Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:50 pm BST

PDB ID	:	6KIA
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

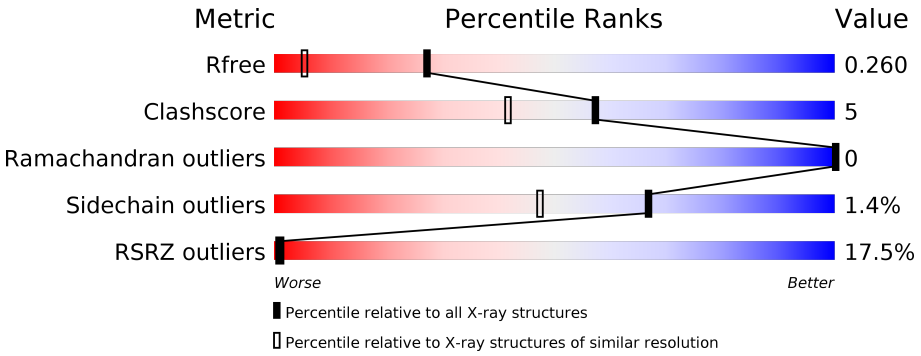
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 on 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 <=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	2% 93% 6%
1	B	446	3% 91% 7%
1	C	446	44% 63% 18% 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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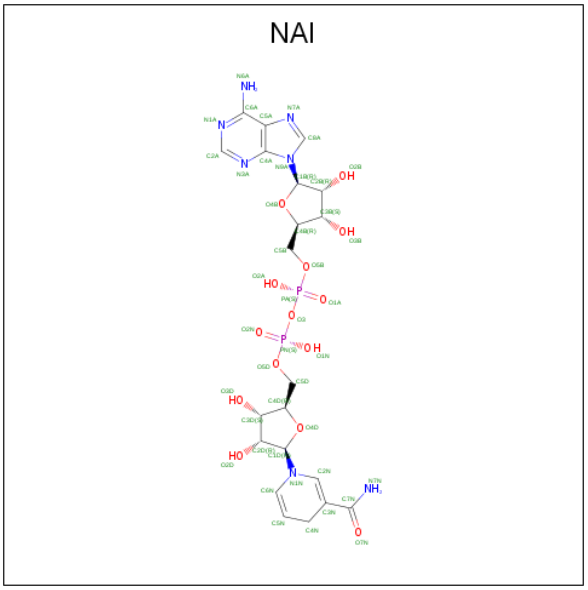
Chain	Residue	Modelled	Actual	Comment	Reference
C	446	HIS	-	expression tag	UNP A0A1C9HA64

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by author).



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.

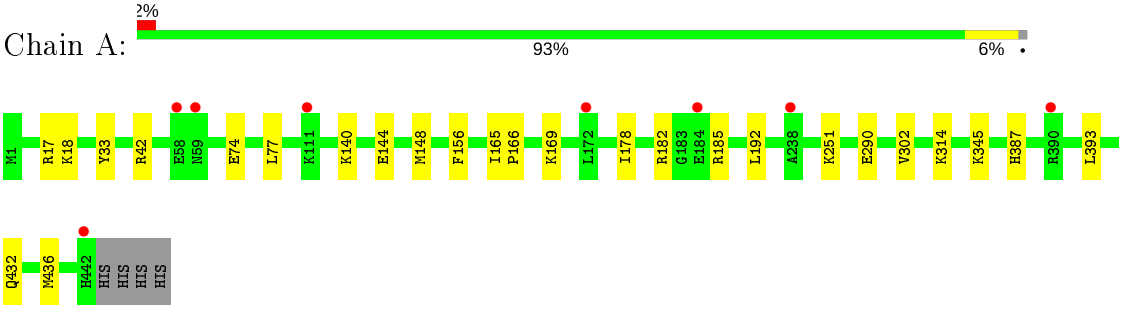
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	397	Total	O	0	0
			397	397		
3	B	417	Total	O	0	0
			417	417		
3	C	49	Total	O	0	0
			49	49		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

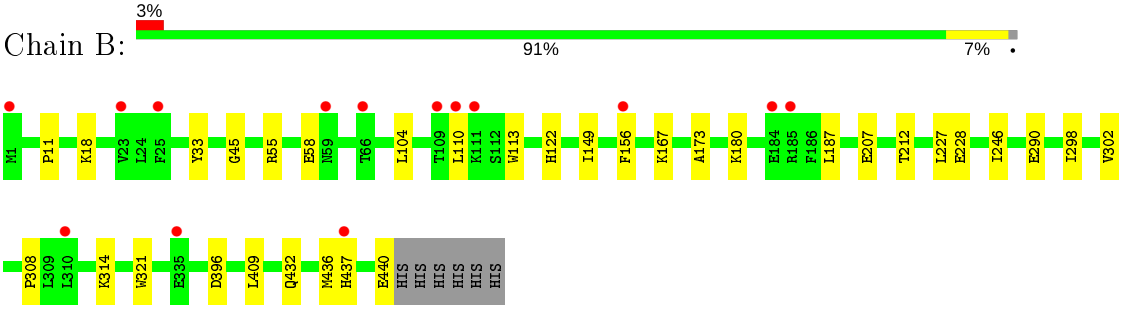
- Molecule 1: Enoyl-acyl carrier protein reductase

Chain A:



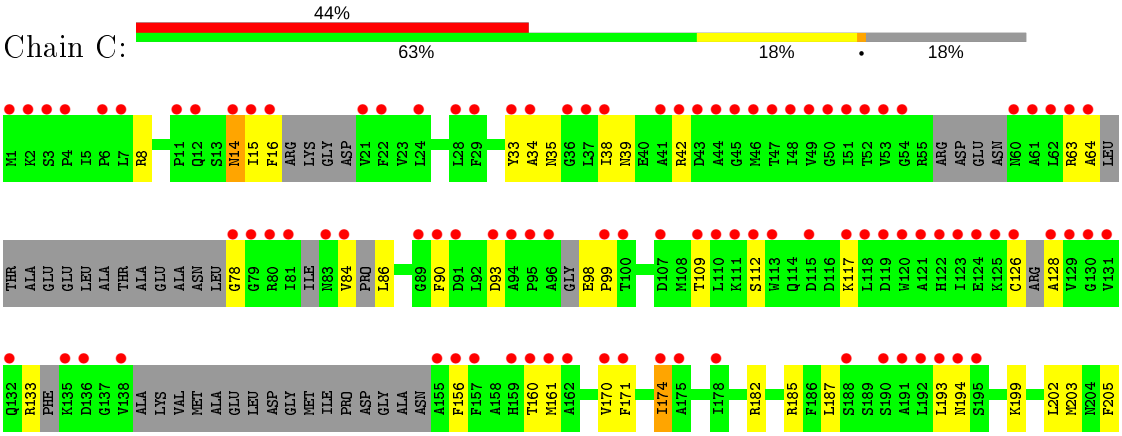
- Molecule 1: Enoyl-acyl carrier protein reductase

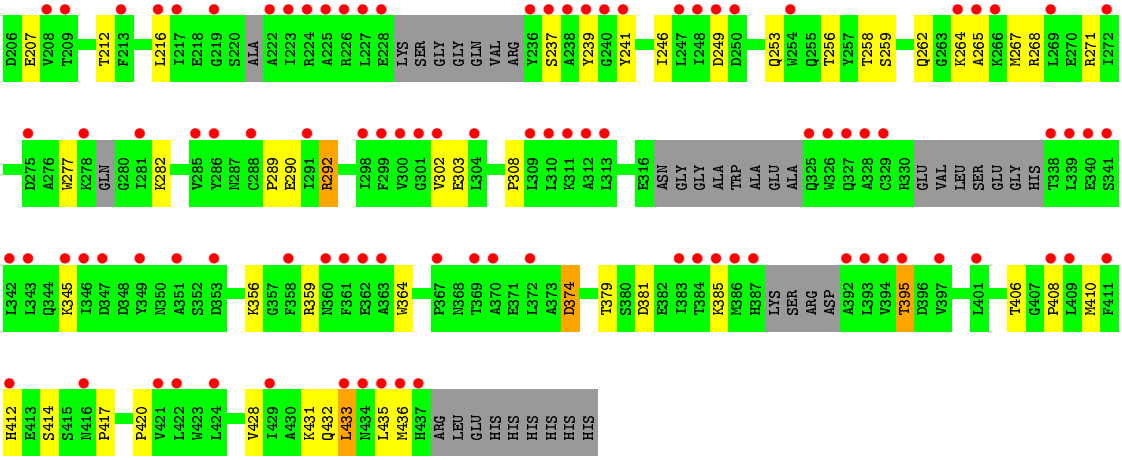
Chain B:



- Molecule 1: Enoyl-acyl carrier protein reductase

Chain C:




D206 E207 V208 T209 T212 F213 L216 I217 E218 G219 S220 ALA A222 I223 R224 A225 R226 L227 E228 LYS SER GLY GLY GLN VAL ARG Y236 S237 A238 Y239 G240 Y241 I246 L247 I248 D249 D250 Q253 W254 Q255 T256 Y257 T258 S259 Q262 G263 K264 A265 K266 M267 R268 L269 E270 R271 I272
D275 A276 W277 K278 GLN G280 I281 K282 V285 Y286 M287 C288 P289 E290 I291 R292 I298 F299 V300 G301 V302 E303 L304 P308 L309 L310 K311 A312 L313 E316 ASN GLY GLY ALA TRP ALA GLU ALA Q325 W326 Q327 A328 C329 R330 GLU VAL LEU SER GLU GLY HIS T338 L339 E340 S341
L342 L343 Q344 K345 I346 D347 D348 Y349 N350 A351 S352 D353 K356 G357 F358 R359 N360 F361 E362 A363 W364 F367 N368 T369 A370 E371 L372 A373 D374 T379 S380 D381 E382 I383 T384 K385 N386 H387 LYS SER ARG ASP A392 L393 V394 T395 D396 V397 L401 T406 G407 P408 L409 M410 F411
H412 E413 S414 S415 N416 P417 P420 V421 L422 W423 L424 V428 I429 A430 K431 Q432 L433 N434 L435 M436 H437 ARG LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	0.85 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.224 , 0.259 0.225 , 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)	0.36 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.43	0/3501	0.57	0/4735
1	B	0.44	0/3479	0.59	0/4705
1	C	0.31	0/2871	0.52	0/3872
All	All	0.40	0/9851	0.56	0/13312

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	17	0
1	B	3412	0	3405	21	0
1	C	2825	0	2769	59	0
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	6	0
3	B	417	0	0	5	0
3	C	49	0	0	0	0
All	All	10664	0	9673	95	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 (95) 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	0.87
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: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:C:428:VAL:HA	1:C:431:LYS:HZ3	1.60	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	0.65
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:A:345:LYS:NZ	3:A:607:HOH:O	2.32	0.58
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:8:ARG:O	1:C:431:LYS:NZ	2.22	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:LEU:HG	1:C:436:MET:HE2	1.95	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:277:TRP:HB2	1:C:420:PRO:HB3	1.96	0.46
1:C:98:GLU:HG3	1:C:99:PRO:HD2	1.97	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: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:HE2	1:C:431:LYS:HB2	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:HE3	1:A:251:LYS:HB2	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:THR:O	1:C:410:MET:HE2	2.18	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: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:90:PHE:HZ	1:C:203:MET:HE2	1.86	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:194:ASN:O	1:C:199:LYS:NZ	2.54	0.41
1:A:314:LYS:NZ	3:A:608:HOH:O	2.34	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

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	359/363 (99%)	355 (99%)	4 (1%)	73 57
1	B	357/363 (98%)	355 (99%)	2 (1%)	86 77
1	C	294/363 (81%)	286 (97%)	8 (3%)	44 20
All	All	1010/1089 (93%)	996 (99%)	14 (1%)	67 47

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TYR
1	A	140	LYS
1	A	156	PHE
1	A	169	LYS
1	B	33	TYR
1	B	156	PHE
1	C	14	ASN
1	C	174	ILE
1	C	216	LEU
1	C	292	ARG
1	C	374	ASP
1	C	395	THR
1	C	433	LEU
1	C	435	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	GLN
1	B	122	HIS
1	C	14	ASN
1	C	60	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 carbohydrates 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	C	501	-	42,48,48	4.61	17 (40%)	47,73,73	2.59	7 (14%)
2	NAI	B	501	-	42,48,48	4.12	15 (35%)	47,73,73	2.15	7 (14%)
2	NAI	A	501	-	42,48,48	4.21	19 (45%)	47,73,73	2.10	7 (14%)

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	C	501	-	-	6/25/72/72	0/5/5/5
2	NAI	B	501	-	-	7/25/72/72	0/5/5/5
2	NAI	A	501	-	-	11/25/72/72	0/5/5/5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAI	C2B-C1B	-17.38	1.27	1.53
2	A	501	NAI	C2B-C1B	-16.16	1.29	1.53
2	B	501	NAI	C2B-C1B	-16.09	1.29	1.53
2	C	501	NAI	C3B-C4B	-10.81	1.25	1.53
2	B	501	NAI	C3B-C4B	-9.67	1.28	1.53
2	C	501	NAI	O4B-C1B	9.56	1.54	1.41
2	A	501	NAI	C3B-C4B	-9.43	1.28	1.53
2	A	501	NAI	O4B-C1B	9.01	1.53	1.41
2	C	501	NAI	O4D-C1D	8.87	1.63	1.42
2	B	501	NAI	O4B-C1B	7.98	1.52	1.41
2	C	501	NAI	C2D-C1D	-7.91	1.28	1.53
2	B	501	NAI	C2D-C1D	-7.21	1.30	1.53
2	A	501	NAI	C2D-C1D	-6.96	1.31	1.53
2	A	501	NAI	O4D-C1D	6.96	1.58	1.42
2	B	501	NAI	O4D-C1D	6.85	1.58	1.42
2	C	501	NAI	O4D-C4D	-5.93	1.31	1.45
2	C	501	NAI	C4N-C3N	-5.91	1.38	1.49
2	A	501	NAI	O4D-C4D	-5.66	1.32	1.45
2	B	501	NAI	C4N-C3N	-5.50	1.39	1.49
2	A	501	NAI	C4N-C3N	-5.46	1.39	1.49
2	C	501	NAI	O4B-C4B	5.40	1.57	1.45
2	C	501	NAI	C2B-C3B	5.05	1.67	1.53
2	B	501	NAI	O4B-C4B	4.89	1.55	1.45
2	B	501	NAI	C2B-C3B	4.88	1.66	1.53
2	A	501	NAI	O4B-C4B	4.76	1.55	1.45
2	B	501	NAI	O4D-C4D	-4.69	1.34	1.45
2	A	501	NAI	C2B-C3B	4.60	1.65	1.53
2	B	501	NAI	C2A-N3A	4.39	1.39	1.32
2	A	501	NAI	C2A-N3A	4.28	1.39	1.32
2	C	501	NAI	C2A-N3A	4.21	1.38	1.32
2	C	501	NAI	C6N-C5N	3.99	1.40	1.33
2	A	501	NAI	C6N-C5N	3.96	1.40	1.33
2	C	501	NAI	C4N-C5N	-3.81	1.38	1.48
2	B	501	NAI	C6N-C5N	3.68	1.39	1.33
2	C	501	NAI	C7N-N7N	3.62	1.43	1.33
2	B	501	NAI	C7N-N7N	3.51	1.42	1.33
2	A	501	NAI	C7N-N7N	3.40	1.42	1.33
2	B	501	NAI	C4N-C5N	-3.27	1.40	1.48
2	A	501	NAI	C4N-C5N	-3.24	1.40	1.48
2	C	501	NAI	C7N-C3N	2.88	1.54	1.48
2	A	501	NAI	C6A-N6A	2.76	1.44	1.34
2	A	501	NAI	O3B-C3B	2.59	1.49	1.43
2	C	501	NAI	C6A-N6A	2.54	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAI	C6A-N6A	2.52	1.43	1.34
2	C	501	NAI	O2D-C2D	2.51	1.48	1.43
2	C	501	NAI	O3D-C3D	-2.24	1.37	1.43
2	A	501	NAI	C5A-C4A	-2.15	1.35	1.40
2	A	501	NAI	C7N-C3N	2.12	1.53	1.48
2	A	501	NAI	O2B-C2B	2.11	1.47	1.43
2	B	501	NAI	O3B-C3B	2.10	1.47	1.43
2	A	501	NAI	C2N-C3N	2.03	1.40	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	NAI	C5A-C6A-N6A	10.56	136.40	120.35
2	A	501	NAI	C5A-C6A-N6A	8.70	133.57	120.35
2	B	501	NAI	C5A-C6A-N6A	8.59	133.41	120.35
2	C	501	NAI	C1B-N9A-C4A	-7.87	112.81	126.64
2	C	501	NAI	N6A-C6A-N1A	-7.07	103.90	118.57
2	B	501	NAI	C1B-N9A-C4A	-6.18	115.79	126.64
2	A	501	NAI	C1B-N9A-C4A	-5.90	116.28	126.64
2	C	501	NAI	N3A-C2A-N1A	-5.56	119.98	128.68
2	B	501	NAI	N3A-C2A-N1A	-4.95	120.94	128.68
2	A	501	NAI	N6A-C6A-N1A	-4.94	108.32	118.57
2	B	501	NAI	N6A-C6A-N1A	-4.93	108.34	118.57
2	A	501	NAI	N3A-C2A-N1A	-4.63	121.44	128.68
2	B	501	NAI	O4B-C1B-C2B	-3.71	101.51	106.93
2	A	501	NAI	O4D-C1D-C2D	-3.44	99.14	106.64
2	C	501	NAI	C3B-C2B-C1B	3.10	105.64	100.98
2	C	501	NAI	PN-O3-PA	-2.80	123.23	132.83
2	C	501	NAI	C5D-C4D-C3D	-2.67	105.18	115.18
2	B	501	NAI	O4D-C1D-C2D	-2.52	101.16	106.64
2	A	501	NAI	C3N-C2N-N1N	-2.31	119.80	123.10
2	B	501	NAI	C4D-O4D-C1D	-2.03	104.99	109.47
2	A	501	NAI	O4B-C1B-C2B	-2.02	103.98	106.93

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	A	501	NAI	C5D-O5D-PN-O1N
2	A	501	NAI	C5D-O5D-PN-O2N
2	C	501	NAI	C3D-C4D-C5D-O5D
2	C	501	NAI	O4D-C4D-C5D-O5D
2	B	501	NAI	PN-O3-PA-O5B
2	A	501	NAI	PN-O3-PA-O5B
2	A	501	NAI	O4D-C1D-N1N-C6N
2	B	501	NAI	C2D-C1D-N1N-C6N
2	A	501	NAI	C2D-C1D-N1N-C6N
2	C	501	NAI	O4D-C1D-N1N-C6N
2	B	501	NAI	O4D-C1D-N1N-C6N
2	C	501	NAI	C2D-C1D-N1N-C6N
2	B	501	NAI	O4B-C4B-C5B-O5B
2	B	501	NAI	C5D-O5D-PN-O3
2	A	501	NAI	C5B-O5B-PA-O3
2	A	501	NAI	C5D-O5D-PN-O3
2	A	501	NAI	O4B-C4B-C5B-O5B
2	A	501	NAI	C5B-O5B-PA-O1A
2	C	501	NAI	O4B-C4B-C5B-O5B
2	A	501	NAI	C2D-C1D-N1N-C2N

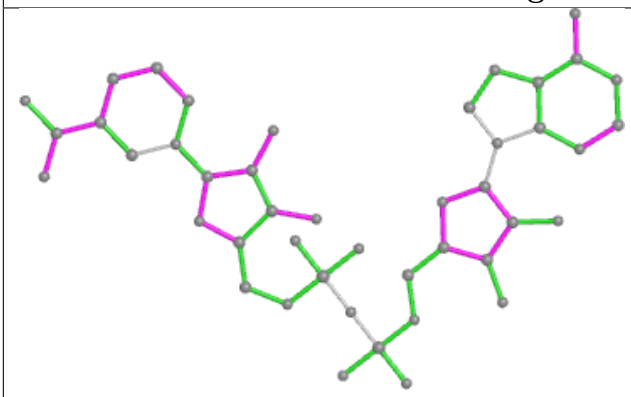
There are no ring outliers.

1 monomer is involved in 3 short contacts:

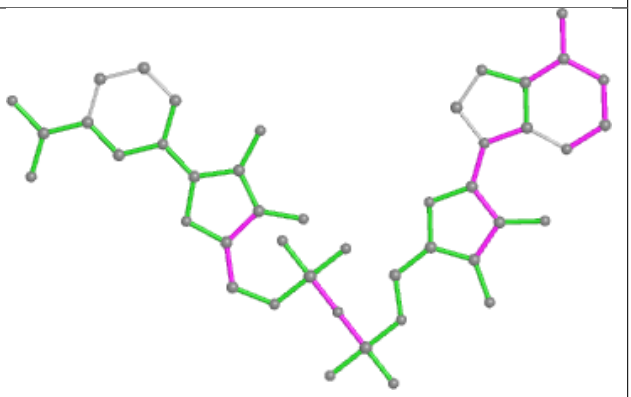
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAI	3	0

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 then 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.

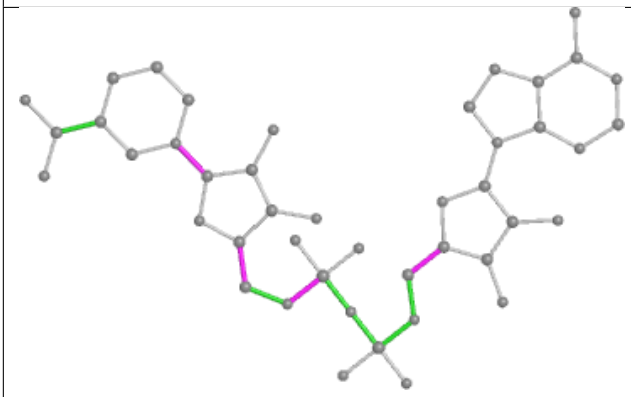
Ligand NAI C 501



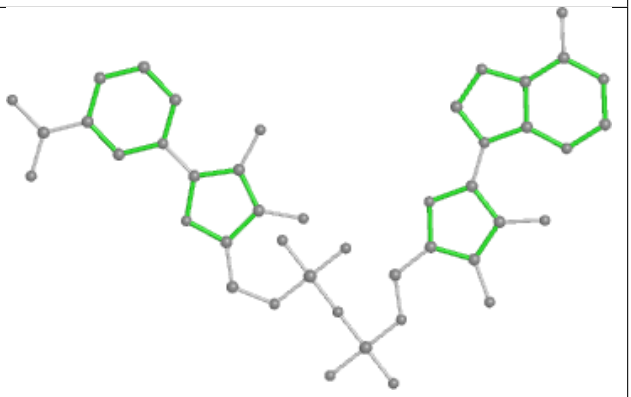
Bond lengths



Bond angles

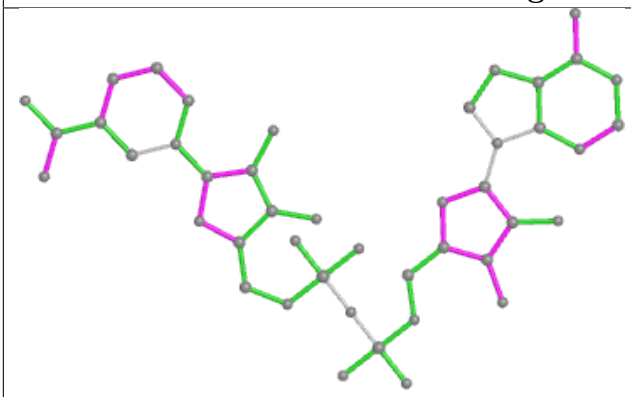


Torsions

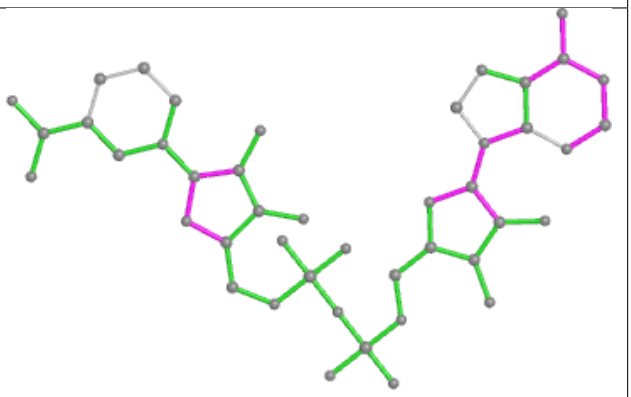


Rings

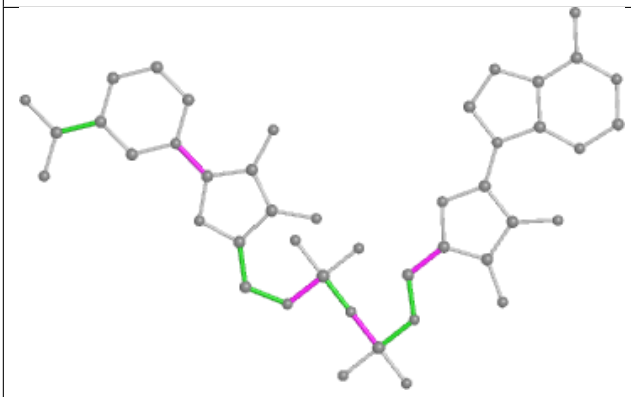
Ligand NAI B 501



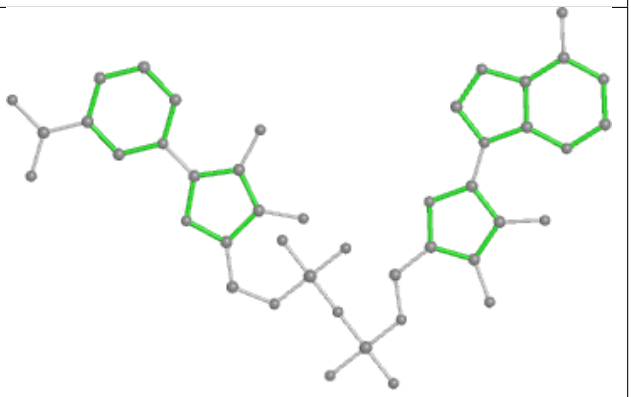
Bond lengths



Bond angles

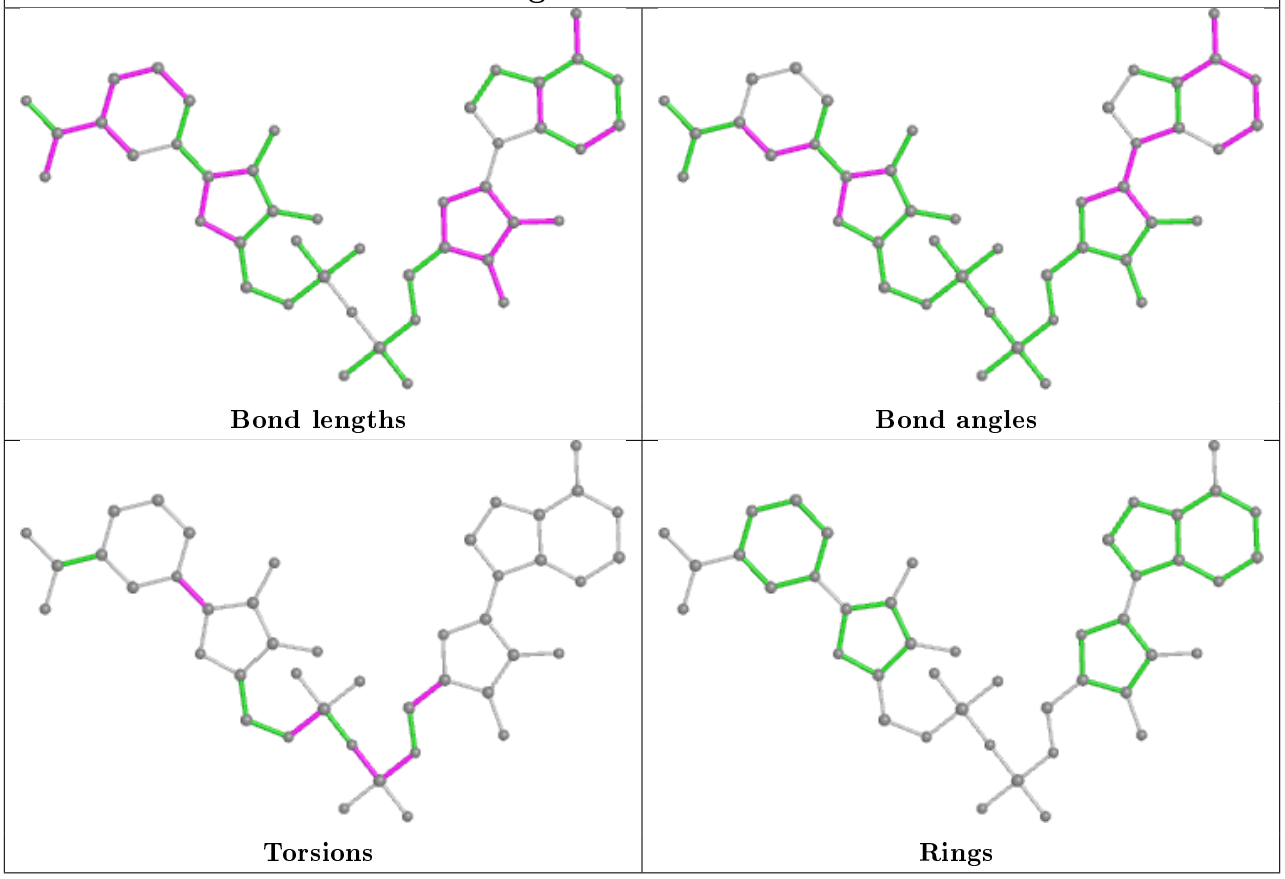


Torsions



Rings

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

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, 95^{th} 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%)	0.12	8 (1%) 68 67	17, 27, 49, 109	0
1	B	440/446 (98%)	0.19	14 (3%) 47 44	15, 26, 47, 78	0
1	C	367/446 (82%)	2.46	197 (53%) 0 0	41, 65, 87, 105	0
All	All	1249/1338 (93%)	0.83	219 (17%) 1 1	15, 32, 78, 109	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	ALA	8.7
1	C	227	LEU	8.5
1	C	120	TRP	7.6
1	C	121	ALA	7.6
1	C	21	VAL	7.2
1	C	33	TYR	7.0
1	C	47	THR	6.9
1	C	392	ALA	6.4
1	C	84	VAL	6.4
1	C	29	PHE	6.3
1	A	442	HIS	6.3
1	C	225	ALA	6.0
1	C	42	ARG	5.9
1	C	269	LEU	5.8
1	A	58	GLU	5.7
1	C	62	LEU	5.7
1	C	239	TYR	5.6
1	C	328	ALA	5.6
1	C	193	LEU	5.6
1	C	123	ILE	5.6
1	C	138	VAL	5.6
1	C	49	VAL	5.5
1	C	326	TRP	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	156	PHE	5.4
1	C	96	ALA	5.3
1	C	90	PHE	5.3
1	C	329	CYS	5.3
1	C	435	LEU	5.2
1	C	81	ILE	5.2
1	C	126	CYS	5.1
1	C	433	LEU	5.1
1	C	386	MET	5.0
1	C	222	ALA	5.0
1	C	22	PHE	4.8
1	C	363	ALA	4.8
1	C	155	ALA	4.7
1	C	393	LEU	4.7
1	C	78	GLY	4.7
1	C	41	ALA	4.7
1	C	110	LEU	4.6
1	C	38	ILE	4.6
1	C	48	ILE	4.5
1	C	249	ASP	4.5
1	C	436	MET	4.4
1	C	99	PRO	4.4
1	C	63	ARG	4.4
1	A	172	LEU	4.4
1	C	95	PRO	4.3
1	C	228	GLU	4.3
1	C	437	HIS	4.3
1	C	394	VAL	4.3
1	C	385	LYS	4.3
1	C	372	LEU	4.2
1	C	281	ILE	4.2
1	C	362	GLU	4.1
1	C	349	TYR	4.1
1	C	226	ARG	4.1
1	C	338	THR	4.1
1	C	24	LEU	4.0
1	C	346	ILE	4.0
1	C	80	ARG	4.0
1	C	325	GLN	4.0
1	C	45	GLY	4.0
1	C	161	MET	4.0
1	C	16	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	28	LEU	4.0
1	C	238	ALA	4.0
1	C	213	PHE	4.0
1	C	395	THR	3.9
1	C	217	ILE	3.9
1	C	1	MET	3.9
1	C	54	GLY	3.9
1	C	79	GLY	3.8
1	C	131	VAL	3.8
1	C	421	VAL	3.8
1	C	171	PHE	3.8
1	C	15	ILE	3.8
1	C	397	VAL	3.8
1	B	184	GLU	3.7
1	C	159	HIS	3.7
1	C	401	LEU	3.6
1	C	162	ALA	3.6
1	C	60	ASN	3.6
1	C	132	GLN	3.6
1	C	412	HIS	3.5
1	C	64	ALA	3.5
1	C	129	VAL	3.5
1	C	2	LYS	3.5
1	C	416	ASN	3.5
1	C	43	ASP	3.5
1	C	387	HIS	3.4
1	C	224	ARG	3.4
1	C	94	ALA	3.4
1	C	112	SER	3.4
1	C	241	TYR	3.3
1	C	61	ALA	3.3
1	C	194	ASN	3.3
1	C	46	MET	3.3
1	C	208	VAL	3.3
1	C	286	TYR	3.2
1	B	25	PHE	3.2
1	C	299	PHE	3.2
1	C	312	ALA	3.2
1	B	110	LEU	3.2
1	C	124	GLU	3.2
1	C	272	ILE	3.2
1	C	367	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	191	ALA	3.1
1	C	351	ALA	3.1
1	C	223	ILE	3.1
1	C	434	ASN	3.1
1	C	327	GLN	3.1
1	C	353	ASP	3.1
1	C	157	PHE	3.1
1	C	188	SER	3.1
1	C	358	PHE	3.0
1	C	384	THR	3.0
1	C	340	GLU	3.0
1	B	111	LYS	3.0
1	C	301	GLY	3.0
1	C	411	PHE	3.0
1	B	185	ARG	3.0
1	C	160	THR	3.0
1	C	313	LEU	2.9
1	C	122	HIS	2.9
1	C	34	ALA	2.9
1	C	219	GLY	2.9
1	C	250	ASP	2.9
1	C	170	VAL	2.9
1	C	265	ALA	2.9
1	A	59	ASN	2.8
1	C	361	PHE	2.8
1	C	135	LYS	2.8
1	C	266	LYS	2.8
1	C	248	ILE	2.8
1	C	298	ILE	2.8
1	C	360	ASN	2.8
1	C	429	ILE	2.8
1	C	408	PRO	2.8
1	C	370	ALA	2.8
1	C	174	ILE	2.8
1	C	341	SER	2.8
1	C	128	ALA	2.7
1	C	302	VAL	2.7
1	C	209	THR	2.7
1	C	240	GLY	2.7
1	C	100	THR	2.7
1	C	117	LYS	2.7
1	C	264	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	247	LEU	2.7
1	C	3	SER	2.6
1	C	109	THR	2.6
1	C	236	TYR	2.6
1	C	50	GLY	2.6
1	C	195	SER	2.6
1	B	335	GLU	2.6
1	B	109	THR	2.6
1	C	339	LEU	2.6
1	A	111	LYS	2.6
1	C	12	GLN	2.6
1	C	285	VAL	2.6
1	C	383	ILE	2.6
1	B	437	HIS	2.5
1	C	192	LEU	2.5
1	C	291	ILE	2.5
1	C	52	THR	2.5
1	C	275	ASP	2.5
1	C	310	LEU	2.5
1	C	115	ASP	2.5
1	C	254	TRP	2.4
1	C	6	PRO	2.4
1	C	288	CYS	2.4
1	C	125	LYS	2.4
1	C	11	PRO	2.4
1	C	111	LYS	2.4
1	A	184	GLU	2.4
1	C	178	ILE	2.4
1	C	237	SER	2.3
1	C	53	VAL	2.3
1	C	14	ASN	2.3
1	C	107	ASP	2.3
1	C	36	GLY	2.3
1	C	409	LEU	2.3
1	C	424	LEU	2.3
1	C	136	ASP	2.3
1	C	343	LEU	2.3
1	C	83	ASN	2.3
1	B	59	ASN	2.2
1	C	93	ASP	2.2
1	C	422	LEU	2.2
1	C	311	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	156	PHE	2.2
1	C	118	LEU	2.2
1	C	216	LEU	2.2
1	C	342	LEU	2.2
1	C	89	GLY	2.2
1	C	190	SER	2.1
1	C	347	ASP	2.1
1	C	7	LEU	2.1
1	C	278	LYS	2.1
1	B	1	MET	2.1
1	C	369	THR	2.1
1	C	175	ALA	2.1
1	A	390	ARG	2.1
1	C	309	LEU	2.1
1	C	91	ASP	2.1
1	C	345	LYS	2.1
1	C	130	GLY	2.1
1	C	304	LEU	2.1
1	C	51	ILE	2.1
1	C	119	ASP	2.1
1	C	4	PRO	2.1
1	B	66	THR	2.1
1	C	113	TRP	2.1
1	C	37	LEU	2.1
1	B	23	VAL	2.0
1	C	300	VAL	2.0
1	B	310	LEU	2.0
1	A	238	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

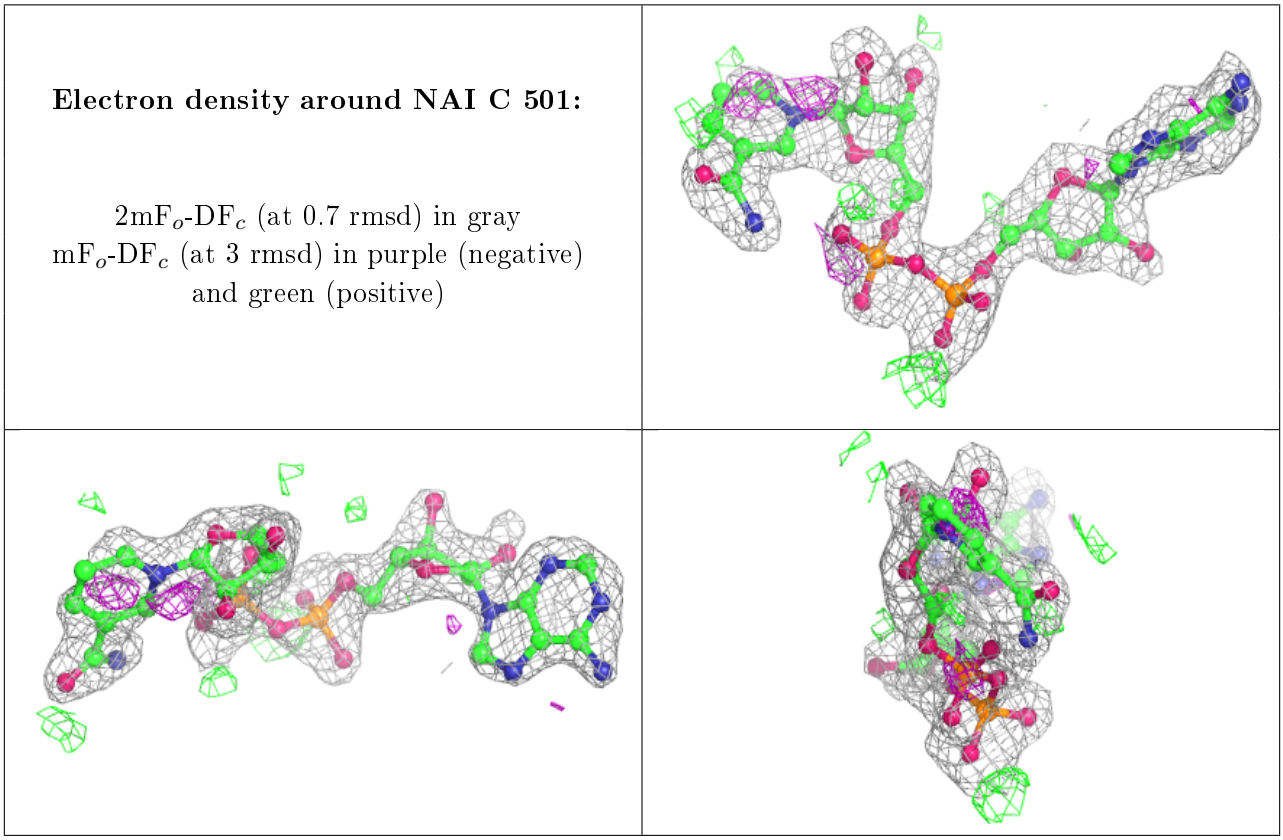
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAI	C	501	44/44	0.84	0.14	42,58,67,119	0
2	NAI	A	501	44/44	0.96	0.09	16,19,22,23	0
2	NAI	B	501	44/44	0.97	0.10	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.

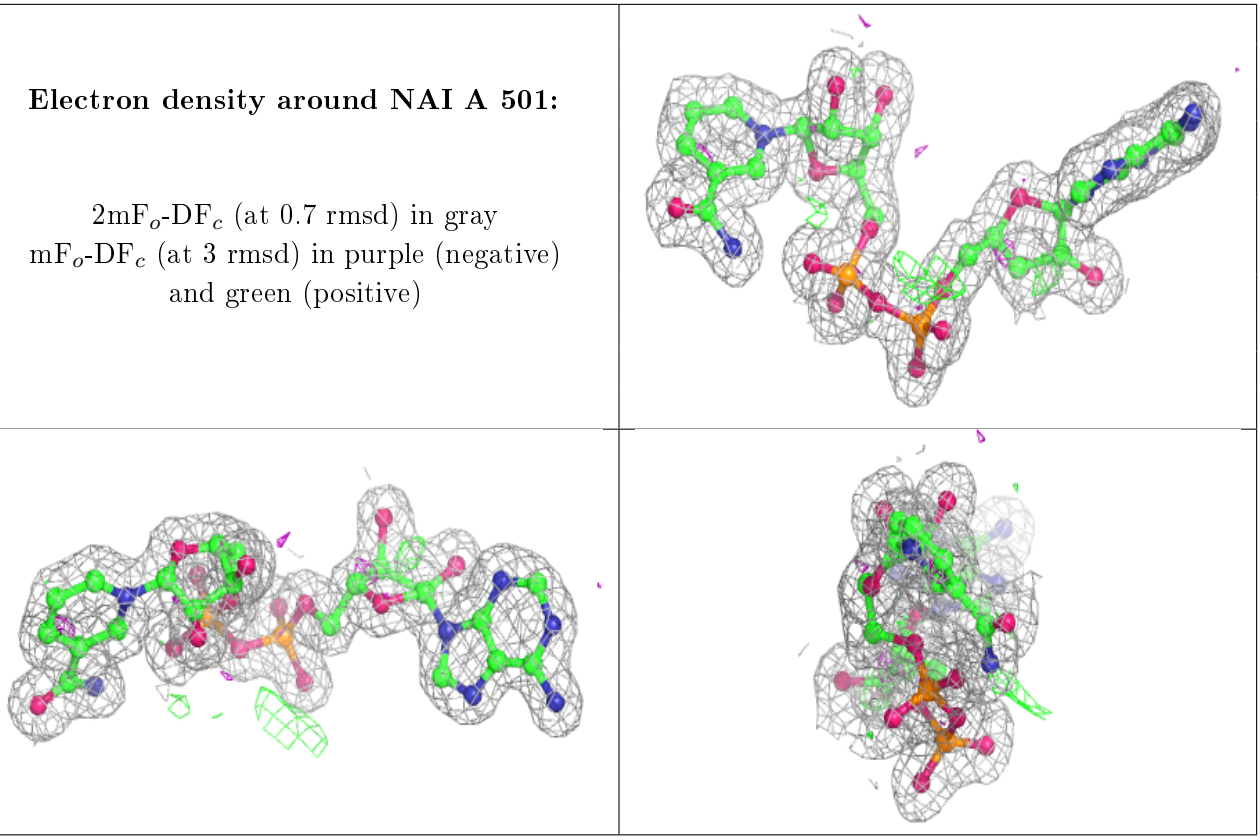
Electron density around NAI C 501:

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



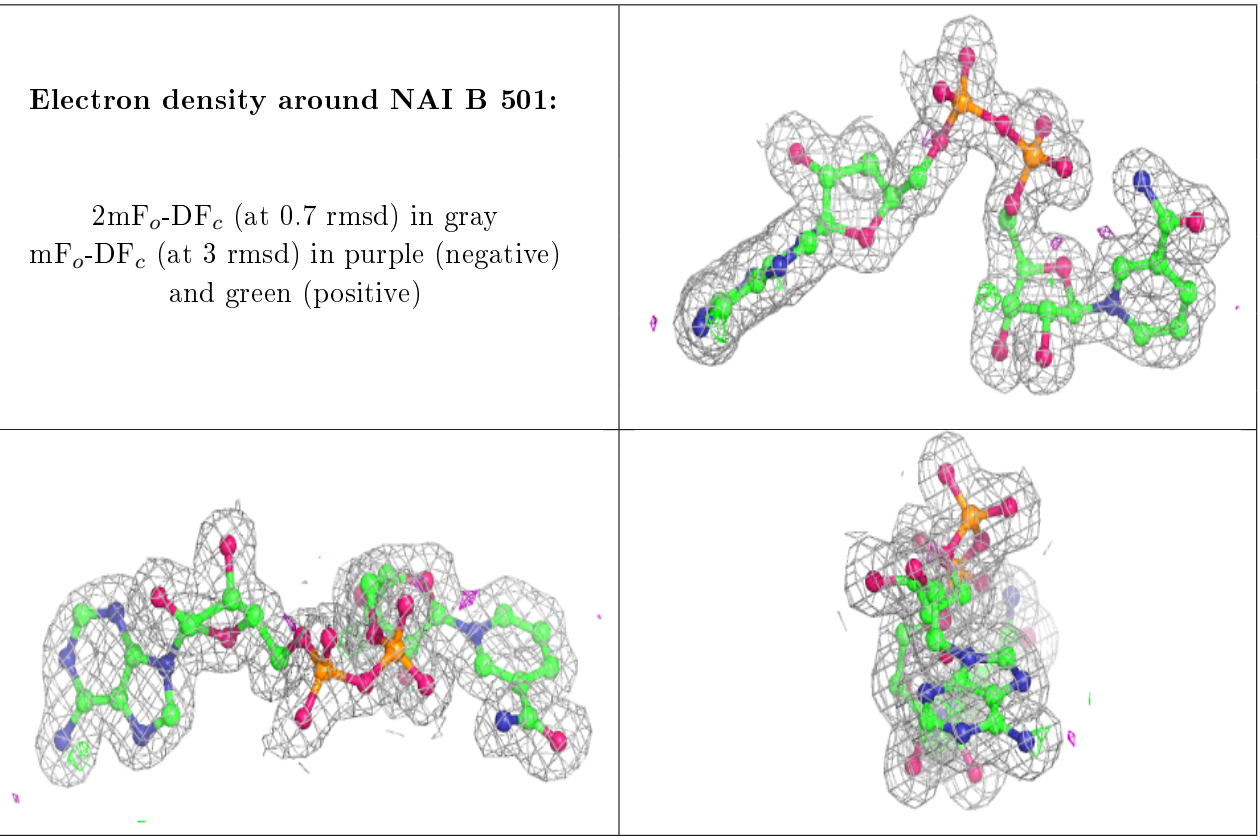
Electron density around NAI A 501:

$2mF_o$-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.