Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 03:24 AM EDT

PDB ID	:	5BSG
Title	:	Crystal structure of Medicago truncatula (delta)1-Pyrroline-5-Carboxylate Reductase (MtP5CR) in complex with NADP+
Authors	:	Ruszkowski, M.; Nocek, B.; Forlani, G.; Dauter, Z.
Deposited on	:	2015-06-02
Resolution	:	1.95 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:

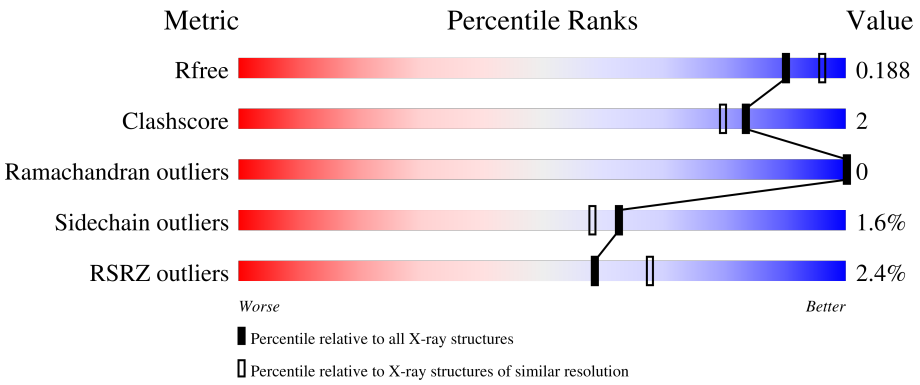
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	277	94%
1	B	277	2% 95%
1	C	277	% 93% 5%
1	D	277	4% 94%
1	E	277	2% 91% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	277	% 91% 7%
1	G	277	2% 93%
1	H	277	2% 91% 6%
1	I	277	3% 93% 5%
1	J	277	6% 91% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22670 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 Pyrroline-5-carboxylate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	2020	1274	348	392	6	0	5	0
1	B	272	2011	1268	349	388	6	0	3	0
1	C	270	2008	1263	350	389	6	0	5	0
1	D	271	2012	1267	350	389	6	0	4	0
1	E	272	2032	1281	353	392	6	0	6	0
1	F	272	2034	1283	354	391	6	0	6	0
1	G	269	1990	1252	347	385	6	0	4	0
1	H	272	2002	1265	346	385	6	0	3	0
1	I	272	2001	1263	348	384	6	0	2	0
1	J	270	1976	1246	342	382	6	0	1	0

There are 30 discrepancies between the modelled and reference sequences:

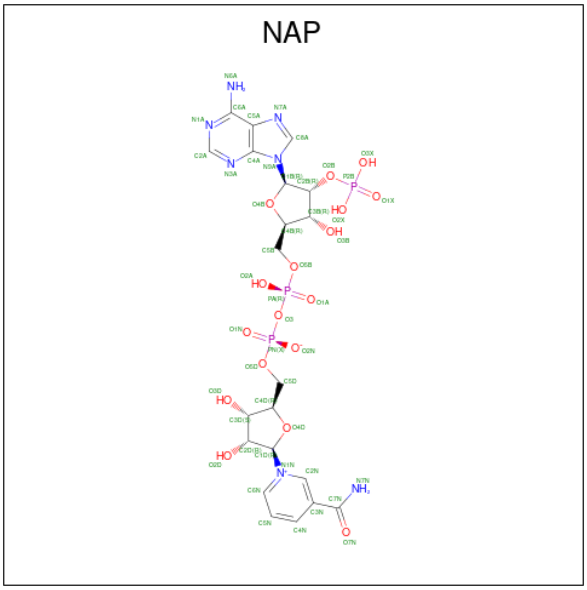
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7KRM5
A	-1	ASN	-	expression tag	UNP G7KRM5
A	0	ALA	-	expression tag	UNP G7KRM5
B	-2	SER	-	expression tag	UNP G7KRM5
B	-1	ASN	-	expression tag	UNP G7KRM5
B	0	ALA	-	expression tag	UNP G7KRM5
C	-2	SER	-	expression tag	UNP G7KRM5
C	-1	ASN	-	expression tag	UNP G7KRM5
C	0	ALA	-	expression tag	UNP G7KRM5

Continued on next page...

Continued from previous page...

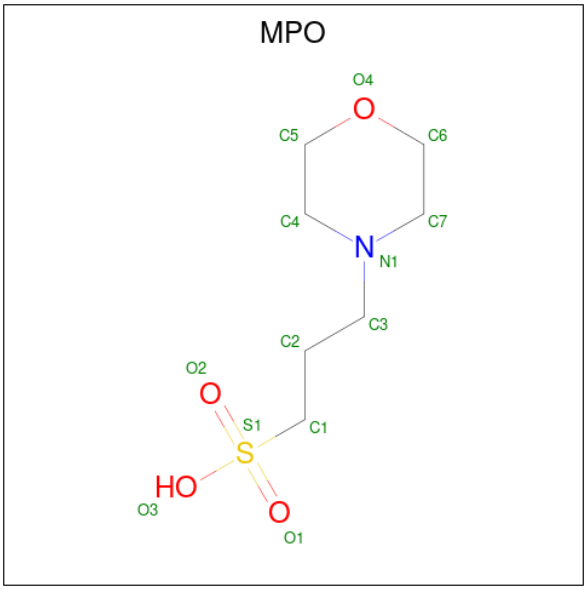
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP G7KRM5
D	-1	ASN	-	expression tag	UNP G7KRM5
D	0	ALA	-	expression tag	UNP G7KRM5
E	-2	SER	-	expression tag	UNP G7KRM5
E	-1	ASN	-	expression tag	UNP G7KRM5
E	0	ALA	-	expression tag	UNP G7KRM5
F	-2	SER	-	expression tag	UNP G7KRM5
F	-1	ASN	-	expression tag	UNP G7KRM5
F	0	ALA	-	expression tag	UNP G7KRM5
G	-2	SER	-	expression tag	UNP G7KRM5
G	-1	ASN	-	expression tag	UNP G7KRM5
G	0	ALA	-	expression tag	UNP G7KRM5
H	-2	SER	-	expression tag	UNP G7KRM5
H	-1	ASN	-	expression tag	UNP G7KRM5
H	0	ALA	-	expression tag	UNP G7KRM5
I	-2	SER	-	expression tag	UNP G7KRM5
I	-1	ASN	-	expression tag	UNP G7KRM5
I	0	ALA	-	expression tag	UNP G7KRM5
J	-2	SER	-	expression tag	UNP G7KRM5
J	-1	ASN	-	expression tag	UNP G7KRM5
J	0	ALA	-	expression tag	UNP G7KRM5

- Molecule 2 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		
2	A	1	48	21	7	17	3	0	0
2	B	1	48	21	7	17	3	0	0
2	C	1	48	21	7	17	3	0	0
2	D	1	48	21	7	17	3	0	0
2	E	1	48	21	7	17	3	0	0
2	F	1	48	21	7	17	3	0	0
2	G	1	48	21	7	17	3	0	0
2	H	1	48	21	7	17	3	0	0
2	I	1	48	21	7	17	3	0	0
2	J	1	48	21	7	17	3	0	0

- Molecule 3 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	13	7	1	4	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	B	1	13	7	1	4	1	0	0
3	C	1	13	7	1	4	1	0	0
3	D	1	13	7	1	4	1	0	0
3	E	1	13	7	1	4	1	0	0
3	F	1	13	7	1	4	1	0	0
3	G	1	13	7	1	4	1	0	0
3	H	1	13	7	1	4	1	0	0
3	I	1	13	7	1	4	1	0	0
3	J	1	13	7	1	4	1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0
4	E	1	1	1	0	0
4	F	1	1	1	0	0
4	G	1	1	1	0	0
4	H	1	1	1	0	0
4	I	1	1	1	0	0
4	J	1	1	1	0	0

- Molecule 5 is water.

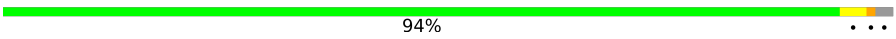
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	248	Total O 248 248	0	0
5	B	202	Total O 203 203	0	1
5	C	205	Total O 206 206	0	1
5	D	158	Total O 159 159	0	1
5	E	203	Total O 205 205	0	2
5	F	231	Total O 231 231	0	0
5	G	155	Total O 155 155	0	0
5	H	193	Total O 194 194	0	1
5	I	194	Total O 194 194	0	0
5	J	169	Total O 169 169	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.

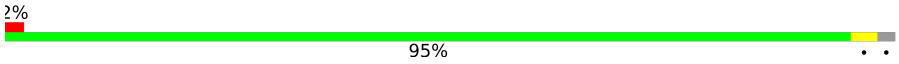
- Molecule 1: Pyrroline-5-carboxylate reductase

Chain A:



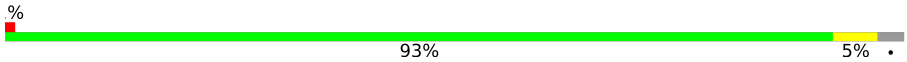
- Molecule 1: Pyrroline-5-carboxylate reductase

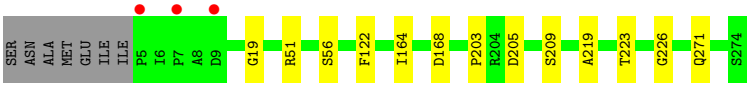
Chain B:



- Molecule 1: Pyrroline-5-carboxylate reductase

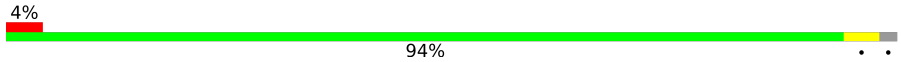
Chain C:

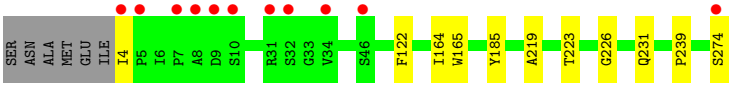




- Molecule 1: Pyrroline-5-carboxylate reductase

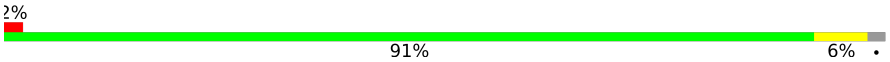
Chain D:

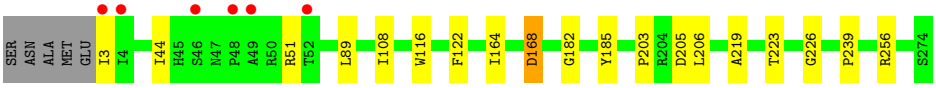




- Molecule 1: Pyrroline-5-carboxylate reductase

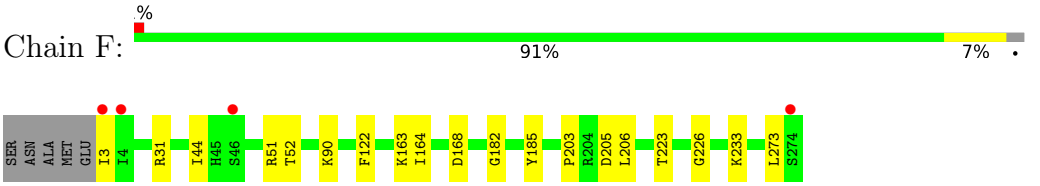
Chain E:





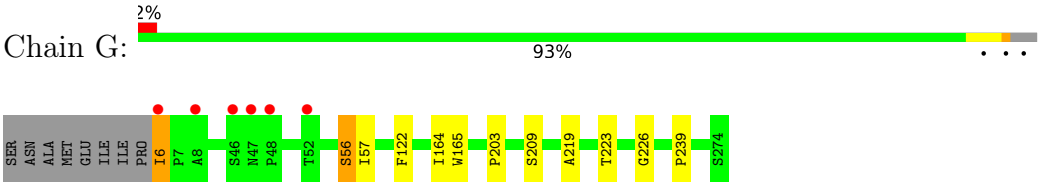
- Molecule 1: Pyrroline-5-carboxylate reductase

Chain F:



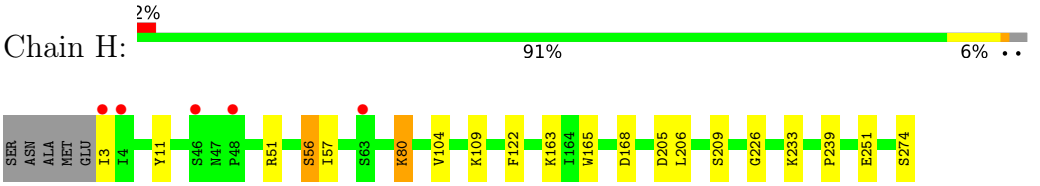
• Molecule 1: Pyrroline-5-carboxylate reductase

Chain G:



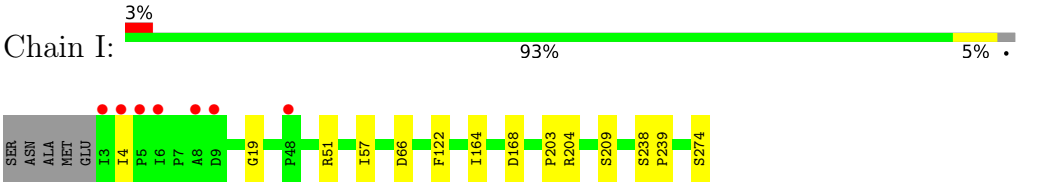
• Molecule 1: Pyrroline-5-carboxylate reductase

Chain H:



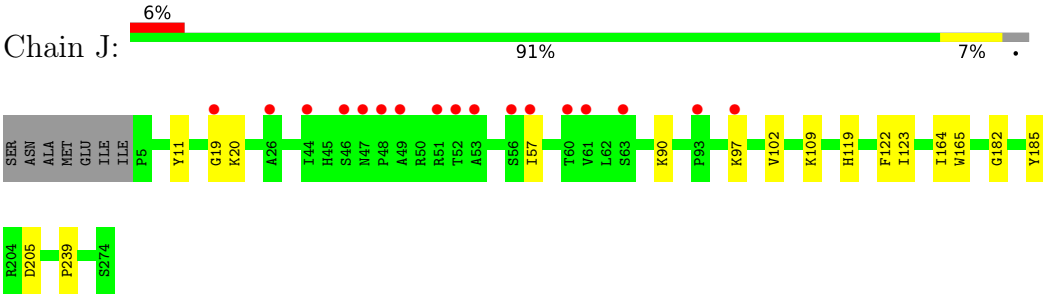
• Molecule 1: Pyrroline-5-carboxylate reductase

Chain I:



• Molecule 1: Pyrroline-5-carboxylate reductase

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	87.24Å 100.30Å 100.79Å 68.13° 85.76° 89.30°	Depositor
Resolution (Å)	39.39 – 1.95 39.39 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.39-1.95) 97.0 (39.39-1.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.155 , 0.178 0.167 , 0.188	Depositor DCC
R_{free} test set	2257 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22670	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MPO, CL, 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	0.95	1/2049 (0.0%)	0.87	4/2774 (0.1%)
1	B	0.92	0/2040	0.89	3/2760 (0.1%)
1	C	0.90	0/2037	0.87	3/2754 (0.1%)
1	D	0.81	0/2041	0.86	1/2761 (0.0%)
1	E	0.90	0/2061	0.87	5/2788 (0.2%)
1	F	0.92	0/2065	0.88	4/2788 (0.1%)
1	G	0.87	0/2018	0.84	1/2728 (0.0%)
1	H	0.96	2/2034 (0.1%)	0.88	3/2751 (0.1%)
1	I	0.87	0/2030	0.88	2/2747 (0.1%)
1	J	0.95	2/2005 (0.1%)	0.86	1/2712 (0.0%)
All	All	0.91	5/20380 (0.0%)	0.87	27/27563 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	191	GLU	CD-OE1	5.64	1.31	1.25
1	H	251	GLU	CD-OE1	5.29	1.31	1.25
1	J	11	TYR	CE1-CZ	5.25	1.45	1.38
1	A	155	SER	CB-OG	-5.10	1.35	1.42
1	H	11	TYR	CE1-CZ	5.07	1.45	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	274	SER	N-CA-CB	5.98	119.47	110.50
1	E	108	ILE	CG1-CB-CG2	-5.91	98.40	111.40
1	C	51	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	F	31	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	H	51	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	I	51	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	F	90	LYS	CA-CB-CG	5.63	125.78	113.40
1	B	205[A]	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	205[B]	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	274	SER	N-CA-CB	5.45	118.67	110.50
1	A	238[A]	SER	CB-CA-C	-5.44	99.77	110.10
1	A	238[B]	SER	CB-CA-C	-5.44	99.77	110.10
1	D	274	SER	N-CA-CB	5.43	118.65	110.50
1	A	66	ASP	CB-CG-OD1	5.34	123.11	118.30
1	H	274	SER	N-CA-CB	5.34	118.50	110.50
1	E	256	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	F	51	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	F	51	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	H	56	SER	N-CA-CB	5.24	118.35	110.50
1	A	274	SER	N-CA-CB	5.19	118.29	110.50
1	J	109	LYS	CD-CE-NZ	5.17	123.58	111.70
1	E	168[A]	ASP	CB-CG-OD1	5.16	122.95	118.30
1	E	168[B]	ASP	CB-CG-OD1	5.16	122.95	118.30
1	E	51	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	G	56	SER	N-CA-CB	5.11	118.17	110.50
1	C	205[A]	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	205[B]	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	273	LEU	Peptide

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	2020	0	2077	9	0
1	B	2011	0	2070	5	0
1	C	2008	0	2058	13	0
1	D	2012	0	2066	7	0
1	E	2032	0	2089	14	0
1	F	2034	0	2104	10	0
1	G	1990	0	2044	11	0
1	H	2002	0	2070	14	0
1	I	2001	0	2069	11	0
1	J	1976	0	2034	15	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
2	E	48	0	25	0	0
2	F	48	0	25	0	0
2	G	48	0	25	0	0
2	H	48	0	25	1	0
2	I	48	0	25	1	0
2	J	48	0	25	2	0
3	A	13	0	14	0	0
3	B	13	0	14	3	0
3	C	13	0	15	0	0
3	D	13	0	14	0	0
3	E	13	0	15	0	0
3	F	13	0	14	1	0
3	G	13	0	14	1	0
3	H	13	0	15	0	0
3	I	13	0	14	0	0
3	J	13	0	15	2	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	1	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	1	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	A	248	0	0	1	0
5	B	203	0	0	1	0
5	C	206	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	159	0	0	5	0
5	E	205	0	0	8	0
5	F	231	0	0	6	0
5	G	155	0	0	5	0
5	H	194	0	0	4	0
5	I	194	0	0	3	0
5	J	169	0	0	2	0
All	All	22670	0	21075	100	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 (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168[B]:ASP:OD1	5:C:402:HOH:O	1.72	1.05
1:E:168[A]:ASP:OD1	5:E:402:HOH:O	1.90	0.89
1:E:89[A]:LEU:HD21	5:E:572:HOH:O	1.78	0.83
1:J:97:LYS:HE3	1:J:119:HIS:HB3	1.62	0.82
1:F:163[B]:LYS:HE2	5:F:401:HOH:O	1.83	0.78
1:J:57:ILE:HG22	1:J:57:ILE:O	1.83	0.78
1:I:57:ILE:HG22	1:I:57:ILE:O	1.82	0.77
1:H:57:ILE:HG22	1:H:57:ILE:O	1.84	0.75
1:J:97:LYS:HE3	1:J:119:HIS:CB	2.16	0.75
1:F:52:THR:HB	5:F:502:HOH:O	1.87	0.74
1:G:57:ILE:O	1:G:57:ILE:HG22	1.87	0.72
1:C:226[B]:GLY:N	5:C:403:HOH:O	2.23	0.70
1:C:226[A]:GLY:N	5:C:403:HOH:O	2.25	0.68
2:A:301:NAP:O2X	5:A:403:HOH:O	2.13	0.67
1:E:89[A]:LEU:CD2	5:E:572:HOH:O	2.38	0.67
1:D:231[A]:GLN:HG2	5:D:529:HOH:O	1.95	0.67
3:G:302:MPO:H72	4:H:303:CL:CL	2.32	0.66
1:C:223:THR:HG21	5:D:404:HOH:O	1.96	0.64
1:C:223:THR:CG2	5:D:404:HOH:O	2.46	0.63
1:A:239:PRO:HG3	1:I:203:PRO:HA	1.80	0.62
1:C:226[B]:GLY:CA	5:C:403:HOH:O	2.49	0.60
1:F:168:ASP:HB3	5:F:543:HOH:O	2.01	0.60
1:G:203:PRO:HA	1:I:239:PRO:HG3	1.83	0.59
1:G:226[B]:GLY:N	5:G:404:HOH:O	2.29	0.59
5:G:420:HOH:O	1:H:163:LYS:HE2	2.03	0.58
1:E:89[A]:LEU:CG	5:E:572:HOH:O	2.51	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205[A]:ASP:OD1	1:E:206:LEU:N	2.37	0.58
1:I:57:ILE:O	1:I:57:ILE:CG2	2.53	0.57
1:A:82:GLN:NE2	1:A:82:GLN:H	2.03	0.56
1:I:204:ARG:HB2	5:I:409:HOH:O	2.05	0.56
1:J:97:LYS:CE	1:J:119:HIS:HB3	2.35	0.56
1:G:6:ILE:HD12	5:G:505:HOH:O	2.07	0.55
1:H:109:LYS:NZ	5:H:407:HOH:O	2.38	0.55
1:J:57:ILE:O	1:J:57:ILE:CG2	2.54	0.54
1:H:57:ILE:O	1:H:57:ILE:CG2	2.56	0.53
1:H:168:ASP:HB3	5:H:539:HOH:O	2.09	0.53
1:H:205[A]:ASP:OD1	1:H:206:LEU:N	2.41	0.53
1:E:89[A]:LEU:HG	5:E:572:HOH:O	2.07	0.53
1:G:226[A]:GLY:N	5:G:404:HOH:O	2.32	0.52
1:C:203:PRO:HA	1:E:239:PRO:HG3	1.92	0.52
1:D:226:GLY:N	5:D:406:HOH:O	2.43	0.52
4:E:303:CL:CL	3:F:302:MPO:H72	2.46	0.52
1:G:57:ILE:O	1:G:57:ILE:CG2	2.57	0.51
1:F:205[A]:ASP:OD1	1:F:206:LEU:N	2.43	0.51
1:I:238[A]:SER:OG	3:J:302:MPO:C1	2.58	0.51
1:C:226[A]:GLY:CA	5:C:403:HOH:O	2.60	0.50
1:F:226:GLY:C	5:F:476:HOH:O	2.49	0.50
1:J:20:LYS:NZ	2:J:301:NAP:O1A	2.44	0.50
1:D:239:PRO:HG3	1:F:203:PRO:HA	1.93	0.49
1:F:223:THR:HG21	5:F:571:HOH:O	2.12	0.49
1:C:209:SER:HB3	1:D:165:TRP:CZ2	2.48	0.48
1:C:226[B]:GLY:C	5:C:403:HOH:O	2.52	0.47
1:B:219:ALA:O	1:B:223:THR:HG23	2.14	0.47
1:J:90:LYS:HG3	5:J:403:HOH:O	2.14	0.47
1:J:19:GLY:HA3	2:J:301:NAP:O5B	2.16	0.46
1:E:226[B]:GLY:N	5:E:407:HOH:O	2.35	0.46
1:H:80:LYS:HA	1:H:80:LYS:HD2	1.78	0.46
1:H:226[B]:GLY:N	5:H:403:HOH:O	2.30	0.45
1:A:219:ALA:O	1:A:223:THR:HG23	2.16	0.45
1:C:271:GLN:HG3	5:C:579:HOH:O	2.16	0.45
1:E:226[A]:GLY:N	5:E:407:HOH:O	2.36	0.45
1:E:219:ALA:O	1:E:223:THR:HG23	2.16	0.45
1:D:231[A]:GLN:CG	5:D:529:HOH:O	2.59	0.44
1:I:238[A]:SER:OG	3:J:302:MPO:H12	2.16	0.44
1:C:219:ALA:O	1:C:223:THR:HG23	2.17	0.43
1:J:97:LYS:HE3	1:J:119:HIS:HB2	1.95	0.43
1:H:226[A]:GLY:N	5:H:403:HOH:O	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:TRP:O	5:E:403:HOH:O	2.21	0.43
1:G:226[B]:GLY:CA	5:G:404:HOH:O	2.64	0.43
1:A:216[A]:LEU:HD12	1:B:216:LEU:HD12	2.00	0.43
1:D:219:ALA:O	1:D:223:THR:HG23	2.19	0.43
4:A:303:CL:CL	3:B:302:MPO:H72	2.56	0.43
1:D:4:ILE:HD13	1:D:4:ILE:HA	1.85	0.42
1:I:168:ASP:HB3	5:I:535:HOH:O	2.18	0.42
1:B:203:PRO:HA	1:J:239:PRO:HG3	2.01	0.42
1:F:226:GLY:N	5:F:403:HOH:O	2.27	0.42
1:J:182:GLY:HA2	1:J:185:TYR:CD2	2.55	0.42
1:A:82:GLN:H	1:A:82:GLN:HE21	1.68	0.42
1:G:209:SER:HB3	1:H:165:TRP:CZ2	2.55	0.42
1:J:102:VAL:HA	1:J:123:ILE:O	2.19	0.42
1:G:219:ALA:O	1:G:223:THR:HG23	2.19	0.42
1:I:209:SER:HB3	1:J:165:TRP:CZ2	2.55	0.42
1:F:182:GLY:HA2	1:F:185:TYR:CD2	2.55	0.41
1:A:163:LYS:HE2	5:B:481:HOH:O	2.19	0.41
1:I:19:GLY:HA3	2:I:301:NAP:O5B	2.21	0.41
1:B:44:ILE:HD12	1:B:44:ILE:HA	1.86	0.41
1:H:239:PRO:HG3	1:J:203:PRO:HA	2.01	0.41
1:E:203:PRO:HA	1:G:239:PRO:HG3	2.02	0.41
1:E:3:ILE:HG22	1:E:3:ILE:O	2.21	0.41
1:I:66:ASP:OD1	5:I:402:HOH:O	2.21	0.41
1:J:205:ASP:HB2	5:J:517:HOH:O	2.20	0.41
1:E:182:GLY:HA2	1:E:185:TYR:CD2	2.56	0.40
1:H:3:ILE:HG22	1:H:3:ILE:O	2.21	0.40
1:A:216[A]:LEU:HD12	1:B:216:LEU:CD1	2.51	0.40
1:F:3:ILE:HG22	1:F:3:ILE:O	2.21	0.40
1:A:238[A]:SER:OG	3:B:302:MPO:C1	2.69	0.40
1:C:19:GLY:HA3	2:C:301:NAP:O5B	2.21	0.40
1:G:165:TRP:CZ2	1:H:209:SER:HB3	2.57	0.40
1:H:104:VAL:O	2:H:301:NAP:H1D	2.22	0.40
1:A:238[A]:SER:OG	3:B:302:MPO:H11	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	275/277 (99%)	271 (98%)	4 (2%)	0	100	100
1	B	273/277 (99%)	268 (98%)	5 (2%)	0	100	100
1	C	273/277 (99%)	266 (97%)	7 (3%)	0	100	100
1	D	273/277 (99%)	267 (98%)	6 (2%)	0	100	100
1	E	276/277 (100%)	271 (98%)	5 (2%)	0	100	100
1	F	275/277 (99%)	270 (98%)	5 (2%)	0	100	100
1	G	271/277 (98%)	268 (99%)	3 (1%)	0	100	100
1	H	273/277 (99%)	268 (98%)	5 (2%)	0	100	100
1	I	272/277 (98%)	267 (98%)	5 (2%)	0	100	100
1	J	269/277 (97%)	266 (99%)	3 (1%)	0	100	100
All	All	2730/2770 (99%)	2682 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/212 (100%)	209 (98%)	4 (2%)	57	50
1	B	211/212 (100%)	208 (99%)	3 (1%)	67	62
1	C	210/212 (99%)	207 (99%)	3 (1%)	67	62
1	D	211/212 (100%)	208 (99%)	3 (1%)	67	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	213/212 (100%)	210 (99%)	3 (1%)	67	62
1	F	214/212 (101%)	210 (98%)	4 (2%)	57	50
1	G	208/212 (98%)	204 (98%)	4 (2%)	57	50
1	H	210/212 (99%)	206 (98%)	4 (2%)	57	50
1	I	210/212 (99%)	207 (99%)	3 (1%)	67	62
1	J	207/212 (98%)	205 (99%)	2 (1%)	76	74
All	All	2107/2120 (99%)	2074 (98%)	33 (2%)	62	58

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	122	PHE
1	A	164	ILE
1	A	274	SER
1	B	44	ILE
1	B	122	PHE
1	B	164	ILE
1	C	56	SER
1	C	122	PHE
1	C	164	ILE
1	D	122	PHE
1	D	164	ILE
1	D	185	TYR
1	E	44	ILE
1	E	122	PHE
1	E	164	ILE
1	F	44	ILE
1	F	122	PHE
1	F	164	ILE
1	F	233	LYS
1	G	6	ILE
1	G	56	SER
1	G	122	PHE
1	G	164	ILE
1	H	56	SER
1	H	80	LYS
1	H	122	PHE
1	H	233	LYS
1	I	4	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	122	PHE
1	I	164	ILE
1	J	122	PHE
1	J	164	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
2	NAP	B	301	-	45,52,52	1.54	10 (22%)	56,80,80	1.32	7 (12%)
3	MPO	F	302	-	13,13,13	2.27	4 (30%)	17,17,17	0.94	1 (5%)
2	NAP	H	301	-	45,52,52	1.47	11 (24%)	56,80,80	1.37	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	G	301	-	45,52,52	1.20	4 (8%)	56,80,80	1.34	9 (16%)
3	MPO	A	302	-	13,13,13	2.46	4 (30%)	17,17,17	1.12	2 (11%)
2	NAP	C	301	-	45,52,52	1.42	8 (17%)	56,80,80	1.30	9 (16%)
3	MPO	B	302	-	13,13,13	2.55	3 (23%)	17,17,17	1.54	3 (17%)
2	NAP	I	301	-	45,52,52	1.39	8 (17%)	56,80,80	1.27	6 (10%)
3	MPO	C	302	-	13,13,13	2.36	4 (30%)	17,17,17	1.14	1 (5%)
3	MPO	H	302	-	13,13,13	2.05	3 (23%)	17,17,17	1.22	2 (11%)
3	MPO	G	302	-	13,13,13	2.69	4 (30%)	17,17,17	1.83	4 (23%)
3	MPO	J	302	-	13,13,13	2.63	4 (30%)	17,17,17	1.70	5 (29%)
2	NAP	A	301	-	45,52,52	1.43	10 (22%)	56,80,80	1.41	11 (19%)
3	MPO	I	302	-	13,13,13	2.56	4 (30%)	17,17,17	1.48	2 (11%)
2	NAP	J	301	-	45,52,52	1.27	9 (20%)	56,80,80	1.18	5 (8%)
3	MPO	D	302	-	13,13,13	2.29	4 (30%)	17,17,17	1.81	4 (23%)
2	NAP	E	301	-	45,52,52	1.49	10 (22%)	56,80,80	1.19	5 (8%)
3	MPO	E	302	-	13,13,13	2.50	3 (23%)	17,17,17	1.71	3 (17%)
2	NAP	D	301	-	45,52,52	1.24	5 (11%)	56,80,80	1.36	9 (16%)
2	NAP	F	301	-	45,52,52	1.33	8 (17%)	56,80,80	1.26	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
2	NAP	B	301	-	-	3/31/67/67	0/5/5/5
3	MPO	F	302	-	-	0/7/15/15	0/1/1/1
2	NAP	H	301	-	-	3/31/67/67	0/5/5/5
2	NAP	G	301	-	-	1/31/67/67	0/5/5/5
3	MPO	A	302	-	-	0/7/15/15	0/1/1/1
2	NAP	C	301	-	-	2/31/67/67	0/5/5/5
3	MPO	B	302	-	-	1/7/15/15	0/1/1/1
2	NAP	I	301	-	-	1/31/67/67	0/5/5/5
3	MPO	C	302	-	-	0/7/15/15	0/1/1/1
3	MPO	H	302	-	-	0/7/15/15	0/1/1/1
3	MPO	G	302	-	-	0/7/15/15	0/1/1/1
3	MPO	J	302	-	-	2/7/15/15	0/1/1/1
2	NAP	A	301	-	-	1/31/67/67	0/5/5/5
3	MPO	I	302	-	-	0/7/15/15	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	J	301	-	-	5/31/67/67	0/5/5/5
3	MPO	D	302	-	-	0/7/15/15	0/1/1/1
2	NAP	E	301	-	-	4/31/67/67	0/5/5/5
3	MPO	E	302	-	-	1/7/15/15	0/1/1/1
2	NAP	D	301	-	-	2/31/67/67	0/5/5/5
2	NAP	F	301	-	-	1/31/67/67	0/5/5/5

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	302	MPO	C1-S1	-8.41	1.65	1.77
3	E	302	MPO	C1-S1	-7.74	1.66	1.77
3	G	302	MPO	C1-S1	-7.71	1.66	1.77
3	I	302	MPO	C1-S1	-7.64	1.66	1.77
3	B	302	MPO	C1-S1	-7.43	1.66	1.77
3	C	302	MPO	C1-S1	-6.95	1.67	1.77
3	D	302	MPO	C1-S1	-6.45	1.68	1.77
3	A	302	MPO	C1-S1	-6.20	1.68	1.77
3	F	302	MPO	C1-S1	-5.91	1.69	1.77
3	H	302	MPO	C1-S1	-5.82	1.69	1.77
3	G	302	MPO	O2-S1	4.11	1.57	1.45
3	B	302	MPO	O1-S1	4.10	1.57	1.45
3	A	302	MPO	O2-S1	-3.70	1.34	1.45
3	A	302	MPO	O1-S1	3.63	1.55	1.45
3	F	302	MPO	O1-S1	-3.57	1.34	1.45
3	A	302	MPO	O3-S1	-3.54	1.35	1.47
3	F	302	MPO	O3-S1	-3.36	1.35	1.47
2	D	301	NAP	O7N-C7N	-3.32	1.17	1.24
3	D	302	MPO	O1-S1	3.25	1.54	1.45
3	I	302	MPO	O3-S1	-3.21	1.36	1.47
3	C	302	MPO	O1-S1	-3.15	1.35	1.45
2	H	301	NAP	O7N-C7N	-3.09	1.18	1.24
2	I	301	NAP	P2B-O3X	-3.02	1.43	1.54
3	H	302	MPO	O1-S1	-2.99	1.36	1.45
2	C	301	NAP	P2B-O3X	-2.96	1.43	1.54
2	A	301	NAP	P2B-O3X	-2.93	1.43	1.54
2	B	301	NAP	P2B-O2B	-2.92	1.53	1.59
3	E	302	MPO	O2-S1	-2.89	1.36	1.45
3	G	302	MPO	O1-S1	-2.88	1.36	1.45
3	D	302	MPO	O3-S1	-2.88	1.37	1.47
3	B	302	MPO	O3-S1	-2.87	1.37	1.47
3	E	302	MPO	O1-S1	-2.85	1.36	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	PN-O2N	-2.85	1.41	1.55
2	E	301	NAP	P2B-O2X	-2.84	1.43	1.54
2	B	301	NAP	PA-O2A	-2.84	1.42	1.55
2	A	301	NAP	PN-O2N	-2.83	1.42	1.55
3	I	302	MPO	O1-S1	-2.82	1.36	1.45
3	G	302	MPO	O3-S1	-2.80	1.37	1.47
2	I	301	NAP	PN-O1N	-2.79	1.41	1.50
3	C	302	MPO	O2-S1	-2.79	1.36	1.45
2	B	301	NAP	P2B-O3X	-2.74	1.44	1.54
2	F	301	NAP	PN-O2N	-2.74	1.42	1.55
2	C	301	NAP	PA-O2A	-2.73	1.42	1.55
3	J	302	MPO	O3-S1	2.73	1.57	1.47
2	C	301	NAP	C4A-N3A	-2.73	1.31	1.35
2	A	301	NAP	O7N-C7N	-2.73	1.18	1.24
2	C	301	NAP	O7N-C7N	-2.71	1.19	1.24
2	C	301	NAP	PN-O2N	-2.70	1.42	1.55
2	H	301	NAP	PN-O2N	-2.68	1.42	1.55
2	E	301	NAP	P2B-O2B	-2.68	1.54	1.59
2	E	301	NAP	O7N-C7N	-2.66	1.19	1.24
2	I	301	NAP	PA-O2A	-2.65	1.42	1.55
2	B	301	NAP	C4A-N3A	-2.65	1.32	1.35
2	C	301	NAP	P2B-O2X	-2.64	1.44	1.54
2	A	301	NAP	PA-O2A	-2.64	1.42	1.55
3	H	302	MPO	O2-S1	-2.62	1.37	1.45
2	F	301	NAP	P2B-O3X	-2.61	1.44	1.54
2	B	301	NAP	P2B-O2X	-2.60	1.44	1.54
3	D	302	MPO	O2-S1	-2.59	1.37	1.45
2	H	301	NAP	PA-O1A	-2.59	1.41	1.50
2	F	301	NAP	PA-O2A	-2.58	1.43	1.55
3	I	302	MPO	O2-S1	2.58	1.52	1.45
2	H	301	NAP	PA-O2A	-2.54	1.43	1.55
2	G	301	NAP	P2B-O3X	-2.52	1.45	1.54
3	F	302	MPO	O2-S1	2.48	1.52	1.45
2	F	301	NAP	P2B-O2X	-2.47	1.45	1.54
2	I	301	NAP	P2B-O2X	-2.45	1.45	1.54
2	E	301	NAP	C5A-N7A	-2.44	1.30	1.39
2	F	301	NAP	PA-O1A	-2.44	1.42	1.50
2	G	301	NAP	PN-O2N	-2.44	1.43	1.55
2	B	301	NAP	PN-O1N	-2.44	1.42	1.50
2	D	301	NAP	PN-O2N	-2.42	1.43	1.55
2	F	301	NAP	O7N-C7N	-2.41	1.19	1.24
2	C	301	NAP	PA-O1A	-2.41	1.42	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	NAP	C2N-N1N	-2.39	1.32	1.35
2	F	301	NAP	C5A-N7A	-2.39	1.31	1.39
2	H	301	NAP	P2B-O3X	-2.38	1.45	1.54
2	D	301	NAP	P2B-O3X	-2.38	1.45	1.54
2	A	301	NAP	PA-O1A	-2.38	1.42	1.50
2	I	301	NAP	PN-O2N	-2.37	1.44	1.55
2	F	301	NAP	PN-O1N	-2.36	1.42	1.50
2	I	301	NAP	C4A-N3A	-2.35	1.32	1.35
2	E	301	NAP	PN-O2N	-2.34	1.44	1.55
2	G	301	NAP	PA-O2A	-2.34	1.44	1.55
2	G	301	NAP	O7N-C7N	-2.32	1.19	1.24
2	A	301	NAP	O4D-C4D	-2.32	1.39	1.45
2	E	301	NAP	PA-O2A	-2.32	1.44	1.55
2	D	301	NAP	PA-O2A	-2.29	1.44	1.55
2	J	301	NAP	PA-O2A	-2.29	1.44	1.55
2	J	301	NAP	C3N-C7N	-2.27	1.47	1.50
2	J	301	NAP	P2B-O3X	-2.23	1.46	1.54
2	A	301	NAP	PN-O1N	-2.23	1.43	1.50
2	B	301	NAP	O7N-C7N	-2.22	1.19	1.24
2	A	301	NAP	O4B-C4B	-2.21	1.40	1.45
2	E	301	NAP	PN-O1N	-2.21	1.43	1.50
2	H	301	NAP	P2B-O2X	-2.19	1.46	1.54
2	I	301	NAP	O7N-C7N	-2.19	1.20	1.24
2	J	301	NAP	O4B-C4B	-2.18	1.40	1.45
2	I	301	NAP	C5A-N7A	-2.18	1.31	1.39
2	B	301	NAP	PA-O1A	-2.17	1.43	1.50
2	H	301	NAP	PN-O1N	-2.16	1.43	1.50
2	B	301	NAP	O4D-C4D	-2.15	1.40	1.45
2	J	301	NAP	P2B-O2X	-2.14	1.46	1.54
3	J	302	MPO	O1-S1	-2.14	1.38	1.45
2	J	301	NAP	C5A-C4A	2.14	1.46	1.40
2	E	301	NAP	P2B-O3X	-2.13	1.46	1.54
2	H	301	NAP	C2N-N1N	-2.12	1.32	1.35
3	J	302	MPO	O2-S1	-2.12	1.38	1.45
2	J	301	NAP	O7N-C7N	-2.11	1.20	1.24
2	E	301	NAP	C6N-N1N	-2.10	1.30	1.35
2	A	301	NAP	P2B-O2X	-2.10	1.46	1.54
2	C	301	NAP	C5A-N7A	-2.10	1.32	1.39
2	D	301	NAP	C5A-N7A	-2.08	1.32	1.39
2	H	301	NAP	O4B-C4B	-2.08	1.40	1.45
2	J	301	NAP	PN-O2N	-2.07	1.45	1.55
2	H	301	NAP	C5A-N7A	-2.04	1.32	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	NAP	O4B-C1B	2.03	1.43	1.41
2	J	301	NAP	O4B-C1B	2.03	1.43	1.41
2	A	301	NAP	C5A-N7A	-2.03	1.32	1.39
3	C	302	MPO	O3-S1	2.03	1.54	1.47

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	MPO	O3-S1-C1	4.86	113.64	105.77
3	D	302	MPO	O1-S1-C1	4.38	112.19	106.92
3	G	302	MPO	O2-S1-C1	4.35	112.15	106.92
3	D	302	MPO	O3-S1-C1	3.84	111.97	105.77
2	B	301	NAP	C4A-C5A-N7A	-3.80	105.44	109.40
3	B	302	MPO	O3-S1-C1	3.79	111.89	105.77
2	F	301	NAP	C3N-C7N-N7N	3.78	122.28	117.75
3	G	302	MPO	O1-S1-C1	3.77	111.45	106.92
2	D	301	NAP	N3A-C2A-N1A	-3.62	123.01	128.68
2	I	301	NAP	C4A-C5A-N7A	-3.48	105.77	109.40
2	I	301	NAP	N3A-C2A-N1A	-3.46	123.27	128.68
2	G	301	NAP	C4A-C5A-N7A	-3.34	105.92	109.40
2	D	301	NAP	C1B-N9A-C4A	-3.29	120.87	126.64
3	J	302	MPO	C6-C7-N1	-3.26	105.16	110.10
3	D	302	MPO	O2-S1-O1	-3.21	102.85	113.95
3	J	302	MPO	O3-S1-C1	3.20	110.95	105.77
2	H	301	NAP	C4A-C5A-N7A	-3.15	106.11	109.40
3	B	302	MPO	C2-C1-S1	-3.14	108.43	113.25
2	C	301	NAP	O3X-P2B-O1X	3.13	122.92	110.68
2	H	301	NAP	C3B-C2B-C1B	-3.01	97.23	102.89
2	C	301	NAP	N3A-C2A-N1A	-3.00	124.00	128.68
2	H	301	NAP	C1B-N9A-C4A	-2.95	121.46	126.64
2	A	301	NAP	N6A-C6A-N1A	2.93	124.66	118.57
2	E	301	NAP	N3A-C2A-N1A	-2.90	124.14	128.68
2	G	301	NAP	O2B-P2B-O1X	-2.88	98.26	109.39
2	C	301	NAP	O3B-C3B-C4B	-2.88	102.73	111.05
2	D	301	NAP	O3X-P2B-O1X	2.83	121.75	110.68
3	I	302	MPO	O2-S1-C1	2.82	110.32	106.92
2	A	301	NAP	C6N-C5N-C4N	-2.79	115.38	119.44
3	J	302	MPO	O1-S1-C1	2.79	110.27	106.92
2	H	301	NAP	O3X-P2B-O2X	2.77	118.23	107.64
2	B	301	NAP	N3A-C2A-N1A	-2.77	124.35	128.68
2	H	301	NAP	PN-O3-PA	-2.75	123.37	132.83
2	I	301	NAP	C3N-C7N-N7N	2.75	121.05	117.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	NAP	C5N-C6N-N1N	2.65	124.21	120.40
2	G	301	NAP	O3B-C3B-C4B	-2.63	103.44	111.05
2	B	301	NAP	C1B-N9A-C4A	-2.62	122.03	126.64
3	G	302	MPO	O4-C5-C4	-2.61	106.04	111.80
2	J	301	NAP	C3B-C2B-C1B	-2.60	98.01	102.89
2	E	301	NAP	O4B-C1B-C2B	-2.58	102.11	106.59
2	F	301	NAP	C4A-C5A-N7A	-2.57	106.72	109.40
2	H	301	NAP	C3N-C7N-N7N	2.55	120.81	117.75
2	D	301	NAP	C3N-C7N-N7N	2.55	120.81	117.75
2	G	301	NAP	N3A-C2A-N1A	-2.54	124.70	128.68
2	I	301	NAP	O7N-C7N-C3N	-2.52	116.62	119.63
2	F	301	NAP	N3A-C2A-N1A	-2.52	124.75	128.68
2	D	301	NAP	C4A-C5A-N7A	-2.50	106.79	109.40
2	H	301	NAP	N3A-C2A-N1A	-2.50	124.77	128.68
2	B	301	NAP	O3X-P2B-O2X	2.48	117.11	107.64
2	J	301	NAP	N3A-C2A-N1A	-2.47	124.82	128.68
2	G	301	NAP	C3N-C7N-N7N	2.47	120.71	117.75
2	C	301	NAP	C4A-C5A-N7A	-2.46	106.84	109.40
3	C	302	MPO	O1-S1-C1	2.44	109.86	106.92
3	B	302	MPO	O2-S1-C1	-2.42	104.01	106.92
3	F	302	MPO	C7-N1-C4	2.42	114.27	108.83
2	G	301	NAP	O2N-PN-O1N	2.41	124.14	112.24
3	G	302	MPO	C7-N1-C4	2.39	114.22	108.83
2	F	301	NAP	O7N-C7N-N7N	-2.39	119.18	122.58
2	J	301	NAP	PN-O3-PA	-2.39	124.64	132.83
2	B	301	NAP	C5B-C4B-C3B	-2.38	106.25	115.18
2	A	301	NAP	N3A-C2A-N1A	-2.37	124.97	128.68
2	B	301	NAP	O3B-C3B-C4B	-2.34	104.27	111.05
3	H	302	MPO	O3-S1-C1	2.31	109.50	105.77
2	H	301	NAP	C2B-C3B-C4B	2.30	107.00	101.99
2	A	301	NAP	O2B-P2B-O1X	-2.28	100.59	109.39
2	E	301	NAP	C2A-N1A-C6A	2.27	122.64	118.75
2	A	301	NAP	PN-O3-PA	-2.26	125.07	132.83
2	C	301	NAP	O2A-PA-O1A	2.26	123.40	112.24
2	E	301	NAP	O2B-P2B-O1X	-2.23	100.77	109.39
2	I	301	NAP	C1B-N9A-C4A	-2.22	122.74	126.64
2	A	301	NAP	O3X-P2B-O1X	2.20	119.30	110.68
2	H	301	NAP	N6A-C6A-N1A	2.20	123.14	118.57
2	A	301	NAP	O3B-C3B-C4B	-2.19	104.71	111.05
2	J	301	NAP	C1B-N9A-C4A	-2.18	122.80	126.64
3	J	302	MPO	O4-C6-C7	-2.18	106.99	111.80
2	B	301	NAP	C2N-C3N-C4N	2.18	120.73	118.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	302	MPO	O3-S1-O1	-2.18	105.95	111.27
2	H	301	NAP	C2A-N1A-C6A	2.17	122.47	118.75
2	G	301	NAP	C2A-N1A-C6A	2.16	122.45	118.75
2	F	301	NAP	C2A-N1A-C6A	2.15	122.43	118.75
2	J	301	NAP	C4A-C5A-N7A	-2.12	107.19	109.40
2	D	301	NAP	PN-O3-PA	-2.11	125.58	132.83
2	E	301	NAP	N6A-C6A-N1A	2.10	122.94	118.57
2	D	301	NAP	O2B-P2B-O1X	-2.10	101.28	109.39
2	A	301	NAP	C1B-N9A-C4A	-2.10	122.96	126.64
2	C	301	NAP	C1B-N9A-C4A	-2.09	122.97	126.64
2	C	301	NAP	C3N-C7N-N7N	2.08	120.25	117.75
3	J	302	MPO	O2-S1-O1	-2.08	106.77	113.95
2	I	301	NAP	O3D-C3D-C4D	-2.07	105.05	111.05
2	D	301	NAP	O2A-PA-O1A	2.07	122.49	112.24
3	A	302	MPO	C7-N1-C4	2.07	113.49	108.83
3	D	302	MPO	C7-N1-C4	2.07	113.48	108.83
3	I	302	MPO	O3-S1-C1	2.07	109.11	105.77
3	E	302	MPO	C6-O4-C5	2.06	116.78	109.89
2	D	301	NAP	C3B-C2B-C1B	-2.05	99.03	102.89
2	C	301	NAP	N6A-C6A-N1A	2.05	122.83	118.57
2	G	301	NAP	C5A-C6A-N1A	-2.05	115.71	120.35
2	C	301	NAP	C3B-C2B-C1B	-2.04	99.06	102.89
2	F	301	NAP	C6N-N1N-C2N	-2.04	120.12	121.97
2	G	301	NAP	PN-O3-PA	-2.04	125.84	132.83
3	A	302	MPO	C6-O4-C5	2.03	116.67	109.89
2	A	301	NAP	O4D-C4D-C3D	2.02	109.11	105.11
2	A	301	NAP	C4A-C5A-N7A	-2.02	107.30	109.40
3	H	302	MPO	O1-S1-C1	2.02	109.34	106.92

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAP	C2B-O2B-P2B-O2X
2	H	301	NAP	C2B-O2B-P2B-O3X
2	J	301	NAP	C2B-O2B-P2B-O1X
3	J	302	MPO	C2-C3-N1-C4
2	H	301	NAP	C1B-C2B-O2B-P2B
2	J	301	NAP	C1B-C2B-O2B-P2B
2	B	301	NAP	O4B-C4B-C5B-O5B
2	E	301	NAP	C2B-O2B-P2B-O1X
2	J	301	NAP	C2B-O2B-P2B-O3X

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	302	MPO	S1-C1-C2-C3
2	E	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	O4B-C4B-C5B-O5B
3	J	302	MPO	S1-C1-C2-C3
2	C	301	NAP	O4B-C4B-C5B-O5B
2	G	301	NAP	O4B-C4B-C5B-O5B
2	I	301	NAP	O4B-C4B-C5B-O5B
2	J	301	NAP	C3B-C2B-O2B-P2B
2	B	301	NAP	C3B-C4B-C5B-O5B
2	E	301	NAP	C3B-C4B-C5B-O5B
3	E	302	MPO	C2-C3-N1-C7
2	H	301	NAP	O4B-C4B-C5B-O5B
2	C	301	NAP	C5D-O5D-PN-O3
2	E	301	NAP	C2B-O2B-P2B-O3X
2	F	301	NAP	O4B-C4B-C5B-O5B
2	A	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	C3B-C4B-C5B-O5B
2	J	301	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

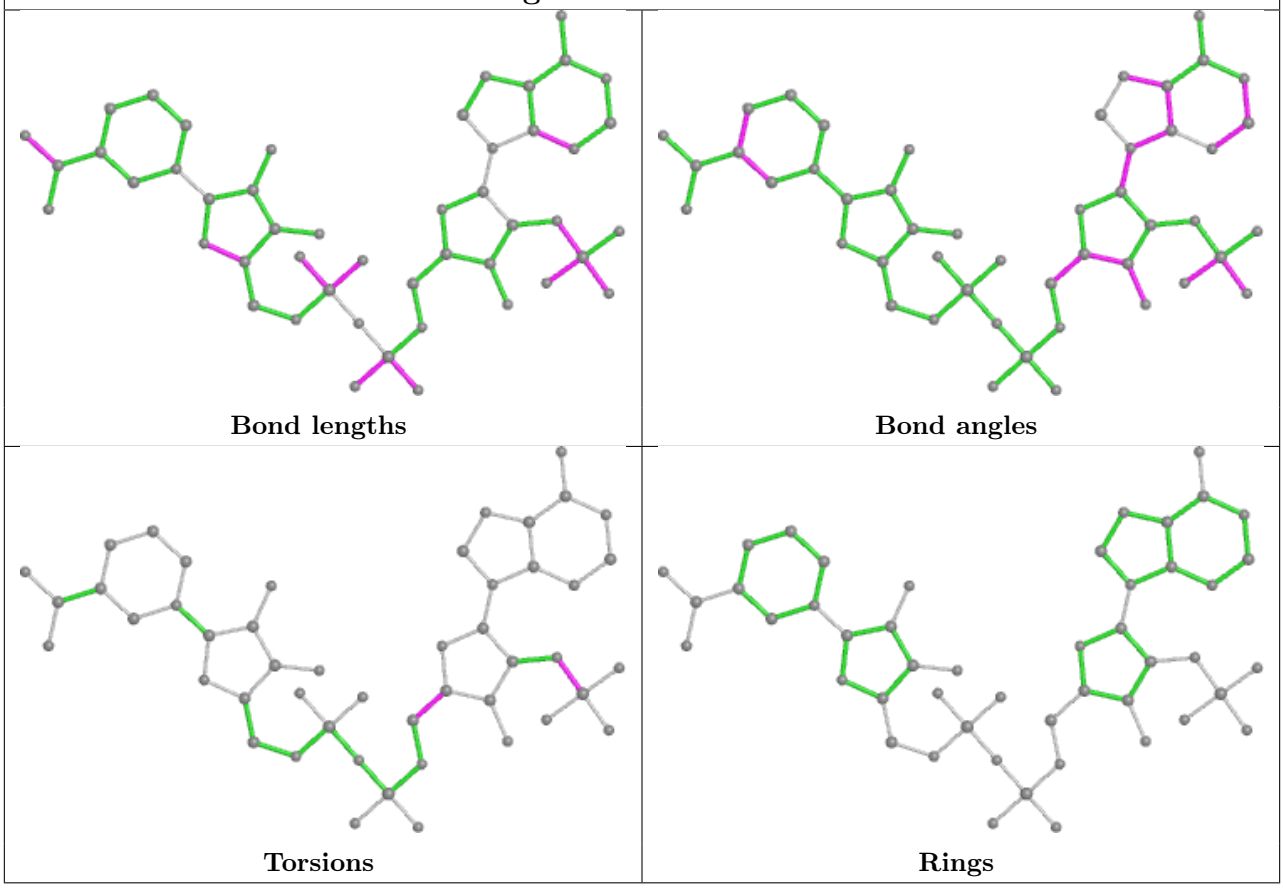
9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	MPO	1	0
2	H	301	NAP	1	0
2	C	301	NAP	1	0
3	B	302	MPO	3	0
2	I	301	NAP	1	0
3	G	302	MPO	1	0
3	J	302	MPO	2	0
2	A	301	NAP	1	0
2	J	301	NAP	2	0

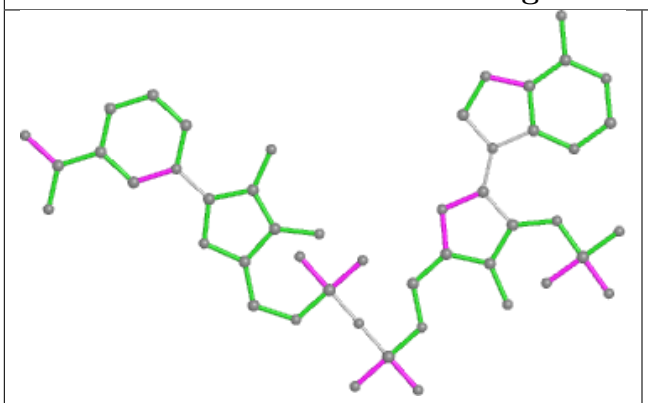
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

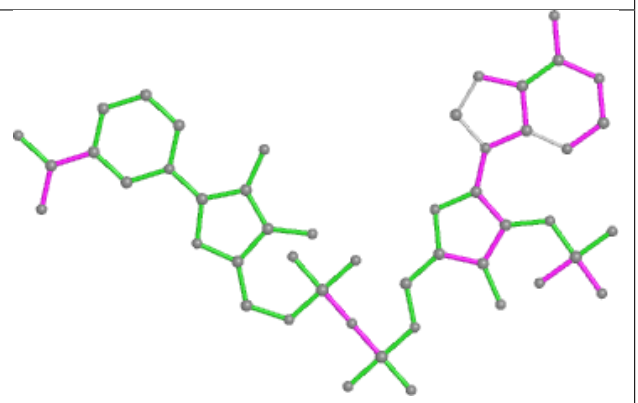
Ligand NAP B 301



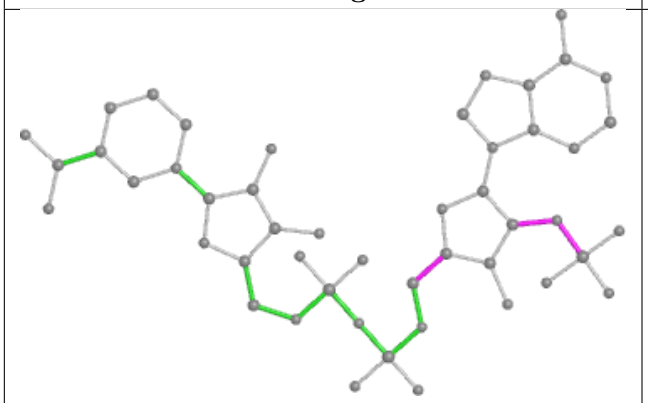
Ligand NAP H 301



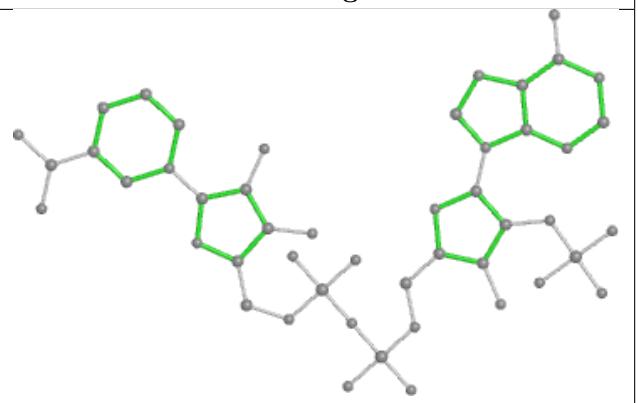
Bond lengths



Bond angles

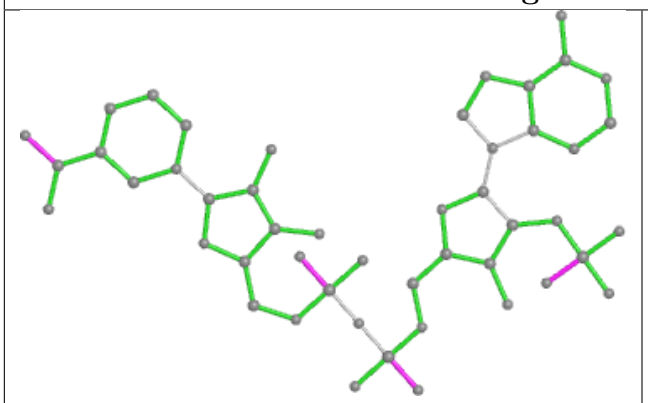


Torsions

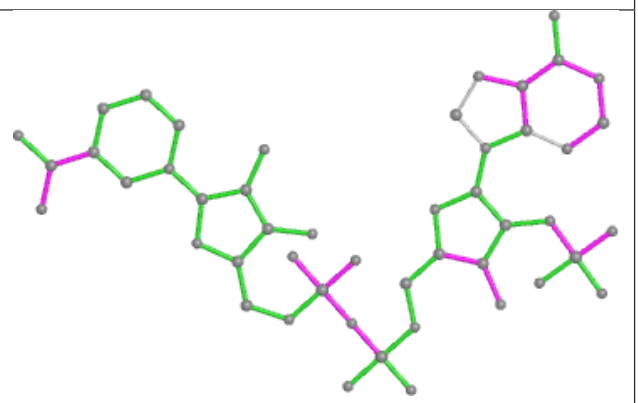


Rings

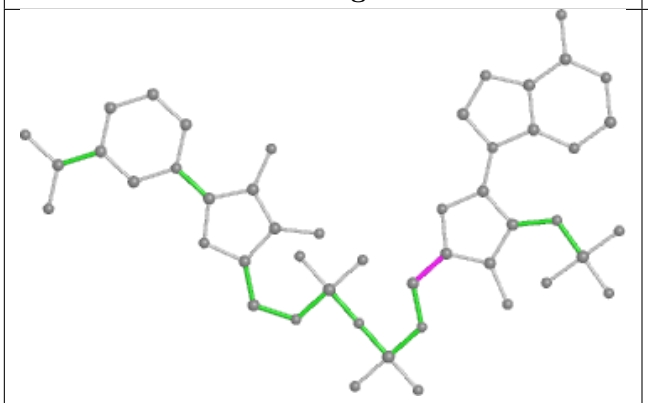
Ligand NAP G 301



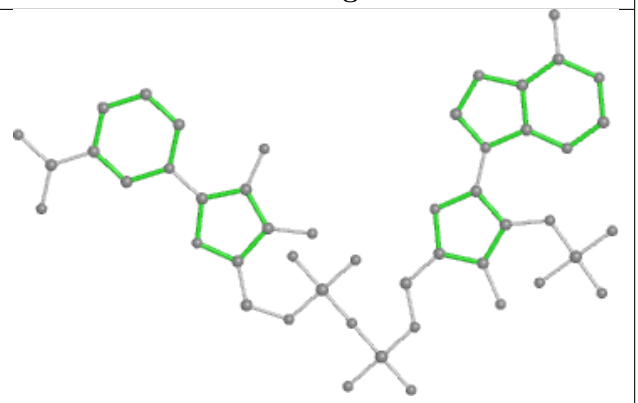
Bond lengths



Bond angles

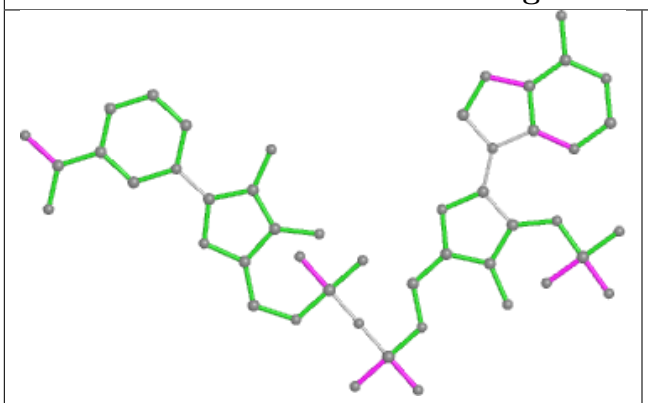


Torsions

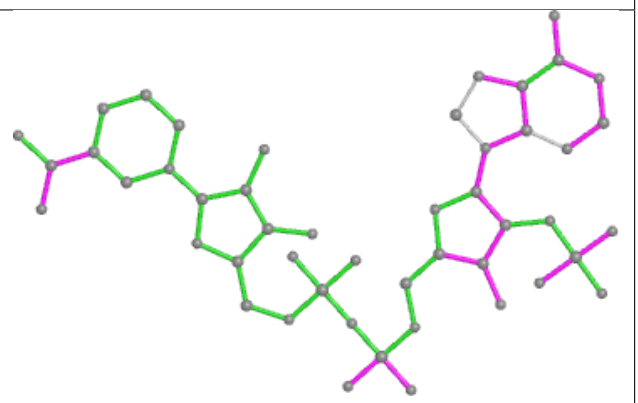


Rings

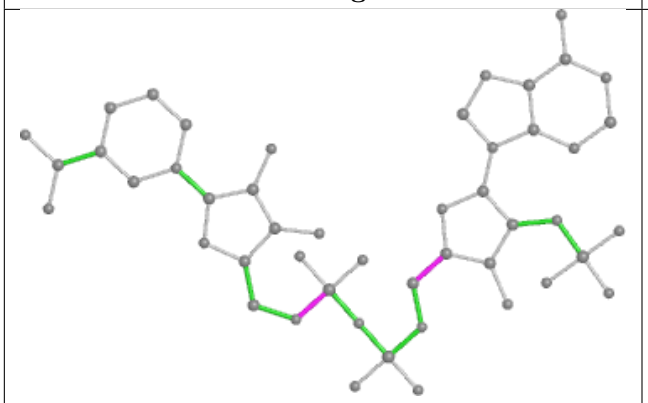
Ligand NAP C 301



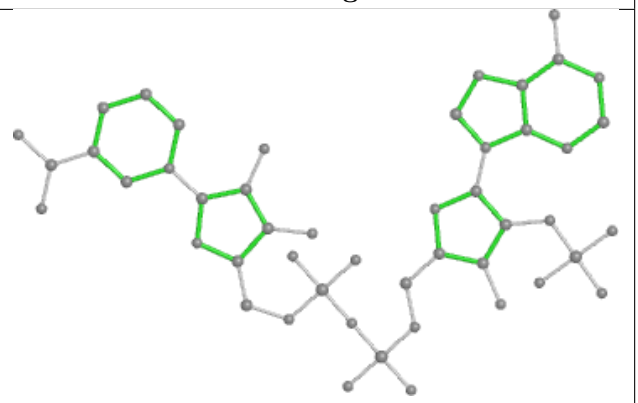
Bond lengths



Bond angles

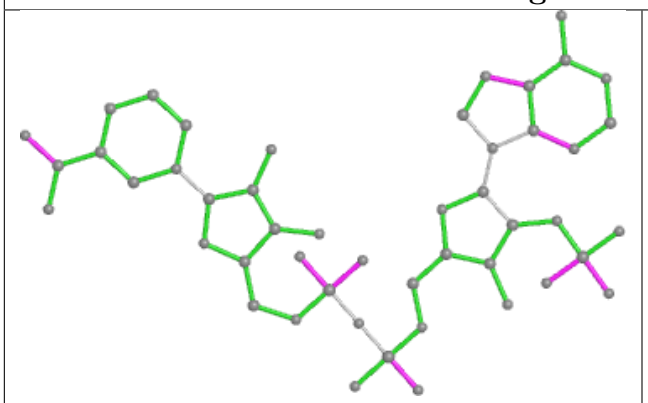


Torsions

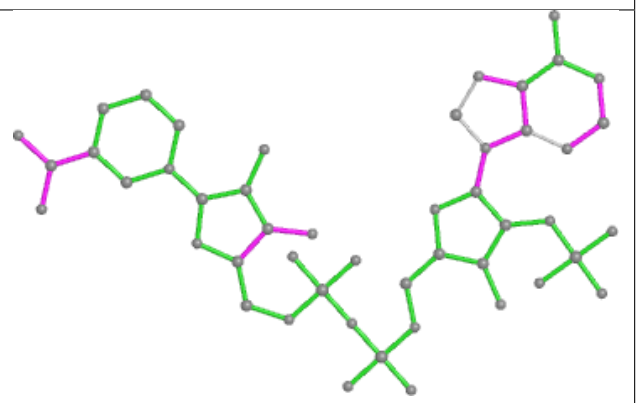


Rings

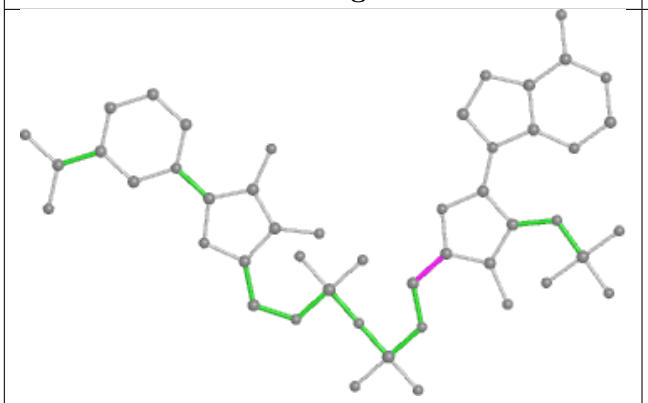
Ligand NAP I 301



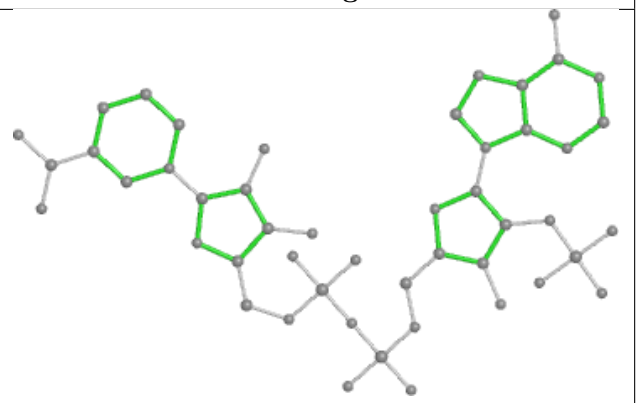
Bond lengths



Bond angles

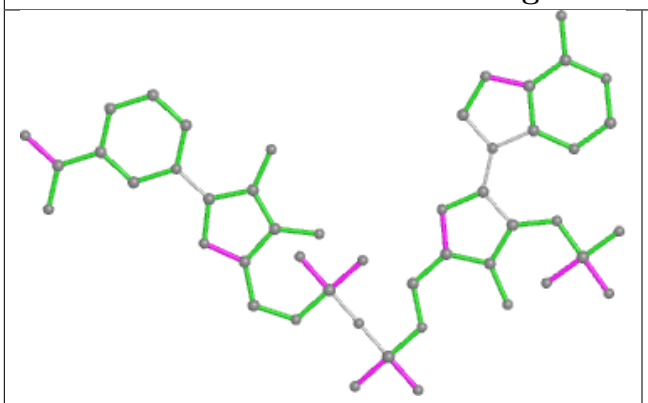


Torsions

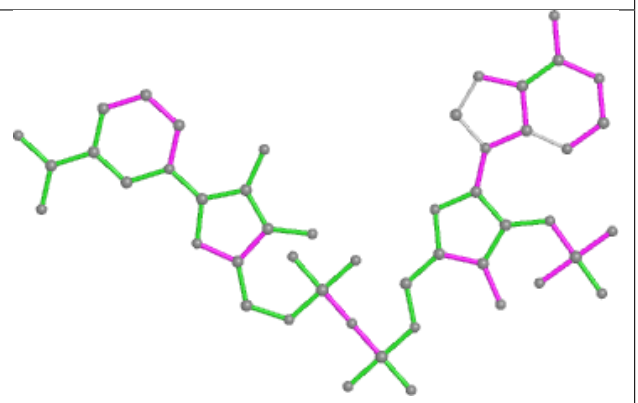


Rings

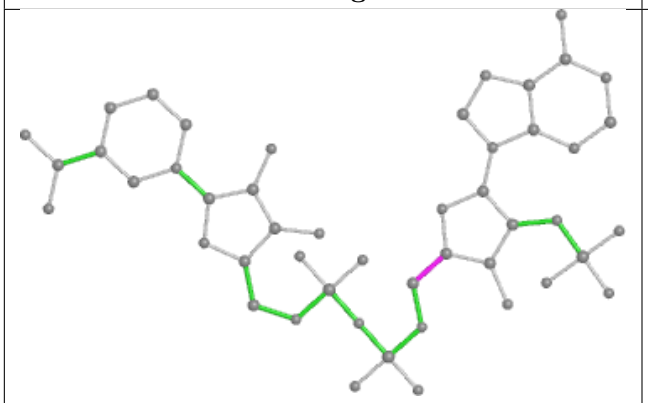
Ligand NAP A 301



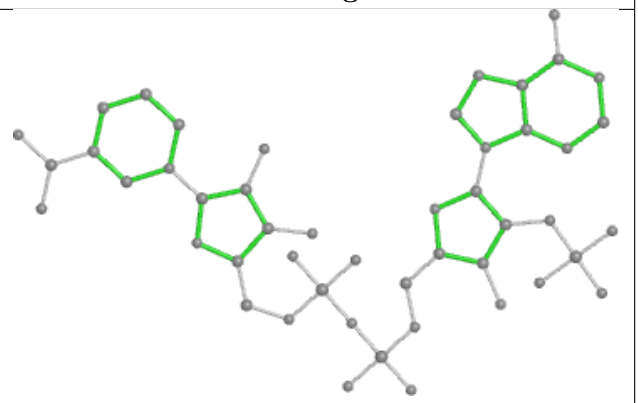
Bond lengths



Bond angles

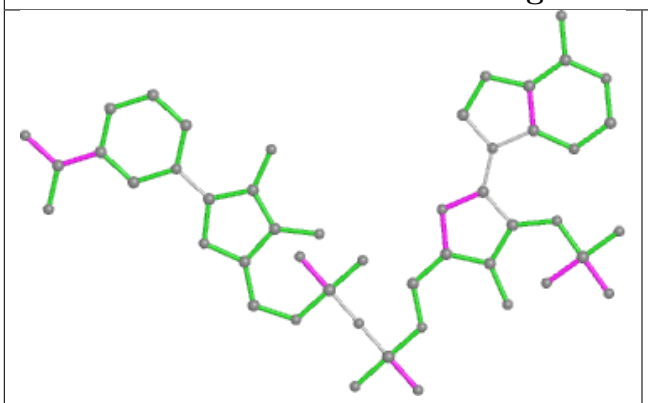


Torsions

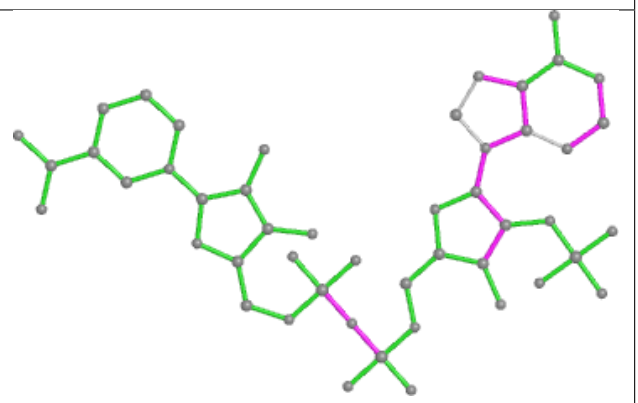


Rings

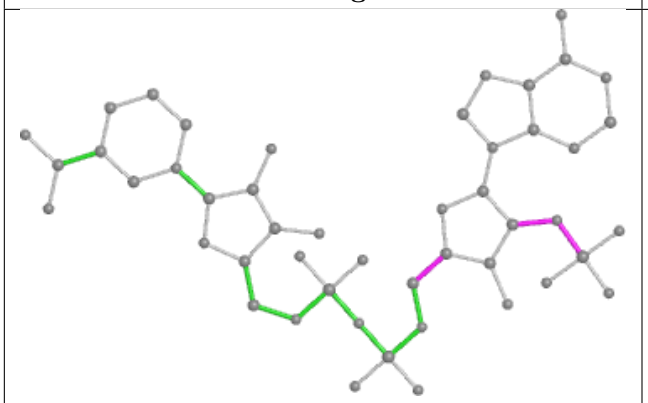
Ligand NAP J 301



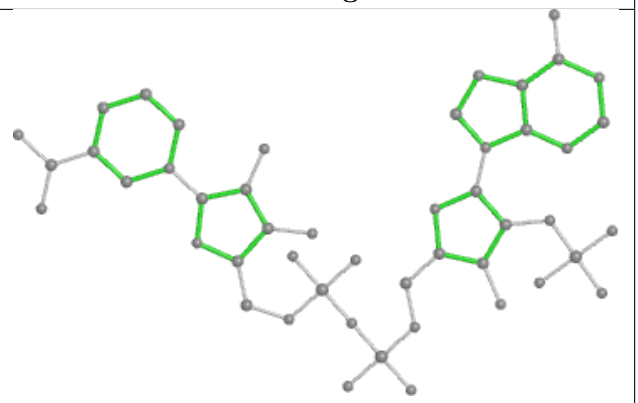
Bond lengths



Bond angles

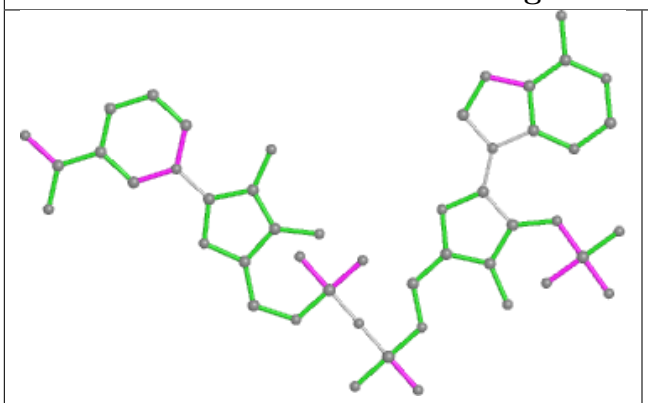


Torsions

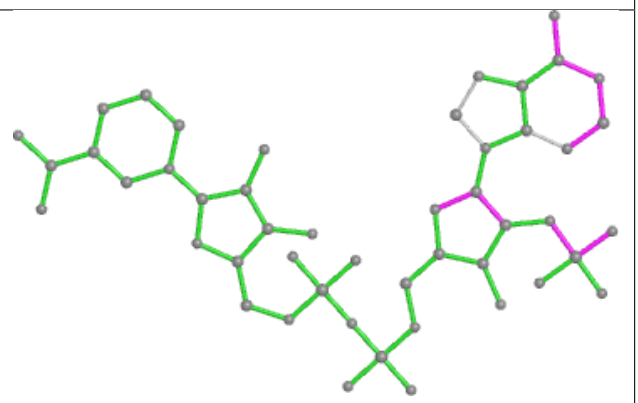


Rings

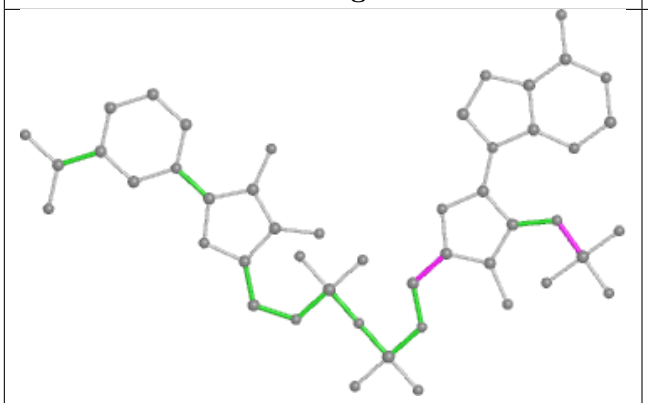
Ligand NAP E 301



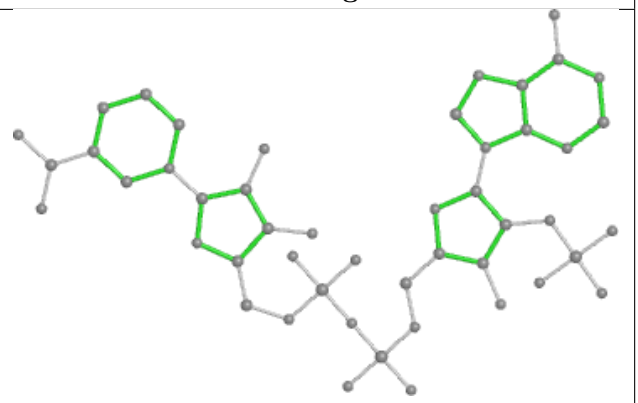
Bond lengths



Bond angles

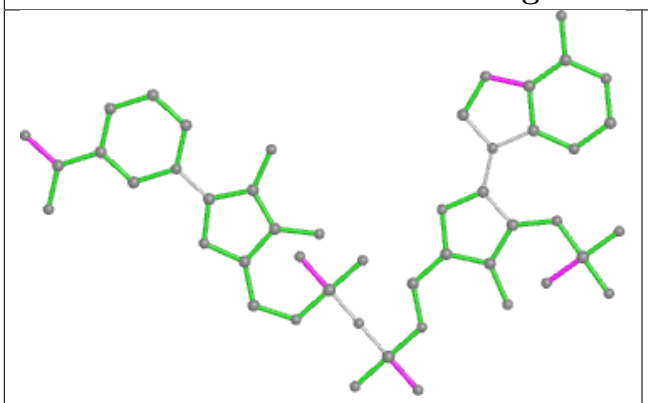


Torsions

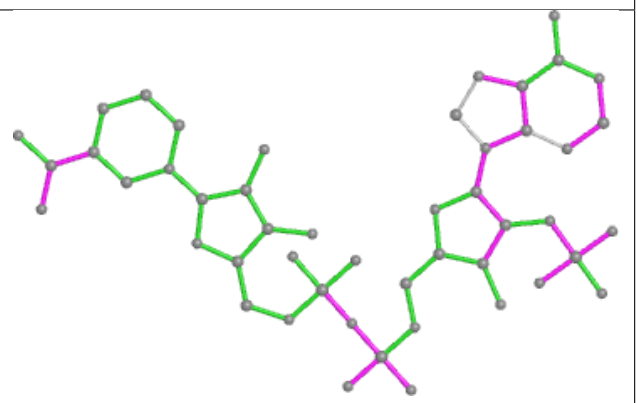


Rings

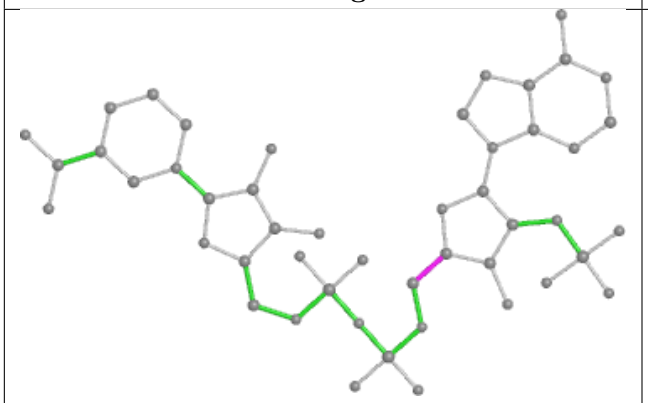
Ligand NAP D 301



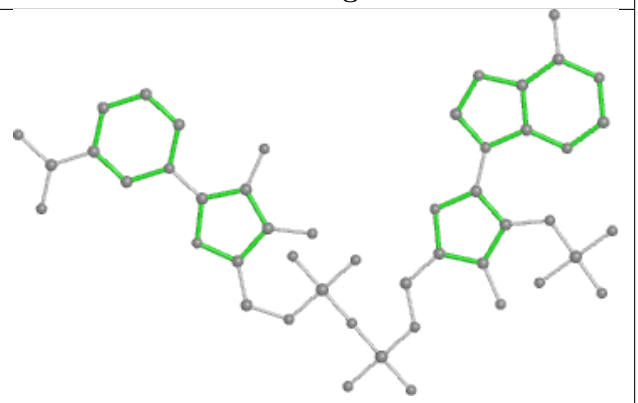
Bond lengths



Bond angles

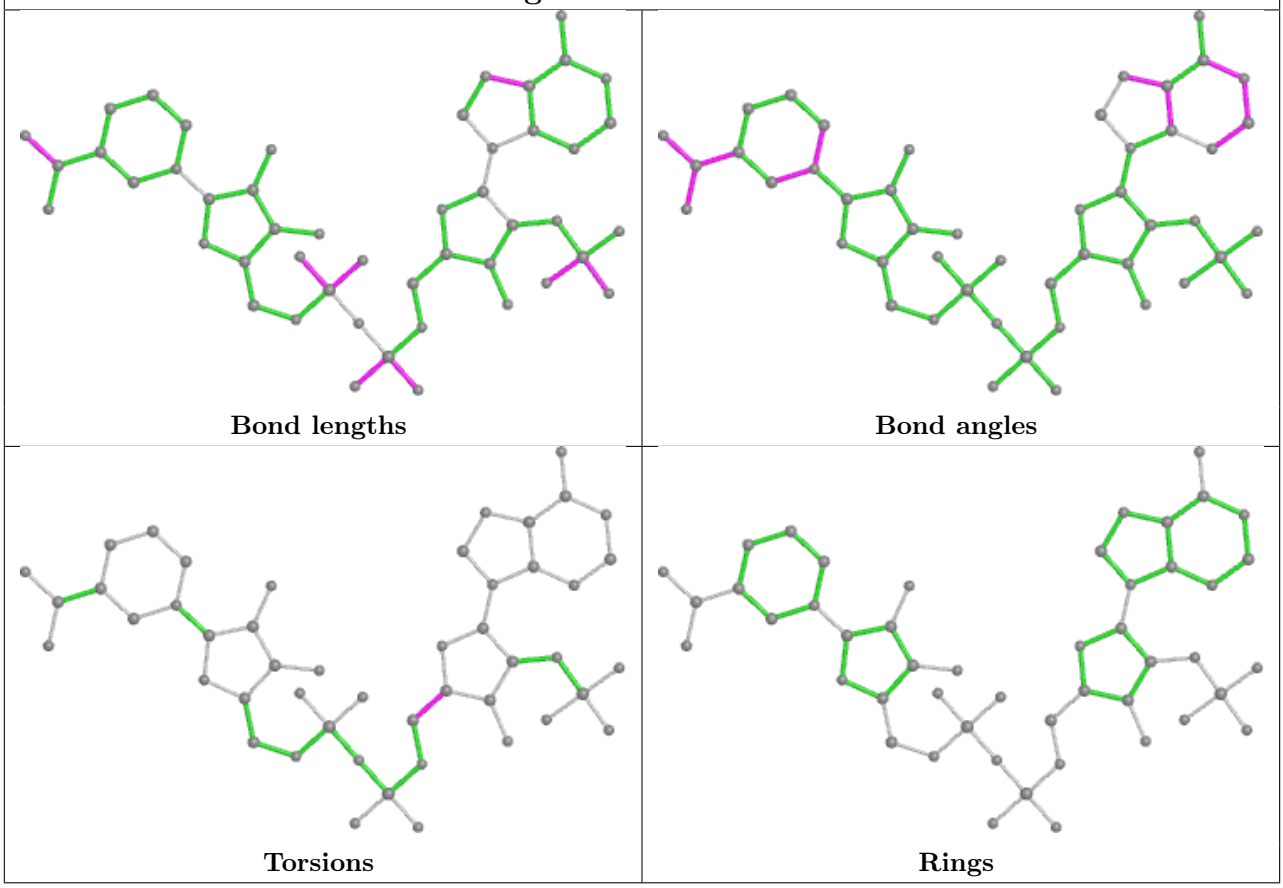


Torsions



Rings

Ligand NAP F 301



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	272/277 (98%)	-0.58	0	100	100	14, 22, 40, 62	0
1	B	272/277 (98%)	-0.20	5 (1%)	68	76	14, 26, 58, 86	0
1	C	270/277 (97%)	-0.37	3 (1%)	80	85	14, 25, 47, 77	0
1	D	271/277 (97%)	-0.09	11 (4%)	37	46	14, 33, 66, 96	0
1	E	272/277 (98%)	-0.22	6 (2%)	62	70	14, 25, 51, 74	0
1	F	272/277 (98%)	-0.46	4 (1%)	73	81	14, 23, 48, 69	0
1	G	269/277 (97%)	-0.00	6 (2%)	62	70	14, 35, 73, 89	0
1	H	272/277 (98%)	-0.27	5 (1%)	68	76	14, 27, 59, 85	0
1	I	272/277 (98%)	-0.31	7 (2%)	56	65	14, 28, 57, 82	0
1	J	270/277 (97%)	0.00	17 (6%)	20	28	14, 34, 67, 89	0
All	All	2712/2770 (97%)	-0.25	64 (2%)	59	68	14, 27, 60, 96	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	3	ILE	6.9
1	H	4	ILE	6.8
1	D	4	ILE	6.7
1	J	57	ILE	5.9
1	E	4	ILE	5.1
1	D	8	ALA	4.9
1	E	3	ILE	4.5
1	J	48	PRO	4.5
1	G	48	PRO	4.3
1	C	5	PRO	3.9
1	B	4	ILE	3.8
1	D	9	ASP	3.8
1	I	4	ILE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	48	PRO	3.8
1	E	49	ALA	3.7
1	J	61	VAL	3.5
1	D	7	PRO	3.5
1	D	5	PRO	3.4
1	J	46	SER	3.4
1	J	52	THR	3.4
1	I	8	ALA	3.3
1	G	47	ASN	3.2
1	J	47	ASN	3.1
1	C	9	ASP	3.1
1	J	97	LYS	3.1
1	B	3	ILE	3.0
1	H	46	SER	3.0
1	E	52	THR	2.9
1	I	9	ASP	2.9
1	G	46	SER	2.9
1	J	44	ILE	2.9
1	F	274[A]	SER	2.8
1	J	60	THR	2.8
1	J	63	SER	2.8
1	H	48	PRO	2.8
1	F	3	ILE	2.7
1	D	31	ARG	2.7
1	D	32	SER	2.7
1	D	10	SER	2.6
1	E	46	SER	2.6
1	I	3	ILE	2.6
1	B	48	PRO	2.6
1	I	5	PRO	2.6
1	B	52	THR	2.5
1	G	6	ILE	2.5
1	J	56	SER	2.4
1	C	7	PRO	2.4
1	G	8	ALA	2.3
1	J	26	ALA	2.3
1	J	93	PRO	2.2
1	H	63	SER	2.2
1	D	34	VAL	2.2
1	B	46	SER	2.1
1	J	49	ALA	2.1
1	F	46	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	51	ARG	2.1
1	F	4	ILE	2.1
1	G	52	THR	2.1
1	I	6	ILE	2.1
1	D	46	SER	2.1
1	D	274	SER	2.1
1	J	53	ALA	2.1
1	I	48	PRO	2.1
1	J	19	GLY	2.1

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 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
3	MPO	B	302	13/13	0.87	0.16	36,45,65,65	0
3	MPO	J	302	13/13	0.91	0.15	36,49,61,62	0
2	NAP	J	301	48/48	0.92	0.15	23,37,60,78	0
2	NAP	G	301	48/48	0.94	0.13	26,39,65,79	0
3	MPO	D	302	13/13	0.94	0.11	26,30,48,51	0
2	NAP	D	301	48/48	0.94	0.10	27,35,56,64	0
3	MPO	G	302	13/13	0.95	0.12	32,43,51,56	0
3	MPO	H	302	13/13	0.95	0.09	22,24,33,35	0
3	MPO	I	302	13/13	0.95	0.10	27,29,41,42	0
3	MPO	F	302	13/13	0.95	0.11	22,25,33,34	0
2	NAP	H	301	48/48	0.96	0.11	17,32,52,74	0
3	MPO	E	302	13/13	0.96	0.09	23,27,36,38	0
2	NAP	I	301	48/48	0.96	0.08	18,27,48,60	0
2	NAP	E	301	48/48	0.96	0.08	21,33,54,67	0

Continued on next page...

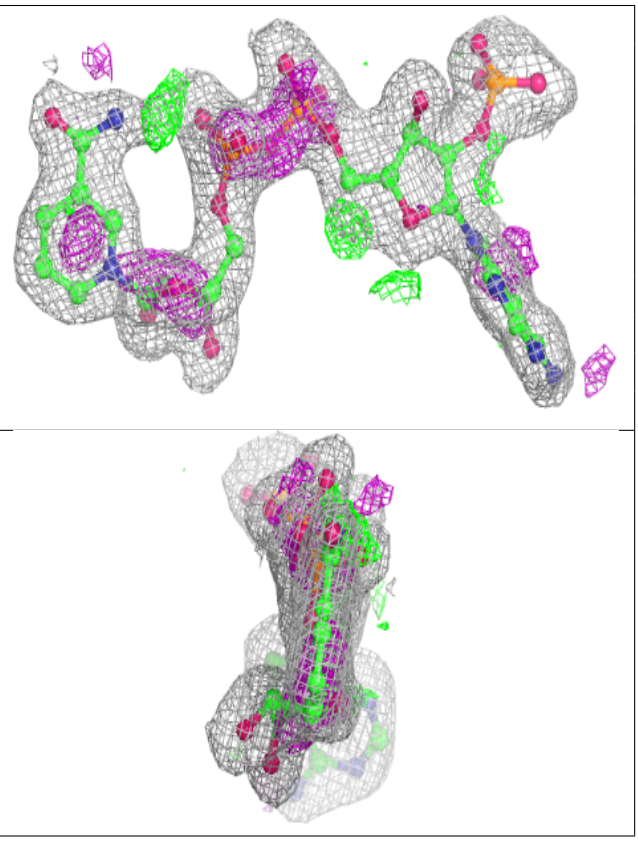
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MPO	A	302	13/13	0.96	0.10	20,24,27,28	0
2	NAP	C	301	48/48	0.96	0.08	22,27,43,51	0
3	MPO	C	302	13/13	0.96	0.08	24,28,36,36	0
2	NAP	F	301	48/48	0.97	0.07	20,29,50,55	0
2	NAP	B	301	48/48	0.97	0.08	20,32,44,64	0
2	NAP	A	301	48/48	0.97	0.08	16,21,34,38	0
4	CL	A	303	1/1	0.98	0.07	31,31,31,31	0
4	CL	H	303	1/1	0.98	0.06	29,29,29,29	0
4	CL	I	303	1/1	0.98	0.05	30,30,30,30	0
4	CL	J	303	1/1	0.98	0.06	28,28,28,28	0
4	CL	G	303	1/1	0.99	0.03	23,23,23,23	0
4	CL	B	303	1/1	0.99	0.04	22,22,22,22	0
4	CL	C	303	1/1	0.99	0.05	25,25,25,25	0
4	CL	E	303	1/1	0.99	0.03	22,22,22,22	0
4	CL	D	303	1/1	1.00	0.04	23,23,23,23	0
4	CL	F	303	1/1	1.00	0.05	24,24,24,24	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.

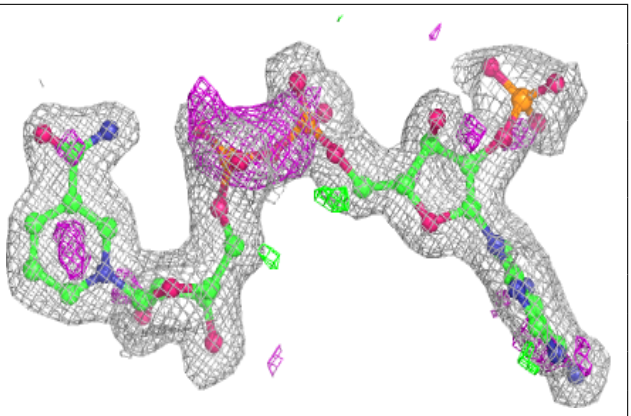
Electron density around NAP J 301:

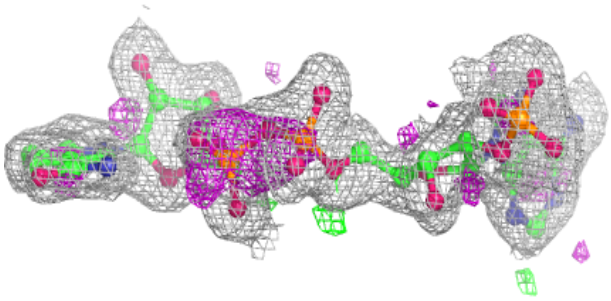
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

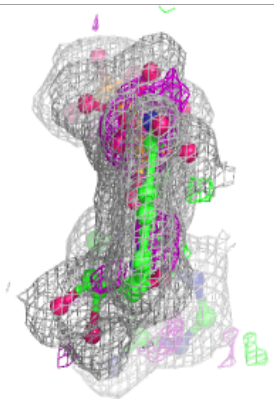


Electron density around NAP G 301:

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

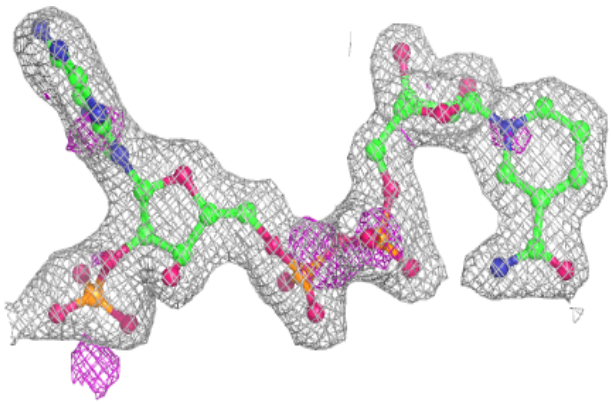


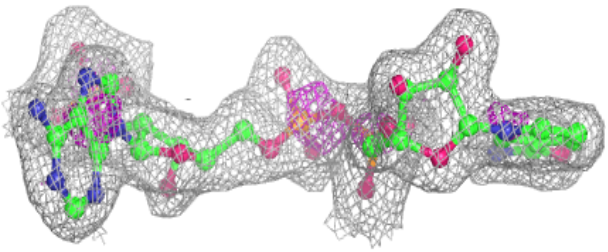


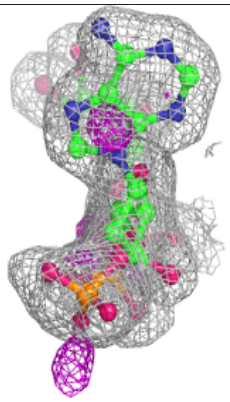


Electron density around NAP D 301:

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

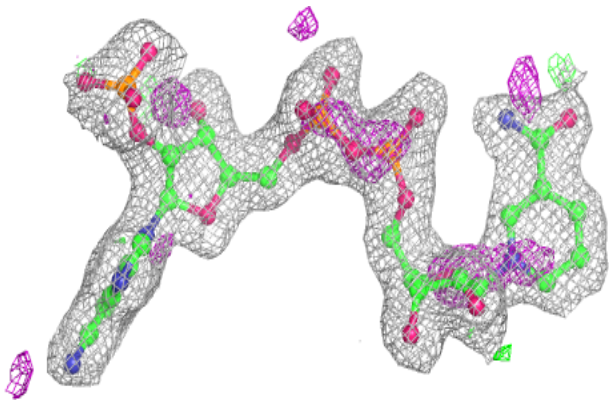


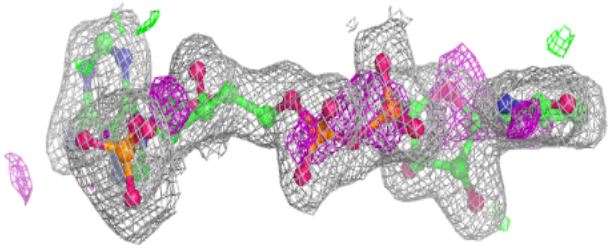


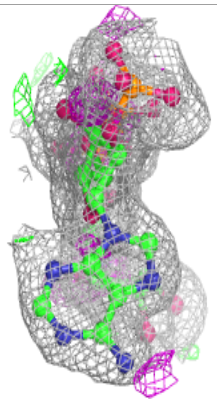


Electron density around NAP H 301:

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

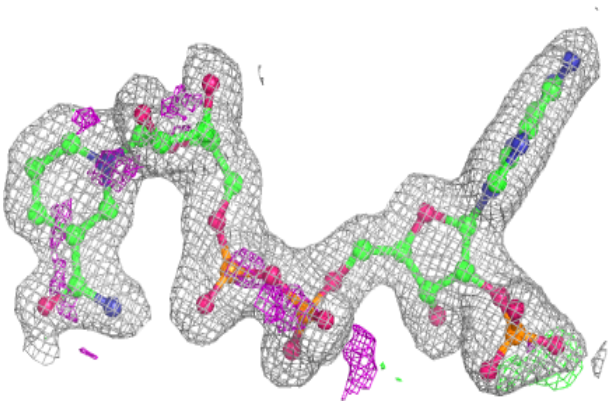


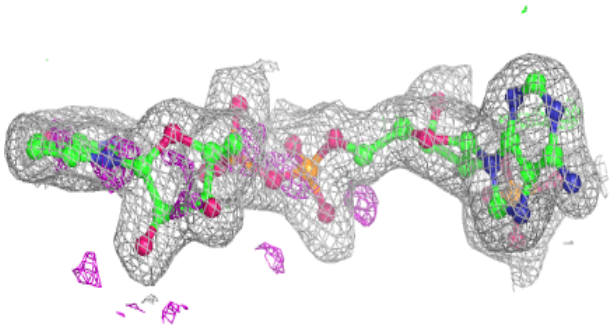


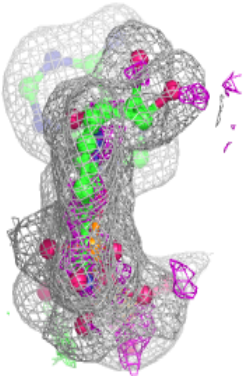


Electron density around NAP I 301:

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

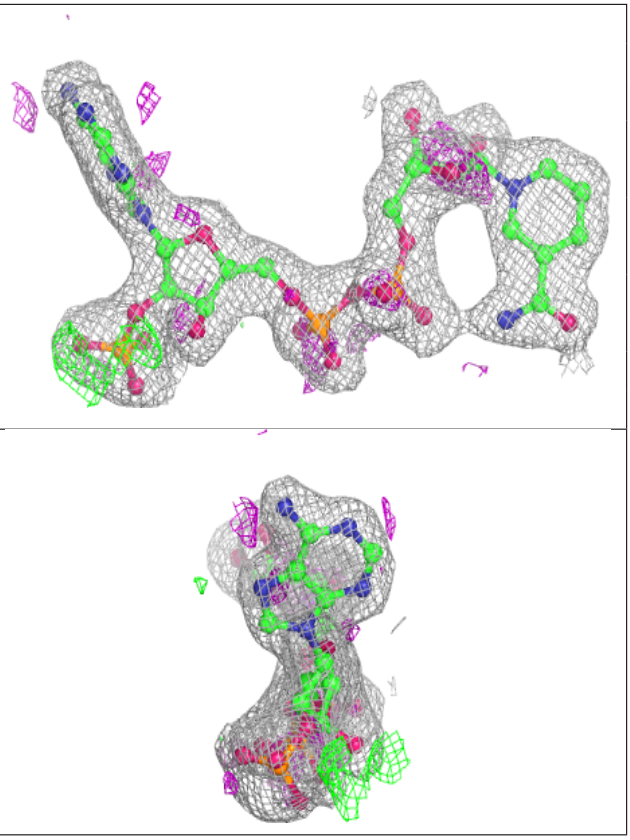






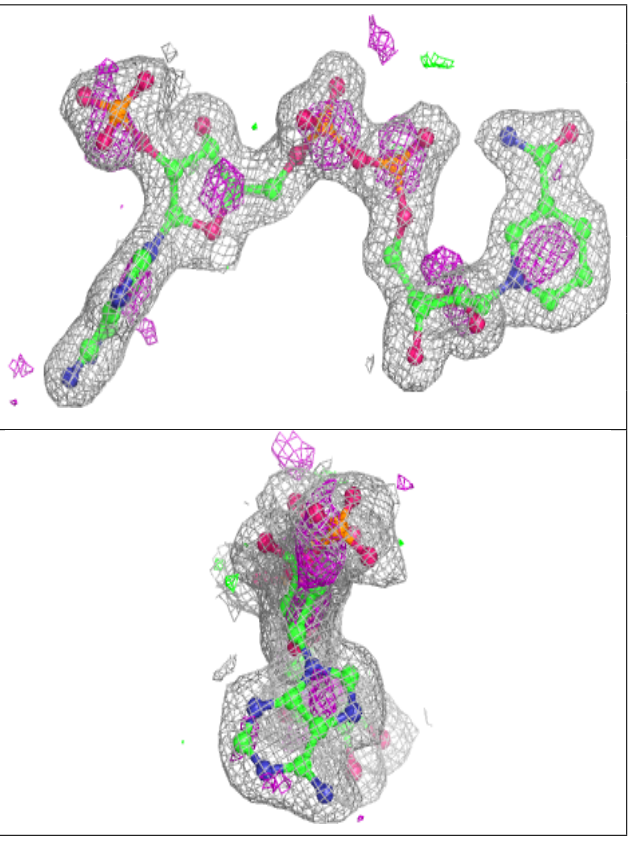
Electron density around NAP E 301:

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



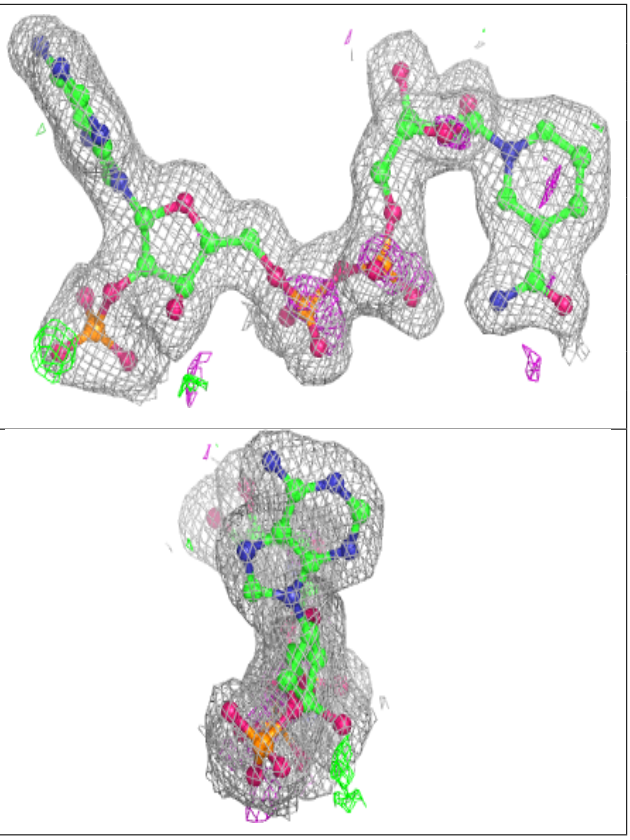
Electron density around NAP C 301:

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



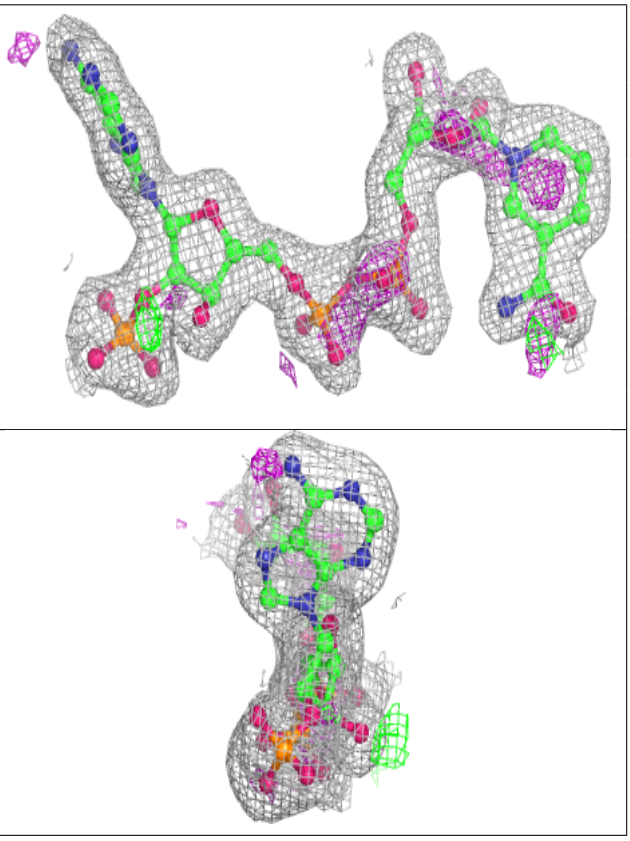
Electron density around NAP F 301:

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



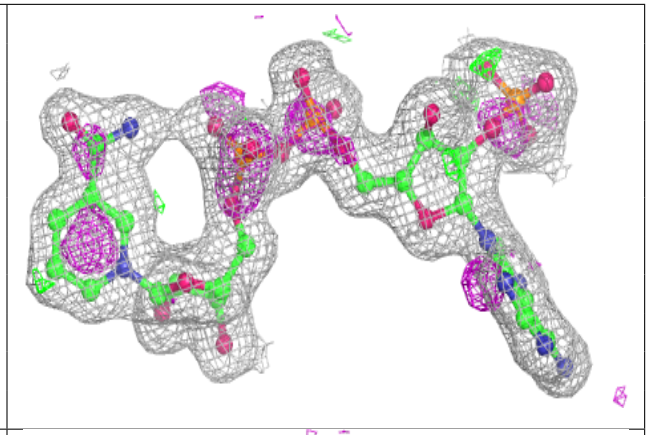
Electron density around NAP B 301:

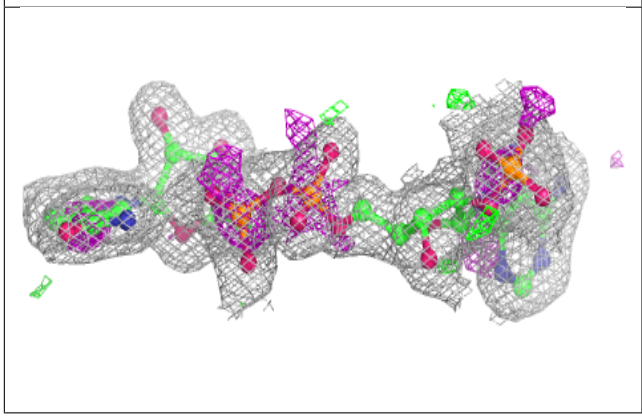
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

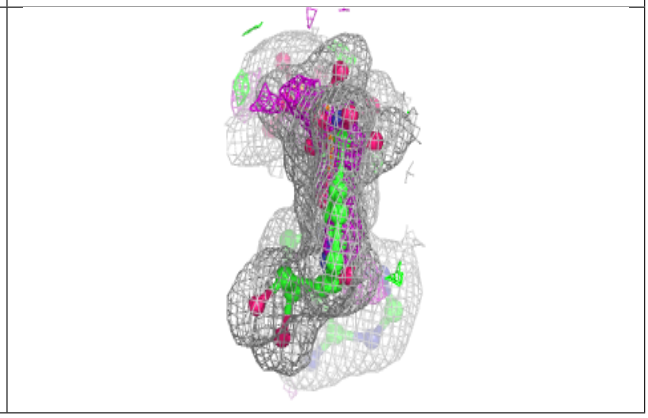


Electron density around NAP A 301:

$2mF_o$-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.