



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:13 AM UTC

PDB ID : 6KIA / pdb_00006kia
Title : NADH bound structure of FabMG, novel type of Enoyl-acyl carrier protein reductase
Authors : Kim, S.; Rhee, S.
Deposited on : 2019-07-17
Resolution : 1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

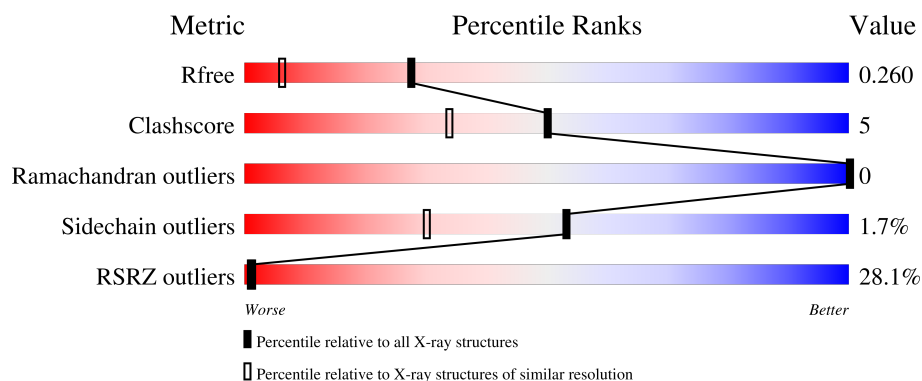
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	446	6% 93% 6%
1	B	446	5% 90% 8%
1	C	446	67% 61% 19% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10664 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 Enoyl-acyl carrier protein reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3432	2173	598	643	18			
1	B	440	Total	C	N	O	S	0	0	0
			3412	2161	592	641	18			
1	C	367	Total	C	N	O	S	0	0	0
			2825	1807	475	527	16			

There are 24 discrepancies between the modelled and reference sequences:

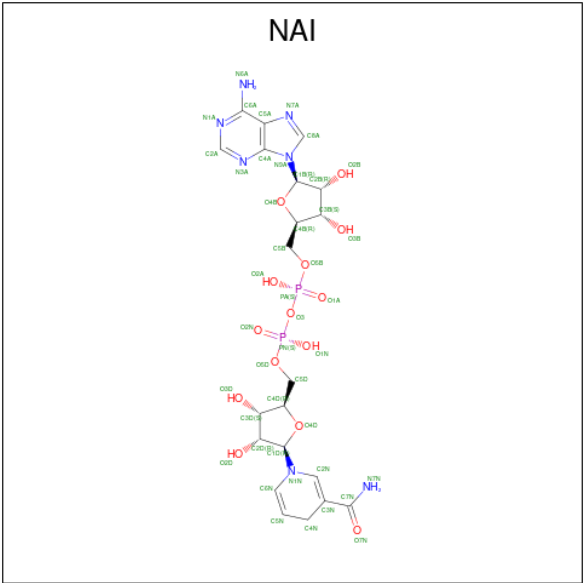
Chain	Residue	Modelled	Actual	Comment	Reference
A	439	LEU	-	expression tag	UNP A0A1C9HA64
A	440	GLU	-	expression tag	UNP A0A1C9HA64
A	441	HIS	-	expression tag	UNP A0A1C9HA64
A	442	HIS	-	expression tag	UNP A0A1C9HA64
A	443	HIS	-	expression tag	UNP A0A1C9HA64
A	444	HIS	-	expression tag	UNP A0A1C9HA64
A	445	HIS	-	expression tag	UNP A0A1C9HA64
A	446	HIS	-	expression tag	UNP A0A1C9HA64
B	439	LEU	-	expression tag	UNP A0A1C9HA64
B	440	GLU	-	expression tag	UNP A0A1C9HA64
B	441	HIS	-	expression tag	UNP A0A1C9HA64
B	442	HIS	-	expression tag	UNP A0A1C9HA64
B	443	HIS	-	expression tag	UNP A0A1C9HA64
B	444	HIS	-	expression tag	UNP A0A1C9HA64
B	445	HIS	-	expression tag	UNP A0A1C9HA64
B	446	HIS	-	expression tag	UNP A0A1C9HA64
C	439	LEU	-	expression tag	UNP A0A1C9HA64
C	440	GLU	-	expression tag	UNP A0A1C9HA64
C	441	HIS	-	expression tag	UNP A0A1C9HA64
C	442	HIS	-	expression tag	UNP A0A1C9HA64
C	443	HIS	-	expression tag	UNP A0A1C9HA64
C	444	HIS	-	expression tag	UNP A0A1C9HA64
C	445	HIS	-	expression tag	UNP A0A1C9HA64

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Chain	Residue	Modelled	Actual	Comment	Reference
C	446	HIS	-	expression tag	UNP A0A1C9HA64

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

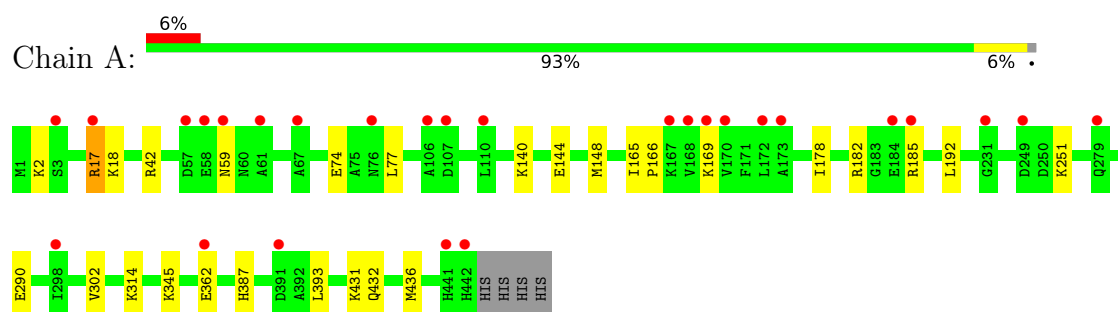
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	397	Total	O	0	0
			397	397		
3	B	417	Total	O	0	0
			417	417		
3	C	49	Total	O	0	0
			49	49		

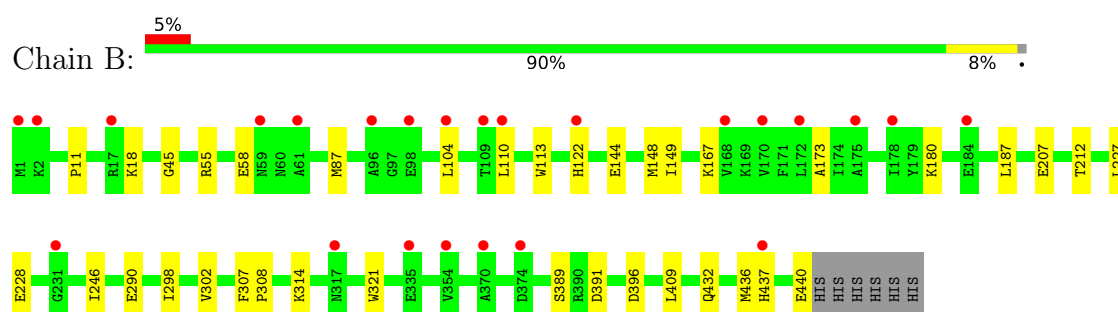
3 Residue-property plots [i](#)

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.

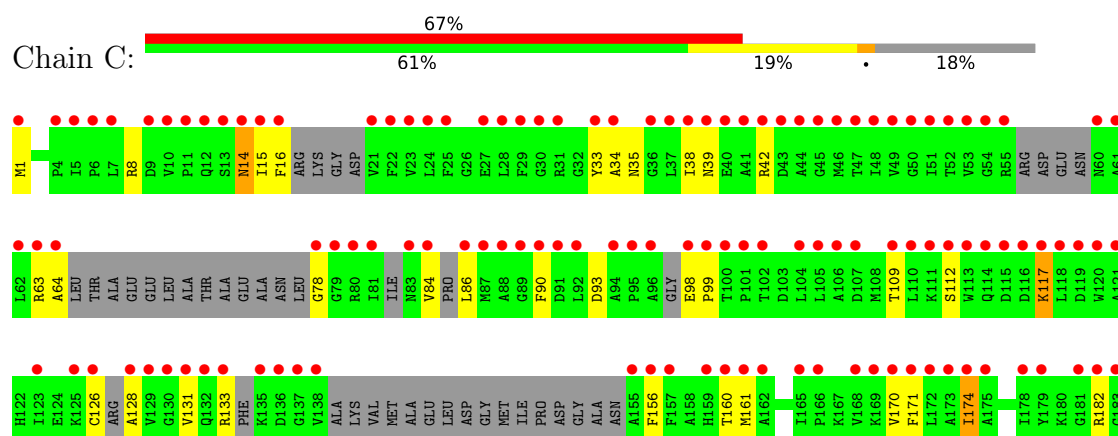
• Molecule 1: Enoyl-acyl carrier protein reductase



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• Molecule 1: Enoyl-acyl carrier protein reductase



V428	I429	A430	K431	Q432	L433	M434	L435	M436	H437	ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
M365	F367	N368	T369	A370	E371	L372	A373	D374	I375	M376	I377	G378	T379	S380	D381	E382	I383	T384
K385	M386	H387	LYS	SER	ARG	ASP	A392	L393	V394	T395	D396	V397	L398	S399	A400	L401	V402	L403
E404	G405	T406	G407	P408	L409	M410	F411	H412	E413	S414	M415	N416	P417	A418	G419	P420	V421	L422
W423	L424																	
L306	F307	P308	L309	L310	K311	A312	L313	K314	K315	E316	ASN	GLY	GLY	ALA	TRP	ALA	GLU	ALA
Q325	W326	Q327	A328	C329	R330	GLU	VAL	L272	A273	SER	E274	D275	GLY	HIS	T338	L339	E340	S341
L281	K282	N283	T284	V285	V286	N287	C288	P289	E290	I291	R292	T293	N294	M355	K356	G357	F358	R359
N360	F361	E362	A363	W364	P365													
L246	L247	D248	D249	Q250	K251	V252	Q253	W254	Q255	T256	V257	T258	S259	V260	T261	Q262	Q263	K264
A265	K266	W267	R268	L269	E270	R271	L272	A273	SER	E274	D275	GLY	HIS	T338	L339	E340	S341	L342
L343	Q344	K345	I346	D347	C348	Y349	N350	A351	S352	D353	V354	M355	K356	G357	F358	R359	N360	F361
E362	A363	W364	P365															
E184	R185	F186	L187	S188	A189	L192	L193	N194	S195	G198	K199	L200	I201	L202	M203	M204	F205	D206
E207	V208	T209	A210	N211	T212	F213	L214	H215	L216	T217	E218	G219	S220	ALA	A222	I223	R224	A225
R226	L227	E228	LYS	SER	GLY	GLY	GLN	VAL	ARG	Y236	S237	A238	Y239	G240	Y241	H242	G243	T244
E245																		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.56Å 138.22Å 157.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 1.60 29.81 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.81-1.60) 85.0 (29.81-1.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.224 , 0.259 0.226 , 0.260	Depositor DCC
R_{free} test set	2000 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10664	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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:
NAI

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	0.53	0/3501	0.78	1/4735 (0.0%)
1	B	0.54	0/3479	0.80	2/4705 (0.0%)
1	C	0.37	0/2871	0.78	2/3872 (0.1%)
All	All	0.49	0/9851	0.79	5/13312 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	419	GLY	CA-C-N	5.25	124.86	119.56
1	C	419	GLY	C-N-CA	5.25	124.86	119.56
1	A	59	ASN	N-CA-C	-5.23	106.74	113.02
1	B	307	PHE	CA-C-N	-5.18	114.48	119.87
1	B	307	PHE	C-N-CA	-5.18	114.48	119.87

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	3432	0	3419	19	0
1	B	3412	0	3405	26	0
1	C	2825	0	2769	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	26	0	0
2	B	44	0	27	0	0
2	C	44	0	27	3	0
3	A	397	0	0	7	0
3	B	417	0	0	5	0
3	C	49	0	0	0	0
All	All	10664	0	9673	103	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 5.

The worst 5 of 103 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:14:ASN:C	1:C:14:ASN:HD22	1.78	0.92
1:B:55:ARG:NH2	3:B:601:HOH:O	2.14	0.81
1:B:104:LEU:HD11	1:B:122:HIS:HD2	1.47	0.78
1:B:58:GLU:HB2	1:C:185:ARG:HH12	1.48	0.77
1:B:58:GLU:O	1:C:185:ARG:NH1	2.18	0.76

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	440/446 (99%)	432 (98%)	8 (2%)	0	100	100
1	B	438/446 (98%)	430 (98%)	8 (2%)	0	100	100
1	C	335/446 (75%)	331 (99%)	4 (1%)	0	100	100
All	All	1213/1338 (91%)	1193 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	359/363 (99%)	354 (99%)	5 (1%)	59	38
1	B	357/363 (98%)	357 (100%)	0	100	100
1	C	294/363 (81%)	282 (96%)	12 (4%)	27	8
All	All	1010/1089 (93%)	993 (98%)	17 (2%)	53	30

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	431	LYS
1	C	435	LEU
1	C	131	VAL
1	C	174	ILE
1	C	216	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	122	HIS
1	C	14	ASN
1	C	176	ASN
1	A	432	GLN
1	A	325	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAI	A	501	-	47,48,48	3.34	20 (42%)	64,73,73	2.05	17 (26%)
2	NAI	C	501	-	47,48,48	3.64	19 (40%)	64,73,73	2.18	16 (25%)
2	NAI	B	501	-	47,48,48	3.27	18 (38%)	64,73,73	1.93	16 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	A	501	-	-	7/29/72/72	0/5/5/5
2	NAI	C	501	-	-	5/29/72/72	0/5/5/5
2	NAI	B	501	-	-	7/29/72/72	0/5/5/5

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAI	C3B-C4B	-10.89	1.25	1.53
2	B	501	NAI	C3B-C4B	-9.74	1.28	1.53
2	A	501	NAI	C3B-C4B	-9.50	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAI	O4D-C1D	9.09	1.63	1.42
2	C	501	NAI	C2B-C1B	-8.30	1.27	1.53

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAI	N6A-C6A-N1A	-6.50	103.91	118.38
2	C	501	NAI	C4A-N9A-C1B	-5.91	112.81	126.63
2	C	501	NAI	N3A-C2A-N1A	-5.68	119.98	128.58
2	C	501	NAI	C1B-N9A-C8A	5.36	138.99	127.09
2	C	501	NAI	C5A-C6A-N6A	5.30	136.40	123.29

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAI	C5B-O5B-PA-O2A
2	A	501	NAI	C5D-O5D-PN-O3
2	A	501	NAI	C5D-O5D-PN-O1N
2	A	501	NAI	C5D-O5D-PN-O2N
2	B	501	NAI	C5D-O5D-PN-O3

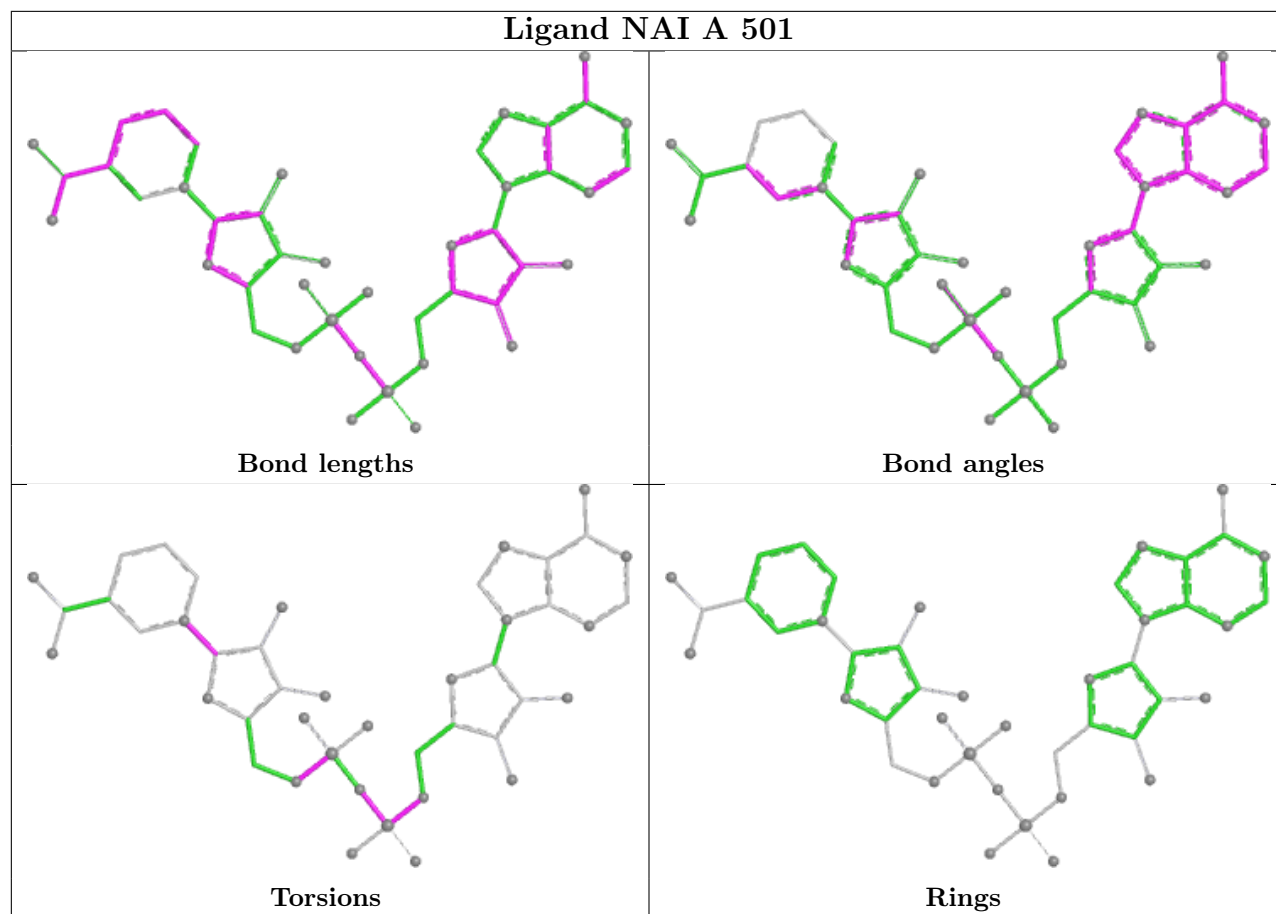
There are no ring outliers.

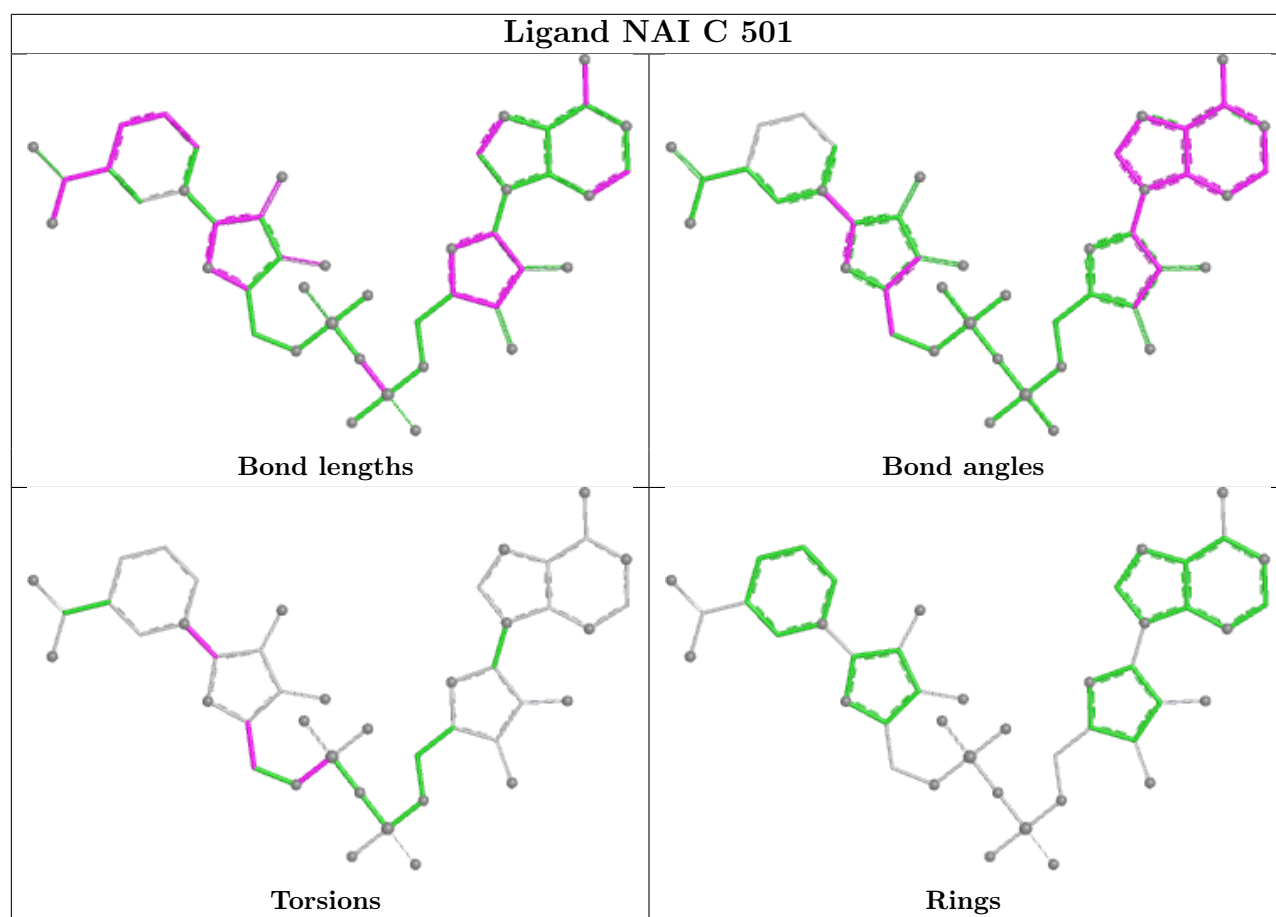
1 monomer is involved in 3 short contacts:

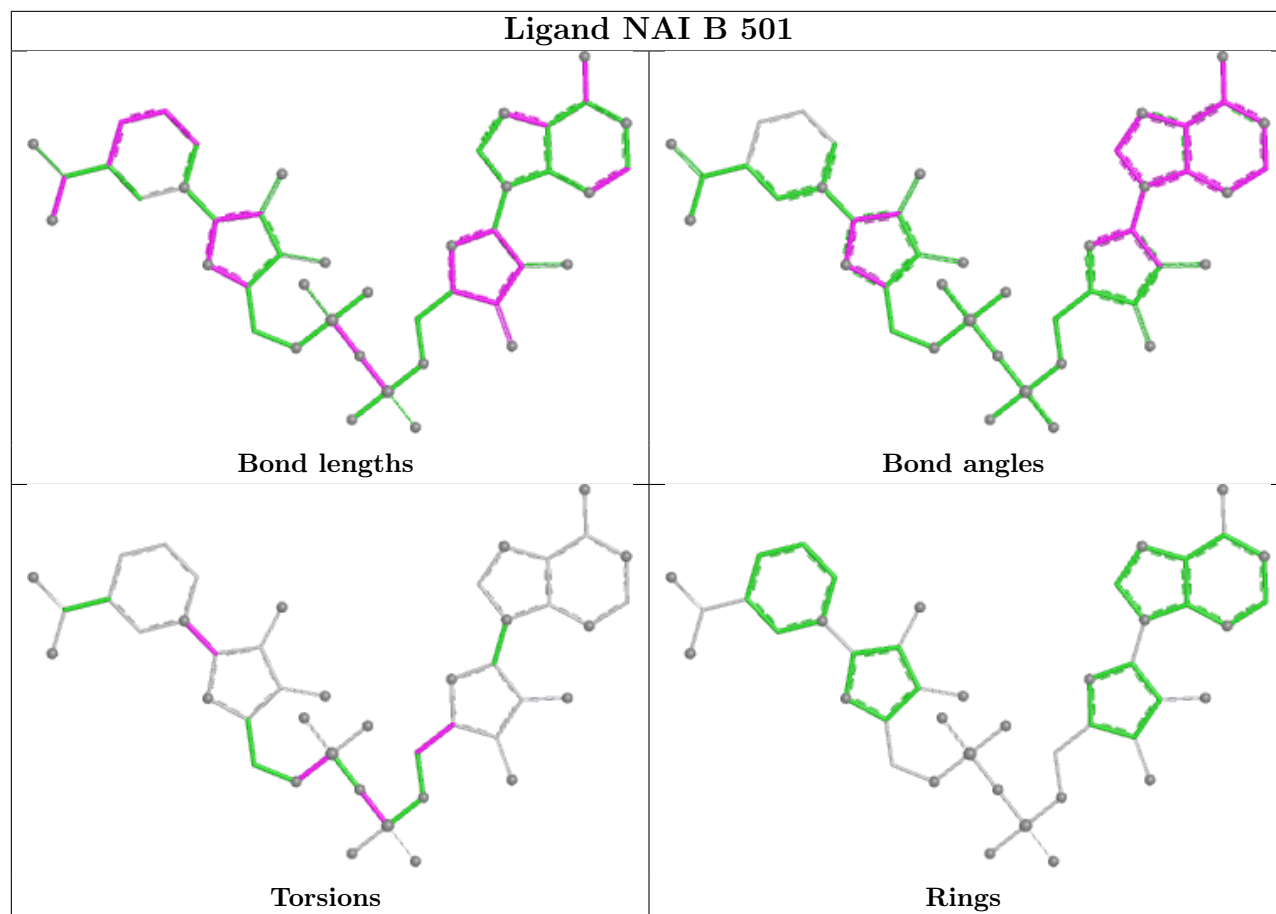
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAI	3	0

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.

Ligand NAI A 501







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	442/446 (99%)	0.51	27 (6%)	27 27	16, 27, 49, 109	0
1	B	440/446 (98%)	0.44	24 (5%)	30 31	15, 26, 47, 78	0
1	C	367/446 (82%)	3.09	300 (81%)	0 0	41, 65, 87, 105	0
All	All	1249/1338 (93%)	1.24	351 (28%)	1 1	15, 32, 78, 109	0

The worst 5 of 351 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	96	ALA	7.2
1	C	156	PHE	7.1
1	C	412	HIS	6.8
1	B	437	HIS	6.6
1	C	81	ILE	6.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

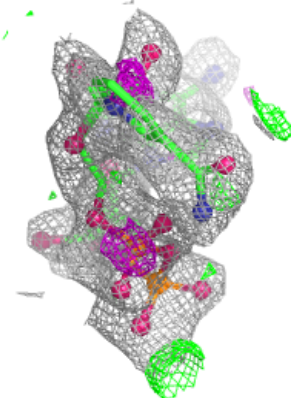
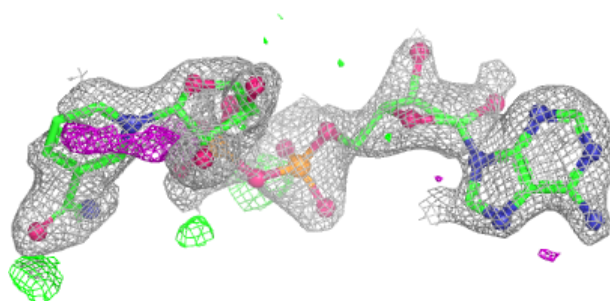
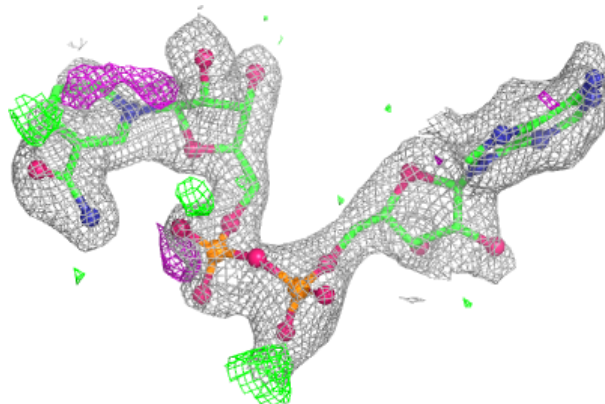
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAI	C	501	44/44	0.85	0.14	42,58,67,119	0
2	NAI	A	501	44/44	0.97	0.06	16,19,22,23	0
2	NAI	B	501	44/44	0.98	0.05	14,19,22,24	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.

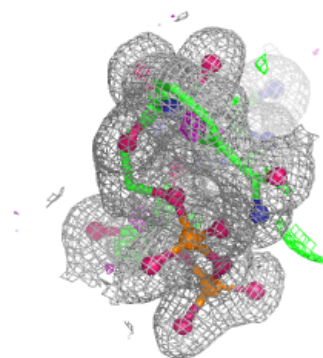
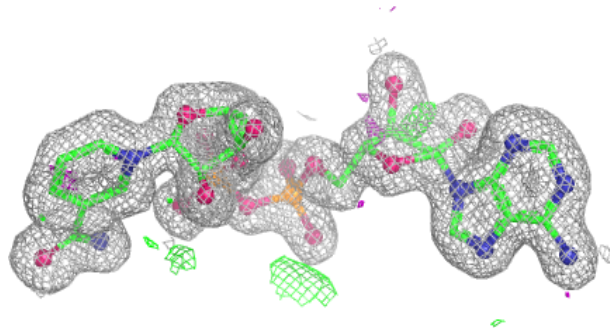
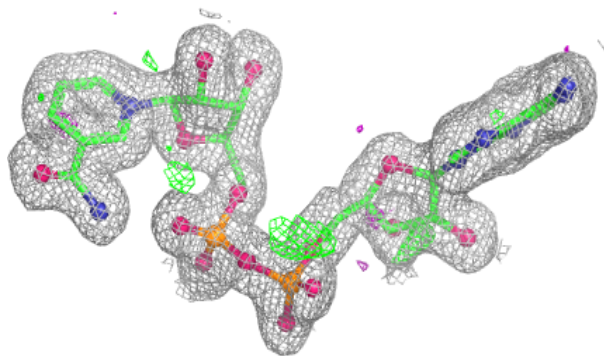
Electron density around NAI C 501:

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

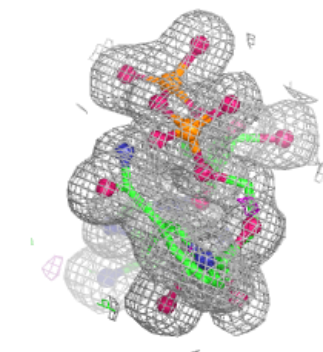
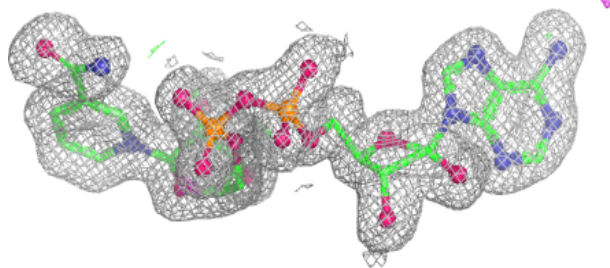
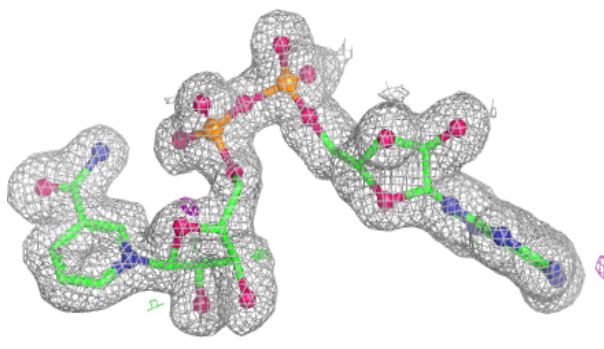


Electron density around NAI A 501:

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

**Electron density around NAI 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.