



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:28 am BST

PDB ID : 2BFP  
Title : Leishmania major pteridine reductase 1 in complex with NADP and tetrahydrobiopterin  
Authors : Schuettelkopf, A.W.; Hunter, W.N.  
Deposited on : 2004-12-10  
Resolution : 2.55 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](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

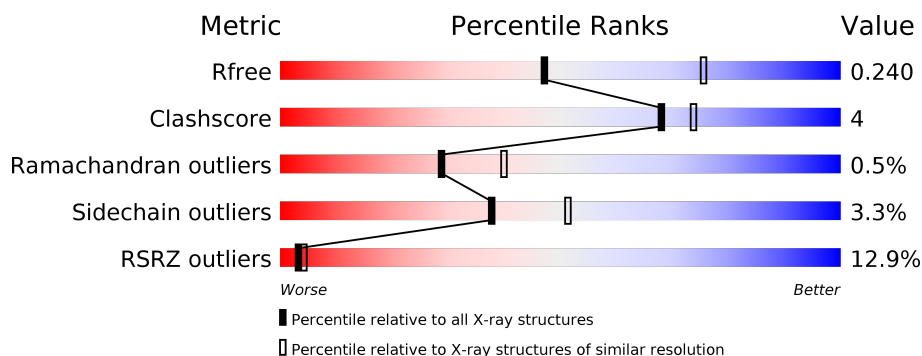
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	288	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 7%</div> </div> </div>
1	B	288	<div> <div>13%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 8%</div> </div> </div>
1	C	288	<div> <div>13%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>11%</div> </div> </div>
1	D	288	<div> <div>14%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>• 11%</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	1293	-	-	X	-

2 Entry composition ⓘ

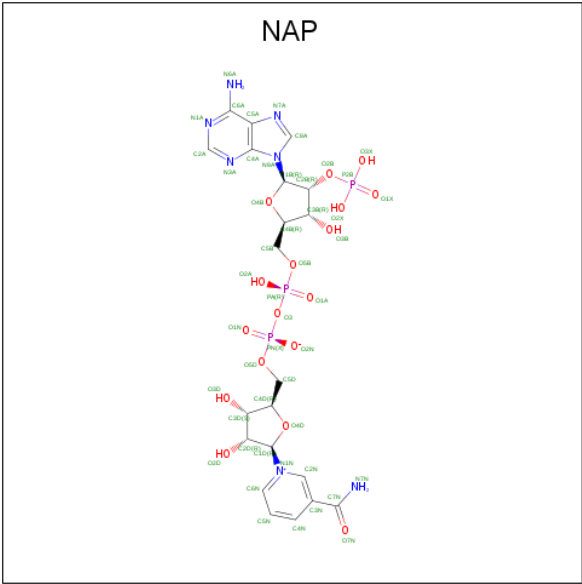
There are 5 unique types of molecules in this entry. The entry contains 8235 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	267	Total	C	N	O	S	0	0	0
			1992	1254	355	372	11			
1	B	266	Total	C	N	O	S	0	1	0
			1984	1251	350	371	12			
1	C	256	Total	C	N	O	S	0	1	0
			1910	1204	342	353	11			
1	D	257	Total	C	N	O	S	0	0	0
			1913	1206	343	354	10			

- Molecule 2 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>).



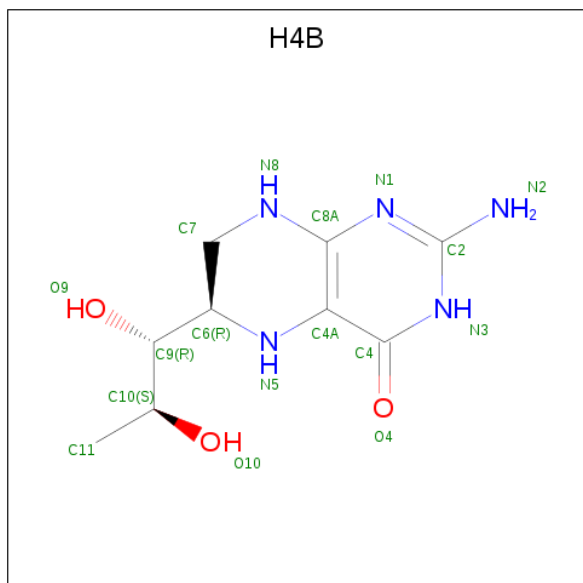
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	B	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

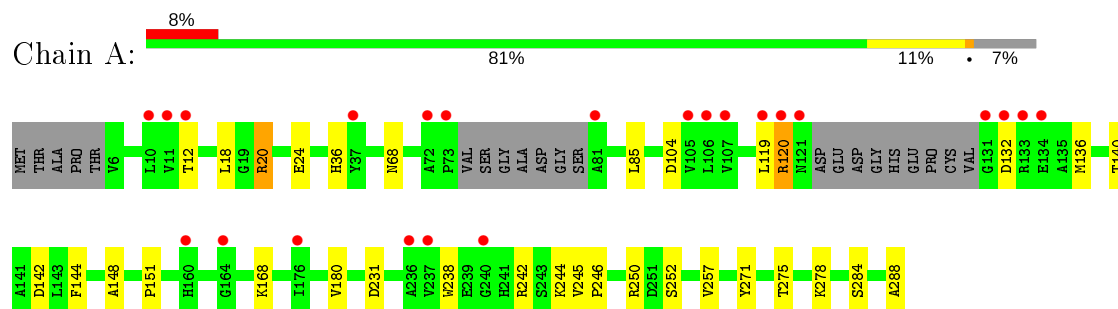
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	44	Total O 44 44	0	0
5	B	35	Total O 35 35	0	0
5	C	42	Total O 42 42	0	0
5	D	31	Total O 31 31	0	0

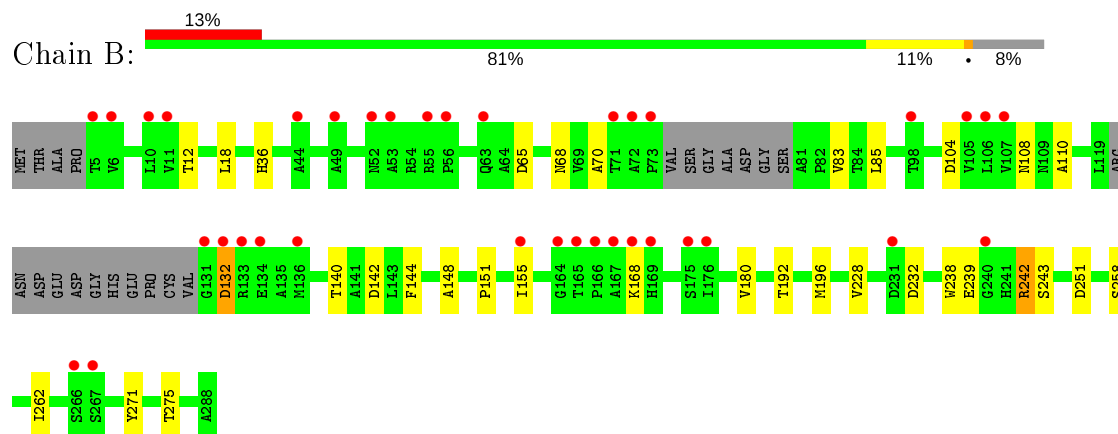
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

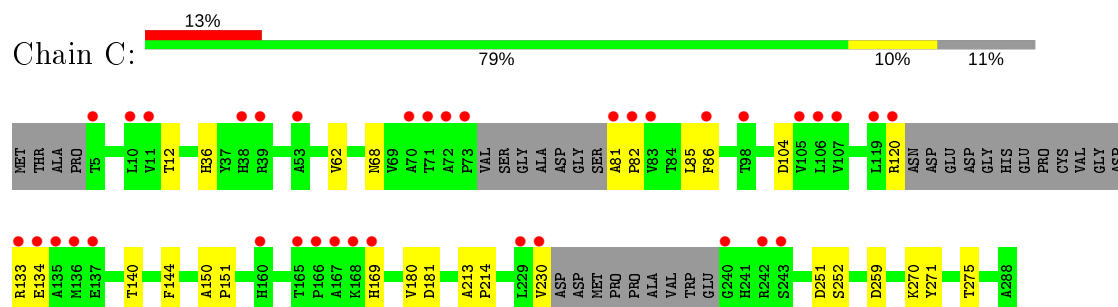
#### • Molecule 1: PTERIDINE REDUCTASE 1



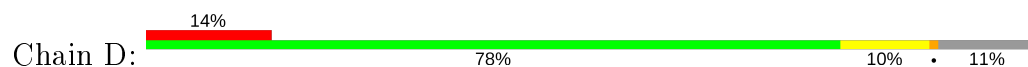
#### • Molecule 1: PTERIDINE REDUCTASE 1

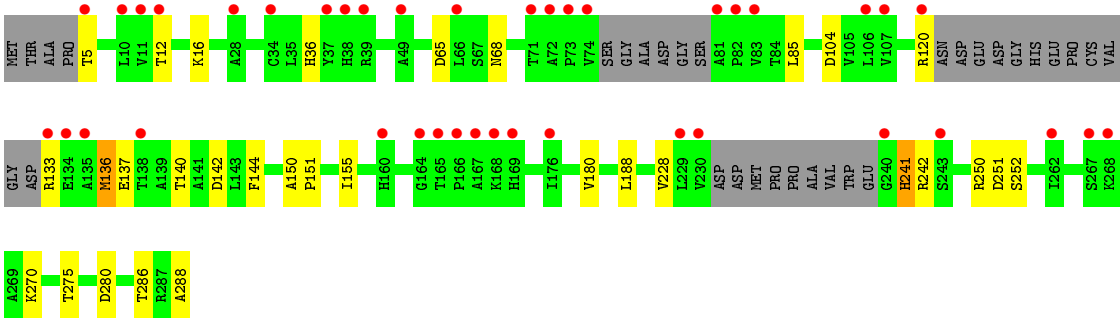


#### • Molecule 1: PTERIDINE REDUCTASE 1



#### • Molecule 1: PTERIDINE REDUCTASE 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.10Å 103.57Å 137.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.50 – 2.55 24.99 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.50-2.55) 97.7 (24.99-2.55)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.72 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.198 , 0.238 0.205 , 0.240	Depositor DCC
$R_{free}$ test set	2185 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8235	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	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 31.33 % 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 1.1269e-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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, H4B, EDO

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	0.44	0/2031	0.80	4/2766 (0.1%)
1	B	0.44	0/2027	0.83	6/2761 (0.2%)
1	C	0.43	0/1948	0.80	4/2648 (0.2%)
1	D	0.43	0/1947	0.80	5/2648 (0.2%)
All	All	0.43	0/7953	0.81	19/10823 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	251	ASP	CB-CG-OD2	7.29	124.87	118.30
1	C	104	ASP	CB-CG-OD2	7.23	124.81	118.30
1	D	65	ASP	CB-CG-OD2	7.21	124.79	118.30
1	B	104	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	251	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	142	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	104	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	132	ASP	CB-CG-OD2	5.65	123.38	118.30
1	D	104	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	232	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	259	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	132	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	142	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	65	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	181	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	231	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	142	ASP	CB-CG-OD2	5.17	122.96	118.30
1	D	280	ASP	CB-CG-OD2	5.17	122.96	118.30
1	C	251	ASP	CB-CG-OD2	5.10	122.89	118.30

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	1992	0	1996	17	0
1	B	1984	0	1989	19	0
1	C	1910	0	1933	9	0
1	D	1913	0	1937	14	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
2	C	48	0	25	2	0
2	D	48	0	25	2	0
3	A	17	0	15	2	0
3	B	17	0	15	2	0
3	C	17	0	15	2	0
3	D	17	0	15	2	0
4	B	12	0	18	7	0
4	C	4	0	6	0	0
4	D	8	0	12	0	0
5	A	44	0	0	1	0
5	B	35	0	0	1	0
5	C	42	0	0	0	0
5	D	31	0	0	0	0
All	All	8235	0	8051	61	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 4.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:HB3	4:B:1293:EDO:H12	1.29	1.12
1:B:151:PRO:HG3	4:B:1293:EDO:H11	1.22	1.11
1:D:241:HIS:H	1:D:241:HIS:CD2	1.88	0.87
2:D:1289:NAP:C4N	3:D:1290:H4B:H6	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:PRO:HG3	4:B:1293:EDO:C1	2.06	0.84
1:A:278:LYS:HE2	1:A:284:SER:OG	1.81	0.80
1:B:108:ASN:CB	4:B:1293:EDO:H12	2.12	0.79
1:D:12:THR:HA	1:D:36:HIS:HB3	1.65	0.79
2:C:1289:NAP:C4N	3:C:1290:H4B:H6	2.16	0.75
2:A:1289:NAP:C4N	3:A:1290:H4B:H6	2.18	0.74
2:B:1289:NAP:C4N	3:B:1290:H4B:H6	2.18	0.73
1:C:12:THR:HA	1:C:36:HIS:HB3	1.71	0.73
1:D:242:ARG:HG2	1:D:250:ARG:HA	1.73	0.71
2:D:1289:NAP:H4N	3:D:1290:H4B:H6	1.72	0.70
1:D:241:HIS:HD2	1:D:241:HIS:H	1.39	0.70
1:B:151:PRO:CG	4:B:1293:EDO:H11	2.13	0.69
1:B:12:THR:HA	1:B:36:HIS:HB3	1.72	0.69
1:A:242:ARG:HB2	1:A:250:ARG:HA	1.74	0.69
1:B:12:THR:OG1	4:B:1293:EDO:H21	2.02	0.60
1:A:238:TRP:O	1:A:242:ARG:HG2	2.03	0.59
2:C:1289:NAP:H4N	3:C:1290:H4B:H6	1.84	0.57
1:A:136:MET:HG2	5:B:2004:HOH:O	2.06	0.55
1:A:271:TYR:CE2	1:C:252:SER:HB3	2.42	0.54
1:B:238:TRP:O	1:B:242:ARG:HG3	2.08	0.53
2:B:1289:NAP:H4N	3:B:1290:H4B:H6	1.91	0.52
1:A:18:LEU:HD13	1:A:257:VAL:HG11	1.93	0.50
1:A:288:ALA:HB2	1:D:286:THR:HB	1.94	0.50
1:B:271:TYR:CE2	1:D:252:SER:HB3	2.46	0.50
1:A:148:ALA:C	1:A:151:PRO:HD2	2.33	0.48
1:B:192:THR:O	1:B:196:MET:HG3	2.13	0.48
2:A:1289:NAP:H4N	3:A:1290:H4B:H6	1.95	0.48
1:B:140:THR:O	1:B:144:PHE:HB2	2.13	0.47
1:B:110:ALA:O	4:B:1293:EDO:O1	2.27	0.47
1:A:12:THR:HA	1:A:36:HIS:HB3	1.95	0.47
1:D:150:ALA:HB3	1:D:151:PRO:HD3	1.96	0.47
1:B:68:ASN:HA	1:B:85:LEU:HD22	1.97	0.47
1:A:252:SER:HB3	1:C:271:TYR:CE2	2.50	0.46
1:C:150:ALA:HB3	1:C:151:PRO:HD3	1.98	0.46
1:C:140:THR:O	1:C:144:PHE:HB2	2.16	0.46
1:A:20:ARG:HD3	1:A:24:GLU:OE2	2.17	0.45
1:B:258:SER:O	1:B:262:ILE:HD13	2.16	0.45
1:A:140:THR:O	1:A:144:PHE:HB2	2.17	0.45
1:D:151:PRO:O	1:D:155:ILE:HG13	2.17	0.45
1:C:81:ALA:HA	1:C:82:PRO:HD3	1.87	0.44
1:B:239:GLU:O	1:B:243:SER:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:PHE:CD2	1:D:136:MET:HE1	2.54	0.43
1:C:213:ALA:N	1:C:214:PRO:CD	2.82	0.43
1:D:68:ASN:HA	1:D:85:LEU:HD22	2.01	0.43
1:D:140:THR:O	1:D:144:PHE:HB2	2.19	0.42
1:A:120:ARG:HG2	1:A:120:ARG:H	1.37	0.42
1:D:241:HIS:N	1:D:241:HIS:CD2	2.68	0.42
1:A:68:ASN:HA	1:A:85:LEU:HD22	2.01	0.42
1:A:244:LYS:HD2	1:D:288:ALA:O	2.20	0.41
1:B:148:ALA:C	1:B:151:PRO:HD2	2.40	0.41
1:B:18:LEU:HB2	2:B:1289:NAP:H51N	2.01	0.41
1:B:70:ALA:HA	1:B:83:VAL:O	2.20	0.41
1:C:68:ASN:HA	1:C:85:LEU:HD22	2.03	0.41
1:A:244:LYS:HA	1:A:244:LYS:HD3	1.97	0.40
5:A:2043:HOH:O	1:D:188:LEU:HD22	2.21	0.40
1:A:245:VAL:HA	1:A:246:PRO:HD3	1.98	0.40
1:B:151:PRO:O	1:B:155:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	261/288 (91%)	246 (94%)	14 (5%)	1 (0%)	34	46
1	B	261/288 (91%)	250 (96%)	9 (3%)	2 (1%)	19	27
1	C	249/288 (86%)	237 (95%)	11 (4%)	1 (0%)	34	46
1	D	249/288 (86%)	237 (95%)	11 (4%)	1 (0%)	34	46
All	All	1020/1152 (88%)	970 (95%)	45 (4%)	5 (0%)	29	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	VAL
1	B	132	ASP
1	B	180	VAL
1	C	180	VAL
1	D	180	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	207/223 (93%)	202 (98%)	5 (2%)	49	64
1	B	207/223 (93%)	203 (98%)	4 (2%)	57	72
1	C	199/223 (89%)	191 (96%)	8 (4%)	31	43
1	D	199/223 (89%)	189 (95%)	10 (5%)	24	33
All	All	812/892 (91%)	785 (97%)	27 (3%)	38	51

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	119	LEU
1	A	120	ARG
1	A	168	LYS
1	A	275	THR
1	B	168	LYS
1	B	228	VAL
1	B	242	ARG
1	B	275	THR
1	C	62	VAL
1	C	120	ARG
1	C	133	ARG
1	C	134	GLU
1	C	169	HIS
1	C	230	VAL
1	C	270	LYS
1	C	275	THR

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Mol	Chain	Res	Type
1	D	5	THR
1	D	16	LYS
1	D	120	ARG
1	D	133	ARG
1	D	136	MET
1	D	137	GLU
1	D	228	VAL
1	D	241	HIS
1	D	270	LYS
1	D	275	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	216	GLN
1	B	216	GLN
1	C	216	GLN
1	D	216	GLN
1	D	241	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

14 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
4	EDO	D	1292	-	3,3,3	0.29	0	2,2,2	0.25	0
2	NAP	C	1289	-	45,52,52	1.70	4 (8%)	56,80,80	1.38	5 (8%)
2	NAP	B	1289	-	45,52,52	1.57	3 (6%)	56,80,80	1.29	5 (8%)
3	H4B	C	1290	-	16,18,18	1.80	4 (25%)	11,26,26	4.42	8 (72%)
2	NAP	A	1289	-	45,52,52	1.60	4 (8%)	56,80,80	1.33	4 (7%)
4	EDO	C	1291	-	3,3,3	0.32	0	2,2,2	0.24	0
4	EDO	B	1292	-	3,3,3	0.34	0	2,2,2	0.09	0
3	H4B	A	1290	-	16,18,18	1.90	3 (18%)	11,26,26	3.84	8 (72%)
4	EDO	B	1293	-	3,3,3	0.35	0	2,2,2	0.49	0
3	H4B	D	1290	-	16,18,18	1.94	4 (25%)	11,26,26	3.87	8 (72%)
4	EDO	B	1291	-	3,3,3	0.31	0	2,2,2	0.59	0
4	EDO	D	1291	-	3,3,3	0.26	0	2,2,2	0.37	0
3	H4B	B	1290	-	16,18,18	1.92	4 (25%)	11,26,26	3.89	8 (72%)
2	NAP	D	1289	-	45,52,52	1.61	2 (4%)	56,80,80	1.30	5 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	1292	-	-	1/1/1/1	-
2	NAP	C	1289	-	-	0/31/67/67	0/5/5/5
2	NAP	B	1289	-	-	4/31/67/67	0/5/5/5
3	H4B	C	1290	-	-	4/8/17/17	0/2/2/2
2	NAP	A	1289	-	-	1/31/67/67	0/5/5/5
4	EDO	C	1291	-	-	1/1/1/1	-
4	EDO	B	1292	-	-	1/1/1/1	-
3	H4B	A	1290	-	-	2/8/17/17	0/2/2/2
4	EDO	B	1293	-	-	0/1/1/1	-
3	H4B	D	1290	-	-	2/8/17/17	0/2/2/2
4	EDO	B	1291	-	-	0/1/1/1	-
4	EDO	D	1291	-	-	0/1/1/1	-
3	H4B	B	1290	-	-	1/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	D	1289	-	-	2/31/67/67	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1289	NAP	O7N-C7N	8.67	1.40	1.24
2	A	1289	NAP	O7N-C7N	8.53	1.40	1.24
2	D	1289	NAP	O7N-C7N	8.48	1.40	1.24
2	B	1289	NAP	O7N-C7N	8.33	1.40	1.24
3	D	1290	H4B	C4-N3	4.65	1.41	1.33
3	C	1290	H4B	C4-N3	4.56	1.41	1.33
3	B	1290	H4B	C4-N3	4.47	1.40	1.33
3	A	1290	H4B	C4-N3	4.45	1.40	1.33
2	C	1289	NAP	C2A-N3A	4.13	1.38	1.32
3	A	1290	H4B	C4A-N5	4.12	1.46	1.38
3	B	1290	H4B	C4A-N5	4.08	1.46	1.38
2	D	1289	NAP	C2A-N3A	3.95	1.38	1.32
3	D	1290	H4B	C4A-N5	3.90	1.46	1.38
3	C	1290	H4B	C4A-N5	3.46	1.45	1.38
3	D	1290	H4B	C6-N5	3.34	1.52	1.45
3	B	1290	H4B	C6-N5	3.29	1.52	1.45
3	A	1290	H4B	C6-N5	3.21	1.52	1.45
2	B	1289	NAP	C2A-N3A	3.10	1.37	1.32
2	A	1289	NAP	C2A-N3A	3.07	1.37	1.32
2	C	1289	NAP	C2N-N1N	2.83	1.38	1.35
3	C	1290	H4B	C6-N5	2.81	1.51	1.45
2	C	1289	NAP	C2A-N1A	2.50	1.38	1.33
2	A	1289	NAP	C2N-N1N	2.41	1.37	1.35
2	A	1289	NAP	C2A-N1A	2.38	1.38	1.33
3	C	1290	H4B	C4A-C8A	-2.29	1.37	1.41
2	B	1289	NAP	C2A-N1A	2.24	1.38	1.33
3	D	1290	H4B	C4A-C8A	-2.15	1.37	1.41
3	B	1290	H4B	C8A-N1	2.02	1.38	1.34

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1290	H4B	C4-C4A-C8A	9.40	122.92	114.57
3	D	1290	H4B	C4-C4A-C8A	8.44	122.07	114.57
3	B	1290	H4B	C4-C4A-C8A	8.26	121.91	114.57
3	A	1290	H4B	C4-C4A-C8A	8.09	121.75	114.57
2	D	1289	NAP	N3A-C2A-N1A	-6.03	119.25	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1289	NAP	N3A-C2A-N1A	-5.64	119.87	128.68
3	C	1290	H4B	C4-C4A-N5	-5.52	114.49	119.12
2	B	1289	NAP	N3A-C2A-N1A	-5.52	120.05	128.68
3	A	1290	H4B	C4-N3-C2	5.24	124.25	115.93
2	C	1289	NAP	C3N-C7N-N7N	5.23	124.03	117.75
3	C	1290	H4B	C4-N3-C2	5.10	124.04	115.93
2	C	1289	NAP	N3A-C2A-N1A	-5.09	120.73	128.68
3	C	1290	H4B	N3-C2-N1	-4.92	117.71	125.42
3	B	1290	H4B	C4-N3-C2	4.82	123.59	115.93
3	D	1290	H4B	C4-N3-C2	4.52	123.11	115.93
3	A	1290	H4B	N3-C2-N1	-4.49	118.38	125.42
3	D	1290	H4B	N3-C2-N1	-4.47	118.40	125.42
3	B	1290	H4B	N3-C2-N1	-4.41	118.51	125.42
2	A	1289	NAP	C3N-C7N-N7N	4.14	122.72	117.75
3	D	1290	H4B	C2-N1-C8A	3.92	123.33	114.54
3	B	1290	H4B	N2-C2-N1	3.83	123.22	117.25
3	C	1290	H4B	C2-N1-C8A	3.79	123.05	114.54
3	A	1290	H4B	C2-N1-C8A	3.69	122.82	114.54
3	B	1290	H4B	C2-N1-C8A	3.56	122.52	114.54
2	D	1289	NAP	C3N-C7N-N7N	3.51	121.97	117.75
3	B	1290	H4B	C4-C4A-N5	-3.40	116.27	119.12
3	C	1290	H4B	C4A-C4-N3	-3.33	114.54	124.01
3	A	1290	H4B	C4A-C4-N3	-3.30	114.64	124.01
2	C	1289	NAP	O7N-C7N-N7N	-3.13	118.13	122.58
3	D	1290	H4B	C4-C4A-N5	-3.11	116.52	119.12
3	C	1290	H4B	N2-C2-N1	3.05	122.00	117.25
2	B	1289	NAP	C3N-C7N-N7N	3.02	121.38	117.75
3	D	1290	H4B	C4A-C4-N3	-3.01	115.46	124.01
3	B	1290	H4B	C4A-C4-N3	-3.00	115.49	124.01
3	A	1290	H4B	N2-C2-N1	2.97	121.88	117.25
2	B	1289	NAP	C3N-C2N-N1N	-2.84	117.65	120.43
3	D	1290	H4B	N2-C2-N1	2.82	121.64	117.25
2	D	1289	NAP	C1B-N9A-C4A	-2.64	122.00	126.64
2	A	1289	NAP	O7N-C7N-C3N	-2.63	116.49	119.63
2	D	1289	NAP	O7N-C7N-N7N	-2.62	118.85	122.58
3	B	1290	H4B	C4A-N5-C6	-2.61	114.07	121.16
2	D	1289	NAP	C4A-C5A-N7A	-2.60	106.69	109.40
2	C	1289	NAP	PN-O3-PA	-2.49	124.29	132.83
3	C	1290	H4B	C4A-N5-C6	-2.41	114.60	121.16
3	A	1290	H4B	C4-C4A-N5	-2.41	117.10	119.12
3	A	1290	H4B	C4A-N5-C6	-2.35	114.77	121.16
2	C	1289	NAP	C4A-C5A-N7A	-2.32	106.98	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1289	NAP	C1B-N9A-C4A	-2.22	122.73	126.64
3	D	1290	H4B	C4A-N5-C6	-2.20	115.19	121.16
2	A	1289	NAP	PN-O3-PA	-2.05	125.78	132.83
2	B	1289	NAP	PN-O3-PA	-2.00	125.96	132.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1290	H4B	C11-C10-C9-C6
3	C	1290	H4B	O10-C10-C9-C6
3	C	1290	H4B	C11-C10-C9-O9
3	C	1290	H4B	O10-C10-C9-O9
2	D	1289	NAP	C5B-O5B-PA-O3
3	D	1290	H4B	C11-C10-C9-C6
2	B	1289	NAP	C5B-O5B-PA-O3
2	B	1289	NAP	C5B-O5B-PA-O2A
2	D	1289	NAP	C5B-O5B-PA-O2A
3	A	1290	H4B	C11-C10-C9-C6
3	B	1290	H4B	C11-C10-C9-C6
3	D	1290	H4B	C11-C10-C9-O9
4	B	1292	EDO	O1-C1-C2-O2
4	D	1292	EDO	O1-C1-C2-O2
2	B	1289	NAP	O4B-C4B-C5B-O5B
4	C	1291	EDO	O1-C1-C2-O2
2	A	1289	NAP	C5B-O5B-PA-O3
3	A	1290	H4B	N5-C6-C9-C10
2	B	1289	NAP	C5B-O5B-PA-O1A

There are no ring outliers.

9 monomers are involved in 16 short contacts:

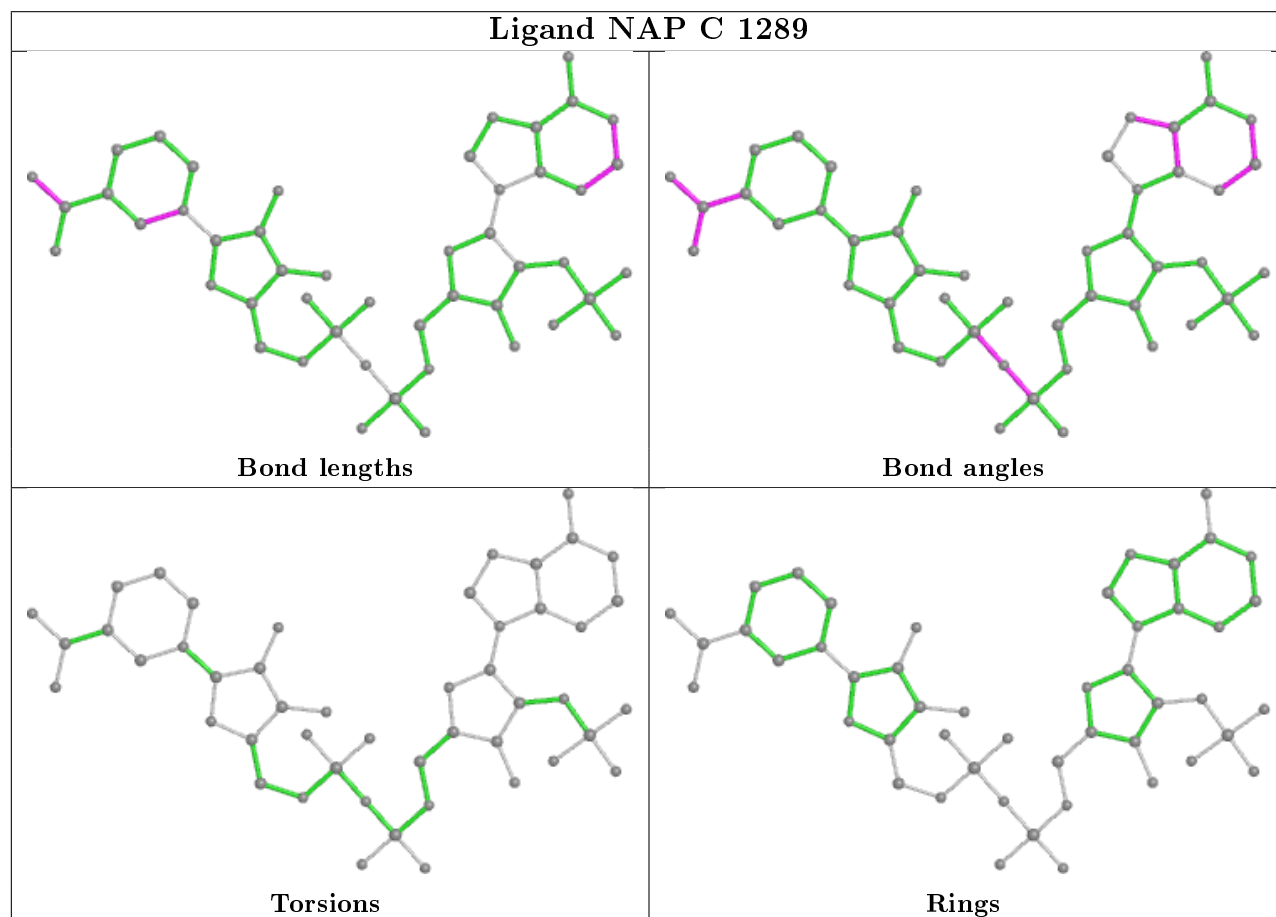
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1289	NAP	2	0
2	B	1289	NAP	3	0
3	C	1290	H4B	2	0
2	A	1289	NAP	2	0
3	A	1290	H4B	2	0
4	B	1293	EDO	7	0
3	D	1290	H4B	2	0
3	B	1290	H4B	2	0

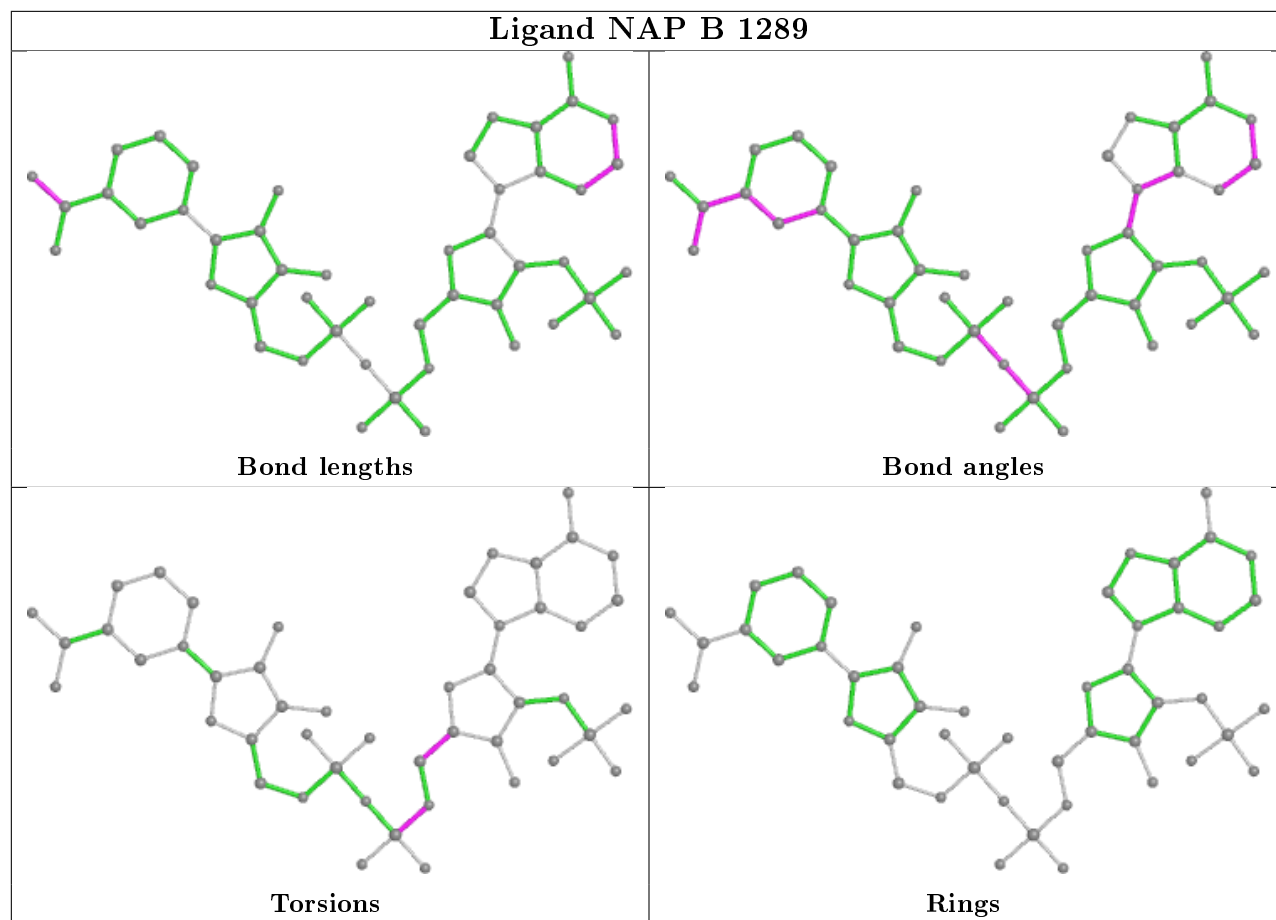
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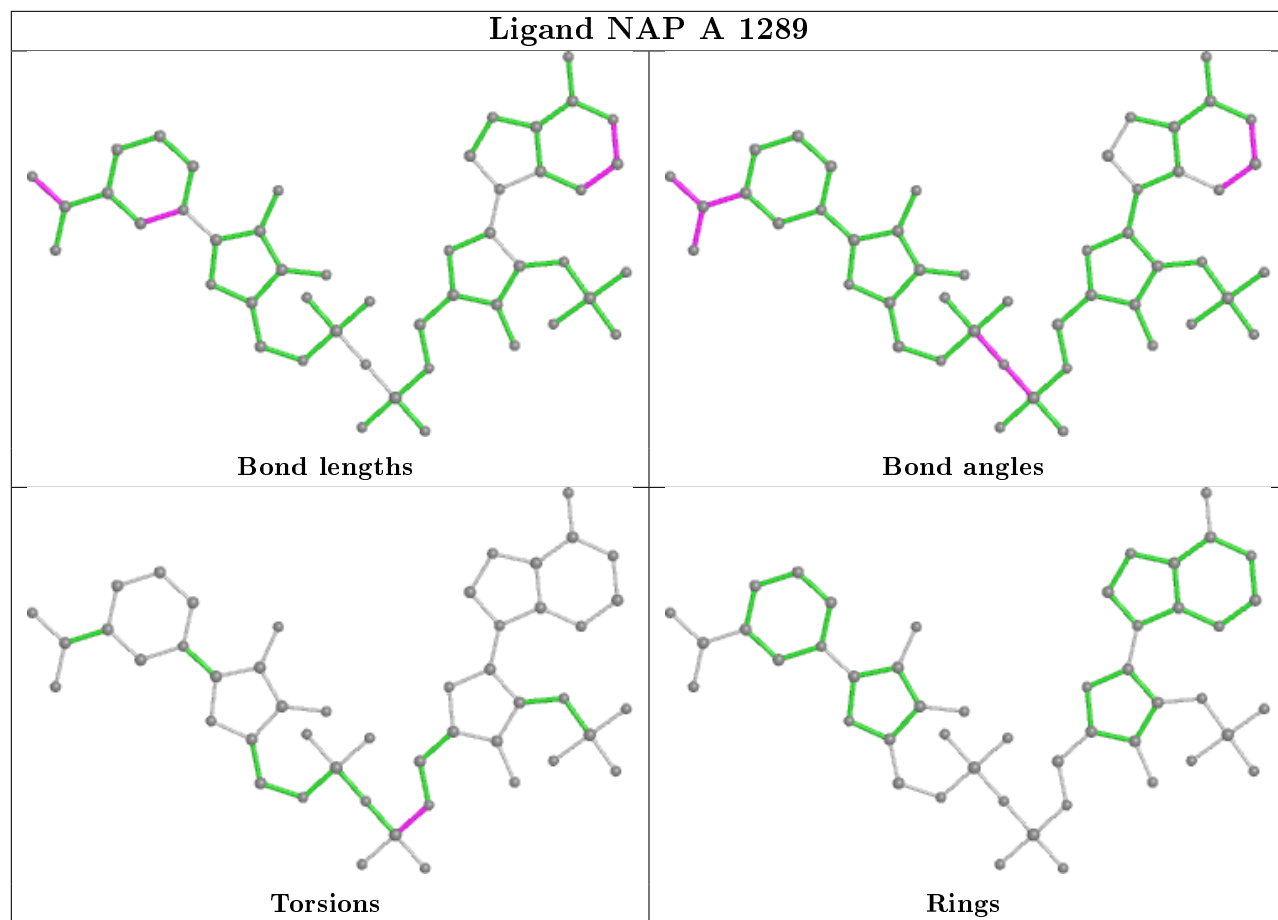
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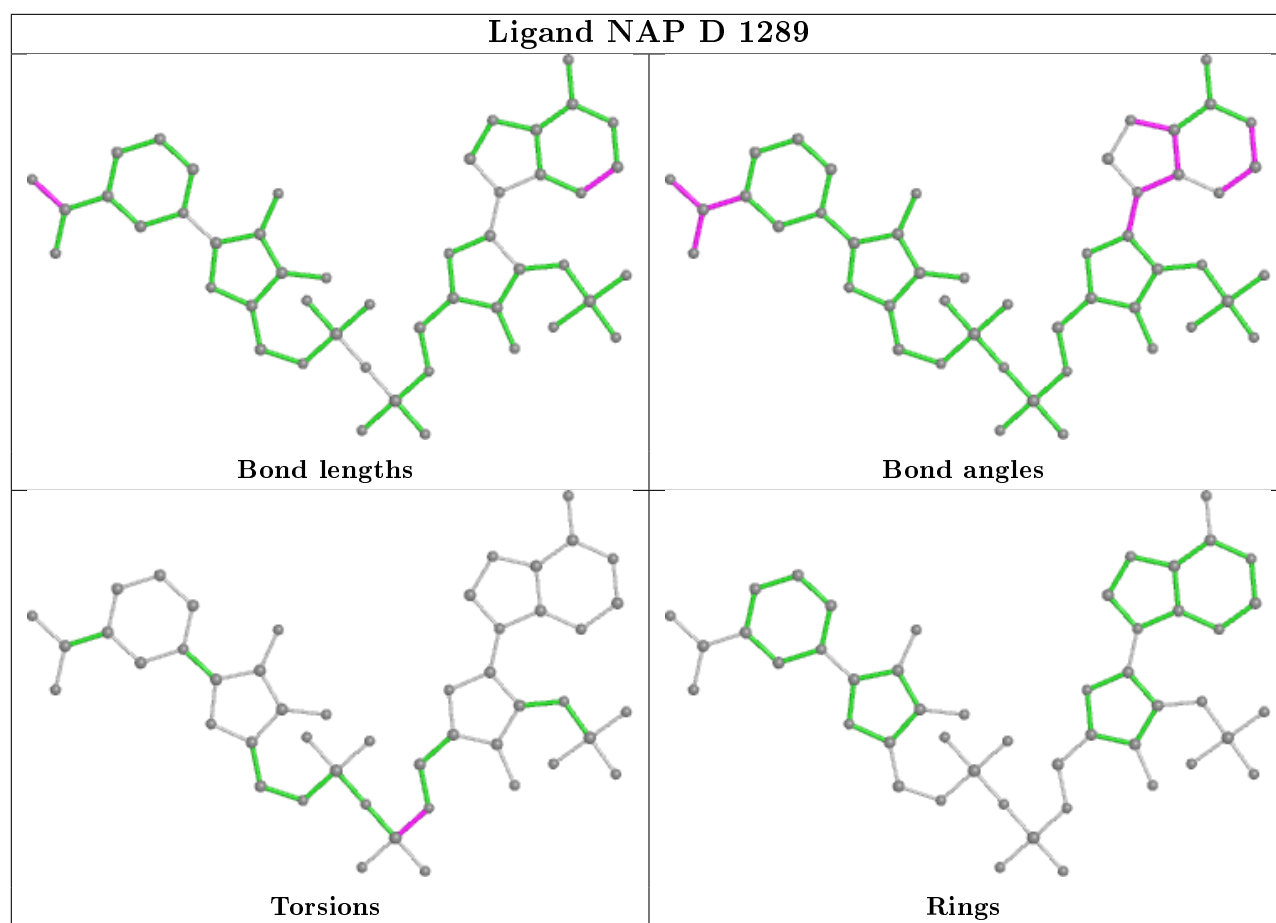
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1289	NAP	2	0

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	267/288 (92%)	0.51	23 (8%) 10 12	36, 44, 64, 90	2 (0%)
1	B	266/288 (92%)	0.66	36 (13%) 3 4	36, 44, 62, 80	2 (0%)
1	C	256/288 (88%)	0.63	36 (14%) 2 3	36, 44, 64, 87	5 (1%)
1	D	257/288 (89%)	0.67	40 (15%) 2 2	36, 44, 70, 92	5 (1%)
All	All	1046/1152 (90%)	0.62	135 (12%) 3 4	36, 44, 65, 92	14 (1%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	ASP	7.2
1	A	121	ASN	6.5
1	A	131	GLY	6.3
1	D	81	ALA	6.3
1	B	72	ALA	6.1
1	C	134	GLU	6.0
1	C	82	PRO	5.9
1	B	133	ARG	5.9
1	C	81	ALA	5.9
1	D	72	ALA	5.7
1	D	133	ARG	5.7
1	B	165	THR	5.5
1	B	5	THR	5.5
1	A	120	ARG	5.4
1	C	120	ARG	5.4
1	D	71	THR	5.1
1	D	83	VAL	5.1
1	C	107	VAL	5.0
1	C	72	ALA	4.9
1	D	135	ALA	4.7
1	A	72	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	176	ILE	4.5
1	C	39	ARG	4.3
1	B	164	GLY	4.2
1	B	49	ALA	4.2
1	B	52	ASN	4.1
1	B	105	VAL	4.1
1	D	10	LEU	4.1
1	C	73	PRO	4.1
1	B	98	THR	4.0
1	D	82	PRO	4.0
1	C	166	PRO	4.0
1	D	240	GLY	4.0
1	A	134	GLU	3.9
1	B	71	THR	3.9
1	B	169	HIS	3.9
1	D	120	ARG	3.9
1	B	166	PRO	3.8
1	D	134	GLU	3.8
1	D	73	PRO	3.8
1	B	132	ASP	3.7
1	C	83	VAL	3.7
1	D	74	VAL	3.7
1	C	230	VAL	3.6
1	D	107	VAL	3.6
1	B	176	ILE	3.6
1	D	106	LEU	3.6
1	A	81	ALA	3.5
1	C	5	THR	3.4
1	D	169	HIS	3.4
1	D	168	LYS	3.4
1	D	49	ALA	3.3
1	A	164	GLY	3.3
1	D	167	ALA	3.3
1	D	39	ARG	3.3
1	D	267	SER	3.3
1	C	71	THR	3.3
1	B	53	ALA	3.3
1	B	134	GLU	3.3
1	D	229	LEU	3.2
1	B	131	GLY	3.2
1	C	169	HIS	3.2
1	A	37	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	137	GLU	3.1
1	C	135	ALA	3.1
1	C	242	ARG	3.1
1	C	11	VAL	3.1
1	C	136[A]	MET	3.0
1	D	28	ALA	3.0
1	D	166	PRO	2.9
1	D	230	VAL	2.9
1	C	165	THR	2.9
1	D	262	ILE	2.8
1	A	10	LEU	2.8
1	B	10	LEU	2.8
1	C	160	HIS	2.8
1	C	105	VAL	2.7
1	D	37	TYR	2.7
1	D	164	GLY	2.7
1	D	12	THR	2.7
1	D	268	LYS	2.7
1	B	240	GLY	2.7
1	B	155	ILE	2.6
1	A	240	GLY	2.6
1	C	133	ARG	2.6
1	D	165	THR	2.5
1	D	5	THR	2.5
1	A	73	PRO	2.5
1	D	138	THR	2.5
1	A	107	VAL	2.5
1	C	243	SER	2.5
1	B	107	VAL	2.4
1	B	56	PRO	2.4
1	A	133	ARG	2.4
1	A	236	ALA	2.4
1	B	11	VAL	2.4
1	D	243	SER	2.4
1	D	11	VAL	2.4
1	A	160	HIS	2.4
1	A	105	VAL	2.4
1	A	12	THR	2.4
1	A	11	VAL	2.3
1	C	86	PHE	2.3
1	B	167	ALA	2.3
1	C	167	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	70	ALA	2.3
1	C	98	THR	2.3
1	D	160	HIS	2.3
1	C	168	LYS	2.3
1	B	175	SER	2.3
1	B	266	SER	2.3
1	B	267	SER	2.3
1	C	38	HIS	2.3
1	C	10	LEU	2.2
1	C	119	LEU	2.2
1	B	168	LYS	2.2
1	D	38	HIS	2.2
1	B	44	ALA	2.2
1	B	106	LEU	2.2
1	B	6	VAL	2.1
1	B	55	ARG	2.1
1	D	176	ILE	2.1
1	B	63	GLN	2.1
1	C	106	LEU	2.1
1	C	229	LEU	2.1
1	B	136[A]	MET	2.1
1	A	119	LEU	2.1
1	C	53	ALA	2.1
1	B	73	PRO	2.1
1	D	66	LEU	2.1
1	C	240	GLY	2.1
1	A	237	VAL	2.1
1	D	34	CYS	2.0
1	B	231	ASP	2.0
1	A	106	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

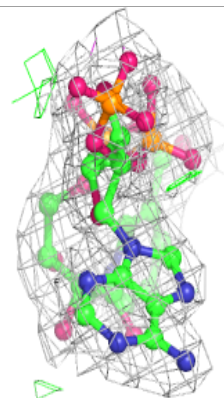
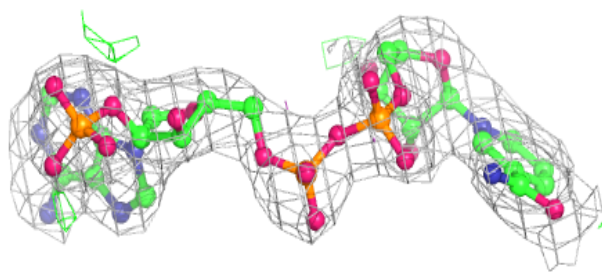
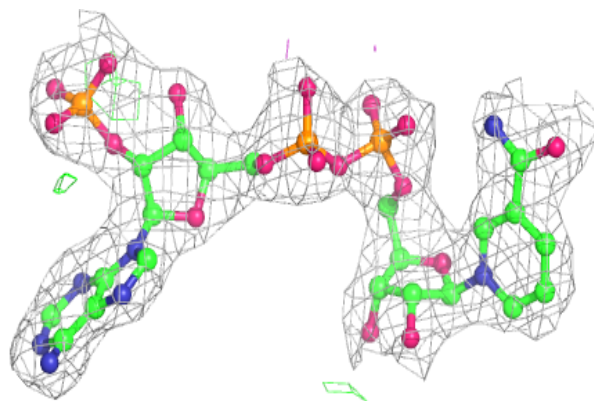
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	C	1291	4/4	0.81	0.28	71,75,77,78	0
4	EDO	D	1292	4/4	0.92	0.31	49,50,51,51	0
4	EDO	B	1292	4/4	0.93	0.48	42,43,43,49	0
3	H4B	A	1290	17/17	0.93	0.17	42,45,48,48	0
3	H4B	C	1290	17/17	0.94	0.14	46,50,64,66	0
4	EDO	B	1293	4/4	0.94	0.21	43,49,49,49	0
3	H4B	B	1290	17/17	0.94	0.16	38,41,50,53	0
3	H4B	D	1290	17/17	0.95	0.16	41,49,60,61	0
4	EDO	B	1291	4/4	0.95	0.14	46,46,47,49	0
2	NAP	C	1289	48/48	0.95	0.14	40,42,44,46	0
2	NAP	D	1289	48/48	0.95	0.14	40,42,44,46	0
2	NAP	A	1289	48/48	0.96	0.15	39,42,44,46	0
2	NAP	B	1289	48/48	0.96	0.14	39,42,43,46	0
4	EDO	D	1291	4/4	0.97	0.27	44,45,46,47	0

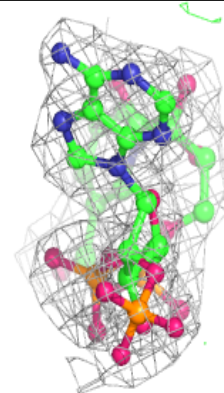
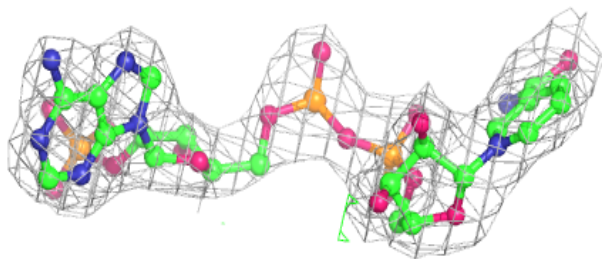
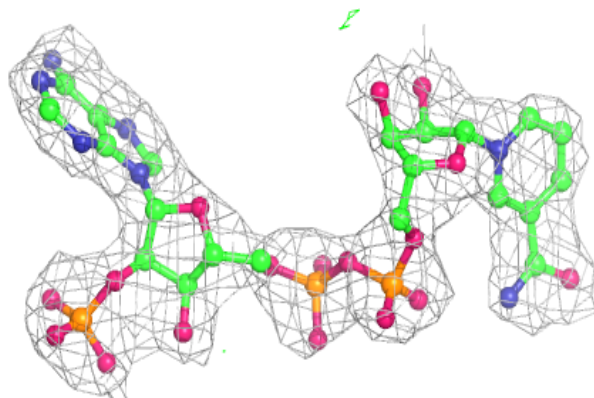
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP C 1289:**

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

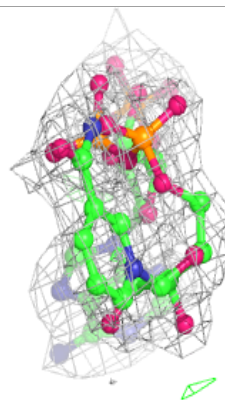
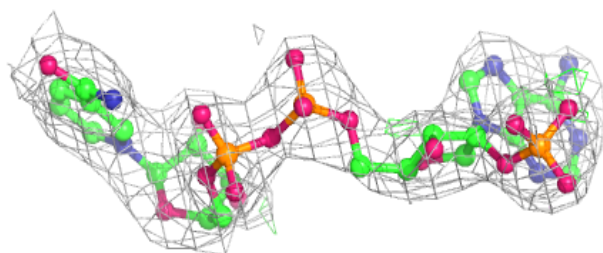
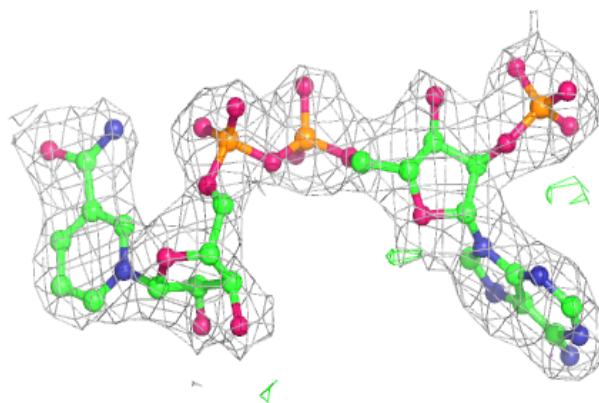
**Electron density around NAP D 1289:**

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

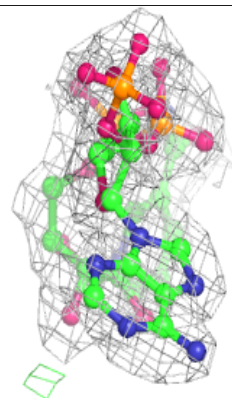
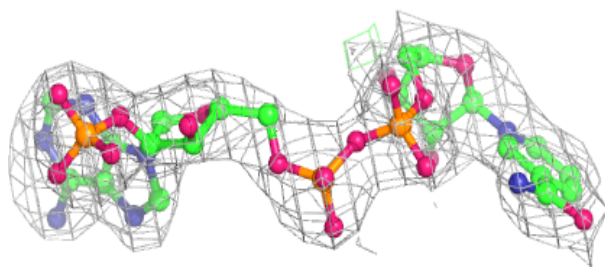
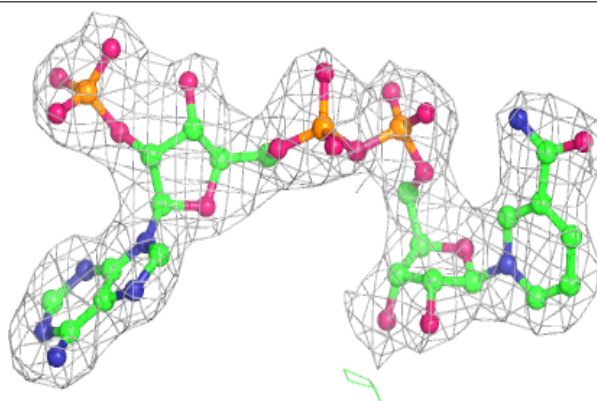


**Electron density around NAP A 1289:**

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

**Electron density around NAP B 1289:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.