



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:25 pm BST

PDB ID : 6F3Q  
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *Pseudomonas aeruginosa* in complex with adenine and Rb<sup>+</sup> cation  
Authors : Czyrko, J.; Brzezinski, K.  
Deposited on : 2017-11-28  
Resolution : 1.45 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.

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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 : 1.8.5 (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

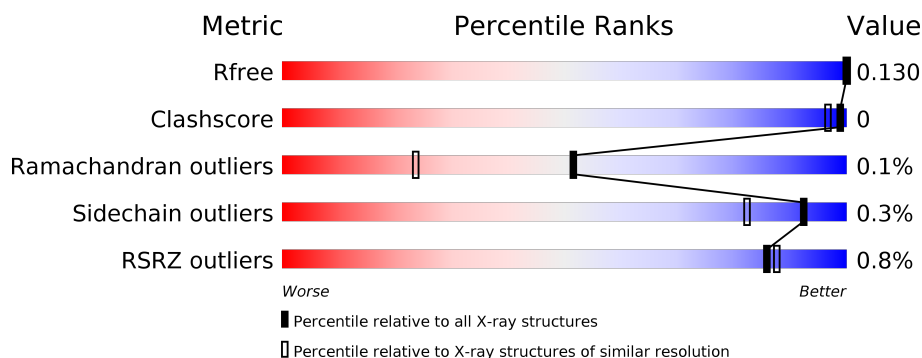
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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  $\geq 3$ , 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	<div> <div>%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div>• •</div> </div>
1	B	472	<div> <div>%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div>• •</div> </div>
1	C	472	<div> <div>%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div>• •</div> </div>
1	D	472	<div> <div></div> <div>95%</div> <div></div> </div> <div>• •</div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 16994 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	460	Total	C	N	O	S	0	15	0
			3644	2303	634	684	23			
1	B	460	Total	C	N	O	S	0	12	0
			3612	2282	623	684	23			
1	C	460	Total	C	N	O	S	0	16	0
			3650	2308	628	690	24			
1	D	461	Total	C	N	O	S	0	16	0
			3648	2301	631	694	22			

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 RUBIDIUM ION (three-letter code: Rb) (formula: Rb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Rb	0	0
			2	2		
2	A	1	Total	Rb	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Rb	0	0
			1	1		
2	C	1	Total	Rb	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



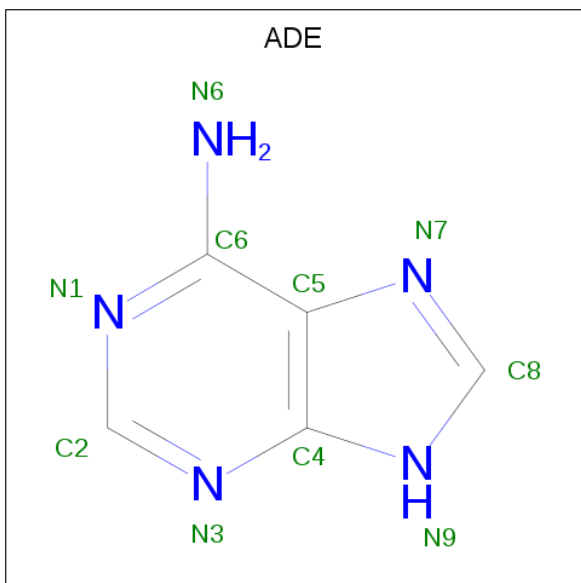
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 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>).



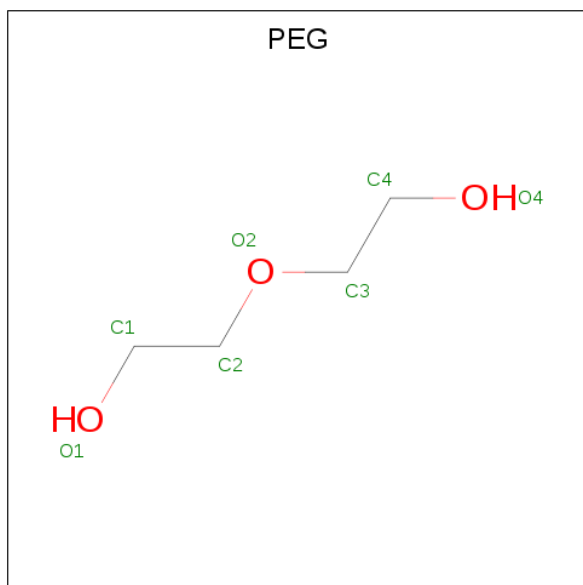
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

- 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 DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

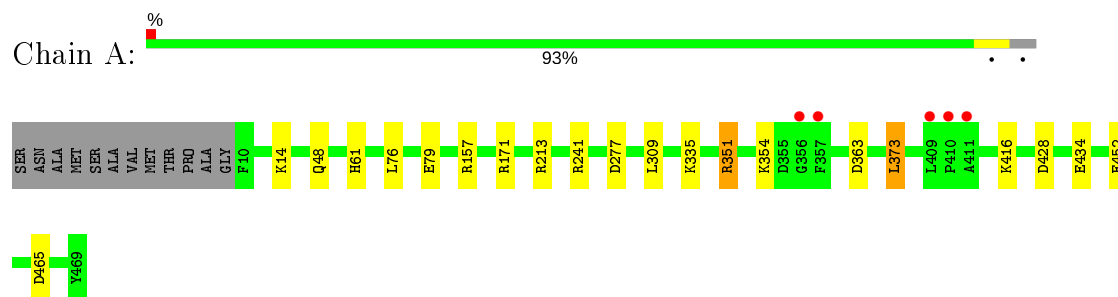
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	519	Total	O	0	17
			526	526		
8	B	588	Total	O	0	28
			604	604		
8	C	468	Total	O	0	13
			474	474		
8	D	553	Total	O	0	21
			562	562		

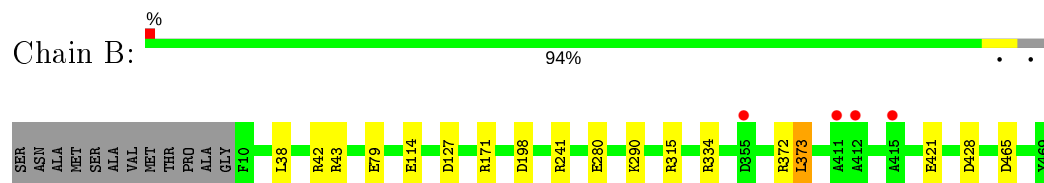
### 3 Residue-property plots [i](#)

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.

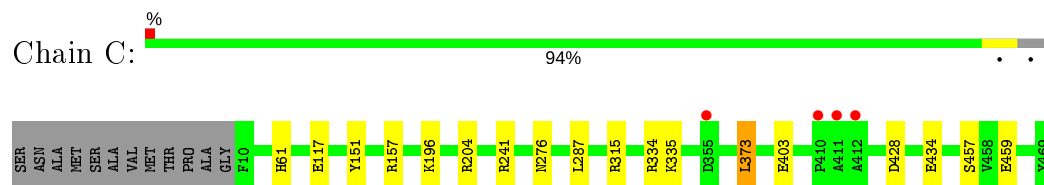
- Molecule 1: Adenosylhomocysteinase



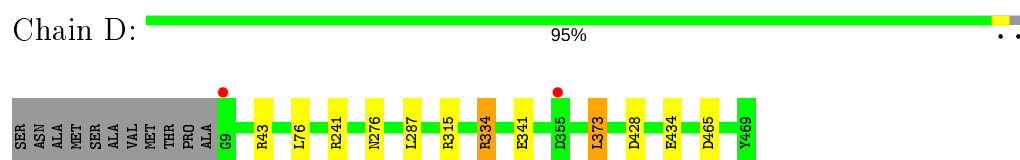
- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.49Å 99.44Å 111.71Å 90.00° 101.93° 90.00°	Depositor
Resolution (Å)	48.53 – 1.45 48.53 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.53-1.45) 98.6 (48.53-1.45)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.093 , 0.124 0.098 , 0.130	Depositor DCC
$R_{free}$ test set	3343 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.2	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	16994	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0998e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAD, PO4, ADE, RB, 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	0.84	3/3728 (0.1%)	0.99	16/5034 (0.3%)
1	B	0.90	6/3696 (0.2%)	0.95	13/4994 (0.3%)
1	C	0.86	6/3737 (0.2%)	0.95	11/5048 (0.2%)
1	D	0.85	4/3729 (0.1%)	0.92	12/5038 (0.2%)
All	All	0.86	19/14890 (0.1%)	0.95	52/20114 (0.3%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	GLU	CD-OE1	10.63	1.37	1.25
1	A	434	GLU	CD-OE2	8.20	1.34	1.25
1	C	276	ASN	CG-ND2	8.17	1.53	1.32
1	A	79	GLU	CD-OE2	-7.78	1.17	1.25
1	B	79	GLU	CD-OE2	-7.75	1.17	1.25
1	A	452	GLU	CD-OE1	7.64	1.34	1.25
1	D	434	GLU	CD-OE2	6.74	1.33	1.25
1	D	334	ARG	CZ-NH1	6.02	1.40	1.33
1	D	341	GLU	CD-OE1	-6.02	1.19	1.25
1	C	151	TYR	CE2-CZ	5.88	1.46	1.38
1	C	151	TYR	CE1-CZ	-5.64	1.31	1.38
1	B	421	GLU	CG-CD	-5.58	1.43	1.51
1	C	117	GLU	CD-OE1	-5.41	1.19	1.25
1	C	403	GLU	CD-OE2	5.36	1.31	1.25
1	C	434	GLU	CD-OE2	5.22	1.31	1.25
1	B	38	LEU	CB-CG	-5.19	1.37	1.52
1	B	42	ARG	CB-CG	-5.13	1.38	1.52
1	D	276	ASN	CG-OD1	5.12	1.35	1.24
1	B	280	GLU	CD-OE1	5.05	1.31	1.25

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	241	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	A	351[A]	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	A	351[B]	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	A	351[A]	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	A	351[B]	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	D	334	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	B	334	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	A	241	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	C	315	ARG	NE-CZ-NH2	9.18	124.89	120.30
1	C	334[A]	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	C	334[B]	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	B	241	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	D	315	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	C	241	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	416	LYS	CD-CE-NZ	-7.62	94.19	111.70
1	C	157	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	B	465	ASP	CB-CG-OD1	7.13	124.71	118.30
1	A	428	ASP	CB-CG-OD1	7.05	124.65	118.30
1	D	428	ASP	CB-CG-OD1	7.05	124.64	118.30
1	D	373[A]	LEU	CA-CB-CG	6.80	130.94	115.30
1	D	373[B]	LEU	CA-CB-CG	6.80	130.94	115.30
1	A	465	ASP	CB-CG-OD1	6.65	124.28	118.30
1	B	171	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	C	373[A]	LEU	CA-CB-CG	6.54	130.34	115.30
1	C	373[B]	LEU	CA-CB-CG	6.54	130.34	115.30
1	B	428	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	373[A]	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	373[B]	LEU	CA-CB-CG	6.31	129.81	115.30
1	B	372	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	315	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	B	171	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	D	241	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	277	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	D	465	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	373[A]	LEU	CA-CB-CG	6.07	129.25	115.30
1	B	373[B]	LEU	CA-CB-CG	6.07	129.25	115.30
1	B	127	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	A	171	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	213	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	D	43[A]	ARG	CG-CD-NE	-5.83	99.56	111.80
1	D	76	LEU	CB-CG-CD2	5.73	120.74	111.00
1	A	213	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	198	ASP	CB-CG-OD2	-5.63	113.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	428	ASP	CB-CG-OD1	5.61	123.34	118.30
1	B	43	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	76	LEU	CB-CG-CD2	5.42	120.21	111.00
1	A	157	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	334	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	43[A]	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	196[A]	LYS	CB-CG-CD	5.08	124.81	111.60
1	C	196[B]	LYS	CB-CG-CD	5.08	124.81	111.60
1	C	204	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3644	0	3687	5	0
1	B	3612	0	3638	1	0
1	C	3650	0	3686	5	0
1	D	3648	0	3658	2	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	44	0	26	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	7	0	10	0	0
7	D	6	0	7	0	0
8	A	526	0	0	1	0
8	B	604	0	0	1	0
8	C	474	0	0	3	0
8	D	562	0	0	2	0
All	All	16994	0	14806	13	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 0.

All (13) 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:459:GLU:HG3	8:C:971:HOH:O	1.84	0.76
1:A:14[B]:LYS:HE2	8:A:1019:HOH:O	1.86	0.75
1:D:287:LEU:HD12	8:D:731:HOH:O	1.88	0.74
1:C:287:LEU:HD12	8:C:924:HOH:O	1.91	0.71
1:C:457[B]:SER:OG	1:C:459:GLU:OE1	2.23	0.57
1:D:334:ARG:NH1	8:D:603:HOH:O	2.38	0.57
1:C:457[B]:SER:OG	1:C:459:GLU:CD	2.44	0.56
1:A:309:LEU:O	1:A:351[A]:ARG:NH2	2.40	0.50
1:C:335:LYS:HG3	8:C:872:HOH:O	2.11	0.50
1:B:290:LYS:HD3	8:B:601[A]:HOH:O	2.14	0.47
1:A:335:LYS:O	1:A:354:LYS:HD2	2.16	0.46
1:A:351[A]:ARG:HD3	1:A:363:ASP:OD1	2.19	0.42
1:A:48[A]:GLN:O	1:A:48[A]:GLN:HG2	2.19	0.41

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	471/472 (100%)	463 (98%)	7 (2%)	1 (0%)	47	22
1	B	468/472 (99%)	460 (98%)	8 (2%)	0	100	100
1	C	473/472 (100%)	464 (98%)	8 (2%)	1 (0%)	47	22
1	D	472/472 (100%)	464 (98%)	8 (2%)	0	100	100
All	All	1884/1888 (100%)	1851 (98%)	31 (2%)	2 (0%)	51	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	C	61	HIS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/385 (101%)	388 (100%)	2 (0%)	88	75
1	B	387/385 (100%)	385 (100%)	2 (0%)	88	75
1	C	392/385 (102%)	390 (100%)	2 (0%)	88	75
1	D	390/385 (101%)	388 (100%)	2 (0%)	88	75
All	All	1559/1540 (101%)	1551 (100%)	8 (0%)	92	75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373[A]	LEU
1	A	373[B]	LEU
1	B	373[A]	LEU
1	B	373[B]	LEU
1	C	373[A]	LEU
1	C	373[B]	LEU
1	D	373[A]	LEU
1	D	373[B]	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 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
3	PO4	C	503	-	4,4,4	2.19	2 (50%)	6,6,6	1.34	1 (16%)
5	ADE	D	506	-	9,11,11	0.74	0	7,15,15	0.85	0
3	PO4	D	503	-	4,4,4	1.28	0	6,6,6	0.95	0
3	PO4	B	504	-	4,4,4	2.23	1 (25%)	6,6,6	1.59	1 (16%)
3	PO4	C	502	-	4,4,4	1.53	1 (25%)	6,6,6	1.88	2 (33%)
4	NAD	C	504	-	42,48,48	0.80	1 (2%)	50,73,73	1.04	2 (4%)
4	NAD	D	505	-	42,48,48	0.84	1 (2%)	50,73,73	1.05	3 (6%)
5	ADE	B	507	-	9,11,11	0.78	0	7,15,15	0.98	0
3	PO4	B	503	-	4,4,4	1.29	0	6,6,6	0.66	0
4	NAD	A	504	-	42,48,48	0.80	1 (2%)	50,73,73	0.97	0
3	PO4	A	502	-	4,4,4	1.16	0	6,6,6	1.37	0
3	PO4	D	504	-	4,4,4	1.79	1 (25%)	6,6,6	1.97	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ADE	A	505	-	9,11,11	0.68	0	7,15,15	1.36	1 (14%)
5	ADE	C	505	-	9,11,11	0.92	1 (11%)	7,15,15	1.05	1 (14%)
4	NAD	B	506	-	42,48,48	1.01	3 (7%)	50,73,73	1.04	4 (8%)
3	PO4	A	503	-	4,4,4	1.32	1 (25%)	6,6,6	0.25	0
7	GOL	D	502	-	5,5,5	1.45	1 (20%)	5,5,5	1.74	2 (40%)
6	PEG	B	505	-	6,6,6	0.56	0	5,5,5	1.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADE	D	506	-	-	-	0/2/2/2
4	NAD	A	504	-	-	5/26/62/62	0/5/5/5
4	NAD	C	504	-	-	5/26/62/62	0/5/5/5
4	NAD	D	505	-	-	5/26/62/62	0/5/5/5
5	ADE	B	507	-	-	-	0/2/2/2
5	ADE	A	505	-	-	-	0/2/2/2
5	ADE	C	505	-	-	-	0/2/2/2
4	NAD	B	506	-	-	5/26/62/62	0/5/5/5
7	GOL	D	502	-	-	0/4/4/4	-
6	PEG	B	505	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	504	PO4	P-O1	3.83	1.59	1.50
3	C	503	PO4	P-O1	3.63	1.59	1.50
3	D	504	PO4	P-O1	3.42	1.58	1.50
4	B	506	NAD	C4N-C3N	2.62	1.43	1.39
4	A	504	NAD	C4N-C3N	2.46	1.43	1.39
3	A	503	PO4	P-O1	2.37	1.56	1.50
4	B	506	NAD	O4B-C1B	2.36	1.44	1.41
3	C	502	PO4	P-O1	2.32	1.56	1.50
7	D	502	GOL	O2-C2	2.18	1.49	1.43
4	C	504	NAD	C2A-N3A	2.16	1.35	1.32
4	B	506	NAD	C2A-N3A	2.15	1.35	1.32
3	C	503	PO4	P-O4	2.06	1.60	1.54
4	D	505	NAD	C2A-N3A	2.01	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	505	ADE	C2-N3	2.01	1.35	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	PO4	O2-P-O1	-3.31	98.77	110.89
7	D	502	GOL	C3-C2-C1	-3.00	100.02	111.70
3	D	504	PO4	O3-P-O1	-2.92	100.20	110.89
3	B	504	PO4	O4-P-O2	-2.83	98.88	107.97
3	D	504	PO4	O4-P-O2	2.82	117.01	107.97
4	B	506	NAD	O4B-C1B-C2B	-2.77	102.87	106.93
5	A	505	ADE	C5-C6-N6	2.73	124.50	120.35
4	D	505	NAD	C3N-C7N-N7N	2.61	120.88	117.75
3	C	502	PO4	O4-P-O3	2.60	116.32	107.97
4	C	504	NAD	C3N-C7N-N7N	2.57	120.84	117.75
4	B	506	NAD	C3N-C7N-N7N	2.36	120.59	117.75
7	D	502	GOL	O2-C2-C3	2.31	119.31	109.12
4	C	504	NAD	C2N-N1N-C1D	-2.23	114.17	119.14
3	C	503	PO4	O4-P-O3	2.13	114.81	107.97
4	D	505	NAD	C5N-C4N-C3N	-2.13	117.82	120.34
4	B	506	NAD	O2A-PA-O1A	2.12	122.73	112.24
4	D	505	NAD	C2N-N1N-C1D	-2.10	114.46	119.14
4	B	506	NAD	PN-O3-PA	-2.06	125.77	132.83
5	C	505	ADE	C5-C6-N6	2.01	123.41	120.35

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	505	NAD	O4D-C1D-N1N-C2N
4	D	505	NAD	O4D-C1D-N1N-C6N
4	D	505	NAD	C2D-C1D-N1N-C2N
4	D	505	NAD	C2D-C1D-N1N-C6N
4	A	504	NAD	O4D-C1D-N1N-C2N
4	A	504	NAD	O4D-C1D-N1N-C6N
4	A	504	NAD	C2D-C1D-N1N-C2N
4	A	504	NAD	C2D-C1D-N1N-C6N
4	C	504	NAD	O4D-C1D-N1N-C2N
4	C	504	NAD	O4D-C1D-N1N-C6N
4	C	504	NAD	C2D-C1D-N1N-C2N
4	C	504	NAD	C2D-C1D-N1N-C6N
4	B	506	NAD	O4D-C1D-N1N-C2N

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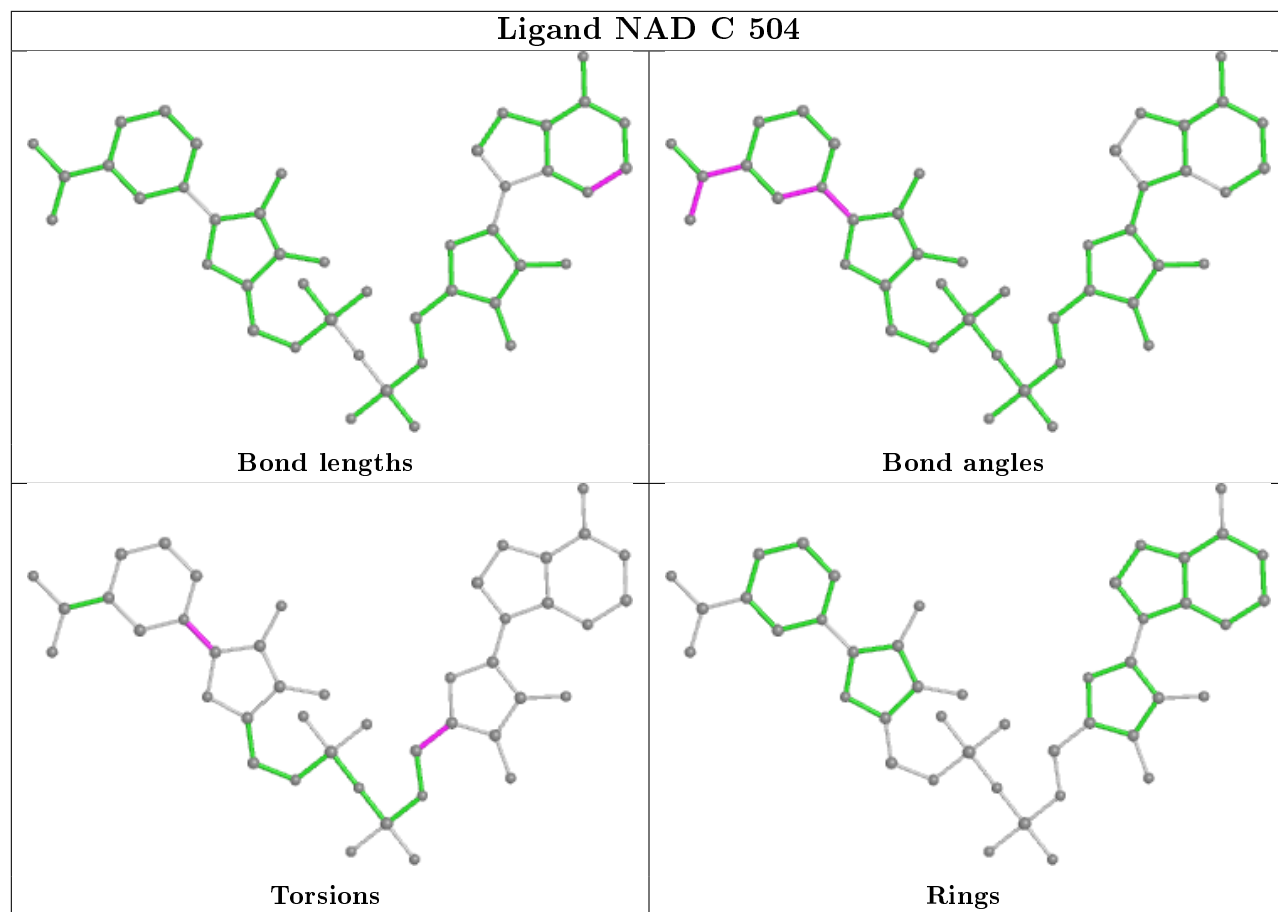
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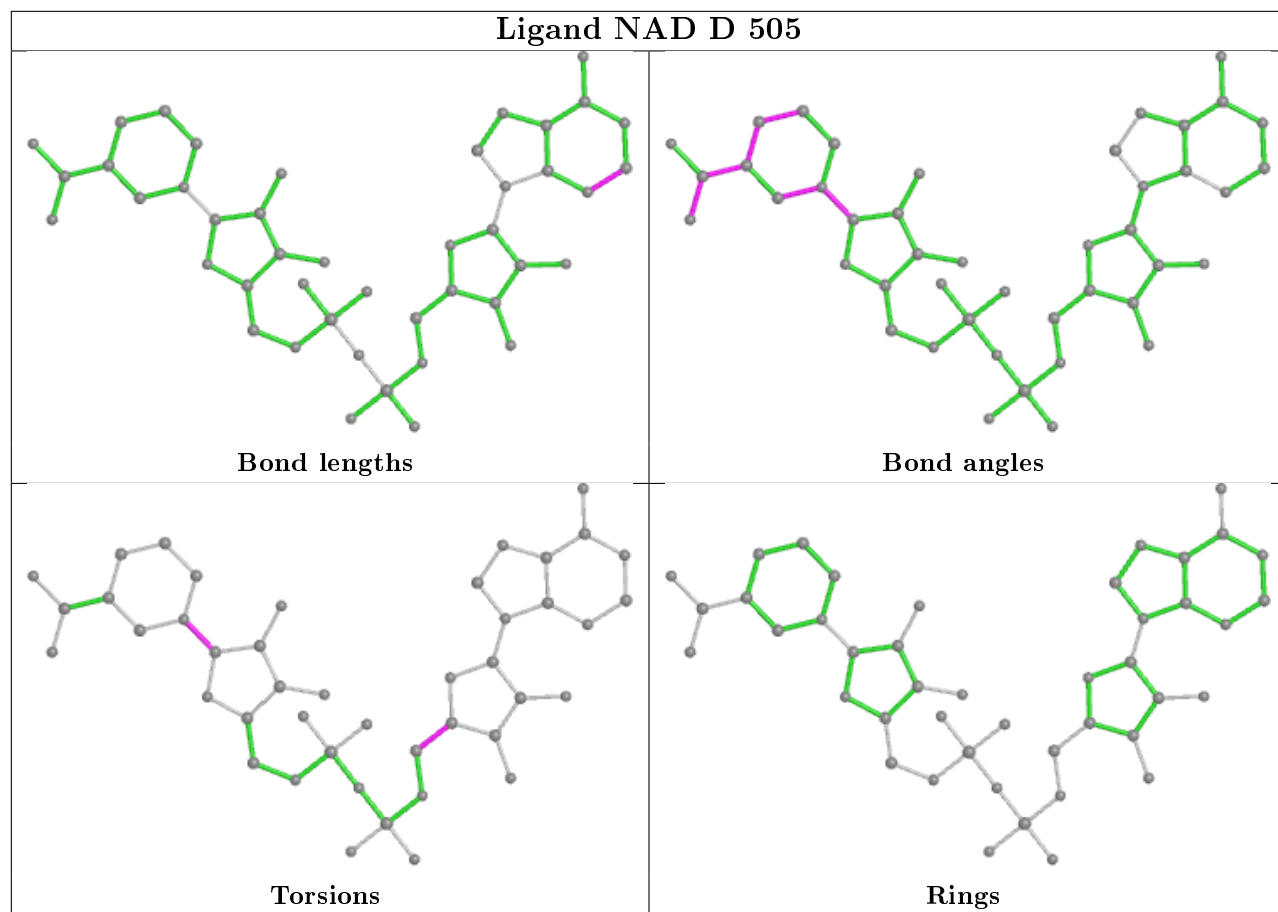
Mol	Chain	Res	Type	Atoms
4	B	506	NAD	O4D-C1D-N1N-C6N
4	B	506	NAD	C2D-C1D-N1N-C2N
4	B	506	NAD	C2D-C1D-N1N-C6N
6	B	505	PEG	O2-C3-C4-O4
6	B	505	PEG	C1-C2-O2-C3
4	D	505	NAD	O4B-C4B-C5B-O5B
4	A	504	NAD	O4B-C4B-C5B-O5B
4	C	504	NAD	O4B-C4B-C5B-O5B
4	B	506	NAD	O4B-C4B-C5B-O5B

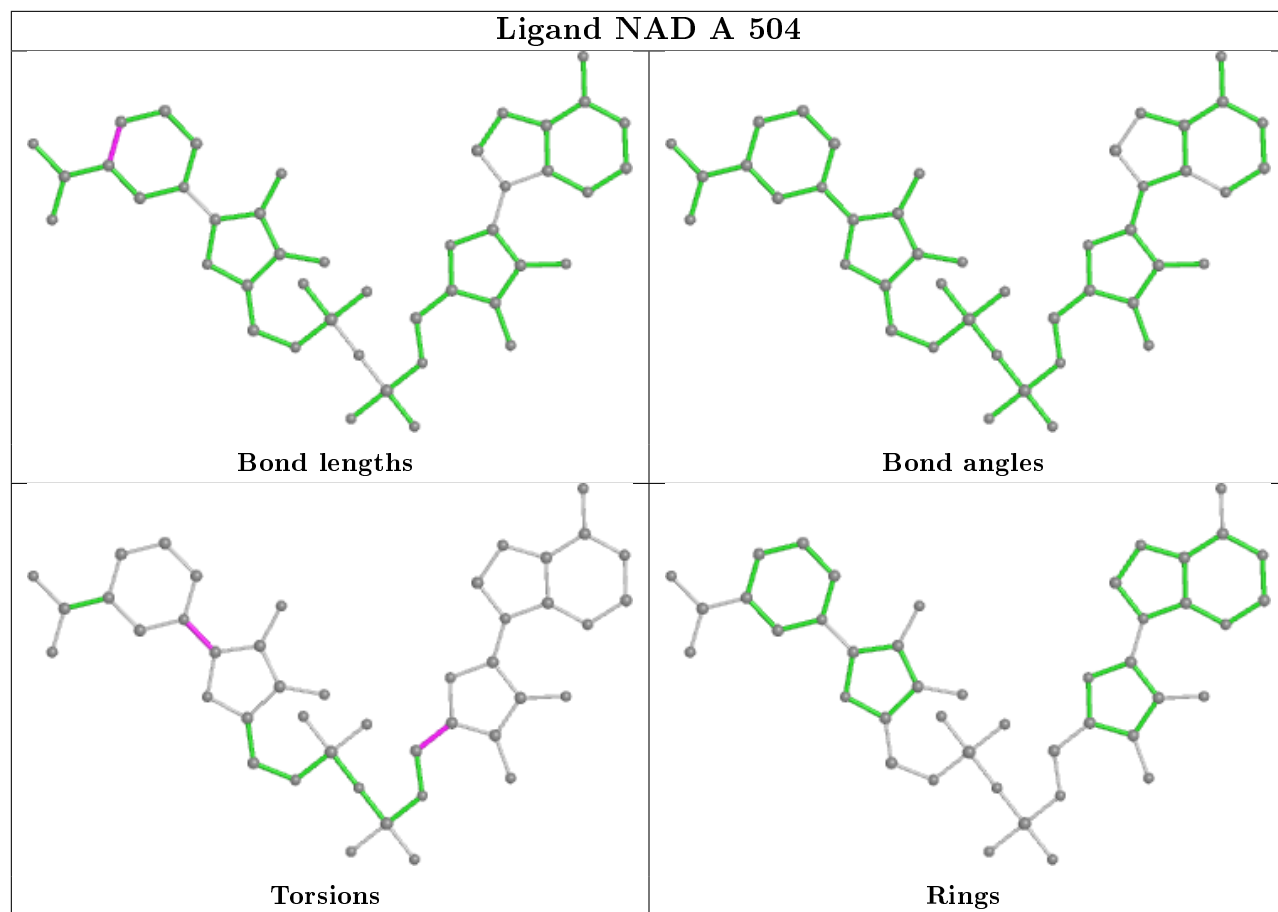
There are no ring outliers.

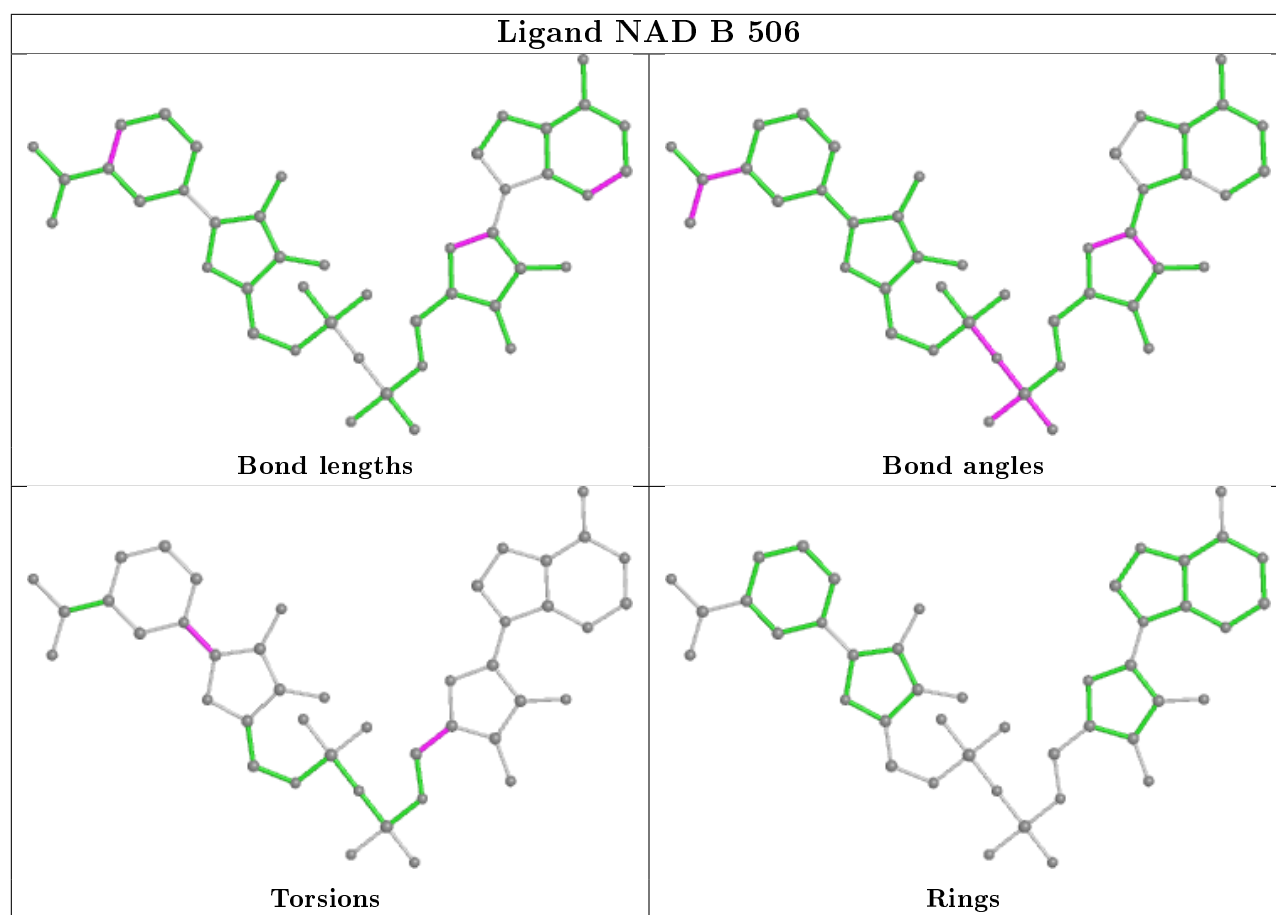
No monomer is involved in short contacts.

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 [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	460/472 (97%)	-0.34	5 (1%) 80 82	9, 15, 28, 42	13 (2%)
1	B	460/472 (97%)	-0.40	4 (0%) 84 86	8, 12, 23, 43	12 (2%)
1	C	460/472 (97%)	-0.36	4 (0%) 84 86	10, 16, 31, 47	17 (3%)
1	D	461/472 (97%)	-0.39	2 (0%) 92 94	9, 13, 24, 52	12 (2%)
All	All	1841/1888 (97%)	-0.37	15 (0%) 86 87	8, 14, 27, 52	54 (2%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	ALA	4.1
1	B	411	ALA	3.8
1	D	9	GLY	3.5
1	B	355	ASP	3.3
1	C	410	PRO	2.9
1	C	355	ASP	2.8
1	D	355	ASP	2.5
1	C	412	ALA	2.5
1	B	412	ALA	2.4
1	A	410	PRO	2.3
1	A	356	GLY	2.3
1	A	357	PHE	2.1
1	A	409	LEU	2.1
1	A	411	ALA	2.1
1	C	411	ALA	2.1

### 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 ⓘ

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, 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.

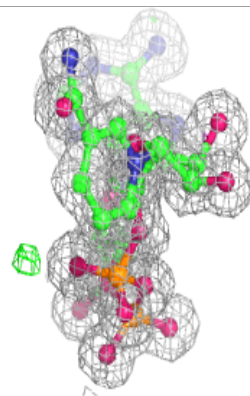
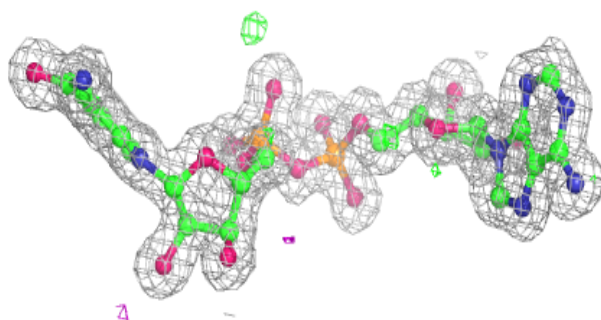
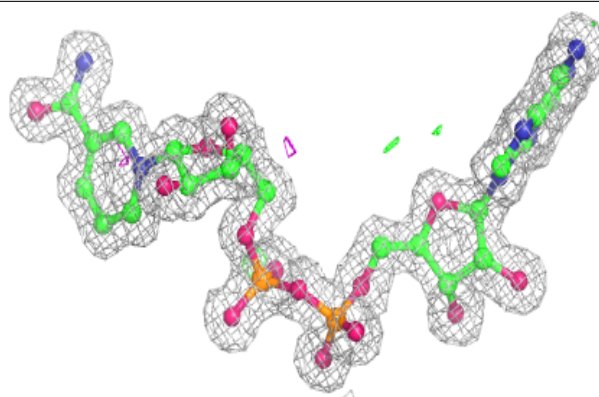
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PEG	B	505	7/7	0.94	0.17	22,23,26,31	7
7	GOL	D	502	6/6	0.96	0.08	19,21,22,27	0
3	PO4	A	503	5/5	0.97	0.14	21,22,26,28	0
3	PO4	B	503	5/5	0.97	0.10	18,18,19,22	0
3	PO4	C	503	5/5	0.97	0.18	24,26,29,31	0
3	PO4	B	504	5/5	0.98	0.07	14,14,15,16	0
3	PO4	D	503	5/5	0.98	0.15	19,20,23,23	0
3	PO4	A	502	5/5	0.98	0.05	16,17,17,18	0
3	PO4	C	502	5/5	0.98	0.07	17,17,19,19	0
3	PO4	D	504	5/5	0.98	0.05	14,15,16,16	0
5	ADE	A	505	10/10	0.98	0.06	9,10,12,12	0
5	ADE	C	505	10/10	0.98	0.06	10,11,12,12	0
4	NAD	C	504	44/44	0.99	0.05	9,11,12,14	0
5	ADE	B	507	10/10	0.99	0.05	7,8,8,8	0
4	NAD	D	505	44/44	0.99	0.06	8,10,12,14	0
5	ADE	D	506	10/10	0.99	0.07	8,9,9,9	0
4	NAD	A	504	44/44	0.99	0.06	9,10,12,15	0
4	NAD	B	506	44/44	0.99	0.06	7,9,11,12	0
2	RB	B	501	1/1	1.00	0.03	9,9,9,9	0
2	RB	B	502	1/1	1.00	0.06	22,22,22,22	1
2	RB	D	501	1/1	1.00	0.03	10,10,10,10	0
2	RB	C	501	1/1	1.00	0.04	12,12,12,12	0
2	RB	A	501	1/1	1.00	0.03	11,11,11,11	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.

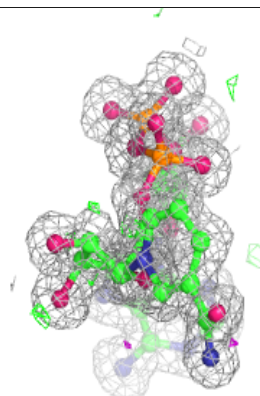
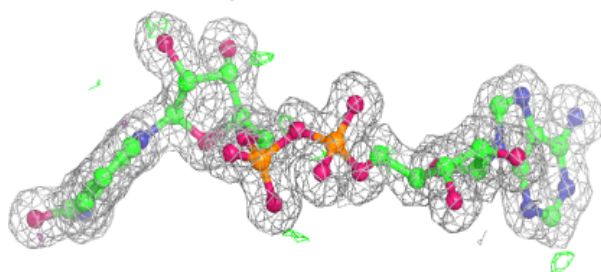
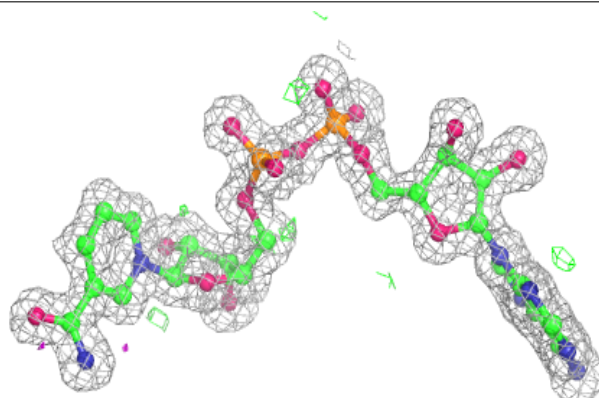


**Electron density around NAD C 504:**

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

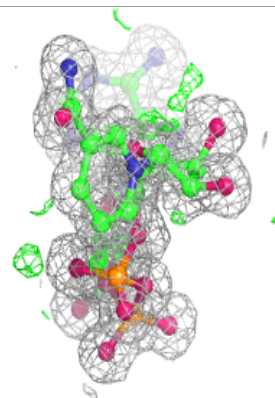
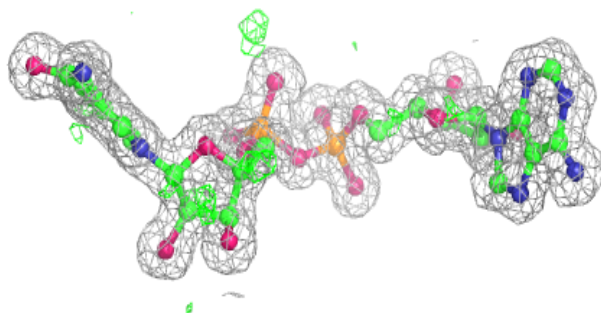
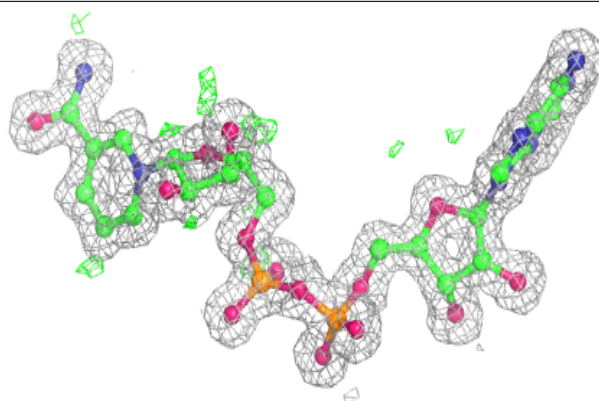
**Electron density around NAD D 505:**

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

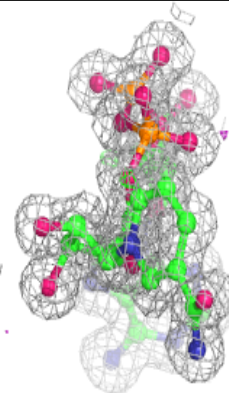
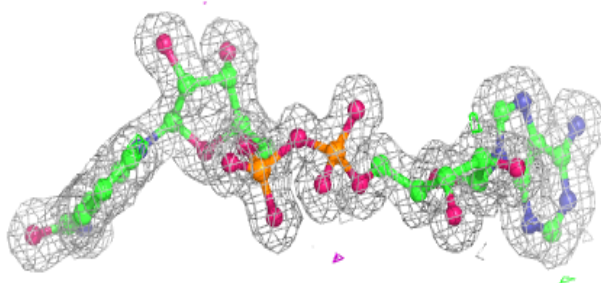
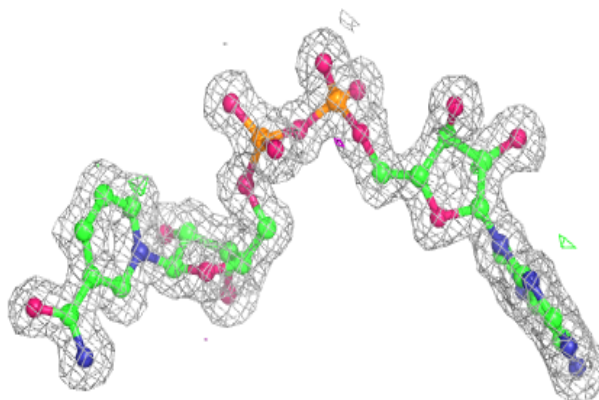


**Electron density around NAD A 504:**

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

**Electron density around NAD B 506:**

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



## 6.5 Other polymers

There are no such residues in this entry.