



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:57 am BST

PDB ID : 5T8K
Title : 1.95 Angstrom Crystal Structure of S-adenosylhomocysteinase from *Cryptosporidium parvum* in Complex with Adenine 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 : 2016-09-07
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

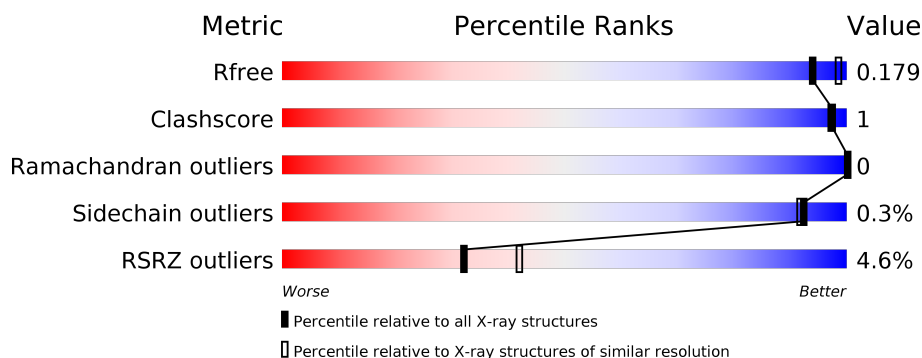
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>4%</div> <div>97%</div> <div>..</div> </div>
1	B	498	<div> <div>7%</div> <div>97%</div> <div>..</div> </div>
1	D	498	<div> <div>4%</div> <div>96%</div> <div>..</div> </div>
2	C	498	<div> <div>4%</div> <div>97%</div> <div>..</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18512 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	491	Total	C	N	O	S	0	25	0
			4070	2583	678	779	30			
1	B	493	Total	C	N	O	S	0	18	0
			4035	2557	676	773	29			
1	D	493	Total	C	N	O	S	0	15	0
			4017	2552	671	765	29			

There are 9 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
D	-2	SER	-	expression tag	UNP Q5CPH1
D	-1	ASN	-	expression tag	UNP Q5CPH1
D	0	ALA	-	expression tag	UNP Q5CPH1

- Molecule 2 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	493	Total	C	N	O	S	0	19	0
			4043	2564	675	773	31			

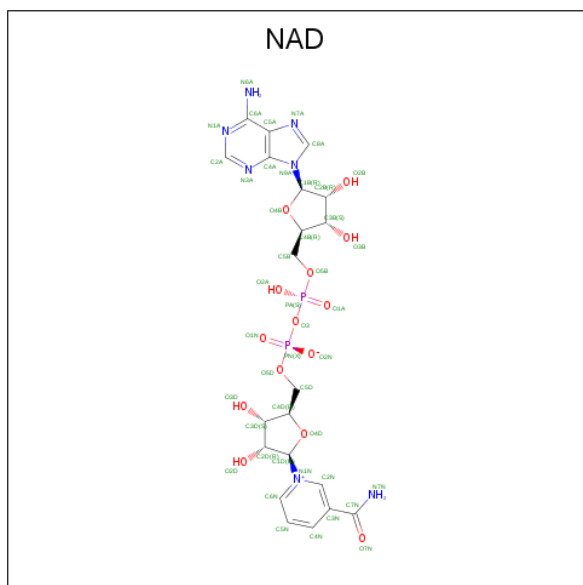
There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

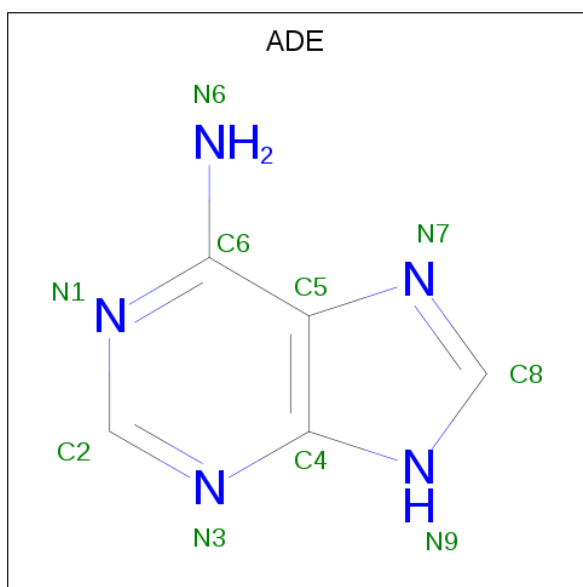
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

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



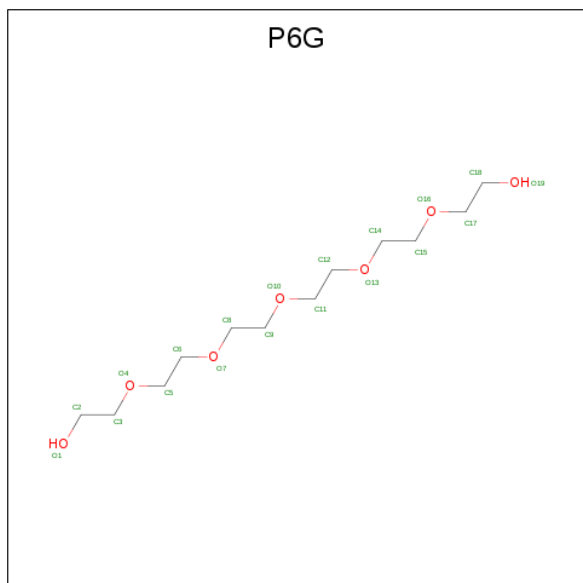
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).



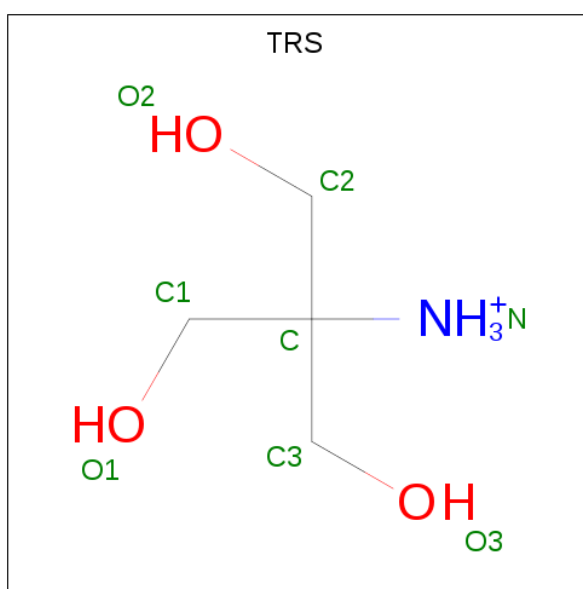
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			10	5	5		
5	B	1	Total	C	N	0	0
			10	5	5		
5	C	1	Total	C	N	0	0
			10	5	5		
5	D	1	Total	C	N	0	0
			10	5	5		

- Molecule 6 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			19	12	7		
6	B	1	Total	C	O	0	0
			19	12	7		
6	C	1	Total	C	O	0	0
			19	12	7		
6	C	1	Total	C	O	0	0
			19	12	7		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



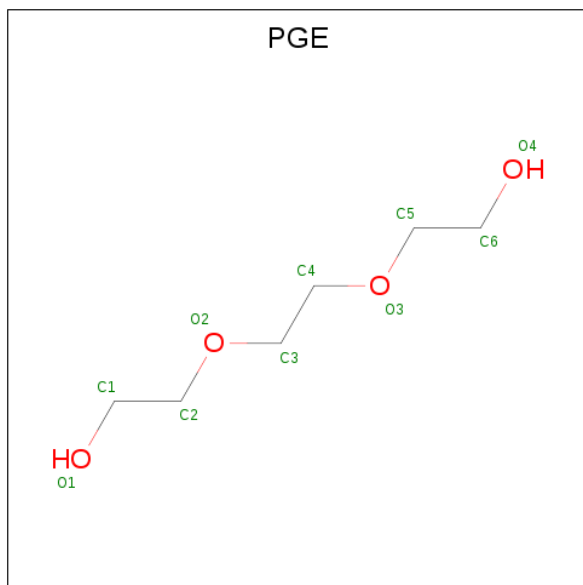
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	466	Total	O	0	28
			486	486		
11	B	468	Total	O	0	23
			481	481		
11	C	508	Total	O	0	23
			523	523		
11	D	483	Total	O	0	19
			493	493		

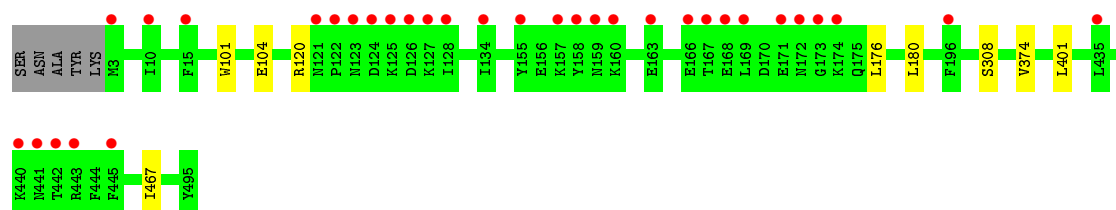
3 Residue-property plots [i](#)

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

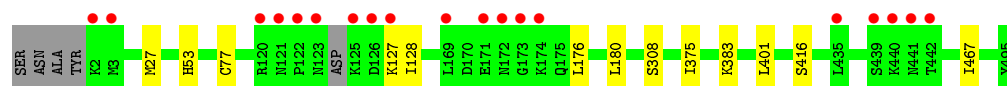
- Molecule 1: Adenosylhomocysteinase



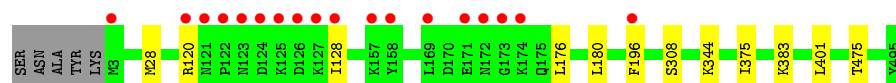
- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase



- Molecule 2: Adenosylhomocysteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.69 Å 182.78 Å 96.25 Å 90.00° 100.58° 90.00°	Depositor
Resolution (Å)	29.92 – 1.95 29.81 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.92-1.95) 100.0 (29.81-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.95 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.141 , 0.173 0.151 , 0.179	Depositor DCC
R_{free} test set	8283 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.6	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	0.97	EDS
Total number of atoms	18512	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: GOL, PGE, NAD, NA, CME, ADE, P6G, TRS, PEG

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	0.45	0/4134	0.69	0/5569
1	B	0.45	0/4100	0.68	0/5528
1	D	0.45	0/4082	0.68	0/5499
2	C	0.46	0/4097	0.70	0/5522
All	All	0.45	0/16413	0.69	0/22118

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	4070	0	4102	8	0
1	B	4035	0	4066	5	0
1	D	4017	0	4060	7	0
2	C	4043	0	4082	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	44	0	26	0	0
4	C	44	0	26	0	0
4	D	44	0	26	0	0
5	A	10	0	4	0	0
5	B	10	0	4	0	0
5	C	10	0	4	0	0
5	D	10	0	4	0	0
6	A	19	0	26	0	0
6	B	19	0	26	0	0
6	C	38	0	52	0	0
7	A	8	0	12	0	0
8	A	6	0	8	0	0
8	B	6	0	8	0	0
9	B	7	0	10	0	0
9	C	14	0	20	0	0
9	D	7	0	10	0	0
10	D	20	0	28	0	0
11	A	486	0	0	1	0
11	B	481	0	0	0	0
11	C	523	0	0	3	0
11	D	493	0	0	0	0
All	All	18512	0	16630	26	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 (26) 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)
2:C:176:LEU:HD22	2:C:180[A]:LEU:HD23	1.81	0.62
1:B:176:LEU:HD22	1:B:180:LEU:HD23	1.82	0.62
1:A:375[A]:ILE:HD11	1:A:383:LYS:HE2	1.87	0.55
2:C:28[B]:MET:HE2	11:C:1103:HOH:O	2.07	0.54
1:B:374[B]:VAL:O	1:B:374[B]:VAL:HG13	2.10	0.51
2:C:344:LYS:NZ	11:C:602:HOH:O	2.35	0.50
1:A:334:LYS:CE	2:C:475[B]:THR:HG22	2.43	0.49
1:D:176:LEU:HD22	1:D:180:LEU:HD23	1.96	0.47
2:C:120:ARG:NH1	2:C:128:ILE:HD11	2.31	0.46
1:A:434[B]:GLU:HB2	11:A:602[B]:HOH:O	2.15	0.46
1:D:127:LYS:HG2	1:D:128:ILE:H	1.80	0.46
2:C:28[B]:MET:CE	11:C:1103:HOH:O	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LEU:HD22	1:A:180:LEU:HD23	2.00	0.44
1:B:467:ILE:HD11	1:D:308[B]:SER:OG	2.18	0.44
1:D:375:ILE:HD11	1:D:383:LYS:HE2	1.99	0.44
1:D:53:HIS:CE1	1:D:77:CYS:SG	3.11	0.43
1:A:467:ILE:HD11	2:C:308[B]:SER:OG	2.19	0.43
2:C:196[B]:PHE:O	2:C:196[B]:PHE:CD2	2.72	0.42
1:A:334:LYS:HE3	2:C:475[B]:THR:HG22	2.01	0.42
2:C:375:ILE:HD11	2:C:383:LYS:HE2	2.01	0.42
1:A:128:ILE:HD12	1:A:128:ILE:C	2.41	0.41
1:B:101:TRP:O	1:B:104:GLU:HG3	2.21	0.40
2:C:180[A]:LEU:HA	2:C:180[A]:LEU:HD12	1.91	0.40
1:B:308[B]:SER:OG	1:D:467:ILE:HD11	2.22	0.40
1:A:274:LEU:HD12	1:A:274:LEU:N	2.36	0.40
1:D:27:MET:HA	1:D:416:SER:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/498 (103%)	493 (96%)	19 (4%)	0	100	100
1	B	509/498 (102%)	494 (97%)	15 (3%)	0	100	100
1	D	504/498 (101%)	491 (97%)	13 (3%)	0	100	100
2	C	509/498 (102%)	495 (97%)	14 (3%)	0	100	100
All	All	2034/1992 (102%)	1973 (97%)	61 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	451/435 (104%)	450 (100%)	1 (0%)	93	93
1	B	449/435 (103%)	447 (100%)	2 (0%)	91	90
1	D	446/435 (102%)	445 (100%)	1 (0%)	93	93
2	C	449/434 (104%)	448 (100%)	1 (0%)	93	93
All	All	1795/1739 (103%)	1790 (100%)	5 (0%)	92	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	401	LEU
1	B	120	ARG
1	B	401	LEU
2	C	401	LEU
1	D	401	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CME	C	129	2	8,9,10	1.08	1 (12%)	5,9,11	2.48	1 (20%)

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	CME	C	129	2	-	2/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	129	CME	CB-SG	-2.20	1.74	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	129	CME	CB-SG-SD	-5.44	89.73	103.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	129	CME	SD-CE-CZ-OH
2	C	129	CME	CE-SD-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
9	PEG	D	506	-	6,6,6	0.43	0	5,5,5	0.25	0
4	NAD	D	502	-	42,48,48	0.86	3 (7%)	50,73,73	1.18	6 (12%)
4	NAD	A	502	-	42,48,48	0.80	2 (4%)	50,73,73	1.23	5 (10%)
4	NAD	B	502	-	42,48,48	0.89	3 (7%)	50,73,73	1.23	4 (8%)
4	NAD	C	502	-	42,48,48	0.87	1 (2%)	50,73,73	1.27	4 (8%)
10	PGE	D	504	-	9,9,9	0.47	0	8,8,8	0.22	0
6	P6G	B	504	-	18,18,18	0.53	0	17,17,17	0.24	0
8	GOL	A	506[A]	-	5,5,5	0.25	0	5,5,5	0.20	0
6	P6G	A	504	-	18,18,18	0.53	0	17,17,17	0.31	0
5	ADE	C	503	-	9,11,11	1.09	1 (11%)	7,15,15	2.07	2 (28%)
5	ADE	A	503	-	9,11,11	1.12	0	7,15,15	1.98	2 (28%)
5	ADE	D	503	-	9,11,11	1.24	2 (22%)	7,15,15	1.98	2 (28%)
5	ADE	B	503	-	9,11,11	1.18	1 (11%)	7,15,15	2.14	2 (28%)
7	TRS	A	505	-	7,7,7	0.32	0	9,9,9	0.19	0
6	P6G	C	505	-	18,18,18	0.51	0	17,17,17	0.21	0
9	PEG	C	506	-	6,6,6	0.42	0	5,5,5	0.35	0
9	PEG	C	507	-	6,6,6	0.50	0	5,5,5	0.22	0
9	PEG	B	505	-	6,6,6	0.44	0	5,5,5	0.19	0
8	GOL	B	506[A]	-	5,5,5	0.23	0	5,5,5	0.26	0
6	P6G	C	504	-	18,18,18	0.52	0	17,17,17	0.14	0
10	PGE	D	505	-	9,9,9	0.49	0	8,8,8	0.20	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
9	PEG	D	506	-	-	3/4/4/4	-
4	NAD	D	502	-	-	5/26/62/62	0/5/5/5
4	NAD	A	502	-	-	5/26/62/62	0/5/5/5
4	NAD	B	502	-	-	5/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	C	502	-	-	5/26/62/62	0/5/5/5
10	PGE	D	504	-	-	2/7/7/7	-
6	P6G	B	504	-	-	3/16/16/16	-
8	GOL	A	506[A]	-	-	0/4/4/4	-
5	ADE	D	503	-	-	-	0/2/2/2
6	P6G	A	504	-	-	9/16/16/16	-
5	ADE	C	503	-	-	-	0/2/2/2
5	ADE	A	503	-	-	-	0/2/2/2
7	TRS	A	505	-	-	4/9/9/9	-
10	PGE	D	505	-	-	3/7/7/7	-
6	P6G	C	505	-	-	5/16/16/16	-
9	PEG	C	506	-	-	1/4/4/4	-
9	PEG	C	507	-	-	3/4/4/4	-
9	PEG	B	505	-	-	2/4/4/4	-
8	GOL	B	506[A]	-	-	2/4/4/4	-
6	P6G	C	504	-	-	5/16/16/16	-
5	ADE	B	503	-	-	-	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	NAD	O4D-C1D	3.18	1.45	1.41
4	B	502	NAD	O4D-C1D	2.73	1.44	1.41
4	D	502	NAD	O4D-C1D	2.40	1.44	1.41
4	A	502	NAD	C5A-C4A	2.39	1.47	1.40
4	D	502	NAD	C5A-C4A	2.28	1.47	1.40
4	B	502	NAD	C2A-N3A	2.21	1.35	1.32
5	D	503	ADE	C2-N3	2.18	1.35	1.32
4	B	502	NAD	C5A-C4A	2.16	1.46	1.40
5	B	503	ADE	C5-C4	2.14	1.46	1.40
4	D	502	NAD	C2A-N3A	2.12	1.35	1.32
5	D	503	ADE	C5-C4	2.09	1.46	1.40
5	C	503	ADE	C5-C4	2.07	1.46	1.40
4	A	502	NAD	O4D-C1D	2.01	1.43	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	NAD	N3A-C2A-N1A	-3.90	122.58	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	503	ADE	C2-N3-C4	3.74	122.21	113.45
5	B	503	ADE	C2-N3-C4	3.71	122.13	113.45
5	B	503	ADE	N3-C2-N1	-3.70	122.89	128.68
4	A	502	NAD	N3A-C2A-N1A	-3.67	122.95	128.68
4	B	502	NAD	N3A-C2A-N1A	-3.63	123.00	128.68
5	C	503	ADE	N3-C2-N1	-3.50	123.21	128.68
5	D	503	ADE	C2-N3-C4	3.47	121.58	113.45
5	A	503	ADE	C2-N3-C4	3.47	121.57	113.45
4	D	502	NAD	N3A-C2A-N1A	-3.44	123.30	128.68
5	A	503	ADE	N3-C2-N1	-3.42	123.34	128.68
5	D	503	ADE	N3-C2-N1	-3.30	123.52	128.68
4	A	502	NAD	C3N-C7N-N7N	2.93	121.26	117.75
4	C	502	NAD	C1B-N9A-C4A	-2.91	121.53	126.64
4	B	502	NAD	PN-O3-PA	-2.89	122.89	132.83
4	C	502	NAD	C3N-C7N-N7N	2.88	121.21	117.75
4	A	502	NAD	PN-O3-PA	-2.81	123.19	132.83
4	C	502	NAD	PN-O3-PA	-2.73	123.45	132.83
4	D	502	NAD	PN-O3-PA	-2.61	123.86	132.83
4	B	502	NAD	C1B-N9A-C4A	-2.53	122.20	126.64
4	B	502	NAD	C3N-C7N-N7N	2.52	120.77	117.75
4	D	502	NAD	C3N-C7N-N7N	2.47	120.71	117.75
4	D	502	NAD	C1B-N9A-C4A	-2.38	122.46	126.64
4	D	502	NAD	C4A-C5A-N7A	-2.30	107.01	109.40
4	D	502	NAD	C2N-N1N-C1D	-2.14	114.37	119.14
4	A	502	NAD	C1B-N9A-C4A	-2.10	122.96	126.64
4	A	502	NAD	C4A-C5A-N7A	-2.09	107.22	109.40

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	502	NAD	O4D-C1D-N1N-C2N
4	D	502	NAD	O4D-C1D-N1N-C6N
4	D	502	NAD	C2D-C1D-N1N-C2N
4	D	502	NAD	C2D-C1D-N1N-C6N
4	A	502	NAD	O4D-C1D-N1N-C2N
4	A	502	NAD	O4D-C1D-N1N-C6N
4	A	502	NAD	C2D-C1D-N1N-C2N
4	A	502	NAD	C2D-C1D-N1N-C6N
8	B	506[A]	GOL	C1-C2-C3-O3
8	B	506[A]	GOL	O2-C2-C3-O3
4	B	502	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
4	B	502	NAD	O4D-C1D-N1N-C6N
4	B	502	NAD	C2D-C1D-N1N-C2N
4	B	502	NAD	C2D-C1D-N1N-C6N
7	A	505	TRS	N-C-C1-O1
4	C	502	NAD	O4D-C1D-N1N-C2N
4	C	502	NAD	O4D-C1D-N1N-C6N
4	C	502	NAD	C2D-C1D-N1N-C2N
4	C	502	NAD	C2D-C1D-N1N-C6N
10	D	505	PGE	O2-C3-C4-O3
6	C	504	P6G	O4-C5-C6-O7
6	A	504	P6G	O10-C11-C12-O13
6	B	504	P6G	O13-C14-C15-O16
6	B	504	P6G	O16-C17-C18-O19
6	C	504	P6G	O16-C17-C18-O19
9	D	506	PEG	O2-C3-C4-O4
6	C	505	P6G	O16-C17-C18-O19
6	C	505	P6G	O7-C8-C9-O10
10	D	504	PGE	O3-C5-C6-O4
10	D	505	PGE	O1-C1-C2-O2
10	D	505	PGE	O3-C5-C6-O4
6	A	504	P6G	O7-C8-C9-O10
9	D	506	PEG	O1-C1-C2-O2
9	B	505	PEG	O1-C1-C2-O2
6	A	504	P6G	O16-C17-C18-O19
9	C	507	PEG	O2-C3-C4-O4
6	C	504	P6G	O1-C2-C3-O4
6	B	504	P6G	O10-C11-C12-O13
6	C	505	P6G	O10-C11-C12-O13
9	B	505	PEG	O2-C3-C4-O4
10	D	504	PGE	C4-C3-O2-C2
6	C	504	P6G	C2-C3-O4-C5
7	A	505	TRS	C1-C-C2-O2
7	A	505	TRS	C3-C-C2-O2
6	A	504	P6G	C14-C15-O16-C17
9	C	506	PEG	O2-C3-C4-O4
6	C	505	P6G	C15-C14-O13-C12
6	A	504	P6G	C5-C6-O7-C8
6	A	504	P6G	O1-C2-C3-O4
6	C	505	P6G	O4-C5-C6-O7
4	A	502	NAD	O4B-C4B-C5B-O5B
9	C	507	PEG	C4-C3-O2-C2
6	A	504	P6G	C11-C12-O13-C14

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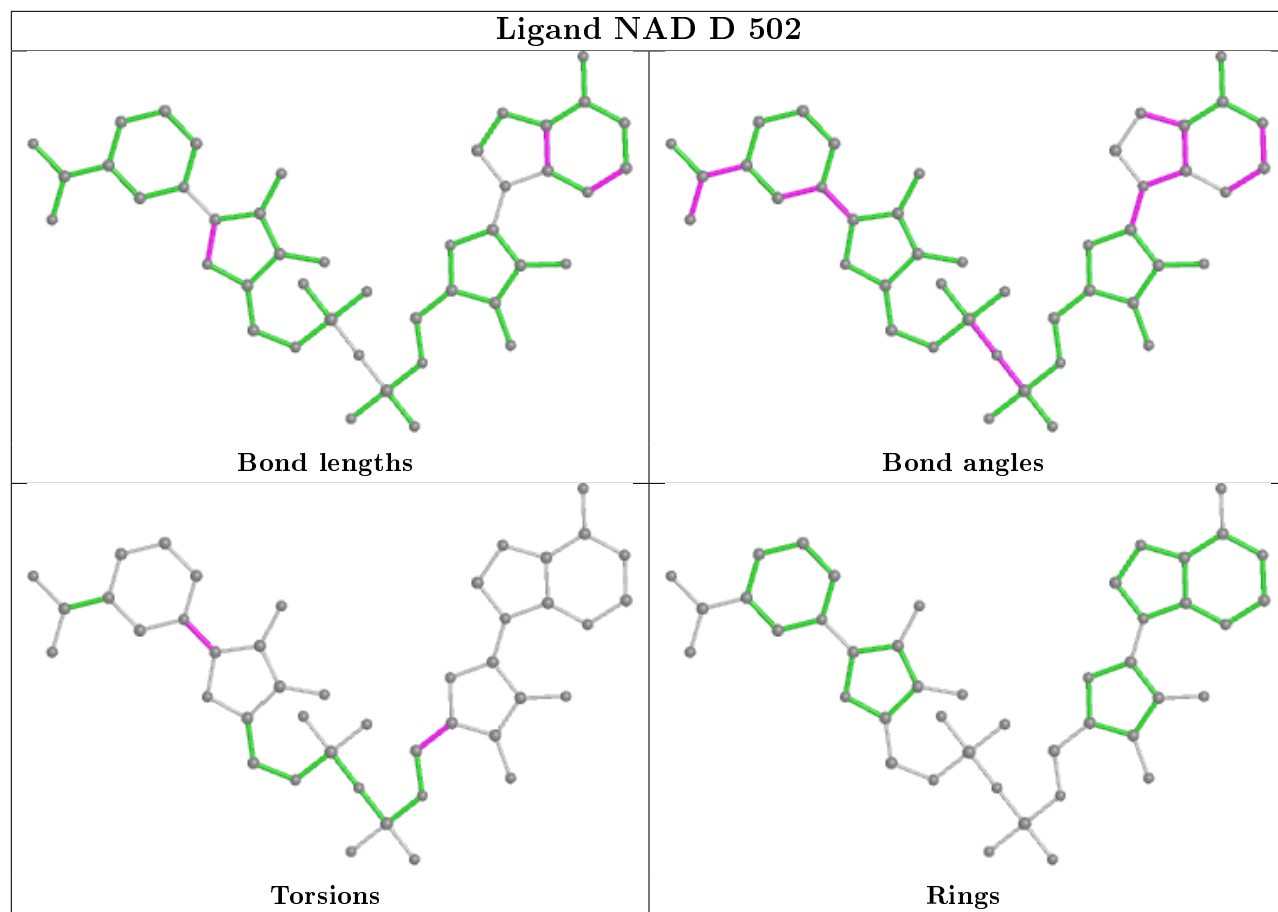
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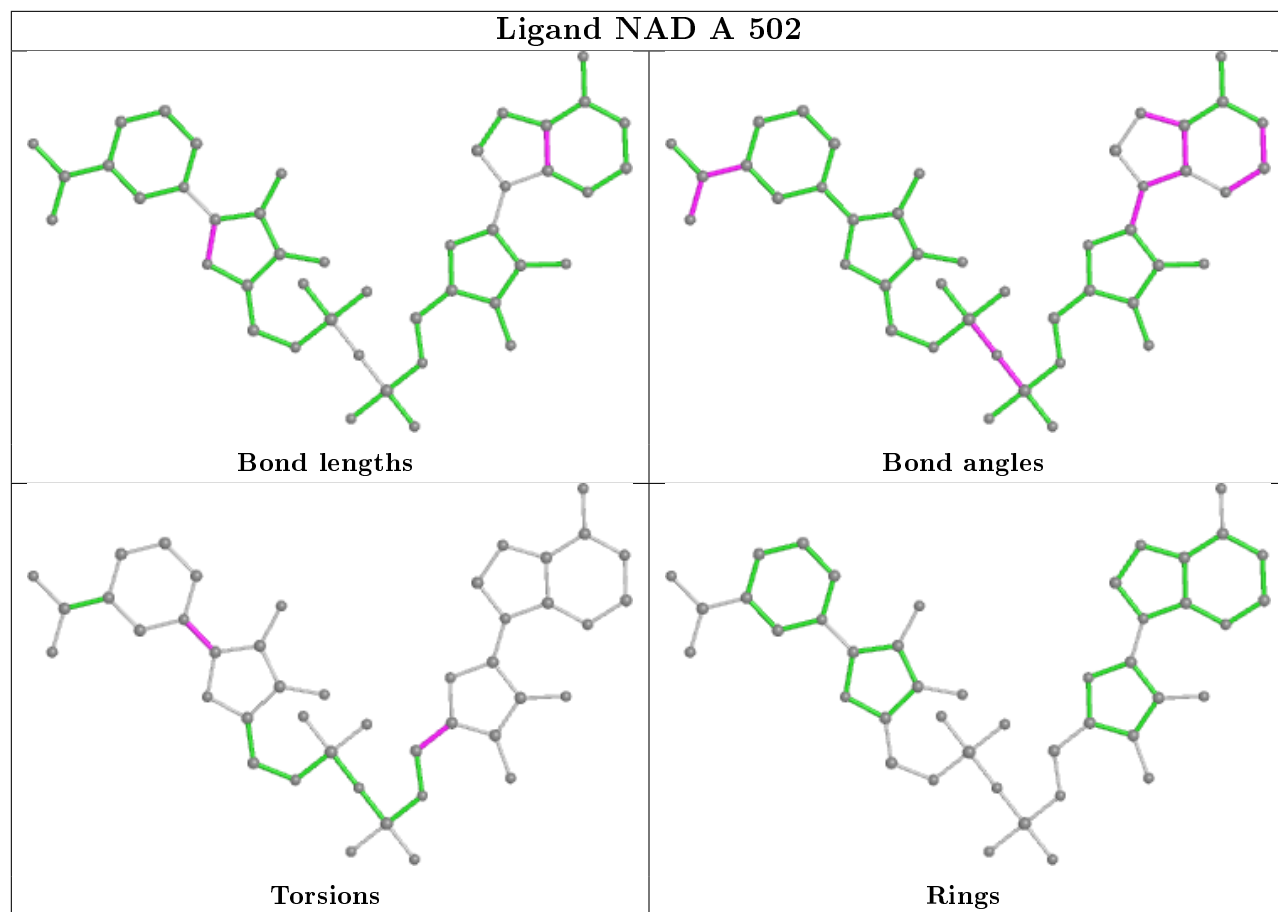
Mol	Chain	Res	Type	Atoms
4	D	502	NAD	O4B-C4B-C5B-O5B
6	A	504	P6G	C15-C14-O13-C12
6	A	504	P6G	C18-C17-O16-C15
4	B	502	NAD	O4B-C4B-C5B-O5B
9	D	506	PEG	C1-C2-O2-C3
7	A	505	TRS	N-C-C2-O2
4	C	502	NAD	O4B-C4B-C5B-O5B
9	C	507	PEG	O1-C1-C2-O2
6	C	504	P6G	O13-C14-C15-O16

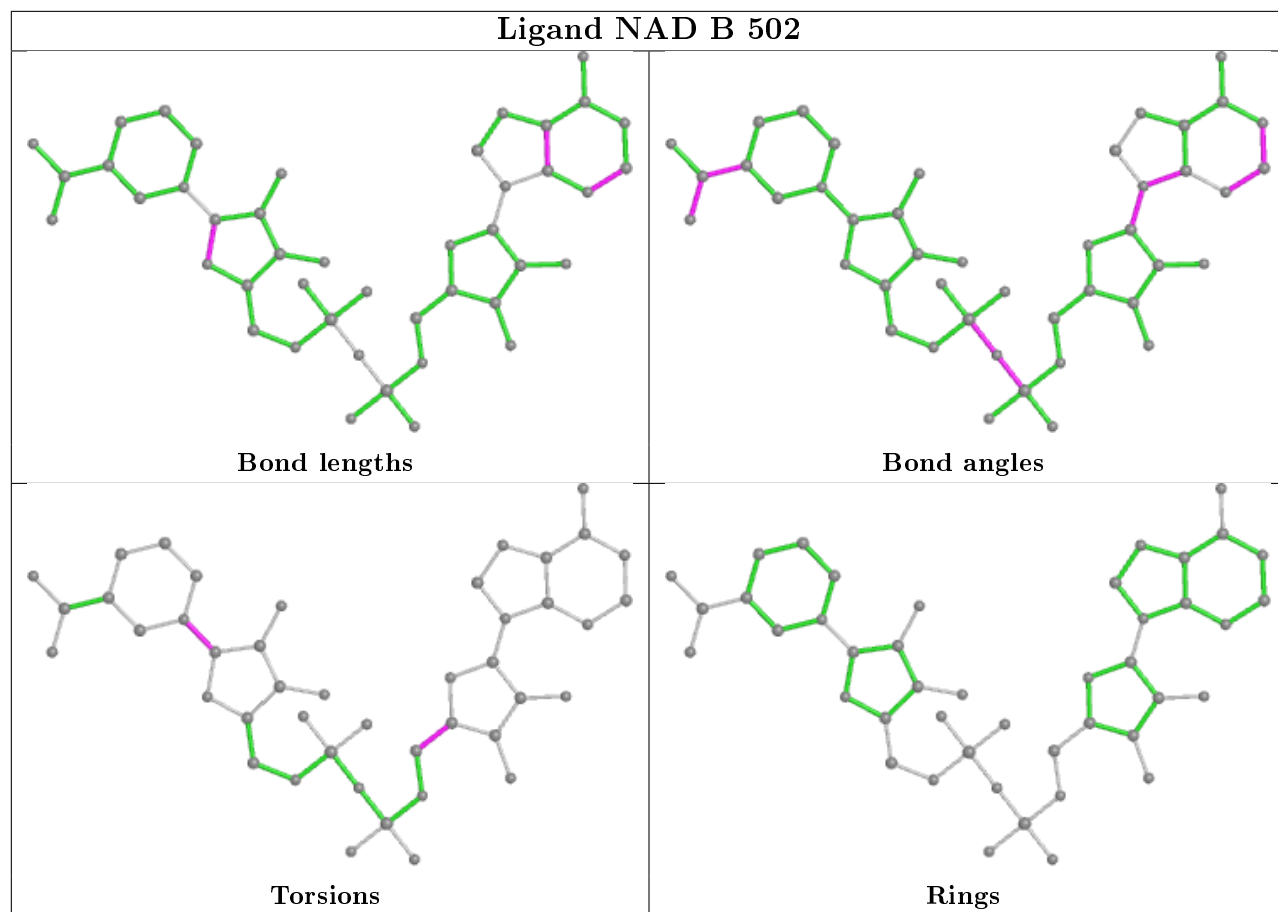
There are no ring outliers.

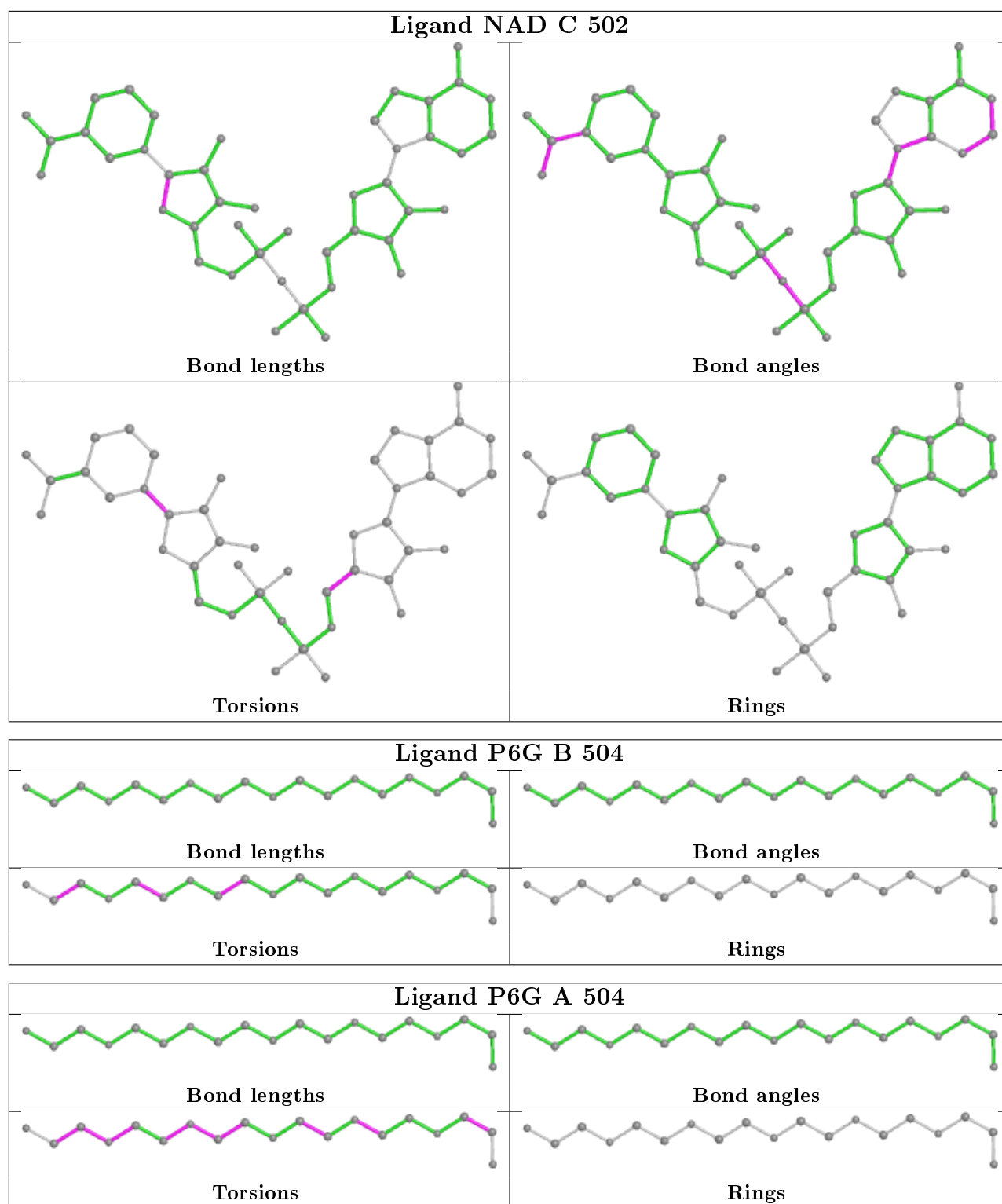
No monomer is involved in short contacts.

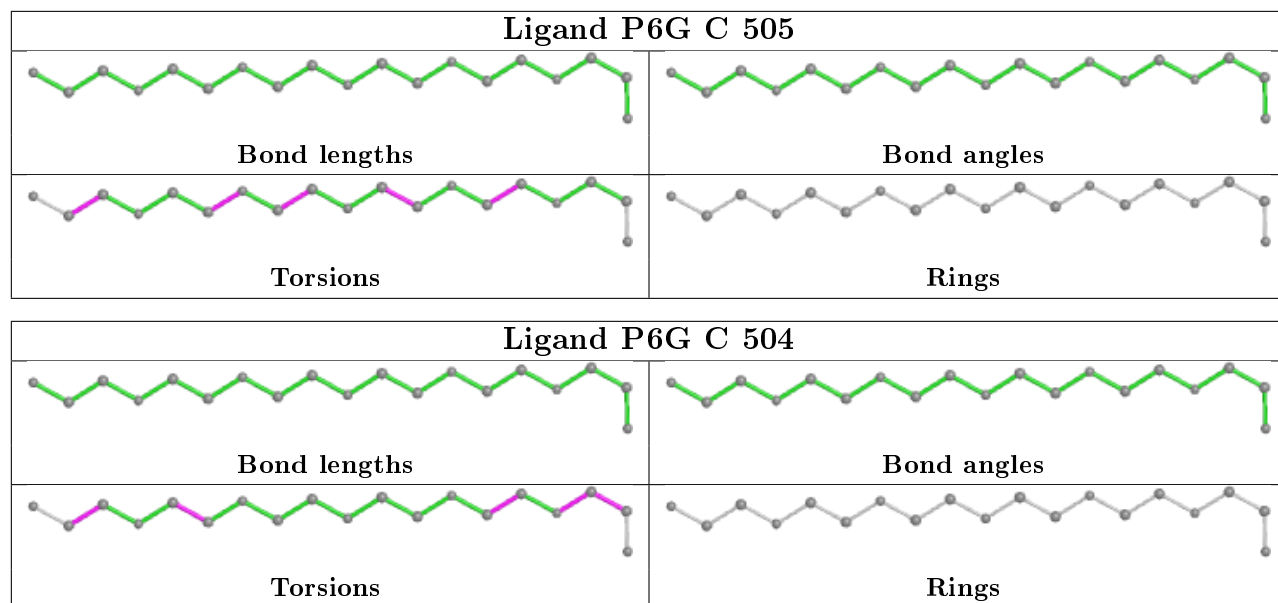
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	491/498 (98%)	-0.22	20 (4%) 37 46	19, 28, 57, 109	0
1	B	493/498 (98%)	-0.06	33 (6%) 17 26	18, 29, 70, 121	0
1	D	493/498 (98%)	-0.30	19 (3%) 39 49	18, 28, 57, 121	0
2	C	492/498 (98%)	-0.30	18 (3%) 41 51	16, 26, 56, 97	0
All	All	1969/1992 (98%)	-0.22	90 (4%) 32 42	16, 28, 61, 121	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	PRO	9.4
1	D	125	LYS	9.2
1	B	123	ASN	7.4
1	B	158	TYR	6.6
1	A	125	LYS	6.6
1	A	3	MET	6.4
2	C	123	ASN	6.4
1	A	126	ASP	6.4
1	B	441	ASN	6.2
2	C	122	PRO	6.0
2	C	3	MET	5.9
1	D	123	ASN	5.8
1	A	172	ASN	5.7
1	A	441	ASN	5.4
1	D	172	ASN	5.4
1	D	441	ASN	5.4
1	B	125	LYS	5.1
1	D	121	ASN	4.8
1	D	3	MET	4.5
1	A	440	LYS	4.5
1	D	126	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	124	ASP	4.3
1	B	121	ASN	4.2
1	A	158	TYR	4.1
1	D	127	LYS	4.1
1	D	174	LYS	4.0
1	D	122	PRO	3.9
1	B	126	ASP	3.9
1	D	439	SER	3.8
2	C	196[A]	PHE	3.8
1	A	439	SER	3.8
1	A	127	LYS	3.8
1	A	443	ARG	3.8
1	B	445	PHE	3.7
1	B	163	GLU	3.7
1	B	3	MET	3.6
2	C	158	TYR	3.5
2	C	125	LYS	3.4
2	C	172	ASN	3.4
1	B	169	LEU	3.4
1	A	173	GLY	3.4
2	C	126	ASP	3.4
1	D	171	GLU	3.3
2	C	120	ARG	3.2
1	A	196[A]	PHE	3.2
1	B	440	LYS	3.2
1	B	196	PHE	3.2
1	B	124	ASP	3.1
1	B	168	GLU	3.1
2	C	173	GLY	3.1
1	B	171	GLU	3.1
1	A	174	LYS	3.0
1	D	440	LYS	3.0
2	C	127	LYS	3.0
1	B	127	LYS	2.9
1	B	166	GLU	2.8
2	C	171	GLU	2.8
1	B	159	ASN	2.8
2	C	121	ASN	2.8
1	B	443	ARG	2.8
1	D	442	THR	2.7
2	C	128	ILE	2.7
2	C	169	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	10	ILE	2.7
1	B	155	TYR	2.7
1	B	167	THR	2.7
2	C	174	LYS	2.7
1	B	134	ILE	2.6
1	D	173	GLY	2.6
1	B	442	THR	2.6
1	D	435	LEU	2.5
1	B	173	GLY	2.5
1	D	2	LYS	2.5
1	B	160	LYS	2.5
1	D	120	ARG	2.5
1	A	171	GLU	2.4
1	A	437	ASP	2.3
1	B	174	LYS	2.3
1	A	442	THR	2.3
1	B	435	LEU	2.2
1	B	157	LYS	2.2
1	D	169	LEU	2.2
2	C	124	ASP	2.2
1	A	224	SER	2.1
1	B	172	ASN	2.1
1	B	15[A]	PHE	2.1
2	C	157	LYS	2.1
1	B	128	ILE	2.0
1	A	434[A]	GLU	2.0
1	A	121	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	CME	C	129	10/11	0.87	0.17	39,54,71,71	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

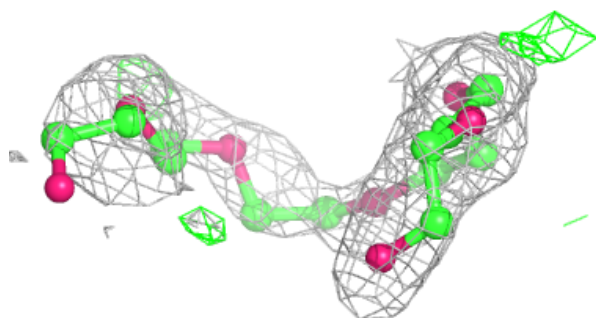
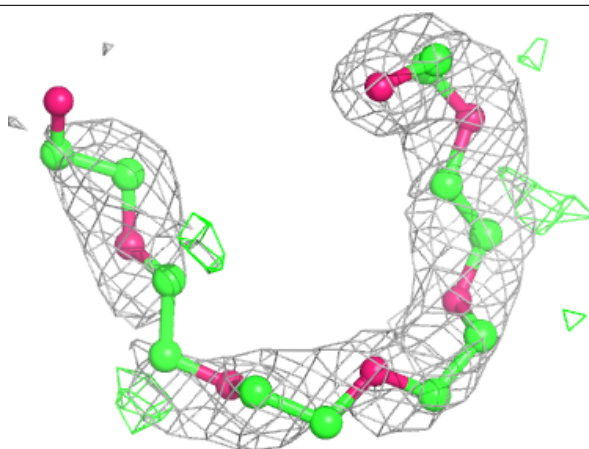
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	P6G	C	504	19/19	0.65	0.24	59,75,93,93	0
6	P6G	C	505	19/19	0.73	0.25	71,77,86,86	0
6	P6G	A	504	19/19	0.75	0.32	53,72,81,83	0
9	PEG	C	507	7/7	0.75	0.19	68,69,71,72	0
6	P6G	B	504	19/19	0.77	0.24	52,69,81,81	0
10	PGE	D	504	10/10	0.78	0.20	58,62,65,66	0
7	TRS	A	505	8/8	0.79	0.26	67,73,74,77	0
9	PEG	D	506	7/7	0.81	0.14	63,64,66,66	0
8	GOL	B	506[A]	6/6	0.82	0.39	39,40,41,42	6
8	GOL	A	506[A]	6/6	0.83	0.22	45,47,49,50	6
3	NA	D	501	1/1	0.84	0.17	39,39,39,39	0
9	PEG	C	506	7/7	0.87	0.11	54,56,59,62	0
9	PEG	B	505	7/7	0.88	0.11	65,66,68,73	0
10	PGE	D	505	10/10	0.88	0.23	53,64,74,75	0
3	NA	A	501	1/1	0.91	0.09	28,28,28,28	0
3	NA	B	501	1/1	0.92	0.09	26,26,26,26	0
3	NA	C	501	1/1	0.94	0.09	28,28,28,28	0
5	ADE	B	503	10/10	0.96	0.07	23,24,25,25	0
5	ADE	A	503	10/10	0.97	0.09	23,23,24,24	0
5	ADE	C	503	10/10	0.98	0.07	19,20,21,21	0
5	ADE	D	503	10/10	0.98	0.07	25,25,26,27	0
4	NAD	D	502	44/44	0.98	0.08	18,21,22,23	0
4	NAD	C	502	44/44	0.99	0.07	15,17,19,20	0
4	NAD	B	502	44/44	0.99	0.07	19,21,22,23	0
4	NAD	A	502	44/44	0.99	0.07	19,21,24,25	0

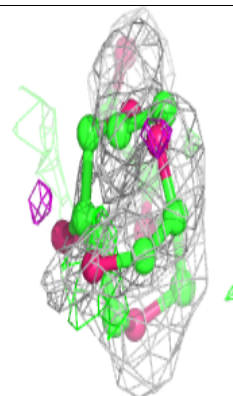
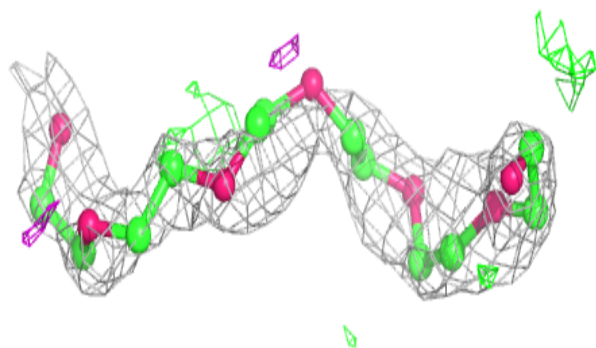
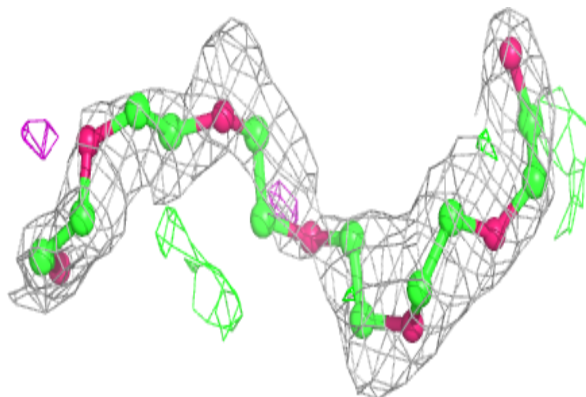
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G C 504:

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

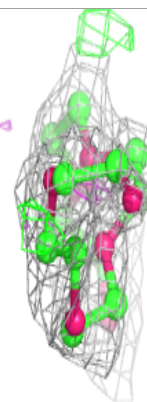
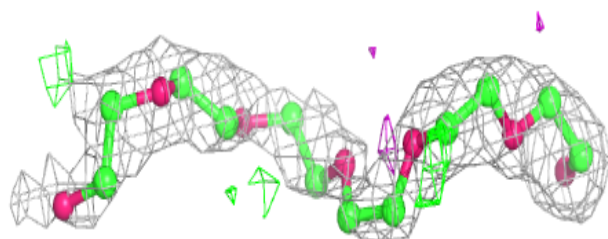
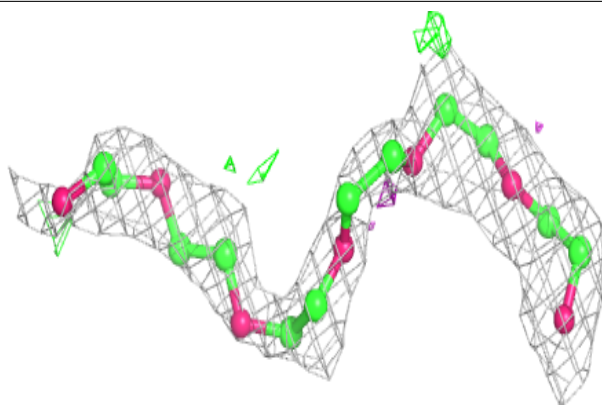
**Electron density around P6G C 505:**

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



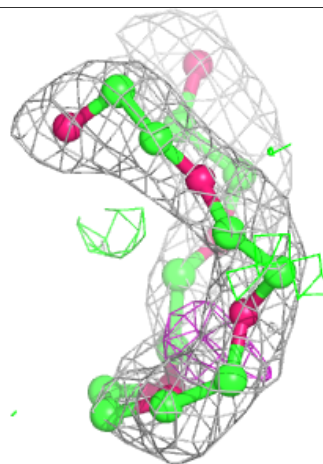
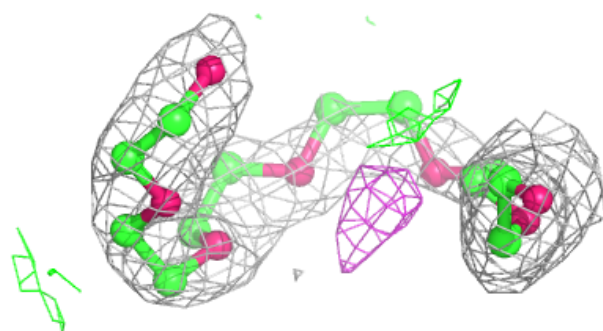
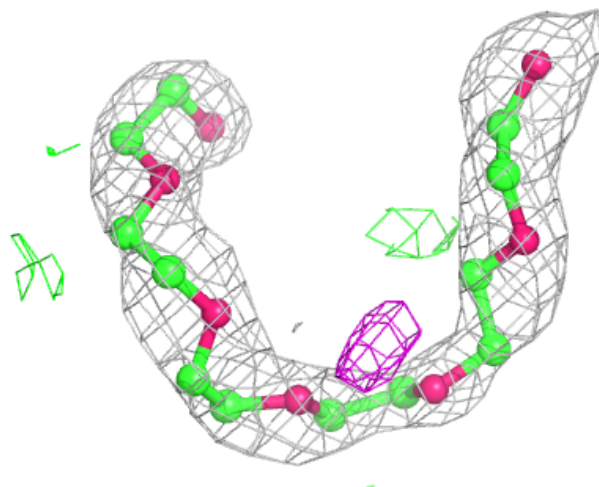
Electron density around P6G A 504:

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



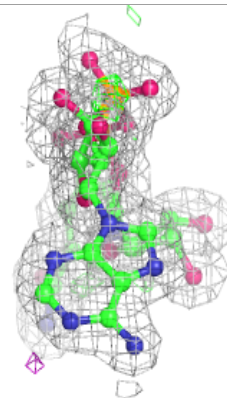
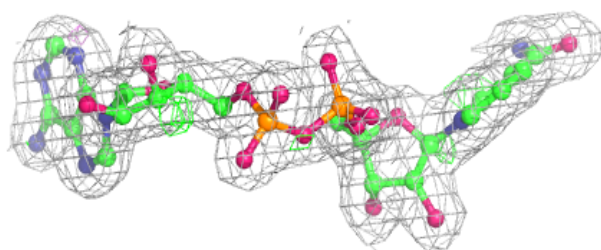
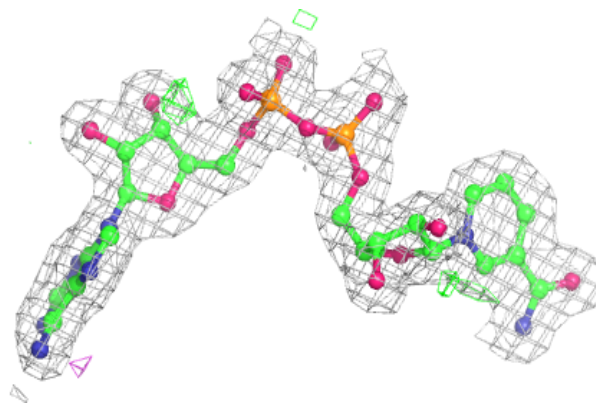
Electron density around P6G B 504:

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

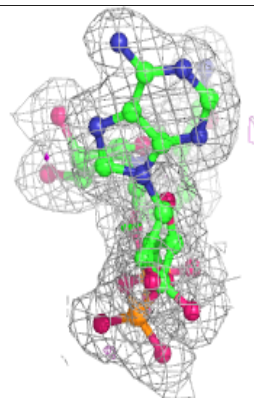
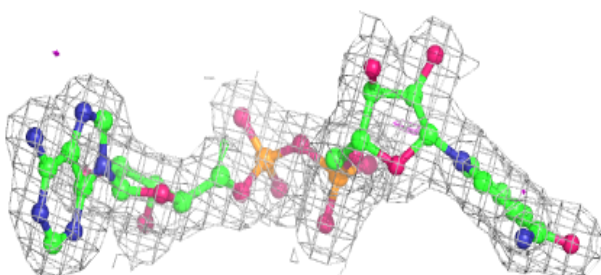
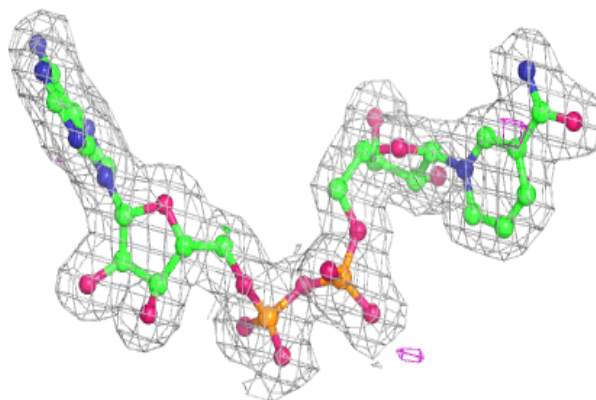


Electron density around NAD D 502:

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

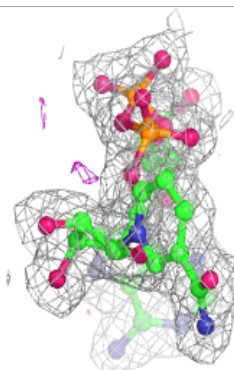
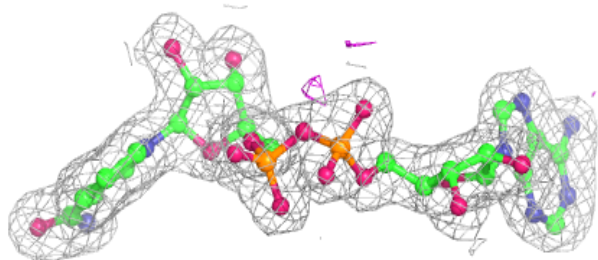
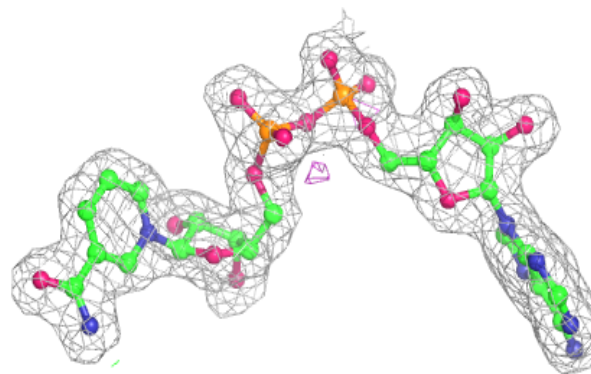
**Electron density around NAD C 502:**

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

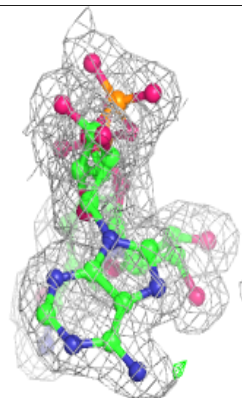
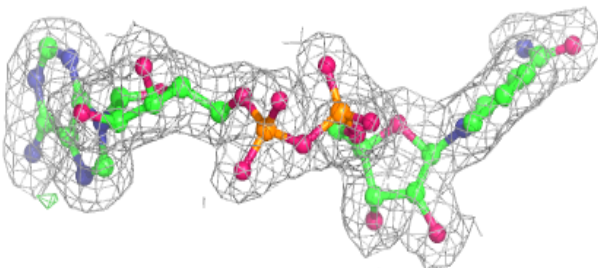
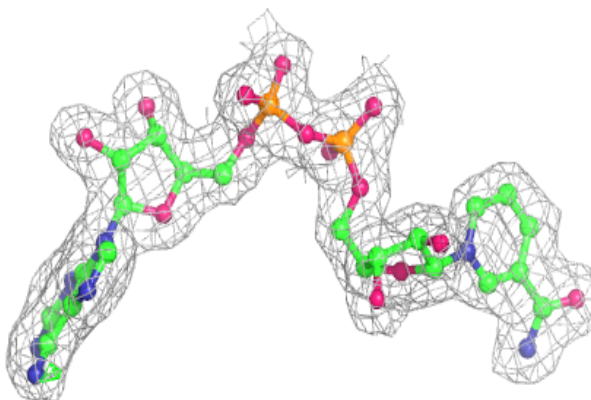


Electron density around NAD B 502:

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

**Electron density around NAD A 502:**

$2mF_o-DF_c$ (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.