



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:14 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)

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<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

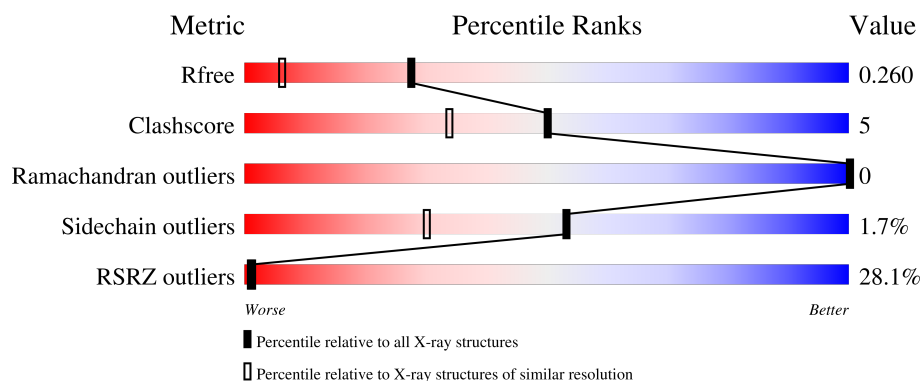
1 Overall quality at a glance

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:

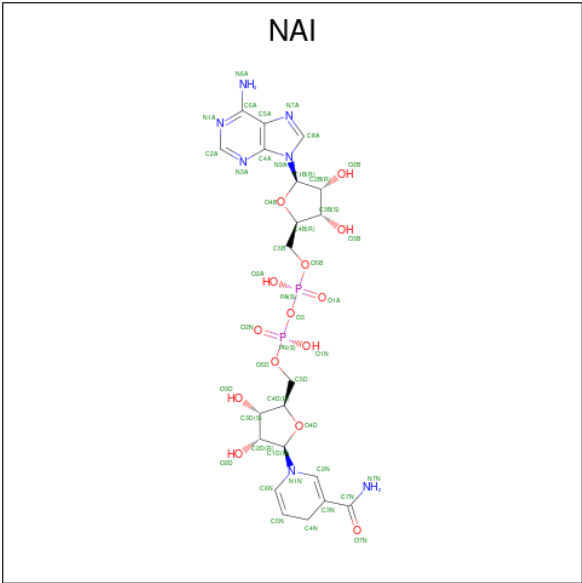
Chain	Residue	Modelled	Actual	Comment	Reference
A	439	LEU	-	expression tag	UNP A0A1C9HA64
A	440	GLU	-	expression tag	UNP A0A1C9HA64
A	441	HIS	-	expression tag	UNP A0A1C9HA64
A	442	HIS	-	expression tag	UNP A0A1C9HA64
A	443	HIS	-	expression tag	UNP A0A1C9HA64
A	444	HIS	-	expression tag	UNP A0A1C9HA64
A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

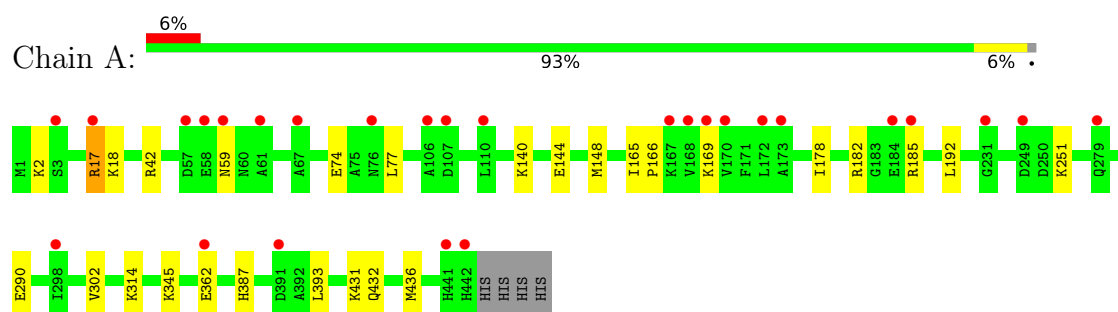
- Molecule 3 is water.

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		

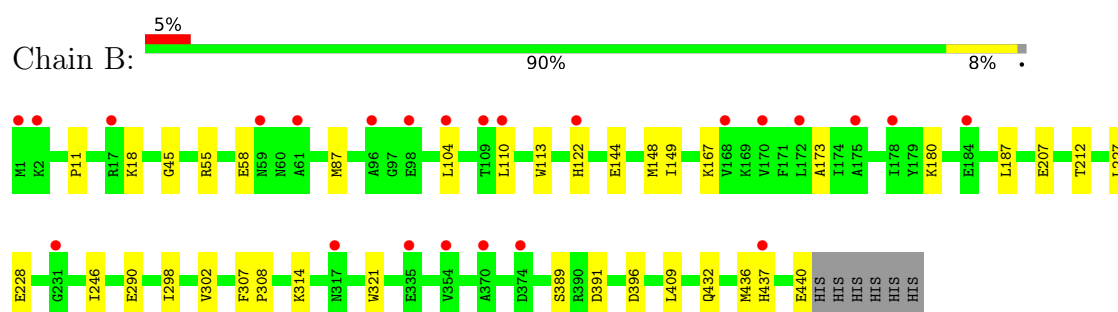
3 Residue-property plots [i](#)

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.

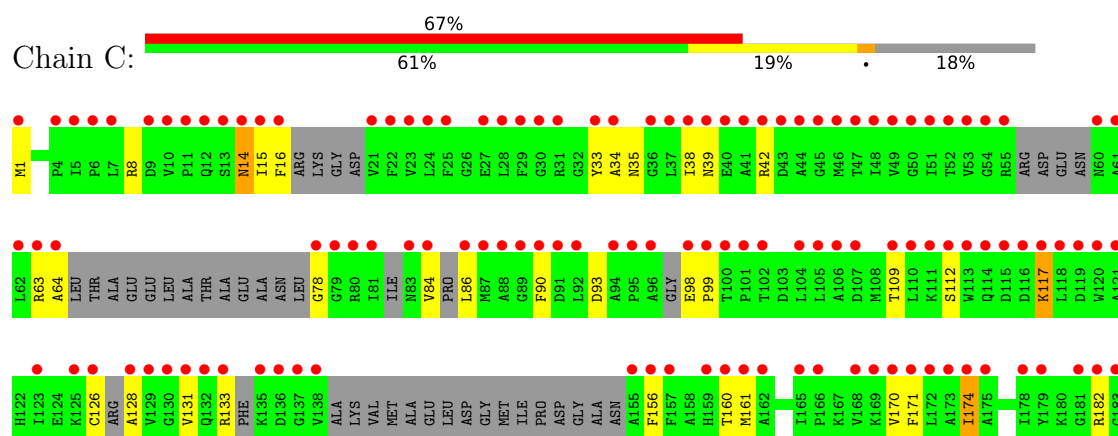
• Molecule 1: Enoyl-acyl carrier protein reductase



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V428	I429	A430	K431	Q432	L433	M434	L435	M436	H437	ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	M366	L306	T246	E184
I429	A430	K431	Q432	L433	M434	L435	M436	H437	ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	M367	F307	T247	E185	
A430	K431	Q432	L433	M434	L435	M436	H437	ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	N368	P308	T248	F186	
K431	Q432	L433	M434	L435	M436	H437	ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	T369	L309	D249	L187	
Q432	L433	M434	L435	M436	H437	ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	A370	L310	D250	S187	
L433	M434	L435	M436	H437	ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	E371	K311	K251	S188	
M434	L435	M436	H437	ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	L372	A312	Y252	A191	
L435	M436	H437	ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	L373	L313	Q253	L192	
M436	H437	ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	D374	K314	W254	L193	
H437	ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	I375	K315	Q255	N194	
ARG	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	E316	T256	T257	S195	
LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ASN	GLY	T258	G198	
GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	GLY	T259	K199	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	ALA	V260	L200	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	TRP	T261	I201	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	Q262	L202	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLU	GLU	Q263	M203	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	K264	N204	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	R265	F205	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	A265	M205	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	K266	D206	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	W267	E207	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	R268	V208	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	L269	T209	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	E270	A210	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	R271	N211	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	I272	T212	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	A273	F213	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	E274	L214	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	D275	H215	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	A276	L216	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	W277	T217	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	R278	E218	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	GLN	G219	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	G280	S220	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	I281	ALA	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	K282	A222	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	N283	I223	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	T284	R224	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	W285	A225	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	Y286	R226	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	N287	L227	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	C288	E228	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	P289	LYS	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	E290	SER	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	I291	GLY	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	K292	GLY	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	T293	GLN	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	N294	VAL	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	S295	ARG	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	S296	Y236	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	D297	S237	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	I298	A238	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	T298	Y239	
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HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	V300	G240	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	G301	Y241	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	V302	H242	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	E303	G243	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	L304	H244	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	S305	T244	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ALA	ALA	R267	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.

All (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
1:C:428:VAL:HA	1:C:431:LYS:HZ3	1.57	0.69
1:C:249:ASP:OD1	1:C:253:GLN:NE2	2.25	0.68
1:C:33:TYR:OH	1:C:289:PRO:O	2.12	0.68
1:B:321:TRP:CD1	1:B:437:HIS:HD1	2.12	0.67
1:C:433:LEU:HG	1:C:436:MET:HE2	1.76	0.67
1:B:321:TRP:NE1	1:B:437:HIS:HD1	1.92	0.67
1:C:84:VAL:O	1:C:86:LEU:N	2.28	0.67
1:C:14:ASN:C	1:C:14:ASN:ND2	2.50	0.63
1:A:345:LYS:NZ	3:A:607:HOH:O	2.32	0.63
1:C:432:GLN:O	1:C:436:MET:HG3	1.98	0.62
1:C:93:ASP:OD1	1:C:133:ARG:NH1	2.32	0.62
1:A:432:GLN:O	1:A:436:MET:HG3	2.02	0.59
1:C:14:ASN:ND2	1:C:16:PHE:H	2.02	0.57
1:C:290:GLU:HB3	1:C:302:VAL:HG22	1.86	0.57
1:C:156:PHE:HZ	1:C:237:SER:HB3	1.69	0.56
1:B:321:TRP:NE1	1:B:437:HIS:ND1	2.55	0.55
1:C:410:MET:O	1:C:414:SER:OG	2.16	0.55
1:A:42:ARG:NH2	1:A:77:LEU:O	2.41	0.54
1:A:314:LYS:NZ	3:A:608:HOH:O	2.34	0.54
1:B:314:LYS:NZ	3:B:608:HOH:O	2.40	0.53
1:B:432:GLN:O	1:B:436:MET:HG3	2.07	0.53
1:C:193:LEU:HD22	1:C:202:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ASN:ND2	1:C:16:PHE:N	2.57	0.53
1:C:202:LEU:HD22	1:C:264:LYS:HD2	1.91	0.52
1:C:42:ARG:NH2	1:C:78:GLY:HA3	2.25	0.52
1:B:104:LEU:HD11	1:B:122:HIS:CD2	2.37	0.52
1:C:345:LYS:HE3	1:C:379:THR:HG23	1.92	0.51
1:C:14:ASN:HD22	1:C:15:ILE:N	2.09	0.51
1:C:33:TYR:HB3	1:C:239:TYR:CE1	2.44	0.51
1:A:144:GLU:HG2	1:A:148:MET:HE3	1.92	0.51
1:C:381:ASP:O	1:C:385:LYS:HG3	2.11	0.51
1:C:171:PHE:HA	1:C:174:ILE:HG22	1.93	0.50
1:C:205:PHE:CD2	1:C:262:GLN:HG3	2.47	0.50
1:C:174:ILE:HG13	1:C:187:LEU:HD23	1.92	0.50
1:C:98:GLU:CG	1:C:99:PRO:HD2	2.41	0.49
1:A:185:ARG:NH2	3:A:615:HOH:O	2.45	0.49
1:C:182:ARG:HD3	1:C:374:ASP:HA	1.95	0.49
1:C:282:LYS:HD2	1:C:417:PRO:HD2	1.95	0.49
1:C:171:PHE:HA	1:C:174:ILE:CG2	2.43	0.49
1:C:170:VAL:O	1:C:174:ILE:HG22	2.14	0.48
1:C:408:PRO:O	1:C:412:HIS:ND1	2.41	0.47
1:A:290:GLU:HB3	1:A:302:VAL:HG22	1.96	0.47
1:C:246:ILE:HD12	1:C:308:PRO:HG2	1.96	0.47
1:C:33:TYR:HE2	2:C:501:NAI:C3N	2.28	0.47
1:C:98:GLU:HG3	1:C:99:PRO:HD2	1.97	0.46
1:C:277:TRP:HB2	1:C:420:PRO:HB3	1.96	0.46
1:B:396:ASP:OD1	3:B:602:HOH:O	2.20	0.46
1:A:178:ILE:HD11	1:A:192:LEU:HB2	1.98	0.46
1:A:431:LYS:NZ	3:A:621:HOH:O	2.49	0.46
1:B:113:TRP:HZ2	1:B:187:LEU:HD21	1.80	0.46
1:C:63:ARG:HG2	1:C:64:ALA:N	2.31	0.45
1:C:431:LYS:HB2	1:C:431:LYS:HE2	1.81	0.45
1:C:39:ASN:O	1:C:42:ARG:HB2	2.16	0.45
1:B:110:LEU:HD11	1:B:173:ALA:HB3	1.99	0.45
1:B:11:PRO:HD2	1:B:409:LEU:HD23	1.99	0.45
1:A:74:GLU:OE2	3:A:602:HOH:O	2.21	0.44
1:B:18:LYS:HD2	1:B:45:GLY:O	2.17	0.44
1:C:258:THR:HA	1:C:259:SER:HA	1.70	0.44
1:A:251:LYS:HB2	1:A:251:LYS:HE3	1.76	0.44
1:B:167:LYS:HB2	3:B:870:HOH:O	2.17	0.44
1:B:149:ILE:HG21	1:B:227:LEU:HD11	1.99	0.44
1:C:356:LYS:HE3	1:C:359:ARG:NH2	2.32	0.43
1:B:228:GLU:HG2	3:B:887:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ASN:O	1:C:38:ILE:HG13	2.19	0.43
1:C:264:LYS:HG3	1:C:265:ALA:H	1.83	0.43
1:C:268:ARG:HA	1:C:271:ARG:HD3	2.00	0.43
1:B:290:GLU:HB3	1:B:302:VAL:HG22	2.00	0.43
1:A:345:LYS:HE2	1:A:345:LYS:HB2	1.84	0.43
1:A:387:HIS:CD2	1:A:393:LEU:HA	2.54	0.43
1:C:1:MET:HE1	1:C:421:VAL:HG11	2.00	0.43
1:B:180:LYS:HE3	1:B:298:ILE:HG13	2.00	0.43
1:C:256:THR:HG21	1:C:364:TRP:HD1	1.84	0.42
1:C:267:MET:O	1:C:271:ARG:HD3	2.19	0.42
1:A:182:ARG:NH2	3:A:601:HOH:O	2.19	0.42
1:B:389:SER:OG	1:B:391:ASP:OD1	2.30	0.42
1:C:109:THR:H	1:C:112:SER:HB3	1.84	0.42
1:C:303:GLU:HB2	1:C:395:THR:HG21	2.00	0.42
1:A:144:GLU:HG2	1:A:148:MET:CE	2.49	0.42
1:B:437:HIS:HB3	1:B:440:GLU:HB3	2.01	0.42
1:B:246:ILE:HD12	1:B:308:PRO:HG2	2.02	0.42
1:C:292:ARG:HD2	1:C:395:THR:HG21	2.02	0.42
1:A:165:ILE:HA	1:A:166:PRO:HD3	1.93	0.41
1:C:126:CYS:O	1:C:128:ALA:N	2.53	0.41
1:C:90:PHE:HZ	1:C:203:MET:HE2	1.85	0.41
1:A:18:LYS:HE2	1:A:18:LYS:HB3	1.74	0.41
1:C:161:MET:HA	2:C:501:NAI:O4B	2.21	0.41
1:C:382:GLU:HG2	1:C:386:MET:HE3	2.01	0.41
1:A:17:ARG:NH1	3:A:626:HOH:O	2.52	0.41
1:C:34:ALA:HB2	1:C:160:THR:HG21	2.02	0.41
1:A:432:GLN:HE21	1:A:436:MET:CG	2.32	0.41
1:C:241:TYR:HB2	2:C:501:NAI:C5N	2.51	0.41
1:C:8:ARG:O	1:C:431:LYS:NZ	2.22	0.41
1:C:194:ASN:O	1:C:199:LYS:NZ	2.54	0.41
1:B:144:GLU:HG2	1:B:148:MET:HE3	2.02	0.40
1:C:207:GLU:O	1:C:212:THR:HG23	2.22	0.40
1:C:117:LYS:HB3	1:C:117:LYS:HE3	1.46	0.40
1:B:207:GLU:O	1:B:212:THR:HG23	2.21	0.40
1:B:87:MET:HE3	1:B:87:MET:HB2	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	17	ARG
1	A	140	LYS
1	A	169	LYS
1	A	362	GLU

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Mol	Chain	Res	Type
1	C	14	ASN
1	C	117	LYS
1	C	131	VAL
1	C	174	ILE
1	C	216	LEU
1	C	264	LYS
1	C	292	ARG
1	C	311	LYS
1	C	395	THR
1	C	431	LYS
1	C	433	LEU
1	C	435	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	GLN
1	A	432	GLN
1	B	12	GLN
1	B	122	HIS
1	C	14	ASN
1	C	176	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

All (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
2	C	501	NAI	O4D-C1D	9.09	1.63	1.42
2	C	501	NAI	C2B-C1B	-8.30	1.27	1.53
2	C	501	NAI	C2D-C1D	-8.05	1.28	1.53
2	A	501	NAI	C2B-C1B	-7.71	1.29	1.53
2	B	501	NAI	C2B-C1B	-7.68	1.29	1.53
2	B	501	NAI	C2D-C1D	-7.33	1.30	1.53
2	A	501	NAI	O4D-C1D	7.14	1.58	1.42
2	A	501	NAI	C2D-C1D	-7.09	1.31	1.53
2	B	501	NAI	O4D-C1D	7.02	1.58	1.42
2	C	501	NAI	C4N-C3N	-6.19	1.38	1.50
2	C	501	NAI	O4D-C4D	-5.96	1.31	1.45
2	A	501	NAI	PA-O3	5.86	1.65	1.59
2	B	501	NAI	C4N-C3N	-5.75	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAI	C4N-C3N	-5.71	1.39	1.50
2	A	501	NAI	O4D-C4D	-5.69	1.32	1.45
2	C	501	NAI	O4B-C4B	5.43	1.57	1.45
2	C	501	NAI	O4B-C1B	5.37	1.54	1.42
2	B	501	NAI	PA-O3	5.26	1.65	1.59
2	C	501	NAI	C2B-C3B	5.09	1.67	1.53
2	A	501	NAI	O4B-C1B	5.04	1.53	1.42
2	B	501	NAI	O4B-C4B	4.92	1.55	1.45
2	B	501	NAI	C2B-C3B	4.92	1.66	1.53
2	A	501	NAI	O4B-C4B	4.78	1.55	1.45
2	B	501	NAI	O4D-C4D	-4.72	1.34	1.45
2	A	501	NAI	C2B-C3B	4.63	1.65	1.53
2	C	501	NAI	PA-O3	4.58	1.64	1.59
2	B	501	NAI	O4B-C1B	4.42	1.52	1.42
2	C	501	NAI	C4N-C5N	-3.88	1.38	1.49
2	A	501	NAI	C6A-N6A	3.88	1.44	1.34
2	C	501	NAI	C6A-N6A	3.56	1.43	1.34
2	B	501	NAI	C6A-N6A	3.53	1.43	1.34
2	B	501	NAI	C4N-C5N	-3.34	1.40	1.49
2	C	501	NAI	C7N-N7N	3.33	1.43	1.33
2	A	501	NAI	C4N-C5N	-3.31	1.40	1.49
2	B	501	NAI	C7N-N7N	3.23	1.42	1.33
2	A	501	NAI	C7N-N7N	3.12	1.42	1.33
2	B	501	NAI	C2A-N3A	2.95	1.39	1.33
2	C	501	NAI	C7N-C3N	2.88	1.54	1.48
2	A	501	NAI	C2A-N3A	2.85	1.39	1.33
2	C	501	NAI	C2A-N3A	2.78	1.38	1.33
2	A	501	NAI	O3B-C3B	2.47	1.49	1.43
2	C	501	NAI	C8A-N7A	2.42	1.36	1.31
2	C	501	NAI	C6N-C5N	2.42	1.40	1.33
2	A	501	NAI	C6N-C5N	2.40	1.40	1.33
2	C	501	NAI	O2D-C2D	2.39	1.48	1.43
2	B	501	NAI	C6N-C5N	2.24	1.39	1.33
2	B	501	NAI	PN-O3	2.18	1.61	1.59
2	A	501	NAI	C5A-C4A	-2.16	1.35	1.39
2	B	501	NAI	C5A-N7A	-2.16	1.35	1.39
2	A	501	NAI	C7N-C3N	2.13	1.53	1.48
2	C	501	NAI	O3D-C3D	-2.12	1.37	1.43
2	A	501	NAI	PN-O3	2.08	1.61	1.59
2	A	501	NAI	O2B-C2B	2.01	1.47	1.43
2	B	501	NAI	O3B-C3B	2.01	1.47	1.43

All (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
2	A	501	NAI	C5A-C4A-N3A	-5.16	119.61	126.72
2	B	501	NAI	N3A-C2A-N1A	-5.05	120.94	128.58
2	C	501	NAI	C5A-C4A-N3A	-4.79	120.12	126.72
2	A	501	NAI	N3A-C2A-N1A	-4.72	121.44	128.58
2	B	501	NAI	C4A-N9A-C1B	-4.64	115.79	126.63
2	A	501	NAI	N6A-C6A-N1A	-4.52	108.32	118.38
2	B	501	NAI	N6A-C6A-N1A	-4.50	108.34	118.38
2	A	501	NAI	C4A-N9A-C1B	-4.43	116.28	126.63
2	A	501	NAI	N3A-C4A-N9A	4.39	134.63	127.17
2	C	501	NAI	N9A-C8A-N7A	-4.29	107.84	113.94
2	A	501	NAI	C5A-C6A-N6A	4.15	133.57	123.29
2	B	501	NAI	C5A-C4A-N3A	-4.15	121.00	126.72
2	A	501	NAI	N9A-C8A-N7A	-4.14	108.06	113.94
2	B	501	NAI	C5A-C6A-N6A	4.09	133.41	123.29
2	B	501	NAI	N9A-C8A-N7A	-3.94	108.34	113.94
2	A	501	NAI	C6A-C5A-C4A	3.89	122.49	117.18
2	B	501	NAI	C1B-N9A-C8A	3.65	135.19	127.09
2	A	501	NAI	O4D-C1D-C2D	-3.49	99.14	106.62
2	B	501	NAI	O4B-C1B-N9A	-3.48	101.41	108.09
2	B	501	NAI	N3A-C4A-N9A	3.46	133.05	127.17
2	A	501	NAI	C1B-N9A-C8A	3.39	134.62	127.09
2	C	501	NAI	C2A-N3A-C4A	3.27	119.81	111.83
2	A	501	NAI	C4A-N9A-C8A	3.20	109.10	105.74
2	B	501	NAI	C4A-N9A-C8A	3.12	109.02	105.74
2	C	501	NAI	N3A-C4A-N9A	2.97	132.22	127.17
2	A	501	NAI	O4B-C1B-N9A	-2.96	102.41	108.09
2	C	501	NAI	C5A-N7A-C8A	2.94	108.08	103.45
2	B	501	NAI	C6A-C5A-C4A	2.83	121.04	117.18
2	C	501	NAI	C5D-C4D-C3D	-2.79	105.18	115.21
2	A	501	NAI	C5A-N7A-C8A	2.78	107.82	103.45
2	A	501	NAI	C4B-O4B-C1B	-2.62	103.69	109.47
2	B	501	NAI	O4D-C1D-C2D	-2.55	101.15	106.62
2	A	501	NAI	C2A-N3A-C4A	2.54	118.03	111.83
2	A	501	NAI	O3-PN-O2N	-2.48	103.24	110.70
2	B	501	NAI	C2A-N3A-C4A	2.41	117.71	111.83
2	B	501	NAI	O4B-C1B-C2B	-2.39	101.51	106.62
2	C	501	NAI	C4A-N9A-C8A	2.34	108.19	105.74
2	B	501	NAI	C5A-N7A-C8A	2.34	107.12	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAI	C3N-C2N-N1N	-2.32	119.80	123.20
2	C	501	NAI	C3B-C2B-C1B	2.21	105.64	101.46
2	C	501	NAI	C4A-C5A-N7A	-2.06	108.22	110.58
2	B	501	NAI	C4D-O4D-C1D	-2.03	104.99	109.47
2	C	501	NAI	C6A-C5A-C4A	2.02	119.93	117.18
2	C	501	NAI	O4D-C1D-N1N	2.01	111.92	108.08

There are no chirality outliers.

All (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
2	B	501	NAI	C5D-O5D-PN-O1N
2	B	501	NAI	C5D-O5D-PN-O2N
2	C	501	NAI	C5D-O5D-PN-O2N
2	C	501	NAI	C3D-C4D-C5D-O5D
2	C	501	NAI	O4D-C4D-C5D-O5D
2	A	501	NAI	PN-O3-PA-O5B
2	B	501	NAI	PN-O3-PA-O5B
2	A	501	NAI	O4D-C1D-N1N-C6N
2	C	501	NAI	O4D-C1D-N1N-C6N
2	B	501	NAI	O4D-C1D-N1N-C6N
2	A	501	NAI	C2D-C1D-N1N-C6N
2	B	501	NAI	C2D-C1D-N1N-C6N
2	C	501	NAI	C2D-C1D-N1N-C6N
2	B	501	NAI	O4B-C4B-C5B-O5B

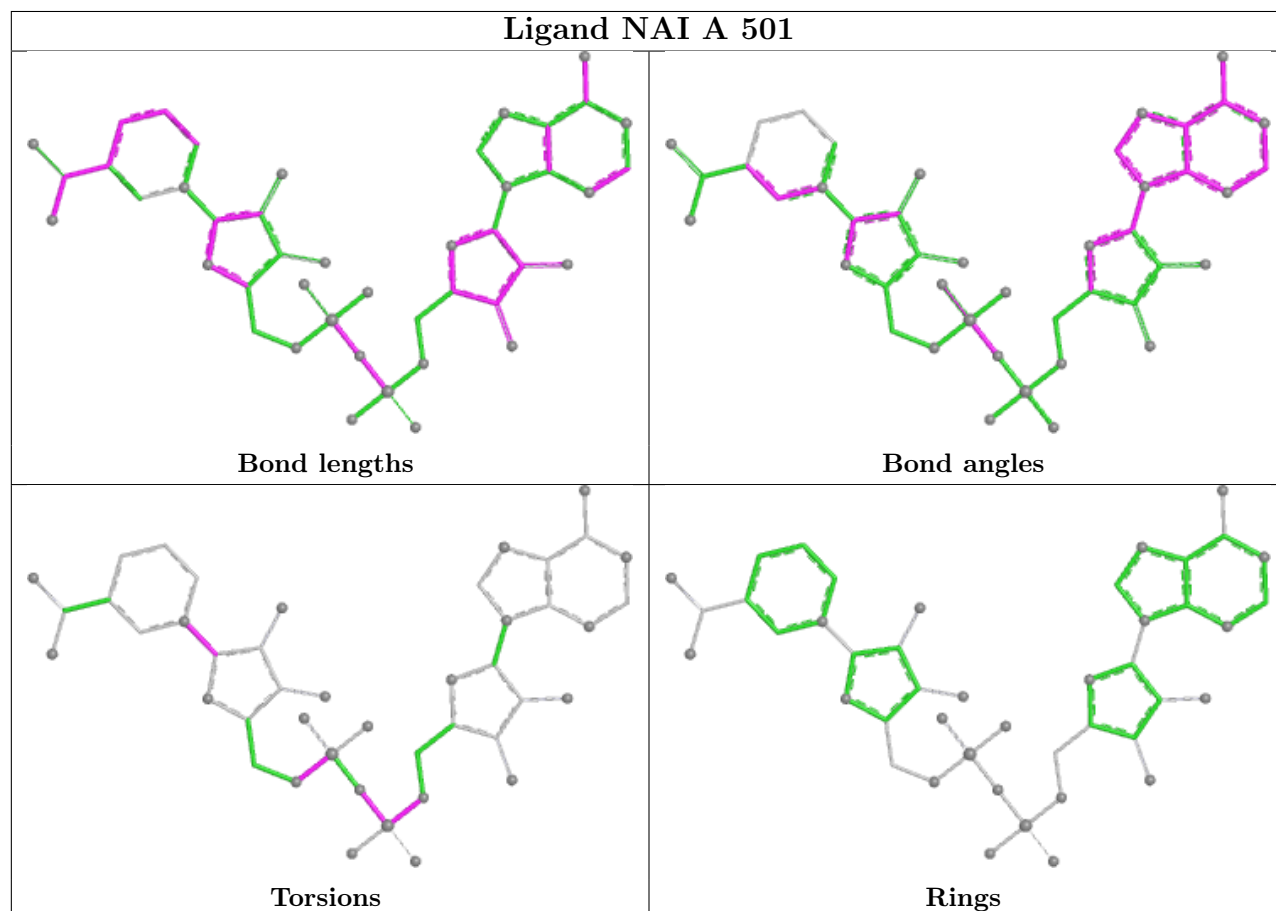
There are no ring outliers.

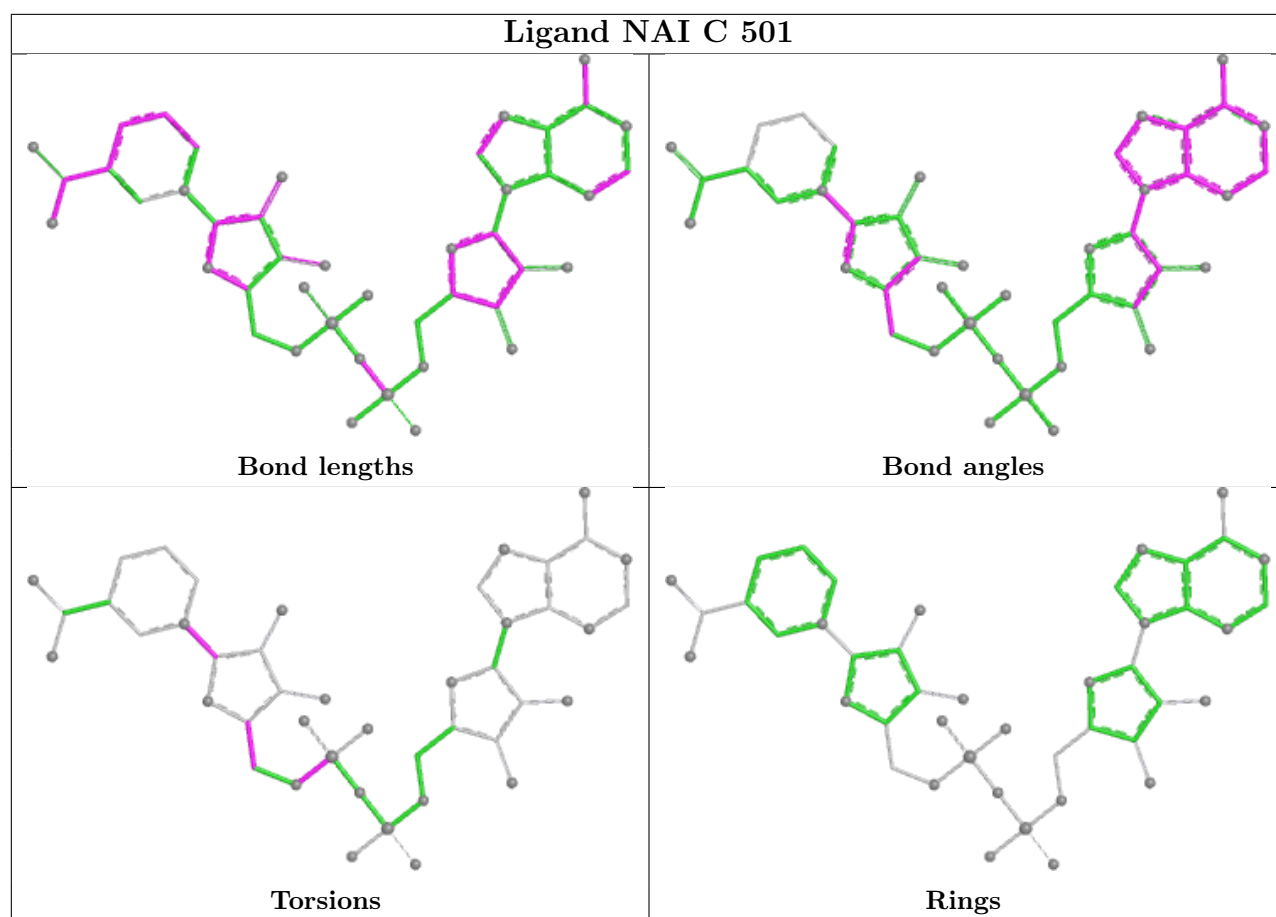
1 monomer is involved in 3 short contacts:

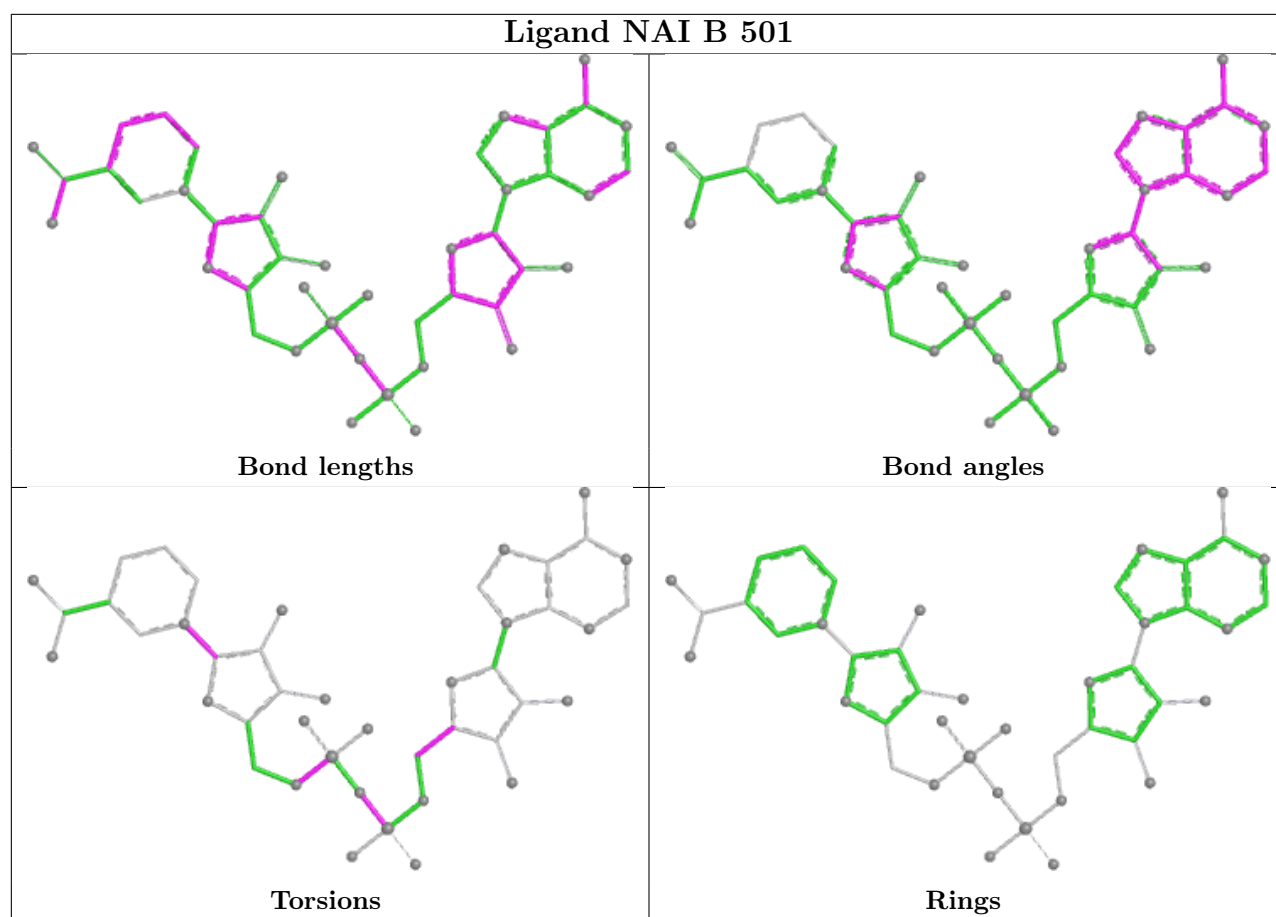
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAI	3	0

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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	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

All (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
1	C	433	LEU	6.4
1	A	442	HIS	6.4
1	C	95	PRO	6.4
1	C	394	VAL	6.3
1	C	84	VAL	6.3
1	C	138	VAL	6.3
1	C	33	TYR	6.1
1	A	172	LEU	6.1
1	B	17	ARG	6.0
1	C	38	ILE	6.0
1	C	90	PHE	5.7
1	C	21	VAL	5.7
1	C	349	TYR	5.7
1	C	129	VAL	5.7
1	C	400	ALA	5.6
1	C	41	ALA	5.5
1	C	251	LYS	5.4
1	C	120	TRP	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	222	ALA	5.4
1	C	272	ILE	5.4
1	C	247	LEU	5.3
1	C	238	ALA	5.3
1	C	223	ILE	5.2
1	C	62	LEU	5.2
1	C	22	PHE	5.1
1	C	401	LEU	5.1
1	C	29	PHE	5.1
1	C	130	GLY	5.0
1	C	409	LEU	5.0
1	C	312	ALA	5.0
1	C	216	LEU	5.0
1	C	283	ALA	4.9
1	C	358	PHE	4.9
1	C	6	PRO	4.9
1	C	113	TRP	4.9
1	C	435	LEU	4.8
1	C	1	MET	4.8
1	C	437	HIS	4.8
1	C	86	LEU	4.8
1	C	421	VAL	4.7
1	C	372	LEU	4.7
1	C	248	ILE	4.7
1	C	15	ILE	4.7
1	C	418	ALA	4.7
1	C	64	ALA	4.6
1	C	276	ALA	4.6
1	C	36	GLY	4.6
1	C	434	ASN	4.6
1	C	309	LEU	4.6
1	C	48	ILE	4.5
1	C	78	GLY	4.5
1	C	128	ALA	4.5
1	C	269	LEU	4.5
1	C	370	ALA	4.5
1	C	10	VAL	4.4
1	C	299	PHE	4.4
1	C	397	VAL	4.4
1	C	403	LEU	4.4
1	C	411	PHE	4.4
1	C	131	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	254	TRP	4.3
1	C	168	VAL	4.3
1	C	354	VAL	4.3
1	C	100	THR	4.2
1	C	416	ASN	4.2
1	C	236	TYR	4.2
1	C	170	VAL	4.2
1	C	110	LEU	4.2
1	C	215	HIS	4.2
1	C	99	PRO	4.2
1	C	342	LEU	4.1
1	C	217	ILE	4.1
1	C	28	LEU	4.1
1	C	186	PHE	4.1
1	A	17	ARG	4.1
1	C	363	ALA	4.1
1	C	285	VAL	4.0
1	C	51	ILE	4.0
1	C	281	ILE	4.0
1	C	61	ALA	4.0
1	C	16	PHE	4.0
1	C	398	LEU	4.0
1	C	44	ALA	4.0
1	C	88	ALA	4.0
1	C	249	ASP	4.0
1	C	37	LEU	4.0
1	C	395	THR	4.0
1	C	47	THR	3.9
1	C	392	ALA	3.9
1	C	205	PHE	3.9
1	C	407	GLY	3.9
1	C	210	ALA	3.9
1	C	343	LEU	3.9
1	C	123	ILE	3.9
1	C	346	ILE	3.9
1	C	34	ALA	3.8
1	C	121	ALA	3.8
1	C	24	LEU	3.8
1	C	172	LEU	3.8
1	C	193	LEU	3.8
1	C	339	LEU	3.8
1	C	277	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	405	GLY	3.7
1	C	341	SER	3.7
1	C	264	LYS	3.7
1	C	417	PRO	3.7
1	C	326	TRP	3.7
1	C	112	SER	3.6
1	C	429	ILE	3.6
1	B	168	VAL	3.6
1	C	213	PHE	3.6
1	C	361	PHE	3.6
1	C	430	ALA	3.6
1	C	92	LEU	3.6
1	C	301	GLY	3.6
1	C	265	ALA	3.6
1	C	241	TYR	3.6
1	C	126	CYS	3.6
1	C	178	ILE	3.6
1	C	246	ILE	3.6
1	C	11	PRO	3.5
1	C	13	SER	3.5
1	C	23	VAL	3.5
1	C	157	PHE	3.5
1	C	109	THR	3.5
1	C	107	ASP	3.5
1	C	227	LEU	3.5
1	C	5	ILE	3.5
1	C	155	ALA	3.5
1	C	300	VAL	3.5
1	C	171	PHE	3.4
1	C	310	LEU	3.4
1	C	364	TRP	3.4
1	B	110	LEU	3.4
1	C	261	THR	3.4
1	A	441	HIS	3.3
1	A	298	ILE	3.3
1	C	83	ASN	3.3
1	C	192	LEU	3.3
1	C	161	MET	3.3
1	C	55	ARG	3.3
1	C	175	ALA	3.3
1	C	313	LEU	3.3
1	C	386	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	298	ILE	3.3
1	C	288	CYS	3.3
1	C	115	ASP	3.2
1	C	79	GLY	3.2
1	C	291	ILE	3.2
1	C	295	SER	3.2
1	C	239	TYR	3.2
1	C	273	ALA	3.2
1	C	387	HIS	3.2
1	C	393	LEU	3.2
1	C	219	GLY	3.2
1	C	160	THR	3.2
1	C	49	VAL	3.2
1	C	375	ILE	3.2
1	C	377	ILE	3.2
1	C	327	GLN	3.2
1	C	94	ALA	3.2
1	C	338	THR	3.1
1	A	173	ALA	3.1
1	C	87	MET	3.1
1	C	356	LYS	3.1
1	C	328	ALA	3.1
1	C	187	LEU	3.1
1	C	408	PRO	3.1
1	C	348	ASP	3.1
1	B	2	LYS	3.0
1	C	119	ASP	3.0
1	C	419	GLY	3.0
1	C	14	ASN	3.0
1	C	162	ALA	3.0
1	C	369	THR	3.0
1	C	302	VAL	3.0
1	C	7	LEU	3.0
1	C	200	LEU	3.0
1	C	42	ARG	3.0
1	A	61	ALA	3.0
1	B	178	ILE	3.0
1	A	362	GLU	3.0
1	B	231	GLY	3.0
1	A	185	ARG	3.0
1	C	224	ARG	3.0
1	C	262	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	111	LYS	3.0
1	C	43	ASP	3.0
1	B	61	ALA	2.9
1	C	240	GLY	2.9
1	C	60	ASN	2.9
1	A	391	ASP	2.9
1	C	202	LEU	2.9
1	B	335	GLU	2.9
1	C	329	CYS	2.9
1	C	282	LYS	2.9
1	C	360	ASN	2.9
1	C	188	SER	2.9
1	C	376	MET	2.9
1	C	117	LYS	2.9
1	C	106	ALA	2.8
1	B	184	GLU	2.8
1	C	209	THR	2.8
1	C	179	TYR	2.8
1	C	208	VAL	2.8
1	C	351	ALA	2.8
1	C	368	ASN	2.8
1	C	330	ARG	2.8
1	C	250	ASP	2.8
1	C	414	SER	2.8
1	C	25	PHE	2.8
1	C	174	ILE	2.8
1	C	159	HIS	2.8
1	C	45	GLY	2.7
1	C	114	GLN	2.7
1	C	244	THR	2.7
1	C	293	THR	2.7
1	C	63	ARG	2.7
1	C	101	PRO	2.7
1	C	260	TYR	2.7
1	C	116	ASP	2.7
1	B	175	ALA	2.7
1	C	225	ALA	2.7
1	C	296	SER	2.7
1	C	340	GLU	2.7
1	C	191	ALA	2.7
1	C	214	LEU	2.7
1	C	80	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	243	GLY	2.7
1	C	280	GLY	2.7
1	A	58	GLU	2.7
1	C	98	GLU	2.7
1	B	96	ALA	2.6
1	C	125	LYS	2.6
1	C	12	GLN	2.6
1	C	132	GLN	2.6
1	C	325	GLN	2.6
1	A	3	SER	2.6
1	C	399	SER	2.6
1	C	292	ARG	2.6
1	C	252	TYR	2.6
1	C	384	THR	2.6
1	C	424	LEU	2.6
1	C	352	SER	2.6
1	C	268	ARG	2.6
1	A	168	VAL	2.6
1	C	137	GLY	2.6
1	A	67	ALA	2.6
1	C	257	TYR	2.6
1	C	422	LEU	2.6
1	C	53	VAL	2.6
1	C	402	VAL	2.6
1	A	279	GLN	2.6
1	C	385	LYS	2.5
1	B	317	ASN	2.5
1	C	133	ARG	2.5
1	C	30	GLY	2.5
1	C	54	GLY	2.5
1	C	9	ASP	2.5
1	C	286	TYR	2.5
1	C	89	GLY	2.5
1	C	166	PRO	2.5
1	C	237	SER	2.5
1	C	428	VAL	2.5
1	C	50	GLY	2.5
1	C	195	SER	2.5
1	C	118	LEU	2.5
1	A	167	LYS	2.4
1	C	226	ARG	2.4
1	C	46	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	203	MET	2.4
1	C	102	THR	2.4
1	C	212	THR	2.4
1	B	370	ALA	2.4
1	C	185	ARG	2.4
1	A	249	ASP	2.4
1	C	104	LEU	2.4
1	C	304	LEU	2.4
1	C	284	THR	2.4
1	B	354	VAL	2.4
1	A	59	ASN	2.4
1	C	396	ASP	2.4
1	C	344	GLN	2.4
1	C	436	MET	2.4
1	C	173	ALA	2.3
1	A	57	ASP	2.3
1	C	423	TRP	2.3
1	C	289	PRO	2.3
1	C	311	LYS	2.3
1	B	98	GLU	2.3
1	C	263	GLY	2.3
1	B	374	ASP	2.3
1	C	91	ASP	2.3
1	B	170	VAL	2.3
1	C	4	PRO	2.3
1	C	256	THR	2.3
1	C	105	LEU	2.3
1	C	383	ILE	2.3
1	C	220	SER	2.3
1	C	169	LYS	2.3
1	C	365	PRO	2.2
1	C	307	PHE	2.2
1	C	406	THR	2.2
1	A	231	GLY	2.2
1	C	135	LYS	2.2
1	A	106	ALA	2.2
1	C	271	ARG	2.2
1	A	184	GLU	2.2
1	B	1	MET	2.2
1	C	316	GLU	2.2
1	C	181	GLY	2.2
1	A	76	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	104	LEU	2.2
1	C	40	GLU	2.2
1	C	373	ALA	2.2
1	C	198	GLY	2.2
1	C	378	GLY	2.2
1	C	275	ASP	2.2
1	C	306	LEU	2.1
1	C	165	ILE	2.1
1	C	52	THR	2.1
1	C	27	GLU	2.1
1	C	381	ASP	2.1
1	C	357	GLY	2.1
1	A	110	LEU	2.1
1	B	109	THR	2.1
1	C	39	ASN	2.1
1	C	314	LYS	2.1
1	C	362	GLU	2.1
1	C	353	ASP	2.1
1	C	258	THR	2.1
1	B	172	LEU	2.1
1	C	359	ARG	2.1
1	A	107	ASP	2.1
1	B	59	ASN	2.1
1	C	367	PRO	2.1
1	C	420	PRO	2.1
1	A	169	LYS	2.0
1	C	404	GLU	2.0
1	C	136	ASP	2.0
1	C	183	GLY	2.0
1	C	31	ARG	2.0
1	C	182	ARG	2.0
1	B	122	HIS	2.0
1	A	170	VAL	2.0
1	C	350	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

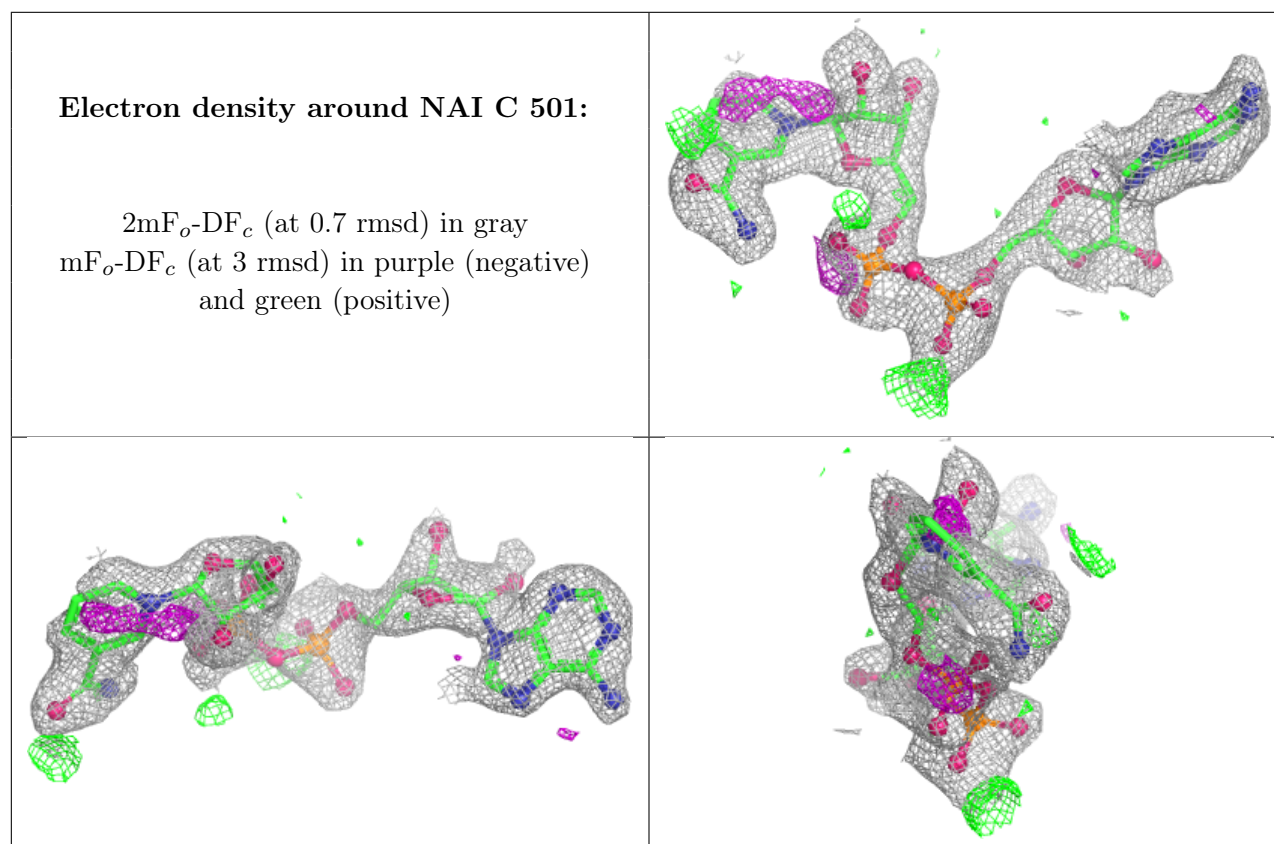
There are no oligosaccharides in this entry.

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.

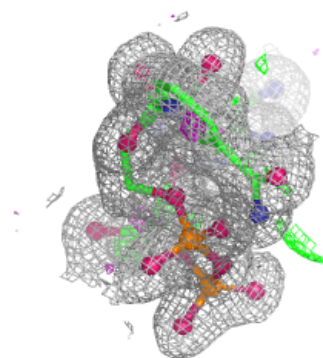
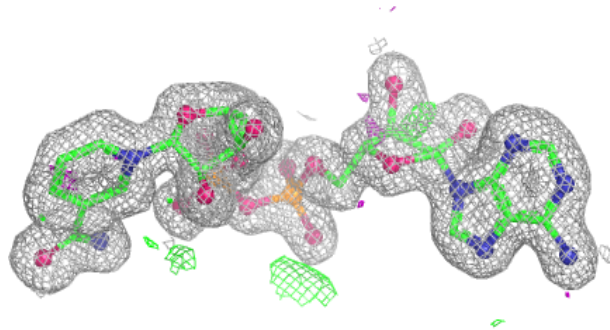
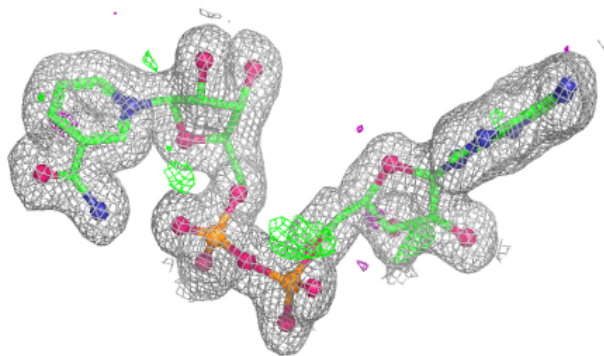
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAI	C	501	44/44	0.85	0.14	42,58,67,119	0
2	NAI	A	501	44/44	0.97	0.06	16,19,22,23	0
2	NAI	B	501	44/44	0.98	0.05	14,19,22,24	0

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.

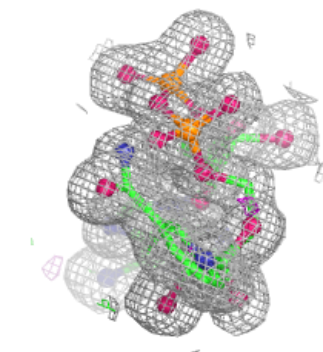
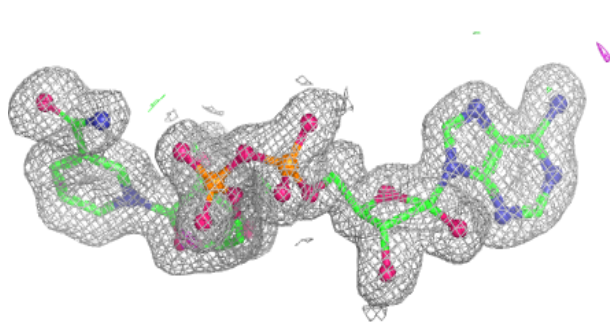
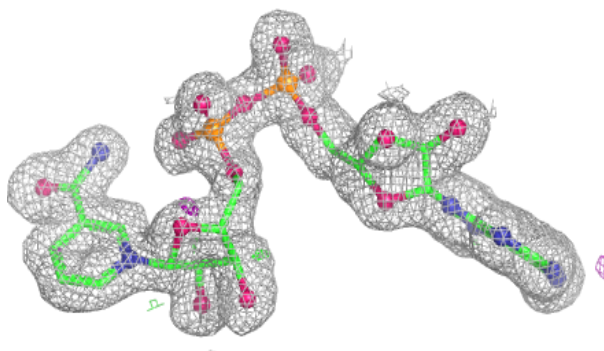


Electron density around NAI A 501:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.