Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 05:31 PM EDT

PDB ID	:	3JQB
Title	:	Crystal structure of pteridine reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor (NADP+) and inhibitor 2-amino-5-(2-phenylethyl)-3,7-dihydro-4H-pyrrolo[2,3-d]pyrimidin-4-one (DX6)
Authors	:	Tulloch, L.B.; Hunter, W.N.
Deposited on	:	2009-09-06
Resolution	:	2.40 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 (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:

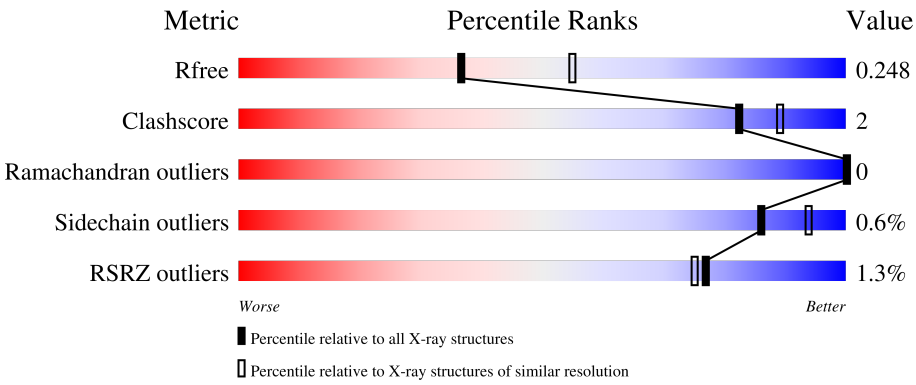
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	288	82% 5% 14%
1	B	288	% 80% 6% 14%
1	D	288	% 78% 8% 14%
2	C	288	2% 81% 6% 14%

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
5	DTT	D	271	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8042 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 Pteridine reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	249	1860	1169	327	353	11	0	2	0
1	B	248	1853	1165	327	350	11	0	1	0
1	D	249	1865	1174	327	353	11	0	2	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q581W1
A	-18	GLY	-	expression tag	UNP Q581W1
A	-17	SER	-	expression tag	UNP Q581W1
A	-16	SER	-	expression tag	UNP Q581W1
A	-15	HIS	-	expression tag	UNP Q581W1
A	-14	HIS	-	expression tag	UNP Q581W1
A	-13	HIS	-	expression tag	UNP Q581W1
A	-12	HIS	-	expression tag	UNP Q581W1
A	-11	HIS	-	expression tag	UNP Q581W1
A	-10	HIS	-	expression tag	UNP Q581W1
A	-9	SER	-	expression tag	UNP Q581W1
A	-8	SER	-	expression tag	UNP Q581W1
A	-7	GLY	-	expression tag	UNP Q581W1
A	-6	LEU	-	expression tag	UNP Q581W1
A	-5	VAL	-	expression tag	UNP Q581W1
A	-4	PRO	-	expression tag	UNP Q581W1
A	-3	ARG	-	expression tag	UNP Q581W1
A	-2	GLY	-	expression tag	UNP Q581W1
A	-1	SER	-	expression tag	UNP Q581W1
A	0	HIS	-	expression tag	UNP Q581W1
B	-19	MET	-	expression tag	UNP Q581W1
B	-18	GLY	-	expression tag	UNP Q581W1
B	-17	SER	-	expression tag	UNP Q581W1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP Q581W1
B	-15	HIS	-	expression tag	UNP Q581W1
B	-14	HIS	-	expression tag	UNP Q581W1
B	-13	HIS	-	expression tag	UNP Q581W1
B	-12	HIS	-	expression tag	UNP Q581W1
B	-11	HIS	-	expression tag	UNP Q581W1
B	-10	HIS	-	expression tag	UNP Q581W1
B	-9	SER	-	expression tag	UNP Q581W1
B	-8	SER	-	expression tag	UNP Q581W1
B	-7	GLY	-	expression tag	UNP Q581W1
B	-6	LEU	-	expression tag	UNP Q581W1
B	-5	VAL	-	expression tag	UNP Q581W1
B	-4	PRO	-	expression tag	UNP Q581W1
B	-3	ARG	-	expression tag	UNP Q581W1
B	-2	GLY	-	expression tag	UNP Q581W1
B	-1	SER	-	expression tag	UNP Q581W1
B	0	HIS	-	expression tag	UNP Q581W1
D	-19	MET	-	expression tag	UNP Q581W1
D	-18	GLY	-	expression tag	UNP Q581W1
D	-17	SER	-	expression tag	UNP Q581W1
D	-16	SER	-	expression tag	UNP Q581W1
D	-15	HIS	-	expression tag	UNP Q581W1
D	-14	HIS	-	expression tag	UNP Q581W1
D	-13	HIS	-	expression tag	UNP Q581W1
D	-12	HIS	-	expression tag	UNP Q581W1
D	-11	HIS	-	expression tag	UNP Q581W1
D	-10	HIS	-	expression tag	UNP Q581W1
D	-9	SER	-	expression tag	UNP Q581W1
D	-8	SER	-	expression tag	UNP Q581W1
D	-7	GLY	-	expression tag	UNP Q581W1
D	-6	LEU	-	expression tag	UNP Q581W1
D	-5	VAL	-	expression tag	UNP Q581W1
D	-4	PRO	-	expression tag	UNP Q581W1
D	-3	ARG	-	expression tag	UNP Q581W1
D	-2	GLY	-	expression tag	UNP Q581W1
D	-1	SER	-	expression tag	UNP Q581W1
D	0	HIS	-	expression tag	UNP Q581W1

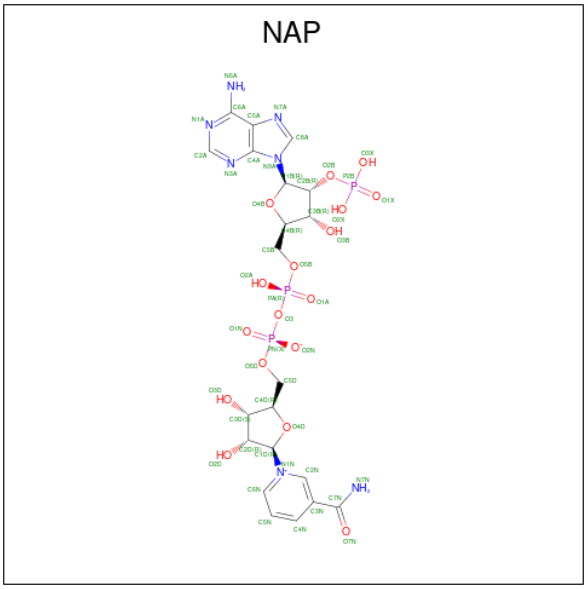
- Molecule 2 is a protein called Pteridine reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	248	1849	1162	326	350	11	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

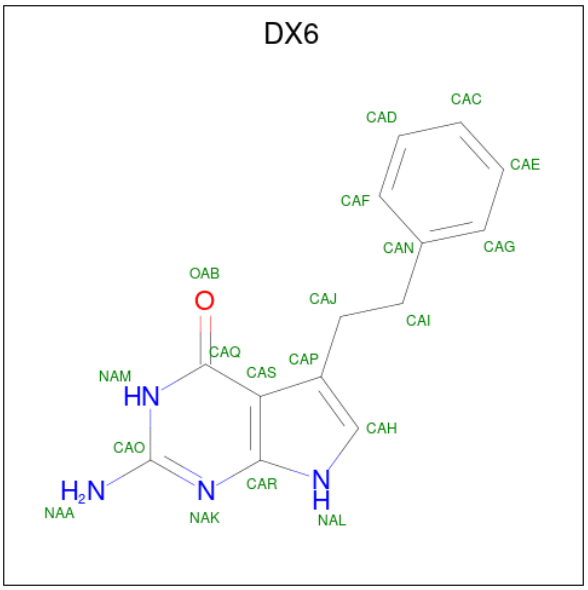
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP Q581W1
C	-18	GLY	-	expression tag	UNP Q581W1
C	-17	SER	-	expression tag	UNP Q581W1
C	-16	SER	-	expression tag	UNP Q581W1
C	-15	HIS	-	expression tag	UNP Q581W1
C	-14	HIS	-	expression tag	UNP Q581W1
C	-13	HIS	-	expression tag	UNP Q581W1
C	-12	HIS	-	expression tag	UNP Q581W1
C	-11	HIS	-	expression tag	UNP Q581W1
C	-10	HIS	-	expression tag	UNP Q581W1
C	-9	SER	-	expression tag	UNP Q581W1
C	-8	SER	-	expression tag	UNP Q581W1
C	-7	GLY	-	expression tag	UNP Q581W1
C	-6	LEU	-	expression tag	UNP Q581W1
C	-5	VAL	-	expression tag	UNP Q581W1
C	-4	PRO	-	expression tag	UNP Q581W1
C	-3	ARG	-	expression tag	UNP Q581W1
C	-2	GLY	-	expression tag	UNP Q581W1
C	-1	SER	-	expression tag	UNP Q581W1
C	0	HIS	-	expression tag	UNP Q581W1

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



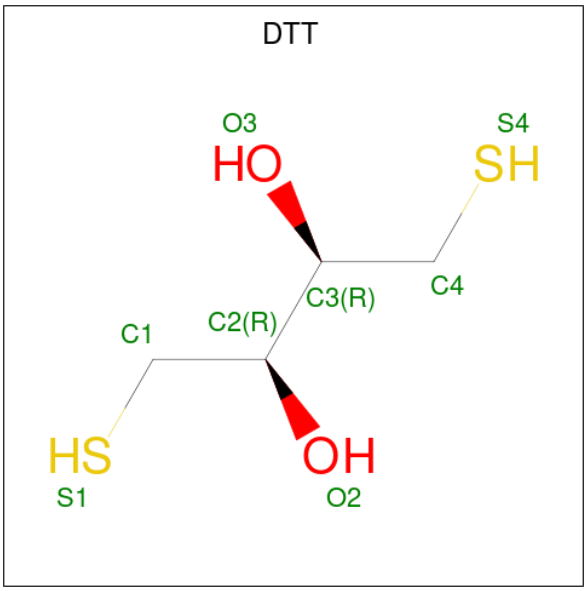
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0
3	B	1	48	21	7	17	3	0	0
3	C	1	48	21	7	17	3	0	0
3	D	1	48	21	7	17	3	0	0

- Molecule 4 is 2-amino-5-(2-phenylethyl)-3,7-dihydro-4H-pyrrolo[2,3-d]pyrimidin-4-one (three-letter code: DX6) (formula: $C_{14}H_{14}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	19	14	4	1	0	0
4	B	1	19	14	4	1	0	0
4	C	1	19	14	4	1	0	0

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	D	1	8	4	2	2	0	0

- Molecule 6 is water.

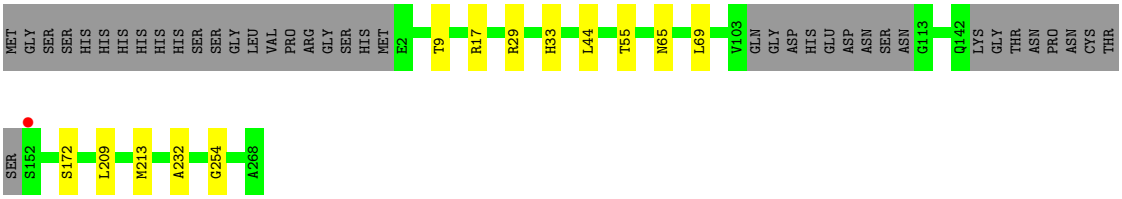
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	98	98	98	0	0
6	B	90	90	90	0	0
6	C	86	86	86	0	0
6	D	84	84	84	0	0

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.

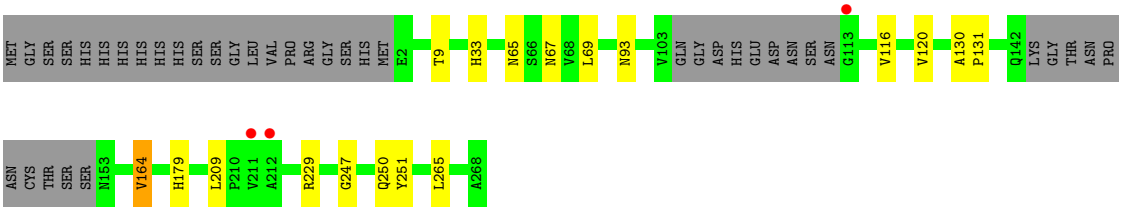
• Molecule 1: Pteridine reductase 1

Chain A:



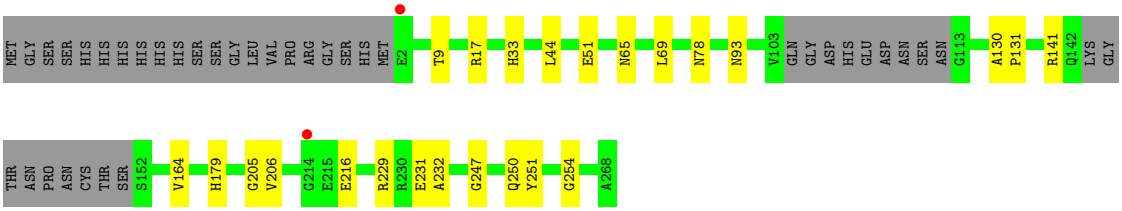
• Molecule 1: Pteridine reductase 1

Chain B:



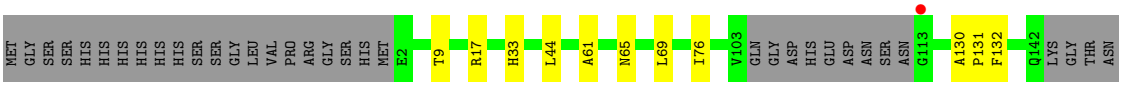
• Molecule 1: Pteridine reductase 1

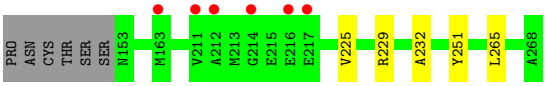
Chain D:



• Molecule 2: Pteridine reductase 1

Chain C:




PRO
ASN
CYS
THR
SER
SER
N153
M163
V211
A212
M213
G214
E215
E216
E217
V225
R229
A232
Y251
L265
A268

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.67Å 90.43Å 82.56Å 90.00° 115.54° 90.00°	Depositor
Resolution (Å)	45.22 – 2.40 45.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.22-2.40) 98.5 (45.22-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	5.74 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.252 0.191 , 0.248	Depositor DCC
R_{free} test set	1952 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	7.9	Xtriage
Anisotropy	2.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 32.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8042	wwPDB-VP
Average B, all atoms (Å^2)	7.0	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 31.08 % 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 1.1748e-03.*

[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: DTT, CSX, NAP, DX6

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	0/1893	0.46	0/2568
1	B	0.35	0/1883	0.47	0/2555
1	D	0.34	0/1898	0.46	0/2575
2	C	0.34	0/1868	0.47	0/2533
All	All	0.34	0/7542	0.47	0/10231

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 (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	1860	0	1887	9	0
1	B	1853	0	1878	11	0
1	D	1865	0	1894	14	0
2	C	1849	0	1872	11	0
3	A	48	0	25	0	0
3	B	48	0	25	0	0
3	C	48	0	25	0	0
3	D	48	0	25	1	0
4	A	19	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	19	0	14	1	0
4	C	19	0	14	0	0
5	D	8	0	10	0	0
6	A	98	0	0	0	0
6	B	90	0	0	0	0
6	C	86	0	0	0	0
6	D	84	0	0	0	0
All	All	8042	0	7683	38	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 (38) 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:A:213:MET:HE1	4:A:270:DX6:HAE	1.65	0.78
1:B:9:THR:HA	1:B:33:HIS:HB3	1.83	0.61
1:A:209:LEU:HD23	4:A:270:DX6:HAG	1.82	0.61
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.82	0.59
2:C:9:THR:HA	2:C:33:HIS:HB3	1.84	0.58
1:A:9:THR:HA	1:A:33:HIS:HB3	1.87	0.57
2:C:232:ALA:HB2	1:D:251:TYR:CE2	2.39	0.56
1:B:67[B]:ASN:H	1:B:67[B]:ASN:HD22	1.53	0.56
1:D:9:THR:HA	1:D:33:HIS:HB3	1.88	0.55
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.44	0.53
1:D:206:VAL:HG12	1:D:231:GLU:HB2	1.92	0.51
1:B:164:VAL:HG22	1:B:179:HIS:CD2	2.46	0.51
1:B:9:THR:O	1:B:93:ASN:HB3	2.13	0.49
1:A:17:ARG:HG3	1:A:44:LEU:HD22	1.95	0.48
2:C:232:ALA:HB2	1:D:251:TYR:CD2	2.49	0.47
1:A:172[A]:SER:HG	2:C:132:PHE:HE1	1.62	0.47
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.96	0.47
1:D:247:GLY:HA2	1:D:250:GLN:HG3	1.97	0.47
1:B:65:ASN:HA	1:B:69:LEU:HD22	1.96	0.47
2:C:251:TYR:CE2	1:D:232:ALA:HB2	2.50	0.46
1:A:254:GLY:HA3	1:B:265:LEU:HD11	1.99	0.45
1:B:116:VAL:O	1:B:120:VAL:HG23	2.17	0.45
1:B:209:LEU:HD23	4:B:270:DX6:HAG	1.99	0.44
1:B:130:ALA:HB3	1:B:131:PRO:HD3	1.99	0.44
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.53	0.43
2:C:65:ASN:HA	2:C:69:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:ARG:HG3	2:C:44:LEU:HD22	1.99	0.43
2:C:130:ALA:HB3	2:C:131:PRO:HD3	2.01	0.42
2:C:265:LEU:HD11	1:D:254:GLY:HA3	2.01	0.42
1:D:130:ALA:HB3	1:D:131:PRO:HD3	2.01	0.42
1:D:9:THR:O	1:D:93:ASN:HB3	2.19	0.42
1:B:247:GLY:HA2	1:B:250:GLN:HG3	2.00	0.42
1:D:205:GLY:O	3:D:269:NAP:H4N	2.20	0.41
1:A:29:ARG:HG2	1:A:55:THR:HG22	2.02	0.41
2:C:61:ALA:HB3	2:C:76:ILE:HD11	2.02	0.41
2:C:225:VAL:O	2:C:229:ARG:HD2	2.19	0.41
1:D:78:ASN:OD1	1:D:141:ARG:NH1	2.53	0.41
1:D:17:ARG:HG3	1:D:44:LEU:HD22	2.02	0.41

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	245/288 (85%)	236 (96%)	9 (4%)	0	100	100
1	B	243/288 (84%)	233 (96%)	10 (4%)	0	100	100
1	D	245/288 (85%)	235 (96%)	10 (4%)	0	100	100
2	C	241/288 (84%)	232 (96%)	9 (4%)	0	100	100
All	All	974/1152 (84%)	936 (96%)	38 (4%)	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	199/231 (86%)	199 (100%)	0	100	100
1	B	197/231 (85%)	195 (99%)	2 (1%)	76	88
1	D	199/231 (86%)	196 (98%)	3 (2%)	65	80
2	C	195/230 (85%)	195 (100%)	0	100	100
All	All	790/923 (86%)	785 (99%)	5 (1%)	86	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	164	VAL
1	B	229	ARG
1	D	51	GLU
1	D	216	GLU
1	D	229	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	B	65	ASN
1	B	179	HIS
2	C	175	ASN
2	C	186	GLN
1	D	67	ASN
1	D	166	GLN
1	D	175	ASN
1	D	186	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CSX	C	168	2	3,6,7	0.63	0	1,6,8	0.43	0

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	CSX	C	168	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	NAP	A	269	-	45,52,52	1.73	4 (8%)	56,80,80	1.07	2 (3%)
3	NAP	C	269	-	45,52,52	1.71	4 (8%)	56,80,80	1.03	1 (1%)
5	DTT	D	271	-	7,7,7	0.43	0	4,8,8	0.51	0
3	NAP	D	269	-	45,52,52	1.71	4 (8%)	56,80,80	1.05	1 (1%)
3	NAP	B	269	-	45,52,52	1.70	4 (8%)	56,80,80	1.06	2 (3%)
4	DX6	A	270	-	20,21,21	1.20	1 (5%)	18,29,29	1.39	2 (11%)
4	DX6	C	270	-	20,21,21	1.21	1 (5%)	18,29,29	1.42	2 (11%)
4	DX6	B	270	-	20,21,21	1.19	1 (5%)	18,29,29	1.39	2 (11%)

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	A	269	-	-	0/31/67/67	0/5/5/5
3	NAP	C	269	-	-	0/31/67/67	0/5/5/5
5	DTT	D	271	-	1/1/2/2	2/8/8/8	-
3	NAP	D	269	-	-	0/31/67/67	0/5/5/5
3	NAP	B	269	-	-	0/31/67/67	0/5/5/5
4	DX6	A	270	-	-	2/5/5/5	0/3/3/3
4	DX6	C	270	-	-	3/5/5/5	0/3/3/3
4	DX6	B	270	-	-	2/5/5/5	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	269	NAP	O7N-C7N	9.09	1.41	1.24
3	D	269	NAP	O7N-C7N	9.01	1.41	1.24
3	B	269	NAP	O7N-C7N	8.86	1.41	1.24
3	C	269	NAP	O7N-C7N	8.84	1.41	1.24
3	C	269	NAP	C2A-N3A	4.14	1.38	1.32
3	B	269	NAP	C2A-N3A	4.03	1.38	1.32
3	A	269	NAP	C2A-N3A	4.00	1.38	1.32
3	D	269	NAP	C2A-N3A	3.96	1.38	1.32
4	A	270	DX6	CAS-CAQ	-3.55	1.39	1.47
4	C	270	DX6	CAS-CAQ	-3.54	1.39	1.47
4	B	270	DX6	CAS-CAQ	-3.51	1.40	1.47
3	C	269	NAP	C2A-N1A	2.66	1.38	1.33
3	B	269	NAP	C2A-N1A	2.65	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	269	NAP	C2A-N1A	2.63	1.38	1.33
3	A	269	NAP	C2A-N1A	2.61	1.38	1.33
3	A	269	NAP	C2N-N1N	2.50	1.38	1.35
3	C	269	NAP	C2N-N1N	2.33	1.37	1.35
3	B	269	NAP	C2N-N1N	2.33	1.37	1.35
3	D	269	NAP	C2N-N1N	2.23	1.37	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	269	NAP	N3A-C2A-N1A	-5.67	119.81	128.68
3	D	269	NAP	N3A-C2A-N1A	-5.65	119.85	128.68
3	A	269	NAP	N3A-C2A-N1A	-5.65	119.86	128.68
3	C	269	NAP	N3A-C2A-N1A	-5.53	120.03	128.68
4	C	270	DX6	CAS-CAQ-NAM	3.95	118.71	115.36
4	A	270	DX6	CAS-CAQ-NAM	3.91	118.67	115.36
4	B	270	DX6	CAS-CAQ-NAM	3.85	118.62	115.36
4	C	270	DX6	CAO-NAM-CAQ	-3.13	119.33	125.10
4	B	270	DX6	CAO-NAM-CAQ	-3.13	119.33	125.10
4	A	270	DX6	CAO-NAM-CAQ	-3.10	119.38	125.10
3	B	269	NAP	C3N-C7N-N7N	2.17	120.35	117.75
3	A	269	NAP	C3D-C2D-C1D	2.07	104.10	100.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	271	DTT	C3

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	270	DX6	CAI-CAJ-CAP-CAH
4	C	270	DX6	CAI-CAJ-CAP-CAS
5	D	271	DTT	C2-C3-C4-S4
5	D	271	DTT	O3-C3-C4-S4
4	A	270	DX6	CAN-CAI-CAJ-CAP
4	B	270	DX6	CAN-CAI-CAJ-CAP
4	C	270	DX6	CAN-CAI-CAJ-CAP
4	A	270	DX6	CAI-CAJ-CAP-CAS
4	B	270	DX6	CAI-CAJ-CAP-CAS

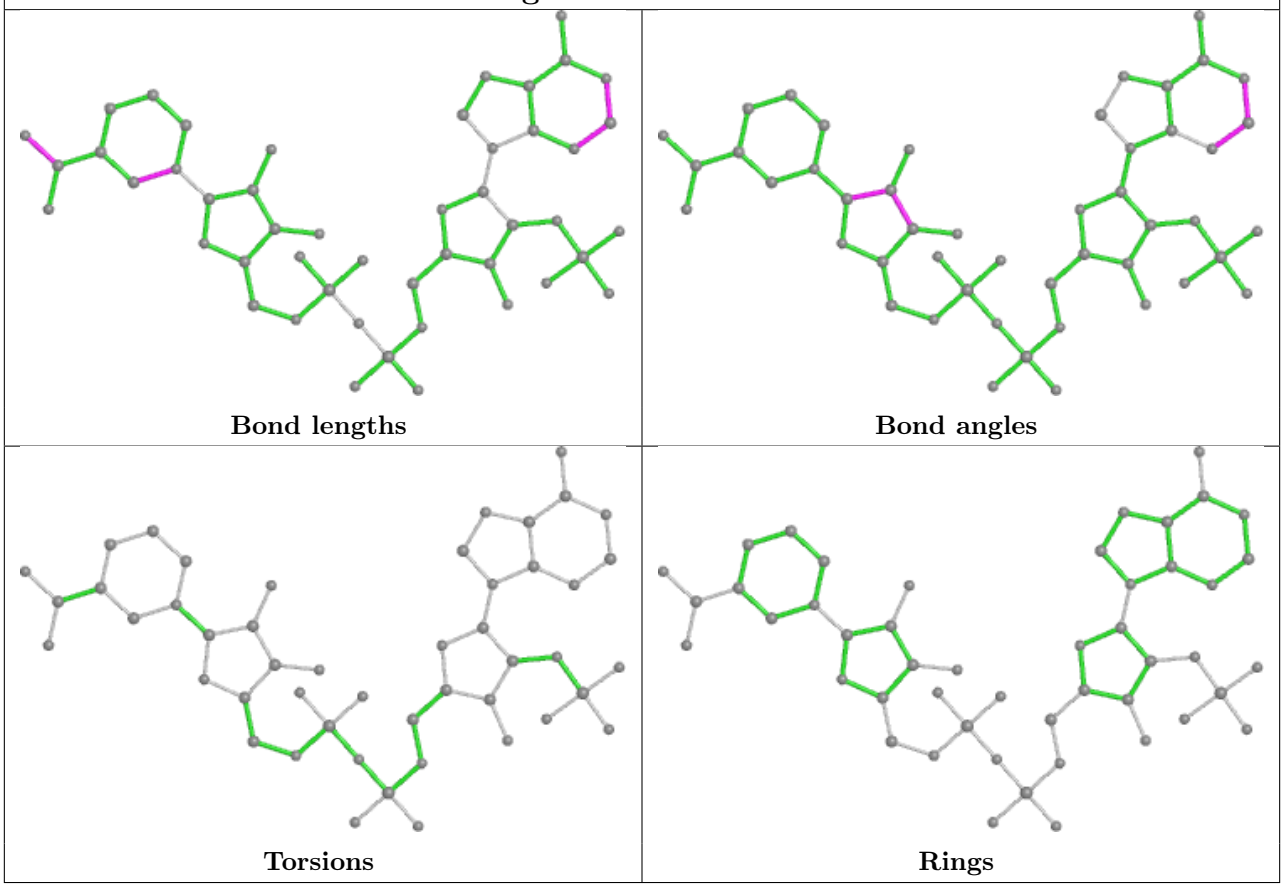
There are no ring outliers.

3 monomers are involved in 4 short contacts:

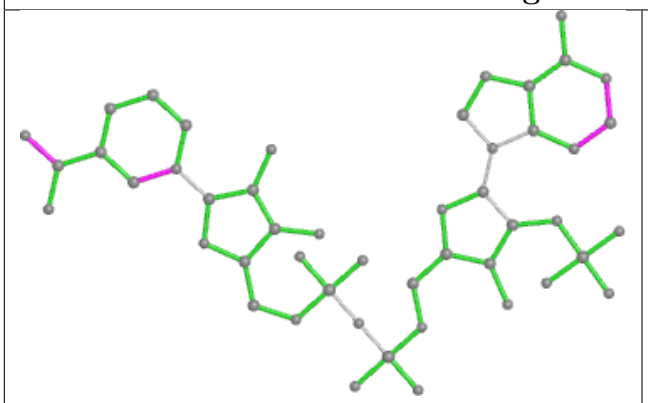
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	269	NAP	1	0
4	A	270	DX6	2	0
4	B	270	DX6	1	0

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.

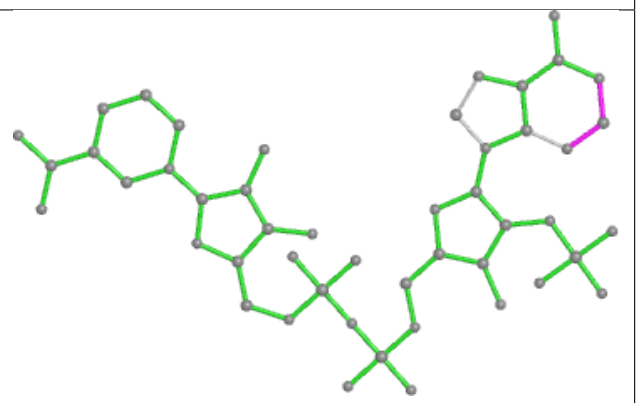
Ligand NAP A 269



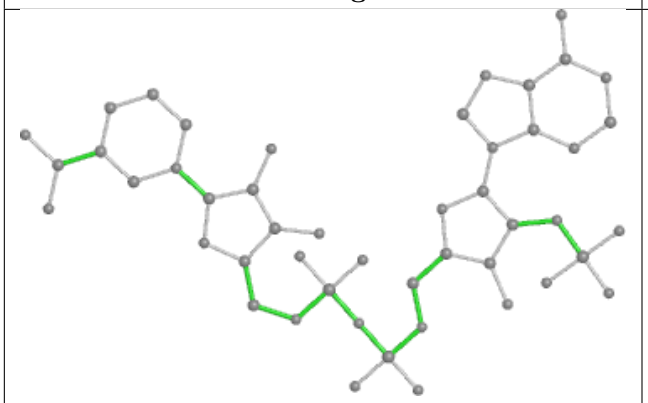
Ligand NAP C 269



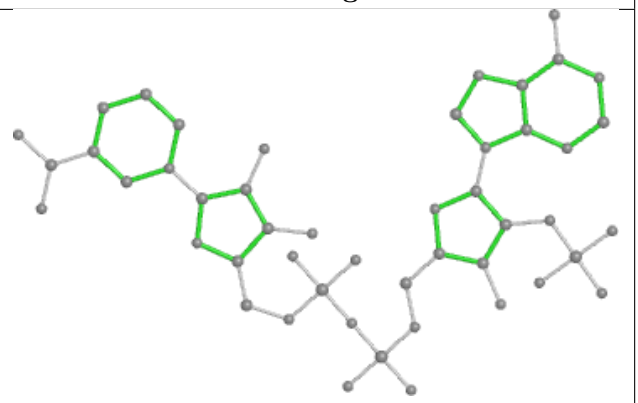
Bond lengths



Bond angles

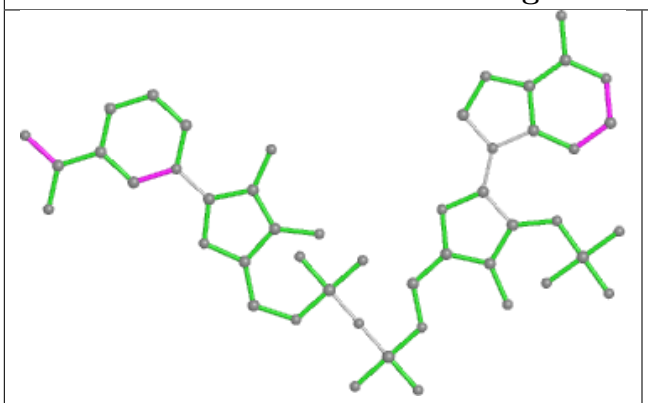


Torsions

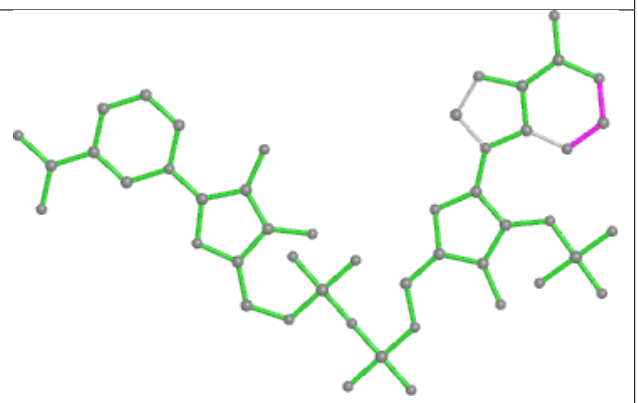


Rings

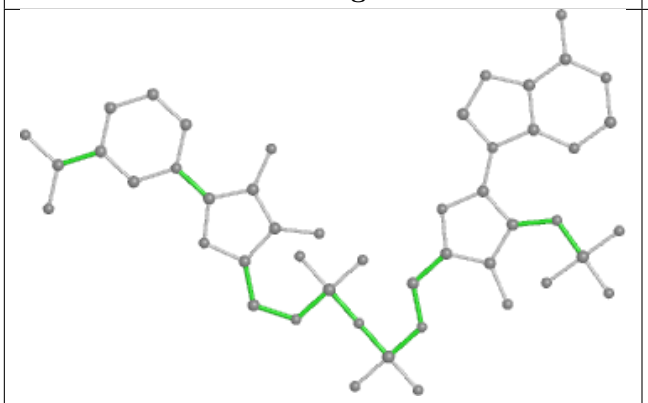
Ligand NAP D 269



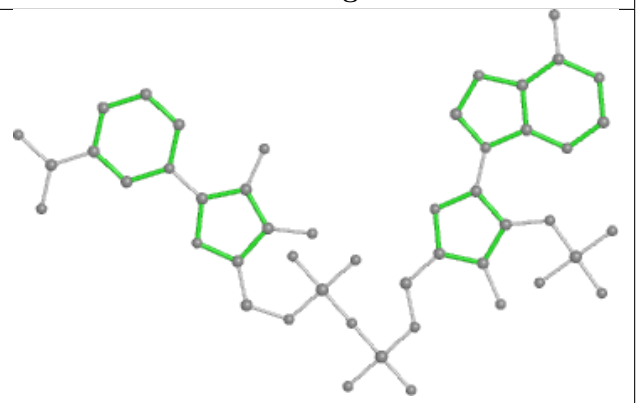
Bond lengths



Bond angles

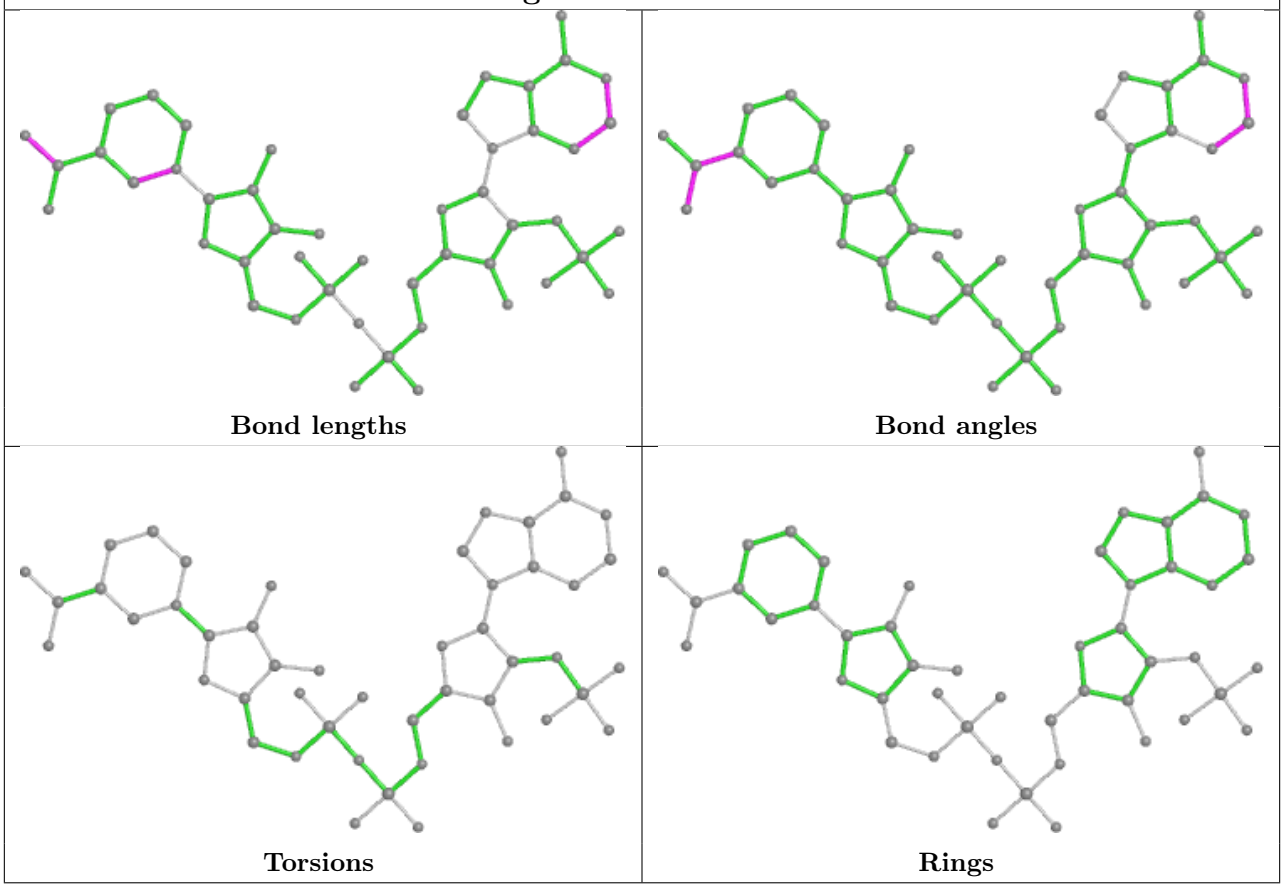


Torsions

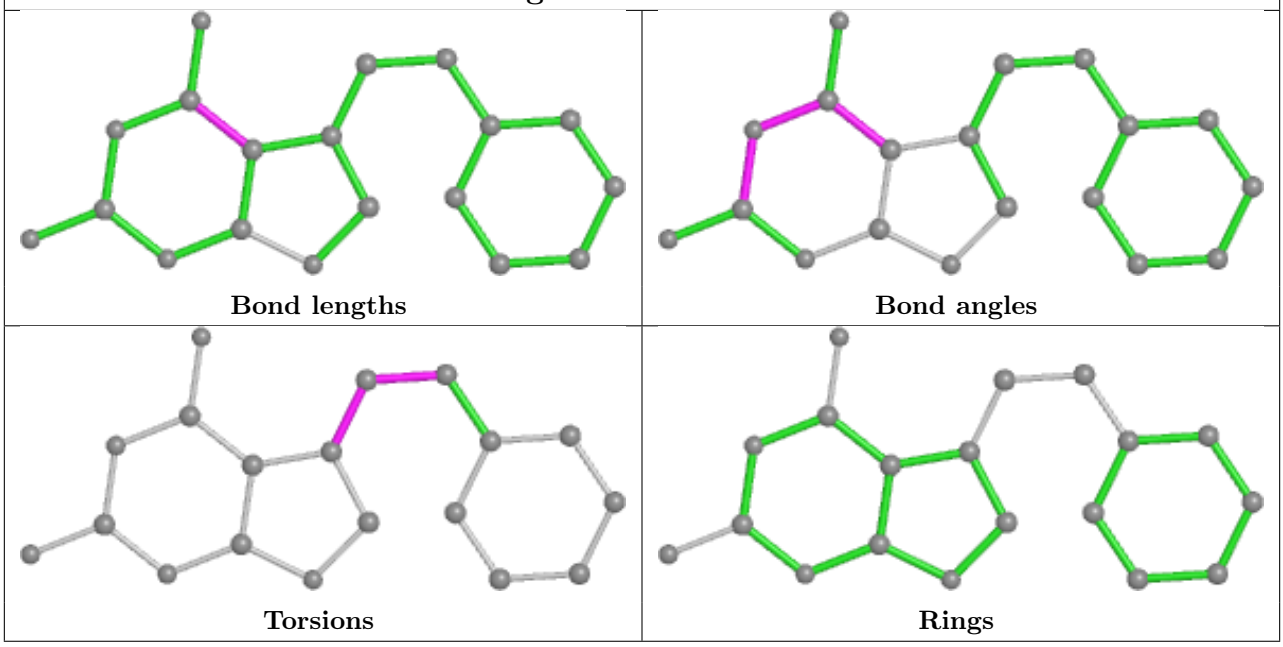


Rings

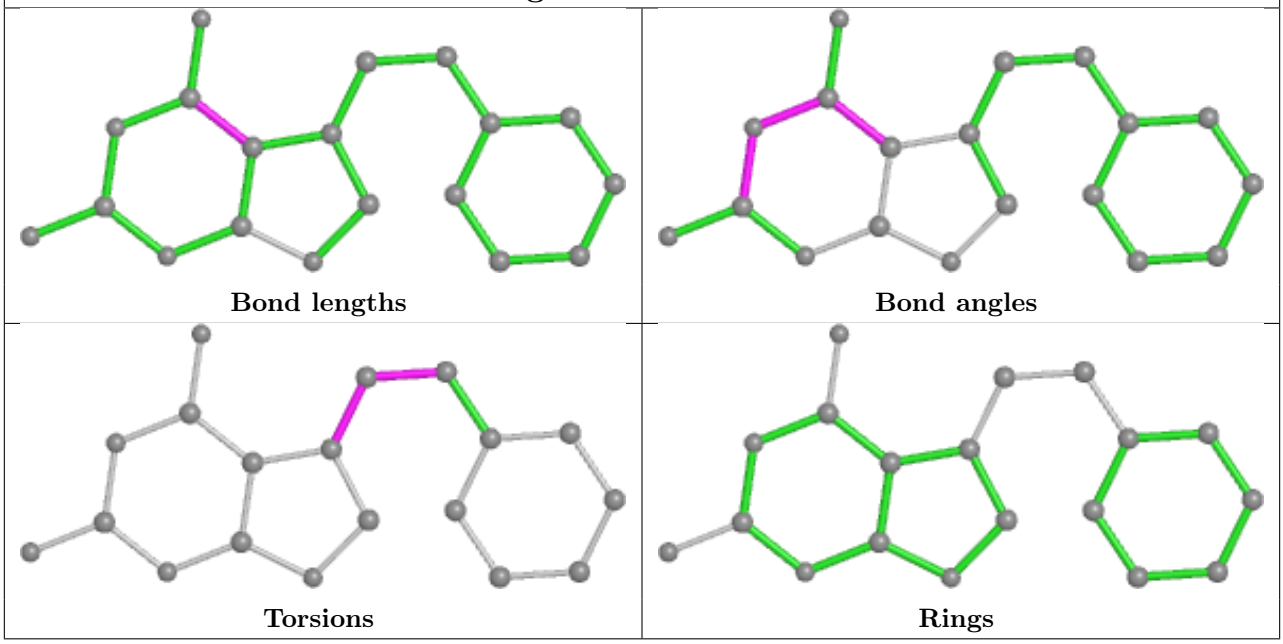
Ligand NAP B 269



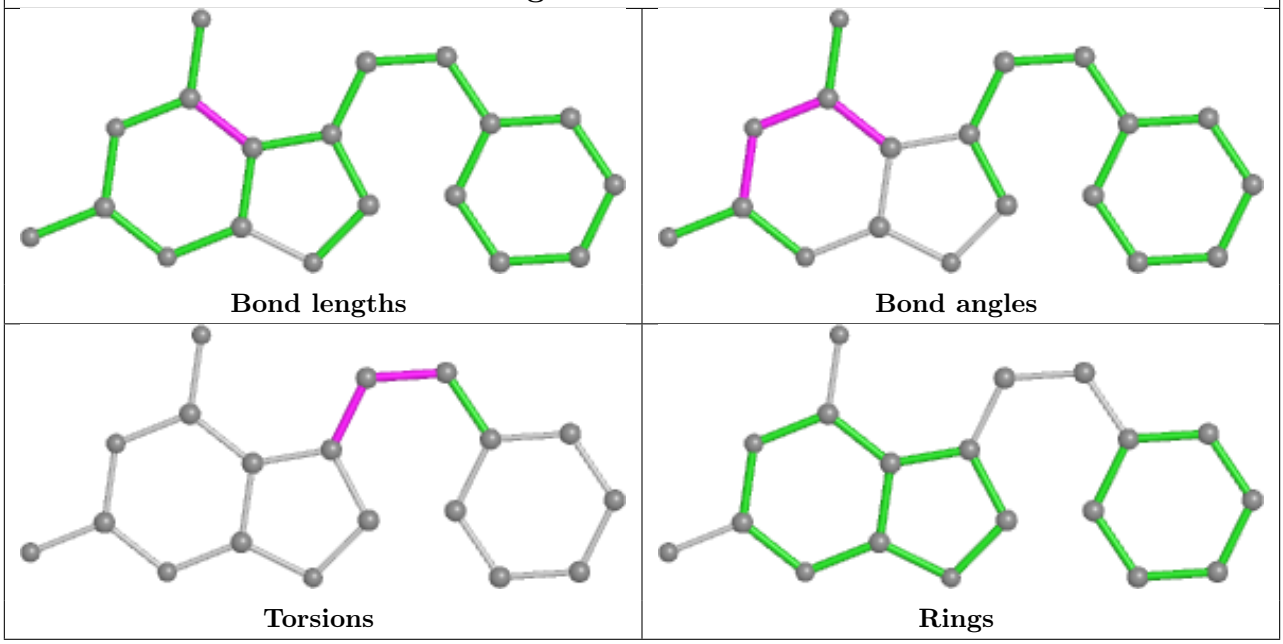
Ligand DX6 A 270



Ligand DX6 C 270



Ligand DX6 B 270



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	249/288 (86%)	-0.20	1 (0%)	92	91	2, 5, 20, 25	9 (3%)
1	B	248/288 (86%)	-0.23	3 (1%)	79	77	2, 4, 19, 27	5 (2%)
1	D	249/288 (86%)	-0.22	2 (0%)	86	84	2, 6, 21, 28	6 (2%)
2	C	247/288 (85%)	-0.13	7 (2%)	53	51	2, 5, 21, 35	5 (2%)
All	All	993/1152 (86%)	-0.19	13 (1%)	77	75	2, 5, 21, 35	25 (2%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	GLY	4.8
1	B	113	GLY	3.4
1	B	211	VAL	3.4
2	C	212	ALA	3.4
1	D	2	GLU	3.2
1	B	212	ALA	3.1
2	C	211	VAL	2.7
1	A	152	SER	2.5
2	C	217	GLU	2.4
2	C	163	MET	2.3
2	C	214	GLY	2.2
2	C	216	GLU	2.2
1	D	214	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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	CSX	C	168	7/8	0.94	0.11	3,5,6,7	1

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

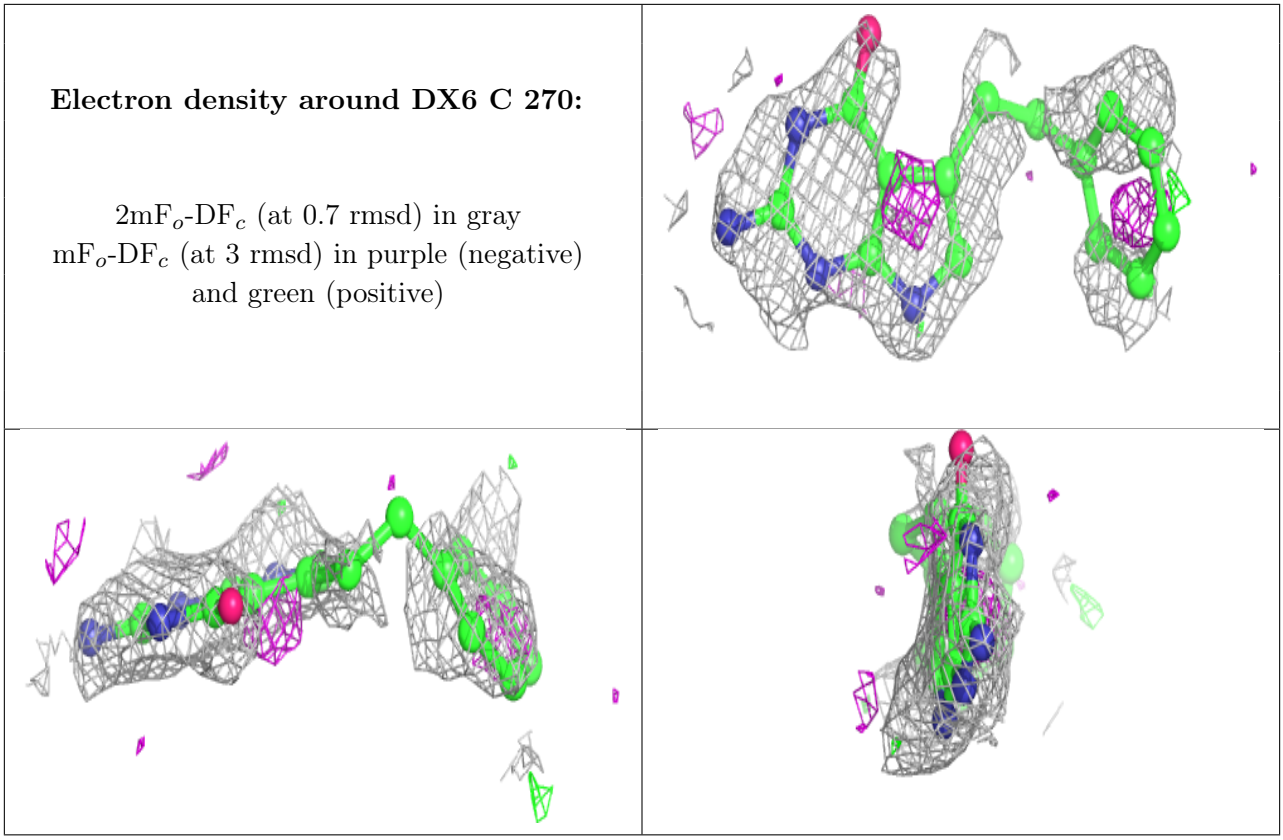
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DTT	D	271	8/8	0.66	0.37	83,84,85,85	0
4	DX6	C	270	19/19	0.72	0.32	41,42,48,48	0
4	DX6	A	270	19/19	0.84	0.24	24,25,36,36	0
4	DX6	B	270	19/19	0.87	0.25	25,26,39,39	0
3	NAP	C	269	48/48	0.94	0.17	5,13,17,22	0
3	NAP	A	269	48/48	0.97	0.13	2,3,6,8	0
3	NAP	D	269	48/48	0.97	0.13	2,5,8,11	0
3	NAP	B	269	48/48	0.97	0.11	2,2,7,9	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.

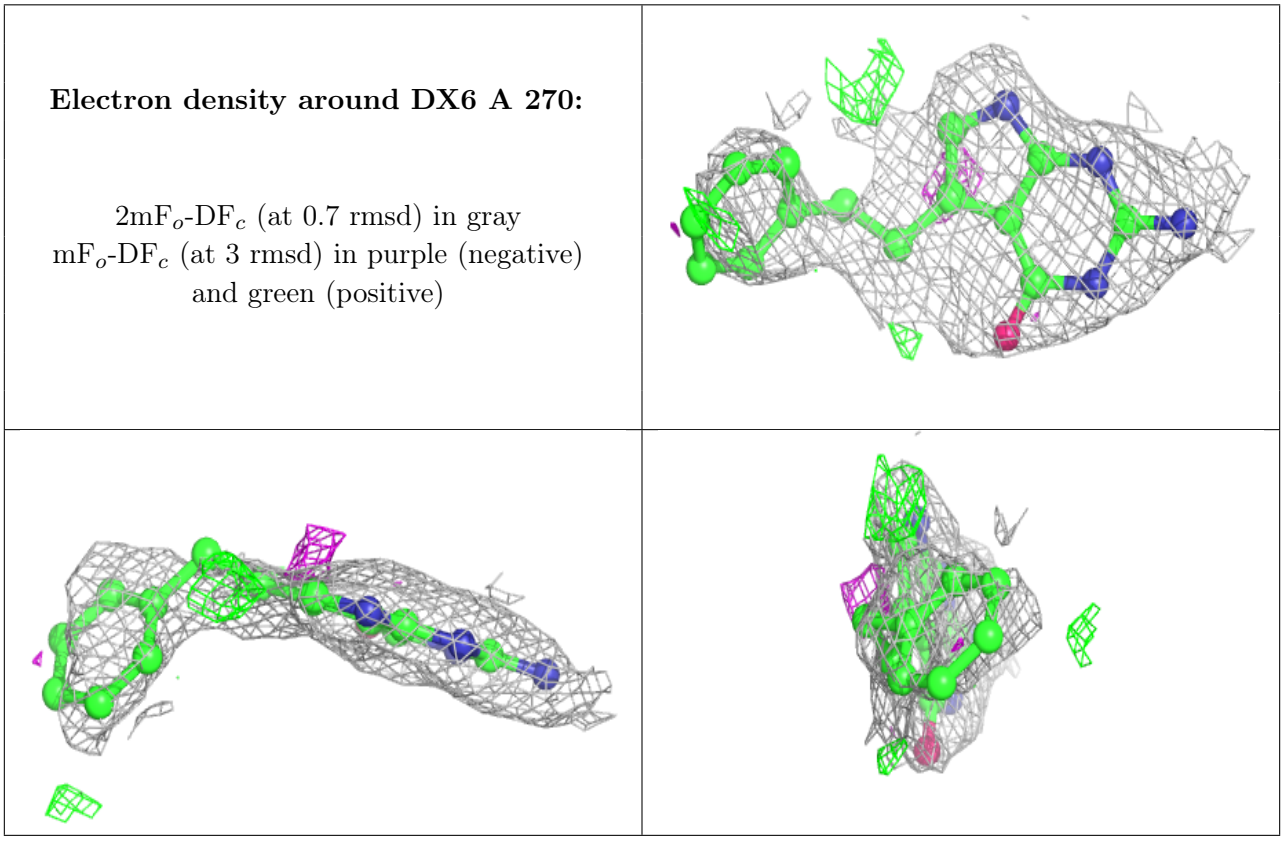
Electron density around DX6 C 270:

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



Electron density around DX6 A 270:

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



Electron density around DX6 B 270:

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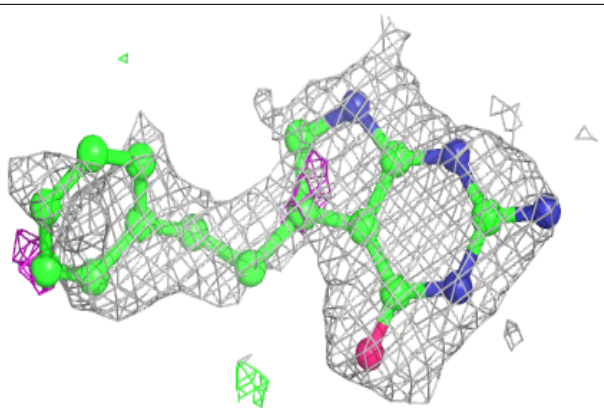
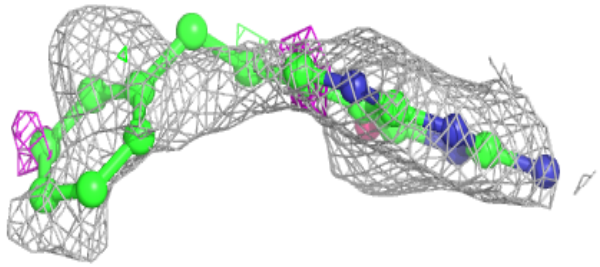
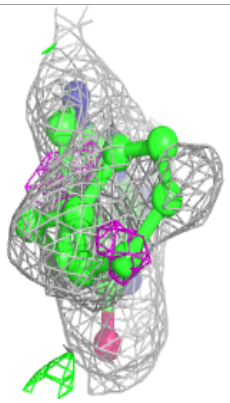
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

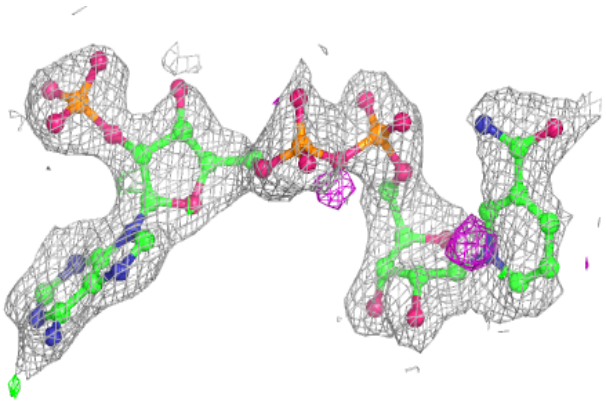


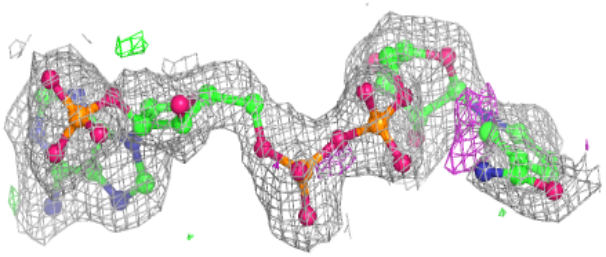


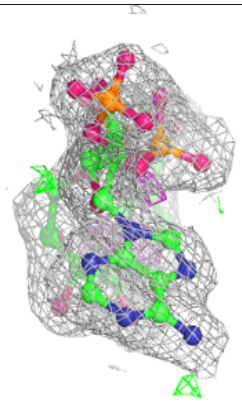


Electron density around NAP C 269:

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

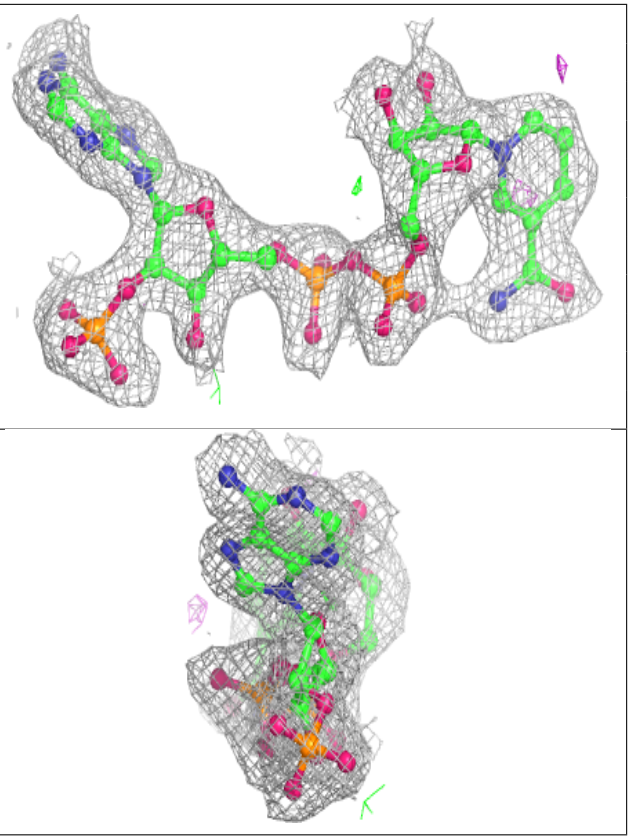


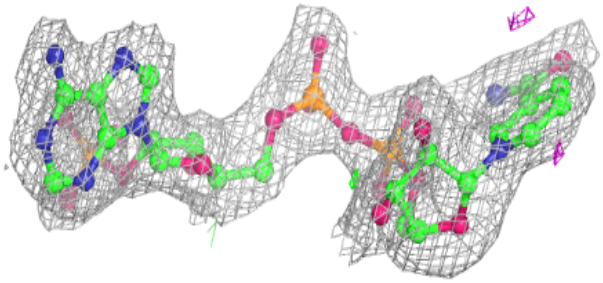




Electron density around NAP A 269:

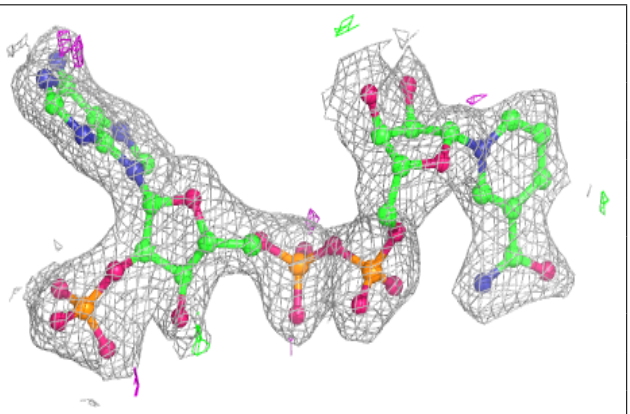
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

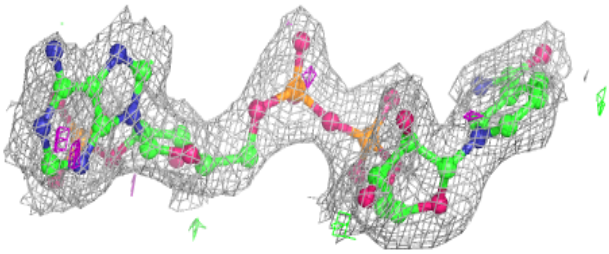


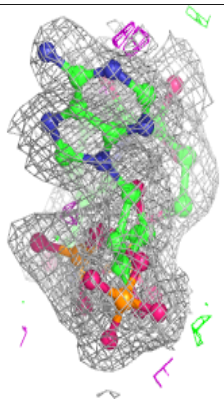


Electron density around NAP D 269:

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

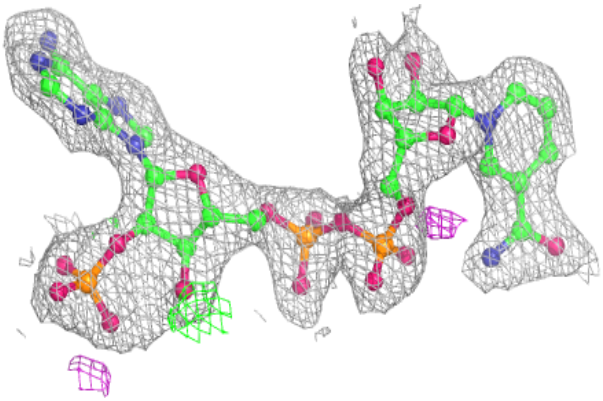


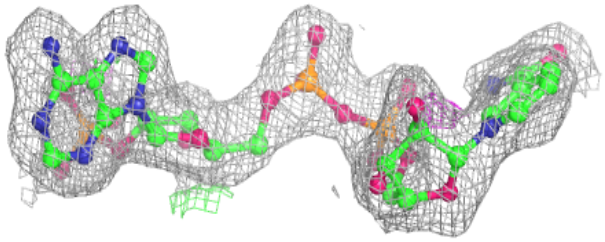


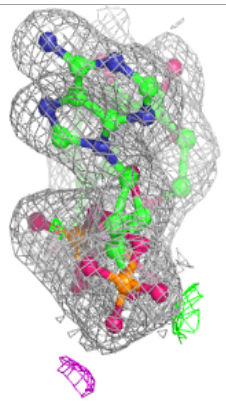


Electron density around NAP B 269:

$2mF_o$-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.