



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 03:31 pm GMT

PDB ID : 8CFM
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *P. aeruginosa* in complex with F2X-Entry library fragment E08
Authors : Malecki, P.H.; Gawel, M.; Stepniewska, M.; Brzezinski, K.
Deposited on : 2023-02-03
Resolution : 1.84 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

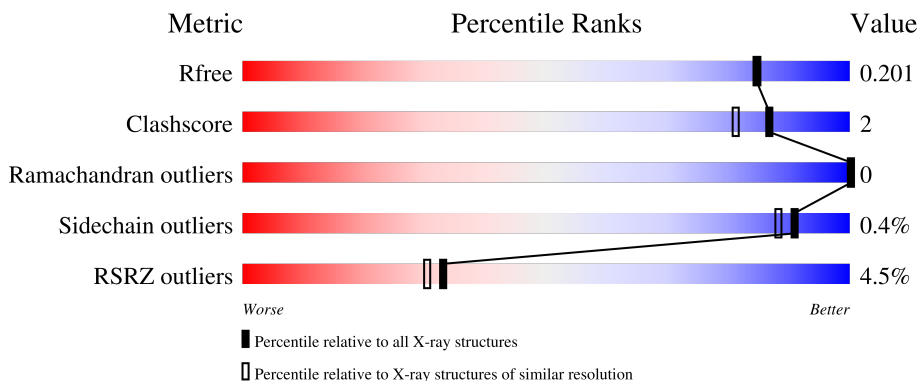
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

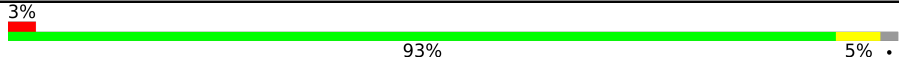
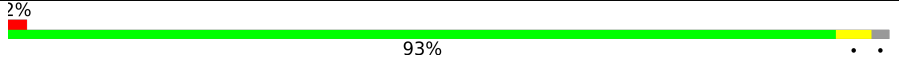
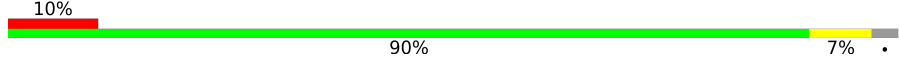
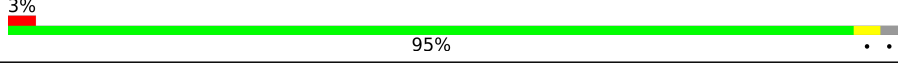
The reported resolution of this entry is 1.84 Å.

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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	472	
1	B	472	
1	C	472	
1	D	472	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 16246 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
			Total	C	N	O	S			
1	A	464	3608	2273	625	687	23	0	5	0
1	B	461	3591	2265	623	681	22	0	6	0
1	C	460	3588	2262	620	683	23	0	6	0
1	D	462	3596	2266	623	684	23	0	6	0

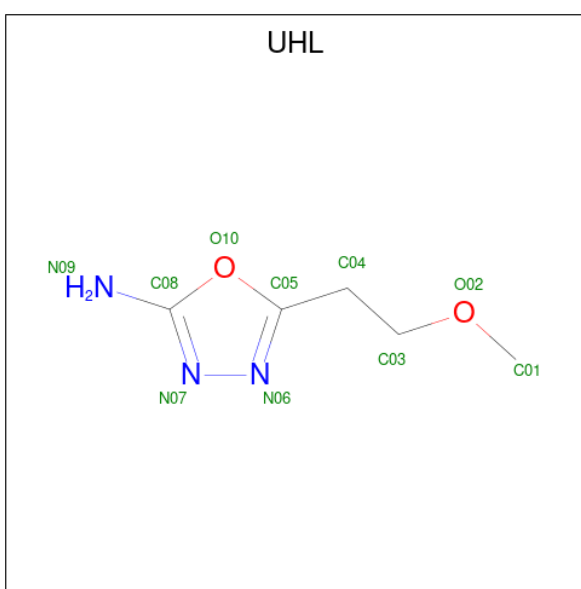
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9I685
A	-1	ASN	-	expression tag	UNP Q9I685
A	0	ALA	-	expression tag	UNP Q9I685
B	-2	SER	-	expression tag	UNP Q9I685
B	-1	ASN	-	expression tag	UNP Q9I685
B	0	ALA	-	expression tag	UNP Q9I685
C	-2	SER	-	expression tag	UNP Q9I685
C	-1	ASN	-	expression tag	UNP Q9I685
C	0	ALA	-	expression tag	UNP Q9I685
D	-2	SER	-	expression tag	UNP Q9I685
D	-1	ASN	-	expression tag	UNP Q9I685
D	0	ALA	-	expression tag	UNP Q9I685

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

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

- Molecule 4 is 5-(2-methoxyethyl)-1,3,4-oxadiazol-2-amine (three-letter code: UHL) (formula: C₅H₉N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 10 5 3 2	0	0
4	C	1	Total C N O 10 5 3 2	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total K 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



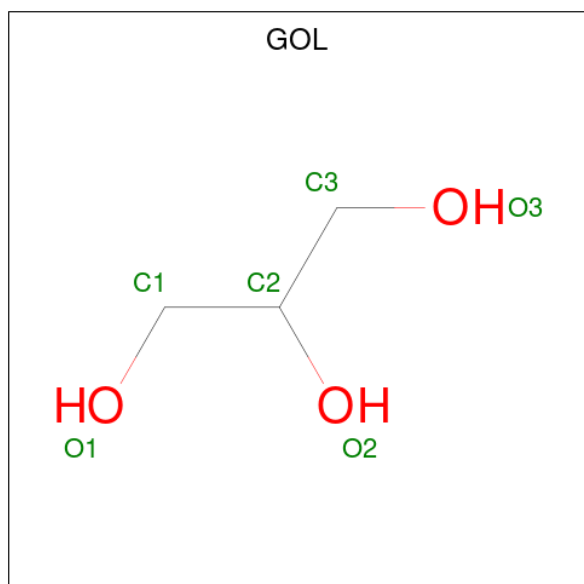
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

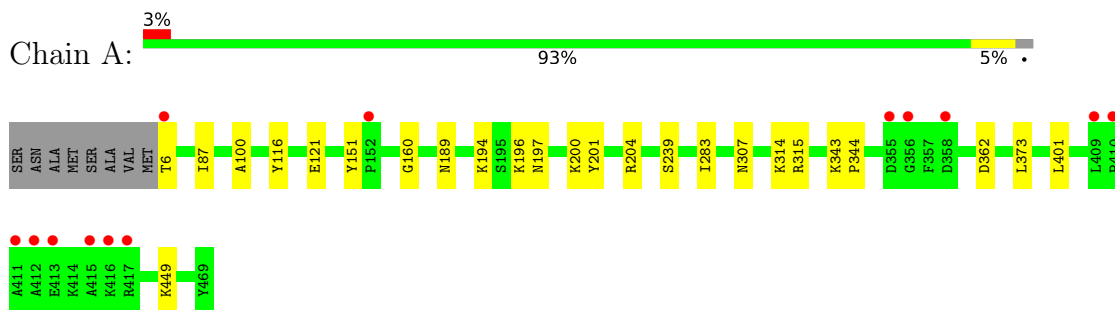
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	370	384	384	0	16
9	B	394	412	412	0	20
9	C	320	328	328	0	11
9	D	383	391	391	0	13

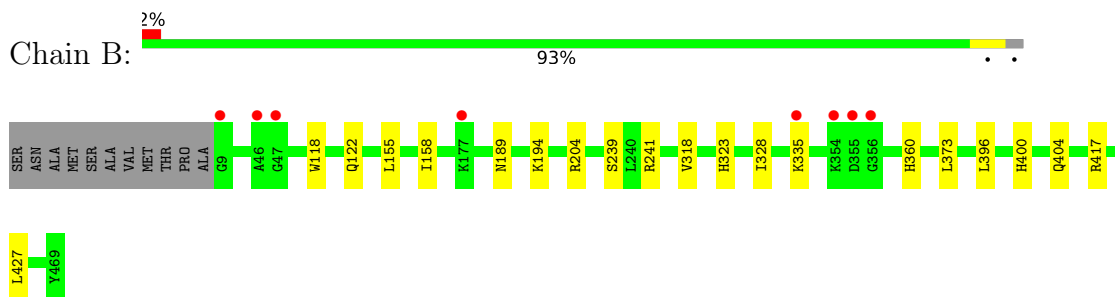
3 Residue-property plots [i](#)

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.

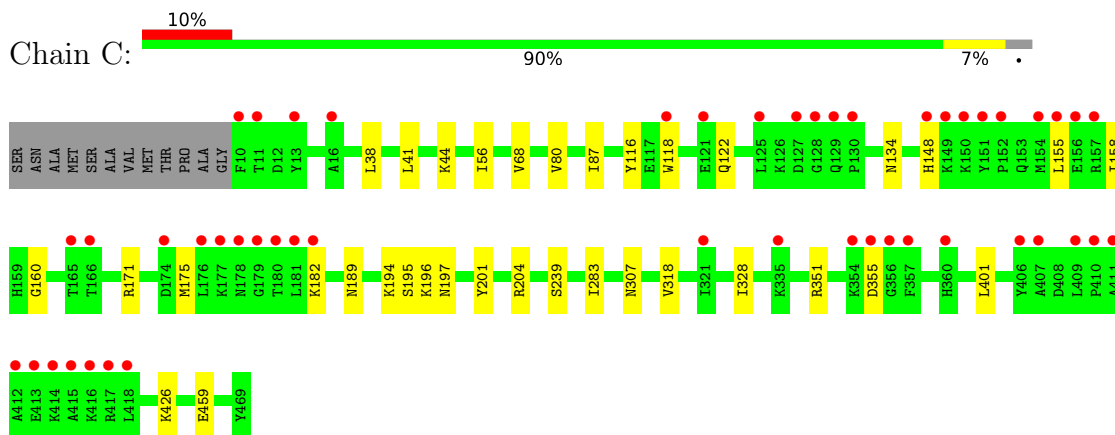
- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase

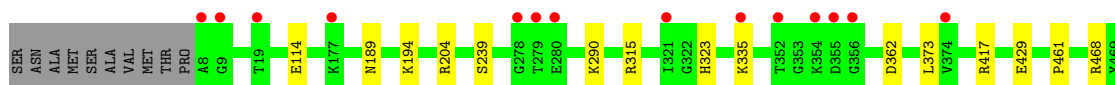


- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase

Chain D:  3% 95%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.05Å 133.22Å 98.28Å 90.00° 100.94° 90.00°	Depositor
Resolution (Å)	36.37 – 1.84 36.37 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.0 (36.37-1.84) 98.0 (36.37-1.84)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.84Å)	Xtrriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.167 , 0.201 0.167 , 0.201	Depositor DCC
R_{free} test set	2101 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtrriage
Anisotropy	0.252	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16246	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, UHL, PO4, ADE, NAD, GOL, K

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	0.28	0/3678	0.50	0/4973
1	B	0.28	0/3669	0.51	0/4958
1	C	0.27	0/3663	0.49	0/4951
1	D	0.28	0/3668	0.50	0/4957
All	All	0.28	0/14678	0.50	0/19839

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	3608	0	3614	16	0
1	B	3591	0	3613	11	0
1	C	3588	0	3599	24	0
1	D	3596	0	3605	9	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	2	0
3	A	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	10	0	0	1	0
4	C	10	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	25	0	0	2	0
6	B	15	0	0	0	0
6	C	20	0	0	1	0
6	D	20	0	0	0	0
7	B	18	0	24	0	0
7	D	6	0	8	0	0
8	D	4	0	6	0	0
9	A	384	0	0	0	0
9	B	412	0	0	1	0
9	C	328	0	0	1	0
9	D	391	0	0	0	0
All	All	16246	0	14589	61	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 2.

All (61) 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:189:ASN:HA	1:C:194:LYS:HD2	1.71	0.71
1:B:189:ASN:HA	1:B:194:LYS:HD2	1.76	0.68
1:A:189:ASN:HA	1:A:194:LYS:HD2	1.77	0.67
1:B:396:LEU:HD13	1:B:427:LEU:HD22	1.86	0.57
1:C:197:ASN:HA	1:C:201:TYR:HD2	1.70	0.57
1:C:351:ARG:NH2	6:C:505:PO4:O1	2.41	0.54
1:C:155:LEU:HD23	1:C:158:ILE:HD12	1.90	0.53
1:A:160:GLY:HA3	1:A:401:LEU:HD13	1.90	0.53
1:A:6:THR:N	1:A:100:ALA:O	2.43	0.52
1:B:204[B]:ARG:HA	1:B:239:SER:HB2	1.91	0.51
1:D:204[B]:ARG:HA	1:D:239:SER:HB2	1.93	0.51
1:D:189:ASN:HA	1:D:194:LYS:HD2	1.91	0.51
1:D:204[A]:ARG:HA	1:D:239:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204[B]:ARG:HA	1:A:239:SER:HB2	1.93	0.50
1:B:155:LEU:HD23	1:B:158:ILE:HD12	1.92	0.50
1:B:204[A]:ARG:HA	1:B:239:SER:HB2	1.92	0.50
1:A:204[A]:ARG:HA	1:A:239:SER:HB2	1.94	0.49
1:C:148:HIS:CD2	1:C:182:LYS:HG2	2.47	0.49
1:C:196:LYS:HE3	9:C:669:HOH:O	2.12	0.49
1:C:197:ASN:HA	1:C:201:TYR:CD2	2.48	0.49
1:A:283:ILE:HG13	1:A:307:ASN:HB3	1.96	0.47
1:A:197:ASN:HA	1:A:201:TYR:HD2	1.78	0.47
1:D:373:LEU:HD22	2:D:502:NAD:N7N	2.30	0.47
1:C:160:GLY:HA3	1:C:401:LEU:HD13	1.97	0.47
1:C:196:LYS:HG2	4:C:501:UHL:N09	2.30	0.46
1:C:189:ASN:O	1:C:195:SER:HB3	2.16	0.46
1:C:56:ILE:HB	1:C:80:VAL:HG12	1.98	0.46
1:D:290:LYS:HB2	1:D:290:LYS:HE3	1.79	0.46
1:C:118:TRP:O	1:C:122:GLN:HG2	2.17	0.45
1:A:121:GLU:OE1	1:A:151:TYR:OH	2.30	0.45
1:B:318:VAL:HG12	1:B:328:ILE:HD13	1.99	0.45
1:B:323:HIS:HA	1:B:373:LEU:HD21	1.99	0.44
1:C:87:ILE:HG22	1:C:116:TYR:HB2	1.98	0.44
1:A:200:LYS:NZ	4:A:503:UHL:O10	2.43	0.44
1:C:197:ASN:O	1:C:201:TYR:HB2	2.18	0.44
1:C:318:VAL:HG12	1:C:328:ILE:HD13	1.98	0.44
1:C:426:LYS:HE2	1:C:459:GLU:HG3	1.99	0.44
1:A:87:ILE:HG22	1:A:116:TYR:HB2	2.00	0.43
1:B:118:TRP:O	1:B:122:GLN:HG2	2.19	0.43
1:C:204[A]:ARG:HA	1:C:239:SER:HB2	2.01	0.43
6:A:506:PO4:P	1:B:360:HIS:HE2	2.41	0.43
1:D:315:ARG:NH1	1:D:362:ASP:HB2	2.33	0.43
1:C:204[B]:ARG:HA	1:C:239:SER:HB2	2.01	0.42
1:D:323:HIS:HA	1:D:373:LEU:HD21	2.00	0.42
1:A:449:LYS:HD3	1:A:449:LYS:HA	1.91	0.42
1:A:314:LYS:HG3	6:A:505:PO4:O2	2.19	0.42
1:A:373:LEU:HD23	2:A:501:NAD:N7N	2.35	0.42
1:C:38:LEU:HD23	1:C:68:VAL:HG12	2.00	0.42
1:A:196:LYS:HE3	1:D:468:ARG:HB2	2.02	0.42
1:C:283:ILE:HG13	1:C:307:ASN:HB3	2.03	0.41
1:A:343:LYS:HB2	1:A:344:PRO:HD2	2.02	0.41
1:C:171:ARG:O	1:C:175:MET:HG3	2.20	0.41
1:D:429:GLU:OE1	1:D:461:PRO:HA	2.20	0.41
1:B:400:HIS:O	1:B:404[B]:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ARG:NH1	1:A:362:ASP:HB2	2.35	0.41
1:B:241:ARG:HD3	9:B:891:HOH:O	2.21	0.41
2:D:502:NAD:H2D	2:D:502:NAD:H6N	1.89	0.41
1:C:134:ASN:HA	1:C:158:ILE:HA	2.03	0.40
1:C:201:TYR:OH	4:C:501:UHL:N09	2.55	0.40
1:C:41:LEU:HD23	1:C:44:LYS:HD3	2.03	0.40
2:C:502:NAD:H2D	2:C:502:NAD:H6N	1.89	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	467/472 (99%)	455 (97%)	12 (3%)	0	100	100
1	B	465/472 (98%)	454 (98%)	11 (2%)	0	100	100
1	C	464/472 (98%)	453 (98%)	11 (2%)	0	100	100
1	D	466/472 (99%)	453 (97%)	13 (3%)	0	100	100
All	All	1862/1888 (99%)	1815 (98%)	47 (2%)	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	384/385 (100%)	384 (100%)	0	100	100
1	B	383/385 (100%)	381 (100%)	2 (0%)	88	85
1	C	383/385 (100%)	382 (100%)	1 (0%)	92	90
1	D	382/385 (99%)	379 (99%)	3 (1%)	81	75
All	All	1532/1540 (100%)	1526 (100%)	6 (0%)	91	88

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

Mol	Chain	Res	Type
1	B	335	LYS
1	B	417	ARG
1	C	355	ASP
1	D	114	GLU
1	D	335	LYS
1	D	417	ARG

Sometimes 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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 4 are monoatomic - leaving 31 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
6	PO4	D	506	-	4,4,4	0.98	0	6,6,6	0.41	0
6	PO4	C	508	-	4,4,4	0.94	0	6,6,6	0.53	0
7	GOL	B	504	-	5,5,5	0.90	0	5,5,5	1.00	0
6	PO4	C	506	-	4,4,4	0.82	0	6,6,6	0.57	0
2	NAD	D	502	-	42,48,48	0.52	0	50,73,73	0.69	1 (2%)
6	PO4	B	509	-	4,4,4	0.89	0	6,6,6	0.52	0
6	PO4	A	507	-	4,4,4	0.97	0	6,6,6	0.37	0
6	PO4	A	506	-	4,4,4	0.98	0	6,6,6	0.44	0
6	PO4	D	509	-	4,4,4	0.87	0	6,6,6	0.41	0
2	NAD	C	502	-	42,48,48	0.54	0	50,73,73	0.66	1 (2%)
3	ADE	A	502	-	9,11,11	0.97	0	7,15,15	1.13	1 (14%)
6	PO4	A	505	-	4,4,4	0.98	0	6,6,6	0.43	0
6	PO4	B	508	-	4,4,4	0.86	0	6,6,6	0.66	0
6	PO4	A	509	-	4,4,4	0.95	0	6,6,6	0.55	0
7	GOL	B	501	-	5,5,5	1.10	0	5,5,5	0.80	0
3	ADE	C	503	-	9,11,11	0.99	0	7,15,15	1.08	0
4	UHL	C	501	-	6,10,10	2.58	2 (33%)	2,12,12	1.17	0
6	PO4	B	507	-	4,4,4	0.97	0	6,6,6	0.46	0
2	NAD	A	501	-	42,48,48	0.56	0	50,73,73	0.66	1 (2%)
6	PO4	A	508	-	4,4,4	0.96	0	6,6,6	0.45	0
6	PO4	C	507	-	4,4,4	0.93	0	6,6,6	0.45	0
4	UHL	A	503	-	6,10,10	2.51	2 (33%)	2,12,12	0.84	0
7	GOL	D	504	-	5,5,5	1.01	0	5,5,5	0.84	0
8	DMS	D	501	-	3,3,3	0.69	0	3,3,3	0.63	0
6	PO4	D	508	-	4,4,4	0.97	0	6,6,6	0.44	0
3	ADE	B	503	-	9,11,11	1.00	0	7,15,15	1.14	1 (14%)
6	PO4	D	507	-	4,4,4	0.93	0	6,6,6	0.46	0
7	GOL	B	505	-	5,5,5	0.92	0	5,5,5	0.97	0
2	NAD	B	502	-	42,48,48	0.52	0	50,73,73	0.67	1 (2%)
3	ADE	D	503	-	9,11,11	1.00	0	7,15,15	1.08	0
6	PO4	C	505	-	4,4,4	0.92	0	6,6,6	0.53	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
3	ADE	B	503	-	-	-	0/2/2/2
2	NAD	C	502	-	-	5/26/62/62	0/5/5/5
7	GOL	B	504	-	-	4/4/4/4	-
7	GOL	B	505	-	-	0/4/4/4	-
7	GOL	B	501	-	-	0/4/4/4	-
3	ADE	A	502	-	-	-	0/2/2/2
2	NAD	B	502	-	-	5/26/62/62	0/5/5/5
2	NAD	D	502	-	-	5/26/62/62	0/5/5/5
4	UHL	C	501	-	-	1/3/4/4	0/1/1/1
3	ADE	C	503	-	-	-	0/2/2/2
3	ADE	D	503	-	-	-	0/2/2/2
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
7	GOL	D	504	-	-	0/4/4/4	-
4	UHL	A	503	-	-	2/3/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	UHL	C04-C05	5.11	1.52	1.49
4	A	503	UHL	C04-C05	4.81	1.52	1.49
4	A	503	UHL	C08-N09	3.73	1.46	1.35
4	C	501	UHL	C08-N09	3.58	1.45	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	NAD	C5A-C6A-N6A	2.36	123.94	120.35
2	D	502	NAD	C5A-C6A-N6A	2.31	123.87	120.35
2	C	502	NAD	C5A-C6A-N6A	2.30	123.84	120.35
2	A	501	NAD	C5A-C6A-N6A	2.29	123.84	120.35
3	B	503	ADE	C5-C6-N6	2.22	123.72	120.35
3	A	502	ADE	C5-C6-N6	2.11	123.56	120.35

There are no chirality outliers.

All (27) 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

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Mol	Chain	Res	Type	Atoms
2	B	502	NAD	O4D-C1D-N1N-C2N
2	B	502	NAD	O4D-C1D-N1N-C6N
2	B	502	NAD	C2D-C1D-N1N-C2N
2	B	502	NAD	C2D-C1D-N1N-C6N
2	C	502	NAD	O4D-C1D-N1N-C2N
2	C	502	NAD	O4D-C1D-N1N-C6N
2	C	502	NAD	C2D-C1D-N1N-C2N
2	C	502	NAD	C2D-C1D-N1N-C6N
2	D	502	NAD	O4D-C1D-N1N-C2N
2	D	502	NAD	O4D-C1D-N1N-C6N
2	D	502	NAD	C2D-C1D-N1N-C2N
2	D	502	NAD	C2D-C1D-N1N-C6N
4	C	501	UHL	O02-C03-C04-C05
7	B	504	GOL	C1-C2-C3-O3
7	B	504	GOL	O1-C1-C2-C3
7	B	504	GOL	O1-C1-C2-O2
4	A	503	UHL	C04-C03-O02-C01
7	B	504	GOL	O2-C2-C3-O3
4	A	503	UHL	O02-C03-C04-C05
2	B	502	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	O4B-C4B-C5B-O5B
2	C	502	NAD	O4B-C4B-C5B-O5B
2	D	502	NAD	O4B-C4B-C5B-O5B

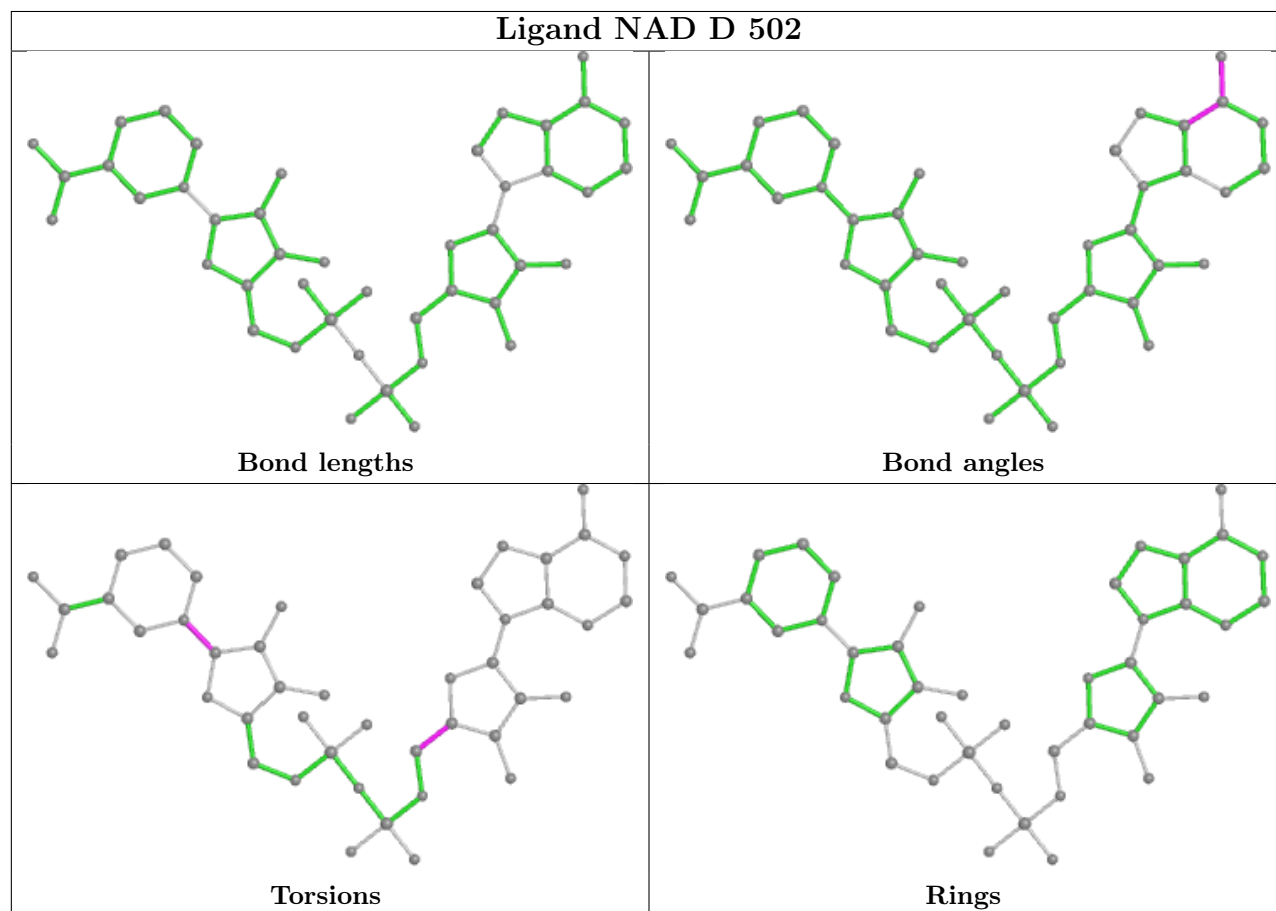
There are no ring outliers.

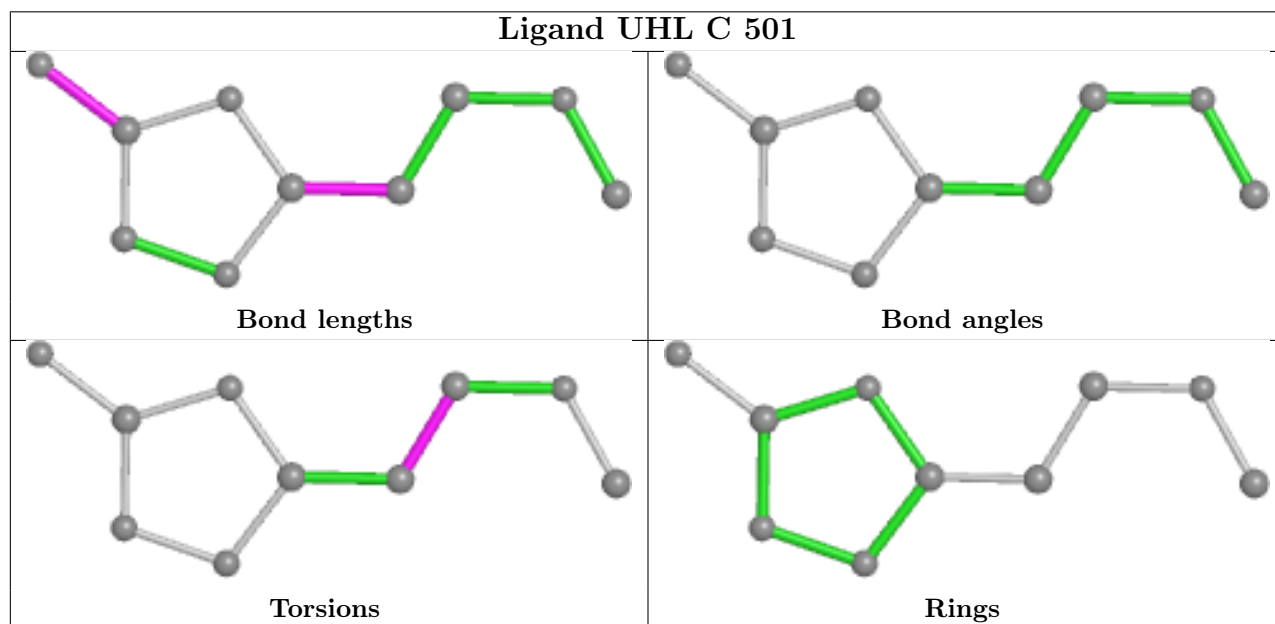
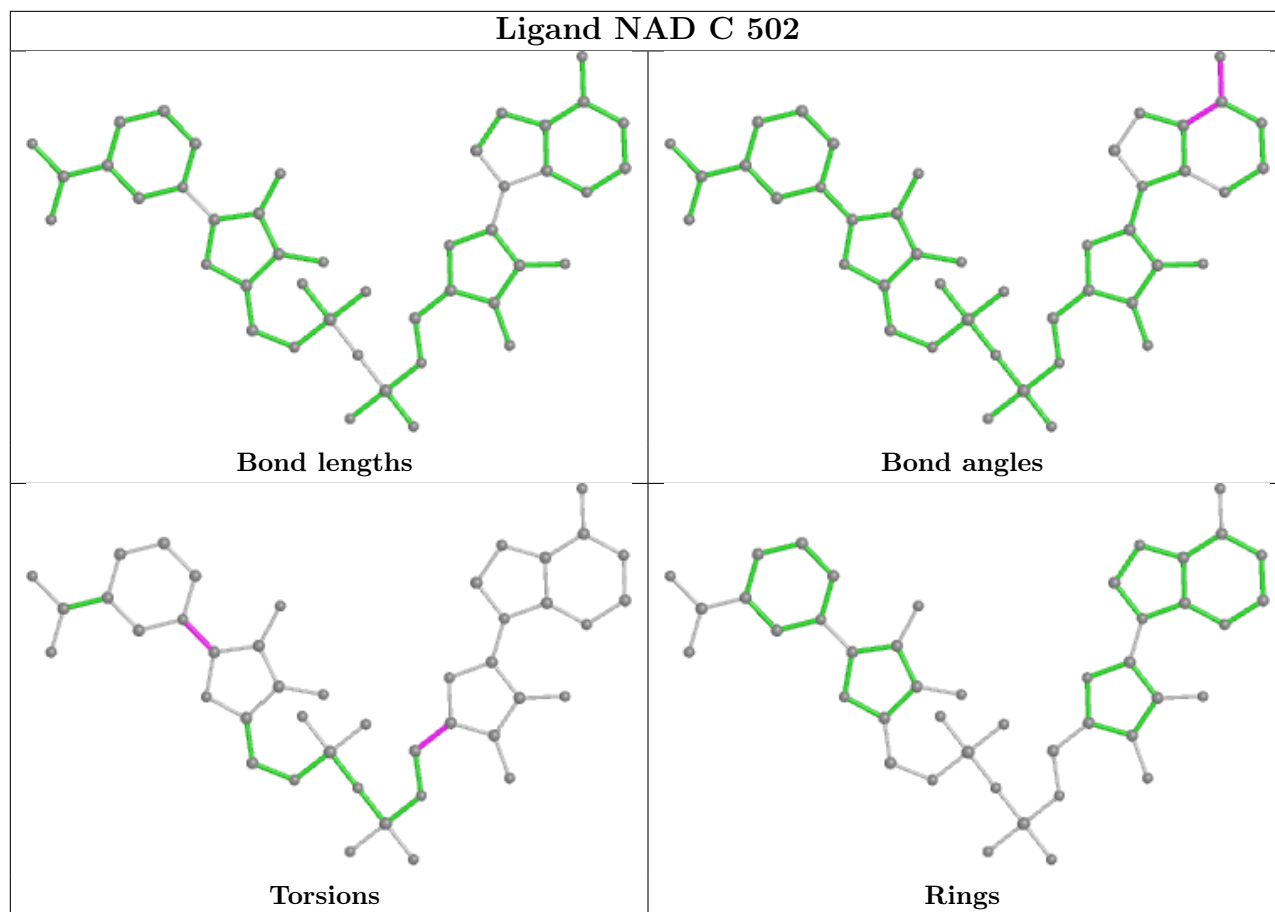
8 monomers are involved in 10 short contacts:

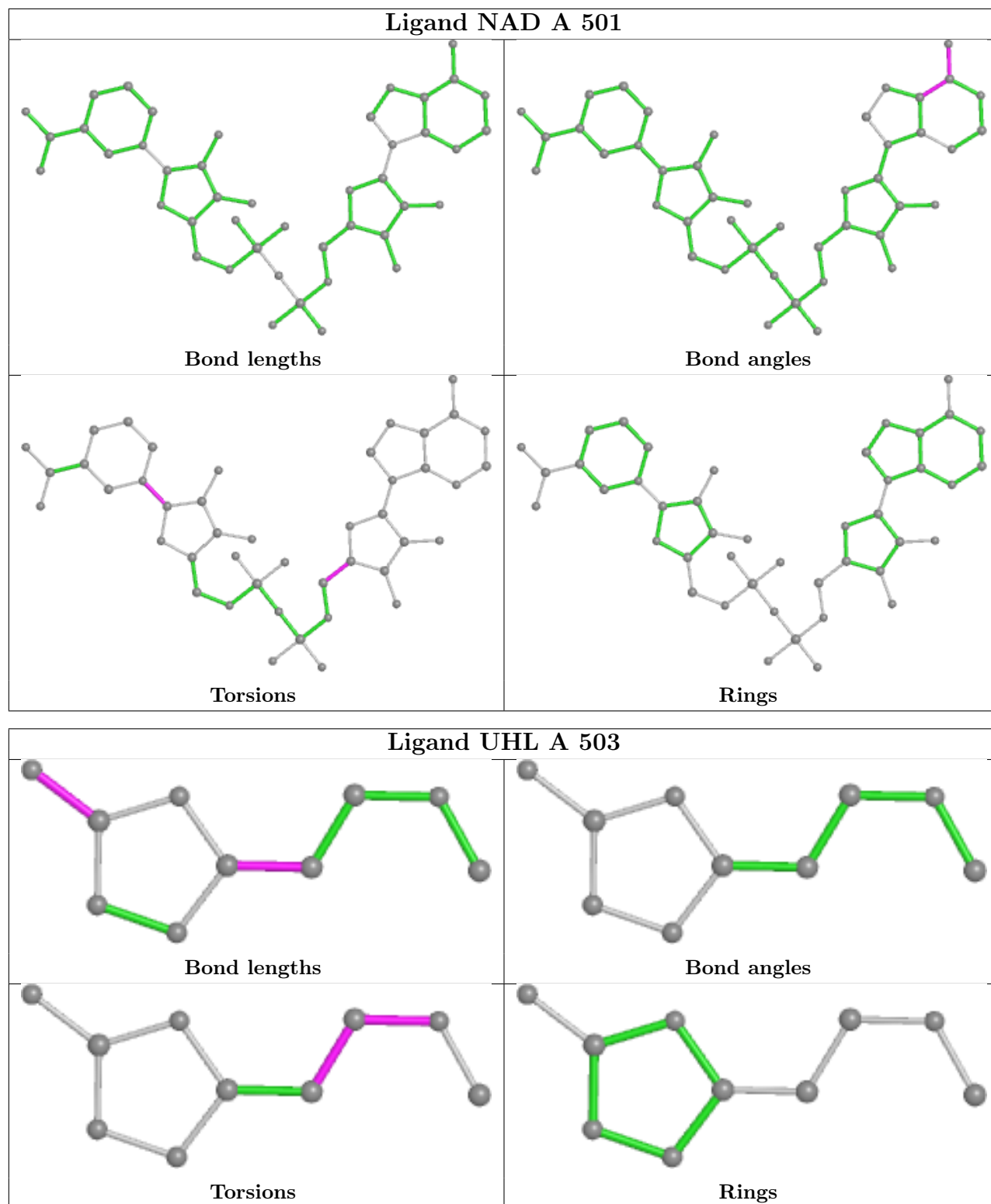
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	NAD	2	0
6	A	506	PO4	1	0
2	C	502	NAD	1	0
6	A	505	PO4	1	0
4	C	501	UHL	2	0
2	A	501	NAD	1	0
4	A	503	UHL	1	0
6	C	505	PO4	1	0

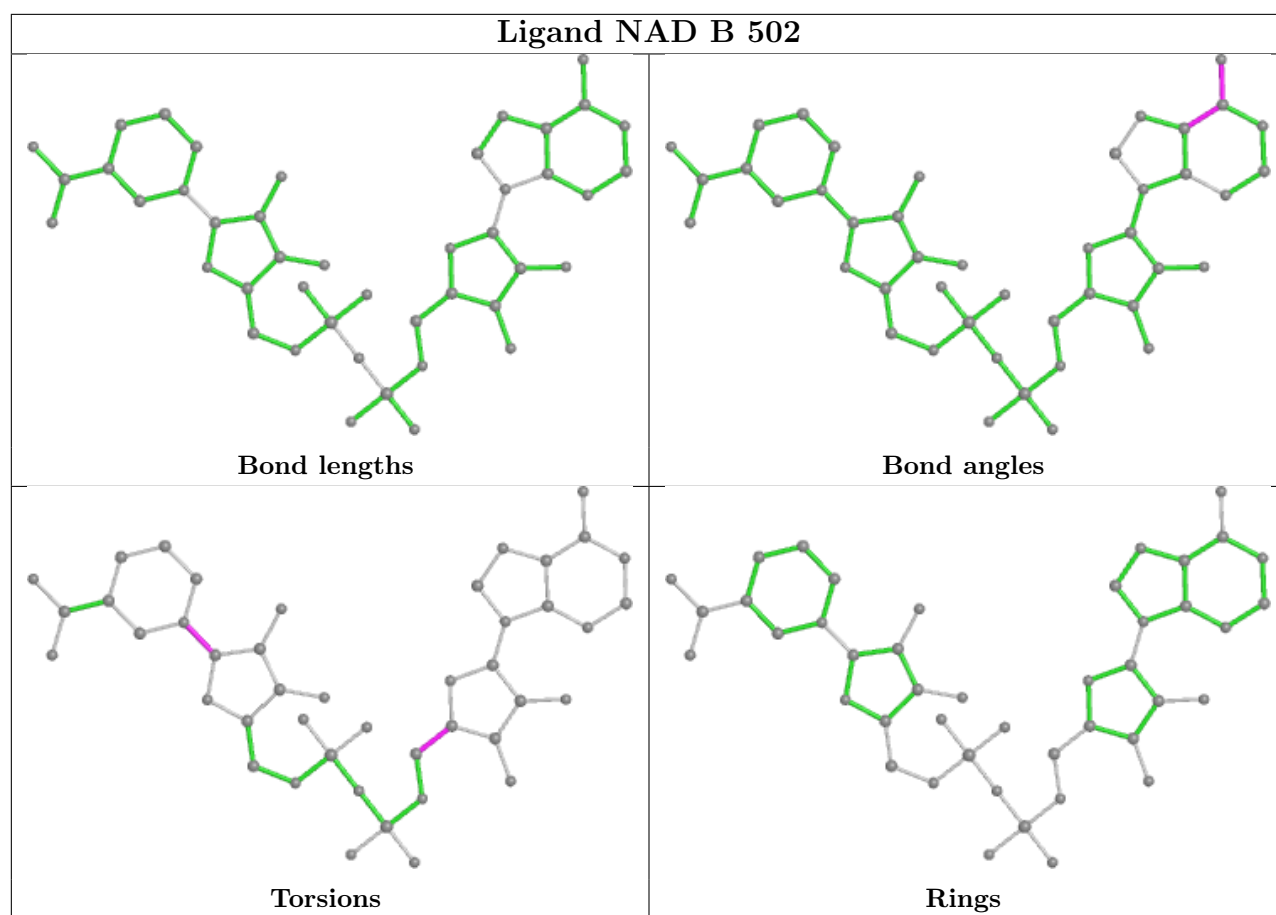
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	464/472 (98%)	-0.09	13 (2%) 53 51	19, 29, 52, 99	0
1	B	461/472 (97%)	-0.27	8 (1%) 70 69	19, 27, 45, 77	0
1	C	460/472 (97%)	0.40	49 (10%) 6 4	18, 34, 71, 111	0
1	D	462/472 (97%)	-0.04	14 (3%) 50 47	20, 29, 48, 77	0
All	All	1847/1888 (97%)	-0.00	84 (4%) 33 30	18, 29, 56, 111	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	411	ALA	10.1
1	A	412	ALA	10.0
1	C	415	ALA	9.8
1	C	412	ALA	8.8
1	C	410	PRO	7.4
1	A	411	ALA	6.4
1	D	8	ALA	6.2
1	C	416	LYS	6.1
1	C	152	PRO	5.6
1	A	415	ALA	5.6
1	C	176	LEU	5.5
1	C	413	GLU	5.4
1	B	355	ASP	5.3
1	C	418	LEU	5.2
1	C	409	LEU	5.1
1	C	125	LEU	5.0
1	C	414	LYS	4.7
1	A	416	LYS	4.6
1	C	417	ARG	4.4
1	C	355	ASP	4.3
1	C	129	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	180	THR	4.3
1	C	149	LYS	4.2
1	A	413	GLU	4.1
1	C	130	PRO	4.1
1	A	355	ASP	4.1
1	C	179	GLY	4.0
1	C	128	GLY	4.0
1	C	178	ASN	4.0
1	A	417	ARG	4.0
1	C	407	ALA	4.0
1	C	11	THR	3.9
1	C	181	LEU	3.8
1	C	127	ASP	3.7
1	C	155	LEU	3.7
1	B	354	LYS	3.6
1	C	10	PHE	3.6
1	A	410	PRO	3.5
1	C	406	TYR	3.5
1	C	177	LYS	3.4
1	C	151	TYR	3.3
1	D	355	ASP	3.2
1	A	409	LEU	3.1
1	C	148	HIS	3.0
1	C	354	LYS	3.0
1	D	279	THR	3.0
1	C	156	GLU	3.0
1	C	16	ALA	3.0
1	D	177	LYS	2.9
1	B	356	GLY	2.9
1	A	6	THR	2.9
1	C	157	ARG	2.8
1	C	150	LYS	2.8
1	D	9	GLY	2.8
1	C	118	TRP	2.7
1	D	335	LYS	2.7
1	D	354	LYS	2.7
1	D	321	ILE	2.6
1	D	280	GLU	2.6
1	C	357	PHE	2.6
1	D	278	GLY	2.6
1	C	121[A]	GLU	2.6
1	C	182	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	356	GLY	2.5
1	B	9	GLY	2.4
1	C	165	THR	2.4
1	C	13	TYR	2.4
1	A	356	GLY	2.4
1	D	19	THR	2.3
1	C	335	LYS	2.3
1	C	174[A]	ASP	2.3
1	D	352	THR	2.3
1	D	356	GLY	2.3
1	D	374	VAL	2.2
1	B	335	LYS	2.2
1	B	47	GLY	2.2
1	C	321	ILE	2.2
1	C	154	MET	2.1
1	C	166	THR	2.1
1	B	177	LYS	2.1
1	A	152	PRO	2.0
1	C	360	HIS	2.0
1	B	46	ALA	2.0
1	A	358	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.

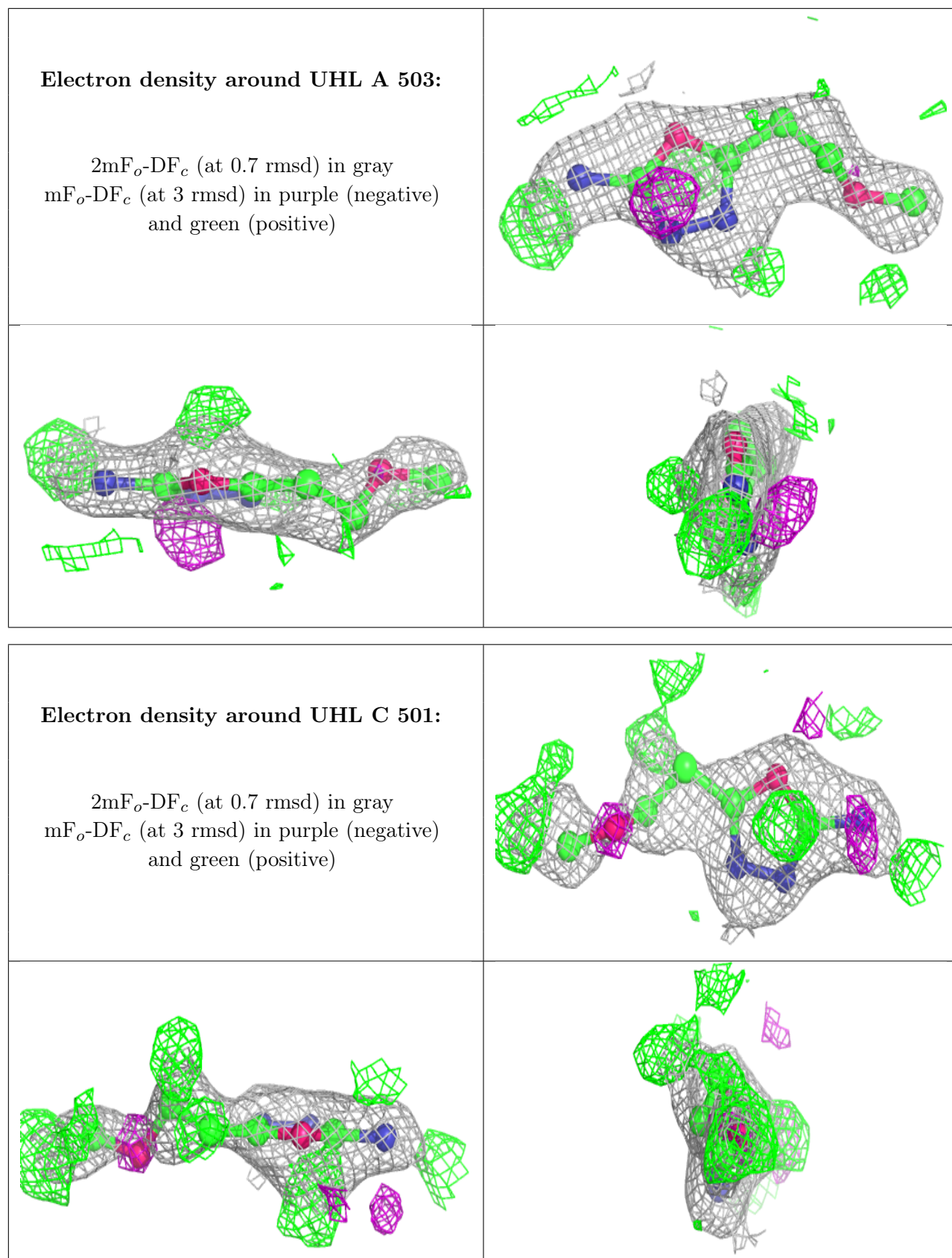
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	DMS	D	501	4/4	0.74	0.20	32,37,55,71	0
4	UHL	A	503	10/10	0.80	0.18	28,34,40,43	10

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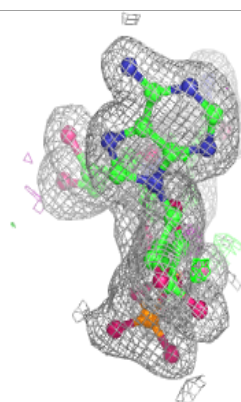
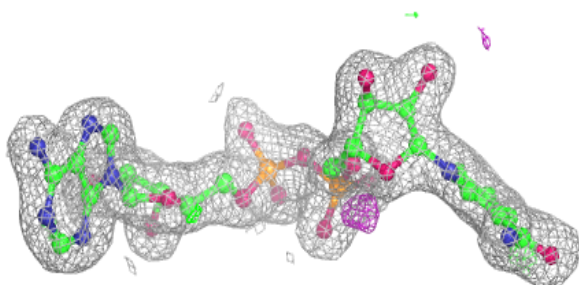
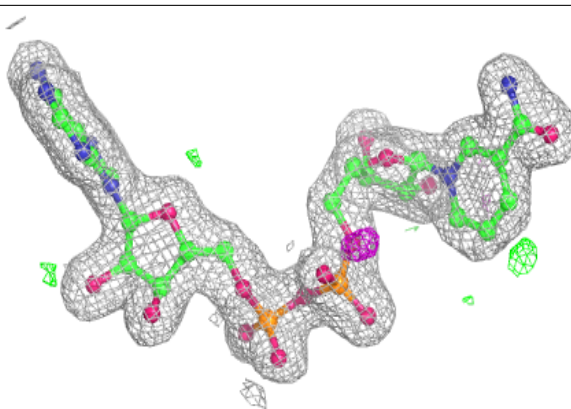
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PO4	C	506	5/5	0.85	0.17	47,49,50,64	0
7	GOL	D	504	6/6	0.86	0.21	32,44,45,47	0
4	UHL	C	501	10/10	0.88	0.16	27,34,42,51	10
7	GOL	B	505	6/6	0.88	0.30	33,40,42,42	0
7	GOL	B	501	6/6	0.89	0.14	30,39,40,41	0
7	GOL	B	504	6/6	0.91	0.16	38,39,42,43	0
6	PO4	B	509	5/5	0.91	0.17	31,37,43,47	5
6	PO4	B	508	5/5	0.92	0.13	25,25,28,33	5
6	PO4	A	505	5/5	0.92	0.14	36,36,44,44	5
6	PO4	C	507	5/5	0.93	0.15	37,39,41,48	5
6	PO4	C	505	5/5	0.93	0.16	35,36,39,40	5
6	PO4	B	507	5/5	0.95	0.14	37,38,45,50	5
6	PO4	A	507	5/5	0.95	0.10	34,36,38,48	0
6	PO4	A	508	5/5	0.95	0.11	39,40,41,48	5
6	PO4	D	506	5/5	0.95	0.20	36,39,40,40	5
6	PO4	D	508	5/5	0.95	0.13	38,39,42,44	5
3	ADE	D	503	10/10	0.96	0.17	25,27,28,28	0
6	PO4	D	507	5/5	0.96	0.10	30,34,36,43	0
3	ADE	B	503	10/10	0.96	0.14	24,25,25,26	0
6	PO4	C	508	5/5	0.96	0.16	35,39,44,56	0
2	NAD	C	502	44/44	0.97	0.09	17,24,31,34	0
2	NAD	D	502	44/44	0.97	0.09	19,25,29,32	0
6	PO4	D	509	5/5	0.97	0.16	30,36,37,37	0
3	ADE	A	502	10/10	0.97	0.13	23,24,26,26	0
2	NAD	A	501	44/44	0.97	0.07	17,23,27,30	0
3	ADE	C	503	10/10	0.97	0.17	31,36,39,41	0
6	PO4	A	509	5/5	0.97	0.08	23,28,30,33	5
2	NAD	B	502	44/44	0.97	0.07	21,24,28,30	0
6	PO4	A	506	5/5	0.98	0.09	28,36,37,38	5
5	K	C	504	1/1	0.98	0.10	32,32,32,32	0
5	K	B	506	1/1	0.99	0.07	22,22,22,22	0
5	K	D	505	1/1	1.00	0.07	25,25,25,25	0
5	K	A	504	1/1	1.00	0.09	24,24,24,24	0

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

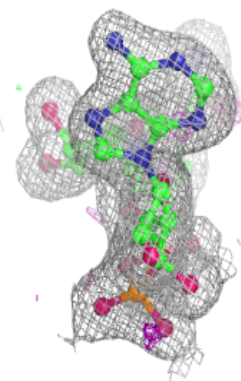
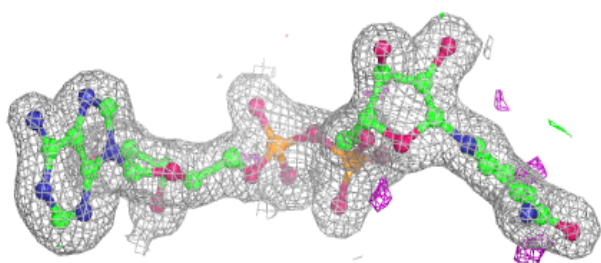
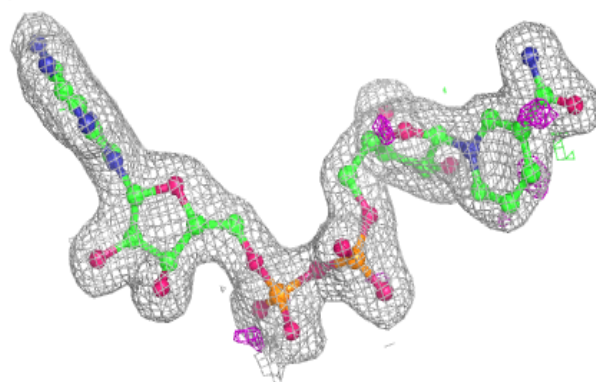


Electron density around NAD C 502:

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

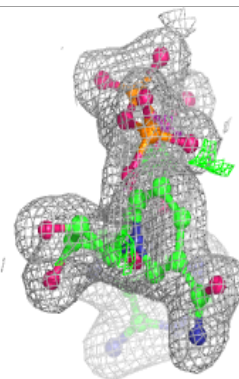
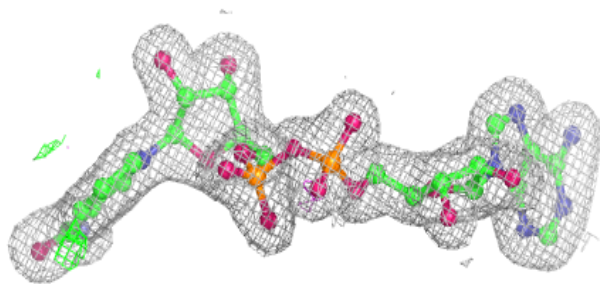
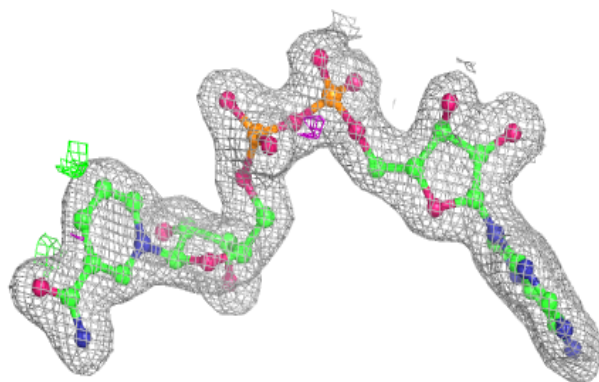
**Electron density around NAD D 502:**

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

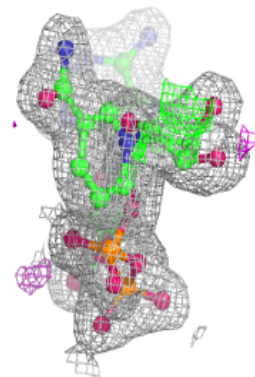
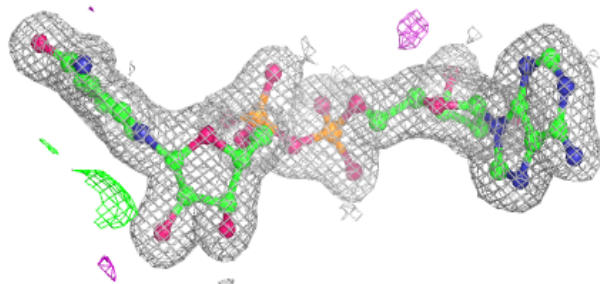
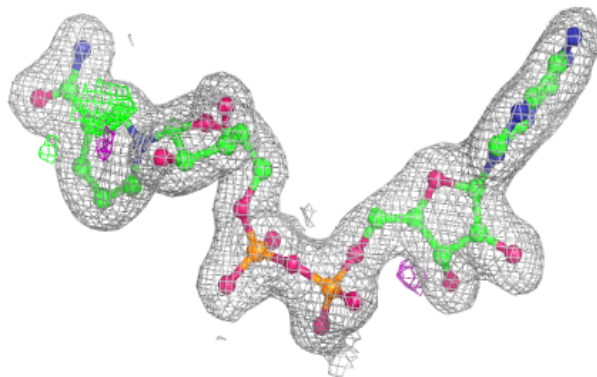


Electron density around NAD A 501:

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

**Electron density around NAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.