



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID : 1YC2 / pdb_00001yc2
Title : Sir2Af2-NAD-ADPribose-nicotinamide
Authors : Avalos, J.L.; Bever, M.K.; Wolberger, C.
Deposited on : 2004-12-21
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

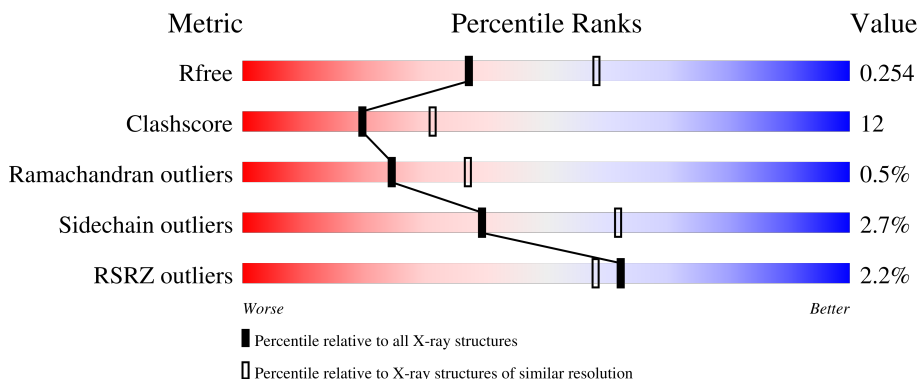
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	253	0% 74% 24% .
1	B	253	85% 14% .
1	C	253	3% 77% 19% .
1	D	253	3% 80% 19% .
1	E	253	4% 61% 33% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	APR	E	504	X	-	-	-
5	NCA	A	506	-	X	-	-
5	NCA	B	508	-	X	-	-
5	NCA	E	509	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 10409 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 NAD-dependent deacetylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1954	1250	333	357	14			
1	B	252	Total	C	N	O	S	0	0	0
			1987	1269	340	364	14			
1	C	252	Total	C	N	O	S	0	0	0
			1967	1258	339	356	14			
1	D	251	Total	C	N	O	S	0	0	0
			1949	1246	334	356	13			
1	E	250	Total	C	N	O	S	0	0	0
			1888	1205	318	352	13			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

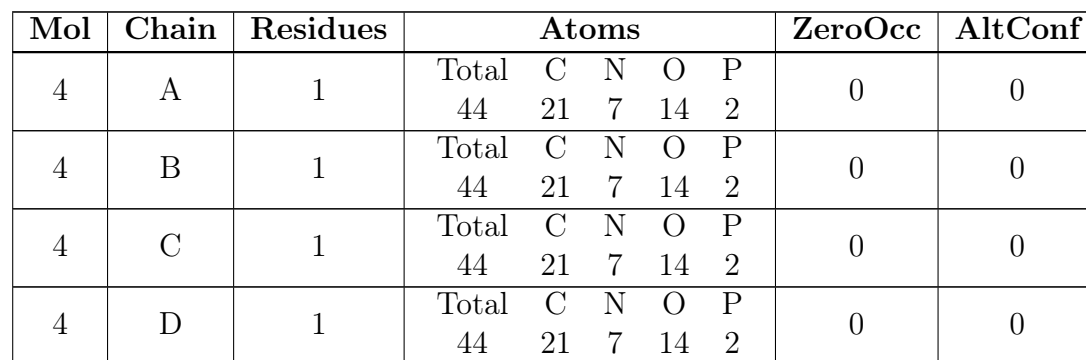
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

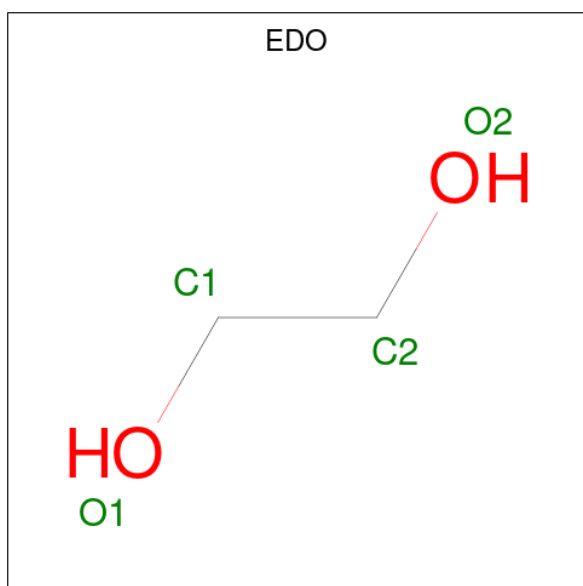
- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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- Chemical structure of NCA (N-cyanoguanidine) showing the molecule with atom labels. The structure consists of a pyrimidine ring (labeled C2, C3, C4, C5, C6) and a cyano group (labeled C7, O7) attached to the ring. The nitrogen atom in the ring is labeled N1. The nitrogen atom in the cyano group is labeled N7. The oxygen atom in the cyano group is labeled O7.

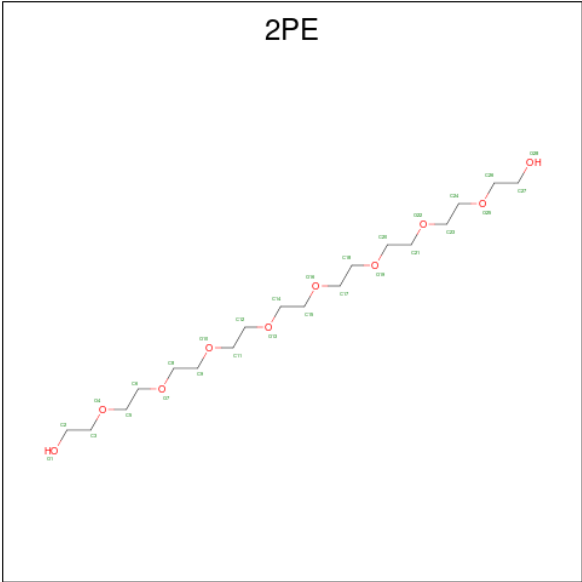
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			9	6	2	1		
5	B	1	Total	C	N	O	0	0
			9	6	2	1		
5	D	1	Total	C	N	O	0	0
			9	6	2	1		
5	E	1	Total	C	N	O	0	0
			9	6	2	1		
5	E	1	Total	C	N	O	0	0
			9	6	2	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



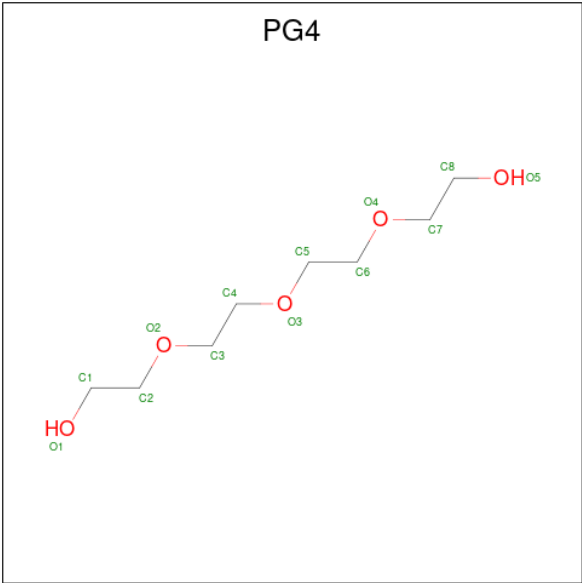
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: $C_{18}H_{38}O_{10}$).



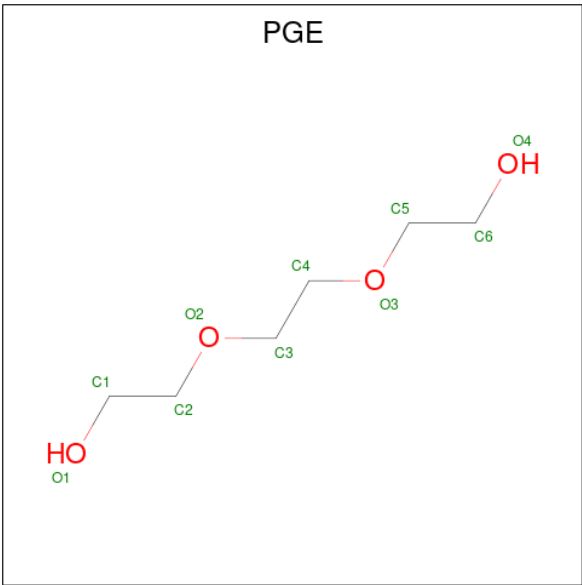
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			28	18	10		
7	C	1	Total	C	O	0	0
			28	18	10		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



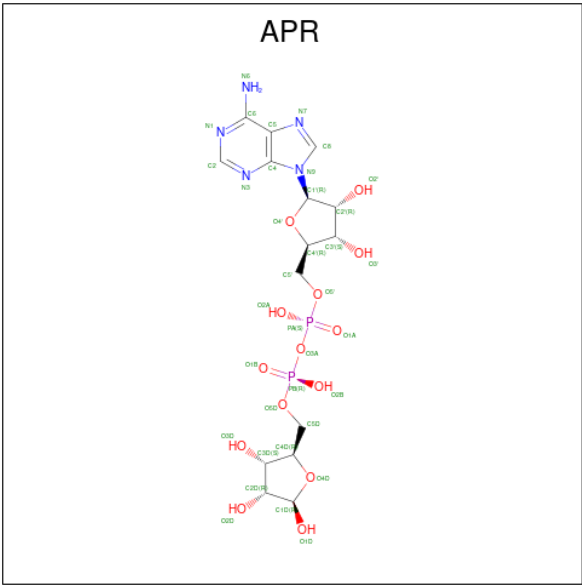
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	E	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

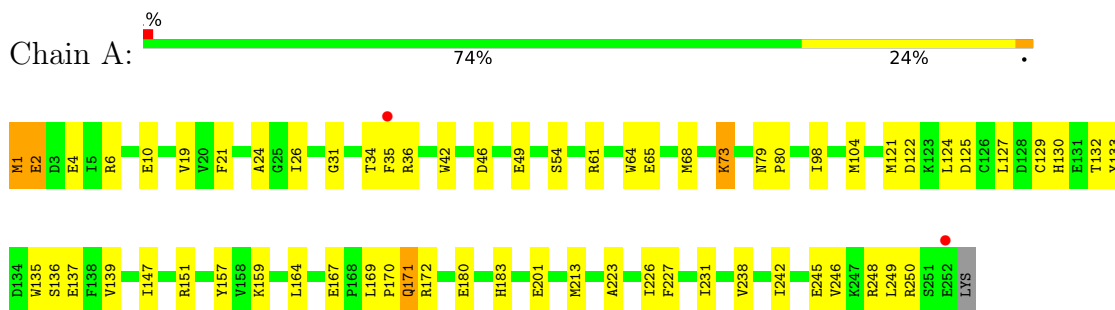
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	47	Total 47	O 47	0	0
11	B	77	Total 77	O 77	0	0
11	C	39	Total 39	O 39	0	0
11	D	64	Total 64	O 64	0	0
11	E	22	Total 22	O 22	0	0

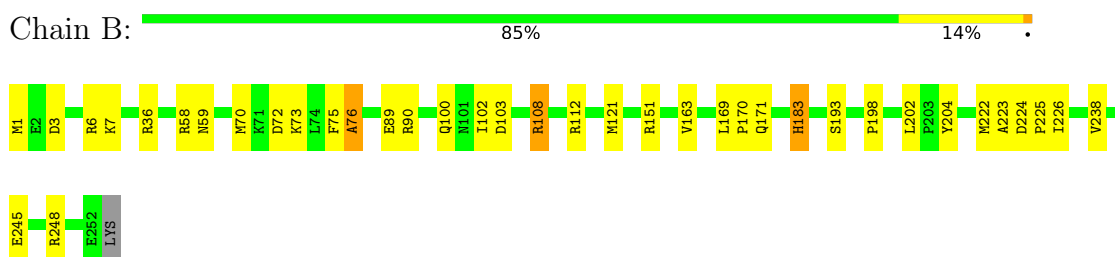
3 Residue-property plots [i](#)

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.

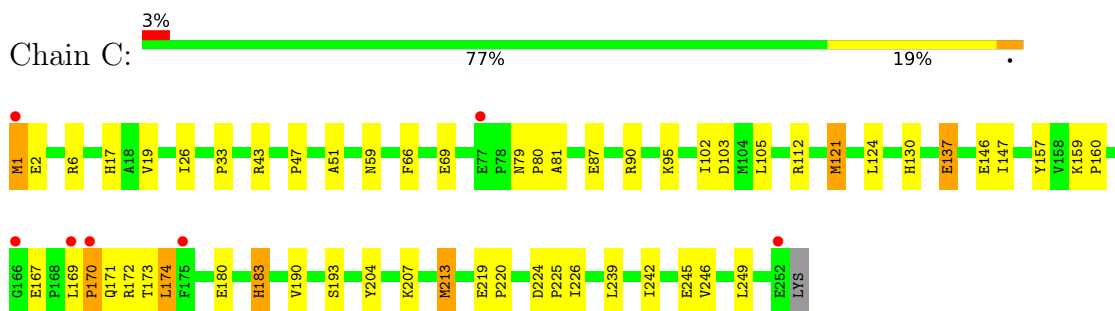
- Molecule 1: NAD-dependent deacetylase 2



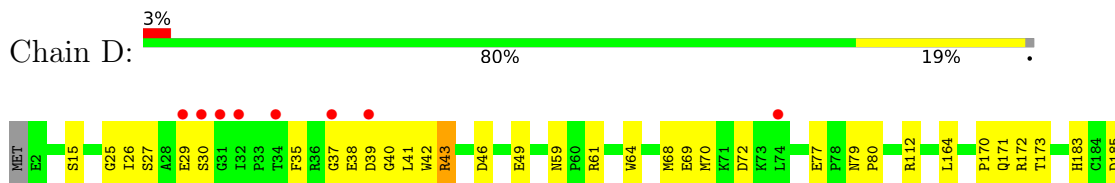
- Molecule 1: NAD-dependent deacetylase 2

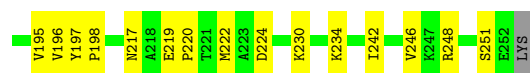


- Molecule 1: NAD-dependent deacetylase 2

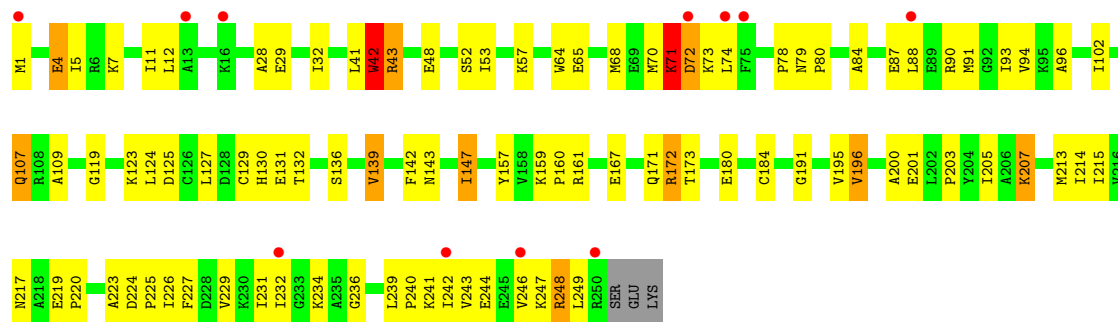


- Molecule 1: NAD-dependent deacetylase 2





• Molecule 1: NAD-dependent deacetylase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.12Å 181.56Å 79.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-2.40) 99.0 (30.00-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.255 0.209 , 0.254	Depositor DCC
R_{free} test set	3043 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10409	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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, PG4, APR, NCA, SO4, EDO, PGE, ZN, 2PE

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	0.42	0/1998	0.88	2/2701 (0.1%)
1	B	0.42	0/2031	0.89	3/2738 (0.1%)
1	C	0.40	0/2011	0.92	4/2714 (0.1%)
1	D	0.41	0/1993	0.89	3/2692 (0.1%)
1	E	0.37	0/1931	0.90	5/2622 (0.2%)
All	All	0.41	0/9964	0.90	17/13467 (0.1%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	73	LYS	N-CA-C	-10.07	101.77	114.56
1	E	74	LEU	N-CA-C	-7.83	103.73	113.20
1	C	213	MET	N-CA-C	6.78	120.46	109.40
1	E	43	ARG	N-CA-C	-6.62	105.09	113.43
1	B	171	GLN	N-CA-C	6.31	118.16	111.28

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	1954	0	1923	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1987	0	1989	26	0
1	C	1967	0	1962	44	0
1	D	1949	0	1920	32	0
1	E	1888	0	1799	76	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
3	A	10	0	0	0	0
3	B	20	0	0	0	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
4	A	44	0	26	6	0
4	B	44	0	26	1	0
4	C	44	0	26	1	0
4	D	44	0	26	2	0
5	A	9	0	6	0	0
5	B	9	0	6	0	0
5	D	9	0	6	0	0
5	E	18	0	12	0	0
6	A	12	0	18	0	0
6	B	8	0	12	0	0
7	B	28	0	38	3	0
7	C	28	0	38	0	0
8	D	13	0	18	0	0
9	D	10	0	14	0	0
10	E	36	0	21	0	0
11	A	47	0	0	1	0
11	B	77	0	0	2	0
11	C	39	0	0	0	0
11	D	64	0	0	0	0
11	E	22	0	0	2	0
All	All	10409	0	9886	231	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 231 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:GLN:H	1:E:107:GLN:HE21	0.93	0.93
1:A:46:ASP:HB3	1:A:49:GLU:HG2	1.50	0.92
1:E:79:ASN:HB2	1:E:80:PRO:HD2	1.56	0.87
1:E:107:GLN:HE21	1:E:107:GLN:N	1.75	0.85
1:E:107:GLN:H	1:E:107:GLN:NE2	1.72	0.85

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	250/253 (99%)	240 (96%)	9 (4%)	1 (0%)	30	43
1	B	250/253 (99%)	245 (98%)	5 (2%)	0	100	100
1	C	250/253 (99%)	244 (98%)	5 (2%)	1 (0%)	30	43
1	D	249/253 (98%)	235 (94%)	13 (5%)	1 (0%)	30	43
1	E	248/253 (98%)	233 (94%)	12 (5%)	3 (1%)	10	16
All	All	1247/1265 (99%)	1197 (96%)	44 (4%)	6 (0%)	24	37

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	71	LYS
1	A	2	GLU
1	D	72	ASP
1	C	170	PRO
1	E	42	TRP

5.3.2 Protein sidechains [i](#)

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	201/212 (95%)	199 (99%)	2 (1%)	68	84
1	B	210/212 (99%)	205 (98%)	5 (2%)	43	65
1	C	205/212 (97%)	197 (96%)	8 (4%)	28	48
1	D	201/212 (95%)	199 (99%)	2 (1%)	68	84
1	E	188/212 (89%)	178 (95%)	10 (5%)	20	36
All	All	1005/1060 (95%)	978 (97%)	27 (3%)	39	62

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	193	SER
1	E	4	GLU
1	E	196	VAL
1	D	217	ASN
1	E	42	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	107	GLN
1	E	171	GLN
1	C	100	GLN
1	C	101	ASN
1	C	171	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 9 are monoatomic - leaving 29 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
4	NAD	B	501	-	46,48,48	2.66	12 (26%)	64,73,73	1.41	9 (14%)
6	EDO	B	708	-	3,3,3	0.67	0	2,2,2	0.29	0
4	NAD	D	505	-	46,48,48	2.89	15 (32%)	64,73,73	1.36	8 (12%)
3	SO4	B	602	-	4,4,4	0.40	0	6,6,6	0.24	0
4	NAD	C	502	-	46,48,48	2.74	12 (26%)	64,73,73	1.42	9 (14%)
5	NCA	E	507	-	9,9,9	3.97	6 (66%)	11,11,11	2.20	3 (27%)
6	EDO	A	704	-	3,3,3	0.63	0	2,2,2	0.34	0
3	SO4	C	612	-	4,4,4	0.43	0	6,6,6	0.10	0
3	SO4	B	604	-	4,4,4	0.37	0	6,6,6	0.13	0
3	SO4	D	603	-	4,4,4	0.39	0	6,6,6	0.12	0
4	NAD	A	503	-	46,48,48	2.75	12 (26%)	64,73,73	1.40	8 (12%)
3	SO4	C	606	-	4,4,4	0.38	0	6,6,6	0.12	0
10	APR	E	504	-	39,39,39	1.66	6 (15%)	56,60,60	1.46	8 (14%)
3	SO4	A	607	-	4,4,4	0.39	0	6,6,6	0.09	0
6	EDO	A	706	-	3,3,3	0.69	0	2,2,2	0.31	0
6	EDO	A	705	-	3,3,3	0.73	0	2,2,2	0.28	0
5	NCA	D	510	-	9,9,9	3.95	6 (66%)	11,11,11	2.15	3 (27%)
7	2PE	B	701	-	27,27,27	0.69	0	26,26,26	0.46	0
9	PGE	D	709	-	9,9,9	0.82	0	8,8,8	0.35	0
5	NCA	E	509	-	9,9,9	3.85	6 (66%)	11,11,11	2.10	4 (36%)
3	SO4	A	605	-	4,4,4	0.39	0	6,6,6	0.11	0
5	NCA	A	506	-	9,9,9	3.91	6 (66%)	11,11,11	2.14	4 (36%)
3	SO4	B	610	-	4,4,4	0.41	0	6,6,6	0.13	0
3	SO4	C	601	-	4,4,4	0.35	0	6,6,6	0.16	0
6	EDO	B	707	-	3,3,3	0.71	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PG4	D	703	-	12,12,12	0.70	0	11,11,11	0.46	0
7	2PE	C	702	-	27,27,27	0.74	0	26,26,26	0.44	0
5	NCA	B	508	-	9,9,9	4.01	6 (66%)	11,11,11	2.18	4 (36%)
3	SO4	B	609	-	4,4,4	0.41	0	6,6,6	0.10	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
4	NAD	B	501	-	-	10/30/62/62	0/5/5/5
6	EDO	B	708	-	-	1/1/1/1	-
4	NAD	D	505	-	-	4/30/62/62	0/5/5/5
4	NAD	C	502	-	-	13/30/62/62	0/5/5/5
5	NCA	E	507	-	-	0/4/4/4	0/1/1/1
6	EDO	A	704	-	-	1/1/1/1	-
4	NAD	A	503	-	-	5/30/62/62	0/5/5/5
10	APR	E	504	-	1/1/10/10	6/22/54/54	0/4/4/4
6	EDO	A	706	-	-	1/1/1/1	-
6	EDO	A	705	-	-	1/1/1/1	-
5	NCA	D	510	-	-	0/4/4/4	0/1/1/1
7	2PE	B	701	-	-	11/25/25/25	-
9	PGE	D	709	-	-	4/7/7/7	-
5	NCA	E	509	-	-	0/4/4/4	0/1/1/1
5	NCA	A	506	-	-	0/4/4/4	0/1/1/1
6	EDO	B	707	-	-	1/1/1/1	-
8	PG4	D	703	-	-	7/10/10/10	-
7	2PE	C	702	-	-	15/25/25/25	-
5	NCA	B	508	-	-	0/4/4/4	0/1/1/1

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	505	NAD	C2N-N1N	10.70	1.46	1.35
4	A	503	NAD	C2N-N1N	9.84	1.45	1.35
4	C	502	NAD	C2N-N1N	9.23	1.45	1.35
4	D	505	NAD	C4N-C3N	8.85	1.52	1.39
4	B	501	NAD	C2N-N1N	8.75	1.44	1.35

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	507	NCA	C5-C4-C3	4.96	125.24	120.36
5	B	508	NCA	C5-C4-C3	4.80	125.08	120.36
5	A	506	NCA	C5-C4-C3	4.79	125.07	120.36
5	D	510	NCA	C5-C4-C3	4.77	125.05	120.36
5	E	509	NCA	C5-C4-C3	4.61	124.90	120.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	E	504	APR	C1D

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	NAD	C5B-O5B-PA-O2A
4	B	501	NAD	C5B-O5B-PA-O3
4	C	502	NAD	C5B-O5B-PA-O2A
4	C	502	NAD	C5B-O5B-PA-O3
4	D	505	NAD	PN-O3-PA-O5B

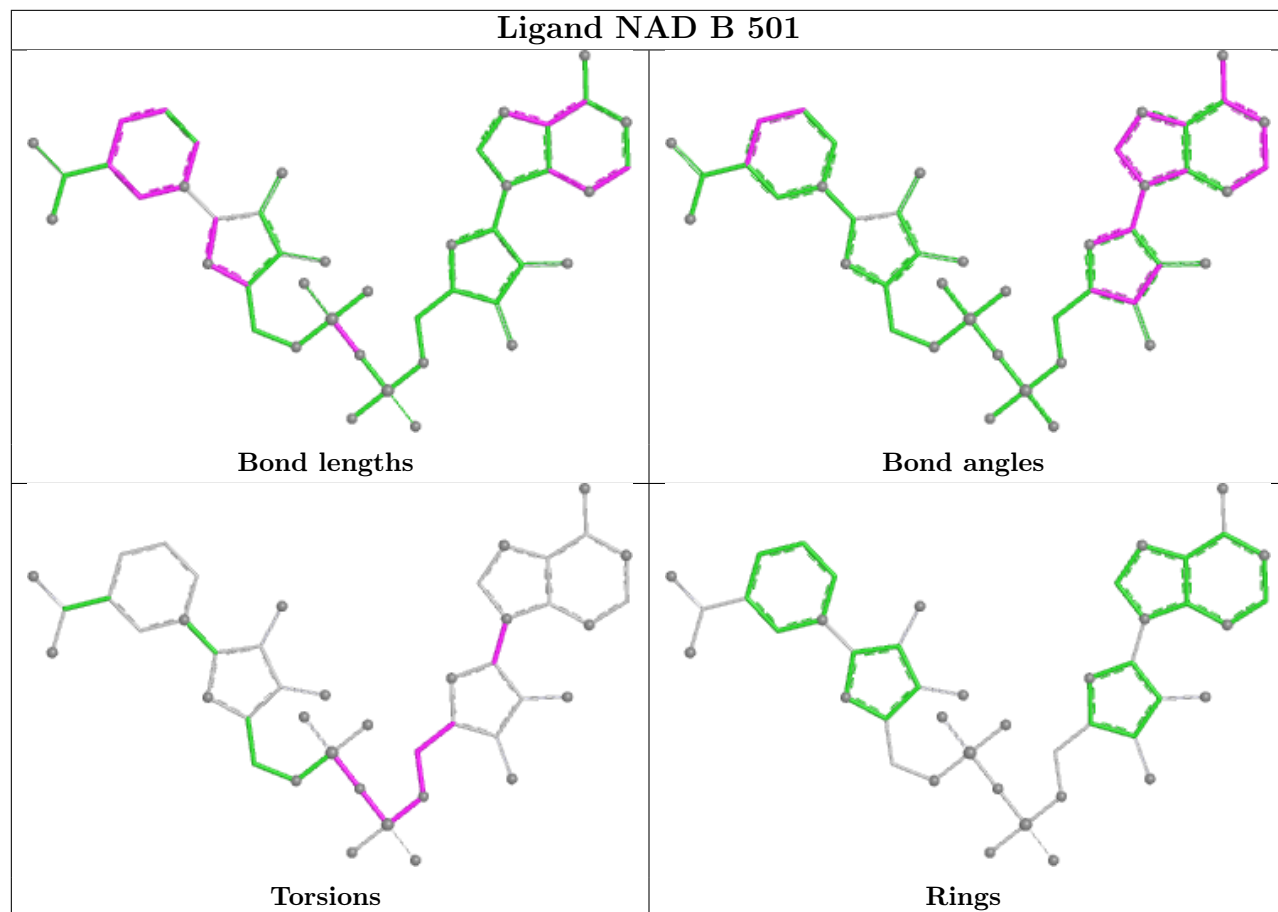
There are no ring outliers.

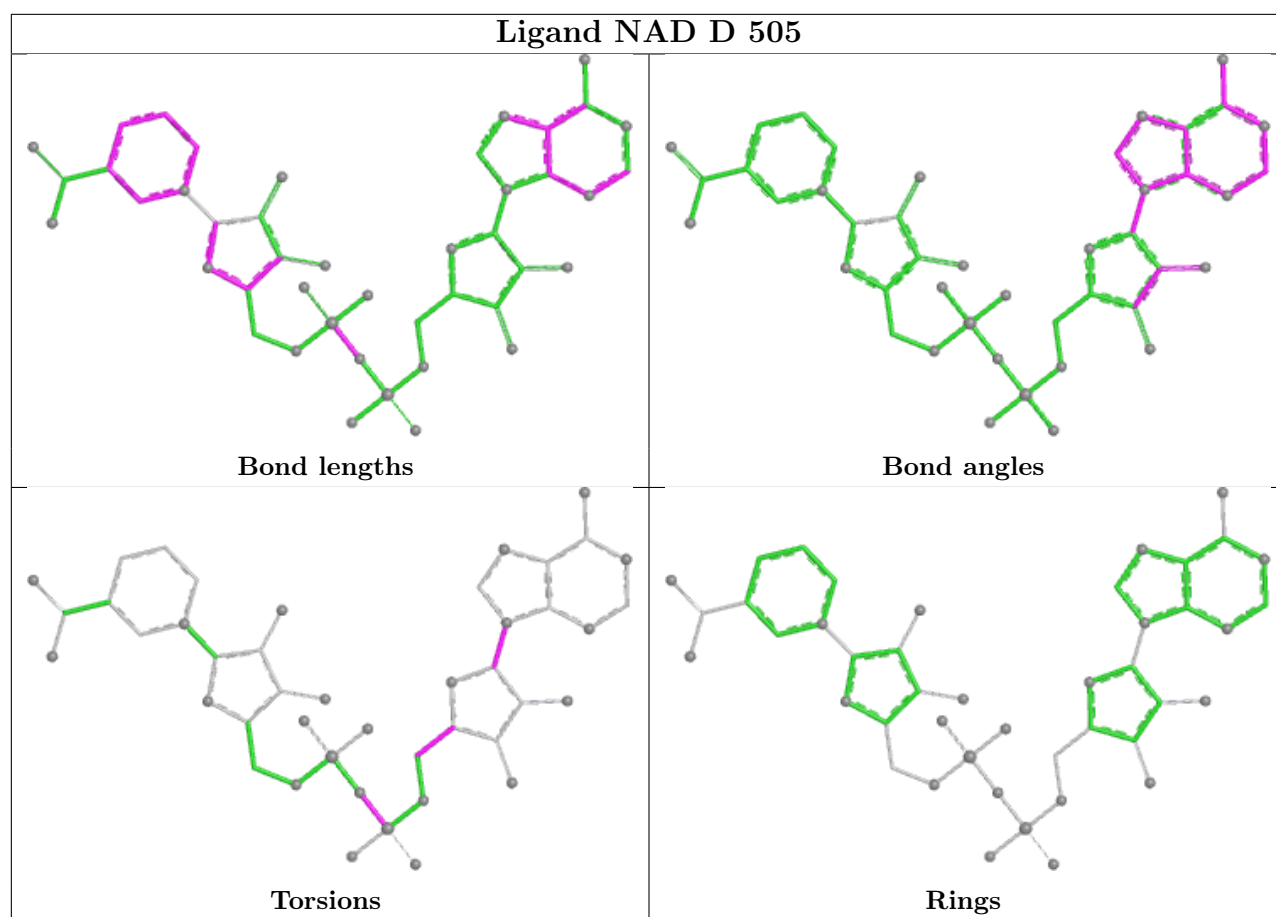
5 monomers are involved in 13 short contacts:

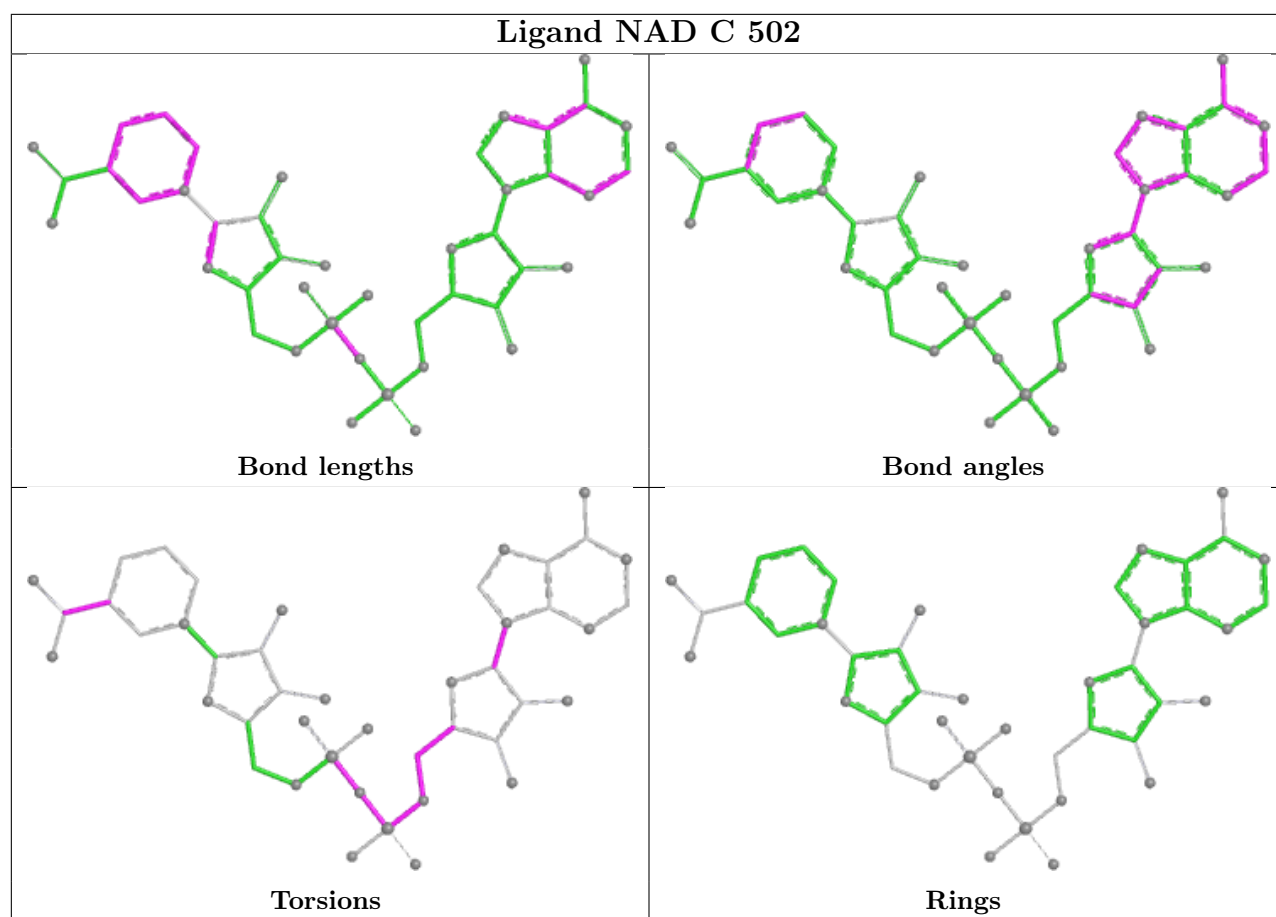
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	NAD	1	0
4	D	505	NAD	2	0
4	C	502	NAD	1	0
4	A	503	NAD	6	0
7	B	701	2PE	3	0

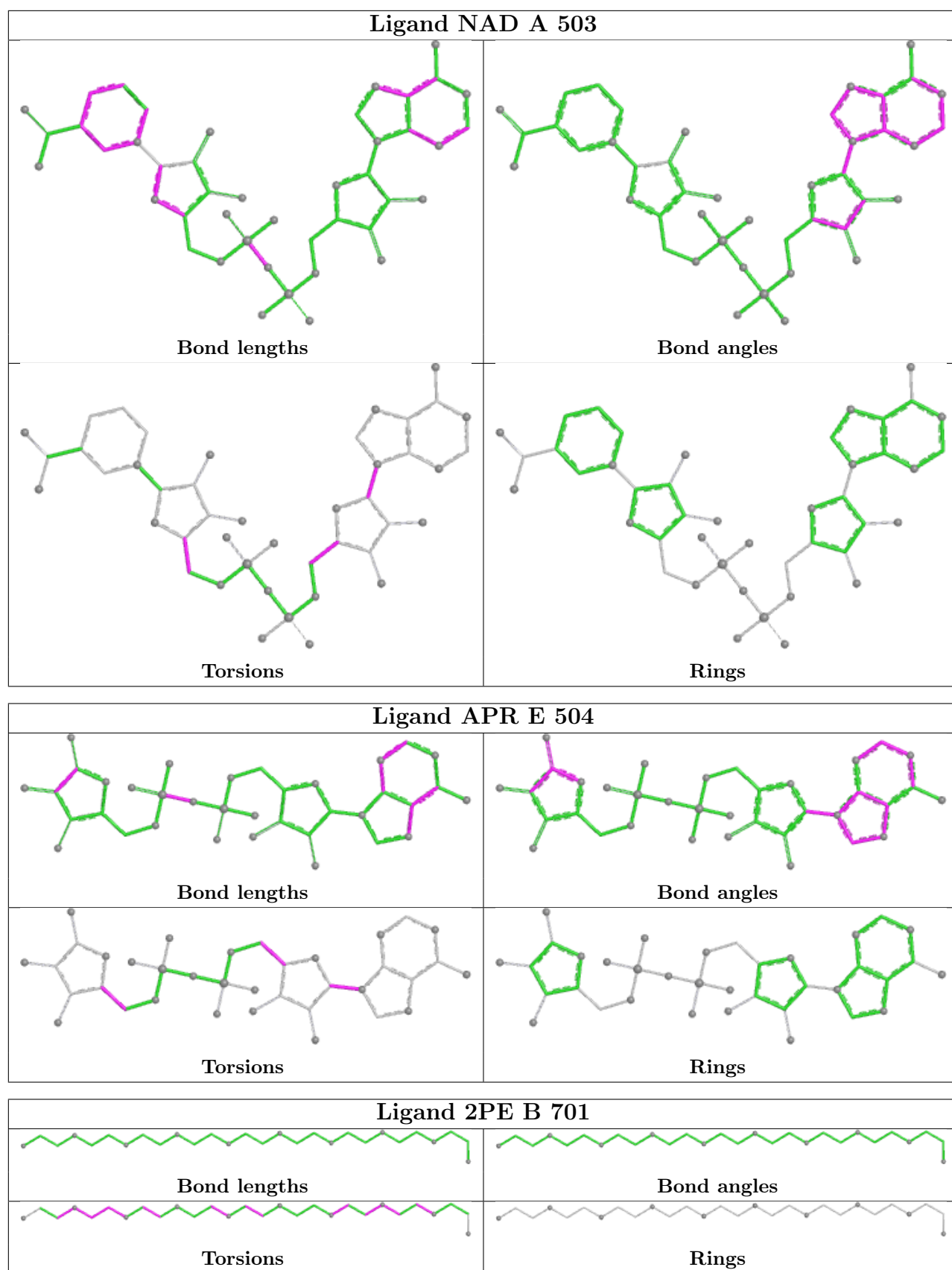
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

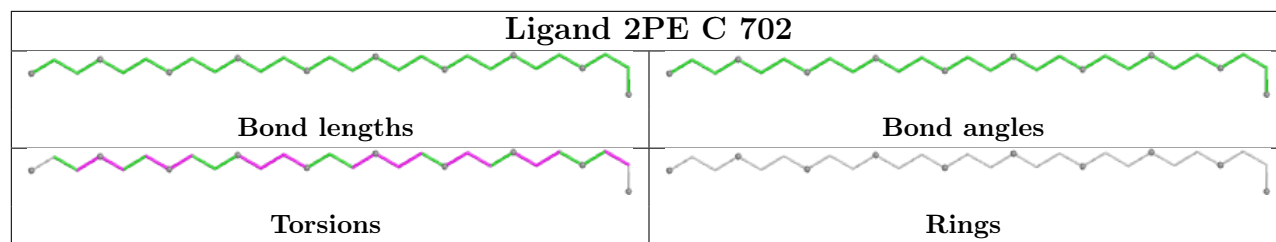
equivalents in the CSD to analyse the geometry.











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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	252/253 (99%)	-0.14	2 (0%) 82 80	19, 37, 67, 83	0
1	B	252/253 (99%)	-0.41	0 100 100	20, 33, 49, 75	0
1	C	252/253 (99%)	0.03	7 (2%) 55 51	26, 43, 69, 93	0
1	D	251/253 (99%)	-0.09	8 (3%) 50 46	20, 38, 80, 98	0
1	E	250/253 (98%)	0.44	11 (4%) 39 34	37, 56, 81, 92	0
All	All	1257/1265 (99%)	-0.04	28 (2%) 62 58	19, 41, 75, 98	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	4.0
1	D	39	ASP	3.9
1	D	32	ILE	3.5
1	C	169	LEU	3.3
1	E	250	ARG	3.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

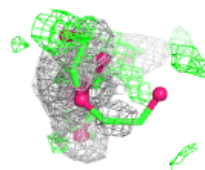
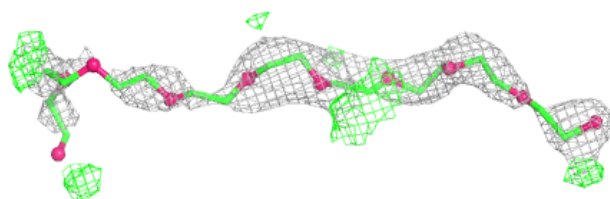
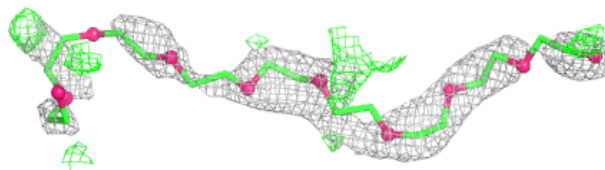
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	610	5/5	0.46	0.13	99,100,100,100	0
3	SO4	C	612	5/5	0.51	0.15	99,100,100,100	0
3	SO4	B	609	5/5	0.67	0.12	100,100,100,100	0
6	EDO	B	707	4/4	0.72	0.21	64,64,64,64	0
7	2PE	C	702	28/28	0.73	0.23	71,87,100,100	0
3	SO4	A	605	5/5	0.76	0.12	99,99,100,100	0
6	EDO	A	706	4/4	0.77	0.21	61,61,64,64	0
3	SO4	C	606	5/5	0.79	0.11	99,99,100,100	0
6	EDO	A	705	4/4	0.80	0.15	61,63,63,63	0
3	SO4	B	604	5/5	0.80	0.12	98,98,99,100	0
4	NAD	D	505	44/44	0.81	0.17	78,87,92,94	0
5	NCA	D	510	9/9	0.81	0.30	67,70,71,71	6
5	NCA	A	506	9/9	0.82	0.23	71,74,76,76	0
9	PGE	D	709	10/10	0.84	0.17	69,70,72,73	0
8	PG4	D	703	13/13	0.85	0.19	66,70,78,80	0
3	SO4	A	607	5/5	0.86	0.11	76,77,78,78	0
6	EDO	A	704	4/4	0.87	0.15	56,56,57,60	0
7	2PE	B	701	28/28	0.88	0.14	49,60,66,67	0
5	NCA	E	509	9/9	0.88	0.19	64,64,65,65	0
3	SO4	D	603	5/5	0.89	0.13	84,84,85,86	0
6	EDO	B	708	4/4	0.89	0.11	61,62,62,64	0
5	NCA	B	508	9/9	0.90	0.17	87,89,90,90	0
4	NAD	A	503	44/44	0.93	0.09	40,46,57,61	0
5	NCA	E	507	9/9	0.93	0.12	53,55,57,58	0
3	SO4	C	601	5/5	0.93	0.08	44,44,46,46	0
10	APR	E	504	36/36	0.93	0.09	43,49,52,53	0
4	NAD	B	501	44/44	0.96	0.07	21,26,31,37	0
4	NAD	C	502	44/44	0.96	0.07	28,33,39,42	0
3	SO4	B	602	5/5	0.98	0.04	34,37,37,38	0
2	ZN	E	409	1/1	0.99	0.04	36,36,36,36	0
2	ZN	C	406	1/1	0.99	0.04	35,35,35,35	0
2	ZN	B	404	1/1	1.00	0.03	31,31,31,31	0
2	ZN	C	405	1/1	1.00	0.02	37,37,37,37	0
2	ZN	A	401	1/1	1.00	0.03	34,34,34,34	0
2	ZN	D	407	1/1	1.00	0.04	27,27,27,27	0
2	ZN	D	408	1/1	1.00	0.04	35,35,35,35	0
2	ZN	A	402	1/1	1.00	0.03	35,35,35,35	0
2	ZN	B	403	1/1	1.00	0.04	37,37,37,37	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.

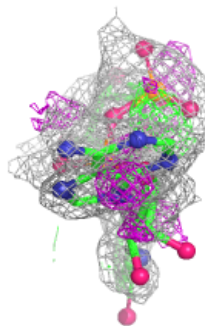
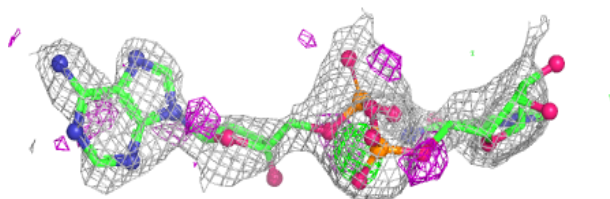
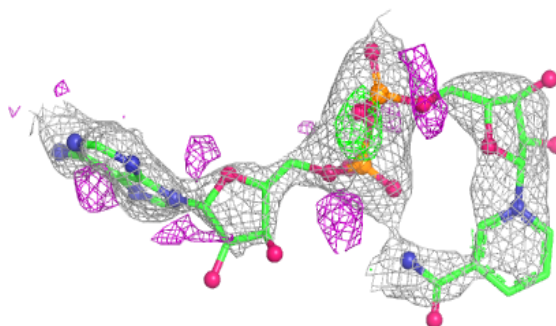
Electron density around 2PE C 702:

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



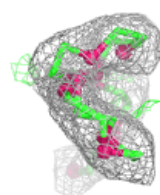
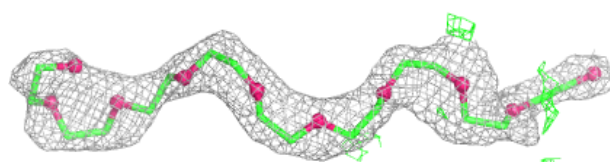
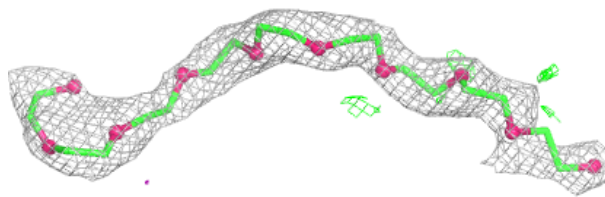
Electron density around NAD D 505:

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

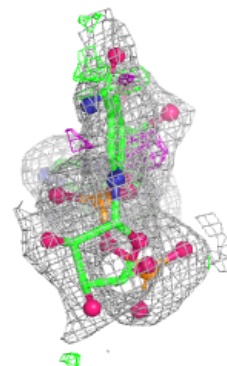
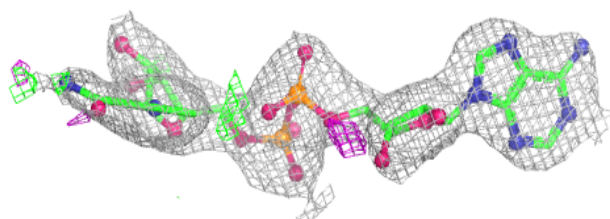
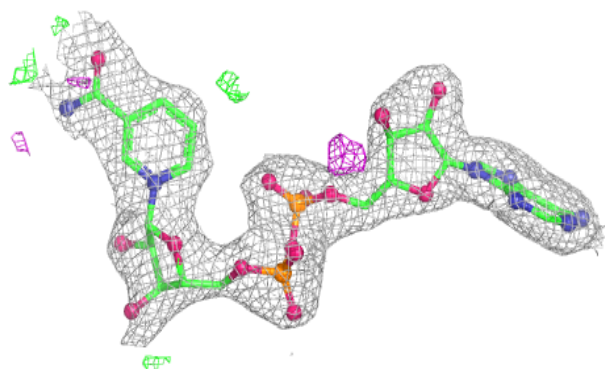


Electron density around 2PE B 701:

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

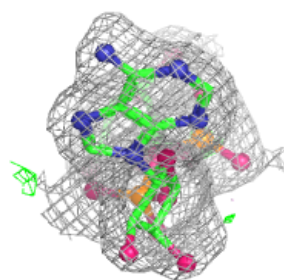
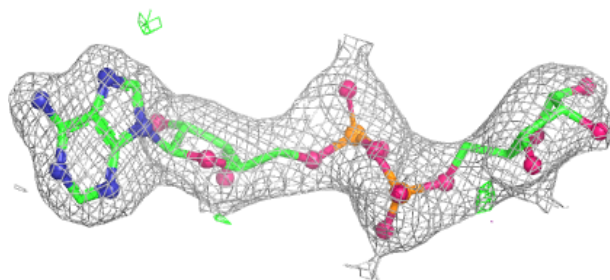
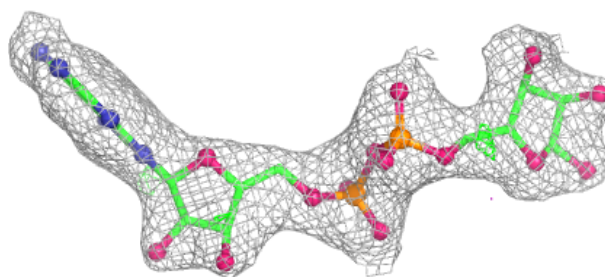
**Electron density around NAD A 503:**

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



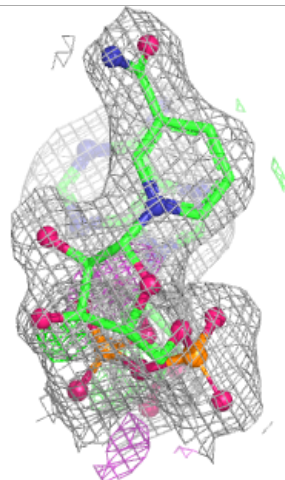
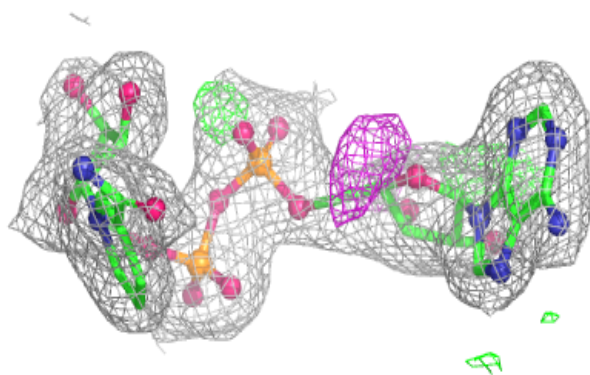
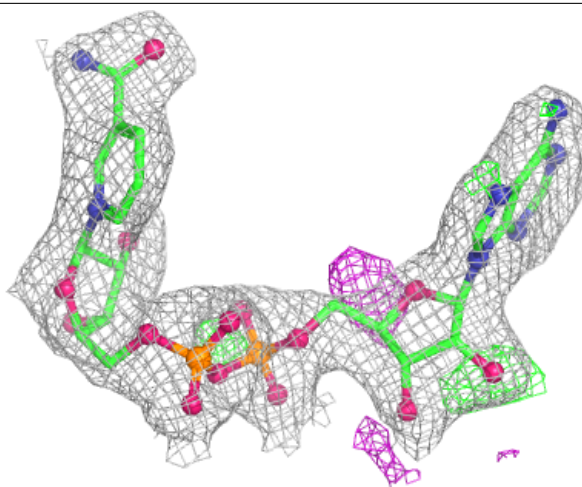
Electron density around APR E 504:

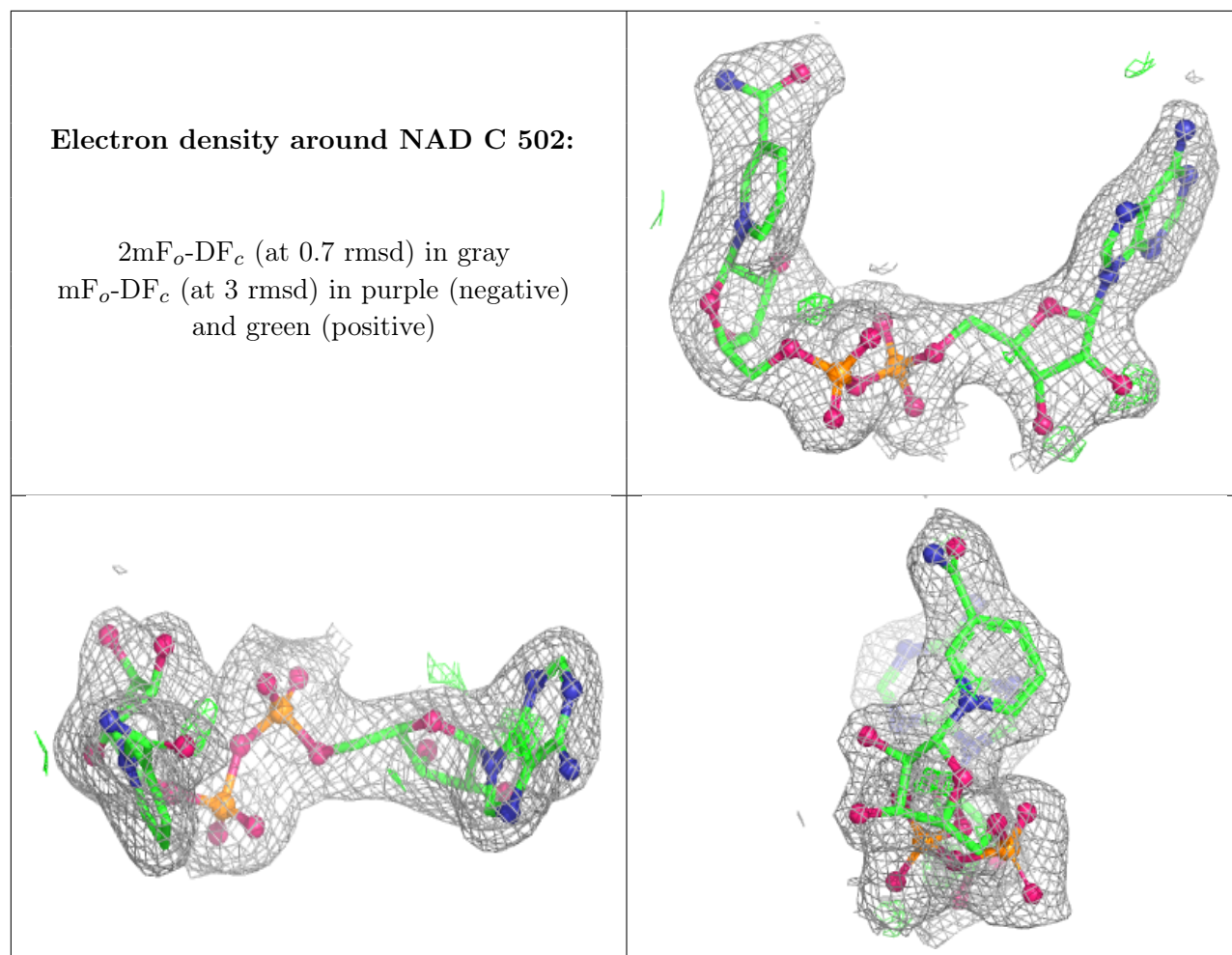
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.