wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 – 08:42 AM EDT

PDB ID	:	3I3O
Title	:	2.06 Angstrom resolution crystal structure of a short chain dehydrogenase from Bacillus anthracis str. 'Ames Ancestor' in complex with NAD-acetone
Authors	:	Halavaty, A.S.; Minasov, G.; Skarina, T.; Onopriyenko, O.; Peterson, S.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2009-06-30
Resolution	:	2.06 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

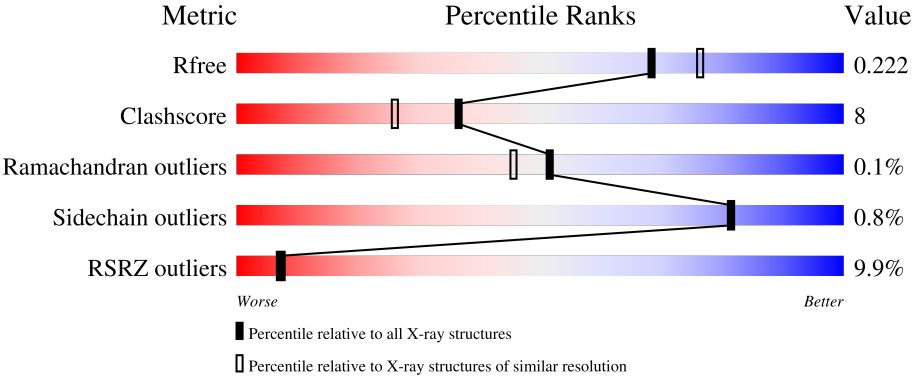
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 <=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	291	9% 89% 8% •
1	B	291	9% 89% 8% •
1	C	291	9% 86% 11% •
1	D	291	7% 87% 11% •
1	E	291	11% 83% 13% •

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Mol	Chain	Length	Quality of chain
1	F	291	10% 82% 11% 7%
1	G	291	8% 73% 11% 16%
1	H	291	12% 78% 14% • 7%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CAC	B	328	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18804 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 Short chain dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2181	1378	367	430	6	0	3	0
1	B	283	2256	1421	380	449	6	0	11	0
1	C	281	2190	1383	369	432	6	0	5	0
1	D	283	2246	1417	381	442	6	0	9	0
1	E	279	2208	1393	372	437	6	0	9	0
1	F	270	2112	1337	354	416	5	0	6	0
1	G	245	1893	1191	320	378	4	0	4	0
1	H	270	2113	1335	357	416	5	0	6	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q81UV8
A	-1	ASN	-	expression tag	UNP Q81UV8
A	0	ALA	-	expression tag	UNP Q81UV8
B	-2	SER	-	expression tag	UNP Q81UV8
B	-1	ASN	-	expression tag	UNP Q81UV8
B	0	ALA	-	expression tag	UNP Q81UV8
C	-2	SER	-	expression tag	UNP Q81UV8
C	-1	ASN	-	expression tag	UNP Q81UV8
C	0	ALA	-	expression tag	UNP Q81UV8
D	-2	SER	-	expression tag	UNP Q81UV8
D	-1	ASN	-	expression tag	UNP Q81UV8
D	0	ALA	-	expression tag	UNP Q81UV8
E	-2	SER	-	expression tag	UNP Q81UV8

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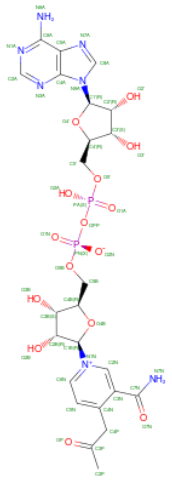
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q81UV8
E	0	ALA	-	expression tag	UNP Q81UV8
F	-2	SER	-	expression tag	UNP Q81UV8
F	-1	ASN	-	expression tag	UNP Q81UV8
F	0	ALA	-	expression tag	UNP Q81UV8
G	-2	SER	-	expression tag	UNP Q81UV8
G	-1	ASN	-	expression tag	UNP Q81UV8
G	0	ALA	-	expression tag	UNP Q81UV8
H	-2	SER	-	expression tag	UNP Q81UV8
H	-1	ASN	-	expression tag	UNP Q81UV8
H	0	ALA	-	expression tag	UNP Q81UV8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0
2	H	1	1	1	0	0

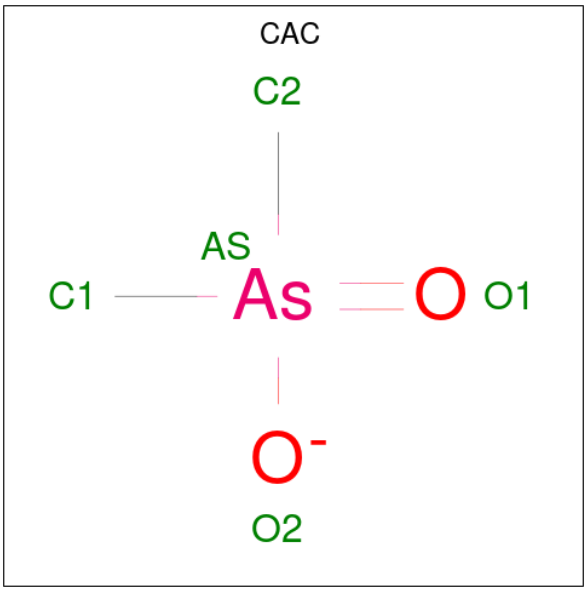
- Molecule 3 is NICOTINAMIDE ADENINE DINUCLEOTIDE ACETONE ADDUCT (three-letter code: NAE) (formula: $C_{24}H_{31}N_7O_{15}P_2$).

NAE



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	24	7	15	2	0	0
3	B	1	48	24	7	15	2	0	0
3	C	1	48	24	7	15	2	0	0
3	D	1	48	24	7	15	2	0	0
3	E	1	48	24	7	15	2	0	0
3	F	1	48	24	7	15	2	0	0
3	H	1	48	24	7	15	2	0	0

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
4	A	1	5	1	2	2	0	0
4	B	1	5	1	2	2	0	0
4	B	1	5	1	2	2	0	0
4	C	1	5	1	2	2	0	0
4	D	1	5	1	2	2	0	0
4	E	1	5	1	2	2	0	0
4	F	1	5	1	2	2	0	0
4	G	1	5	1	2	2	0	0
4	H	1	5	1	2	2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	D	1	1	1	0	0

- Molecule 6 is water.

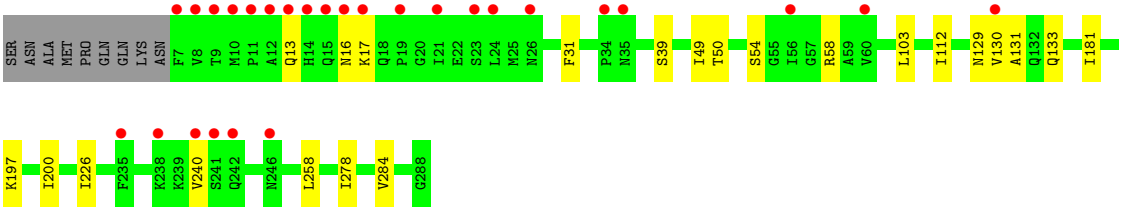
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	178	179	179	0	3
			Total	O		
6	B	221	221	221	0	5
			Total	O		
6	C	190	191	191	0	5
			Total	O		
6	D	169	169	169	0	5
			Total	O		
6	E	171	174	174	0	6
			Total	O		
6	F	100	100	100	0	0
			Total	O		
6	G	66	66	66	0	1
			Total	O		
6	H	115	116	116	0	3

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.

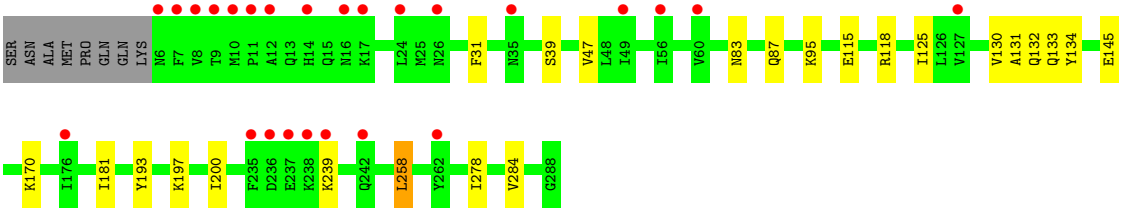
• Molecule 1: Short chain dehydrogenase

Chain A:



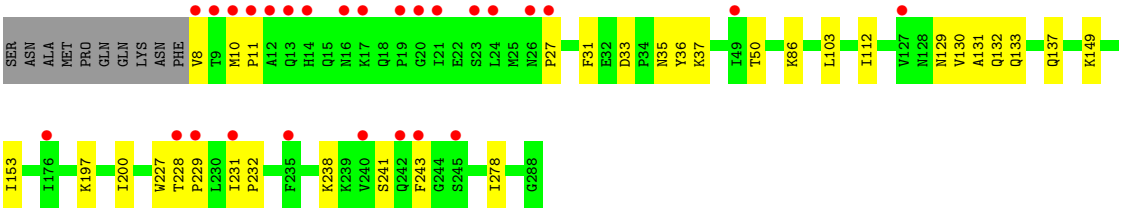
• Molecule 1: Short chain dehydrogenase

Chain B:



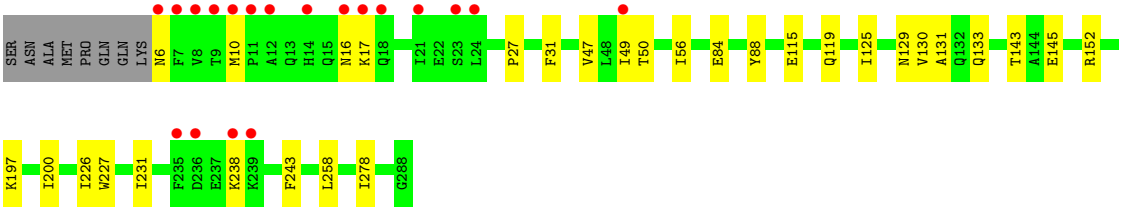
• Molecule 1: Short chain dehydrogenase

Chain C:



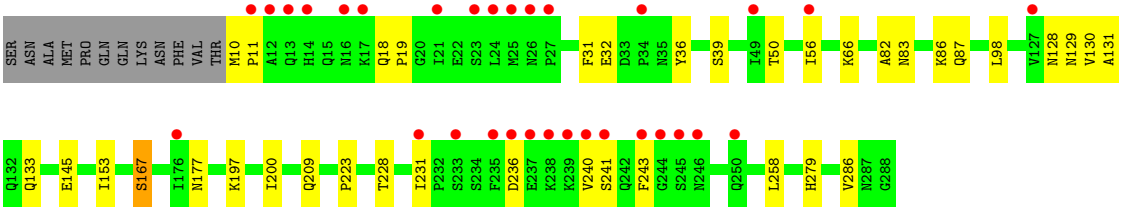
• Molecule 1: Short chain dehydrogenase

Chain D:



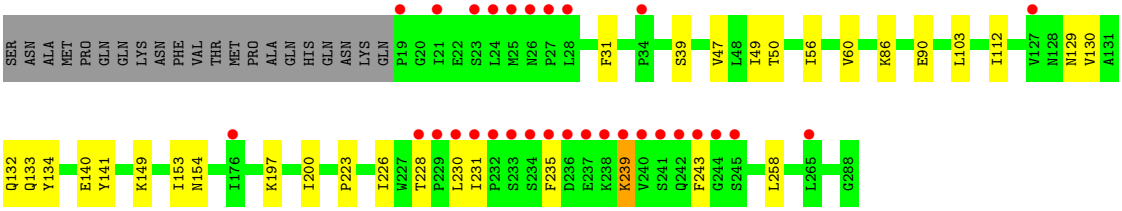
• Molecule 1: Short chain dehydrogenase

Chain E:



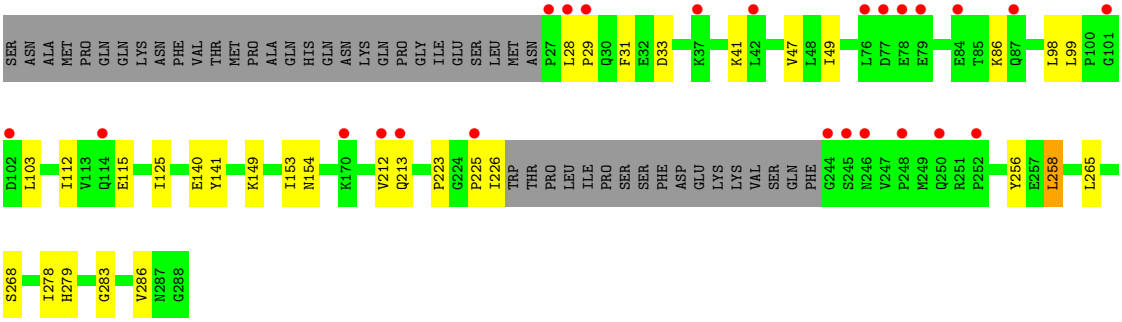
• Molecule 1: Short chain dehydrogenase

Chain F:



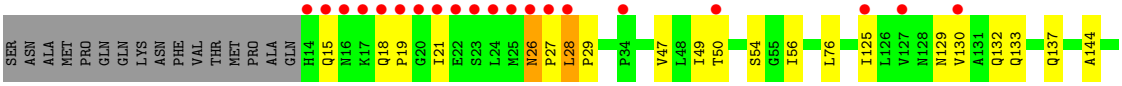
• Molecule 1: Short chain dehydrogenase

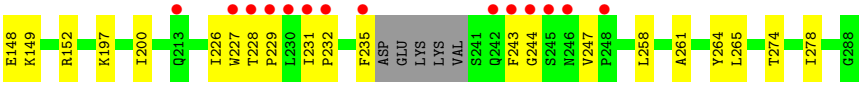
Chain G:



• Molecule 1: Short chain dehydrogenase

Chain H:




E148
K149
R152
K197
I200
Q213
I226
W227
T228
P229
L230
I231
P232
F235
ASP
GLU
LYS
LYS
VAL
S241
Q242
F243
G244
S245
N246
V247
P248
L258
A261
Y264
L265
T274
I278
G288

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	131.76Å 168.16Å 107.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 2.06 29.56 – 2.06	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.95-2.06) 100.0 (29.56-2.06)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.80 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.161 , 0.205 0.182 , 0.222	Depositor DCC
R_{free} test set	7384 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	22.1	Xtriage
Anisotropy	0.947	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.0	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	18804	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6785e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAE, CL, CAC, MG

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	0.73	0/2223	0.74	1/3015 (0.0%)
1	B	0.75	0/2298	0.75	1/3117 (0.0%)
1	C	0.78	0/2231	0.74	0/3025
1	D	0.70	0/2288	0.74	0/3102
1	E	0.70	0/2249	0.74	1/3050 (0.0%)
1	F	0.62	0/2151	0.70	0/2916
1	G	0.66	0/1924	0.71	0/2606
1	H	0.63	0/2152	0.73	0/2918
All	All	0.70	0/17516	0.73	3/23749 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	258	LEU	CA-CB-CG	-7.23	98.67	115.30
1	E	167	SER	CB-CA-C	-5.14	100.33	110.10
1	A	58	ARG	NE-CZ-NH2	-5.08	117.76	120.30

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	2181	0	2157	22	0
1	B	2256	0	2214	24	0
1	C	2190	0	2172	30	0
1	D	2246	0	2218	37	0
1	E	2208	0	2178	46	0
1	F	2112	0	2099	42	0
1	G	1893	0	1871	22	0
1	H	2113	0	2087	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
3	A	48	0	30	13	0
3	B	48	0	29	14	0
3	C	48	0	30	7	0
3	D	48	0	29	8	0
3	E	48	0	29	15	0
3	F	48	0	29	9	0
3	H	48	0	30	7	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
5	D	1	0	0	0	0
6	A	179	0	0	1	0
6	B	221	0	0	3	0
6	C	191	0	0	4	0
6	D	169	0	0	4	0
6	E	174	0	0	1	0
6	F	100	0	0	2	0
6	G	66	0	0	2	0
6	H	116	0	0	2	0
All	All	18804	0	17202	274	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 8.

The worst 5 of 274 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:10:MET:HE3	1:C:27:PRO:HD2	1.48	0.94
1:C:132:GLN:HE22	1:C:149:LYS:HE2	1.34	0.91
1:A:130:VAL:HG23	3:A:311:NAE:C1'	2.01	0.91
1:D:56:ILE:HG12	1:D:258[B]:LEU:HD22	1.55	0.89
1:F:226:ILE:O	1:F:231:ILE:HD11	1.72	0.89

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	283/291 (97%)	274 (97%)	9 (3%)	0	100	100
1	B	292/291 (100%)	280 (96%)	12 (4%)	0	100	100
1	C	284/291 (98%)	272 (96%)	12 (4%)	0	100	100
1	D	290/291 (100%)	281 (97%)	9 (3%)	0	100	100
1	E	286/291 (98%)	273 (96%)	13 (4%)	0	100	100
1	F	274/291 (94%)	263 (96%)	11 (4%)	0	100	100
1	G	245/291 (84%)	235 (96%)	10 (4%)	0	100	100
1	H	272/291 (94%)	260 (96%)	10 (4%)	2 (1%)	22	11
All	All	2226/2328 (96%)	2138 (96%)	86 (4%)	2 (0%)	51	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	26	ASN
1	H	28	LEU

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	239/244 (98%)	238 (100%)	1 (0%)	91	91
1	B	248/244 (102%)	245 (99%)	3 (1%)	71	69
1	C	240/244 (98%)	239 (100%)	1 (0%)	91	91
1	D	246/244 (101%)	242 (98%)	4 (2%)	62	59
1	E	242/244 (99%)	241 (100%)	1 (0%)	91	91
1	F	231/244 (95%)	230 (100%)	1 (0%)	91	91
1	G	205/244 (84%)	203 (99%)	2 (1%)	76	75
1	H	231/244 (95%)	229 (99%)	2 (1%)	78	78
All	All	1882/1952 (96%)	1867 (99%)	15 (1%)	81	81

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	17	LYS
1	H	137[A]	GLN
1	D	238	LYS
1	H	137[B]	GLN
1	G	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	129	ASN
1	E	177	ASN
1	H	132	GLN
1	H	18	GLN
1	H	129	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAE	C	311	2	46,52,52	2.40	7 (15%)	54,79,79	1.91	10 (18%)
4	CAC	A	327	-	0,4,4	-	-	0,6,6	-	-
4	CAC	D	324	-	0,4,4	-	-	0,6,6	-	-
3	NAE	E	311	2	46,52,52	2.26	8 (17%)	54,79,79	2.18	12 (22%)
4	CAC	C	322	-	0,4,4	-	-	0,6,6	-	-
3	NAE	H	311	2	46,52,52	2.25	7 (15%)	54,79,79	1.69	6 (11%)
3	NAE	D	311	2	46,52,52	2.40	9 (19%)	54,79,79	2.02	10 (18%)
3	NAE	B	311	2	46,52,52	2.29	7 (15%)	54,79,79	2.13	11 (20%)
4	CAC	H	323	-	0,4,4	-	-	0,6,6	-	-
4	CAC	E	325	-	0,4,4	-	-	0,6,6	-	-
4	CAC	B	321	-	0,4,4	-	-	0,6,6	-	-
4	CAC	B	328	-	0,4,4	-	-	0,6,6	-	-
3	NAE	F	311	2	46,52,52	2.17	9 (19%)	54,79,79	2.09	9 (16%)
3	NAE	A	311	2	46,52,52	2.55	8 (17%)	54,79,79	1.93	10 (18%)
4	CAC	G	326	-	0,4,4	-	-	0,6,6	-	-
4	CAC	F	329	-	0,4,4	-	-	0,6,6	-	-

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
3	NAE	C	311	2	-	9/30/66/66	0/5/5/5
3	NAE	E	311	2	-	8/30/66/66	0/5/5/5
3	NAE	H	311	2	-	10/30/66/66	0/5/5/5
3	NAE	D	311	2	-	4/30/66/66	0/5/5/5
3	NAE	B	311	2	-	8/30/66/66	0/5/5/5
3	NAE	F	311	2	-	9/30/66/66	0/5/5/5
3	NAE	A	311	2	-	7/30/66/66	0/5/5/5

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	311	NAE	C2N-N1N	9.77	1.46	1.35
3	C	311	NAE	C3N-C4N	9.48	1.52	1.40
3	H	311	NAE	C3N-C4N	9.19	1.52	1.40
3	D	311	NAE	C2N-N1N	8.66	1.45	1.35
3	B	311	NAE	C5N-C4N	8.62	1.54	1.39

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	311	NAE	C4P-C4N-C3N	-8.60	108.88	123.43
3	E	311	NAE	C4P-C4N-C3N	-7.39	110.91	123.43
3	F	311	NAE	C4P-C4N-C3N	-7.13	111.36	123.43
3	F	311	NAE	C5N-C4N-C3N	-6.29	110.94	118.47
3	F	311	NAE	C6N-N1N-C2N	-6.15	116.37	121.97

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	311	NAE	C5B-O5B-PN-O1N
3	A	311	NAE	C3B-C4B-C5B-O5B
3	A	311	NAE	C2P-C3P-C4P-C4N
3	B	311	NAE	PN-OPP-PA-O5'
3	C	311	NAE	C5B-O5B-PN-O1N

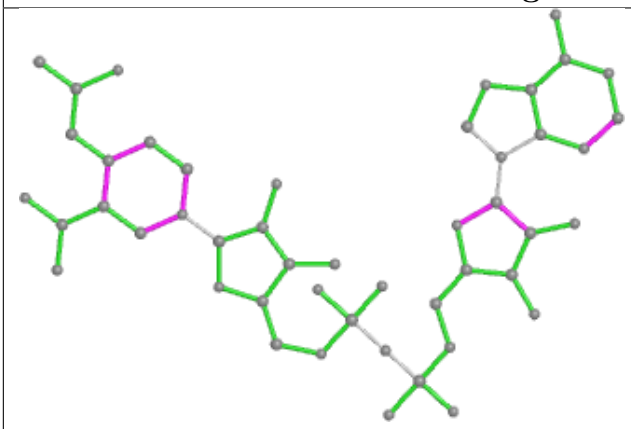
There are no ring outliers.

8 monomers are involved in 74 short contacts:

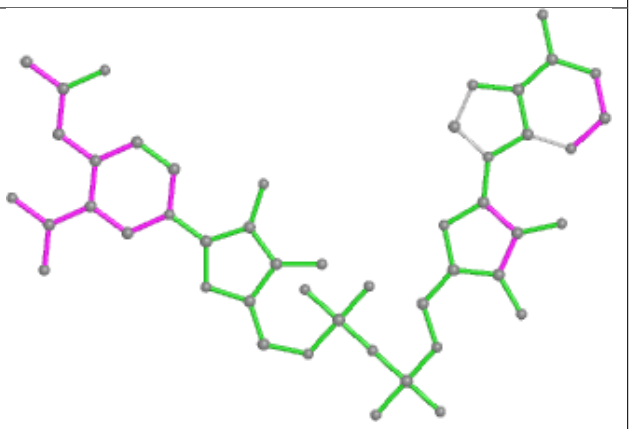
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	311	NAE	7	0
3	E	311	NAE	15	0
4	C	322	CAC	1	0
3	H	311	NAE	7	0
3	D	311	NAE	8	0
3	B	311	NAE	14	0
3	F	311	NAE	9	0
3	A	311	NAE	13	0

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.

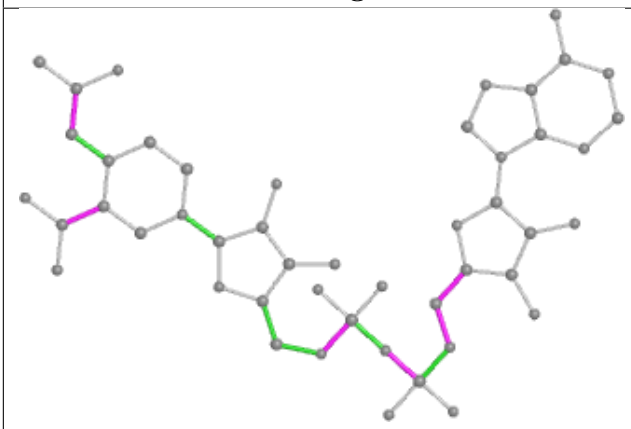
Ligand NAE C 311



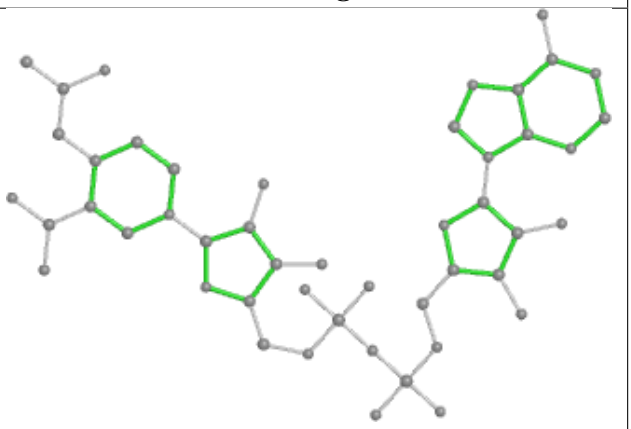
Bond lengths



Bond angles

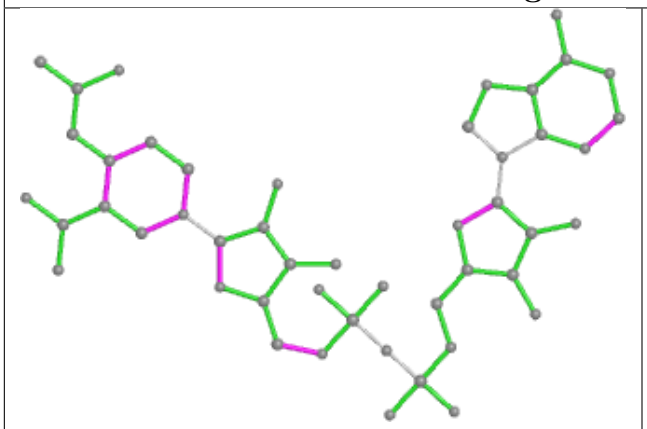


Torsions

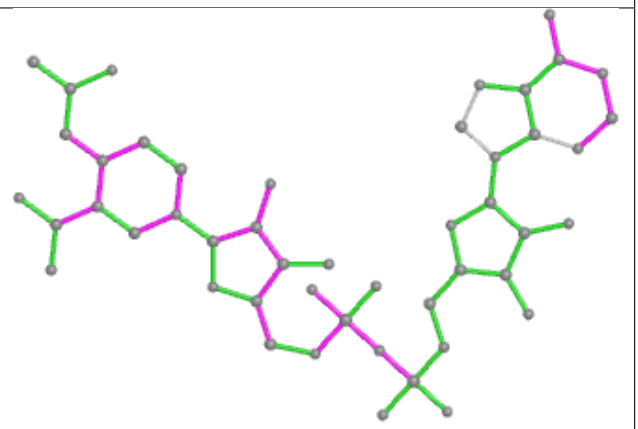


Rings

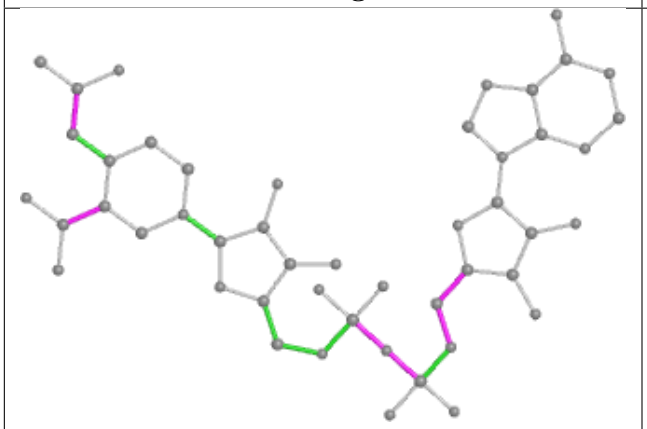
Ligand NAE E 311



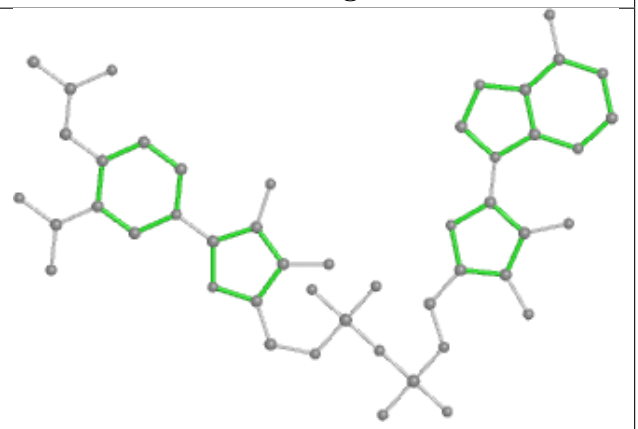
Bond lengths



Bond angles

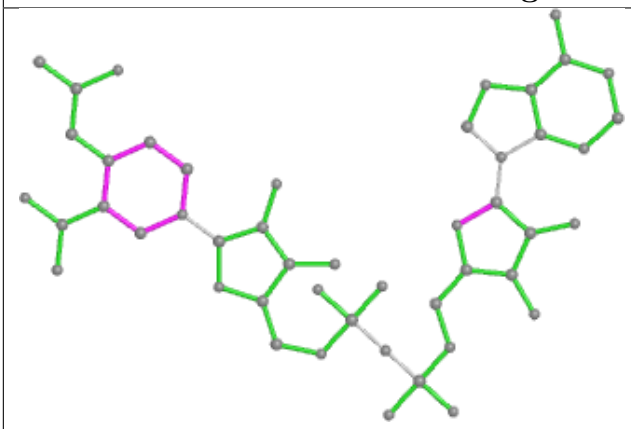


Torsions

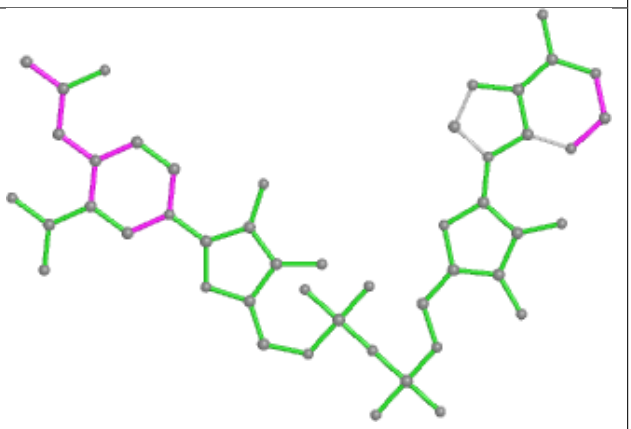


Rings

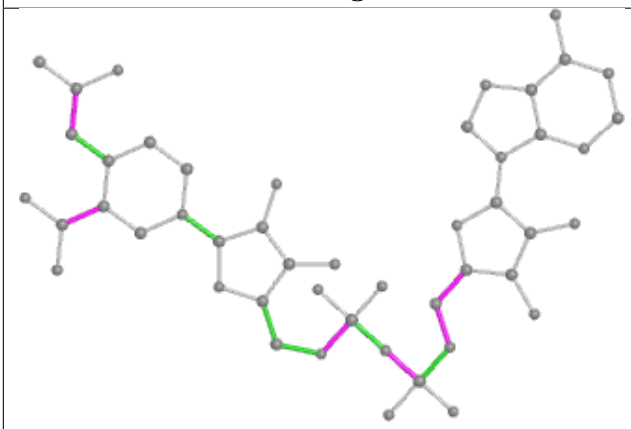
Ligand NAE H 311



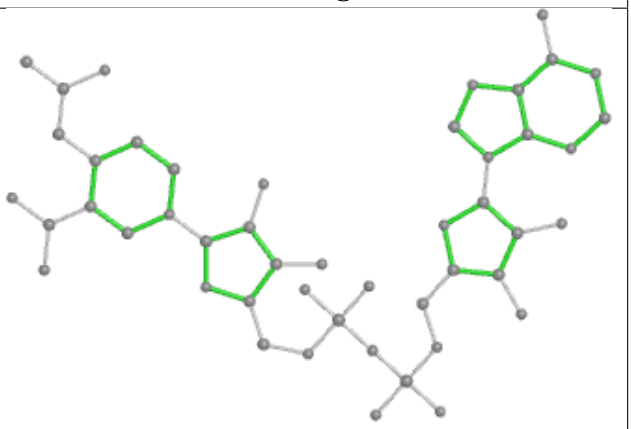
Bond lengths



Bond angles

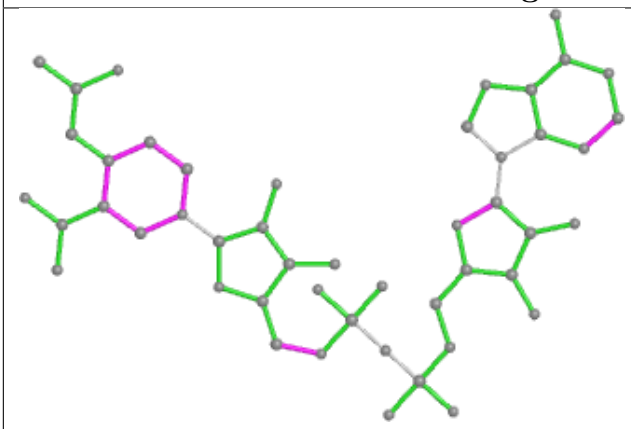


Torsions

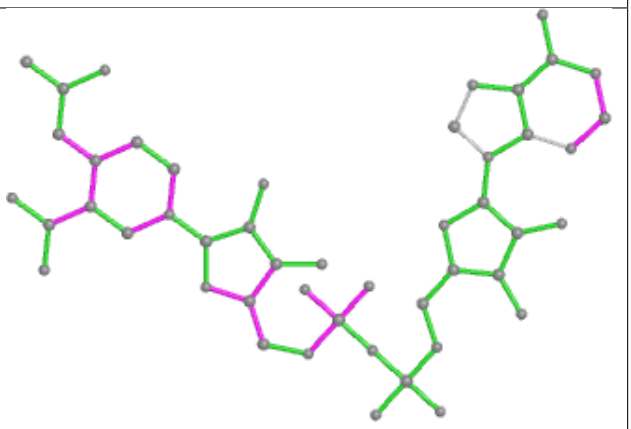


Rings

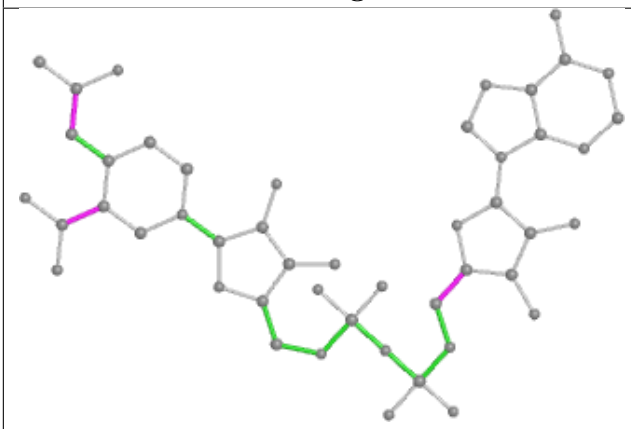
Ligand NAE D 311



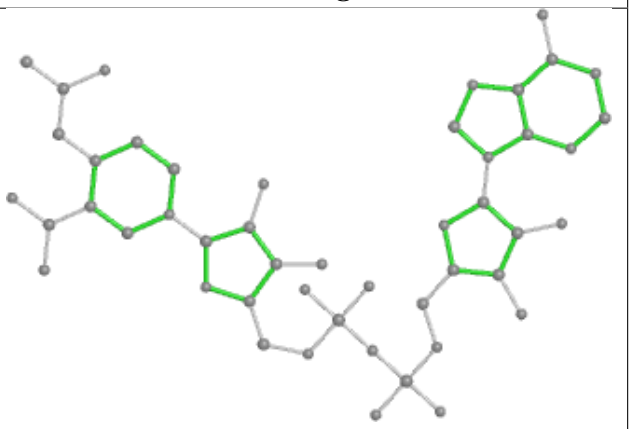
Bond lengths



Bond angles

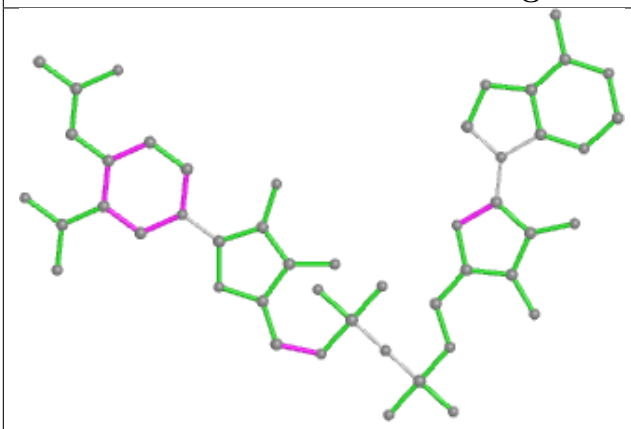


Torsions

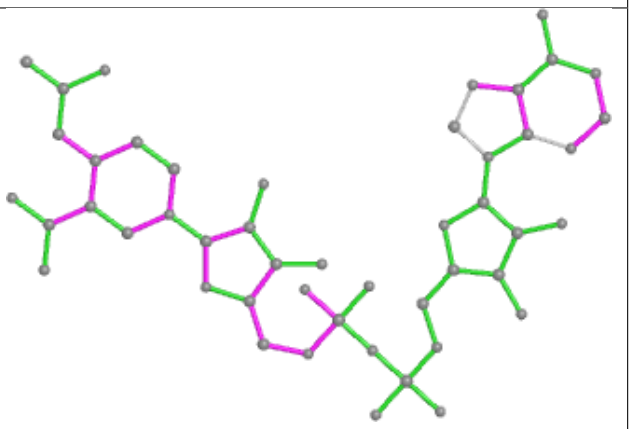


Rings

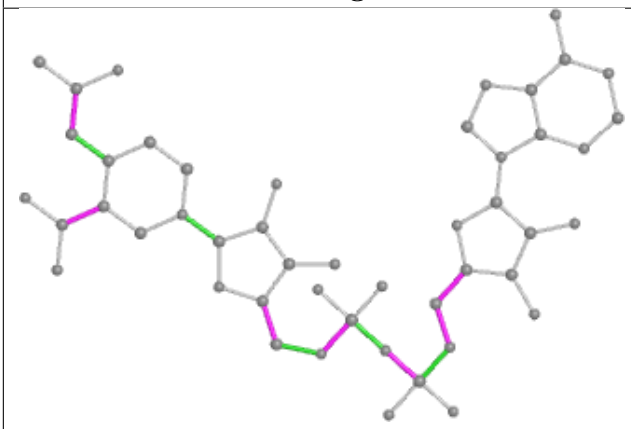
Ligand NAE B 311



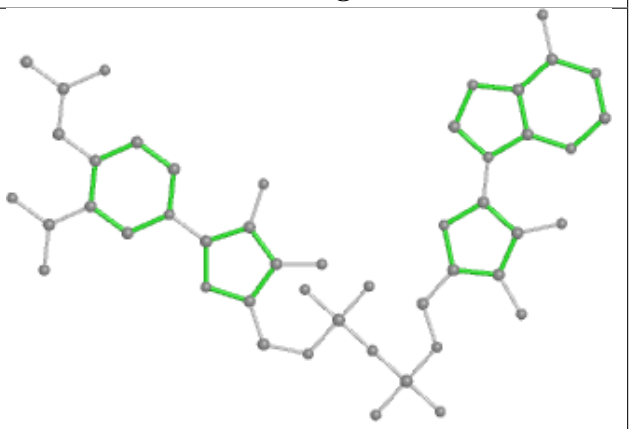
Bond lengths



Bond angles

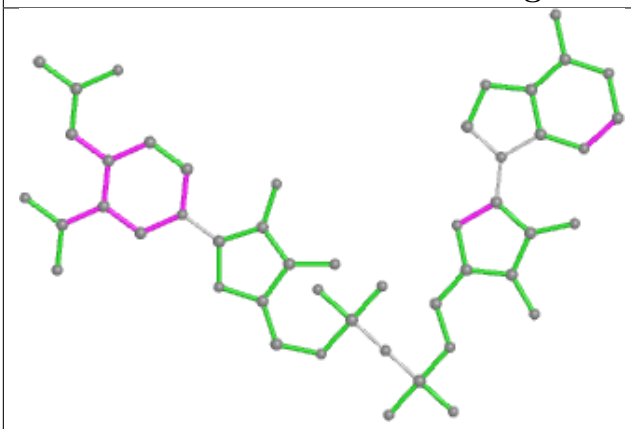


Torsions

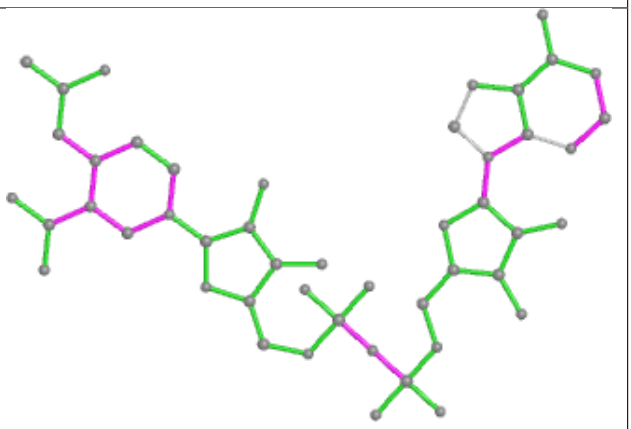


Rings

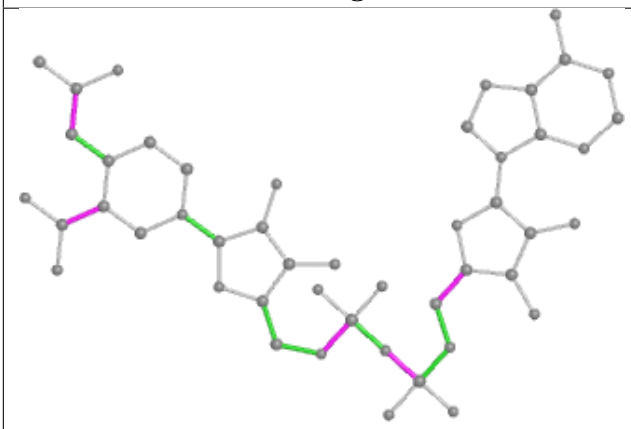
Ligand NAE F 311



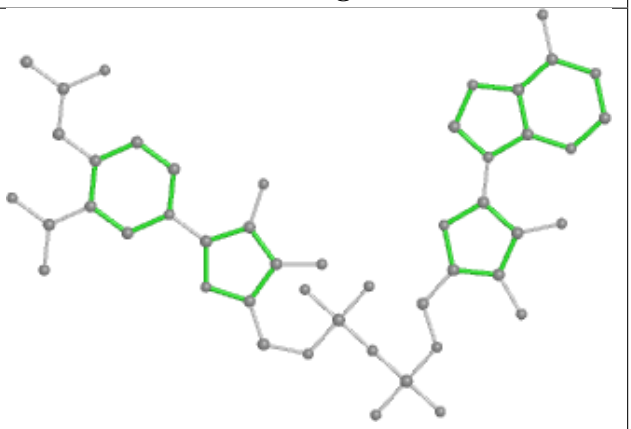
Bond lengths



Bond angles

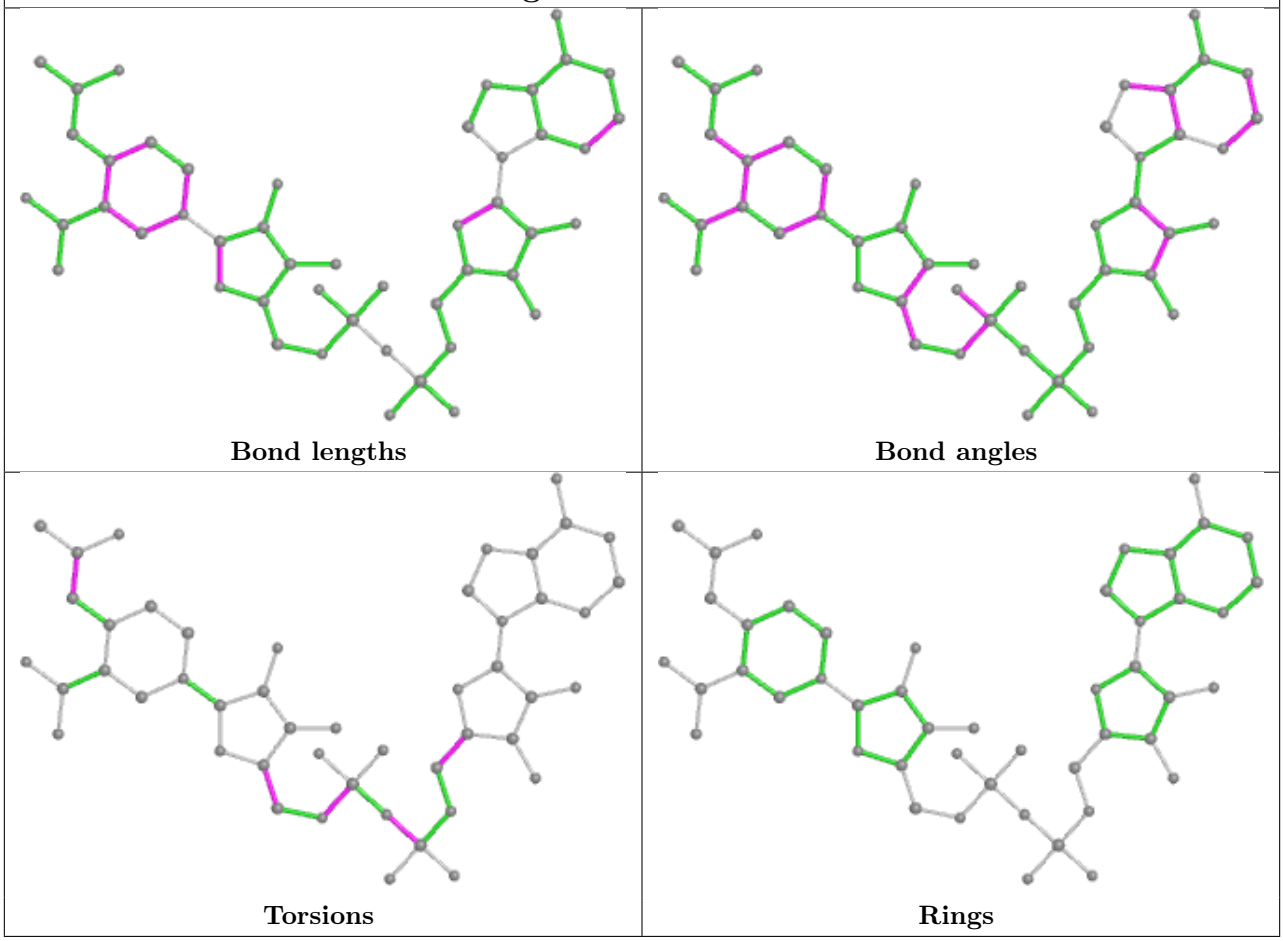


Torsions



Rings

Ligand NAE A 311



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	282/291 (96%)	0.24	27 (9%)	8	8	7, 16, 26, 38	0
1	B	283/291 (97%)	0.19	25 (8%)	10	10	7, 13, 23, 32	0
1	C	281/291 (96%)	0.29	27 (9%)	8	8	8, 14, 24, 31	0
1	D	283/291 (97%)	0.17	19 (6%)	17	18	11, 16, 27, 33	0
1	E	279/291 (95%)	0.37	31 (11%)	5	5	2, 15, 25, 36	0
1	F	270/291 (92%)	0.43	30 (11%)	5	5	12, 18, 27, 31	0
1	G	245/291 (84%)	0.63	24 (9%)	7	7	10, 20, 28, 37	0
1	H	270/291 (92%)	0.48	34 (12%)	3	3	10, 18, 31, 40	0
All	All	2193/2328 (94%)	0.34	217 (9%)	7	7	2, 16, 27, 40	0

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	ASN	9.6
1	A	7	PHE	9.3
1	H	26	ASN	8.6
1	D	7	PHE	8.5
1	B	7	PHE	7.6

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 monosaccharides in this entry.

6.4 Ligands (i)

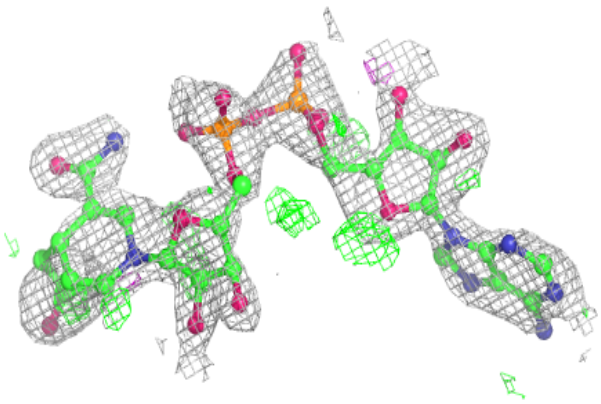
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

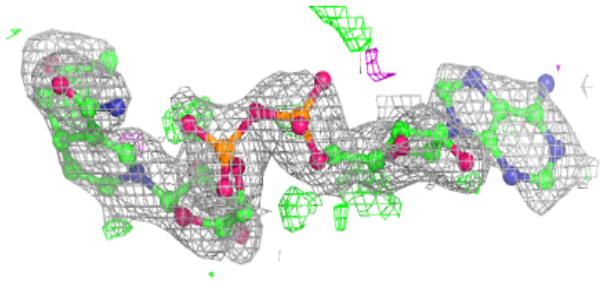
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	E	305	1/1	0.61	0.13	45,45,45,45	0
2	MG	H	307	1/1	0.69	0.09	40,40,40,40	0
4	CAC	B	328	5/5	0.69	0.41	61,61,62,62	5
2	MG	F	303	1/1	0.75	0.10	40,40,40,40	0
3	NAE	H	311	48/48	0.80	0.23	30,40,46,49	48
2	MG	C	304	1/1	0.82	0.11	38,38,38,38	0
2	MG	D	302	1/1	0.84	0.07	39,39,39,39	0
3	NAE	C	311	48/48	0.86	0.17	22,32,39,42	48
2	MG	B	301	1/1	0.87	0.08	34,34,34,34	0
3	NAE	F	311	48/48	0.88	0.17	25,36,40,43	48
4	CAC	A	327	5/5	0.89	0.40	51,53,54,56	5
4	CAC	H	323	5/5	0.89	0.26	48,51,51,58	5
5	CL	D	308	1/1	0.89	0.10	51,51,51,51	0
3	NAE	A	311	48/48	0.90	0.17	23,31,38,44	0
4	CAC	C	322	5/5	0.90	0.27	37,41,46,54	5
4	CAC	F	329	5/5	0.91	0.27	52,53,54,56	5
3	NAE	E	311	48/48	0.92	0.14	21,33,37,42	48
3	NAE	B	311	48/48	0.92	0.13	18,26,35,44	0
3	NAE	D	311	48/48	0.92	0.13	25,30,37,45	48
4	CAC	B	321	5/5	0.93	0.35	54,58,59,61	5
4	CAC	D	324	5/5	0.93	0.30	44,46,48,53	5
4	CAC	E	325	5/5	0.93	0.25	46,50,52,53	5
4	CAC	G	326	5/5	0.94	0.19	46,47,49,50	5
2	MG	A	306	1/1	0.95	0.04	35,35,35,35	0

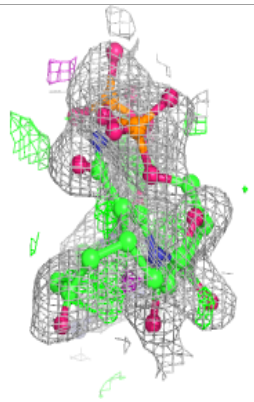
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAE H 311:

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

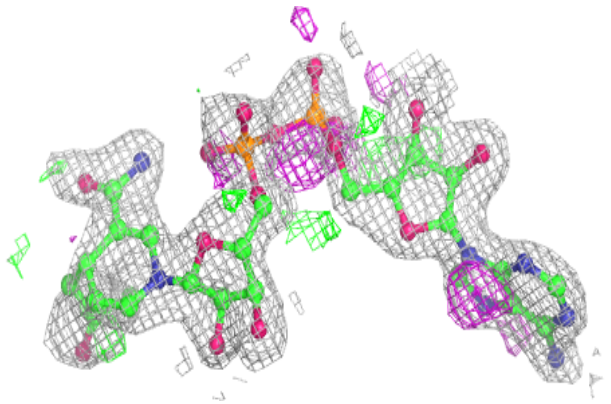


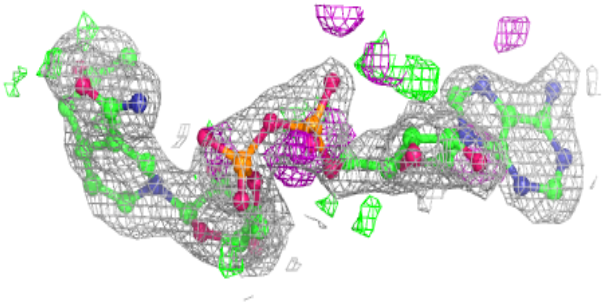


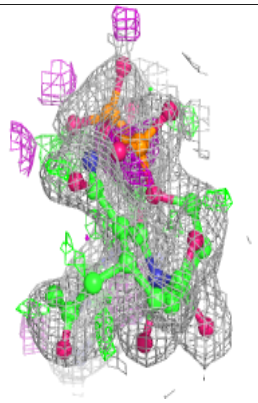


Electron density around NAE C 311:

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

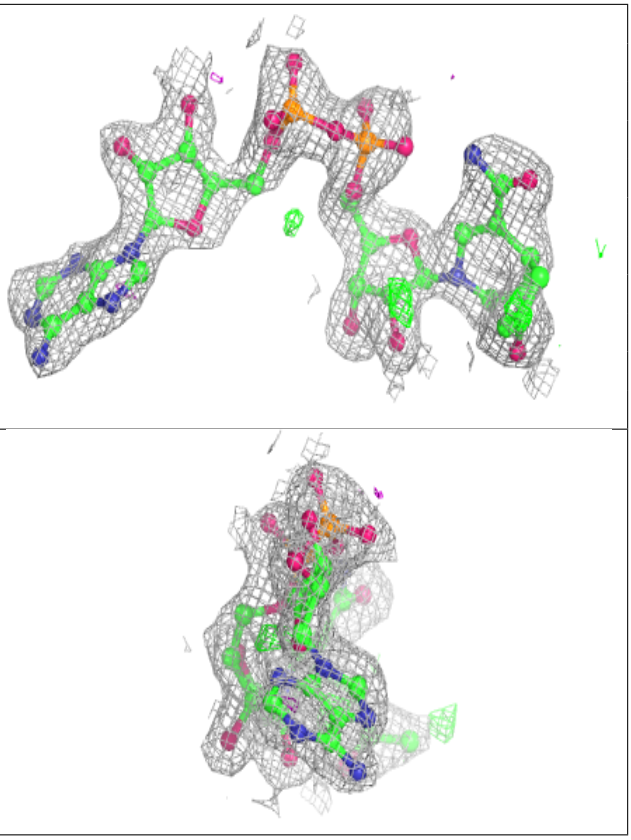






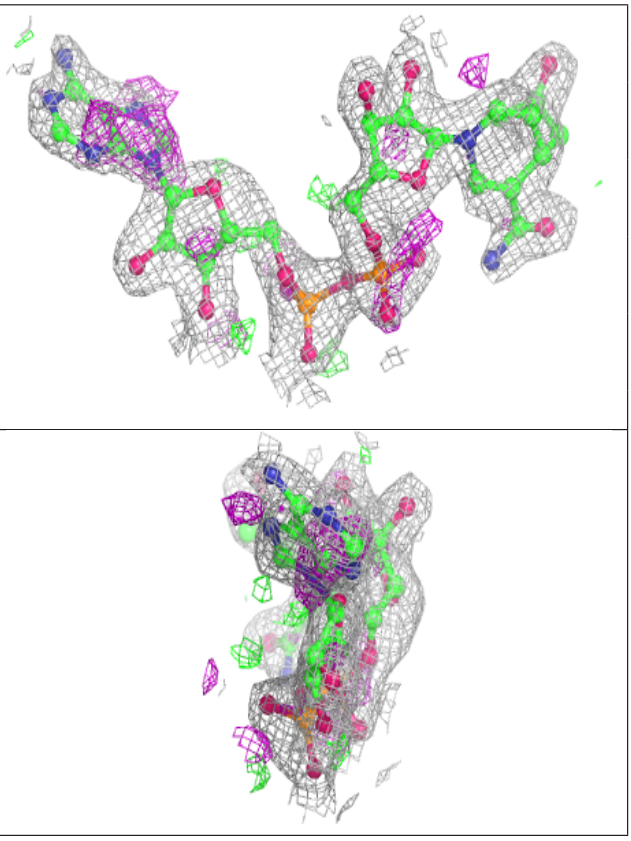
Electron density around NAE F 311:

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



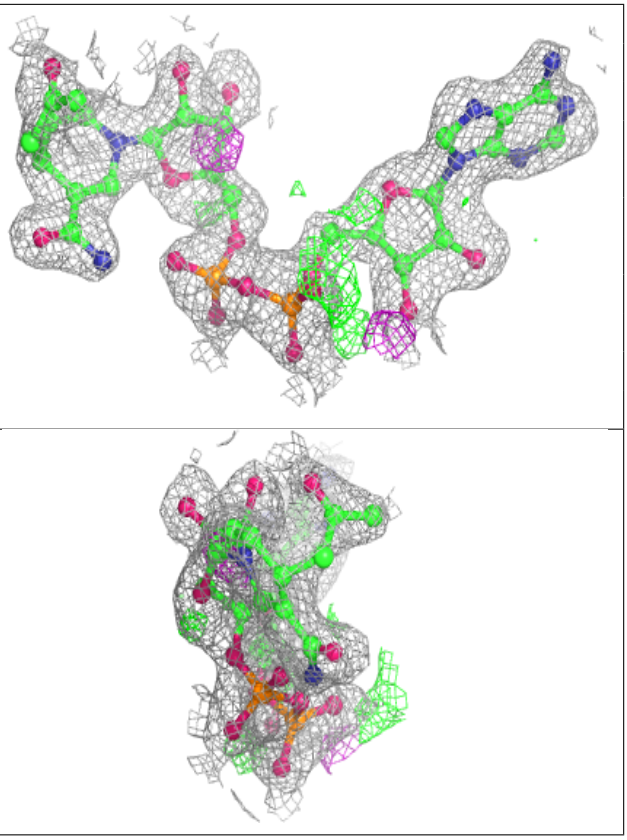
Electron density around NAE A 311:

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



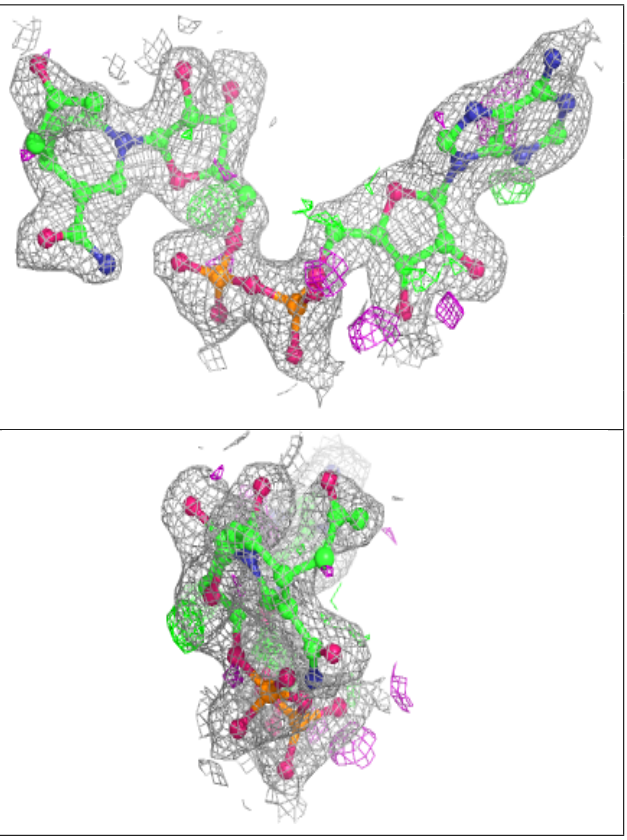
Electron density around NAE E 311:

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



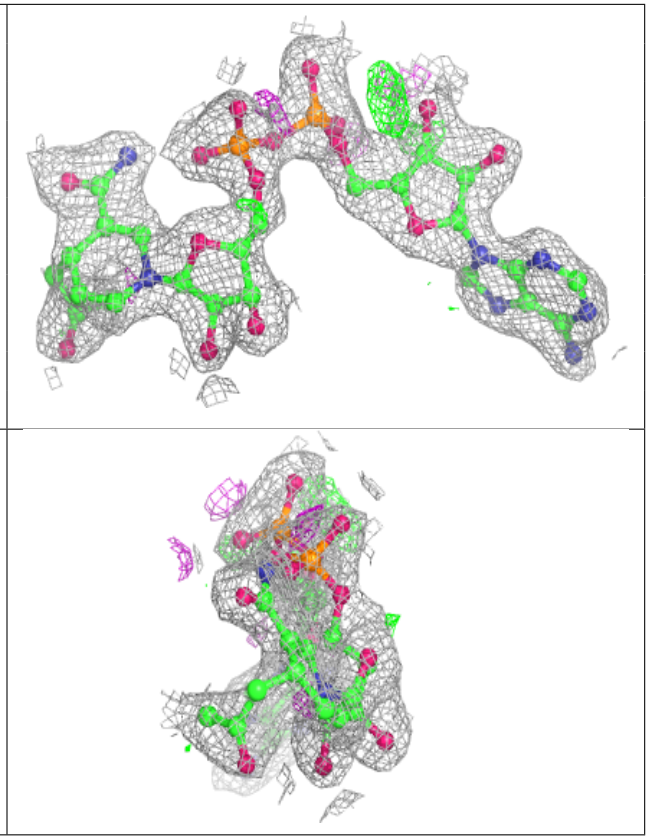
Electron density around NAE B 311:

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



Electron density around NAE D 311:

$2mF_o$-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.