Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 08:11 am BST

PDB ID	:	4WLO
Title	:	Crystal structure of oxaloacetate and NADH bound MDH2
Authors	:	Eo, Y.M.; Han, B.G.; Ahn, H.C.
Deposited on	:	2014-10-07
Resolution	:	2.50 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:

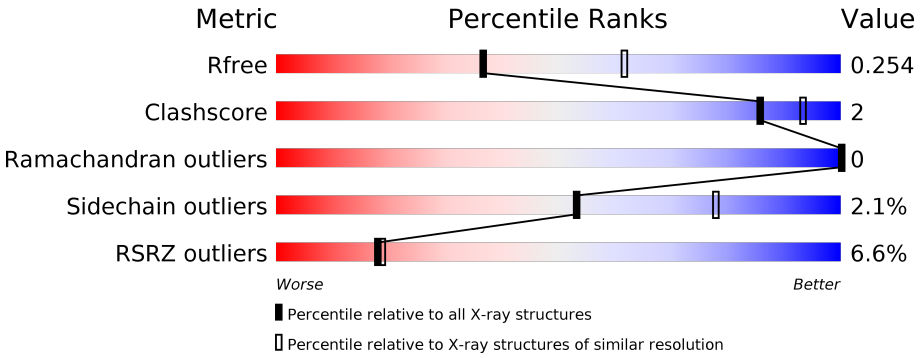
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	340	4% 86% 6% · 8%
1	B	340	3% 88% · 8%
1	C	340	12% 87% · · 8%
1	D	340	5% 88% · 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OAA	A	402	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9488 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 Malate dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2312	1472	390	437	13			
1	B	314	Total	C	N	O	S	0	0	0
			2312	1472	390	437	13			
1	C	314	Total	C	N	O	S	0	0	0
			2312	1472	390	437	13			
1	D	314	Total	C	N	O	S	0	1	0
			2315	1474	390	438	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P40926
A	0	GLY	-	expression tag	UNP P40926
A	1	SER	-	expression tag	UNP P40926
A	2	SER	-	expression tag	UNP P40926
A	3	HIS	-	expression tag	UNP P40926
A	4	HIS	-	expression tag	UNP P40926
A	5	HIS	-	expression tag	UNP P40926
A	6	HIS	-	expression tag	UNP P40926
A	7	HIS	-	expression tag	UNP P40926
A	8	HIS	-	expression tag	UNP P40926
A	9	SER	-	expression tag	UNP P40926
A	10	SER	-	expression tag	UNP P40926
A	11	GLY	-	expression tag	UNP P40926
A	12	LEU	-	expression tag	UNP P40926
A	13	VAL	-	expression tag	UNP P40926
A	14	PRO	-	expression tag	UNP P40926
A	15	ARG	-	expression tag	UNP P40926
A	16	GLY	-	expression tag	UNP P40926
A	17	SER	-	expression tag	UNP P40926
A	18	HIS	-	expression tag	UNP P40926
A	19	MET	-	expression tag	UNP P40926

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	expression tag	UNP P40926
B	0	GLY	-	expression tag	UNP P40926
B	1	SER	-	expression tag	UNP P40926
B	2	SER	-	expression tag	UNP P40926
B	3	HIS	-	expression tag	UNP P40926
B	4	HIS	-	expression tag	UNP P40926
B	5	HIS	-	expression tag	UNP P40926
B	6	HIS	-	expression tag	UNP P40926
B	7	HIS	-	expression tag	UNP P40926
B	8	HIS	-	expression tag	UNP P40926
B	9	SER	-	expression tag	UNP P40926
B	10	SER	-	expression tag	UNP P40926
B	11	GLY	-	expression tag	UNP P40926
B	12	LEU	-	expression tag	UNP P40926
B	13	VAL	-	expression tag	UNP P40926
B	14	PRO	-	expression tag	UNP P40926
B	15	ARG	-	expression tag	UNP P40926
B	16	GLY	-	expression tag	UNP P40926
B	17	SER	-	expression tag	UNP P40926
B	18	HIS	-	expression tag	UNP P40926
B	19	MET	-	expression tag	UNP P40926
C	-1	MET	-	expression tag	UNP P40926
C	0	GLY	-	expression tag	UNP P40926
C	1	SER	-	expression tag	UNP P40926
C	2	SER	-	expression tag	UNP P40926
C	3	HIS	-	expression tag	UNP P40926
C	4	HIS	-	expression tag	UNP P40926
C	5	HIS	-	expression tag	UNP P40926
C	6	HIS	-	expression tag	UNP P40926
C	7	HIS	-	expression tag	UNP P40926
C	8	HIS	-	expression tag	UNP P40926
C	9	SER	-	expression tag	UNP P40926
C	10	SER	-	expression tag	UNP P40926
C	11	GLY	-	expression tag	UNP P40926
C	12	LEU	-	expression tag	UNP P40926
C	13	VAL	-	expression tag	UNP P40926
C	14	PRO	-	expression tag	UNP P40926
C	15	ARG	-	expression tag	UNP P40926
C	16	GLY	-	expression tag	UNP P40926
C	17	SER	-	expression tag	UNP P40926
C	18	HIS	-	expression tag	UNP P40926
C	19	MET	-	expression tag	UNP P40926

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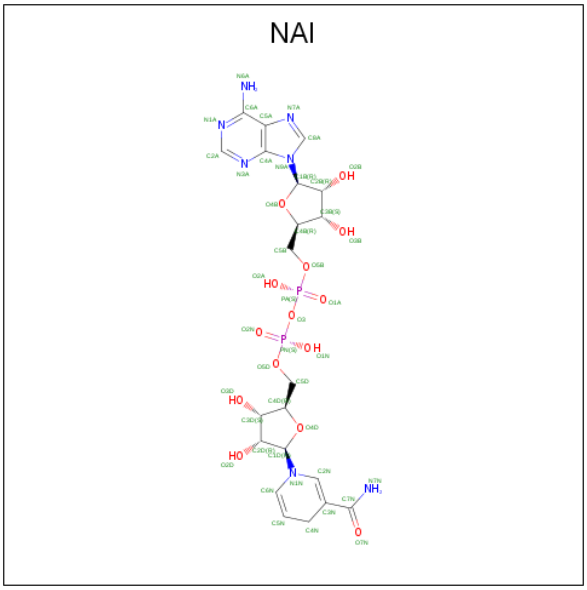
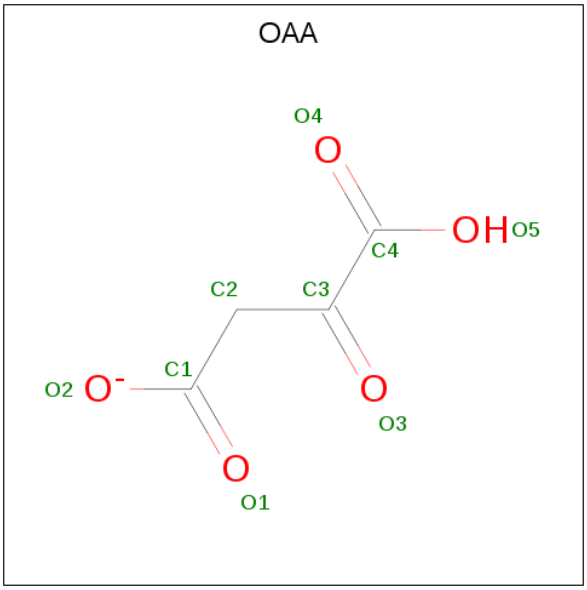
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	MET	-	expression tag	UNP P40926
D	0	GLY	-	expression tag	UNP P40926
D	1	SER	-	expression tag	UNP P40926
D	2	SER	-	expression tag	UNP P40926
D	3	HIS	-	expression tag	UNP P40926
D	4	HIS	-	expression tag	UNP P40926
D	5	HIS	-	expression tag	UNP P40926
D	6	HIS	-	expression tag	UNP P40926
D	7	HIS	-	expression tag	UNP P40926
D	8	HIS	-	expression tag	UNP P40926
D	9	SER	-	expression tag	UNP P40926
D	10	SER	-	expression tag	UNP P40926
D	11	GLY	-	expression tag	UNP P40926
D	12	LEU	-	expression tag	UNP P40926
D	13	VAL	-	expression tag	UNP P40926
D	14	PRO	-	expression tag	UNP P40926
D	15	ARG	-	expression tag	UNP P40926
D	16	GLY	-	expression tag	UNP P40926
D	17	SER	-	expression tag	UNP P40926
D	18	HIS	-	expression tag	UNP P40926
D	19	MET	-	expression tag	UNP P40926

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



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		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			9	4	5			
3	B	1	Total	C	O		0	0
			9	4	5			
3	C	1	Total	C	O		0	0
			9	4	5			
3	D	1	Total	C	O		0	0
			9	4	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	16	Total	O	0	0
			16	16		

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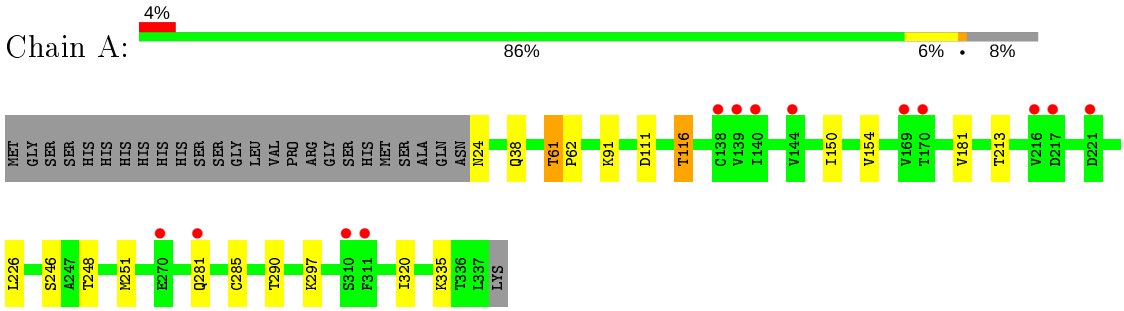
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total O 2 2	0	0
4	D	4	Total O 4 4	0	0

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.

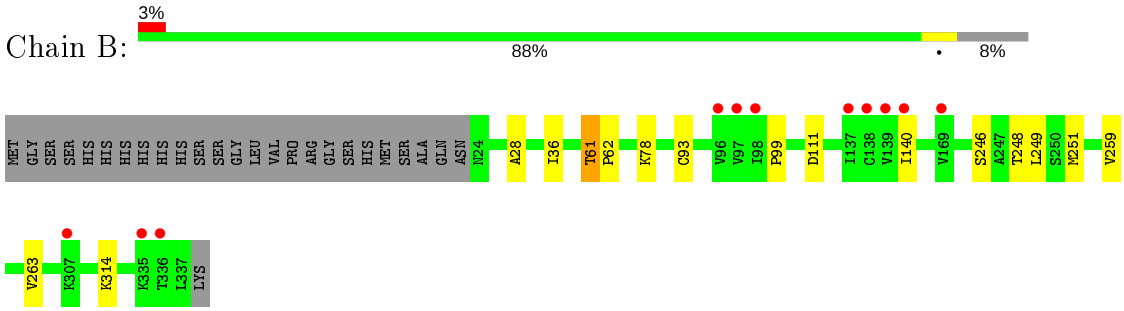
- Molecule 1: Malate dehydrogenase, mitochondrial

Chain A:



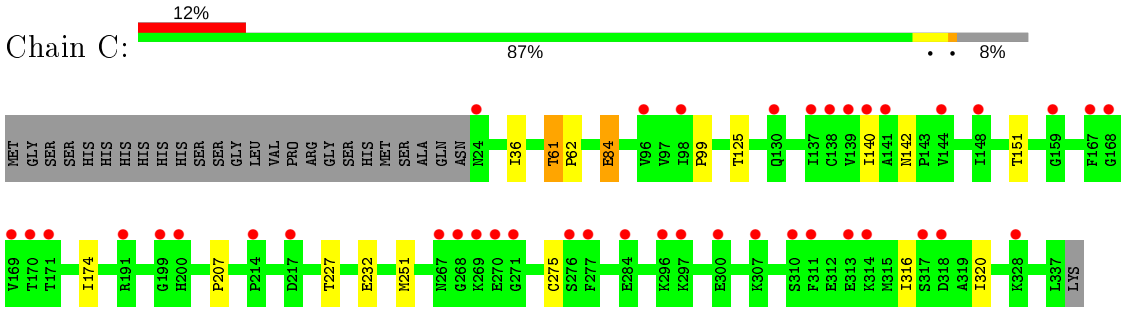
- Molecule 1: Malate dehydrogenase, mitochondrial

Chain B:



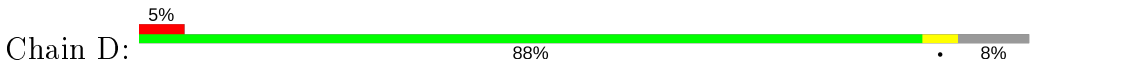
- Molecule 1: Malate dehydrogenase, mitochondrial

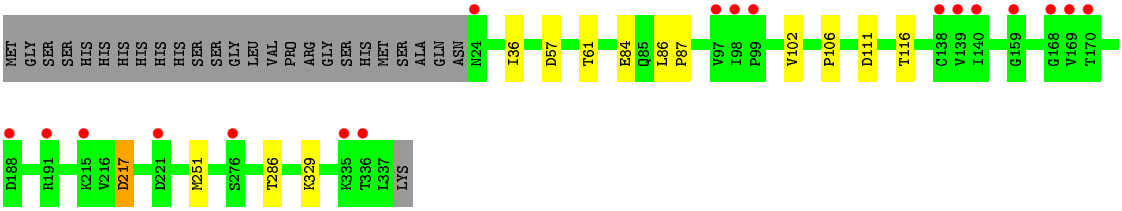
Chain C:



- Molecule 1: Malate dehydrogenase, mitochondrial

Chain D:




MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER ALA GLN ASN N24 I36 D57 T61 E84 Q85 L86 P87 V97 I98 P99 V102 P106 D111 T116 C138 V139 I140 G159 G168 V169 T170
D188 R191 K215 V216 D217 D221 M251 S276 T286 K329 R335 T336 L337 LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.99Å 152.19Å 155.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.35 – 2.50 28.35 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (28.35-2.50) 99.0 (28.35-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.30 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.212 , 0.255 0.216 , 0.254	Depositor DCC
R_{free} test set	2541 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9488	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, OAA

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	0.33	0/2351	0.51	0/3192
1	B	0.33	0/2351	0.51	0/3192
1	C	0.30	0/2351	0.47	0/3192
1	D	0.31	0/2358	0.48	0/3202
All	All	0.32	0/9411	0.50	0/12778

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	2312	0	2400	8	0
1	B	2312	0	2400	9	0
1	C	2312	0	2400	11	0
1	D	2315	0	2403	8	0
2	A	44	0	27	5	0
2	B	44	0	27	5	0
2	C	44	0	27	4	0
2	D	44	0	27	6	0
3	A	9	0	2	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	2	1	0
3	C	9	0	2	2	0
3	D	9	0	2	3	0
4	A	3	0	0	0	0
4	B	16	0	0	0	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
All	All	9488	0	9719	43	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 2.

All (43) 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:B:251:MET:SD	2:B:401:NAI:H4N	2.23	0.79
1:A:116:THR:HG23	1:D:106:PRO:O	1.97	0.64
1:A:251:MET:SD	2:A:401:NAI:H4N	2.41	0.60
1:C:316:ILE:O	1:C:320:ILE:HD12	2.05	0.57
2:B:401:NAI:H42N	3:B:402:OAA:C3	2.38	0.54
1:C:84:GLU:H	1:C:84:GLU:CD	2.13	0.52
2:A:401:NAI:H42N	3:A:402:OAA:C3	2.39	0.52
1:D:251:MET:SD	2:D:401:NAI:H4N	2.51	0.51
1:B:99:PRO:O	2:B:401:NAI:H51N	2.11	0.50
1:C:125:THR:HG21	1:C:151:THR:HG23	1.94	0.50
1:D:111:ASP:OD2	1:D:329:LYS:NZ	2.45	0.50
2:A:401:NAI:H42N	3:A:402:OAA:C4	2.42	0.49
1:C:99:PRO:O	2:C:401:NAI:H51N	2.15	0.47
1:C:174:ILE:HD11	1:C:275:CYS:HB2	1.98	0.46
1:D:102:VAL:HG21	1:D:116:THR:HG21	1.97	0.46
1:A:150:ILE:O	1:A:154:VAL:HG23	2.16	0.46
1:B:36:ILE:HD11	2:B:401:NAI:C6N	2.47	0.45
2:A:401:NAI:C5N	3:A:402:OAA:C2	2.94	0.45
2:C:401:NAI:H42N	3:C:402:OAA:C4	2.46	0.45
2:D:401:NAI:H42N	3:D:402:OAA:C3	2.46	0.45
1:A:285:CYS:SG	1:A:320:ILE:HG23	2.57	0.45
1:B:140:ILE:O	2:B:401:NAI:H2N	2.17	0.45
1:D:86:LEU:HB3	1:D:87:PRO:HD3	1.99	0.44
1:A:181:VAL:HG22	1:A:226:LEU:HD21	1.99	0.44
1:C:36:ILE:HD11	2:C:401:NAI:C6N	2.48	0.44
2:D:401:NAI:H42N	3:D:402:OAA:C4	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ASP:OD2	2:D:401:NAI:O3B	2.35	0.44
1:C:142:ASN:ND2	3:C:402:OAA:O3	2.51	0.43
1:B:28:ALA:HB2	1:B:93:CYS:SG	2.59	0.42
1:D:217:ASP:OD1	1:D:217:ASP:N	2.52	0.42
1:A:246:SER:O	1:A:248:THR:HG23	2.20	0.42
2:A:401:NAI:C5N	3:A:402:OAA:H21	2.49	0.42
1:C:99:PRO:HA	1:C:140:ILE:HB	2.02	0.42
1:B:246:SER:O	1:B:248:THR:HG23	2.19	0.41
1:D:36:ILE:HD11	2:D:401:NAI:C6N	2.50	0.41
1:C:251:MET:SD	2:C:401:NAI:H4N	2.60	0.41
1:B:259:VAL:O	1:B:263:VAL:HG23	2.19	0.41
1:B:61:THR:N	1:B:62:PRO:CD	2.84	0.41
1:C:207:PRO:CG	1:C:227:THR:HG23	2.51	0.41
2:D:401:NAI:C5N	3:D:402:OAA:C2	2.98	0.41
1:A:38:GLN:HB3	1:B:249:LEU:HD21	2.04	0.40
1:A:61:THR:N	1:A:62:PRO:CD	2.84	0.40
1:C:61:THR:N	1:C:62:PRO:CD	2.84	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	312/340 (92%)	305 (98%)	7 (2%)	0	100	100
1	B	312/340 (92%)	303 (97%)	9 (3%)	0	100	100
1	C	312/340 (92%)	304 (97%)	8 (3%)	0	100	100
1	D	313/340 (92%)	307 (98%)	6 (2%)	0	100	100
All	All	1249/1360 (92%)	1219 (98%)	30 (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	253/275 (92%)	243 (96%)	10 (4%)	31	56
1	B	253/275 (92%)	249 (98%)	4 (2%)	62	84
1	C	253/275 (92%)	250 (99%)	3 (1%)	71	88
1	D	254/275 (92%)	249 (98%)	5 (2%)	55	79
All	All	1013/1100 (92%)	991 (98%)	22 (2%)	53	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	61	THR
1	A	91	LYS
1	A	111	ASP
1	A	116	THR
1	A	213	THR
1	A	281	GLN
1	A	290	THR
1	A	297	LYS
1	A	335	LYS
1	B	61	THR
1	B	78	LYS
1	B	111	ASP
1	B	314	LYS
1	C	61	THR
1	C	84	GLU
1	C	232	GLU
1	D	61	THR
1	D	84	GLU
1	D	217	ASP
1	D	286[A]	THR
1	D	286[B]	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	164	ASN
1	A	267	ASN
1	B	164	ASN
1	B	193	ASN
1	B	267	ASN
1	C	24	ASN
1	C	267	ASN
1	D	24	ASN
1	D	164	ASN
1	D	267	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

8 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	401	-	42,48,48	1.83	10 (23%)	47,73,73	1.39	4 (8%)
3	OAA	D	402	-	2,8,8	0.71	0	2,10,10	2.81	1 (50%)
3	OAA	B	402	-	2,8,8	1.21	0	2,10,10	2.66	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OAA	C	402	-	2,8,8	1.63	1 (50%)	2,10,10	1.35	0
3	OAA	A	402	-	2,8,8	1.14	0	2,10,10	2.75	1 (50%)
2	NAI	B	401	-	42,48,48	1.81	10 (23%)	47,73,73	1.40	5 (10%)
2	NAI	D	401	-	42,48,48	1.72	10 (23%)	47,73,73	1.52	6 (12%)
2	NAI	C	401	-	42,48,48	1.81	10 (23%)	47,73,73	1.39	4 (8%)

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	401	-	-	6/25/72/72	0/5/5/5
3	OAA	D	402	-	-	2/2/8/8	-
3	OAA	B	402	-	-	2/2/8/8	-
3	OAA	C	402	-	-	2/2/8/8	-
3	OAA	A	402	-	-	2/2/8/8	-
2	NAI	B	401	-	-	6/25/72/72	0/5/5/5
2	NAI	D	401	-	-	10/25/72/72	0/5/5/5
2	NAI	C	401	-	-	7/25/72/72	0/5/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAI	C2A-N3A	5.18	1.40	1.32
2	A	401	NAI	C2A-N3A	4.99	1.40	1.32
2	C	401	NAI	C2A-N3A	4.87	1.40	1.32
2	D	401	NAI	C2A-N3A	4.40	1.39	1.32
2	C	401	NAI	C4N-C3N	-4.19	1.41	1.49
2	D	401	NAI	C4N-C3N	-4.12	1.41	1.49
2	A	401	NAI	O4B-C1B	4.11	1.46	1.41
2	B	401	NAI	C4N-C3N	-4.11	1.41	1.49
2	A	401	NAI	C4N-C3N	-4.05	1.42	1.49
2	B	401	NAI	C6N-C5N	3.70	1.39	1.33
2	B	401	NAI	C2A-N1A	3.69	1.40	1.33
2	C	401	NAI	C2A-N1A	3.57	1.40	1.33
2	C	401	NAI	C6N-C5N	3.55	1.39	1.33
2	D	401	NAI	C6N-C5N	3.45	1.39	1.33
2	D	401	NAI	C2A-N1A	3.44	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAI	C4N-C5N	-3.39	1.40	1.48
2	C	401	NAI	O4B-C1B	3.39	1.45	1.41
2	C	401	NAI	C7N-C3N	-3.29	1.41	1.48
2	A	401	NAI	C6N-C5N	3.29	1.39	1.33
2	A	401	NAI	C2A-N1A	3.21	1.39	1.33
2	D	401	NAI	C4N-C5N	-3.20	1.40	1.48
2	A	401	NAI	C7N-C3N	-3.20	1.41	1.48
2	B	401	NAI	C7N-C3N	-3.15	1.41	1.48
2	C	401	NAI	C4N-C5N	-3.11	1.40	1.48
2	D	401	NAI	C7N-C3N	-3.04	1.42	1.48
2	B	401	NAI	C4N-C5N	-2.96	1.41	1.48
2	B	401	NAI	O4B-C1B	2.84	1.45	1.41
2	A	401	NAI	C5A-C4A	-2.77	1.33	1.40
2	D	401	NAI	C5A-C4A	-2.68	1.33	1.40
2	B	401	NAI	C5A-C4A	-2.61	1.34	1.40
2	D	401	NAI	C6A-C5A	-2.53	1.33	1.43
2	C	401	NAI	C5A-C4A	-2.51	1.34	1.40
2	D	401	NAI	O4B-C1B	2.36	1.44	1.41
2	B	401	NAI	C6A-C5A	-2.34	1.34	1.43
2	C	401	NAI	C6A-C5A	-2.29	1.34	1.43
3	C	402	OAA	C2-C3	2.25	1.53	1.51
2	A	401	NAI	C6A-C5A	-2.24	1.35	1.43
2	B	401	NAI	C2N-C3N	2.13	1.40	1.34
2	A	401	NAI	C2N-C3N	2.13	1.40	1.34
2	C	401	NAI	C2N-C3N	2.05	1.40	1.34
2	D	401	NAI	C2N-C3N	2.01	1.40	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	NAI	N3A-C2A-N1A	-6.65	118.29	128.68
2	D	401	NAI	N3A-C2A-N1A	-6.54	118.45	128.68
2	B	401	NAI	N3A-C2A-N1A	-6.50	118.51	128.68
2	C	401	NAI	N3A-C2A-N1A	-6.38	118.71	128.68
3	D	402	OAA	C1-C2-C3	-3.95	108.47	115.51
3	A	402	OAA	C1-C2-C3	-3.80	108.73	115.51
3	B	402	OAA	C1-C2-C3	-3.70	108.91	115.51
2	D	401	NAI	C1B-N9A-C4A	-3.41	120.66	126.64
2	D	401	NAI	PN-O3-PA	-2.85	123.05	132.83
2	B	401	NAI	O4B-C1B-C2B	-2.57	103.17	106.93
2	A	401	NAI	PN-O3-PA	-2.53	124.13	132.83
2	C	401	NAI	C1B-N9A-C4A	-2.50	122.26	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	NAI	C1B-N9A-C4A	-2.49	122.27	126.64
2	B	401	NAI	C5A-C6A-N6A	-2.29	116.87	120.35
2	B	401	NAI	C1B-N9A-C4A	-2.27	122.66	126.64
2	D	401	NAI	C5B-C4B-C3B	-2.23	106.83	115.18
2	D	401	NAI	O4B-C1B-C2B	-2.19	103.73	106.93
2	A	401	NAI	C4A-C5A-N7A	-2.15	107.16	109.40
2	C	401	NAI	O4B-C1B-C2B	-2.05	103.92	106.93
2	C	401	NAI	C4A-C5A-N7A	-2.03	107.28	109.40
2	B	401	NAI	O4D-C1D-N1N	2.02	112.01	108.06
2	D	401	NAI	C4A-C5A-N7A	-2.01	107.31	109.40

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	NAI	C5B-O5B-PA-O1A
2	D	401	NAI	O4B-C4B-C5B-O5B
2	D	401	NAI	C3B-C4B-C5B-O5B
3	A	402	OAA	C1-C2-C3-C4
2	A	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	C2D-C1D-N1N-C2N
2	C	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	C5B-O5B-PA-O3
3	D	402	OAA	C1-C2-C3-O3
3	D	402	OAA	C1-C2-C3-C4
3	B	402	OAA	C1-C2-C3-O3
3	B	402	OAA	C1-C2-C3-C4
3	C	402	OAA	C1-C2-C3-O3
3	C	402	OAA	C1-C2-C3-C4
3	A	402	OAA	C1-C2-C3-O3
2	B	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	C5B-O5B-PA-O2A
2	D	401	NAI	O4D-C1D-N1N-C2N
2	C	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	O4D-C1D-N1N-C2N
2	B	401	NAI	O4D-C1D-N1N-C2N
2	B	401	NAI	C2D-C1D-N1N-C6N
2	C	401	NAI	C2D-C1D-N1N-C6N
2	A	401	NAI	C2D-C1D-N1N-C6N
2	D	401	NAI	C2D-C1D-N1N-C6N
2	A	401	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	B	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C6N
2	D	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	C2N-C3N-C7N-N7N
2	B	401	NAI	C2N-C3N-C7N-N7N
2	D	401	NAI	C2N-C3N-C7N-N7N
2	C	401	NAI	C5B-O5B-PA-O1A
2	C	401	NAI	C2N-C3N-C7N-N7N
2	C	401	NAI	O4B-C4B-C5B-O5B

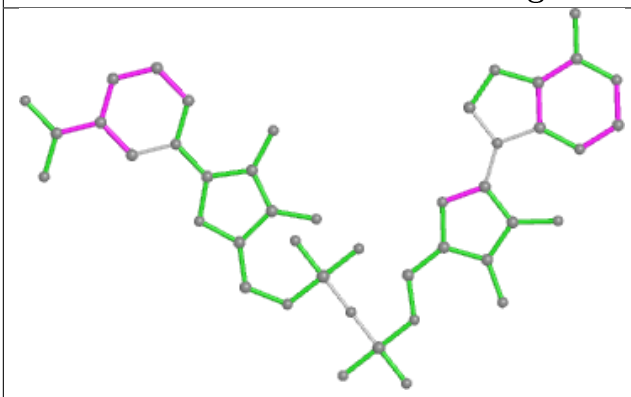
There are no ring outliers.

8 monomers are involved in 21 short contacts:

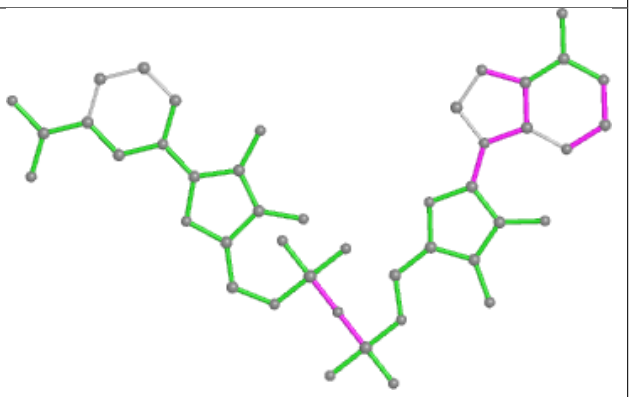
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAI	5	0
3	D	402	OAA	3	0
3	B	402	OAA	1	0
3	C	402	OAA	2	0
3	A	402	OAA	4	0
2	B	401	NAI	5	0
2	D	401	NAI	6	0
2	C	401	NAI	4	0

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.

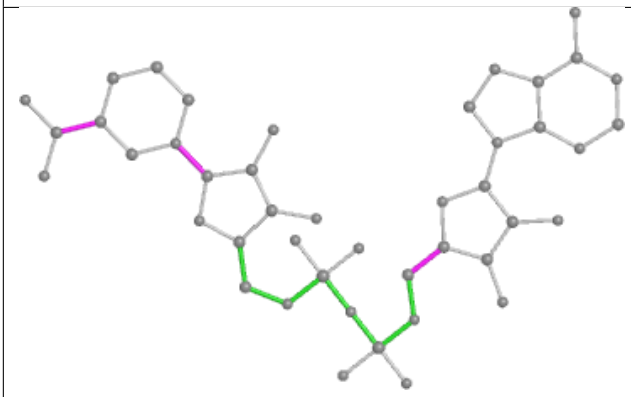
Ligand NAI A 401



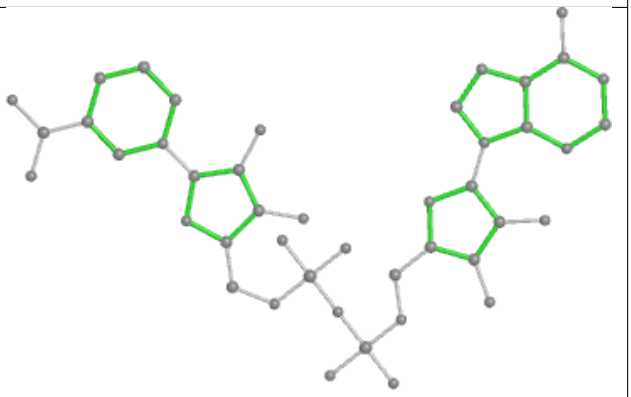
Bond lengths



Bond angles

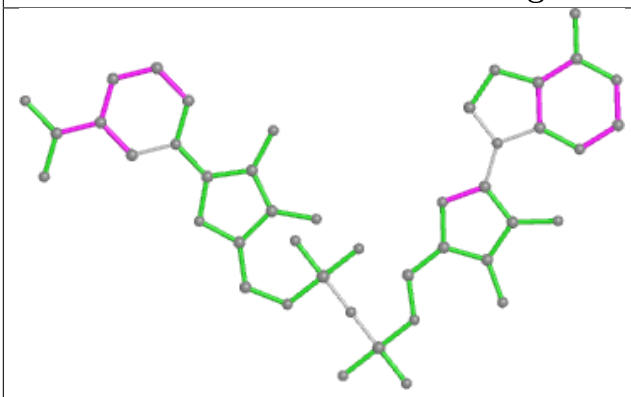


Torsions

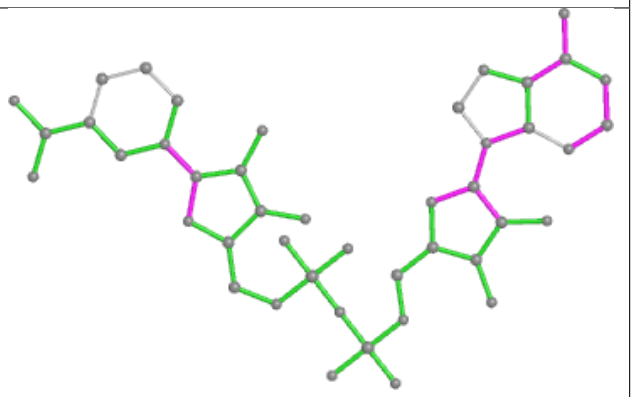


Rings

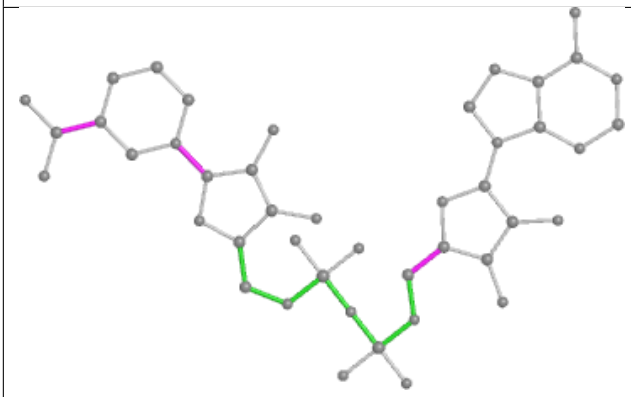
Ligand NAI B 401



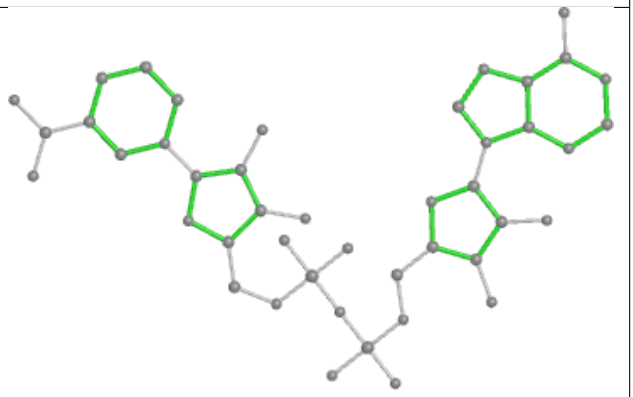
Bond lengths



Bond angles

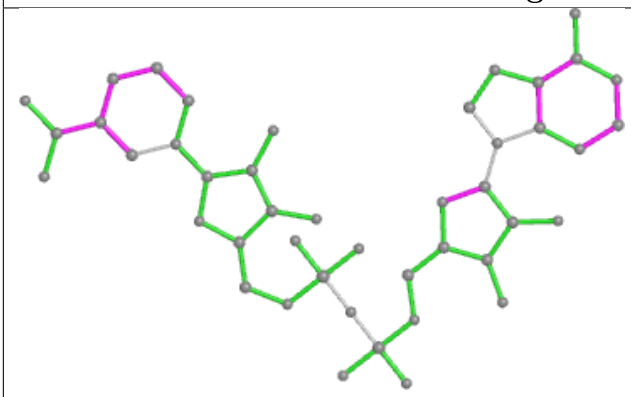


Torsions

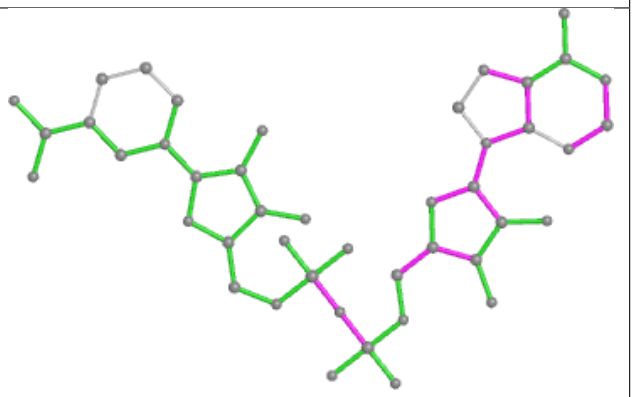


Rings

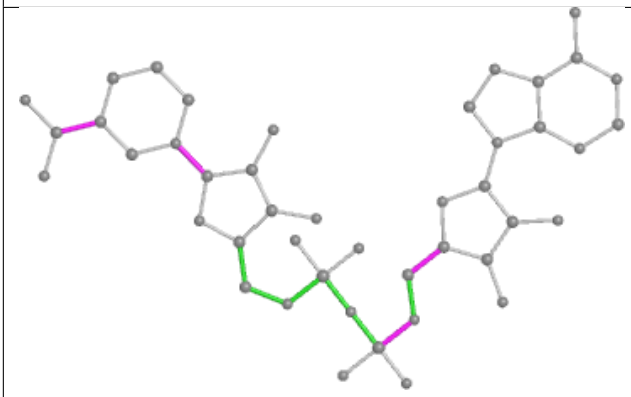
Ligand NAI D 401



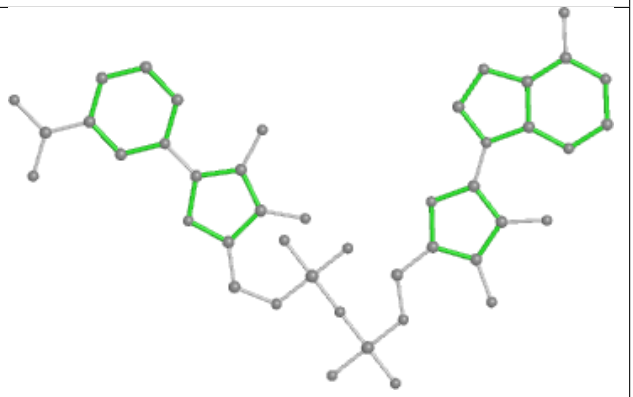
Bond lengths



Bond angles

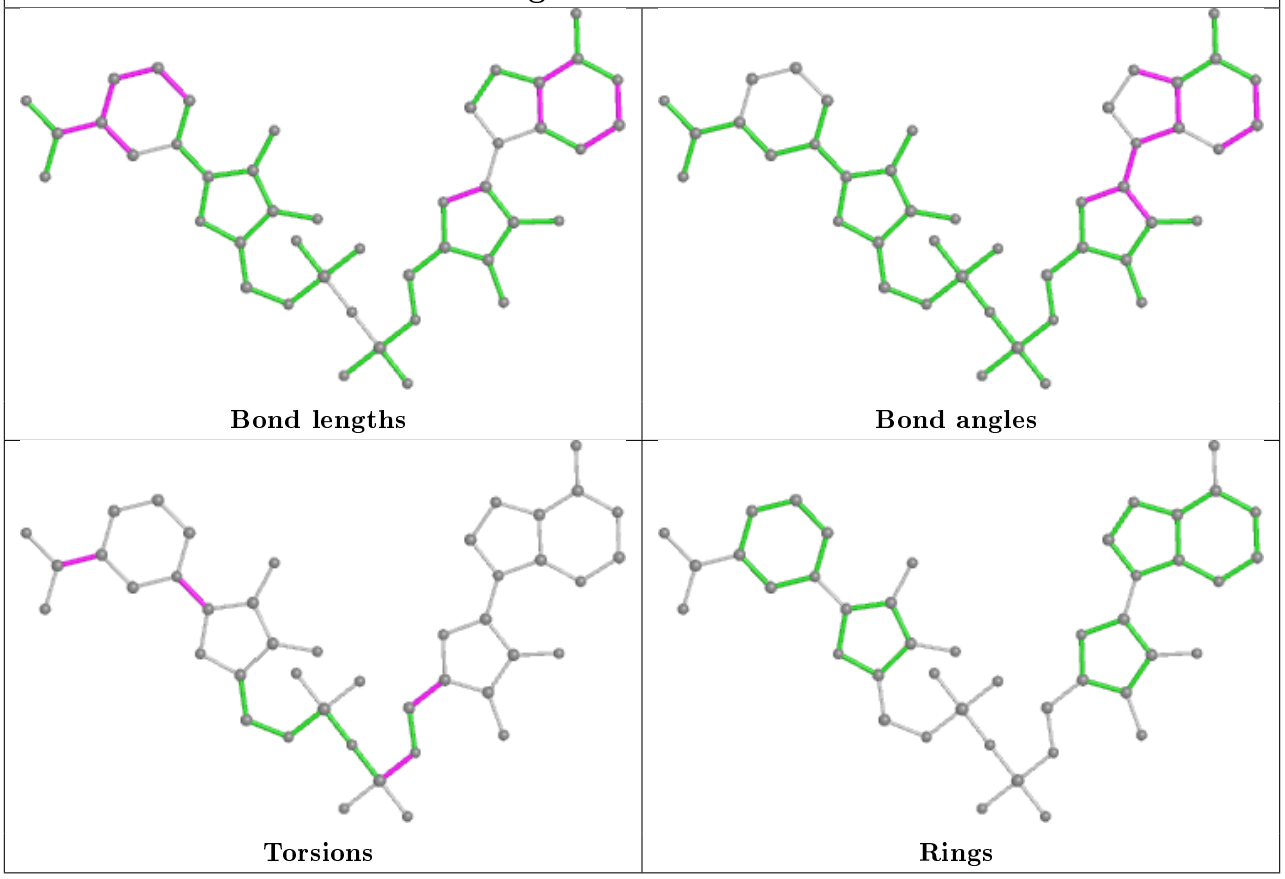


Torsions



Rings

Ligand NAI C 401



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	314/340 (92%)	0.31	13 (4%)	37	40	25, 43, 62, 74	0
1	B	314/340 (92%)	0.13	11 (3%)	44	47	21, 33, 48, 69	0
1	C	314/340 (92%)	0.74	41 (13%)	3	3	36, 56, 76, 81	0
1	D	314/340 (92%)	0.38	18 (5%)	23	25	33, 45, 64, 75	0
All	All	1256/1360 (92%)	0.39	83 (6%)	18	19	21, 44, 69, 81	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	139	VAL	5.9
1	C	169	VAL	5.5
1	C	310	SER	4.3
1	C	168	GLY	4.3
1	D	139	VAL	4.1
1	B	169	VAL	4.0
1	B	139	VAL	3.8
1	D	98	ILE	3.7
1	C	270	GLU	3.7
1	C	276	SER	3.6
1	C	24	ASN	3.5
1	C	271	GLY	3.5
1	A	270	GLU	3.5
1	D	169	VAL	3.5
1	D	24	ASN	3.5
1	C	170	THR	3.4
1	C	140	ILE	3.4
1	B	335	LYS	3.3
1	C	191	ARG	3.2
1	C	98	ILE	3.2
1	C	144	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	140	ILE	3.1
1	D	191	ARG	3.1
1	B	140	ILE	3.1
1	B	138	CYS	3.0
1	C	214	PRO	3.0
1	C	171	THR	2.9
1	C	141	ALA	2.9
1	A	169	VAL	2.9
1	C	284	GLU	2.8
1	C	317	SER	2.8
1	D	97	VAL	2.8
1	C	307	LYS	2.8
1	D	221	ASP	2.8
1	C	159	GLY	2.8
1	B	98	ILE	2.8
1	D	335	LYS	2.8
1	C	138	CYS	2.7
1	A	139	VAL	2.7
1	D	215	LYS	2.7
1	D	336	THR	2.7
1	D	138	CYS	2.7
1	D	170	THR	2.7
1	A	138	CYS	2.6
1	A	216	VAL	2.6
1	C	314	LYS	2.5
1	A	221	ASP	2.5
1	C	217	ASP	2.5
1	C	130	GLN	2.5
1	C	328	LYS	2.5
1	C	268	GLY	2.5
1	C	199	GLY	2.4
1	B	96	VAL	2.4
1	A	140	ILE	2.4
1	D	168	GLY	2.4
1	C	200	HIS	2.4
1	C	296	LYS	2.4
1	A	144	VAL	2.4
1	C	148	ILE	2.4
1	A	310	SER	2.3
1	B	97	VAL	2.3
1	C	277	PHE	2.3
1	C	313	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	167	PHE	2.2
1	C	311	PHE	2.2
1	D	99	PRO	2.2
1	C	300	GLU	2.2
1	A	170	THR	2.2
1	C	269	LYS	2.2
1	C	318	ASP	2.2
1	C	96	VAL	2.2
1	A	217	ASP	2.2
1	B	137	ILE	2.2
1	A	311	PHE	2.1
1	C	137	ILE	2.1
1	C	297	LYS	2.1
1	A	281	GLN	2.1
1	D	276	SER	2.1
1	B	307	LYS	2.1
1	D	188	ASP	2.0
1	D	159	GLY	2.0
1	B	336	THR	2.0
1	C	267	ASN	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
3	OAA	C	402	9/9	0.76	0.29	60,63,64,66	0
2	NAI	B	401	44/44	0.89	0.20	52,56,65,68	0
2	NAI	C	401	44/44	0.89	0.22	51,65,93,94	0

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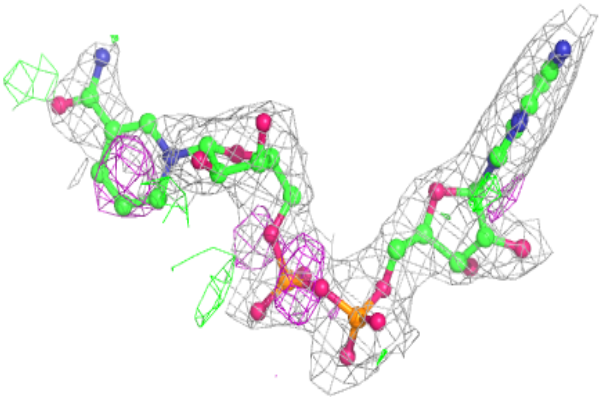
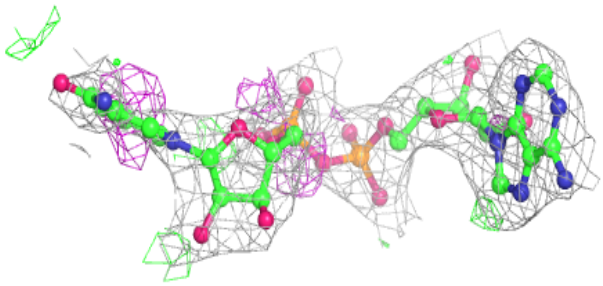
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OAA	B	402	9/9	0.90	0.20	36,38,41,41	0
3	OAA	D	402	9/9	0.90	0.20	49,53,55,58	0
3	OAA	A	402	9/9	0.91	0.20	39,46,49,51	0
2	NAI	D	401	44/44	0.93	0.16	38,44,58,59	0
2	NAI	A	401	44/44	0.93	0.15	36,42,48,49	0

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 B 401:

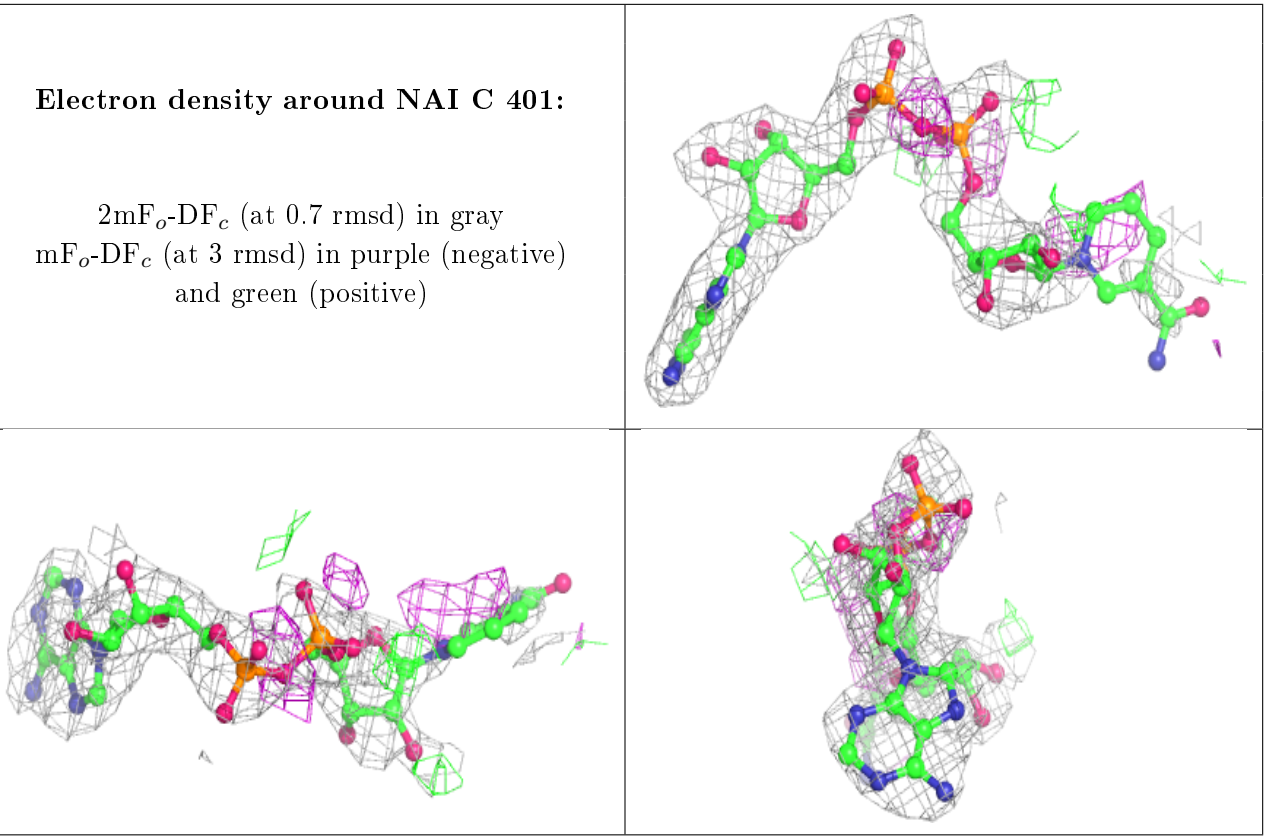
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





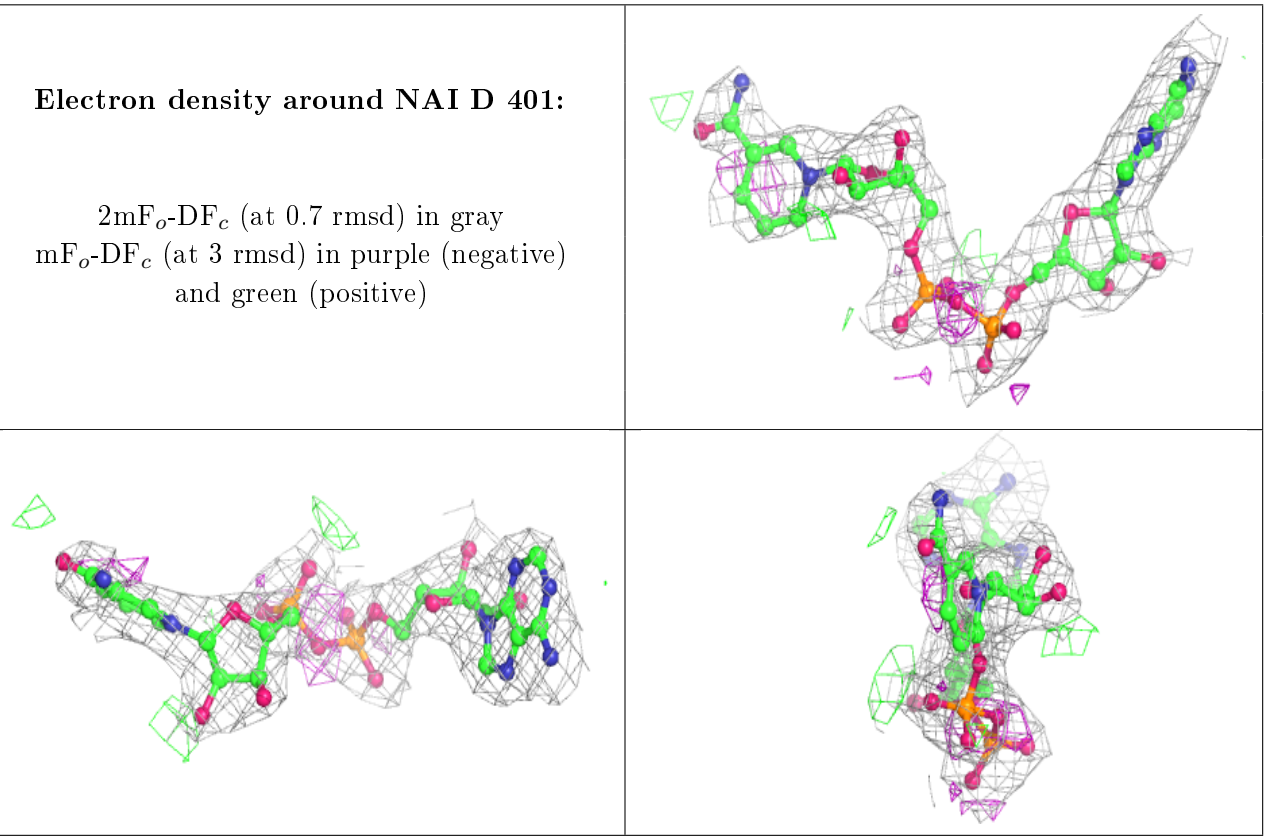
Electron density around NAI C 401:

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



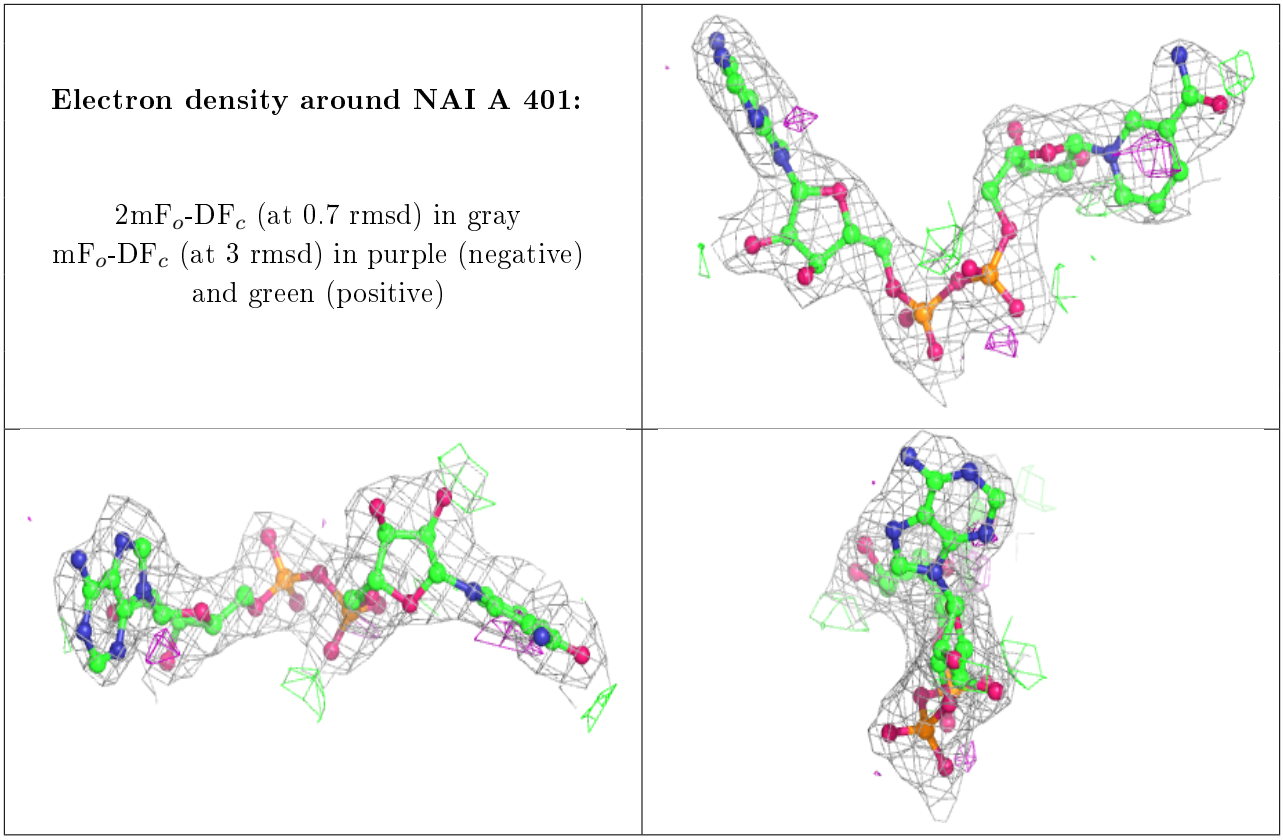
Electron density around NAI D 401:

$2mF_o$-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 401:

$2mF_o$-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.