



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 12:57 pm GMT

PDB ID : 8CFD  
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *P. aeruginosa* in complex with F2X-Entry library fragment A07  
Authors : Malecki, P.H.; Gawel, M.; Stepniewska, M.; Brzezinski, K.  
Deposited on : 2023-02-03  
Resolution : 1.88 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](mailto: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>.

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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

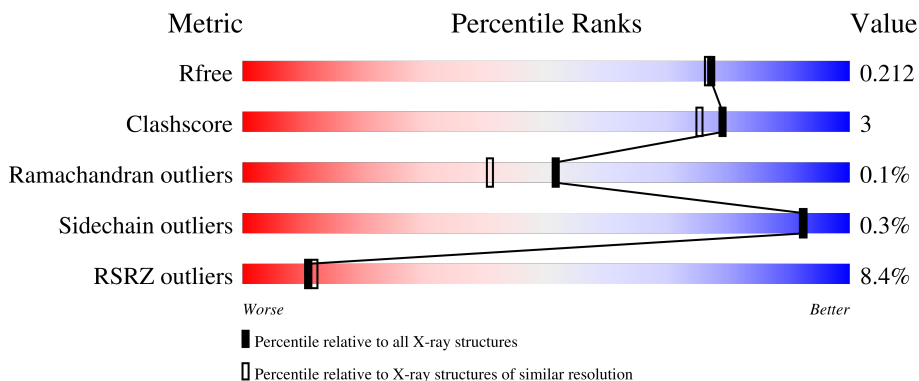
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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  $\geq 3$ , 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 8 unique types of molecules in this entry. The entry contains 16114 atoms, of which 8 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	462	3598	2268	623	684	23	0	6	0
1	B	461	3583	2260	620	681	22	0	5	0
1	C	462	3619	2283	626	687	23	0	10	0
1	D	461	3580	2256	618	684	22	0	5	0

There are 12 discrepancies between the modelled and reference sequences:

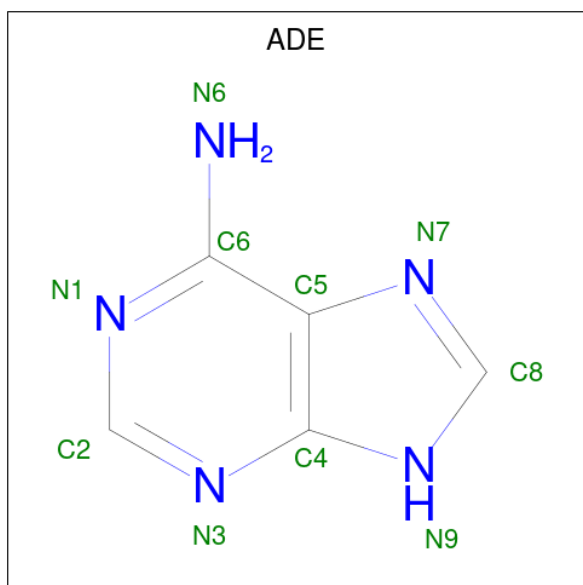
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9I685
A	-1	ASN	-	expression tag	UNP Q9I685
A	0	ALA	-	expression tag	UNP Q9I685
B	-2	SER	-	expression tag	UNP Q9I685
B	-1	ASN	-	expression tag	UNP Q9I685
B	0	ALA	-	expression tag	UNP Q9I685
C	-2	SER	-	expression tag	UNP Q9I685
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: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 3 is ADENINE (three-letter code: ADE) (formula: C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>).

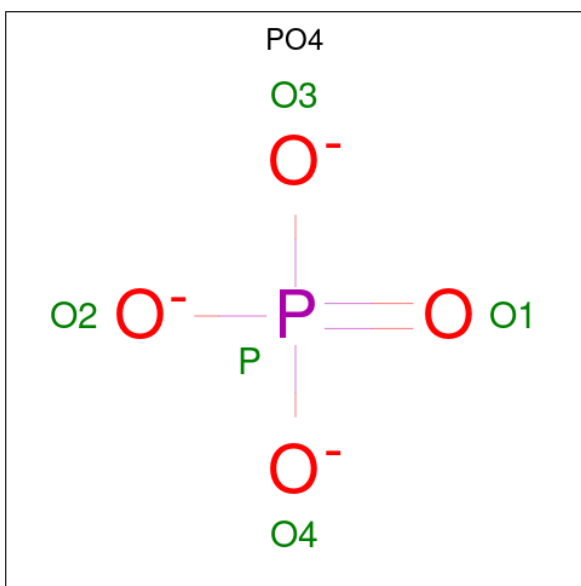


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 10 5 5	0	0
3	B	1	Total C N 10 5 5	0	0
3	C	1	Total C N 10 5 5	0	0
3	D	1	Total C N 10 5 5	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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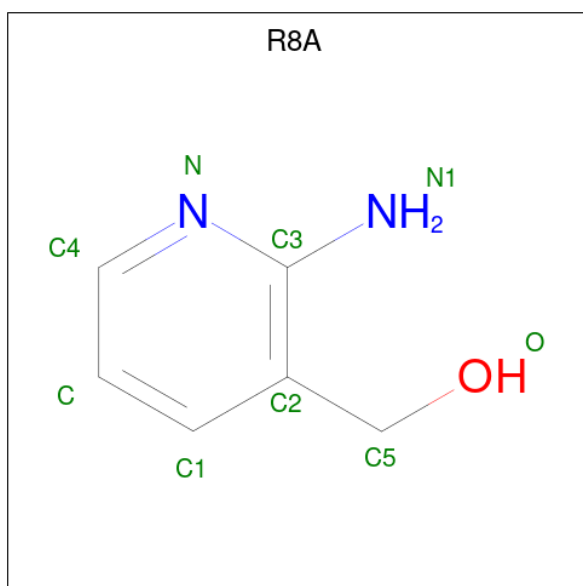
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total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

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

- Molecule 7 is (2-aminopyridin-3-yl)methanol (three-letter code: R8A) (formula: C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
7	D	1	17	6	8	2	1	0	0

- Molecule 8 is water.

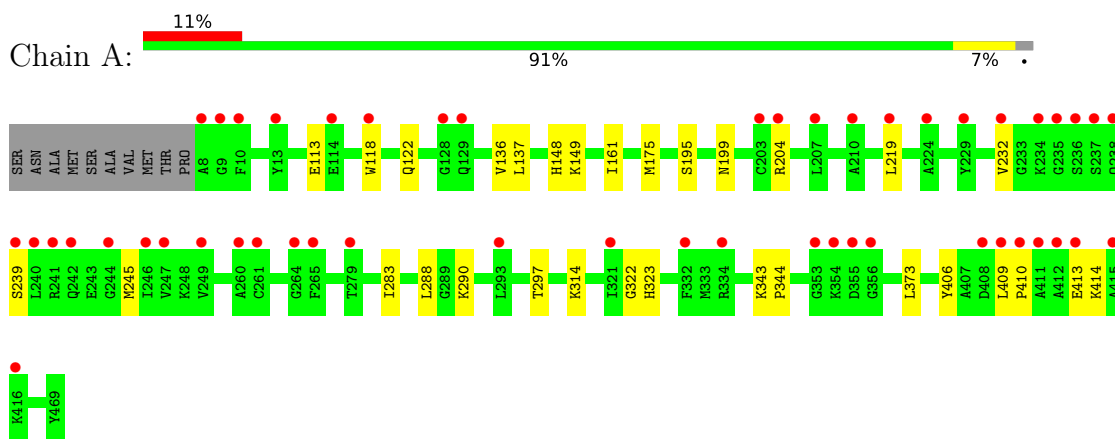
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	362	Total 365	O 365	0	4
8	B	332	Total 335	O 335	0	4
8	C	339	Total 342	O 342	0	3
8	D	365	Total 368	O 368	0	6



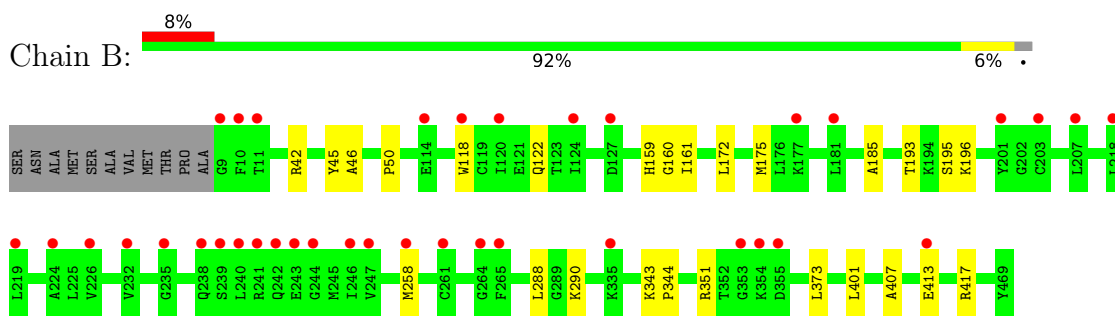
### 3 Residue-property plots [i](#)

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.

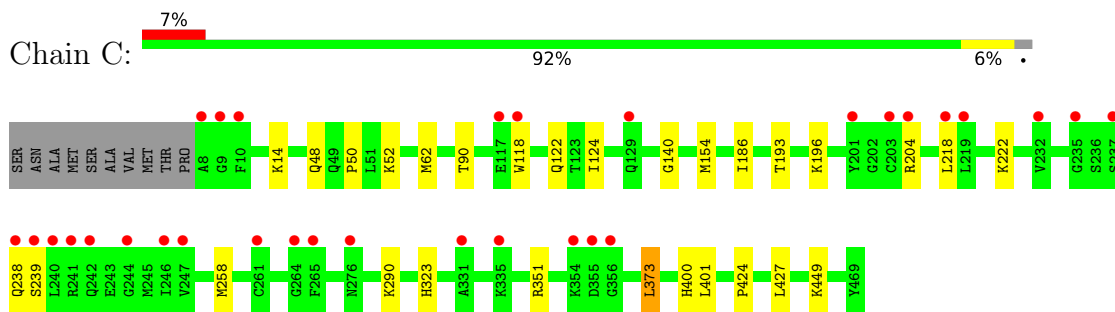
- Molecule 1: Adenosylhomocysteinase



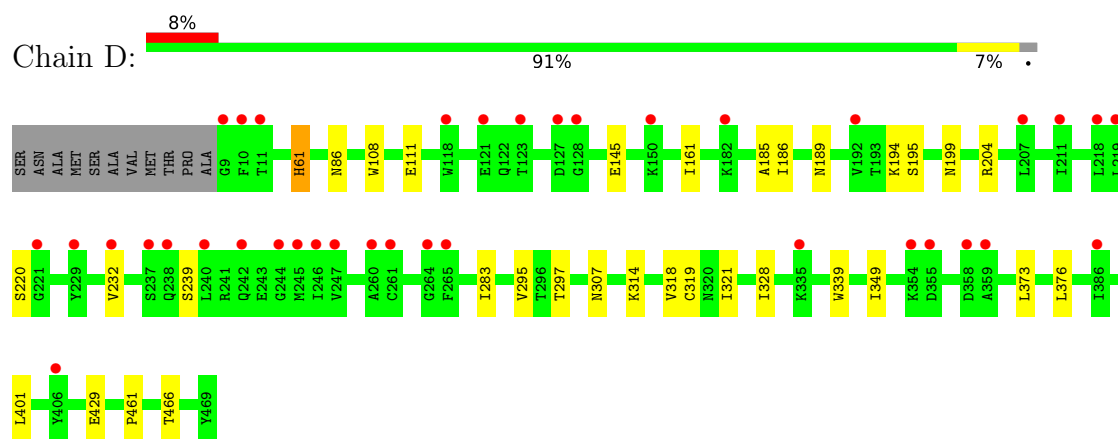
- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.76Å 105.14Å 108.25Å 90.00° 99.71° 90.00°	Depositor
Resolution (Å)	43.38 – 1.88 49.48 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.38-1.88) 98.5 (49.48-1.88)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 1.88Å)	Xtrriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, $R_{free}$	0.174 , 0.216 0.172 , 0.212	Depositor DCC
$R_{free}$ test set	2101 reflections (1.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtrriage
Anisotropy	0.159	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, NAD, K, R8A, ADE, PO4

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	0.35	0/3673	0.54	0/4964
1	B	0.35	0/3658	0.54	0/4944
1	C	0.35	0/3706	0.53	0/5007
1	D	0.34	0/3652	0.54	0/4937
All	All	0.35	0/14689	0.54	0/19852

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	3598	0	3611	25	0
1	B	3583	0	3600	17	0
1	C	3619	0	3645	23	0
1	D	3580	0	3583	19	0
2	A	44	0	26	0	0
2	B	44	0	26	2	0
2	C	44	0	26	1	0
2	D	44	0	26	0	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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	15	0	0	1	0
5	B	15	0	0	1	0
5	C	25	0	0	1	0
5	D	20	0	0	1	0
6	C	4	0	6	0	0
6	D	8	0	12	3	0
7	D	9	8	0	0	0
8	A	365	0	0	3	0
8	B	335	0	0	1	0
8	C	342	0	0	3	0
8	D	368	0	0	0	0
All	All	16106	8	14577	83	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 3.

All (83) 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:A:409:LEU:HB3	1:A:413:GLU:HB2	1.72	0.71
1:A:410:PRO:HD2	1:A:413:GLU:HG2	1.76	0.68
1:A:314:LYS:HG3	5:A:504:PO4:O1	1.95	0.66
1:A:290:LYS:HD2	8:A:719:HOH:O	1.96	0.66
1:D:466:THR:HA	6:D:503:DMS:C2	2.26	0.64
1:C:186:ILE:HG13	1:C:401:LEU:HD11	1.81	0.62
1:A:406:TYR:OH	1:A:414:LYS:HB3	2.00	0.62
1:D:189:ASN:HA	1:D:194:LYS:HD2	1.80	0.62
1:A:113:GLU:HG2	8:A:779:HOH:O	2.00	0.61
1:B:373:LEU:HD22	2:B:501:NAD:N7N	2.15	0.61
1:C:424:PRO:HD2	1:C:427:LEU:HD12	1.83	0.59
1:B:195:SER:OG	1:B:196[B]:LYS:HD2	2.03	0.58
1:A:232:VAL:HG12	1:A:297:THR:HB	1.86	0.57
1:A:323:HIS:HA	1:A:373:LEU:HD21	1.85	0.57
1:A:406:TYR:CZ	1:A:414:LYS:HB3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:PRO:HD2	1:A:413:GLU:CG	2.35	0.57
1:C:48[B]:GLN:HG3	1:C:50:PRO:HD3	1.89	0.55
1:A:195:SER:O	1:A:199:ASN:HB2	2.08	0.54
1:B:172:LEU:HA	1:B:175:MET:HE3	1.88	0.54
1:D:466:THR:HA	6:D:503:DMS:H21	1.89	0.54
1:C:48[A]:GLN:HG3	8:C:721:HOH:O	2.08	0.53
1:C:204[B]:ARG:HA	1:C:239:SER:HB2	1.92	0.52
1:A:322:GLY:O	1:A:373:LEU:HD23	2.10	0.52
1:D:232:VAL:HG12	1:D:297:THR:HB	1.92	0.51
1:B:193:THR:HG22	1:C:258[A]:MET:SD	2.50	0.51
1:C:48[B]:GLN:CG	1:C:50:PRO:HD3	2.40	0.51
1:C:290:LYS:HD2	8:C:867:HOH:O	2.10	0.51
1:A:118:TRP:O	1:A:122:GLN:HG2	2.11	0.51
1:A:283:ILE:CG2	1:A:288:LEU:HD12	2.41	0.51
1:C:449:LYS:HA	1:C:449:LYS:HE2	1.93	0.50
1:B:118:TRP:O	1:B:122:GLN:HG2	2.11	0.50
1:B:351:ARG:NH2	5:B:505:PO4:O2	2.45	0.50
1:D:466:THR:HA	6:D:503:DMS:H22	1.93	0.50
1:C:204[A]:ARG:HA	1:C:239:SER:HB2	1.93	0.49
1:C:400:HIS:HE1	8:C:852:HOH:O	1.96	0.49
1:C:373:LEU:HD22	2:C:501:NAD:N7N	2.28	0.48
1:B:160:GLY:HA3	1:B:401:LEU:HD13	1.95	0.48
1:C:118:TRP:O	1:C:122:GLN:HG2	2.13	0.48
2:B:501:NAD:H8A	8:B:790:HOH:O	2.13	0.48
1:D:86:ASN:ND2	1:D:373:LEU:HD12	2.30	0.47
1:A:148:HIS:CD2	1:A:175:MET:HE2	2.51	0.46
1:A:343:LYS:HB2	1:A:344:PRO:HD2	1.97	0.46
1:A:204[B]:ARG:HA	1:A:239:SER:HB2	1.98	0.46
1:A:204[A]:ARG:HA	1:A:239:SER:HB2	1.98	0.46
1:D:283:ILE:HG13	1:D:307:ASN:HB3	1.99	0.45
1:C:204[B]:ARG:HD3	1:C:238[B]:GLN:OE1	2.17	0.45
1:A:137:LEU:C	1:A:137:LEU:HD23	2.37	0.45
1:D:195:SER:O	1:D:199:ASN:HB2	2.17	0.44
1:D:339:TRP:CE2	1:D:349:ILE:HD12	2.52	0.44
1:B:258[A]:MET:SD	1:C:193:THR:HG22	2.58	0.44
1:C:351:ARG:NH2	5:C:509:PO4:O3	2.50	0.44
1:B:288:LEU:HD13	1:B:288:LEU:HA	1.81	0.44
1:A:148:HIS:CG	1:A:175:MET:HE1	2.53	0.43
1:A:344:PRO:HA	8:A:857:HOH:O	2.19	0.43
1:D:318:VAL:HG12	1:D:328:ILE:HD13	2.00	0.43
1:B:161:ILE:O	1:B:185:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:HB2	1:A:344:PRO:CD	2.48	0.43
1:C:218:LEU:O	1:C:222:LYS:HD2	2.19	0.43
1:D:161:ILE:O	1:D:185:ALA:HA	2.19	0.42
1:D:108:TRP:O	1:D:111:GLU:HG3	2.20	0.42
1:D:429:GLU:OE1	1:D:461:PRO:HA	2.20	0.42
1:C:186:ILE:HG13	1:C:401:LEU:CD1	2.49	0.42
1:A:136:VAL:HB	1:A:161:ILE:HG12	2.01	0.41
1:B:417:ARG:O	1:B:417:ARG:HG3	2.19	0.41
1:C:62:MET:HB3	1:C:90:THR:HG23	2.01	0.41
1:A:219:LEU:O	1:A:245:MET:HG2	2.20	0.41
1:C:52:LYS:HB2	1:C:52:LYS:HE2	1.88	0.41
1:B:159:HIS:CE1	1:B:407:ALA:HB3	2.56	0.41
1:D:314:LYS:HG3	5:D:507:PO4:O2	2.21	0.41
1:B:290:LYS:HB3	1:B:290:LYS:HE3	1.91	0.41
1:C:140:GLY:HA3	1:C:323:HIS:CE1	2.56	0.41
1:D:61:HIS:CE1	1:D:376:LEU:HD13	2.56	0.41
1:B:42:ARG:O	1:B:46:ALA:HB2	2.21	0.41
1:B:45:TYR:CD1	1:B:50:PRO:HG3	2.56	0.41
1:C:124:ILE:HG23	1:C:154:MET:SD	2.61	0.41
1:D:204:ARG:HA	1:D:239:SER:HB2	2.02	0.41
1:A:283:ILE:HG23	1:A:288:LEU:HD12	2.02	0.40
1:D:297:THR:HG22	1:D:321:ILE:CG2	2.51	0.40
1:D:186:ILE:HG13	1:D:401:LEU:HD11	2.03	0.40
1:B:343:LYS:HB2	1:B:344:PRO:HD2	2.04	0.40
1:C:14:LYS:HD3	1:C:118:TRP:CH2	2.56	0.40
1:D:295:VAL:HG22	1:D:319:CYS:SG	2.61	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	466/472 (99%)	457 (98%)	9 (2%)	0	100	100
1	B	464/472 (98%)	452 (97%)	12 (3%)	0	100	100
1	C	470/472 (100%)	457 (97%)	12 (3%)	1 (0%)	47	37
1	D	464/472 (98%)	453 (98%)	10 (2%)	1 (0%)	47	37
All	All	1864/1888 (99%)	1819 (98%)	43 (2%)	2 (0%)	51	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	373	LEU
1	D	61	HIS

### 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	383/385 (100%)	382 (100%)	1 (0%)	92	92
1	B	382/385 (99%)	381 (100%)	1 (0%)	92	92
1	C	387/385 (100%)	385 (100%)	2 (0%)	88	88
1	D	381/385 (99%)	379 (100%)	2 (0%)	88	88
All	All	1533/1540 (100%)	1527 (100%)	6 (0%)	92	90

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

Mol	Chain	Res	Type
1	A	149	LYS
1	B	413	GLU
1	C	196[A]	LYS
1	C	196[B]	LYS
1	D	145	GLU
1	D	220	SER

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 31 ligands modelled in this entry, 4 are monoatomic - leaving 27 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	PO4	C	509	-	4,4,4	1.03	0	6,6,6	0.54	0
3	ADE	C	502	-	9,11,11	1.05	1 (11%)	7,15,15	1.18	1 (14%)
5	PO4	C	508	-	4,4,4	1.04	0	6,6,6	0.46	0
2	NAD	A	501	-	42,48,48	0.58	0	50,73,73	0.68	1 (2%)
5	PO4	B	506	-	4,4,4	0.65	0	6,6,6	0.54	0
5	PO4	C	506	-	4,4,4	0.82	0	6,6,6	0.55	0
7	R8A	D	505	-	9,9,9	1.80	2 (22%)	9,11,11	1.66	2 (22%)
6	DMS	D	503	-	3,3,3	0.69	0	3,3,3	0.69	0
5	PO4	C	505	-	4,4,4	0.88	0	6,6,6	0.43	0
5	PO4	C	507	-	4,4,4	0.98	0	6,6,6	0.47	0
5	PO4	A	505	-	4,4,4	0.89	0	6,6,6	0.54	0
5	PO4	D	509	-	4,4,4	0.75	0	6,6,6	0.70	0
5	PO4	D	507	-	4,4,4	0.94	0	6,6,6	0.42	0
2	NAD	D	501	-	42,48,48	0.57	0	50,73,73	0.74	1 (2%)
3	ADE	A	502	-	9,11,11	1.03	1 (11%)	7,15,15	1.11	1 (14%)
3	ADE	D	502	-	9,11,11	1.03	1 (11%)	7,15,15	1.12	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PO4	B	504	-	4,4,4	0.88	0	6,6,6	0.43	0
6	DMS	C	503	-	3,3,3	0.73	0	3,3,3	0.68	0
6	DMS	D	504	-	3,3,3	0.67	0	3,3,3	0.55	0
5	PO4	D	508	-	4,4,4	0.81	0	6,6,6	0.44	0
5	PO4	D	510	-	4,4,4	0.90	0	6,6,6	0.52	0
2	NAD	B	501	-	42,48,48	0.53	0	50,73,73	0.75	2 (4%)
5	PO4	A	506	-	4,4,4	0.82	0	6,6,6	0.76	0
3	ADE	B	502	-	9,11,11	0.99	1 (11%)	7,15,15	1.14	1 (14%)
5	PO4	B	505	-	4,4,4	0.97	0	6,6,6	0.54	0
5	PO4	A	504	-	4,4,4	0.88	0	6,6,6	0.57	0
2	NAD	C	501	-	42,48,48	0.55	0	50,73,73	0.71	1 (2%)

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	A	502	-	-	-	0/2/2/2
3	ADE	D	502	-	-	-	0/2/2/2
3	ADE	C	502	-	-	-	0/2/2/2
2	NAD	B	501	-	-	5/26/62/62	0/5/5/5
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
3	ADE	B	502	-	-	-	0/2/2/2
7	R8A	D	505	-	-	0/2/2/2	0/1/1/1
2	NAD	D	501	-	-	5/26/62/62	0/5/5/5
2	NAD	C	501	-	-	5/26/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	505	R8A	C3-N1	4.65	1.45	1.34
3	C	502	ADE	C4-N3	-2.24	1.34	1.37
7	D	505	R8A	C2-C3	-2.18	1.39	1.42
3	B	502	ADE	C4-N3	-2.04	1.34	1.37
3	A	502	ADE	C4-N3	-2.03	1.34	1.37
3	D	502	ADE	C4-N3	-2.01	1.34	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	505	R8A	C4-N-C3	3.37	122.55	117.61
7	D	505	R8A	C-C4-N	-2.57	119.23	123.43
2	B	501	NAD	PN-O3-PA	-2.38	124.66	132.83
3	C	502	ADE	C5-C6-N6	2.36	123.93	120.35
2	C	501	NAD	C5A-C6A-N6A	2.28	123.81	120.35
2	B	501	NAD	C5A-C6A-N6A	2.21	123.71	120.35
2	D	501	NAD	C5A-C6A-N6A	2.19	123.68	120.35
2	A	501	NAD	C5A-C6A-N6A	2.19	123.68	120.35
3	D	502	ADE	C5-C6-N6	2.18	123.66	120.35
3	B	502	ADE	C5-C6-N6	2.12	123.57	120.35
3	A	502	ADE	C5-C6-N6	2.09	123.53	120.35

There are no chirality outliers.

All (20) 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
2	D	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

7 monomers are involved in 10 short contacts:

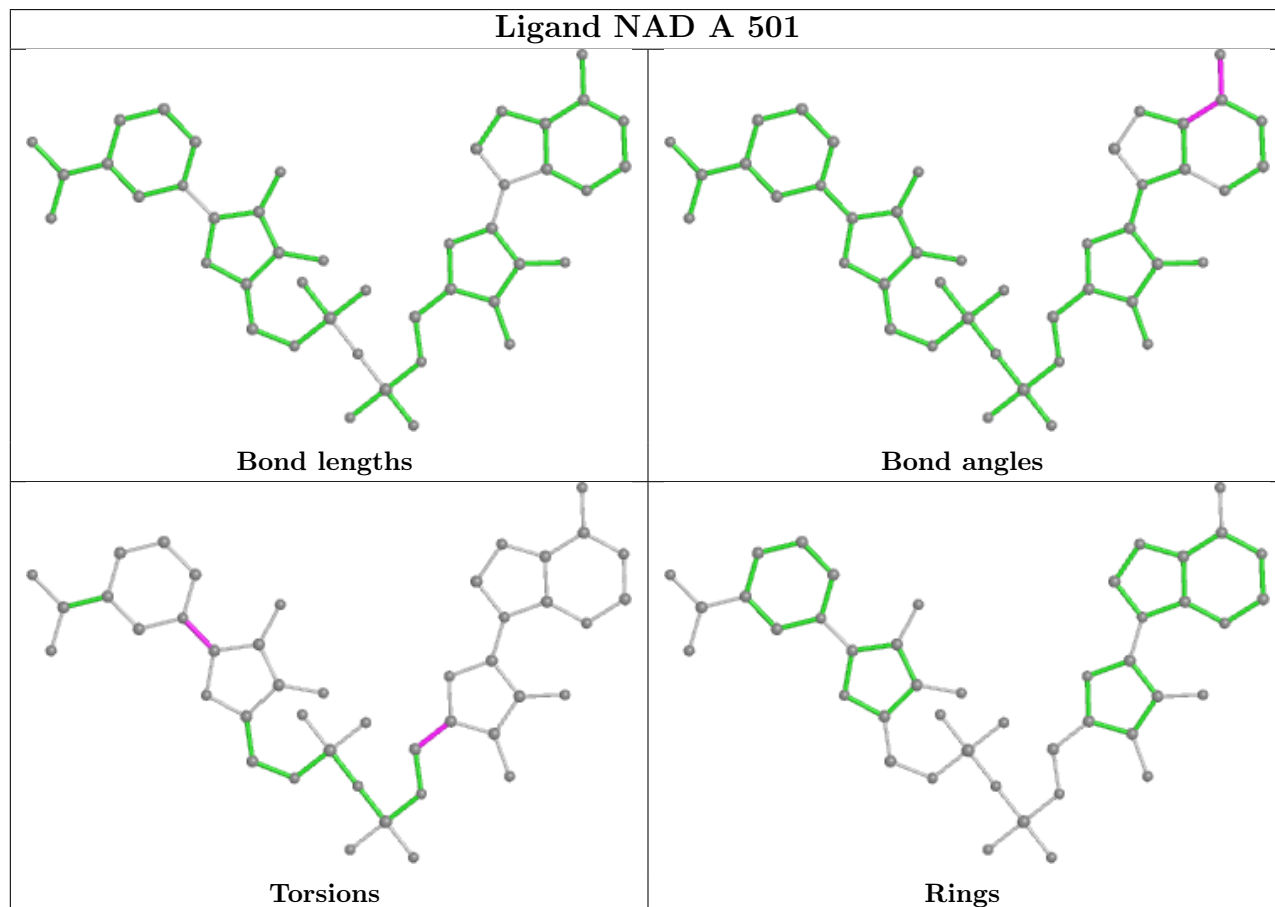
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	509	PO4	1	0

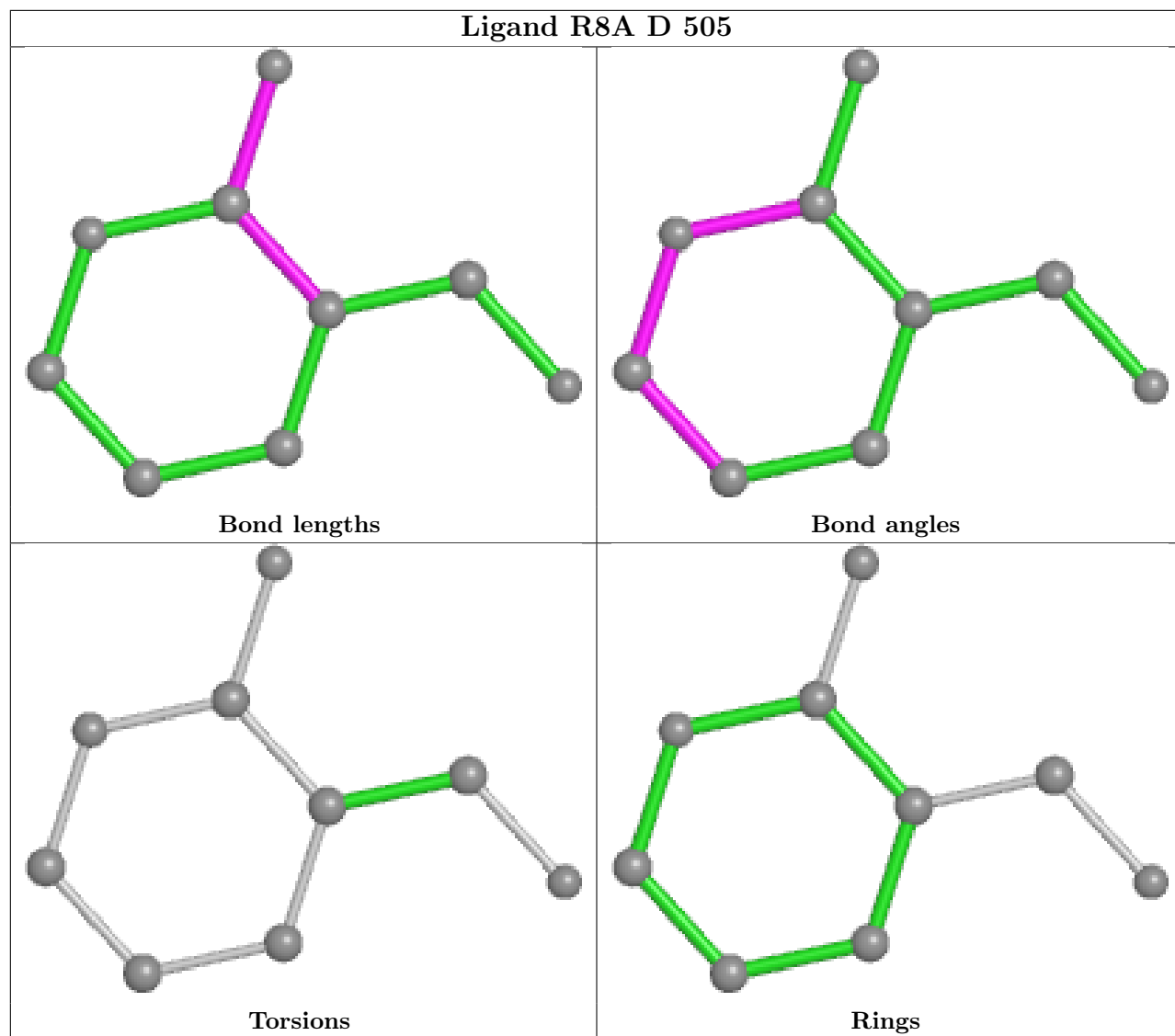
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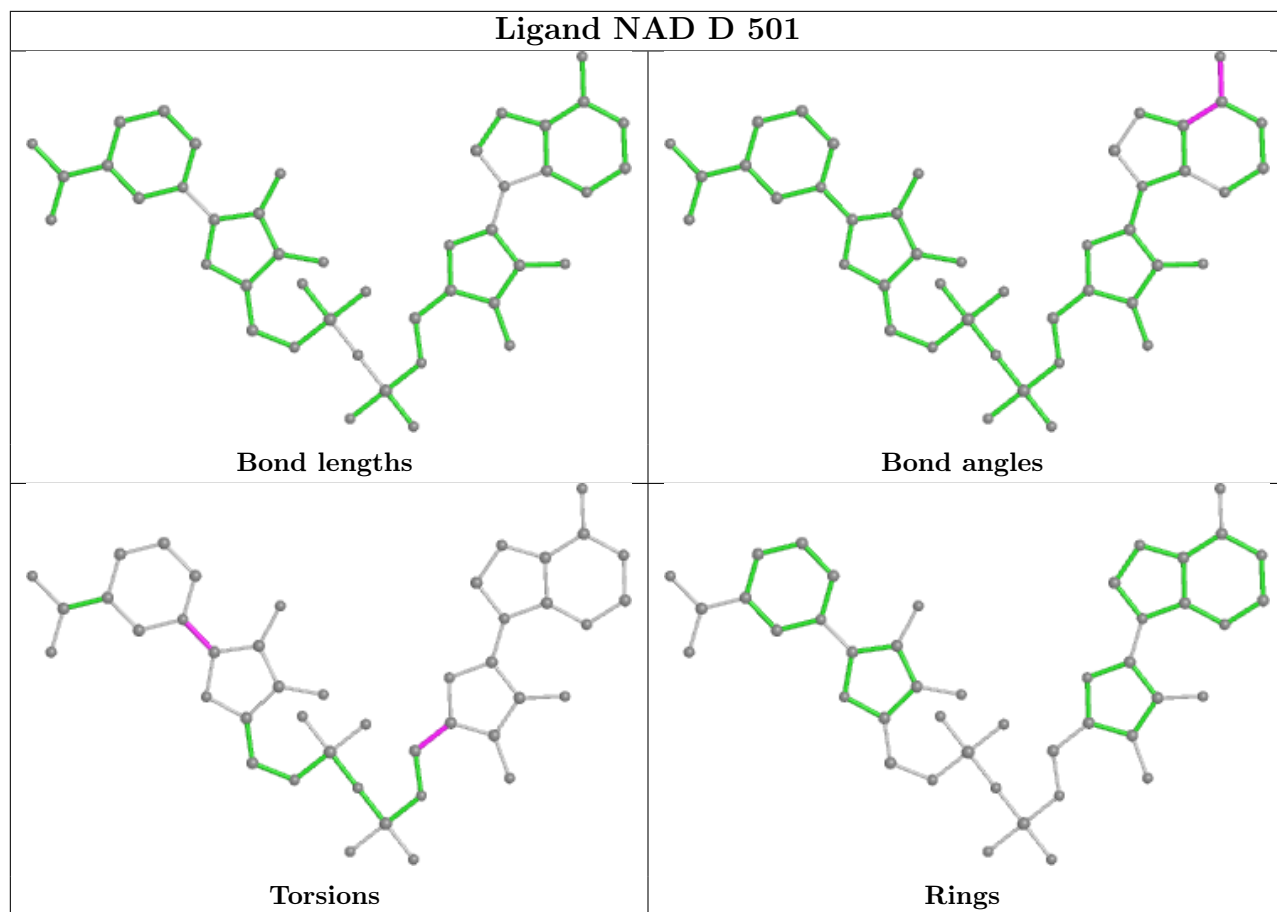
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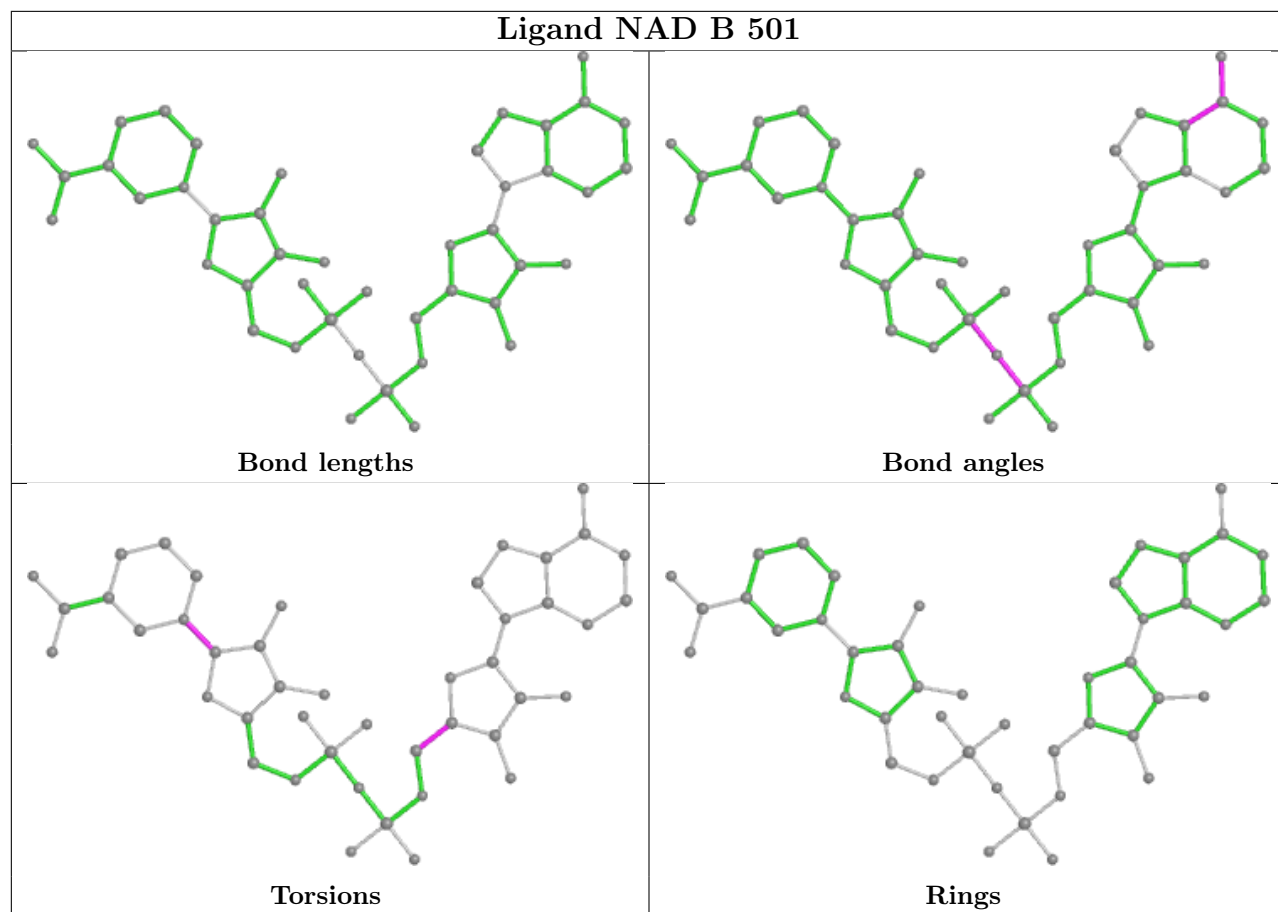
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	503	DMS	3	0
5	D	507	PO4	1	0
2	B	501	NAD	2	0
5	B	505	PO4	1	0
5	A	504	PO4	1	0
2	C	501	NAD	1	0

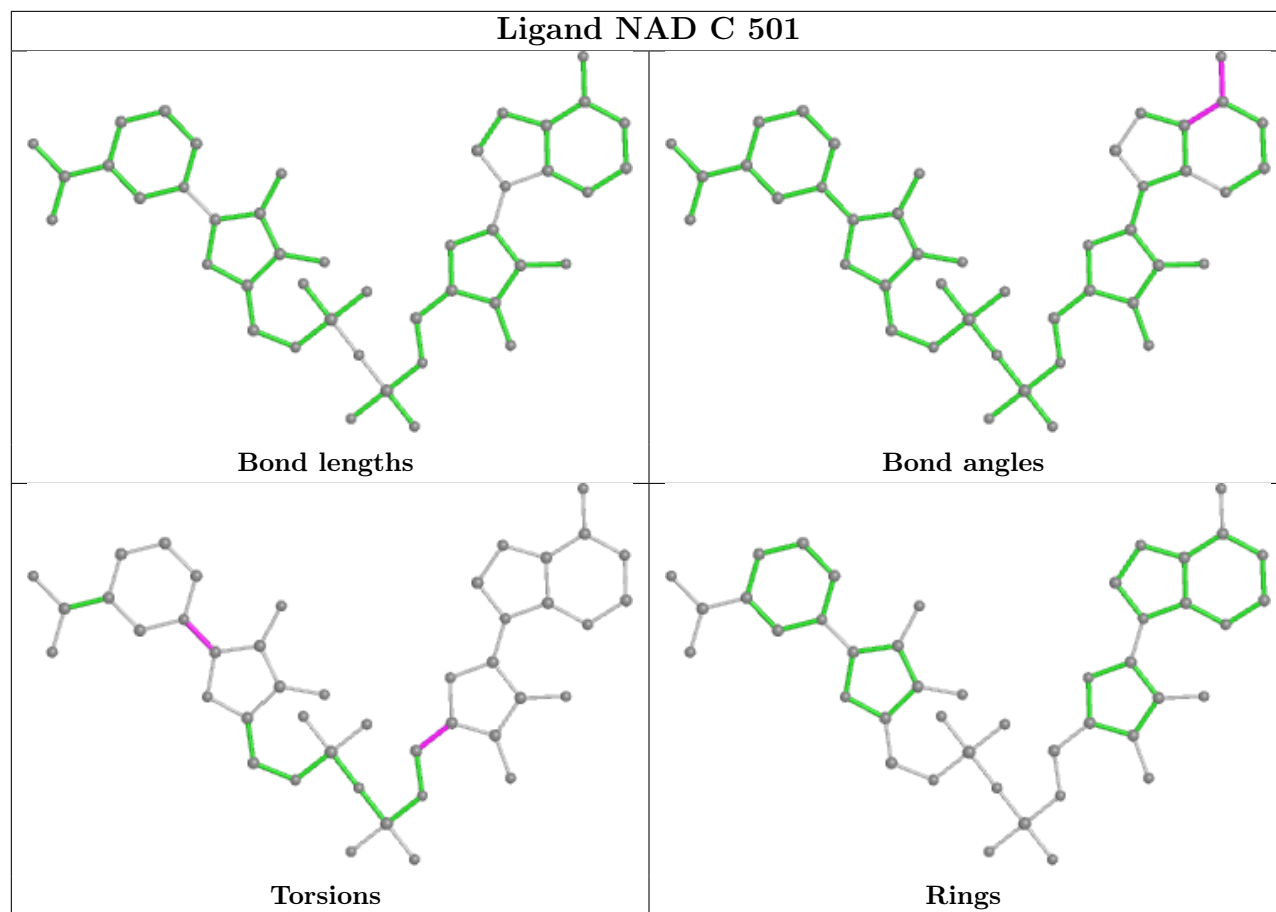
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	462/472 (97%)	0.48	50 (10%) 5 6	28, 39, 58, 100	0
1	B	461/472 (97%)	0.40	37 (8%) 12 13	28, 40, 59, 79	0
1	C	462/472 (97%)	0.31	31 (6%) 17 19	30, 40, 58, 100	0
1	D	461/472 (97%)	0.40	37 (8%) 12 13	28, 40, 60, 83	0
All	All	1846/1888 (97%)	0.40	155 (8%) 11 12	28, 40, 59, 100	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	8	ALA	5.9
1	A	8	ALA	5.7
1	A	410	PRO	5.5
1	A	355	ASP	5.1
1	A	9	GLY	5.1
1	A	411	ALA	4.7
1	D	128	GLY	4.4
1	C	355	ASP	4.3
1	B	240	LEU	4.2
1	C	204[A]	ARG	4.2
1	A	240	LEU	4.1
1	A	409	LEU	4.0
1	C	10	PHE	4.0
1	D	247	VAL	4.0
1	A	265	PHE	3.9
1	D	355	ASP	3.8
1	A	204[A]	ARG	3.8
1	D	240	LEU	3.8
1	B	247	VAL	3.8
1	C	9	GLY	3.8
1	D	127	ASP	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	335	LYS	3.8
1	A	412	ALA	3.7
1	B	118	TRP	3.6
1	B	219	LEU	3.6
1	D	9	GLY	3.6
1	A	354	LYS	3.6
1	A	219	LEU	3.5
1	B	353	GLY	3.5
1	C	241	ARG	3.5
1	C	265	PHE	3.4
1	B	264	GLY	3.3
1	A	129	GLN	3.3
1	A	207	LEU	3.3
1	A	236	SER	3.2
1	A	261	CYS	3.1
1	D	150	LYS	3.1
1	A	232	VAL	3.1
1	D	246	ILE	3.1
1	D	265	PHE	3.1
1	B	10	PHE	3.0
1	D	264	GLY	3.0
1	A	235	GLY	3.0
1	A	242	GLN	3.0
1	B	238	GLN	3.0
1	C	240	LEU	2.9
1	D	358	ASP	2.9
1	D	219	LEU	2.9
1	B	355	ASP	2.9
1	C	242	GLN	2.9
1	A	413	GLU	2.9
1	C	219	LEU	2.9
1	A	415	ALA	2.8
1	C	331	ALA	2.8
1	D	354	LYS	2.8
1	C	264	GLY	2.8
1	A	244	GLY	2.8
1	A	246	ILE	2.7
1	B	177	LYS	2.7
1	A	10	PHE	2.7
1	B	9	GLY	2.7
1	A	260	ALA	2.7
1	B	201	TYR	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	241	ARG	2.7
1	D	244	GLY	2.7
1	D	121	GLU	2.7
1	A	118	TRP	2.7
1	A	239	SER	2.7
1	C	238[A]	GLN	2.6
1	B	207	LEU	2.6
1	C	218	LEU	2.6
1	D	261	CYS	2.6
1	A	237	SER	2.6
1	D	207	LEU	2.6
1	D	118	TRP	2.6
1	C	247	VAL	2.6
1	B	114	GLU	2.6
1	C	201	TYR	2.5
1	B	218	LEU	2.5
1	C	118	TRP	2.5
1	C	276	ASN	2.5
1	B	124	ILE	2.5
1	B	246	ILE	2.5
1	C	235	GLY	2.5
1	C	246	ILE	2.5
1	D	10	PHE	2.4
1	B	243	GLU	2.4
1	B	224	ALA	2.4
1	A	247	VAL	2.4
1	D	11	THR	2.4
1	B	244	GLY	2.4
1	C	244	GLY	2.4
1	C	356	GLY	2.4
1	B	261	CYS	2.4
1	B	239	SER	2.4
1	A	128	GLY	2.4
1	A	353	GLY	2.4
1	A	241	ARG	2.3
1	A	238	GLN	2.3
1	B	226	VAL	2.3
1	C	203	CYS	2.3
1	A	264	GLY	2.3
1	A	408	ASP	2.3
1	D	245	MET	2.3
1	D	218	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	242	GLN	2.3
1	A	229	TYR	2.3
1	B	413	GLU	2.3
1	A	249	VAL	2.3
1	C	232	VAL	2.3
1	A	224	ALA	2.3
1	B	120	ILE	2.3
1	B	242	GLN	2.3
1	A	114	GLU	2.3
1	D	182	LYS	2.3
1	A	210	ALA	2.2
1	C	354	LYS	2.2
1	A	279	THR	2.2
1	B	11	THR	2.2
1	B	127	ASP	2.2
1	C	129	GLN	2.2
1	A	13	TYR	2.2
1	B	203	CYS	2.2
1	B	354	LYS	2.2
1	B	258[A]	MET	2.2
1	B	265	PHE	2.2
1	A	356	GLY	2.2
1	C	117	GLU	2.2
1	D	237	SER	2.2
1	D	386	ILE	2.1
1	B	235	GLY	2.1
1	B	335	LYS	2.1
1	D	359	ALA	2.1
1	D	229	TYR	2.1
1	A	234	LYS	2.1
1	A	293	LEU	2.1
1	D	192	VAL	2.1
1	A	321	ILE	2.1
1	D	260	ALA	2.1
1	C	239	SER	2.1
1	A	416	LYS	2.1
1	D	335	LYS	2.1
1	D	123	THR	2.1
1	D	232	VAL	2.1
1	D	238	GLN	2.1
1	D	221	GLY	2.1
1	A	334	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	332	PHE	2.0
1	B	232	VAL	2.0
1	B	181	LEU	2.0
1	D	406	TYR	2.0
1	D	211	ILE	2.0
1	C	237	SER	2.0
1	A	203	CYS	2.0
1	C	261	CYS	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, 95<sup>th</sup> 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.

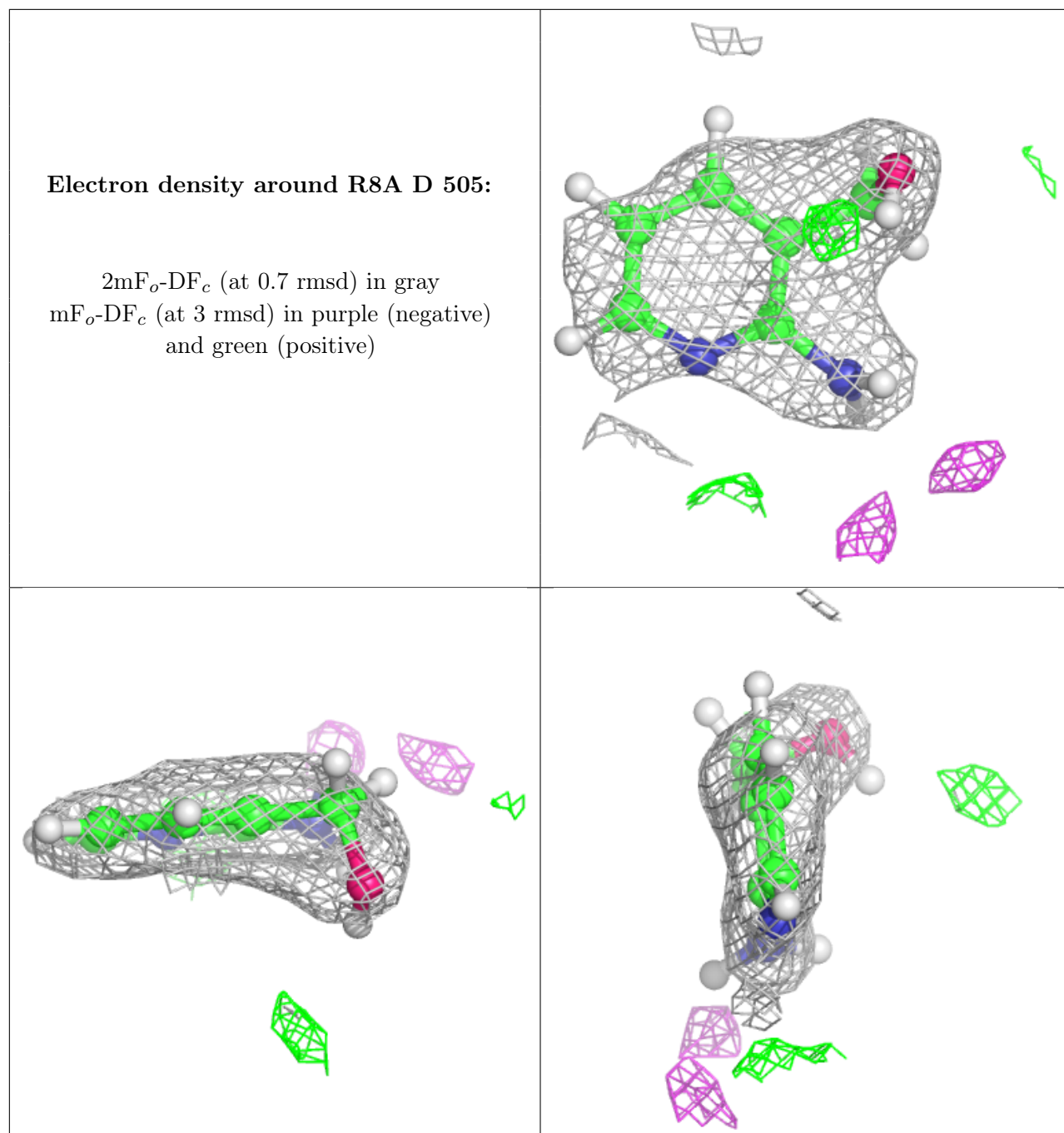
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	DMS	C	503	4/4	0.81	0.22	42,44,55,67	0
7	R8A	D	505	9/9	0.81	0.22	45,50,59,60	17
6	DMS	D	503	4/4	0.83	0.26	38,45,45,57	4
5	PO4	D	510	5/5	0.85	0.22	37,42,44,48	5
5	PO4	C	507	5/5	0.89	0.13	44,47,51,51	5
5	PO4	C	508	5/5	0.89	0.18	43,44,47,48	5
5	PO4	B	505	5/5	0.91	0.21	39,42,44,44	5
6	DMS	D	504	4/4	0.92	0.23	65,70,88,88	0
3	ADE	A	502	10/10	0.92	0.11	30,34,36,37	0
5	PO4	D	507	5/5	0.93	0.17	41,44,44,45	5
5	PO4	A	504	5/5	0.93	0.11	42,44,47,47	5
3	ADE	D	502	10/10	0.94	0.09	36,40,44,46	0
5	PO4	B	506	5/5	0.94	0.10	33,38,38,43	5
2	NAD	C	501	44/44	0.95	0.10	29,34,36,37	0
2	NAD	A	501	44/44	0.95	0.11	29,32,35,37	0

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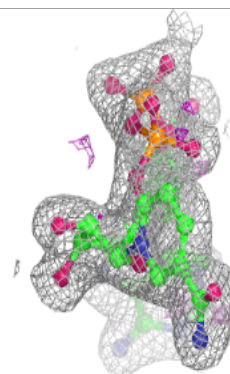
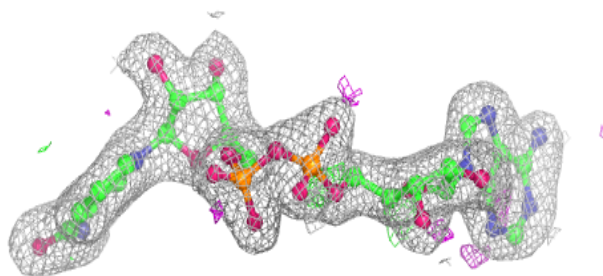
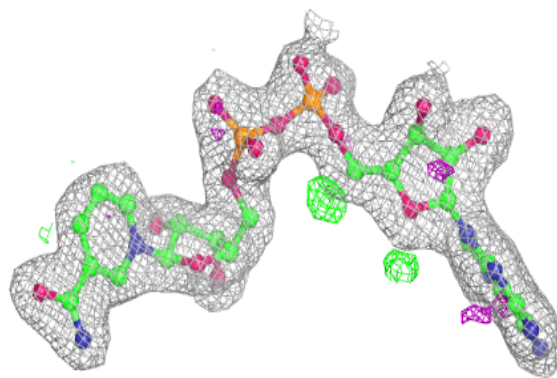
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PO4	C	509	5/5	0.95	0.18	40,44,46,47	5
3	ADE	B	502	10/10	0.96	0.10	34,35,37,37	0
3	ADE	C	502	10/10	0.96	0.11	34,35,39,40	0
5	PO4	C	505	5/5	0.96	0.13	46,47,49,51	5
2	NAD	D	501	44/44	0.96	0.08	26,33,36,37	0
2	NAD	B	501	44/44	0.96	0.09	27,33,35,37	0
5	PO4	A	506	5/5	0.96	0.12	32,33,38,38	5
5	PO4	A	505	5/5	0.97	0.14	44,48,51,54	0
5	PO4	C	506	5/5	0.97	0.10	36,36,40,46	5
5	PO4	B	504	5/5	0.97	0.24	51,53,53,55	0
5	PO4	D	508	5/5	0.97	0.22	49,51,54,55	0
5	PO4	D	509	5/5	0.97	0.10	34,36,40,44	5
4	K	D	506	1/1	0.99	0.15	31,31,31,31	0
4	K	A	503	1/1	0.99	0.11	33,33,33,33	0
4	K	B	503	1/1	1.00	0.11	33,33,33,33	0
4	K	C	504	1/1	1.00	0.15	34,34,34,34	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.

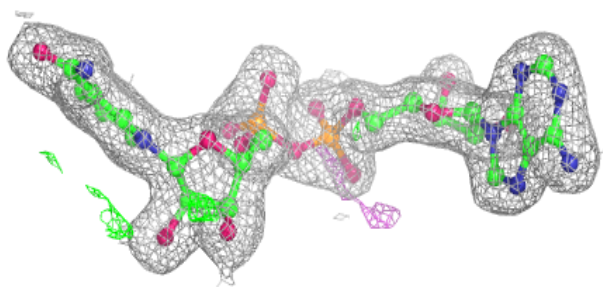
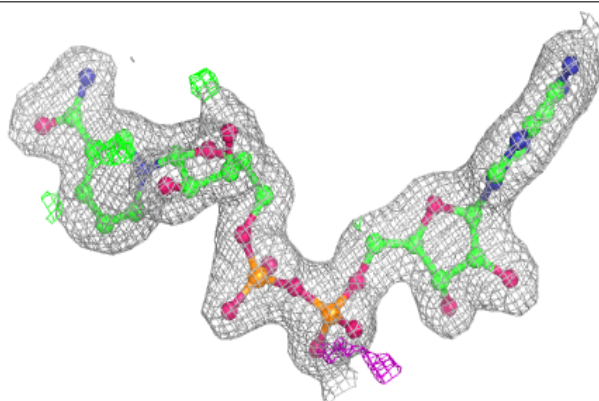


**Electron density around NAD C 501:**

$2mF_o-DF_c$  (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:**

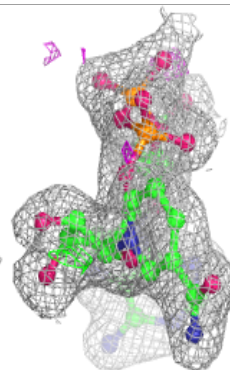
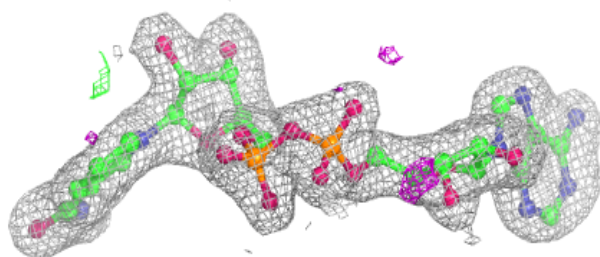
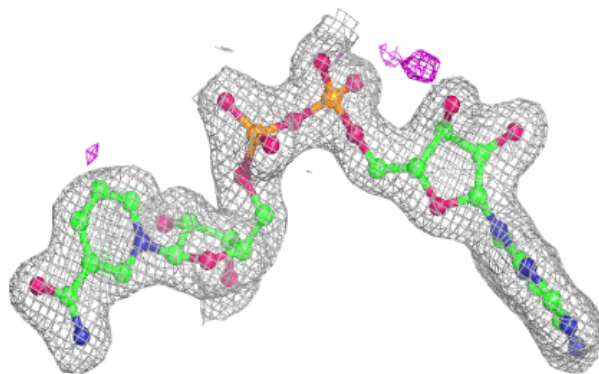
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



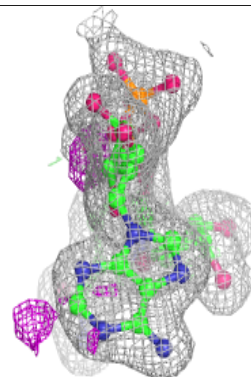
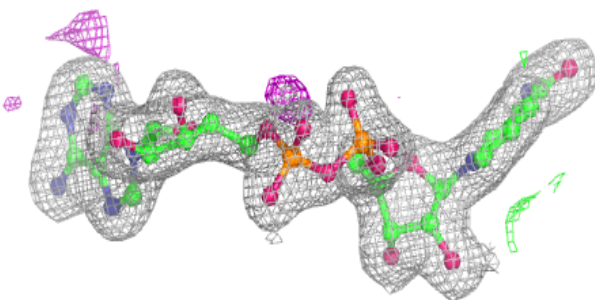
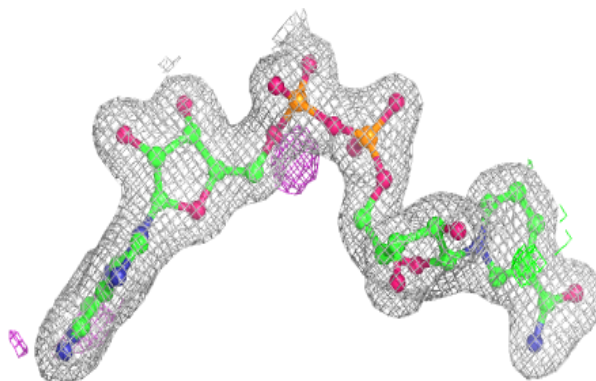


**Electron density around NAD D 501:**

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

**Electron density around NAD B 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.