



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 04:53 pm BST

PDB ID : 2VUU  
Title : Crystal structure of NADP-bound NmrA-AreA zinc finger complex  
Authors : Kotaka, M.; Johnson, C.; Lamb, H.K.; Hawkins, A.R.; Ren, J.; Stammers, D.K.  
Deposited on : 2008-05-30  
Resolution : 2.80 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](mailto: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.

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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

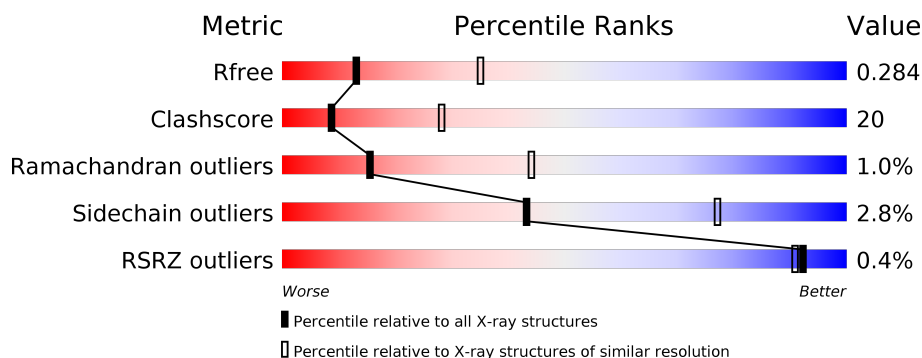
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.







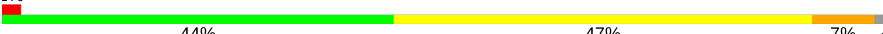
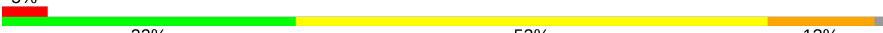




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	352	<div> <div>55%</div> <div>33%</div> <div>10%</div> </div>
1	B	352	<div> <div>51%</div> <div>39%</div> <div>9%</div> </div>
1	C	352	<div> <div>57%</div> <div>32%</div> <div>10%</div> </div>
1	D	352	<div> <div>53%</div> <div>36%</div> <div>9%</div> </div>
1	E	352	<div> <div>59%</div> <div>31%</div> <div>10%</div> </div>
1	F	352	<div> <div>54%</div> <div>35%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	352	
1	H	352	
2	I	43	
2	J	43	
2	K	43	
2	L	43	
2	M	43	
2	N	43	
2	O	43	
2	P	43	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23588 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 NITROGEN METABOLITE REPRESSION REGULATOR NMRA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	B	319	Total	C	N	O	S	0	0	0
			2541	1643	432	458	8			
1	C	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	D	319	Total	C	N	O	S	0	0	0
			2541	1643	432	458	8			
1	E	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	F	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	G	319	Total	C	N	O	S	0	0	0
			2541	1643	432	458	8			
1	H	319	Total	C	N	O	S	0	0	0
			2539	1642	430	459	8			

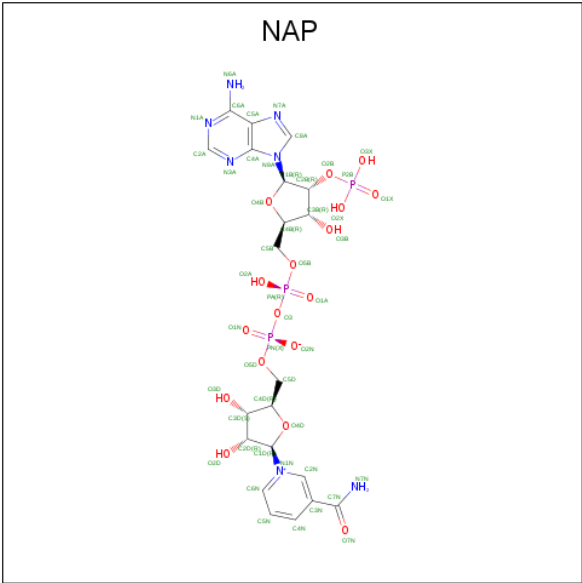
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	ARG	LEU	conflict	UNP O59919
B	238	ARG	LEU	conflict	UNP O59919
C	238	ARG	LEU	conflict	UNP O59919
D	238	ARG	LEU	conflict	UNP O59919
E	238	ARG	LEU	conflict	UNP O59919
F	238	ARG	LEU	conflict	UNP O59919
G	238	ARG	LEU	conflict	UNP O59919
H	238	ARG	LEU	conflict	UNP O59919

- Molecule 2 is a protein called NITROGEN REGULATORY PROTEIN AREA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	J	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	K	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	L	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	M	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	N	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	O	41	Total	C	N	O	S	0	0	0
			318	200	59	55	4			
2	P	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	N	1	Total	Zn	0	0
			1	1		
4	O	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	M	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	26	Total	O	0	0
			26	26		
5	C	39	Total	O	0	0
			39	39		
5	D	36	Total	O	0	0
			36	36		

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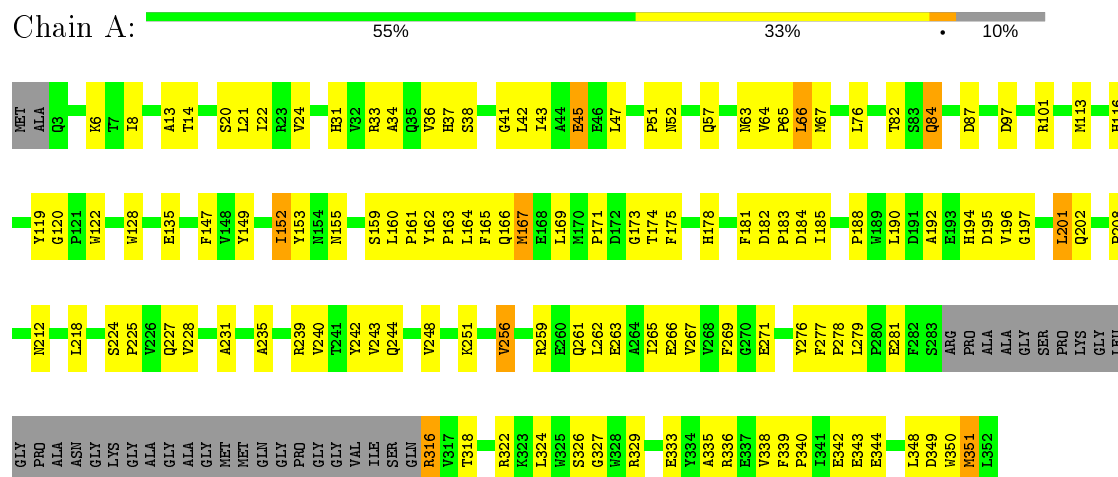
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	42	Total 42	O 42	0	0
5	F	33	Total 33	O 33	0	0
5	G	41	Total 41	O 41	0	0
5	H	33	Total 33	O 33	0	0
5	I	4	Total 4	O 4	0	0
5	J	3	Total 3	O 3	0	0
5	K	4	Total 4	O 4	0	0
5	L	4	Total 4	O 4	0	0
5	M	5	Total 5	O 5	0	0
5	N	3	Total 3	O 3	0	0
5	O	6	Total 6	O 6	0	0
5	P	3	Total 3	O 3	0	0

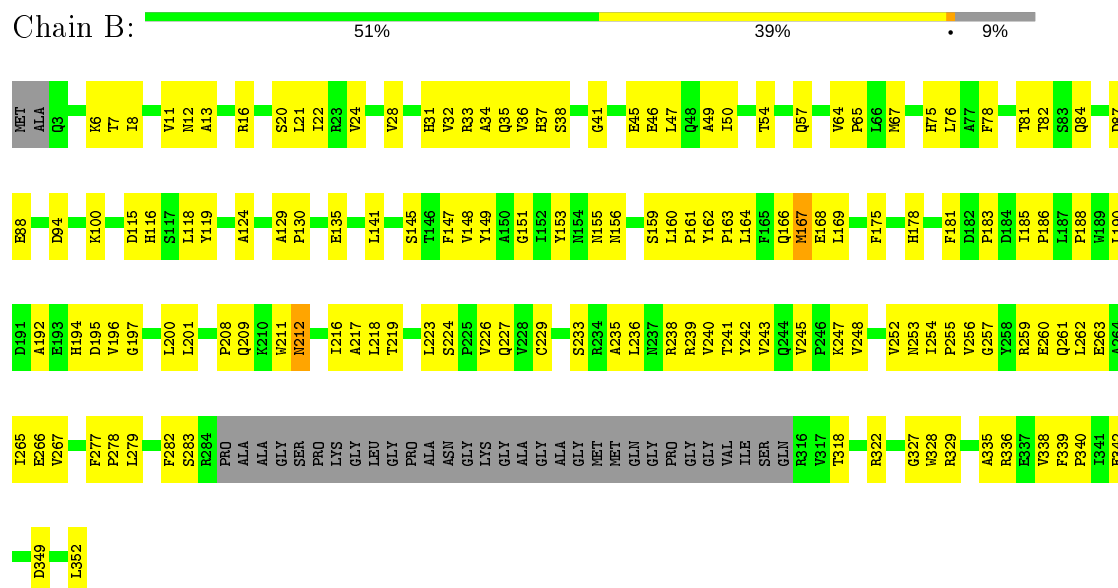
### 3 Residue-property plots

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: NITROGEN METABOLITE REPRESSION REGULATOR NMRA



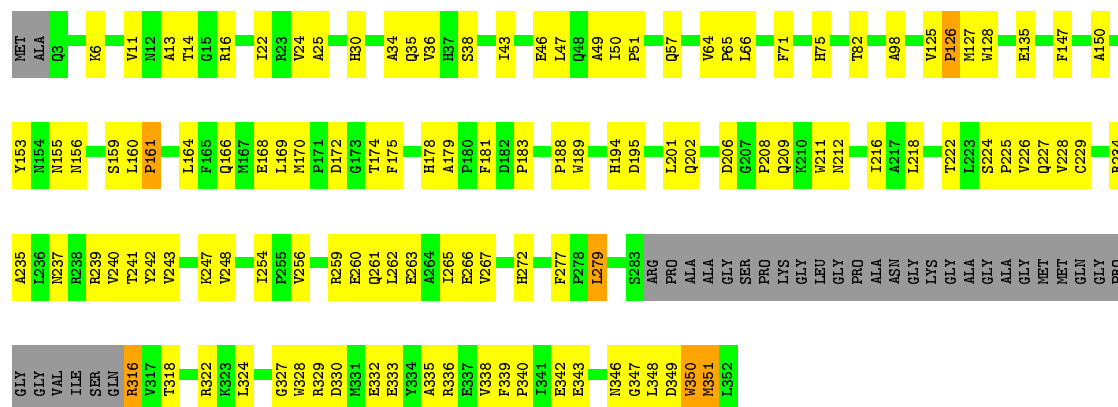
#### • Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA



#### • Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

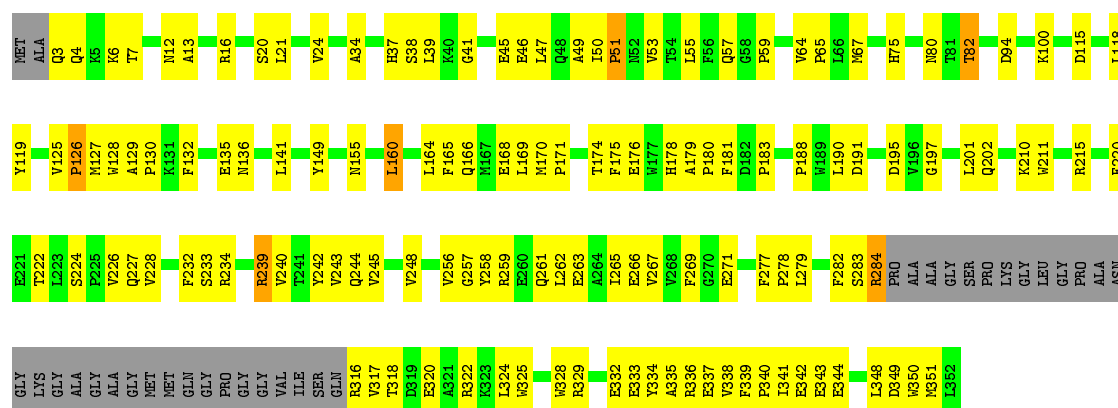






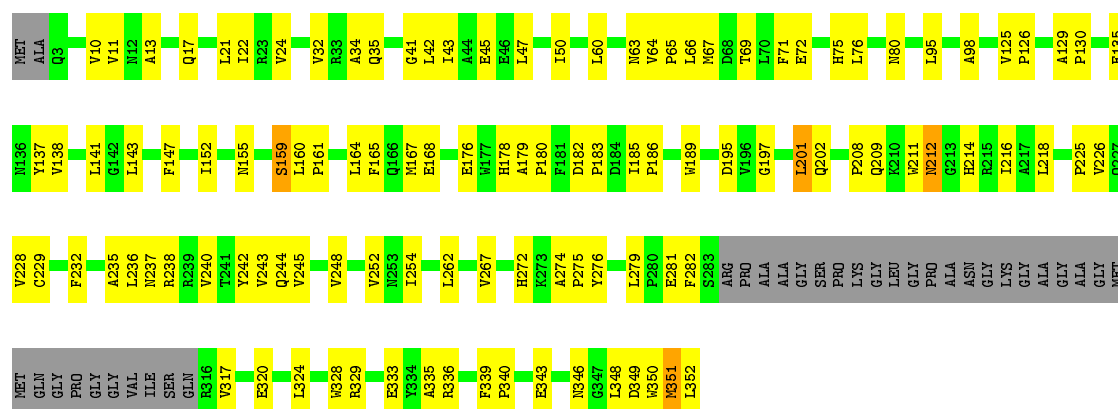
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain D: 53% 36% 9%



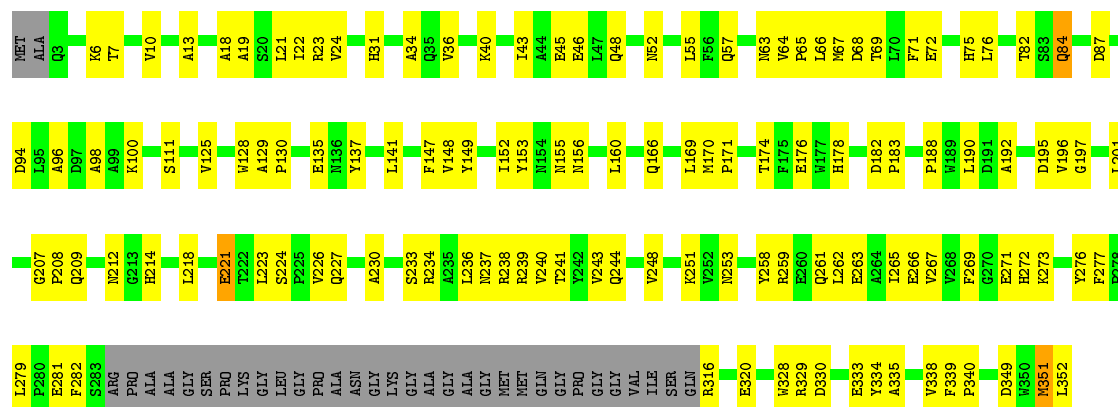
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain E: 59% 31% 10%



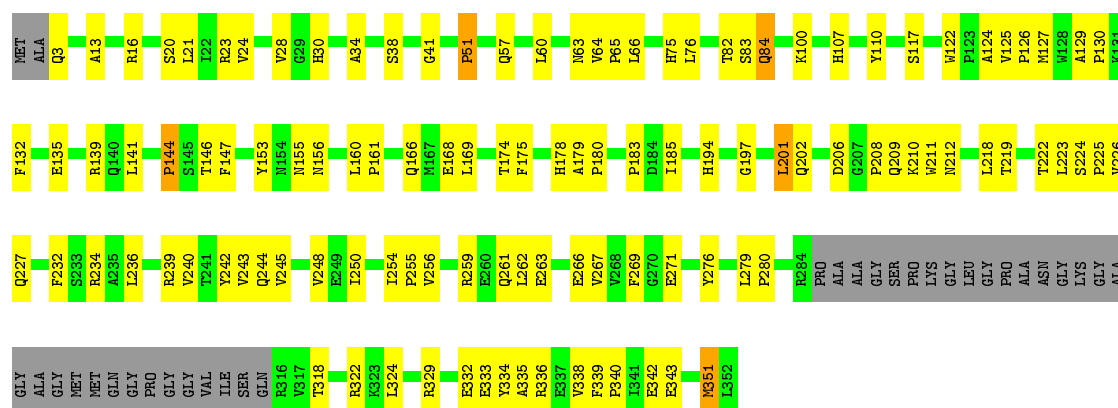
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain F: 54% 35% 10%



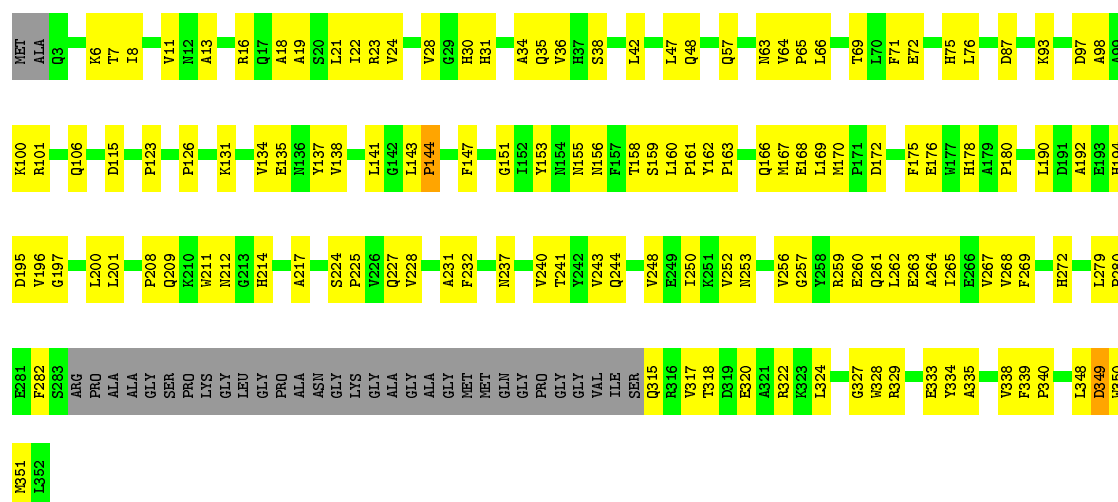
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain G: 58% 31% 9%



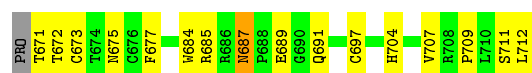
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain H: 52% 38% 9%



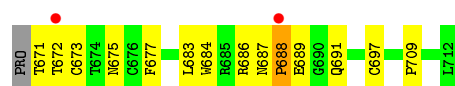
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain I: 




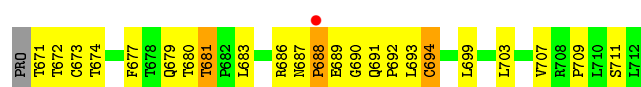
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain J: 



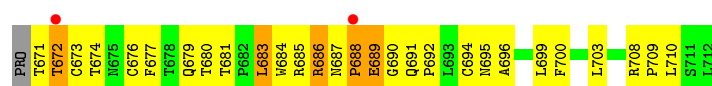
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain K: 



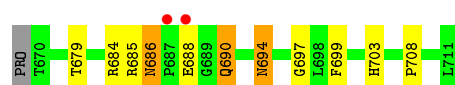
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain L: 



• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain M: 



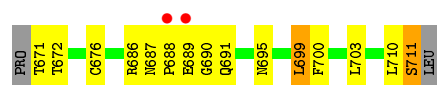
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain N: 



• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain O: 



• Molecule 2: NITROGEN REGULATORY PROTEIN AREA



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.73Å 231.73Å 223.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.86 – 2.80 29.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.86-2.80) 100.0 (29.86-2.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.287 0.228 , 0.284	Depositor DCC
$R_{free}$ test set	5547 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.459 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23588	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	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 21.37 % 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 7.1182e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAP

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	0/2606	0.68	1/3557 (0.0%)
1	B	0.42	0/2617	0.68	0/3571
1	C	0.42	0/2606	0.66	0/3557
1	D	0.44	0/2617	0.71	2/3571 (0.1%)
1	E	0.43	0/2606	0.68	1/3557 (0.0%)
1	F	0.45	0/2606	0.69	0/3557
1	G	0.43	0/2617	0.68	0/3571
1	H	0.42	0/2615	0.67	0/3569
2	I	0.42	0/334	0.65	0/456
2	J	0.41	0/334	0.65	0/456
2	K	0.44	0/334	0.63	0/456
2	L	0.49	0/334	0.77	0/456
2	M	0.44	0/334	0.64	0/456
2	N	0.38	0/334	0.64	0/456
2	O	0.40	0/326	0.64	0/445
2	P	0.39	0/334	0.64	0/456
All	All	0.43	0/23554	0.68	4/32147 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	284	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	D	284	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	E	167	MET	N-CA-C	-5.12	97.19	111.00
1	A	167	MET	N-CA-C	-5.08	97.29	111.00

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	2530	0	2476	98	0
1	B	2541	0	2489	107	0
1	C	2530	0	2476	108	0
1	D	2541	0	2489	106	0
1	E	2530	0	2476	83	0
1	F	2530	0	2476	98	0
1	G	2541	0	2489	101	0
1	H	2539	0	2484	113	0
2	I	326	0	326	20	0
2	J	326	0	326	12	0
2	K	326	0	327	19	0
2	L	326	0	326	30	0
2	M	326	0	326	21	0
2	N	326	0	326	14	0
2	O	318	0	315	17	0
2	P	326	0	326	19	0
3	A	48	0	25	2	0
3	B	48	0	25	1	0
3	C	48	0	25	1	0
3	D	48	0	25	2	0
3	E	48	0	25	0	0
3	F	48	0	25	1	0
3	G	48	0	25	0	0
3	H	48	0	25	2	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	A	32	0	0	0	0
5	B	26	0	0	0	0
5	C	39	0	0	3	0
5	D	36	0	0	3	0
5	E	42	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	33	0	0	1	0
5	G	41	0	0	4	0
5	H	33	0	0	4	0
5	I	4	0	0	1	0
5	J	3	0	0	0	0
5	K	4	0	0	2	0
5	L	4	0	0	0	0
5	M	5	0	0	0	0
5	N	3	0	0	0	0
5	O	6	0	0	0	0
5	P	3	0	0	0	0
All	All	23588	0	22653	939	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 20.

The worst 5 of 939 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)
2:M:686:ASN:HB2	2:M:690:GLN:HB2	1.20	1.11
1:D:239:ARG:HB3	1:D:239:ARG:HH11	1.20	1.06
1:F:82:THR:HG22	3:F:1353:NAP:H51N	1.36	1.03
1:C:82:THR:HG22	3:C:1353:NAP:H51N	1.40	1.02
1:C:166:GLN:HE21	1:C:168:GLU:HB2	1.22	1.01

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	314/352 (89%)	288 (92%)	23 (7%)	3 (1%)	15 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	315/352 (90%)	296 (94%)	18 (6%)	1 (0%)	41 72
1	C	314/352 (89%)	286 (91%)	23 (7%)	5 (2%)	9 31
1	D	315/352 (90%)	286 (91%)	27 (9%)	2 (1%)	25 56
1	E	314/352 (89%)	288 (92%)	25 (8%)	1 (0%)	41 72
1	F	314/352 (89%)	286 (91%)	27 (9%)	1 (0%)	41 72
1	G	315/352 (90%)	284 (90%)	29 (9%)	2 (1%)	25 56
1	H	315/352 (90%)	288 (91%)	23 (7%)	4 (1%)	12 36
2	I	40/43 (93%)	36 (90%)	3 (8%)	1 (2%)	5 19
2	J	40/43 (93%)	35 (88%)	5 (12%)	0	100 100
2	K	40/43 (93%)	34 (85%)	3 (8%)	3 (8%)	1 2
2	L	40/43 (93%)	34 (85%)	4 (10%)	2 (5%)	2 6
2	M	40/43 (93%)	37 (92%)	3 (8%)	0	100 100
2	N	40/43 (93%)	33 (82%)	6 (15%)	1 (2%)	5 19
2	O	39/43 (91%)	33 (85%)	5 (13%)	1 (3%)	5 18
2	P	40/43 (93%)	37 (92%)	3 (8%)	0	100 100
All	All	2835/3160 (90%)	2581 (91%)	227 (8%)	27 (1%)	15 44

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	350	TRP
2	I	711	SER
2	L	689	GLU
1	A	87	ASP
1	A	256	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	266/284 (94%)	254 (96%)	12 (4%)	27 60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	267/284 (94%)	260 (97%)	7 (3%)	46	79
1	C	266/284 (94%)	262 (98%)	4 (2%)	65	89
1	D	267/284 (94%)	260 (97%)	7 (3%)	46	79
1	E	266/284 (94%)	260 (98%)	6 (2%)	50	82
1	F	266/284 (94%)	258 (97%)	8 (3%)	41	75
1	G	267/284 (94%)	259 (97%)	8 (3%)	41	75
1	H	267/284 (94%)	264 (99%)	3 (1%)	73	92
2	I	38/39 (97%)	36 (95%)	2 (5%)	22	54
2	J	38/39 (97%)	37 (97%)	1 (3%)	46	79
2	K	38/39 (97%)	36 (95%)	2 (5%)	22	54
2	L	38/39 (97%)	35 (92%)	3 (8%)	12	34
2	M	38/39 (97%)	35 (92%)	3 (8%)	12	34
2	N	38/39 (97%)	37 (97%)	1 (3%)	46	79
2	O	37/39 (95%)	35 (95%)	2 (5%)	22	53
2	P	38/39 (97%)	38 (100%)	0	100	100
All	All	2435/2584 (94%)	2366 (97%)	69 (3%)	43	77

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	159	SER
1	F	221	GLU
2	M	686	ASN
1	E	201	LEU
1	E	351	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	48	GLN
1	G	57	GLN
2	M	694	ASN
1	F	62	ASN
1	F	166	GLN

### 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 ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	NAP	F	1353	-	45,52,52	2.26	12 (26%)	56,80,80	1.44	6 (10%)
3	NAP	C	1353	-	45,52,52	2.23	13 (28%)	56,80,80	1.41	7 (12%)
3	NAP	E	1353	-	45,52,52	2.20	12 (26%)	56,80,80	1.41	6 (10%)
3	NAP	B	1353	-	45,52,52	2.29	11 (24%)	56,80,80	1.41	7 (12%)
3	NAP	A	1353	-	45,52,52	2.25	10 (22%)	56,80,80	1.37	6 (10%)
3	NAP	H	1353	-	45,52,52	2.34	12 (26%)	56,80,80	1.35	7 (12%)
3	NAP	G	1353	-	45,52,52	2.33	16 (35%)	56,80,80	1.41	7 (12%)
3	NAP	D	1353	-	45,52,52	2.24	9 (20%)	56,80,80	1.40	6 (10%)

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	NAP	F	1353	-	-	2/31/67/67	0/5/5/5
3	NAP	C	1353	-	-	2/31/67/67	0/5/5/5
3	NAP	E	1353	-	-	2/31/67/67	0/5/5/5
3	NAP	B	1353	-	-	2/31/67/67	0/5/5/5
3	NAP	A	1353	-	-	2/31/67/67	0/5/5/5
3	NAP	H	1353	-	-	2/31/67/67	0/5/5/5
3	NAP	G	1353	-	-	2/31/67/67	0/5/5/5
3	NAP	D	1353	-	-	2/31/67/67	0/5/5/5

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1353	NAP	C2N-N1N	10.32	1.47	1.35
3	G	1353	NAP	C2N-N1N	10.21	1.47	1.35
3	F	1353	NAP	C2N-N1N	10.16	1.47	1.35
3	D	1353	NAP	C2N-N1N	10.14	1.47	1.35
3	H	1353	NAP	C2N-N1N	9.98	1.47	1.35

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1353	NAP	O4B-C4B-C5B	5.53	127.55	109.37
3	H	1353	NAP	O4B-C4B-C5B	5.42	127.20	109.37
3	F	1353	NAP	O4B-C4B-C5B	5.39	127.11	109.37
3	B	1353	NAP	O4B-C4B-C5B	5.37	127.05	109.37
3	A	1353	NAP	O4B-C4B-C5B	5.28	126.73	109.37

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

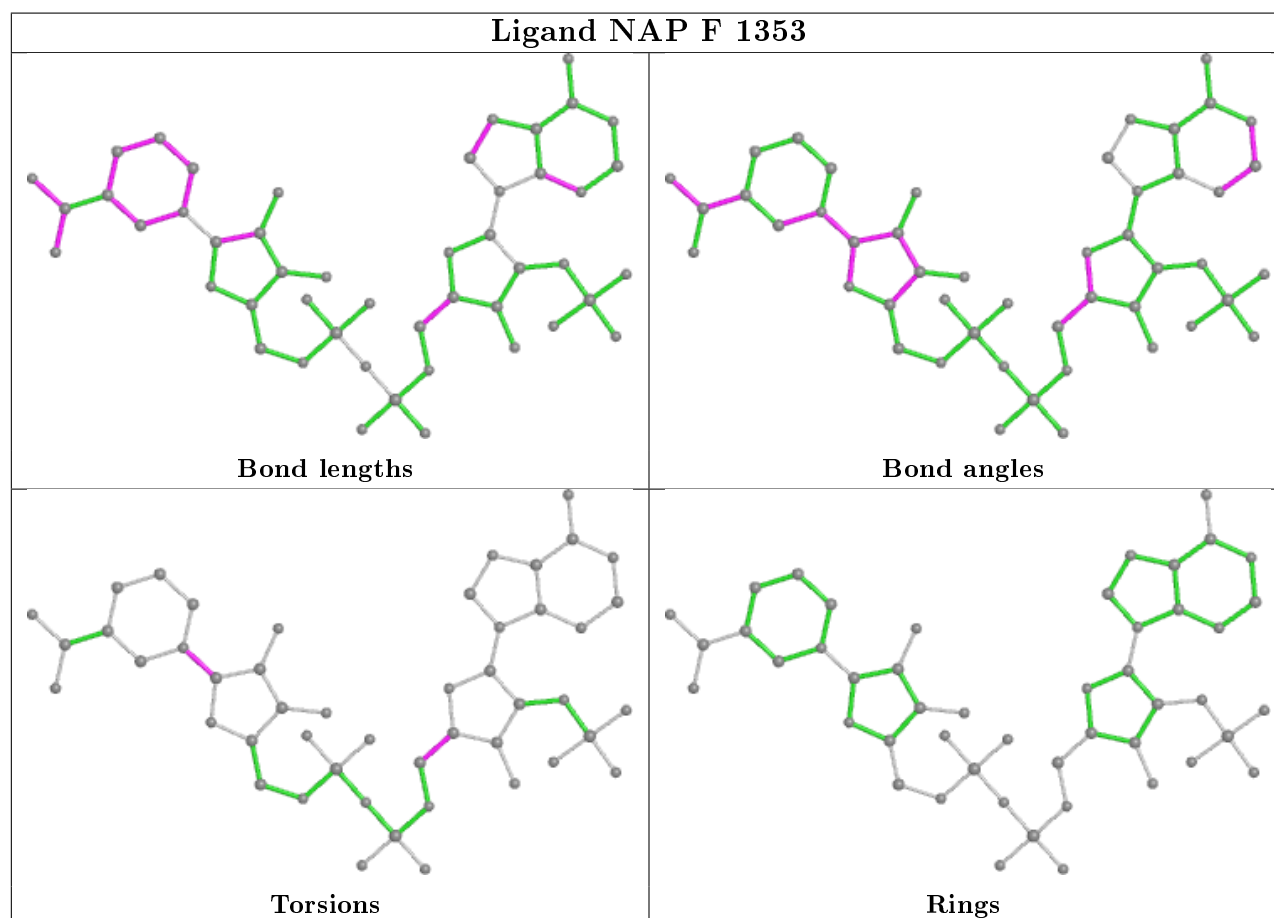
Mol	Chain	Res	Type	Atoms
3	F	1353	NAP	O4D-C1D-N1N-C2N
3	C	1353	NAP	O4D-C1D-N1N-C2N
3	E	1353	NAP	O4D-C1D-N1N-C2N
3	B	1353	NAP	O4D-C1D-N1N-C2N
3	A	1353	NAP	O4D-C1D-N1N-C2N

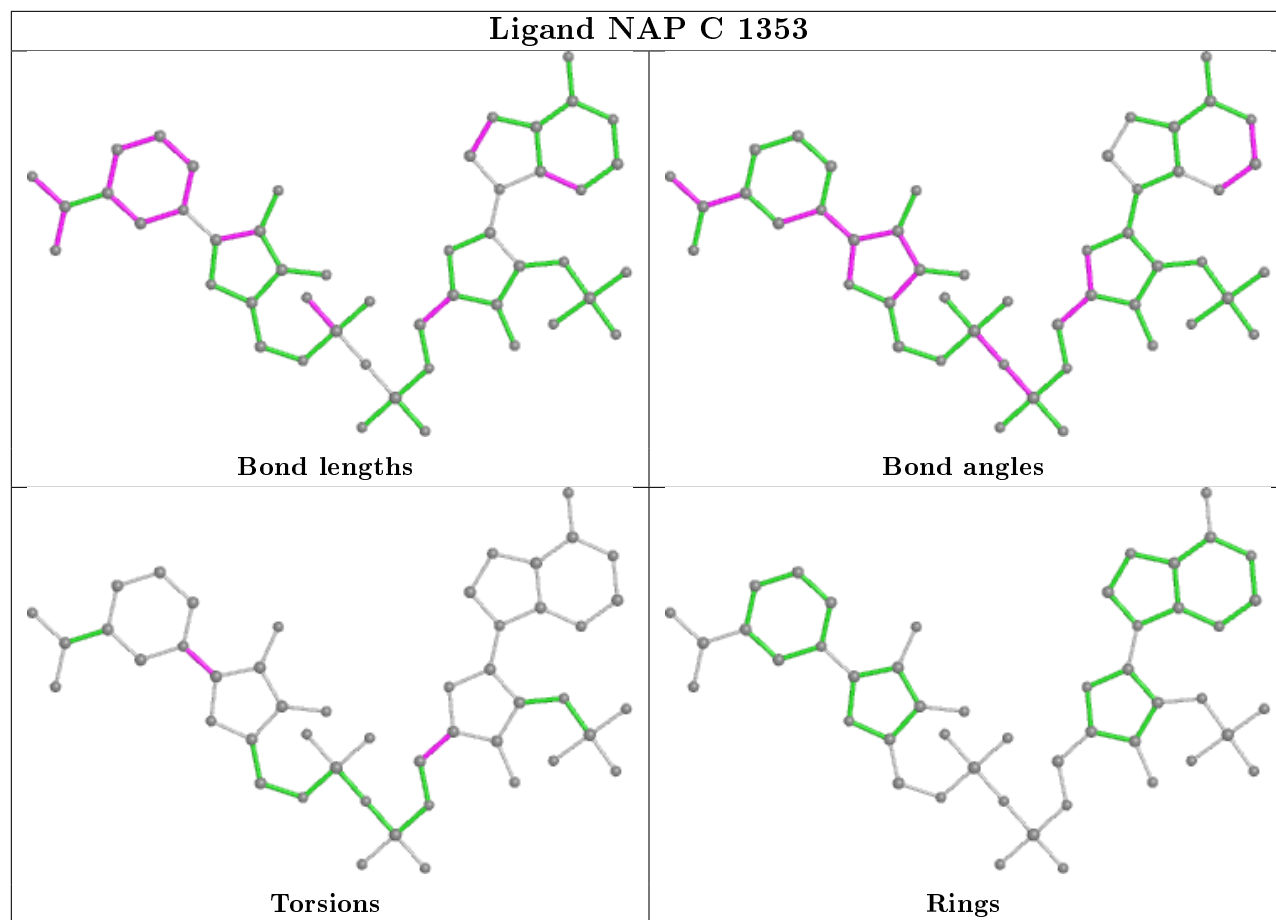
There are no ring outliers.

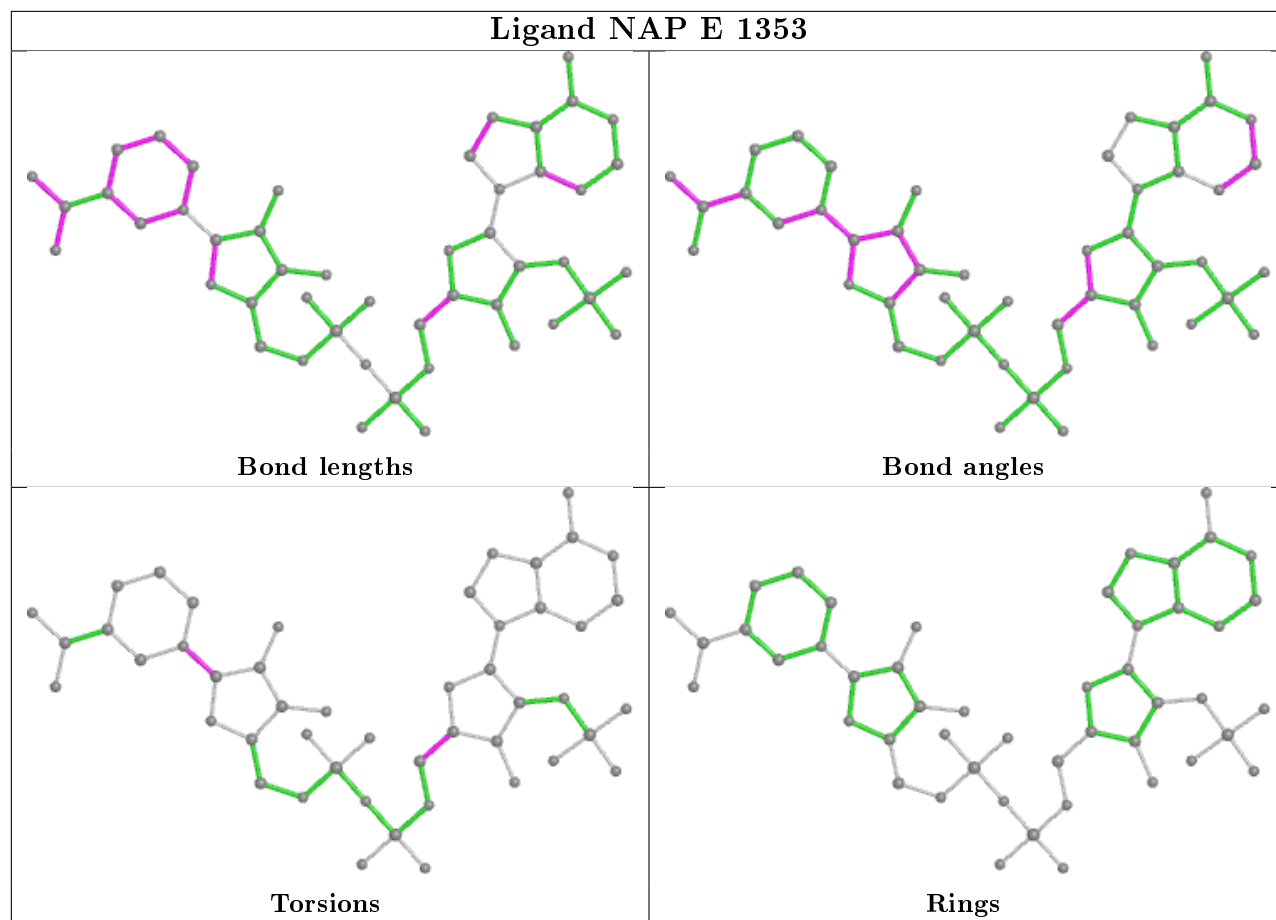
6 monomers are involved in 9 short contacts:

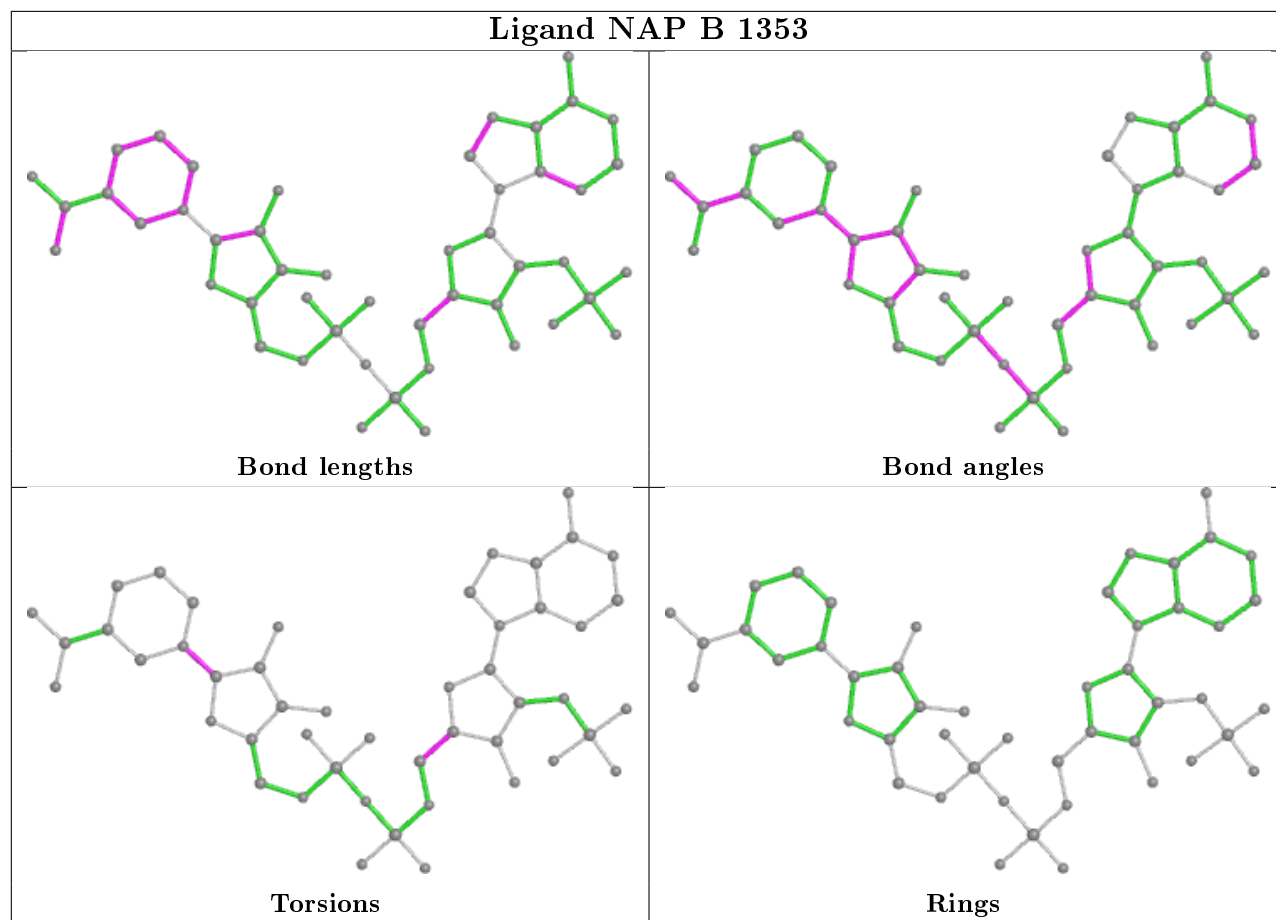
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1353	NAP	1	0
3	C	1353	NAP	1	0
3	B	1353	NAP	1	0
3	A	1353	NAP	2	0
3	H	1353	NAP	2	0
3	D	1353	NAP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

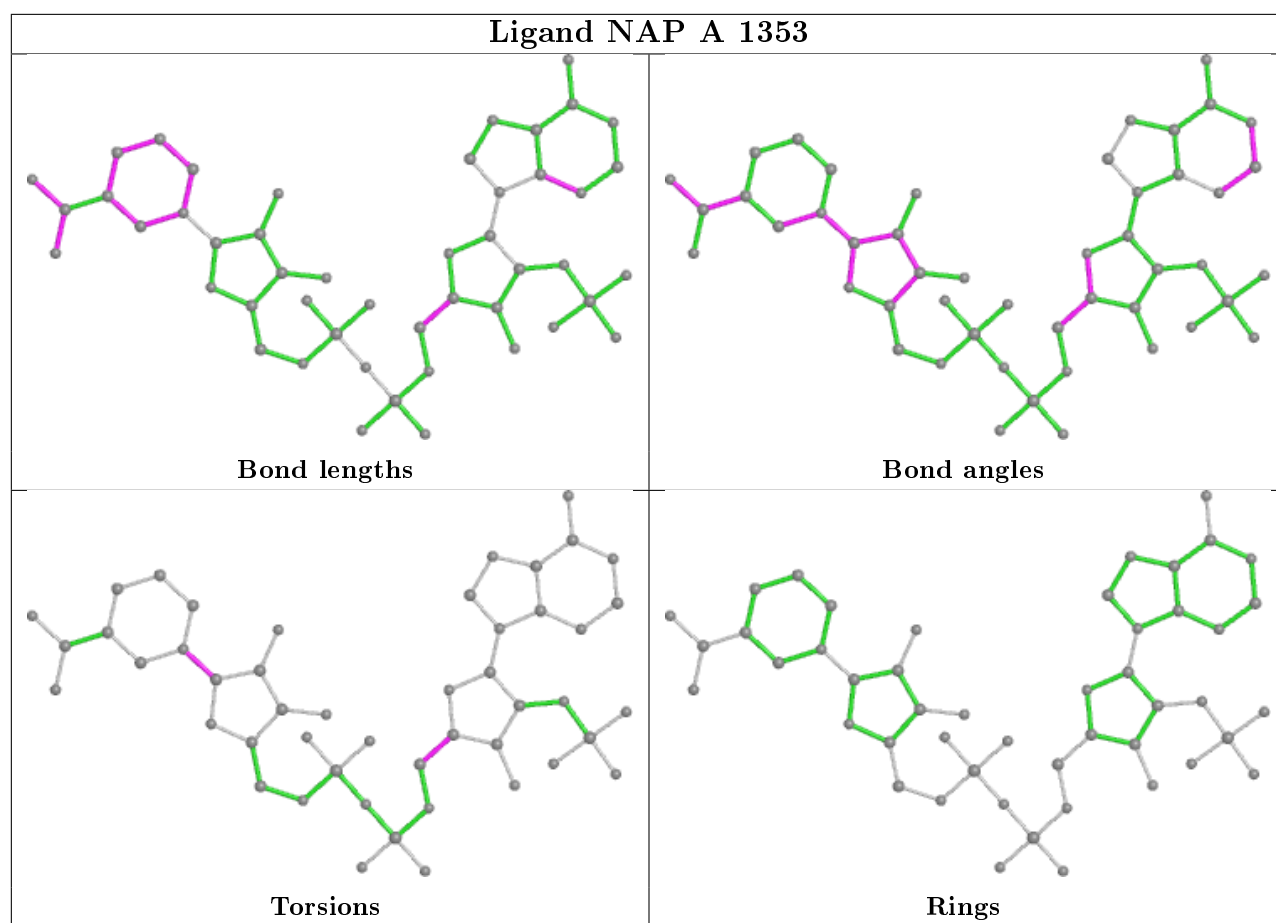


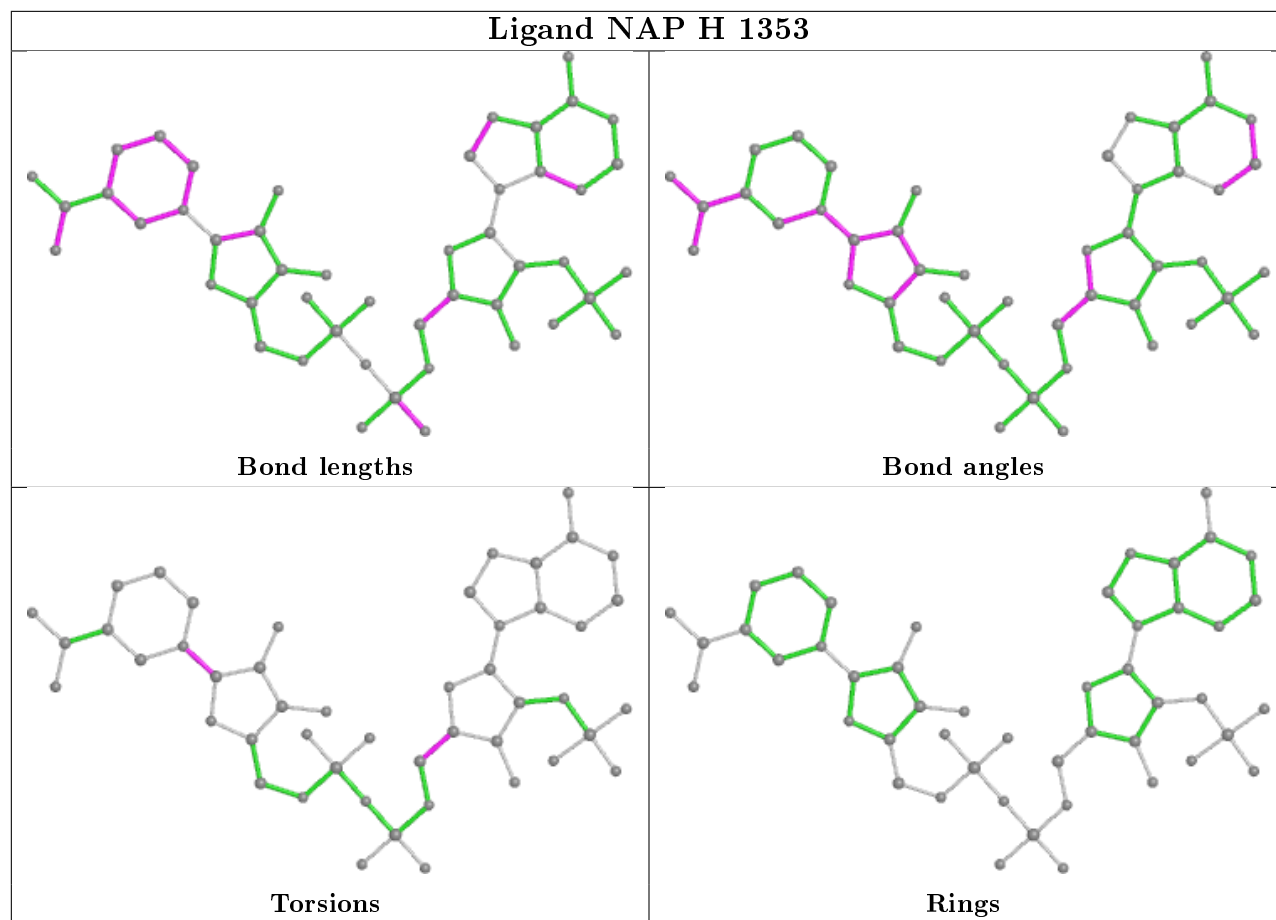


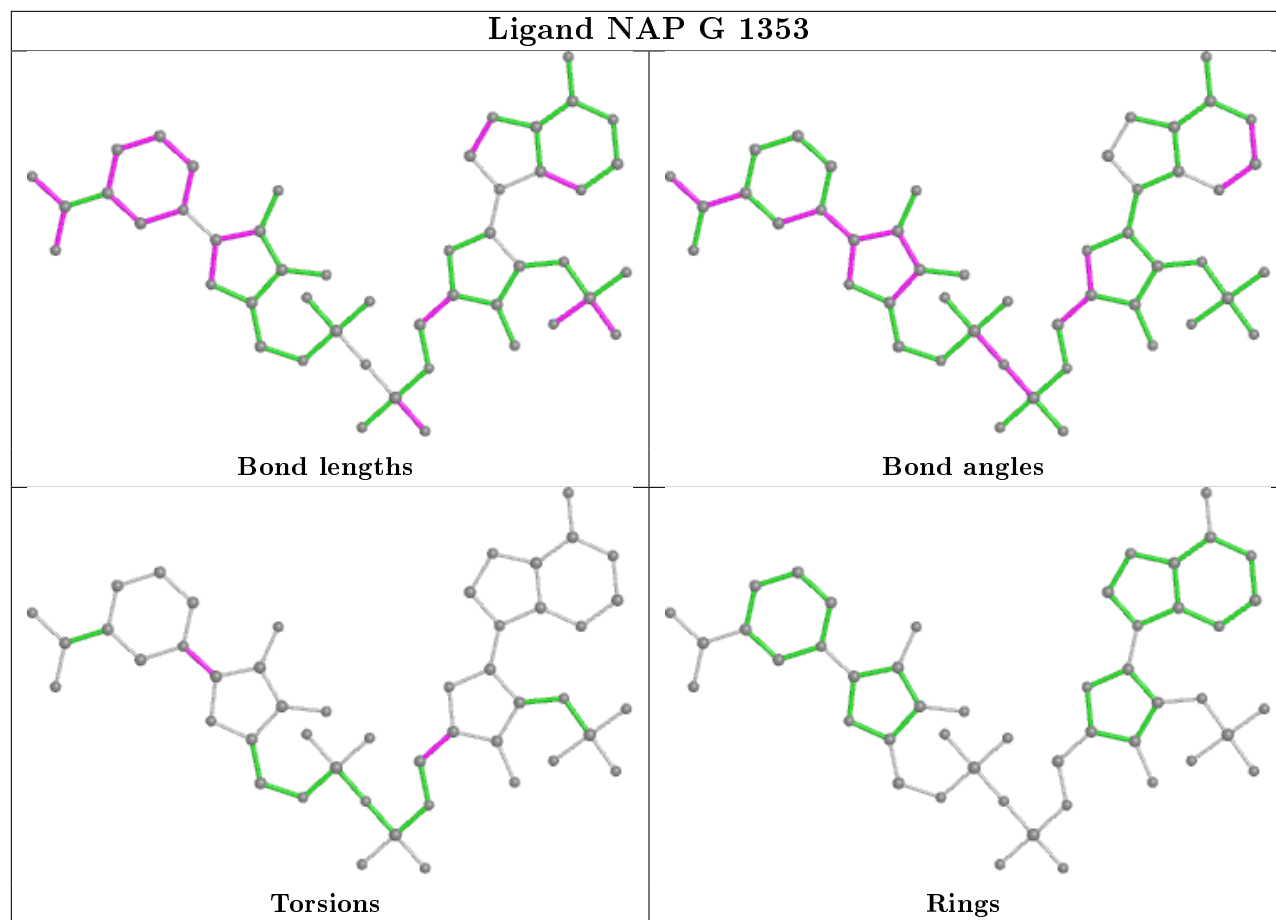


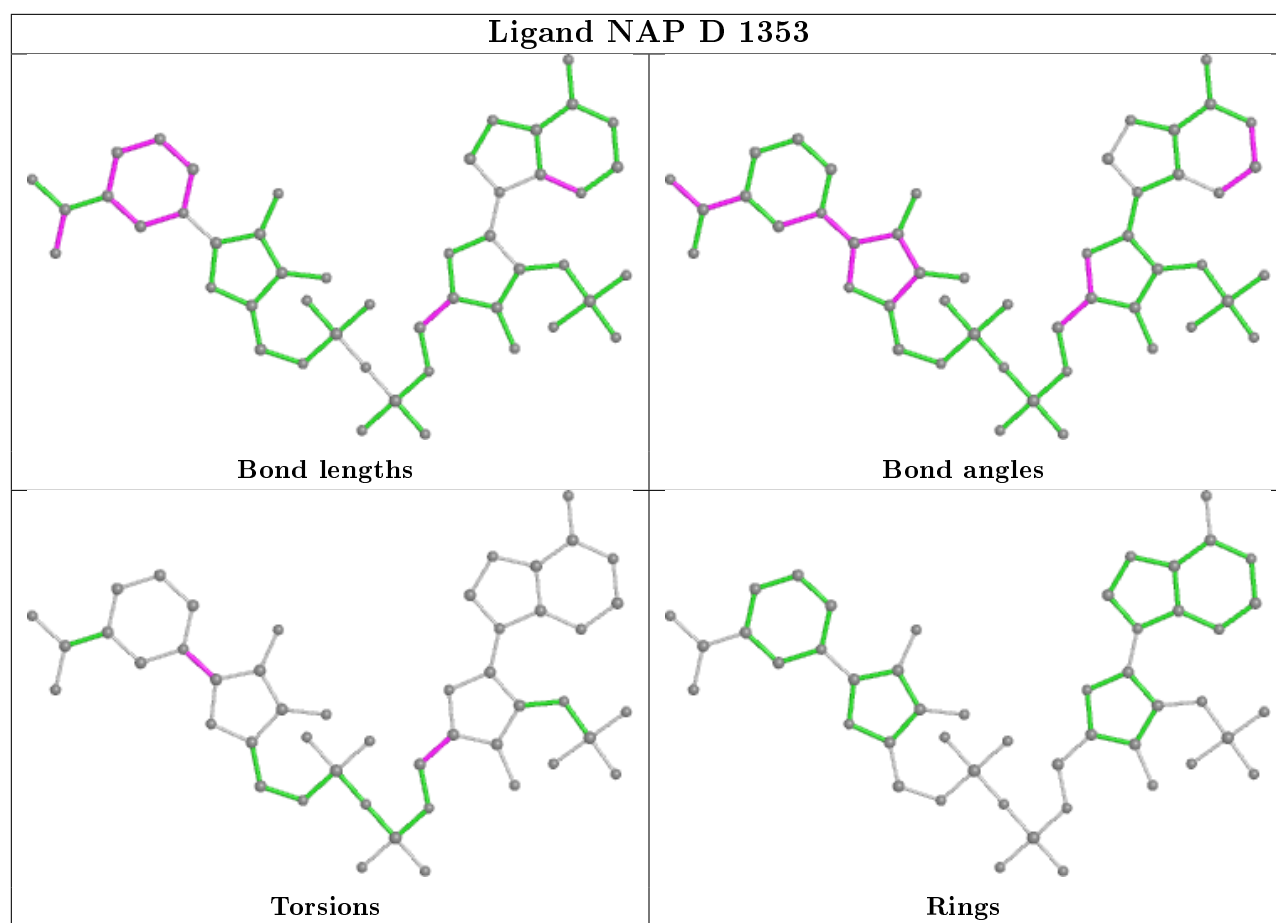












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	318/352 (90%)	-0.32	0 100 100	22, 47, 74, 91	0
1	B	319/352 (90%)	-0.19	0 100 100	21, 49, 78, 99	0
1	C	318/352 (90%)	-0.29	0 100 100	23, 45, 73, 90	0
1	D	319/352 (90%)	-0.28	0 100 100	20, 46, 74, 91	0
1	E	318/352 (90%)	-0.29	0 100 100	18, 43, 71, 83	0
1	F	318/352 (90%)	-0.31	0 100 100	23, 43, 69, 81	0
1	G	319/352 (90%)	-0.25	0 100 100	25, 44, 71, 99	0
1	H	319/352 (90%)	-0.32	0 100 100	21, 43, 73, 85	0
2	I	42/43 (97%)	0.16	0 100 100	30, 60, 121, 126	0
2	J	42/43 (97%)	0.30	2 (4%) 30 21	35, 60, 110, 121	0
2	K	42/43 (97%)	0.18	1 (2%) 59 49	35, 62, 121, 130	0
2	L	42/43 (97%)	0.11	2 (4%) 30 21	29, 57, 114, 139	0
2	M	42/43 (97%)	0.28	2 (4%) 30 21	22, 53, 111, 134	0
2	N	42/43 (97%)	0.10	2 (4%) 30 21	30, 57, 116, 130	0
2	O	41/43 (95%)	0.22	2 (4%) 29 20	36, 54, 108, 124	0
2	P	42/43 (97%)	0.26	1 (2%) 59 49	33, 55, 111, 125	0
All	All	2883/3160 (91%)	-0.22	12 (0%) 92 91	18, 46, 78, 139	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	687	PRO	4.6
2	M	688	GLU	3.7
2	O	688	PRO	3.6
2	J	688	PRO	3.1
2	P	688	PRO	3.1

## 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](#)

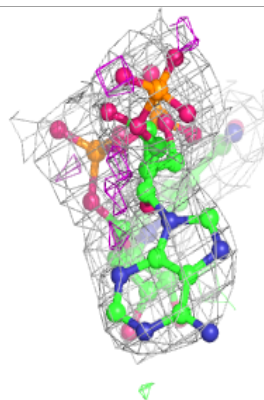
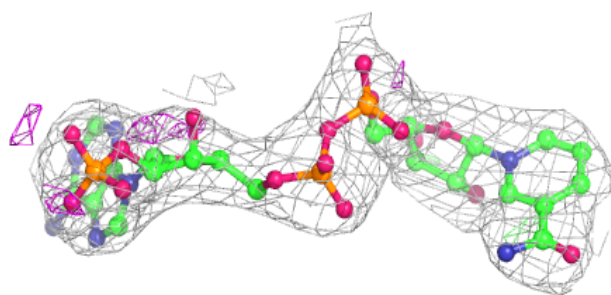
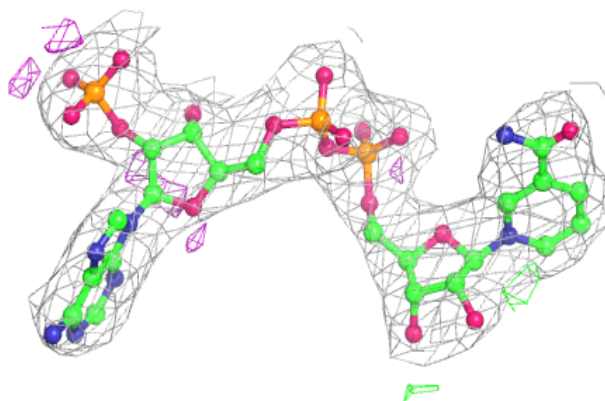
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAP	F	1353	48/48	0.97	0.17	25,49,80,87	0
3	NAP	C	1353	48/48	0.97	0.17	31,57,96,101	0
3	NAP	B	1353	48/48	0.97	0.16	25,55,87,91	0
3	NAP	A	1353	48/48	0.97	0.18	36,54,98,105	0
3	NAP	H	1353	48/48	0.97	0.19	22,61,106,110	0
3	NAP	G	1353	48/48	0.97	0.18	27,51,78,99	0
3	NAP	D	1353	48/48	0.97	0.18	25,53,74,85	0
3	NAP	E	1353	48/48	0.98	0.17	20,48,80,87	0
4	ZN	J	1713	1/1	0.98	0.14	57,57,57,57	0
4	ZN	P	1713	1/1	0.99	0.15	47,47,47,47	0
4	ZN	I	1713	1/1	0.99	0.13	58,58,58,58	0
4	ZN	O	1712	1/1	0.99	0.14	52,52,52,52	0
4	ZN	L	1713	1/1	0.99	0.13	58,58,58,58	0
4	ZN	N	1713	1/1	0.99	0.14	53,53,53,53	0
4	ZN	K	1713	1/1	0.99	0.11	66,66,66,66	0
4	ZN	M	1712	1/1	1.00	0.15	48,48,48,48	0

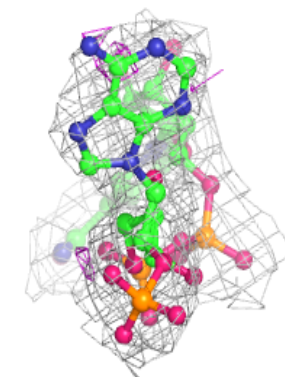
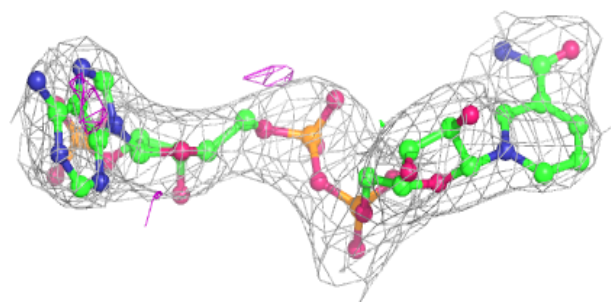
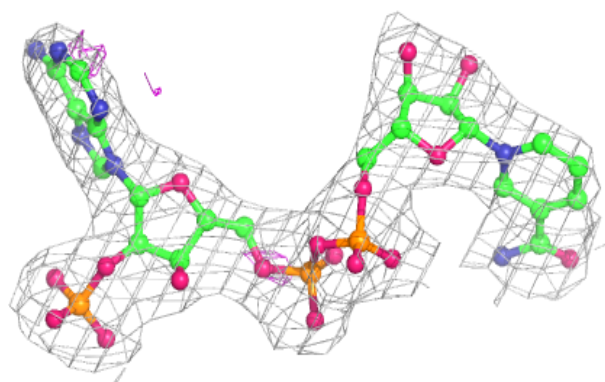
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP F 1353:**

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

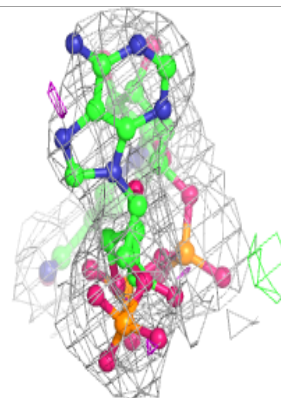
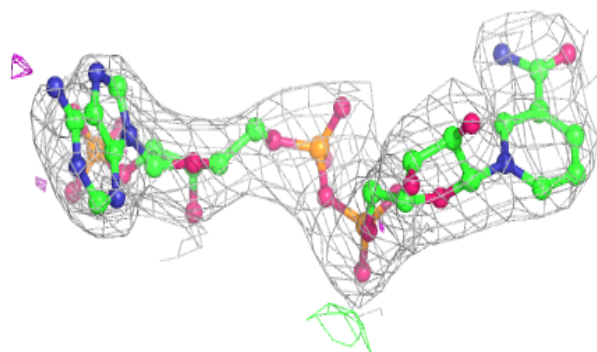
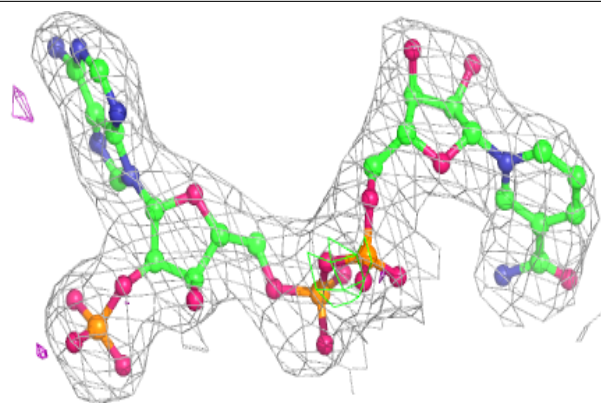
**Electron density around NAP C 1353:**

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

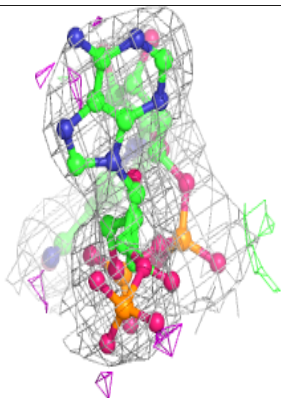
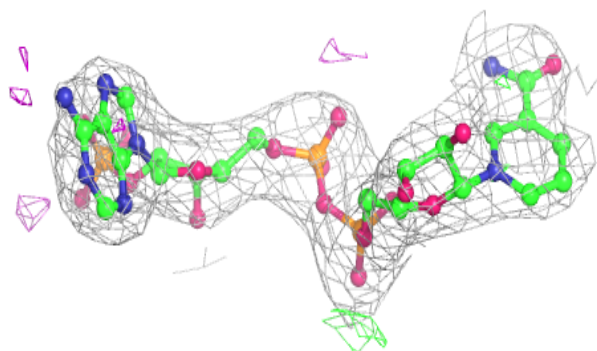
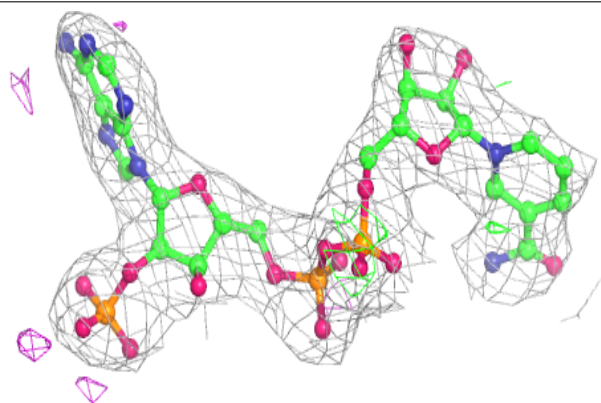


**Electron density around NAP B 1353:**

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

**Electron density around NAP A 1353:**

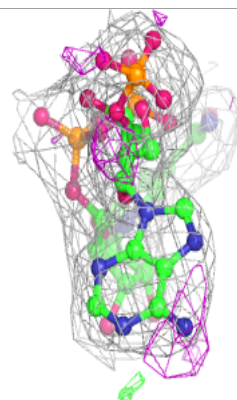
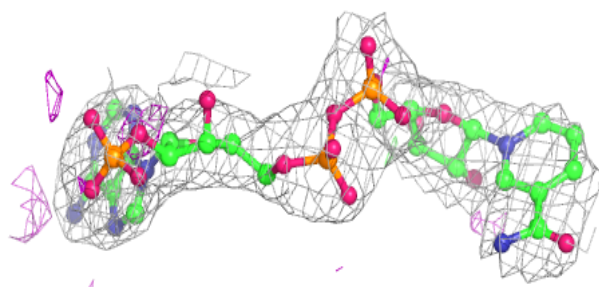
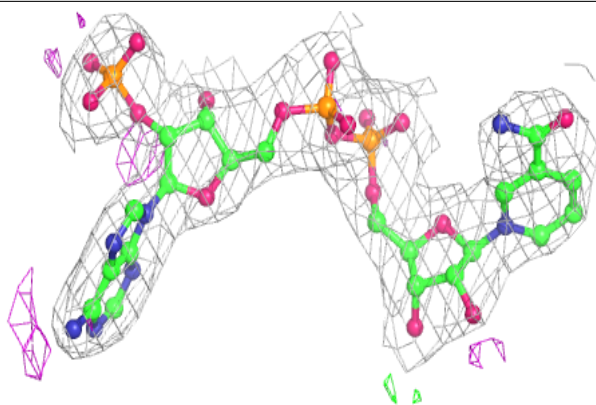
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



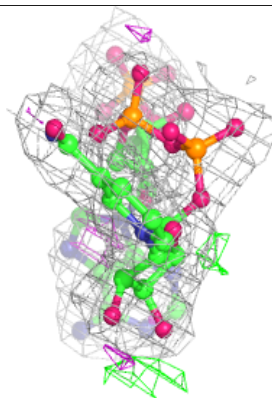
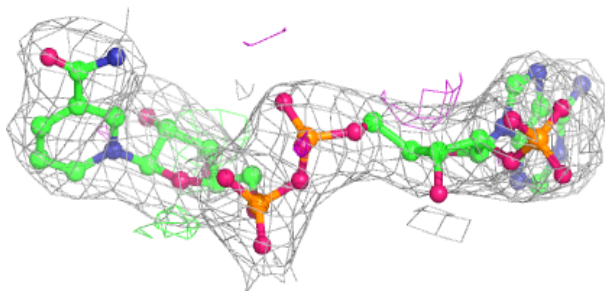
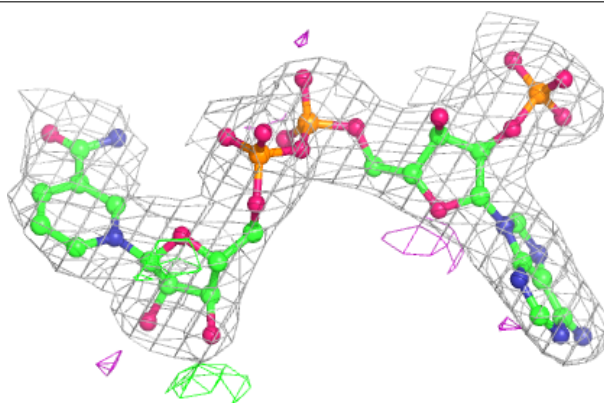


**Electron density around NAP H 1353:**

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

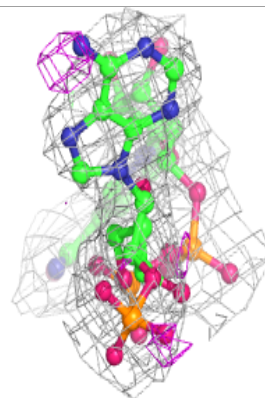
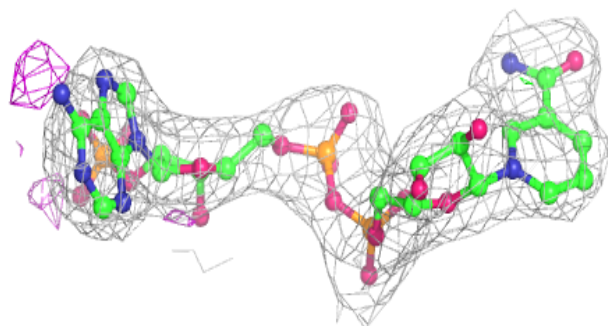
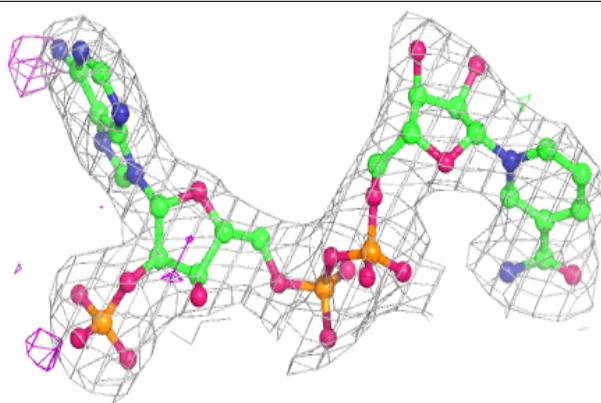
**Electron density around NAP G 1353:**

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

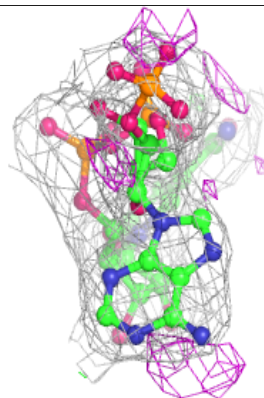
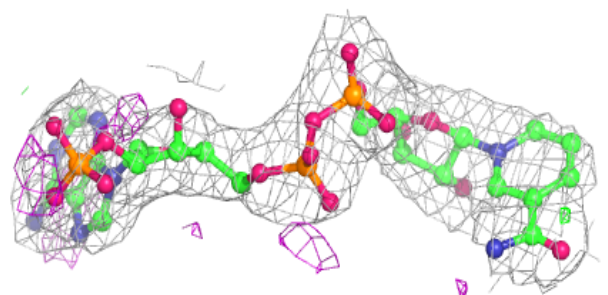
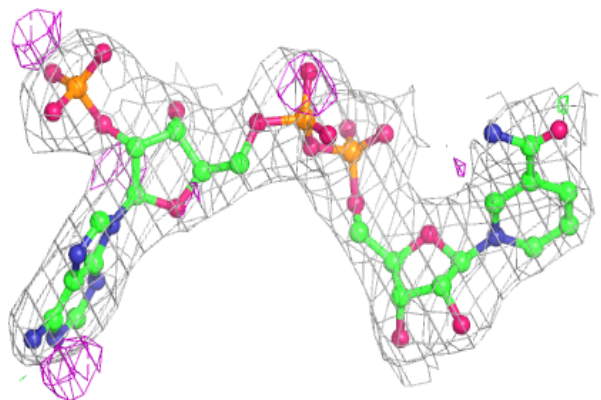


**Electron density around NAP D 1353:**

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

**Electron density around NAP E 1353:**

$2mF_o-DF_c$  (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.