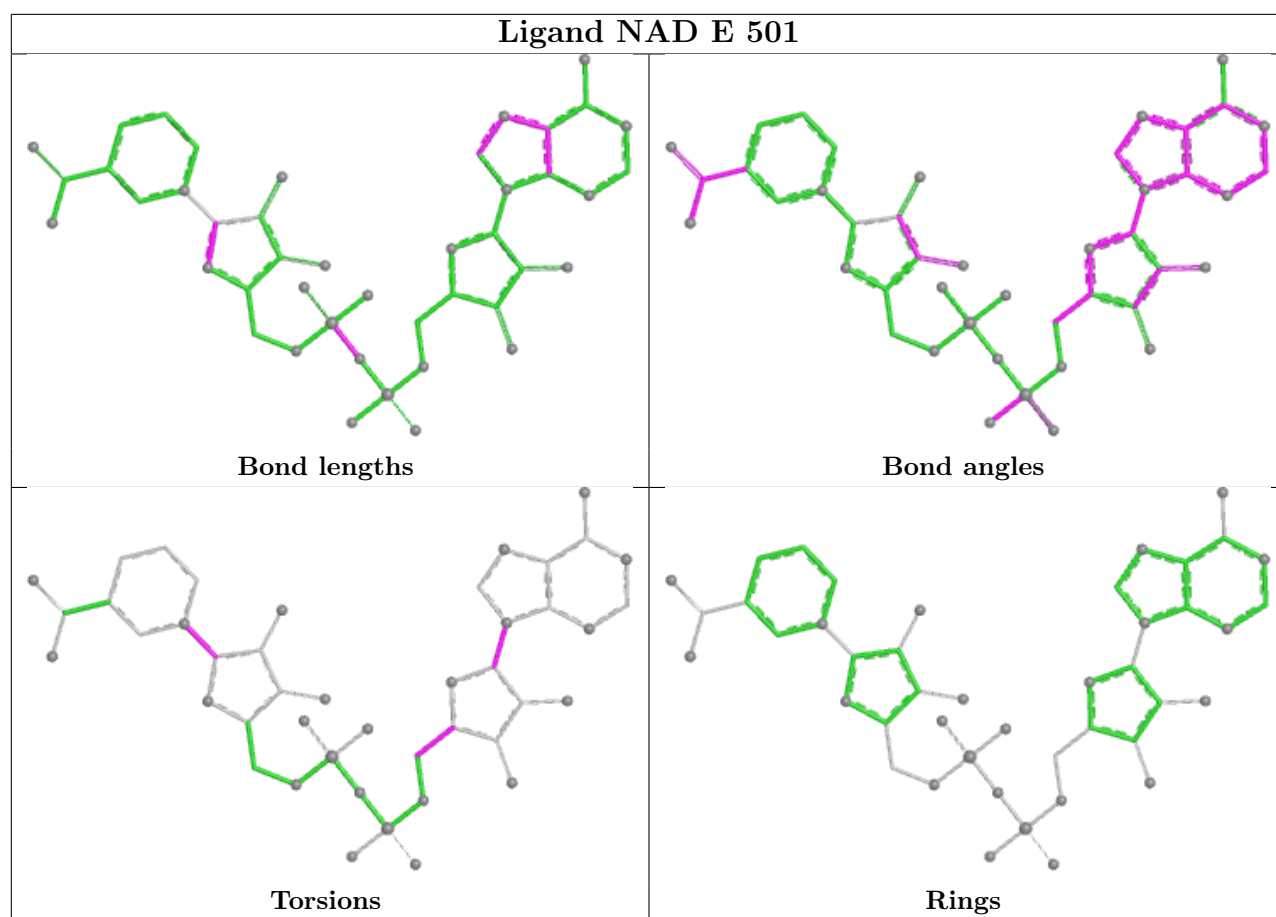












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	470/471 (99%)	0.43	21 (4%)	38 43	20, 39, 64, 74	1 (0%)
1	B	466/471 (98%)	0.44	13 (2%)	55 59	23, 38, 59, 86	0
1	C	454/471 (96%)	0.63	27 (5%)	28 32	25, 42, 68, 86	0
1	D	456/471 (96%)	0.44	14 (3%)	51 55	22, 38, 58, 79	0
1	E	460/471 (97%)	-0.15	8 (1%)	69 73	11, 24, 47, 73	4 (0%)
1	F	458/471 (97%)	0.05	13 (2%)	55 59	15, 29, 58, 74	0
All	All	2764/2826 (97%)	0.31	96 (3%)	47 51	11, 36, 61, 86	5 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	456	ILE	4.9
1	B	456	ILE	4.5
1	E	450	PRO	4.2
1	E	309[A]	GLU	3.7
1	C	6	ASN	3.6
1	D	308	ASP	3.4
1	F	459	ASP	3.4
1	A	56	PHE	3.4
1	A	51	TYR	3.3
1	B	455	ALA	3.3
1	C	448	ASN	3.2
1	B	181	CYS	3.2
1	B	458	SER	3.1
1	C	213	GLN	3.1
1	F	123	THR	3.0
1	B	180	ASP	3.0
1	B	5	ILE	3.0
1	D	215	SER	3.0
1	C	308	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	39	TYR	3.0
1	D	5	ILE	2.9
1	B	4	SER	2.9
1	A	68	ILE	2.8
1	A	455	ALA	2.8
1	C	352	LEU	2.8
1	A	181	CYS	2.8
1	B	182	LYS	2.8
1	D	213	GLN	2.8
1	C	33	LEU	2.8
1	C	183	LYS	2.8
1	C	49	ILE	2.8
1	A	122	PRO	2.7
1	A	38	ILE	2.7
1	F	50	GLU	2.7
1	F	124	ILE	2.6
1	C	307	ALA	2.6
1	A	469	LEU	2.6
1	A	37	GLU	2.6
1	C	53	ALA	2.6
1	B	78	LEU	2.6
1	F	51	TYR	2.6
1	A	65	ILE	2.5
1	A	213	GLN	2.5
1	C	214	LYS	2.5
1	E	449	ASN	2.5
1	C	36	LEU	2.5
1	F	182	LYS	2.5
1	C	51	TYR	2.4
1	B	335	ASN	2.4
1	E	469	LEU	2.4
1	C	52	PHE	2.4
1	F	181	CYS	2.4
1	F	26	LEU	2.3
1	C	56	PHE	2.3
1	C	342	LYS	2.3
1	C	215	SER	2.3
1	E	215	SER	2.3
1	F	34	SER	2.3
1	D	6	ASN	2.3
1	D	448	ASN	2.3
1	C	54	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	469	LEU	2.3
1	E	214	LYS	2.3
1	D	338	MET	2.3
1	A	0	PRO	2.3
1	B	308	ASP	2.3
1	D	307	ALA	2.3
1	E	457	ASP	2.2
1	C	181	CYS	2.2
1	A	458	SER	2.2
1	C	47	PRO	2.2
1	F	180	ASP	2.2
1	C	341	GLU	2.2
1	A	260	CYS	2.2
1	D	341	GLU	2.1
1	F	56	PHE	2.1
1	C	178	LEU	2.1
1	D	352	LEU	2.1
1	B	215	SER	2.1
1	F	4	SER	2.1
1	A	182	LYS	2.1
1	C	50	GLU	2.1
1	B	307	ALA	2.1
1	C	16	LEU	2.1
1	D	260	CYS	2.1
1	A	218[A]	ARG	2.1
1	D	214	LYS	2.1
1	D	442	ASP	2.1
1	F	216	ARG	2.1
1	A	117	GLY	2.1
1	C	179	GLY	2.1
1	A	124	ILE	2.1
1	D	458	SER	2.1
1	C	58	LEU	2.0
1	E	36	LEU	2.0
1	A	118	GLY	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

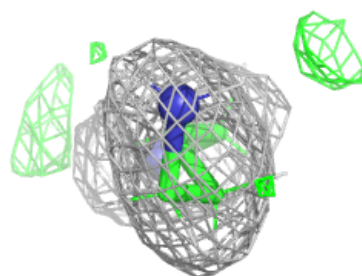
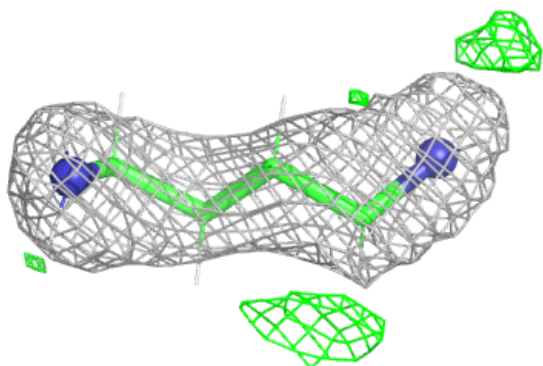
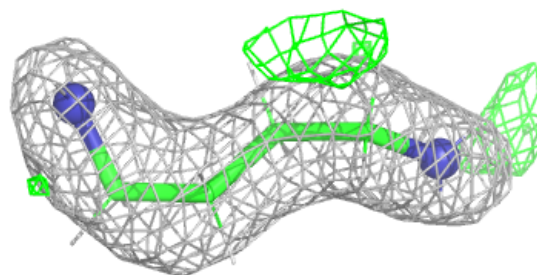
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PUT	A	502	6/6	0.85	0.14	35,45,51,51	0
3	PUT	C	502	6/6	0.85	0.16	41,50,55,55	0
3	PUT	E	502	6/6	0.88	0.12	26,32,38,38	0
2	NAD	B	501	44/44	0.90	0.11	24,39,55,58	0
2	NAD	F	501	44/44	0.92	0.09	20,37,47,54	0
2	NAD	C	501	44/44	0.93	0.09	33,41,50,54	0
2	NAD	D	501	44/44	0.93	0.09	22,40,49,53	0
2	NAD	A	501	44/44	0.95	0.08	31,47,58,61	0
2	NAD	E	501	44/44	0.97	0.05	15,23,30,33	0

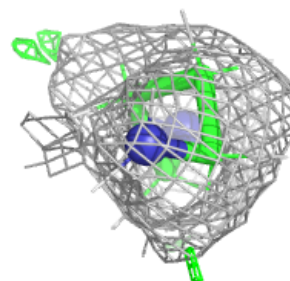
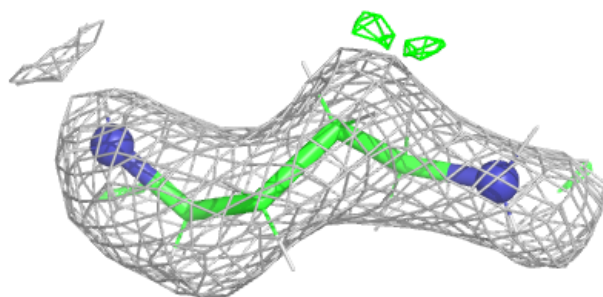
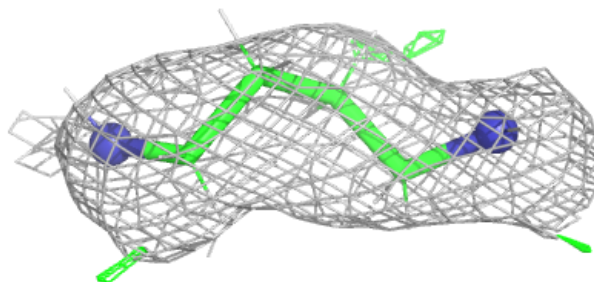
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PUT 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)

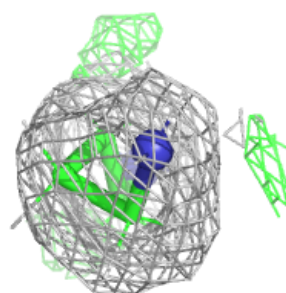
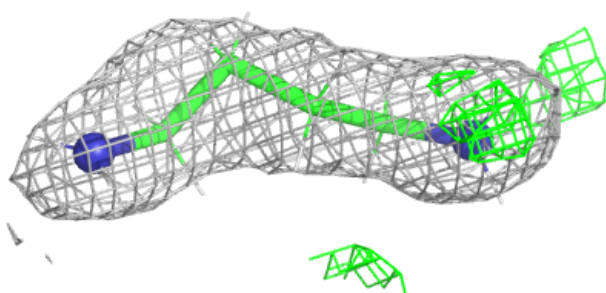
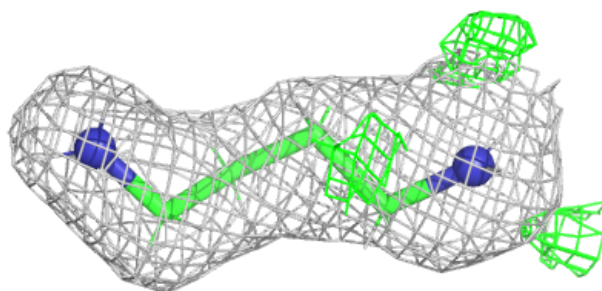
**Electron density around PUT C 502:**

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

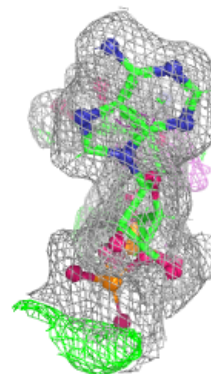
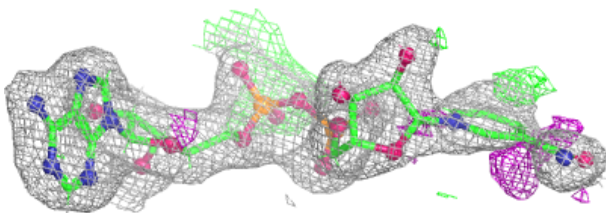
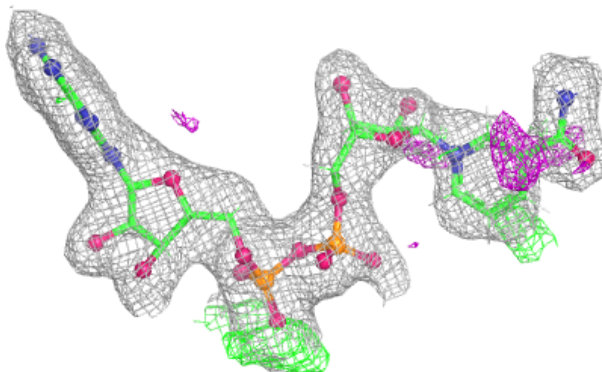


Electron density around PUT E 502:

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

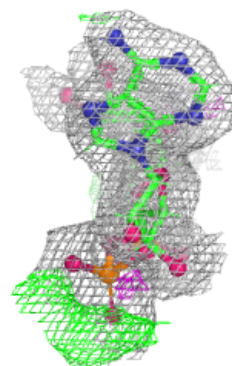
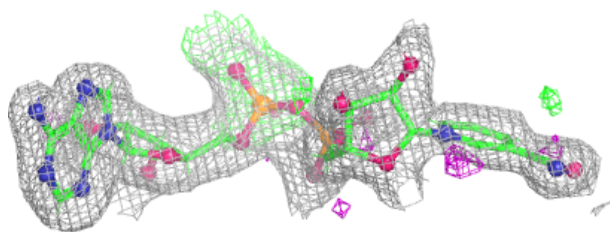
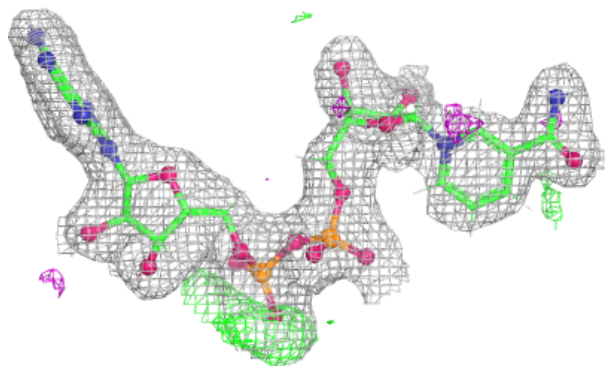
**Electron density around NAD B 501:**

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

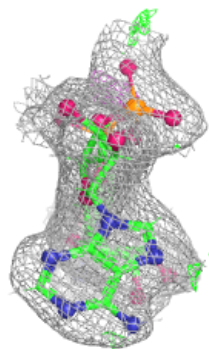
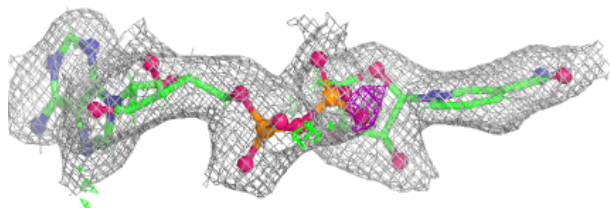
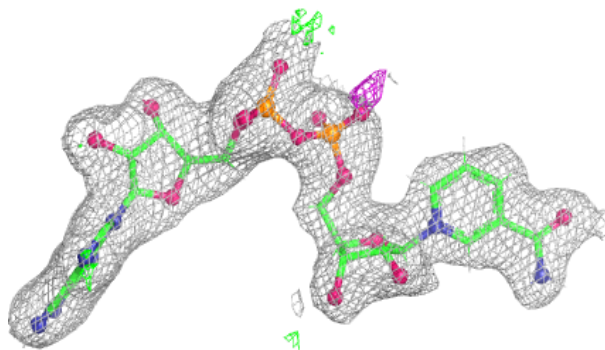


Electron density around NAD F 501:

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

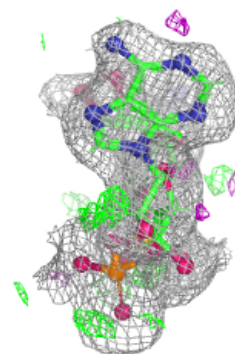
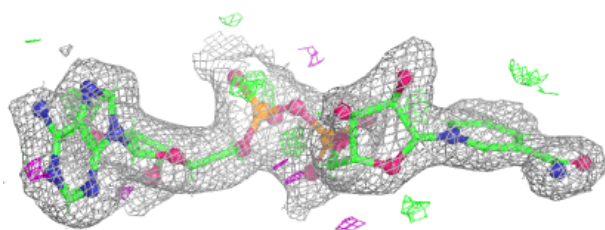
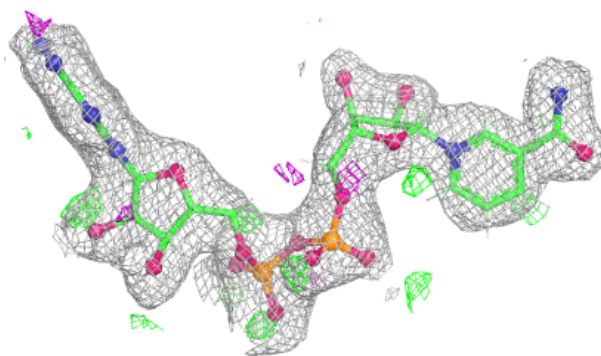
**Electron density around NAD C 501:**

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

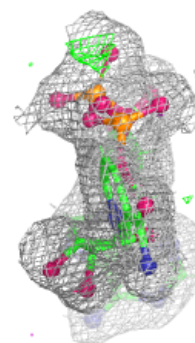
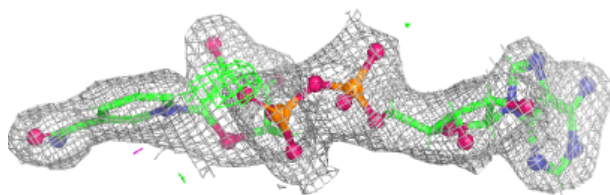
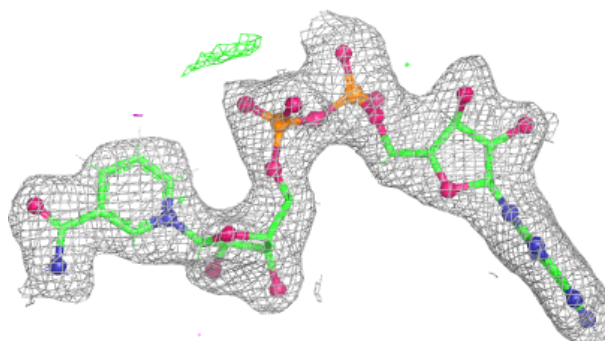


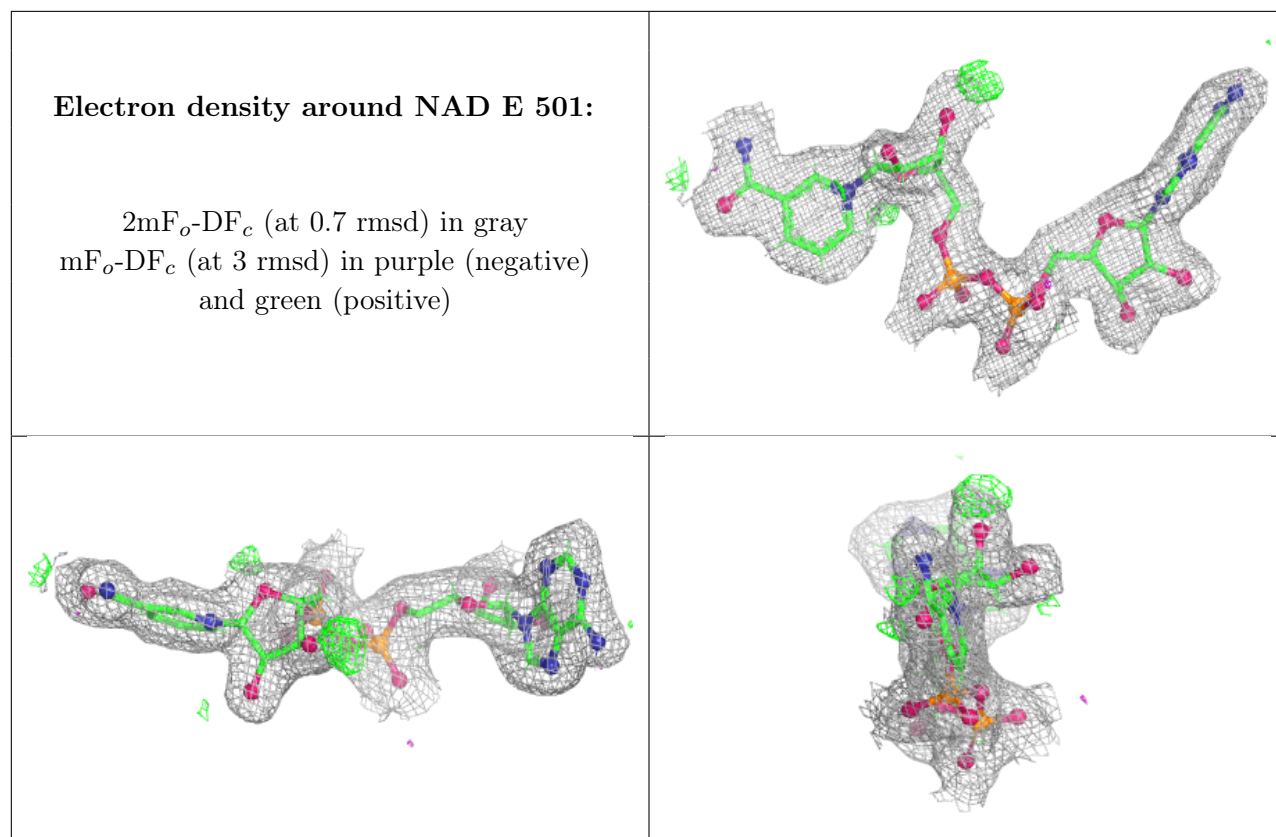
Electron density around NAD D 501:

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

**Electron density around 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.