



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:36 PM UTC

PDB ID : 5JPI / pdb_00005jpi
Title : 2.15 Angstrom Crystal Structure of S-adenosylhomocysteinase from *Cryptosporidium parvum* in Complex with D-Eritadenine and NAD
Authors : Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Dubrovskaya, I.; Bishop, B.; Kwon, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2016-05-03
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](#) ①) 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

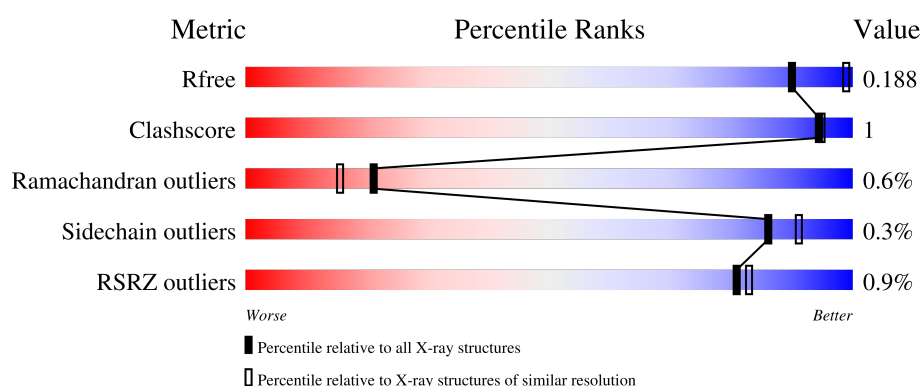
1 Overall quality at a glance

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	498	% 95% 5%
1	B	498	% 92% 6% .
1	C	498	% 92% 7% .
1	D	498	% 95% . .

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17474 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.

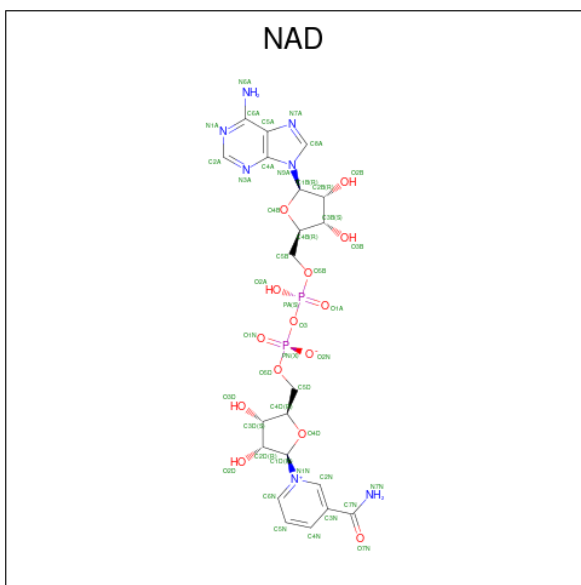
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	13	0
			4024	2554	674	767	29			
1	B	491	Total	C	N	O	S	0	8	0
			3937	2497	660	752	28			
1	C	492	Total	C	N	O	S	0	8	0
			3954	2512	661	752	29			
1	D	491	Total	C	N	O	S	0	10	0
			3961	2515	662	755	29			

There are 12 discrepancies between the modelled and reference sequences:

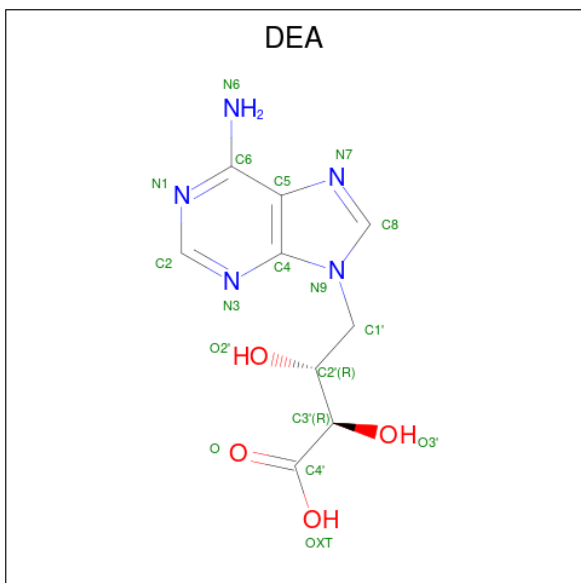
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5CPH1
A	-1	ASN	-	expression tag	UNP Q5CPH1
A	0	ALA	-	expression tag	UNP Q5CPH1
B	-2	SER	-	expression tag	UNP Q5CPH1
B	-1	ASN	-	expression tag	UNP Q5CPH1
B	0	ALA	-	expression tag	UNP Q5CPH1
C	-2	SER	-	expression tag	UNP Q5CPH1
C	-1	ASN	-	expression tag	UNP Q5CPH1
C	0	ALA	-	expression tag	UNP Q5CPH1
D	-2	SER	-	expression tag	UNP Q5CPH1
D	-1	ASN	-	expression tag	UNP Q5CPH1
D	0	ALA	-	expression tag	UNP Q5CPH1

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



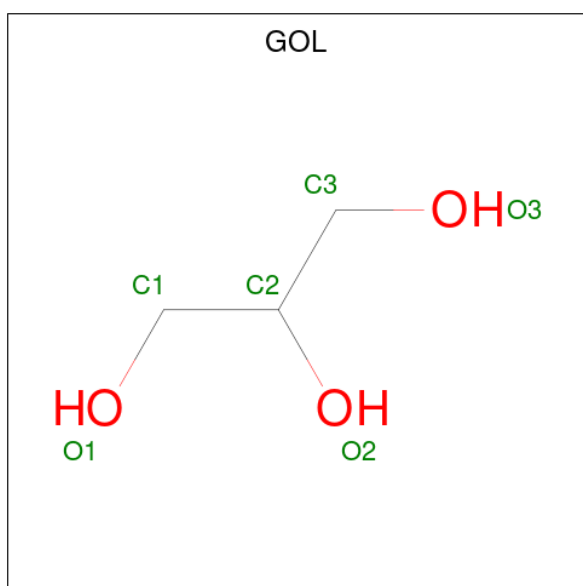
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is D-ERITADENINE (CCD ID: DEA) (formula: $\text{C}_9\text{H}_{11}\text{N}_5\text{O}_4$).



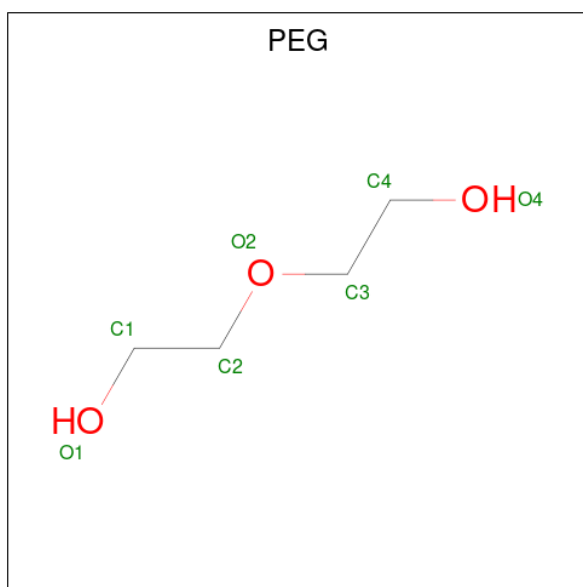
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	9	5	4		
3	B	1	Total	C	N	O	0	0
			18	9	5	4		
3	C	1	Total	C	N	O	0	0
			18	9	5	4		
3	D	1	Total	C	N	O	0	0
			18	9	5	4		

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



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

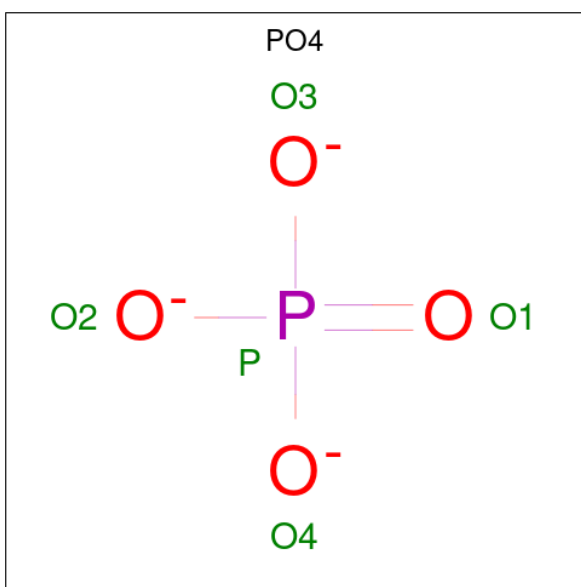


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

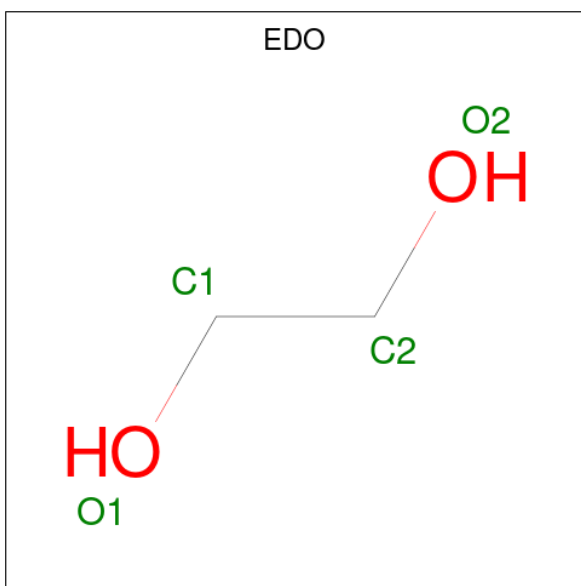
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Cl	0	0
			2	2		
6	C	2	Total	Cl	0	0
			2	2		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	P	0	0
			5	4	1		

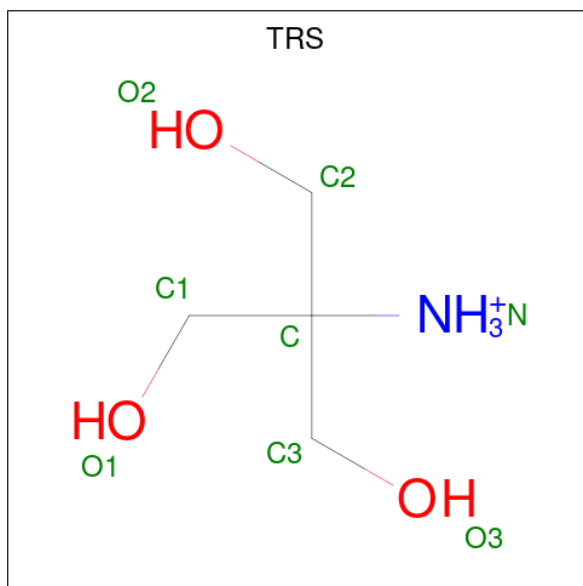
- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS)

(formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	N	O	0	0
			8	4	1	3		

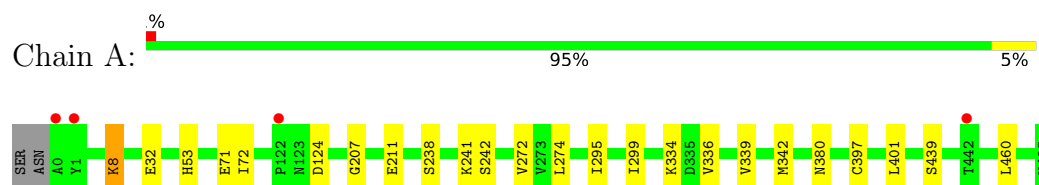
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	295	Total	O	0	13
			308	308		
10	B	299	Total	O	0	14
			313	313		
10	C	344	Total	O	0	11
			354	354		
10	D	285	Total	O	0	9
			293	293		

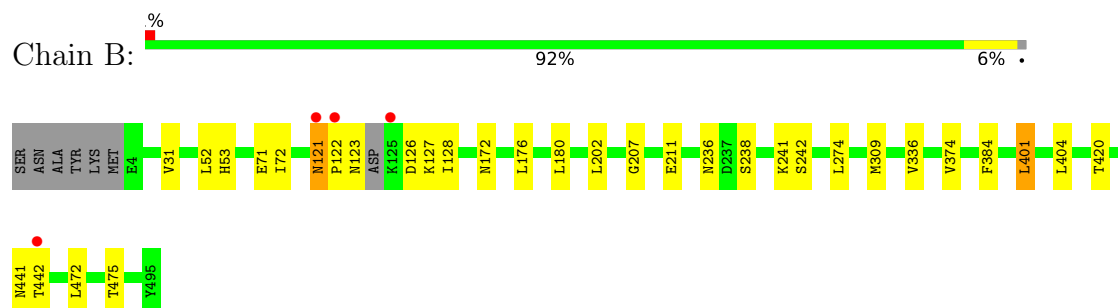
3 Residue-property plots [i](#)

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.

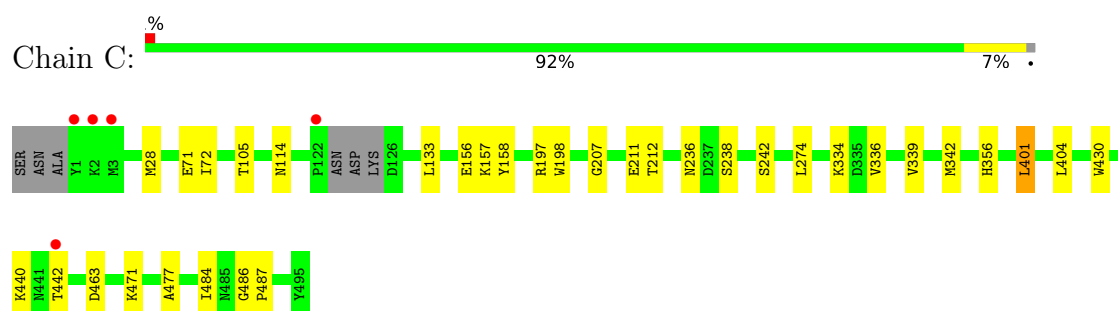
- Molecule 1: Adenosylhomocysteinase



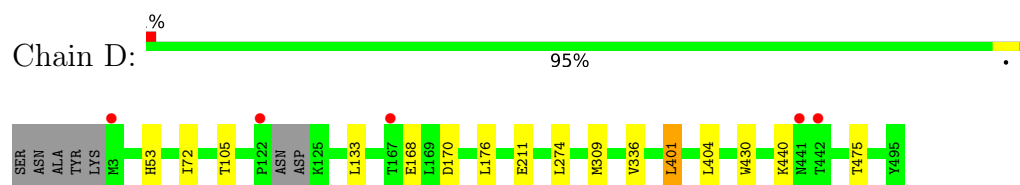
- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.85Å 121.22Å 178.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.15 29.97 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.97-2.15) 99.9 (29.97-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.142 , 0.181 0.155 , 0.188	Depositor DCC
R_{free} test set	6830 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17474	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DEA, PEG, NAD, GOL, EDO, TRS, PO4, CL

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	0.66	0/4089	0.93	9/5510 (0.2%)
1	B	0.66	0/4000	0.92	10/5392 (0.2%)
1	C	0.67	0/4018	0.94	8/5414 (0.1%)
1	D	0.65	0/4024	0.90	3/5424 (0.1%)
All	All	0.66	0/16131	0.92	30/21740 (0.1%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	ILE	N-CA-C	8.72	120.19	109.30
1	A	72	ILE	N-CA-C	7.66	119.86	108.46
1	D	72	ILE	N-CA-C	7.14	119.10	108.46
1	B	72	ILE	N-CA-C	6.68	118.34	108.45
1	B	207	GLY	N-CA-C	6.55	119.80	111.09
1	C	72	ILE	N-CA-C	6.54	118.20	108.46
1	C	207	GLY	N-CA-C	6.06	119.19	111.37
1	C	71	GLU	N-CA-C	-5.79	100.27	109.76
1	B	211	GLU	N-CA-C	5.67	118.67	111.69
1	D	211	GLU	N-CA-C	5.66	118.65	111.69
1	A	242	SER	N-CA-C	5.59	117.37	111.28
1	A	211	GLU	N-CA-C	5.56	118.53	111.69
1	B	127	LYS	N-CA-C	5.53	116.66	108.86
1	C	238	SER	N-CA-C	-5.42	102.25	110.28
1	A	238	SER	N-CA-C	-5.41	102.27	110.28
1	C	356	HIS	N-CA-C	5.32	117.08	111.28
1	A	71[A]	GLU	N-CA-C	-5.32	101.03	109.96
1	A	71[B]	GLU	N-CA-C	-5.32	101.03	109.96
1	C	211	GLU	N-CA-C	5.30	118.21	111.69
1	A	207	GLY	N-CA-C	5.27	118.10	111.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	105	THR	N-CA-C	-5.25	103.46	110.55
1	B	420	THR	N-CA-C	-5.22	105.67	111.36
1	C	156	GLU	N-CA-C	5.17	117.59	111.59
1	C	105	THR	N-CA-C	-5.17	103.58	110.55
1	B	202	LEU	N-CA-C	5.16	116.90	111.28
1	B	238	SER	N-CA-C	-5.09	102.75	110.28
1	B	71	GLU	N-CA-C	-5.03	101.51	109.76
1	A	8[A]	LYS	N-CA-C	5.02	117.87	111.69
1	A	8[B]	LYS	N-CA-C	5.02	117.87	111.69
1	B	441	ASN	N-CA-C	5.01	118.80	111.04

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	4024	0	4078	10	0
1	B	3937	0	3984	14	0
1	C	3954	0	4011	15	0
1	D	3961	0	4010	6	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	18	0	10	0	0
3	B	18	0	10	0	0
3	C	18	0	10	0	0
3	D	18	0	10	0	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	B	7	0	10	1	0
5	C	14	0	20	0	0
6	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	2	0	0	0	0
7	C	5	0	0	0	0
8	C	4	0	6	0	0
8	D	4	0	6	0	0
9	D	8	0	12	0	0
10	A	308	0	0	0	0
10	B	313	0	0	0	0
10	C	354	0	0	0	0
10	D	293	0	0	0	0
All	All	17474	0	16329	41	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 (41) 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:C:28[B]:MET:HE1	1:C:463[B]:ASP:HB3	1.70	0.73
1:B:309:MET:HE2	1:B:309:MET:HA	1.85	0.58
1:C:28[B]:MET:HE1	1:C:463[B]:ASP:OD2	2.04	0.57
1:B:121:ASN:O	1:B:123:ASN:N	2.38	0.55
1:A:339:VAL:HA	1:A:342:MET:HE3	1.90	0.54
1:B:401:LEU:HD13	1:B:404:LEU:HB2	1.90	0.53
1:D:274:LEU:HD22	1:D:336[B]:VAL:HG12	1.90	0.53
1:C:339:VAL:HA	1:C:342:MET:HE3	1.94	0.49
1:C:28[B]:MET:HE1	1:C:463[B]:ASP:CB	2.42	0.48
1:D:309:MET:HA	1:D:309:MET:HE2	1.95	0.48
1:A:334:LYS:CE	1:B:475:THR:HG22	2.43	0.48
1:B:442:THR:O	1:B:442:THR:HG22	2.13	0.48
1:C:197:ARG:NH1	1:C:198:TRP:CZ2	2.81	0.47
1:B:176:LEU:HD22	1:B:180:LEU:HD23	1.97	0.47
1:A:274:LEU:HD22	1:A:336:VAL:HG12	1.97	0.46
1:D:133:LEU:HD11	1:D:430:TRP:HB2	1.98	0.46
1:C:133:LEU:HD11	1:C:430:TRP:HB2	1.97	0.46
1:C:401:LEU:HD13	1:C:404:LEU:HB2	1.97	0.45
1:B:374:VAL:HG22	1:B:384:PHE:CD2	2.52	0.44
1:C:442:THR:HG22	1:C:442:THR:O	2.17	0.44
1:D:401:LEU:HD22	1:D:404:LEU:HD12	1.99	0.43
1:B:31:VAL:HG12	5:B:505:PEG:H11	2.00	0.43
1:C:236:ASN:O	1:C:242:SER:HB3	2.19	0.43
1:C:274:LEU:HD22	1:C:336:VAL:HG12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:LYS:CE	1:D:475:THR:HG22	2.49	0.43
1:C:486:GLY:HA2	1:C:487:PRO:C	2.44	0.43
1:A:32:GLU:HG2	1:A:460:LEU:HD22	2.01	0.42
1:D:170:ASP:HB3	1:D:176:LEU:HD23	2.01	0.42
1:A:334:LYS:HE3	1:B:475:THR:HG22	2.02	0.42
1:A:299:ILE:HD13	1:B:472:LEU:HD21	2.03	0.41
1:C:477:ALA:HB2	1:C:484:ILE:HD13	2.03	0.41
1:B:241:LYS:C	1:B:241:LYS:HD3	2.45	0.41
1:A:380:ASN:HB3	1:A:397:CYS:HB3	2.03	0.41
1:B:274:LEU:HD22	1:B:336:VAL:HG12	2.01	0.41
1:A:8[B]:LYS:O	1:A:8[B]:LYS:HG3	2.20	0.41
1:A:241:LYS:HD3	1:A:241:LYS:C	2.46	0.41
1:C:157[A]:LYS:HG3	1:C:158:TYR:CD2	2.55	0.41
1:B:236:ASN:O	1:B:242:SER:HB3	2.20	0.41
1:C:114:ASN:OD1	1:C:197:ARG:NH1	2.51	0.41
1:A:272:VAL:HA	1:A:295:ILE:O	2.22	0.40
1:B:52:LEU:O	1:B:53:HIS:C	2.64	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	507/498 (102%)	487 (96%)	17 (3%)	3 (1%)	21	15
1	B	495/498 (99%)	473 (96%)	18 (4%)	4 (1%)	16	10
1	C	496/498 (100%)	480 (97%)	15 (3%)	1 (0%)	43	44
1	D	497/498 (100%)	477 (96%)	17 (3%)	3 (1%)	21	15
All	All	1995/1992 (100%)	1917 (96%)	67 (3%)	11 (1%)	21	15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	ASN
1	B	122	PRO
1	A	439	SER
1	B	172	ASN
1	C	440	LYS
1	D	440	LYS
1	A	124	ASP
1	B	126	ASP
1	D	53	HIS
1	A	53	HIS
1	D	168	GLU

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	446/435 (102%)	445 (100%)	1 (0%)	87	92
1	B	437/435 (100%)	436 (100%)	1 (0%)	87	92
1	C	438/435 (101%)	435 (99%)	3 (1%)	76	82
1	D	439/435 (101%)	438 (100%)	1 (0%)	87	92
All	All	1760/1740 (101%)	1754 (100%)	6 (0%)	86	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	401	LEU
1	B	401	LEU
1	C	212	THR
1	C	401	LEU
1	C	471	LYS
1	D	401	LEU

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

Mol	Chain	Res	Type
1	A	481	ASN
1	B	103	ASN
1	B	368	ASN
1	B	379	GLN
1	B	380	ASN
1	C	94	ASN
1	C	159	ASN
1	C	285	GLN
1	C	368	ASN
1	D	114	ASN
1	D	368	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	$\# Z > 2$
5	PEG	C	504	-	6,6,6	0.47	0	5,5,5	0.26	0
4	GOL	A	504	-	5,5,5	0.26	0	5,5,5	0.34	0
4	GOL	B	504	-	5,5,5	0.27	0	5,5,5	0.24	0
3	DEA	B	502	-	19,19,19	1.68	5 (26%)	24,27,27	2.56	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	501	-	46,48,48	1.13	5 (10%)	64,73,73	1.56	12 (18%)
2	NAD	C	501	-	46,48,48	1.17	6 (13%)	64,73,73	1.61	10 (15%)
5	PEG	B	505	-	6,6,6	0.66	0	5,5,5	0.56	0
4	GOL	B	503	-	5,5,5	0.38	0	5,5,5	0.14	0
4	GOL	D	503	-	5,5,5	0.34	0	5,5,5	0.17	0
8	EDO	C	509	-	3,3,3	0.46	0	2,2,2	0.30	0
3	DEA	D	502	-	19,19,19	1.67	4 (21%)	24,27,27	2.69	10 (41%)
4	GOL	A	503	-	5,5,5	0.23	0	5,5,5	0.28	0
2	NAD	D	501	-	46,48,48	1.19	6 (13%)	64,73,73	1.57	12 (18%)
5	PEG	C	508	-	6,6,6	0.44	0	5,5,5	0.30	0
7	PO4	C	505	-	4,4,4	0.91	0	6,6,6	0.47	0
3	DEA	C	502	-	19,19,19	1.71	5 (26%)	24,27,27	2.58	11 (45%)
3	DEA	A	502	-	19,19,19	1.71	4 (21%)	24,27,27	2.71	9 (37%)
8	EDO	D	505	-	3,3,3	0.46	0	2,2,2	0.21	0
2	NAD	A	501	-	46,48,48	1.16	5 (10%)	64,73,73	1.58	13 (20%)
9	TRS	D	504	-	7,7,7	0.31	0	9,9,9	0.27	0
4	GOL	C	503	-	5,5,5	0.35	0	5,5,5	0.22	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
5	PEG	C	504	-	-	3/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	B	504	-	-	1/4/4/4	-
3	DEA	B	502	-	-	0/12/12/12	0/2/2/2
2	NAD	B	501	-	-	5/30/62/62	0/5/5/5
2	NAD	C	501	-	-	5/30/62/62	0/5/5/5
5	PEG	B	505	-	-	2/4/4/4	-
4	GOL	B	503	-	-	2/4/4/4	-
4	GOL	D	503	-	-	0/4/4/4	-
8	EDO	C	509	-	-	0/1/1/1	-
3	DEA	D	502	-	-	0/12/12/12	0/2/2/2
4	GOL	A	503	-	-	2/4/4/4	-
2	NAD	D	501	-	-	5/30/62/62	0/5/5/5
5	PEG	C	508	-	-	3/4/4/4	-
3	DEA	C	502	-	-	0/12/12/12	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DEA	A	502	-	-	0/12/12/12	0/2/2/2
8	EDO	D	505	-	-	1/1/1/1	-
2	NAD	A	501	-	-	5/30/62/62	0/5/5/5
9	TRS	D	504	-	-	2/9/9/9	-
4	GOL	C	503	-	-	2/4/4/4	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAD	C5A-C4A	4.61	1.47	1.39
2	A	501	NAD	C5A-C4A	4.47	1.47	1.39
2	C	501	NAD	C5A-C4A	4.30	1.46	1.39
3	C	502	DEA	C5-C4	4.25	1.46	1.39
2	B	501	NAD	C5A-C4A	4.16	1.46	1.39
3	A	502	DEA	C5-C4	4.11	1.46	1.39
3	D	502	DEA	C5-C4	4.00	1.46	1.39
3	B	502	DEA	C5-C4	3.81	1.45	1.39
3	C	502	DEA	C4-N9	-3.76	1.33	1.37
3	B	502	DEA	C4-N9	-3.65	1.33	1.37
3	D	502	DEA	C4-N9	-3.51	1.33	1.37
3	A	502	DEA	C4-N9	-3.37	1.33	1.37
3	A	502	DEA	C5-N7	-2.68	1.34	1.39
2	C	501	NAD	C5A-N7A	-2.65	1.34	1.39
2	D	501	NAD	C8A-N7A	2.64	1.36	1.31
2	D	501	NAD	C5A-C6A	2.63	1.48	1.41
2	C	501	NAD	O4D-C1D	2.62	1.44	1.40
2	A	501	NAD	C5A-N7A	-2.53	1.34	1.39
3	D	502	DEA	C5-C6	2.53	1.48	1.41
3	B	502	DEA	C5-N7	-2.49	1.34	1.39
2	B	501	NAD	C5A-C6A	2.48	1.47	1.41
3	C	502	DEA	C5-N7	-2.47	1.34	1.39
2	A	501	NAD	C5A-C6A	2.47	1.47	1.41
2	D	501	NAD	C5A-N7A	-2.45	1.34	1.39
2	A	501	NAD	C4A-N9A	-2.42	1.32	1.37
2	C	501	NAD	C4A-N9A	-2.38	1.32	1.37
2	B	501	NAD	C5A-N7A	-2.37	1.34	1.39
2	C	501	NAD	C8A-N7A	2.35	1.36	1.31
3	A	502	DEA	C5-C6	2.33	1.47	1.41
2	B	501	NAD	C4A-N9A	-2.30	1.32	1.37
3	B	502	DEA	C5-C6	2.30	1.47	1.41
3	C	502	DEA	C5-C6	2.25	1.47	1.41
3	D	502	DEA	C5-N7	-2.25	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	O4D-C1D	2.22	1.43	1.40
2	A	501	NAD	O4D-C1D	2.17	1.43	1.40
2	C	501	NAD	C5A-C6A	2.14	1.46	1.41
3	B	502	DEA	C8-N7	2.11	1.35	1.31
2	D	501	NAD	O4D-C1D	2.06	1.43	1.40
3	C	502	DEA	C8-N7	2.03	1.35	1.31
2	D	501	NAD	C4A-N9A	-2.02	1.33	1.37

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	DEA	N3-C4-N9	6.36	134.75	126.87
3	A	502	DEA	N3-C4-N9	6.32	134.69	126.87
3	C	502	DEA	N3-C4-N9	6.04	134.35	126.87
3	B	502	DEA	N3-C4-N9	6.01	134.31	126.87
2	C	501	NAD	C5A-C4A-N3A	-5.47	119.19	126.72
3	D	502	DEA	C5-C4-N3	-5.44	119.22	126.72
3	A	502	DEA	C5-C4-N3	-5.42	119.26	126.72
2	D	501	NAD	C5A-C4A-N3A	-5.37	119.33	126.72
3	B	502	DEA	C5-C4-N3	-5.34	119.36	126.72
3	C	502	DEA	C5-C4-N3	-5.23	119.52	126.72
2	B	501	NAD	C5A-C4A-N3A	-5.01	119.81	126.72
2	A	501	NAD	C5A-C4A-N3A	-4.84	120.05	126.72
3	D	502	DEA	C4-N9-C8	4.63	109.07	105.75
3	A	502	DEA	C4-N9-C8	4.48	108.97	105.75
2	C	501	NAD	N3A-C4A-N9A	4.42	134.68	127.17
3	A	502	DEA	N9-C8-N7	-4.29	110.19	114.16
2	D	501	NAD	N3A-C4A-N9A	4.20	134.31	127.17
2	B	501	NAD	N3A-C4A-N9A	4.18	134.27	127.17
2	A	501	NAD	N3A-C2A-N1A	-4.14	122.32	128.58
3	C	502	DEA	C4-N9-C8	4.13	108.72	105.75
2	A	501	NAD	N3A-C4A-N9A	4.12	134.18	127.17
3	B	502	DEA	C4-N9-C8	4.11	108.70	105.75
3	D	502	DEA	N9-C8-N7	-3.91	110.54	114.16
3	B	502	DEA	N9-C8-N7	-3.86	110.59	114.16
2	B	501	NAD	N3A-C2A-N1A	-3.78	122.85	128.58
2	C	501	NAD	N3A-C2A-N1A	-3.77	122.87	128.58
3	D	502	DEA	C2-N3-C4	3.77	121.04	111.83
2	D	501	NAD	N3A-C2A-N1A	-3.74	122.93	128.58
3	A	502	DEA	N3-C2-N1	-3.70	122.98	128.58
3	A	502	DEA	C2-N3-C4	3.69	120.85	111.83
3	B	502	DEA	C2-N3-C4	3.69	120.84	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAD	C2A-N3A-C4A	3.68	120.82	111.83
3	C	502	DEA	N3-C2-N1	-3.66	123.05	128.58
3	D	502	DEA	N3-C2-N1	-3.64	123.07	128.58
2	C	501	NAD	C2A-N3A-C4A	3.63	120.69	111.83
2	A	501	NAD	C2A-N3A-C4A	3.57	120.56	111.83
3	D	502	DEA	C4-C5-N7	-3.56	106.51	110.58
3	C	502	DEA	C2-N3-C4	3.53	120.45	111.83
3	C	502	DEA	N9-C8-N7	-3.52	110.90	114.16
2	B	501	NAD	C2A-N3A-C4A	3.49	120.34	111.83
3	A	502	DEA	C4-C5-N7	-3.41	106.68	110.58
3	B	502	DEA	N3-C2-N1	-3.39	123.45	128.58
2	D	501	NAD	C4A-C5A-N7A	-3.31	106.79	110.58
2	B	501	NAD	C4A-N9A-C8A	3.28	109.19	105.74
2	A	501	NAD	C4A-N9A-C8A	3.26	109.16	105.74
2	B	501	NAD	C4A-C5A-N7A	-3.24	106.88	110.58
3	B	502	DEA	C4-C5-N7	-3.16	106.97	110.58
3	C	502	DEA	C4-C5-N7	-3.15	106.98	110.58
2	A	501	NAD	C4A-C5A-N7A	-3.09	107.05	110.58
2	C	501	NAD	C3N-C7N-N7N	3.06	121.51	117.74
2	C	501	NAD	C4A-N9A-C8A	3.03	108.92	105.74
2	C	501	NAD	C4A-C5A-N7A	-3.03	107.12	110.58
3	A	502	DEA	C5-N7-C8	2.97	108.11	103.45
2	D	501	NAD	C4A-N9A-C8A	2.83	108.71	105.74
3	D	502	DEA	C5-N7-C8	2.79	107.83	103.45
2	D	501	NAD	C3N-C7N-N7N	2.77	121.15	117.74
2	B	501	NAD	C3N-C7N-N7N	2.75	121.13	117.74
2	B	501	NAD	C5A-N7A-C8A	2.59	107.53	103.45
2	D	501	NAD	C5A-N7A-C8A	2.57	107.49	103.45
3	B	502	DEA	C5-N7-C8	2.52	107.40	103.45
2	C	501	NAD	C5A-N7A-C8A	2.45	107.30	103.45
3	C	502	DEA	OXT-C4'-C3'	2.44	120.10	113.31
2	A	501	NAD	C5A-N7A-C8A	2.44	107.29	103.45
2	B	501	NAD	N9A-C8A-N7A	-2.43	110.49	113.94
3	C	502	DEA	C5-N7-C8	2.43	107.27	103.45
2	A	501	NAD	C3N-C7N-N7N	2.43	120.73	117.74
2	B	501	NAD	C6N-N1N-C1D	2.42	124.47	119.73
2	C	501	NAD	N9A-C8A-N7A	-2.40	110.53	113.94
2	A	501	NAD	C2A-N1A-C6A	2.35	122.60	118.73
2	D	501	NAD	C6N-N1N-C1D	2.35	124.34	119.73
2	A	501	NAD	C6A-C5A-N7A	2.34	136.60	132.09
2	D	501	NAD	N9A-C8A-N7A	-2.32	110.64	113.94
2	A	501	NAD	N9A-C8A-N7A	-2.27	110.71	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAD	C6N-N1N-C1D	2.27	124.18	119.73
2	C	501	NAD	C6N-N1N-C1D	2.27	124.17	119.73
3	D	502	DEA	C6-C5-N7	2.25	136.44	132.09
2	B	501	NAD	C2A-N1A-C6A	2.15	122.26	118.73
3	A	502	DEA	OXT-C4'-C3'	2.14	119.27	113.31
2	D	501	NAD	C6A-C5A-N7A	2.13	136.19	132.09
2	B	501	NAD	C6A-C5A-N7A	2.10	136.13	132.09
3	D	502	DEA	OXT-C4'-C3'	2.06	119.05	113.31
3	C	502	DEA	C2-N1-C6	2.06	122.11	118.73
2	A	501	NAD	O7N-C7N-N7N	-2.02	119.69	122.62
2	D	501	NAD	C2A-N1A-C6A	2.02	122.05	118.73
3	C	502	DEA	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (38) 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	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	C	501	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
4	A	503	GOL	C1-C2-C3-O3
4	B	503	GOL	C1-C2-C3-O3
4	B	503	GOL	O2-C2-C3-O3
4	C	503	GOL	O1-C1-C2-C3
4	C	503	GOL	O1-C1-C2-O2
5	C	504	PEG	O1-C1-C2-O2
4	A	503	GOL	O2-C2-C3-O3
5	B	505	PEG	O2-C3-C4-O4
5	C	508	PEG	O2-C3-C4-O4

Continued on next page...

Continued from previous page...

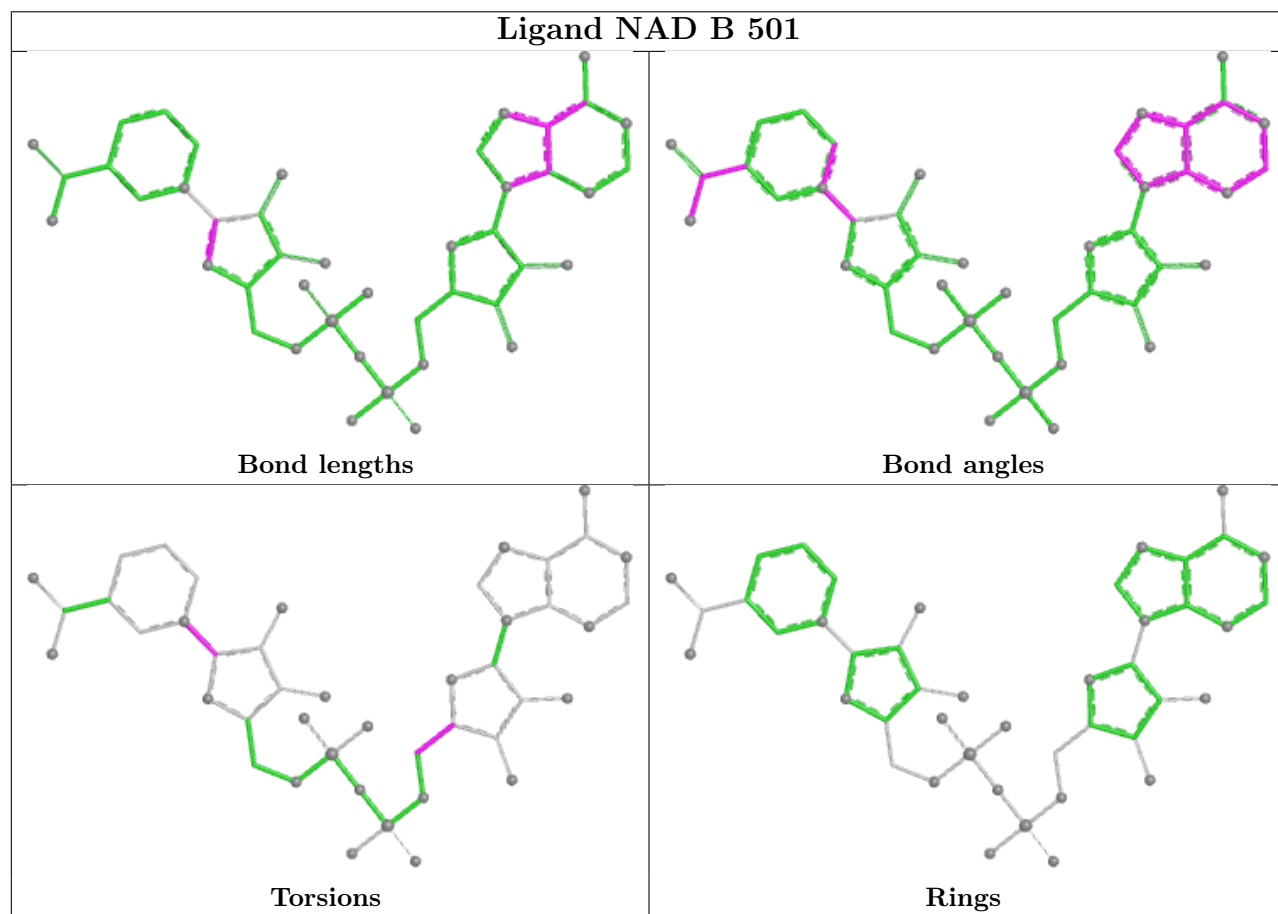
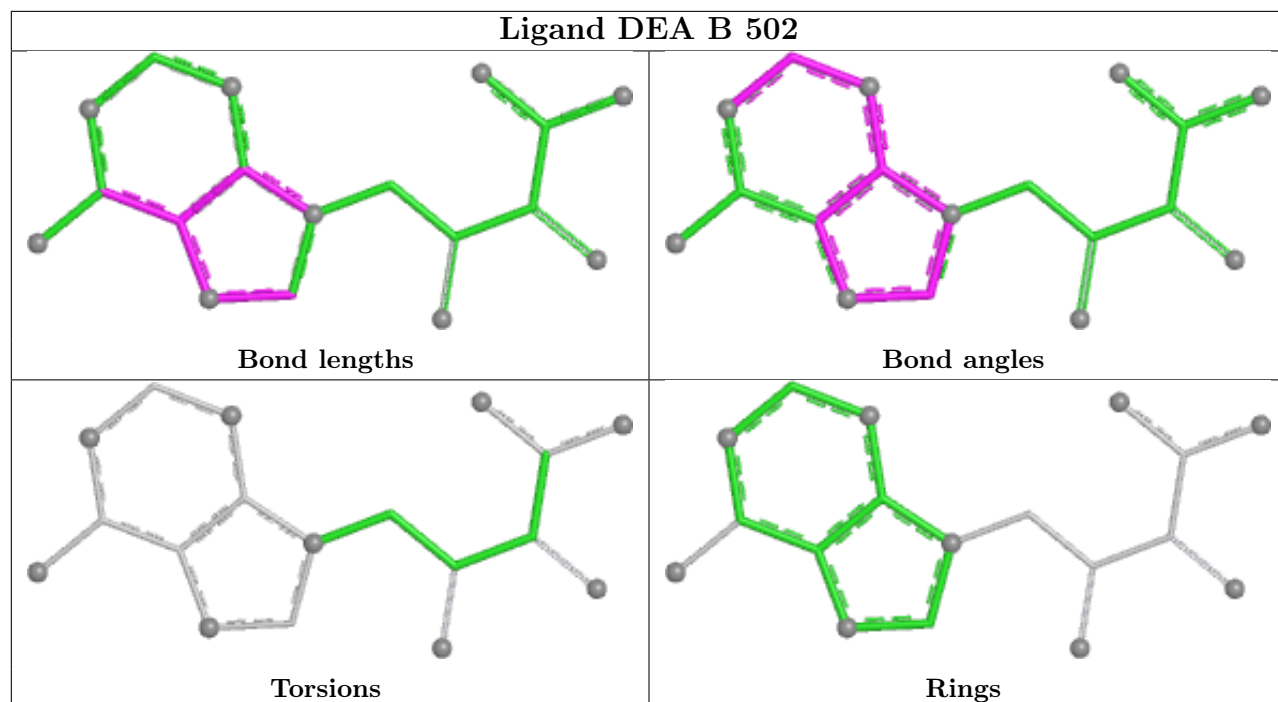
Mol	Chain	Res	Type	Atoms
5	C	504	PEG	O2-C3-C4-O4
5	C	508	PEG	C1-C2-O2-C3
2	B	501	NAD	O4B-C4B-C5B-O5B
5	B	505	PEG	C1-C2-O2-C3
8	D	505	EDO	O1-C1-C2-O2
9	D	504	TRS	C1-C-C3-O3
5	C	508	PEG	O1-C1-C2-O2
2	A	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B
2	D	501	NAD	O4B-C4B-C5B-O5B
9	D	504	TRS	N-C-C3-O3
4	B	504	GOL	O1-C1-C2-O2
5	C	504	PEG	C1-C2-O2-C3

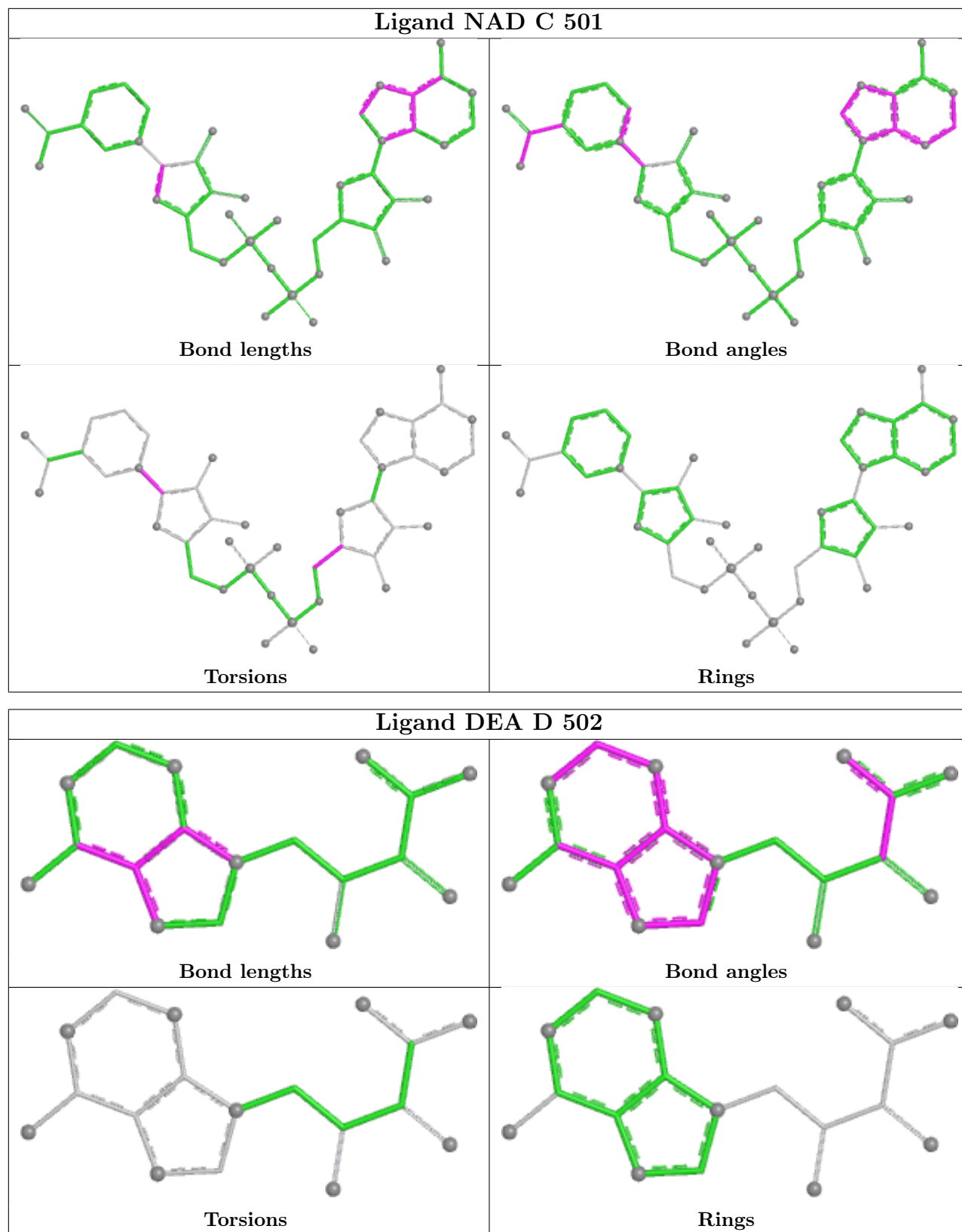
There are no ring outliers.

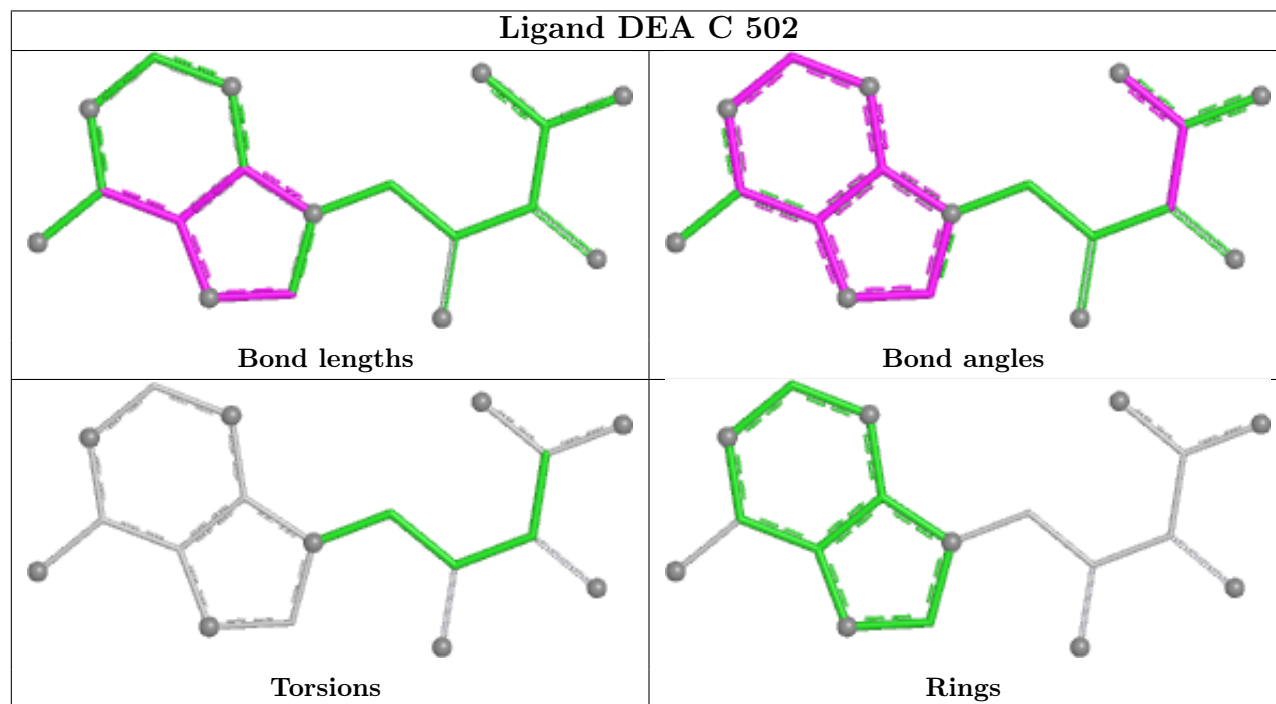
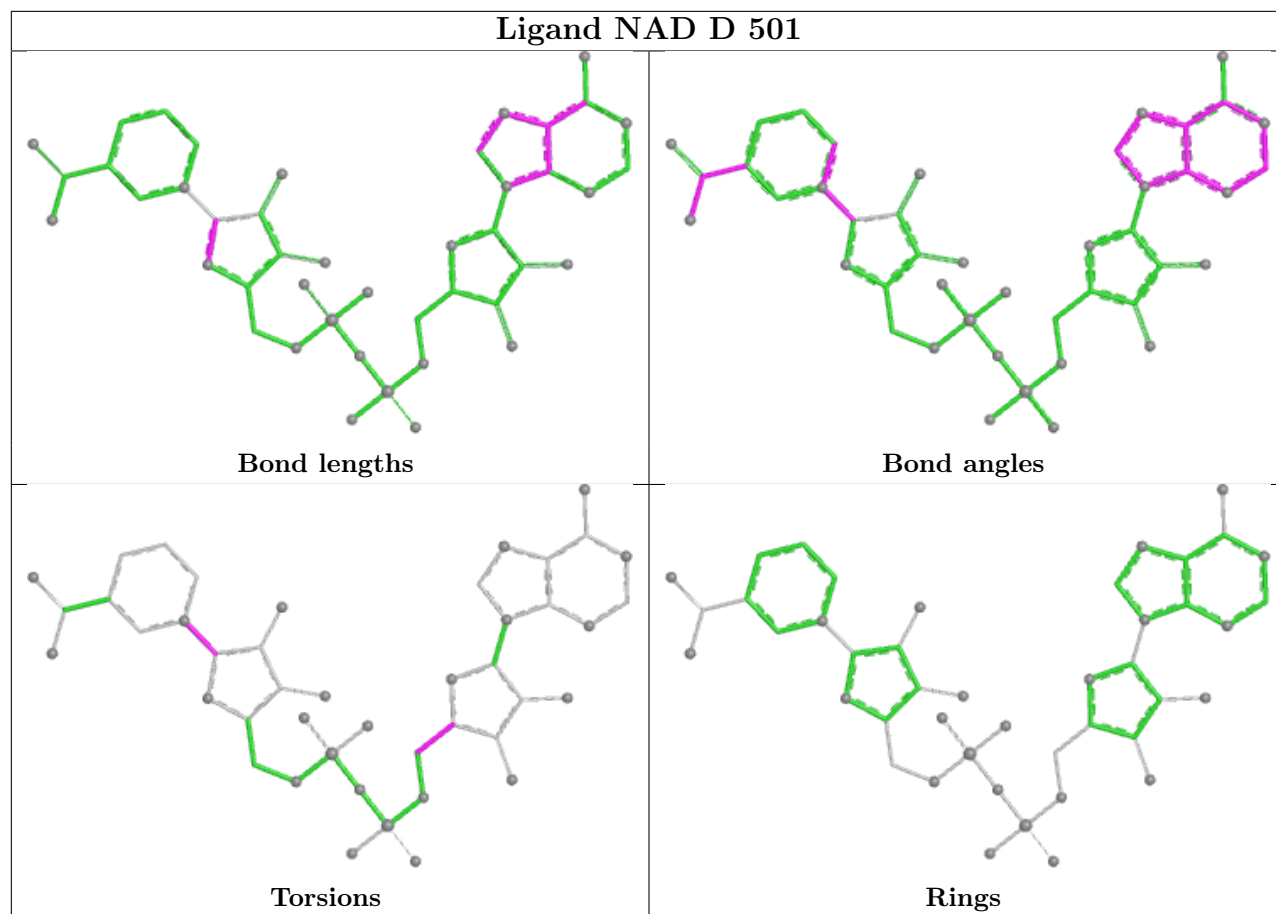
1 monomer is involved in 1 short contact:

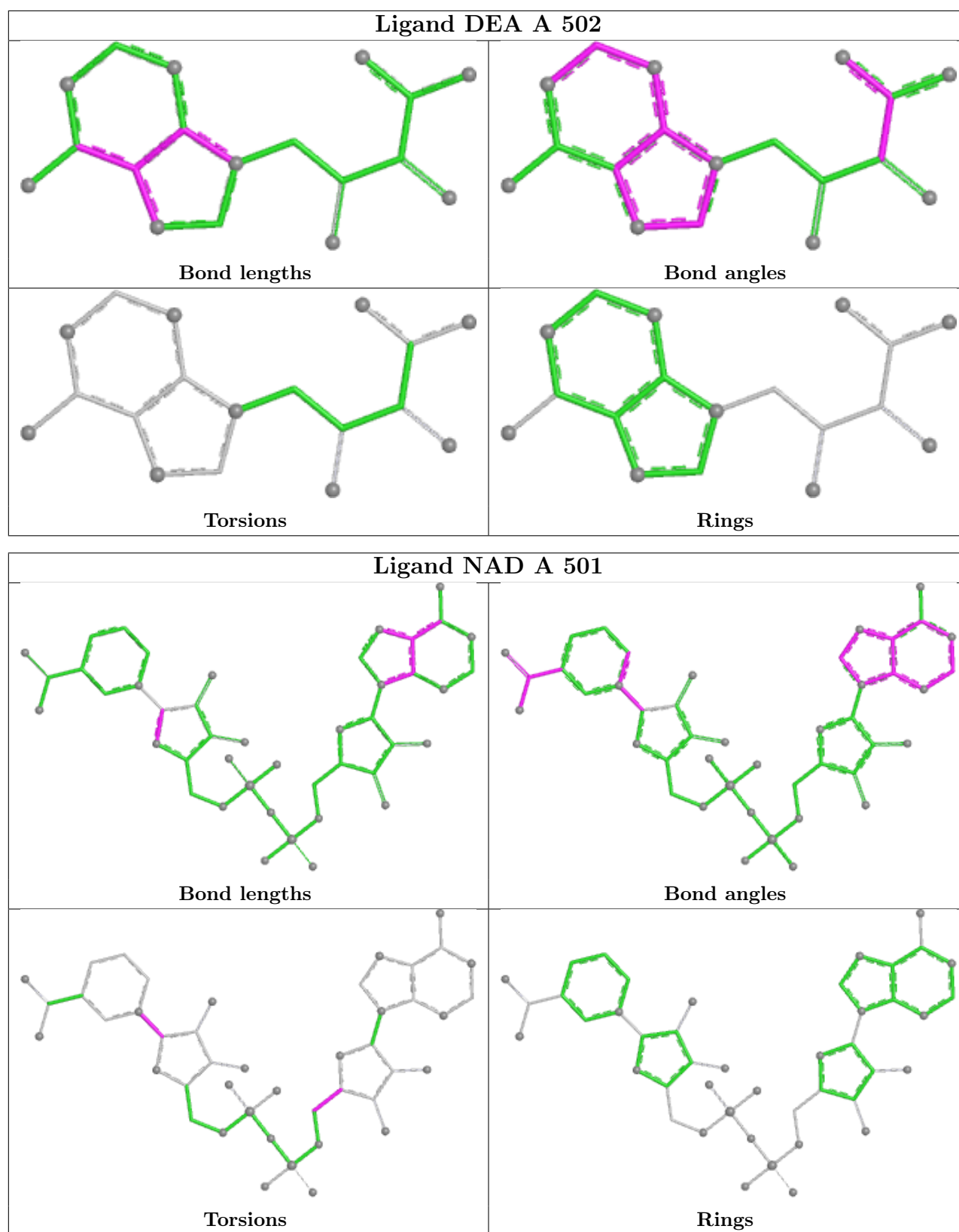
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	PEG	1	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	496/498 (99%)	-0.38	4 (0%) 82 84	12, 34, 81, 131	13 (2%)
1	B	491/498 (98%)	-0.44	4 (0%) 82 84	14, 34, 70, 144	8 (1%)
1	C	492/498 (98%)	-0.46	5 (1%) 79 82	13, 32, 58, 119	8 (1%)
1	D	491/498 (98%)	-0.34	5 (1%) 79 82	14, 38, 84, 123	10 (2%)
All	All	1970/1992 (98%)	-0.40	18 (0%) 81 83	12, 34, 76, 144	39 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	122	PRO	4.9
1	C	3	MET	4.3
1	A	122	PRO	3.7
1	B	122	PRO	3.6
1	D	122	PRO	3.5
1	B	442	THR	3.5
1	A	0	ALA	2.9
1	B	125	LYS	2.8
1	C	442	THR	2.7
1	D	442	THR	2.6
1	A	1	TYR	2.6
1	D	167	THR	2.5
1	C	2	LYS	2.5
1	B	121	ASN	2.4
1	C	1	TYR	2.4
1	D	441	ASN	2.2
1	D	3	MET	2.2
1	A	442	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

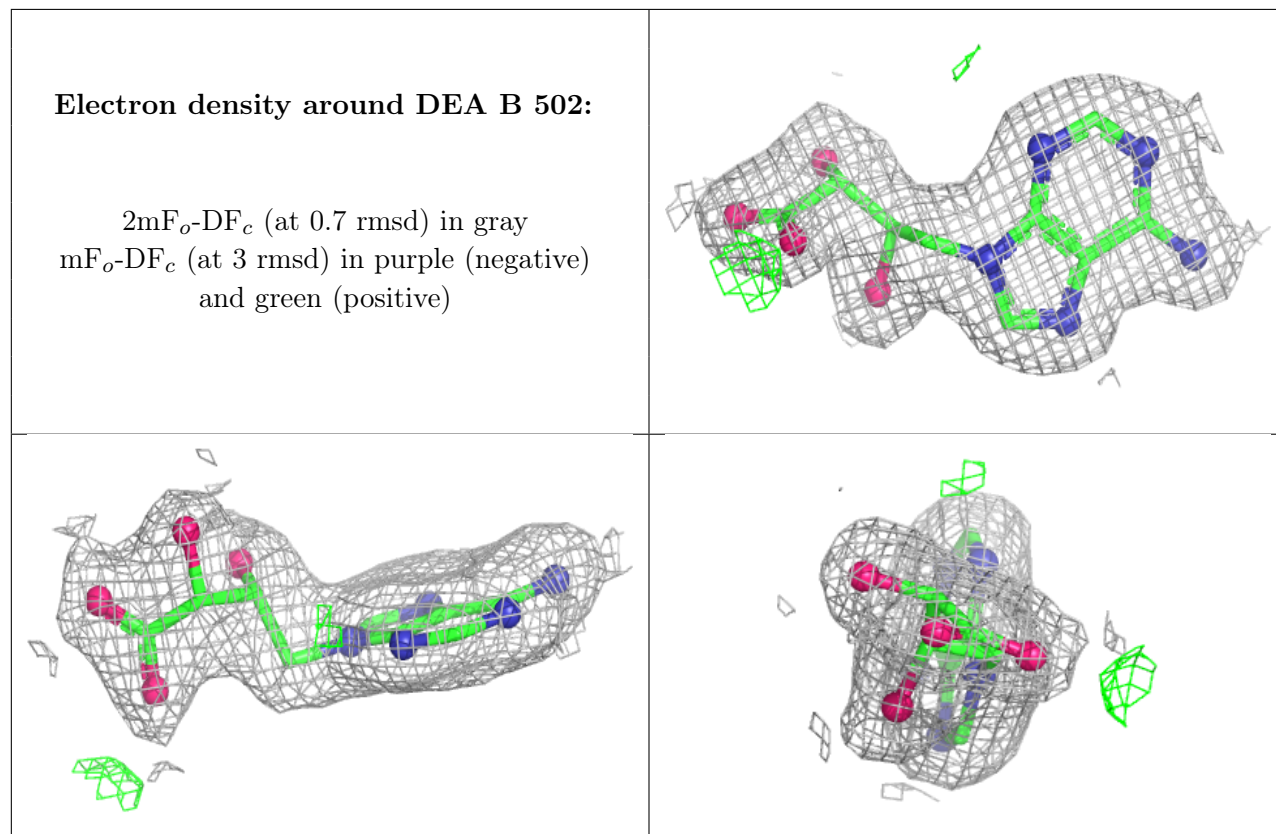
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	EDO	C	509	4/4	0.72	0.26	73,78,78,80	0
5	PEG	C	504	7/7	0.74	0.19	67,73,78,83	0
5	PEG	B	505	7/7	0.81	0.14	42,49,52,56	0
4	GOL	A	503	6/6	0.82	0.17	58,60,67,74	0
5	PEG	C	508	7/7	0.83	0.21	71,72,82,88	0
4	GOL	B	504	6/6	0.83	0.13	63,64,67,67	0
8	EDO	D	505	4/4	0.83	0.23	75,75,76,77	0
7	PO4	C	505	5/5	0.85	0.10	77,78,88,92	0
9	TRS	D	504	8/8	0.85	0.15	54,63,66,72	0
4	GOL	C	503	6/6	0.86	0.11	59,62,63,64	0
4	GOL	A	504	6/6	0.87	0.11	61,69,71,74	0
6	CL	C	506	1/1	0.89	0.16	89,89,89,89	0
6	CL	B	507	1/1	0.90	0.19	80,80,80,80	0
6	CL	C	507	1/1	0.90	0.12	95,95,95,95	0
4	GOL	D	503	6/6	0.91	0.09	44,61,64,68	0
4	GOL	B	503	6/6	0.93	0.09	39,57,60,64	0
3	DEA	B	502	18/18	0.97	0.05	25,27,35,36	0
3	DEA	D	502	18/18	0.97	0.05	27,30,38,41	0
3	DEA	A	502	18/18	0.98	0.04	23,25,34,38	0
2	NAD	C	501	44/44	0.98	0.04	22,24,26,28	0
3	DEA	C	502	18/18	0.98	0.04	23,26,32,36	0
2	NAD	D	501	44/44	0.98	0.04	25,29,34,38	0
2	NAD	A	501	44/44	0.99	0.04	23,26,28,29	0
6	CL	B	506	1/1	0.99	0.07	35,35,35,35	0
2	NAD	B	501	44/44	0.99	0.04	22,27,29,31	0

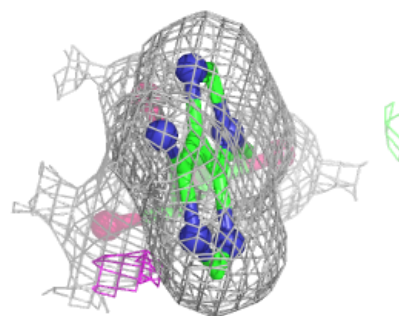
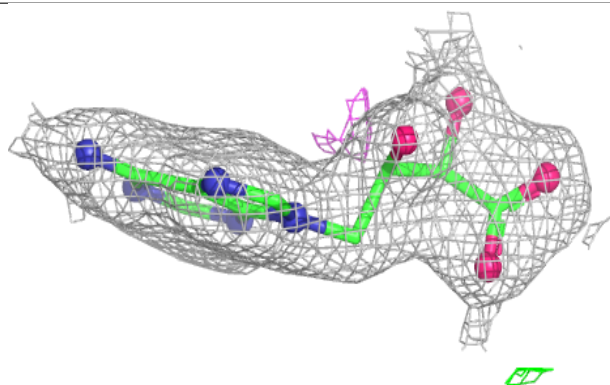
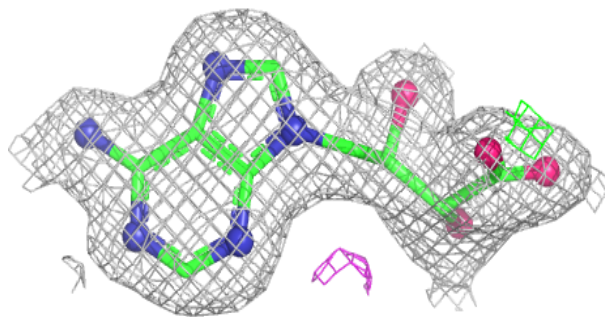
The following is a graphical depiction of the model fit to experimental electron density of all

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.

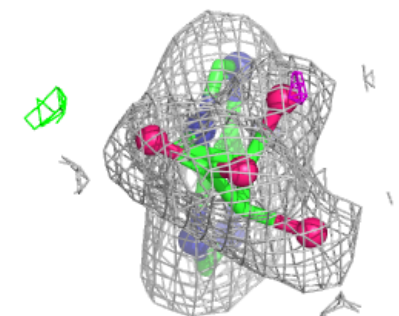
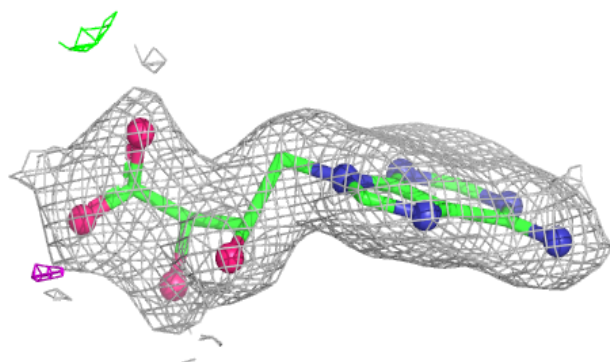
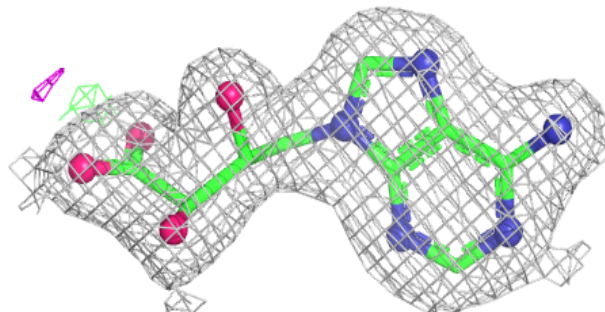


Electron density around DEA D 502:

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

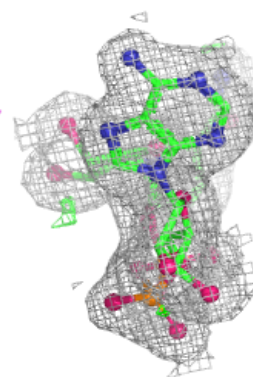
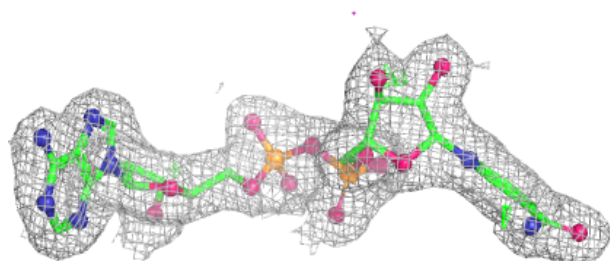
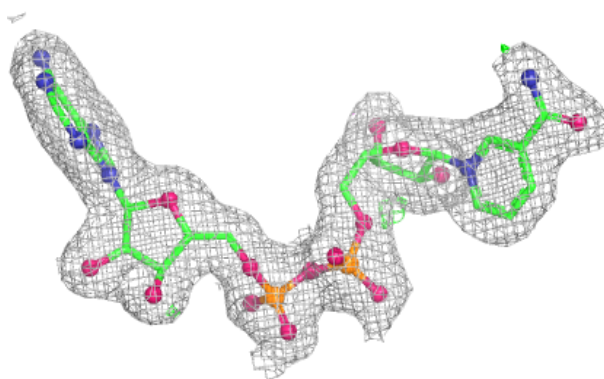
**Electron density around DEA A 502:**

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

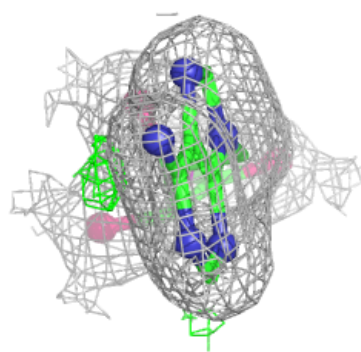
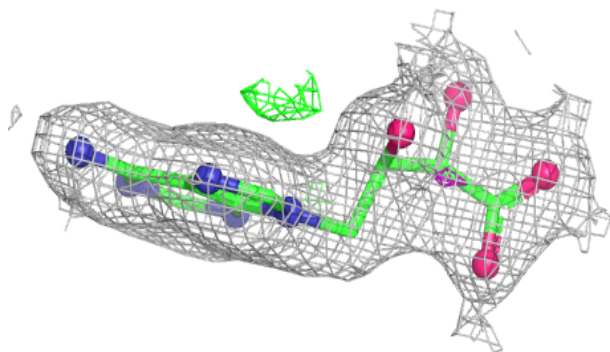
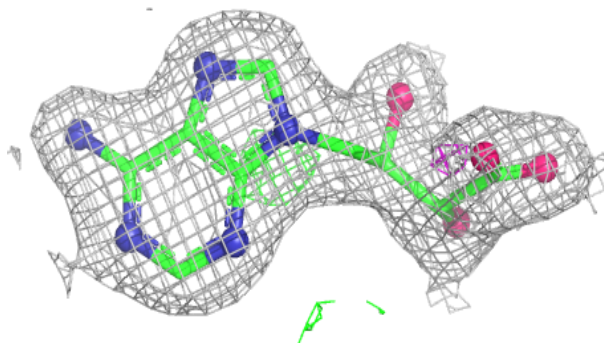


Electron density around NAD C 501:

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

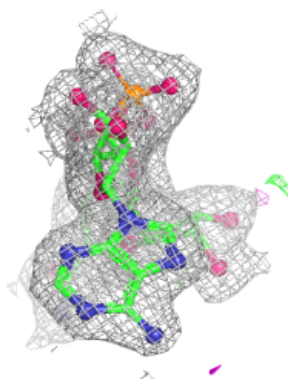
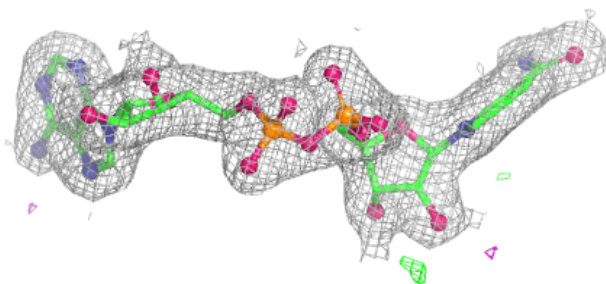
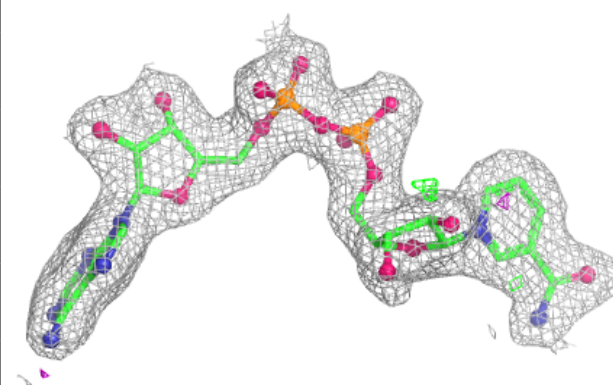
**Electron density around DEA C 502:**

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

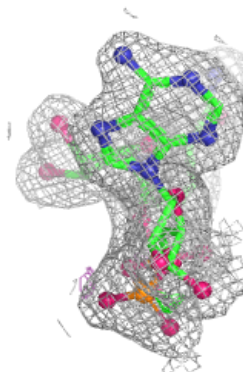
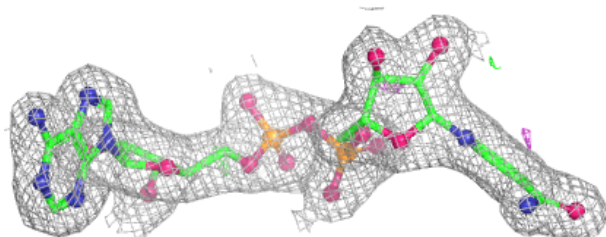
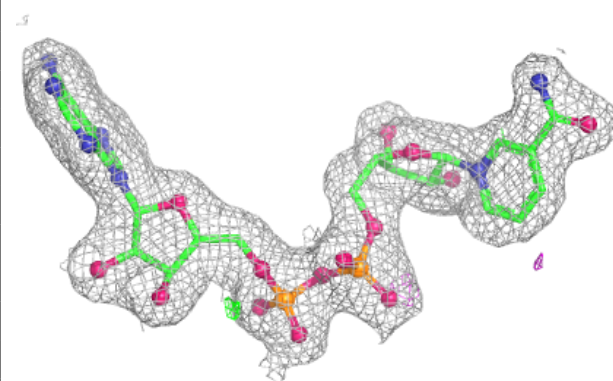


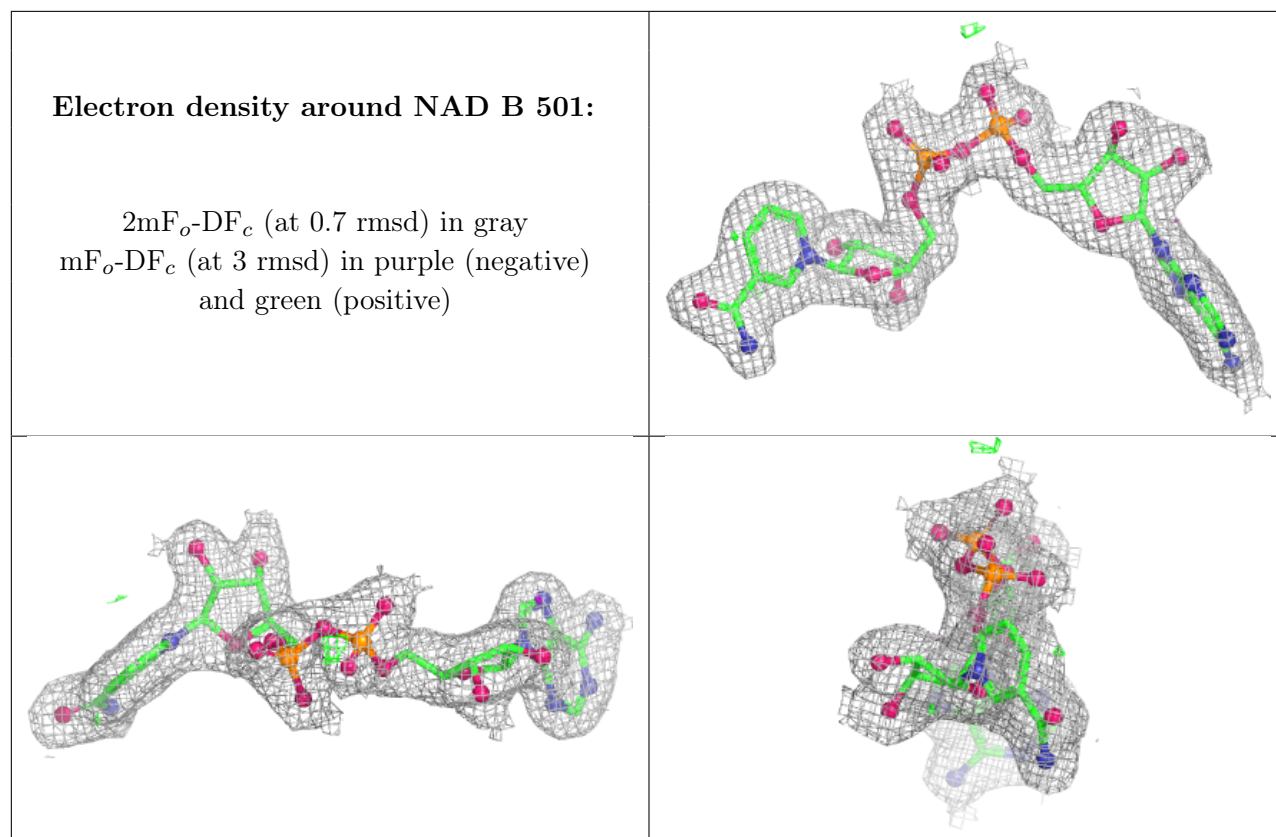
Electron density around NAD D 501:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.