Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 10:19 pm GMT

PDB ID	:	4BMV
Title	:	Short-chain dehydrogenase from Sphingobium yanoikuyae in complex with NADPH
Authors	:	Man, H.; Kedziora, K.; Lavandera-Garcia, I.; Gotor-Fernandez, V.; Grogan, G.
Deposited on	:	2013-05-10
Resolution	:	2.50 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 ⓘ 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 ⓘ) were used in the production of this report:

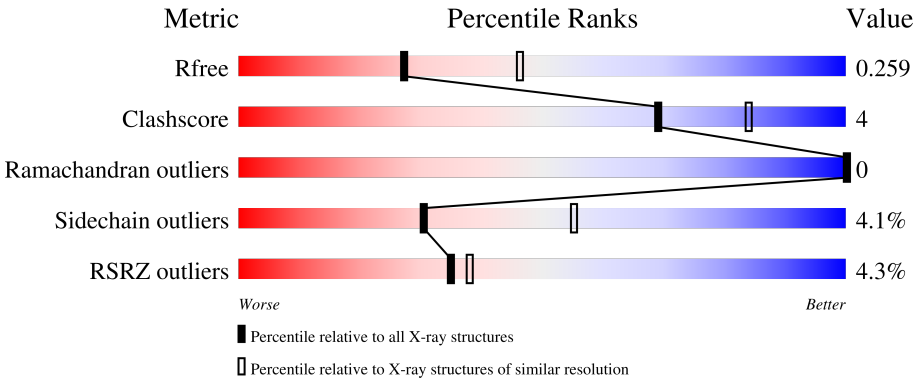
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	262	87% 10% • •
1	B	262	86% 10% • •
1	C	262	87% 10% • •
1	D	262	90% 7% • •

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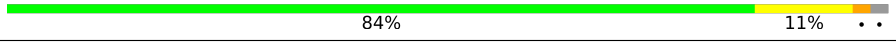
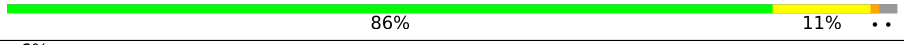
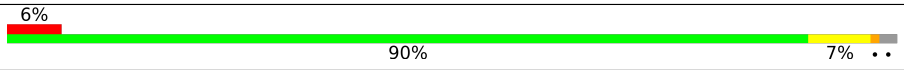
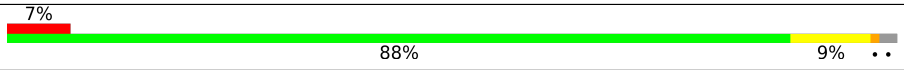
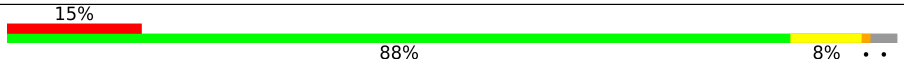
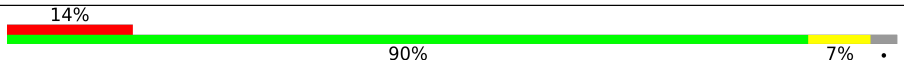
Mol	Chain	Length	Quality of chain
1	E	262	
1	F	262	
1	G	262	
1	H	262	
1	I	262	
1	J	262	

2 Entry composition (i)

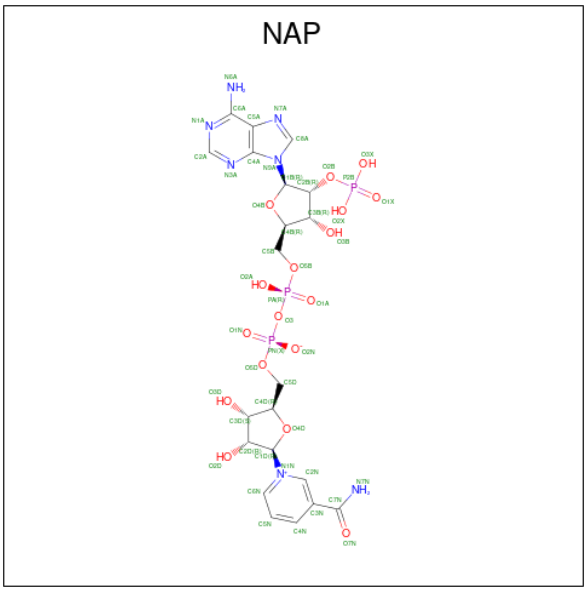
There are 3 unique types of molecules in this entry. The entry contains 19692 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SHORT-CHAIN DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1904	1198	343	359	4			
1	B	257	Total	C	N	O	S	0	0	0
			1922	1208	349	361	4			
1	C	258	Total	C	N	O	S	0	0	0
			1919	1206	347	362	4			
1	D	257	Total	C	N	O	S	0	0	0
			1918	1205	349	360	4			
1	E	257	Total	C	N	O	S	0	0	0
			1922	1208	349	361	4			
1	F	256	Total	C	N	O	S	0	0	0
			1914	1203	348	359	4			
1	G	256	Total	C	N	O	S	0	0	0
			1894	1191	344	355	4			
1	H	256	Total	C	N	O	S	0	0	0
			1880	1183	339	354	4			
1	I	254	Total	C	N	O	S	0	0	0
			1803	1134	321	344	4			
1	J	255	Total	C	N	O	S	0	0	0
			1846	1161	331	350	4			

- 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
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
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		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	48	Total	O	0	0
			48	48		

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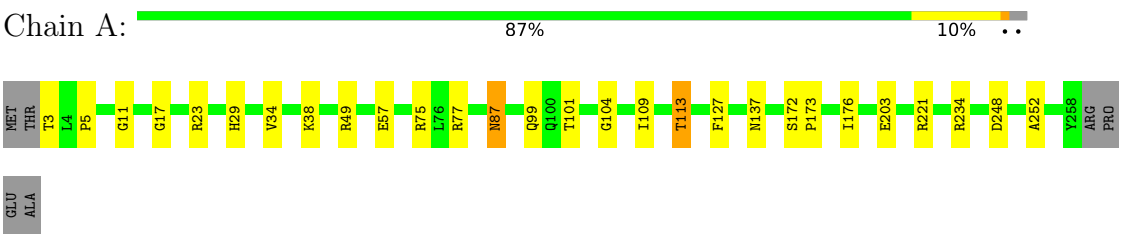
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	49	Total O 49 49	0	0
3	D	20	Total O 20 20	0	0
3	E	65	Total O 65 65	0	0
3	F	28	Total O 28 28	0	0
3	G	12	Total O 12 12	0	0
3	H	7	Total O 7 7	0	0
3	I	1	Total O 1 1	0	0
3	J	2	Total O 2 2	0	0

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.

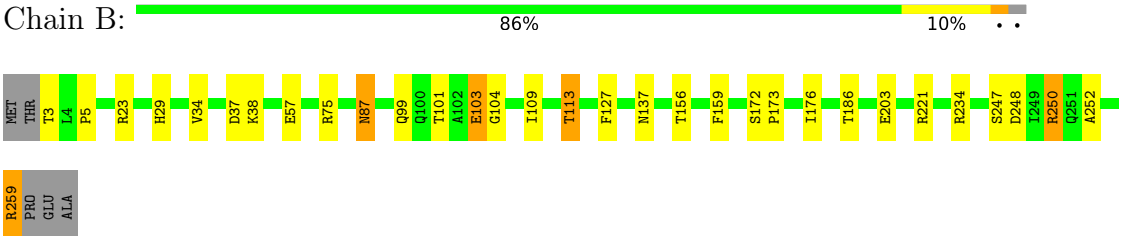
• Molecule 1: SHORT-CHAIN DEHYDROGENASE

Chain A:



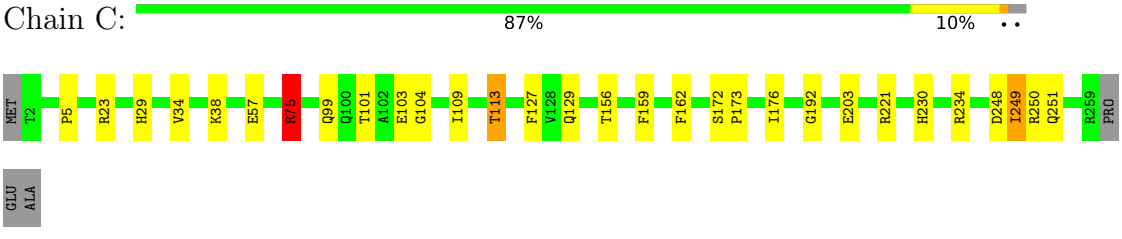
• Molecule 1: SHORT-CHAIN DEHYDROGENASE

Chain B:



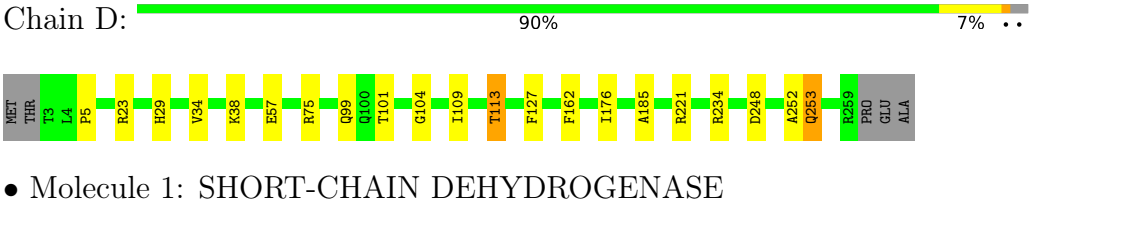
• Molecule 1: SHORT-CHAIN DEHYDROGENASE

Chain C:



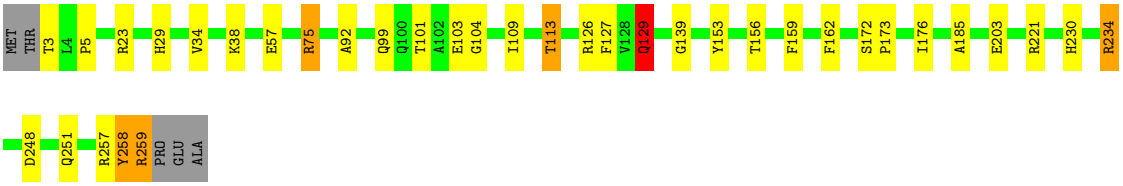
• Molecule 1: SHORT-CHAIN DEHYDROGENASE

Chain D:



• Molecule 1: SHORT-CHAIN DEHYDROGENASE

Chain E:

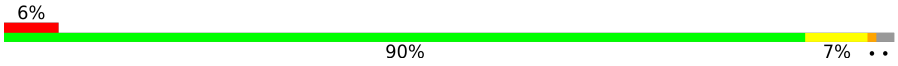


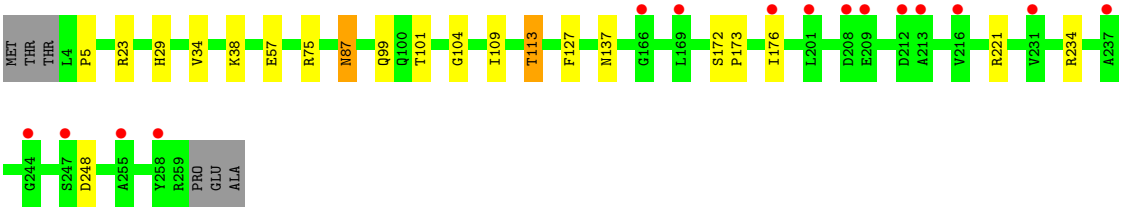
• Molecule 1: SHORT-CHAIN DEHYDROGENASE

Chain F:

• Molecule 1: SHORT-CHAIN DEHYDROGENASE

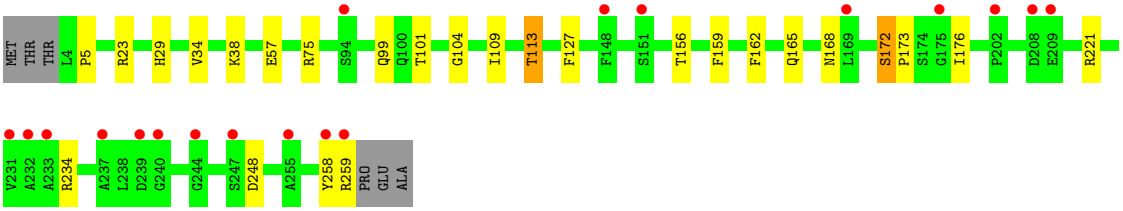
Chain G:





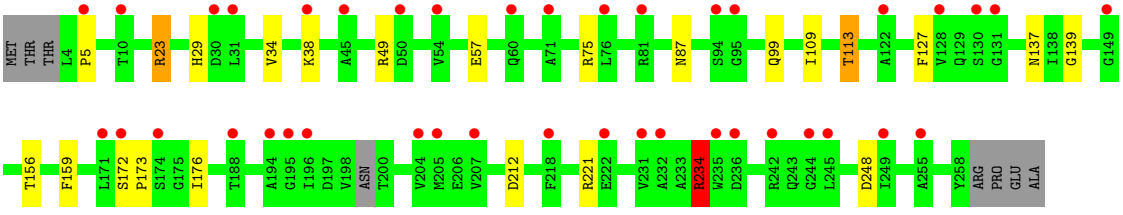
• Molecule 1: SHORT-CHAIN DEHYDROGENASE

Chain H:



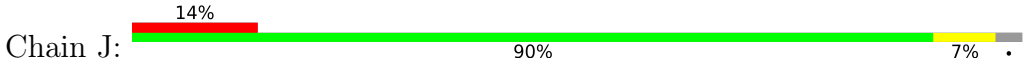
• Molecule 1: SHORT-CHAIN DEHYDROGENASE

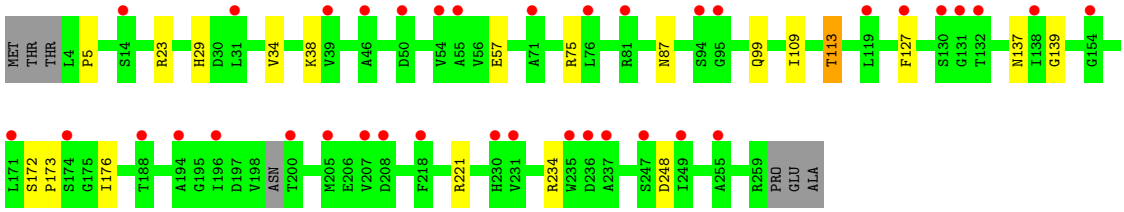
Chain I:



• Molecule 1: SHORT-CHAIN DEHYDROGENASE

Chain J:


14%
90%
7%


MET
THR
THR
L4
P5
S14
R23
H29
D30
L31
V34
K38
V39
A46
D50
V54
A55
V56
E57
A71
R75
L76
R81
N87
S94
G95
Q99
I109
T113
L119
F127
S130
G131
T132
N137
I138
G139
G154
L171
S172
P173
S174
G175
I176
T188
A194
G195
I196
D197
V198
ASN
T200
M205
E206
V207
D208
F218
R221
H230
V231
R234
W235
D236
A237
S247
D248
I249
A255
R259
PRO
GLU
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	144.91Å 86.84Å 155.61Å 90.00° 106.36° 90.00°	Depositor
Resolution (Å)	139.04 – 2.50 139.04 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.8 (139.04-2.50) 99.7 (139.04-2.34)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.234 , 0.251 0.241 , 0.259	Depositor DCC
R_{free} test set	7837 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19692	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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 20.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.3983e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.69	0/1930	0.77	1/2626 (0.0%)
1	B	0.67	0/1948	0.79	1/2648 (0.0%)
1	C	0.75	0/1945	0.80	3/2645 (0.1%)
1	D	0.64	0/1944	0.76	1/2642 (0.0%)
1	E	0.75	0/1948	0.81	2/2648 (0.1%)
1	F	0.66	0/1940	0.78	2/2637 (0.1%)
1	G	0.52	0/1919	0.71	0/2606
1	H	0.49	0/1904	0.71	0/2585
1	I	0.46	0/1826	0.71	2/2479 (0.1%)
1	J	0.48	0/1869	0.71	0/2543
All	All	0.62	0/19173	0.76	12/26059 (0.0%)

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	E	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	253	GLN	CA-CB-CG	6.12	126.87	113.40
1	C	249	ILE	CG1-CB-CG2	-5.80	98.64	111.40
1	A	49	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	250	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	E	129	GLN	CA-CB-CG	5.53	125.56	113.40
1	F	253	GLN	CA-CB-CG	5.29	125.03	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	75	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	129	GLN	CA-CB-CG	5.17	124.77	113.40
1	E	234	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	I	49	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	I	234	ARG	CG-CD-NE	5.06	122.43	111.80
1	F	259	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	258	TYR	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	1904	0	1935	15	0
1	B	1922	0	1959	24	0
1	C	1919	0	1947	17	0
1	D	1918	0	1951	13	0
1	E	1922	0	1959	28	0
1	F	1914	0	1950	19	0
1	G	1894	0	1916	10	0
1	H	1880	0	1901	13	0
1	I	1803	0	1765	13	0
1	J	1846	0	1845	10	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
2	E	48	0	25	1	0
2	F	48	0	25	3	0
2	G	48	0	25	0	0
2	H	48	0	25	0	0
2	I	48	0	25	1	0
2	J	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	58	0	0	2	0
3	B	48	0	0	2	0
3	C	49	0	0	0	0
3	D	20	0	0	0	0
3	E	65	0	0	2	0
3	F	28	0	0	0	0
3	G	12	0	0	0	0
3	H	7	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
All	All	19692	0	19378	142	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 (142) 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:E:113:THR:HG21	3:E:2034:HOH:O	1.67	0.94
1:B:101:THR:HG23	1:B:103:GLU:OE2	1.82	0.79
1:E:259:ARG:HA	1:E:259:ARG:NH1	1.99	0.77
1:E:234:ARG:HD2	1:F:248:ASP:OD2	1.86	0.75
1:E:259:ARG:HA	1:E:259:ARG:HH11	1.52	0.74
1:E:258:TYR:O	1:E:259:ARG:HB2	1.92	0.70
1:C:234:ARG:HD2	1:D:248:ASP:OD2	1.92	0.69
1:B:103:GLU:CD	1:B:103:GLU:H	1.96	0.66
1:J:127:PHE:HB3	1:J:176:ILE:HD12	1.81	0.63
1:E:248:ASP:OD2	1:F:234:ARG:HD2	1.99	0.63
1:F:127:PHE:HB3	1:F:176:ILE:HD12	1.81	0.62
1:I:234:ARG:HG2	1:I:234:ARG:HH11	1.65	0.61
1:D:127:PHE:HB3	1:D:176:ILE:HD12	1.82	0.61
1:C:203:GLU:HG2	1:D:252:ALA:HB2	1.82	0.60
1:E:257:ARG:NE	1:E:258:TYR:CE2	2.70	0.60
1:I:57:GLU:OE1	1:I:75:ARG:NH2	2.34	0.60
1:B:57:GLU:OE1	1:B:75:ARG:NH2	2.34	0.60
1:H:57:GLU:OE1	1:H:75:ARG:NH2	2.35	0.60
1:I:127:PHE:HB3	1:I:176:ILE:HD12	1.83	0.60
1:G:57:GLU:OE1	1:G:75:ARG:NH2	2.33	0.59
1:C:57:GLU:OE1	1:C:75:ARG:NH2	2.33	0.58
1:G:127:PHE:HB3	1:G:176:ILE:HD12	1.84	0.58
1:A:127:PHE:HB3	1:A:176:ILE:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:OE1	1:A:75:ARG:NH2	2.35	0.57
1:B:127:PHE:HB3	1:B:176:ILE:HD12	1.85	0.57
1:E:127:PHE:HB3	1:E:176:ILE:HD12	1.87	0.57
1:H:248:ASP:OD2	1:I:234:ARG:NH1	2.37	0.57
1:J:57:GLU:OE1	1:J:75:ARG:NH2	2.34	0.57
1:E:57:GLU:OE1	1:E:75:ARG:NH2	2.35	0.56
1:F:57:GLU:OE1	1:F:75:ARG:NH2	2.35	0.56
1:A:234:ARG:HD2	1:B:248:ASP:OD2	2.06	0.56
1:H:127:PHE:HB3	1:H:176:ILE:HD12	1.86	0.56
1:E:129:GLN:HE21	1:E:129:GLN:HA	1.70	0.56
1:D:57:GLU:OE1	1:D:75:ARG:NH2	2.37	0.55
1:H:234:ARG:HD2	1:I:248:ASP:OD2	2.05	0.55
1:C:127:PHE:HB3	1:C:176:ILE:HD12	1.87	0.55
1:E:203:GLU:HG2	1:F:252:ALA:HB2	1.87	0.55
1:G:248:ASP:OD2	1:J:234:ARG:HD2	2.06	0.55
1:E:257:ARG:NH2	1:F:229:LEU:O	2.39	0.55
1:A:248:ASP:OD2	1:B:234:ARG:HD2	2.08	0.54
1:E:5:PRO:O	1:E:29:HIS:HD2	1.92	0.53
1:F:256:ASP:OD1	1:F:259:ARG:NH2	2.37	0.53
1:G:234:ARG:HD2	1:J:248:ASP:OD2	2.09	0.53
1:C:248:ASP:OD2	1:D:234:ARG:HD2	2.09	0.52
1:F:127:PHE:HB3	1:F:176:ILE:CD1	2.39	0.52
1:A:252:ALA:HB2	1:B:203:GLU:HG2	1.92	0.52
1:D:127:PHE:HB3	1:D:176:ILE:CD1	2.40	0.52
1:B:101:THR:CG2	1:B:103:GLU:HG2	2.40	0.51
1:G:5:PRO:O	1:G:29:HIS:HD2	1.93	0.51
1:H:5:PRO:O	1:H:29:HIS:HD2	1.93	0.51
1:C:5:PRO:O	1:C:29:HIS:HD2	1.94	0.51
1:A:203:GLU:HG2	1:B:252:ALA:HB2	1.93	0.51
1:B:101:THR:CG2	1:B:103:GLU:OE2	2.57	0.51
1:F:5:PRO:O	1:F:29:HIS:HD2	1.93	0.51
1:J:127:PHE:HB3	1:J:176:ILE:CD1	2.40	0.51
1:D:5:PRO:O	1:D:29:HIS:HD2	1.93	0.51
1:B:5:PRO:O	1:B:29:HIS:HD2	1.94	0.51
1:A:5:PRO:O	1:A:29:HIS:HD2	1.94	0.50
1:I:5:PRO:O	1:I:29:HIS:HD2	1.95	0.50
1:B:101:THR:HG21	1:B:103:GLU:HG2	1.93	0.50
1:J:5:PRO:O	1:J:29:HIS:HD2	1.95	0.49
1:I:127:PHE:HB3	1:I:176:ILE:CD1	2.42	0.48
1:E:129:GLN:HE21	1:E:129:GLN:CA	2.24	0.48
1:G:127:PHE:HB3	1:G:176:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:HB3	1:A:176:ILE:CD1	2.44	0.47
1:B:127:PHE:HB3	1:B:176:ILE:CD1	2.44	0.47
1:E:172:SER:N	1:E:173:PRO:CD	2.78	0.47
2:F:300:NAP:O1N	2:F:300:NAP:H2N	2.15	0.47
1:J:139:GLY:O	2:J:300:NAP:H6N	2.14	0.47
1:H:127:PHE:HB3	1:H:176:ILE:CD1	2.45	0.46
1:C:251:GLN:HE21	1:D:185:ALA:H	1.64	0.46
1:D:162:PHE:CD1	1:D:162:PHE:C	2.88	0.46
1:F:162:PHE:C	1:F:162:PHE:CD1	2.87	0.46
1:J:87:ASN:HB2	1:J:137:ASN:HD22	1.80	0.46
1:I:87:ASN:HB2	1:I:137:ASN:HD22	1.81	0.46
1:E:127:PHE:HB3	1:E:176:ILE:CD1	2.46	0.46
1:F:11:GLY:HA2	2:F:300:NAP:H1B	1.98	0.46
1:C:172:SER:N	1:C:173:PRO:CD	2.79	0.46
1:H:258:TYR:C	1:H:259:ARG:HG3	2.37	0.45
1:I:139:GLY:O	2:I:300:NAP:H6N	2.16	0.45
1:E:162:PHE:C	1:E:162:PHE:CD1	2.90	0.45
1:D:109:ILE:O	1:D:113:THR:HB	2.17	0.45
1:G:109:ILE:O	1:G:113:THR:HB	2.17	0.45
1:I:109:ILE:O	1:I:113:THR:HB	2.17	0.45
1:A:77:ARG:NH1	3:A:2024:HOH:O	2.50	0.45
1:H:109:ILE:O	1:H:113:THR:HB	2.17	0.44
1:B:259:ARG:CZ	1:B:259:ARG:CB	2.96	0.44
1:B:109:ILE:O	1:B:113:THR:HB	2.18	0.44
1:E:185:ALA:H	1:F:251:GLN:HE21	1.66	0.44
1:G:87:ASN:HB2	1:G:137:ASN:HD22	1.82	0.44
1:H:168:ASN:O	1:H:172:SER:HB2	2.17	0.44
1:F:109:ILE:O	1:F:113:THR:HB	2.17	0.44
1:A:109:ILE:O	1:A:113:THR:HB	2.18	0.44
3:B:2008:HOH:O	1:C:192:GLY:HA3	2.16	0.44
1:C:127:PHE:HB3	1:C:176:ILE:CD1	2.47	0.44
1:C:230:HIS:HE1	1:D:253:GLN:O	2.00	0.44
1:B:186:THR:H	2:B:300:NAP:H72N	1.66	0.44
1:C:109:ILE:O	1:C:113:THR:HB	2.18	0.44
1:E:230:HIS:HE1	1:F:253:GLN:O	2.00	0.44
1:B:37:ASP:HA	3:B:2007:HOH:O	2.17	0.43
1:I:172:SER:N	1:I:173:PRO:CD	2.81	0.43
1:J:172:SER:N	1:J:173:PRO:CD	2.81	0.43
1:E:109:ILE:O	1:E:113:THR:HB	2.18	0.43
1:B:87:ASN:HB2	1:B:137:ASN:HD22	1.84	0.43
1:E:101:THR:HG22	1:E:103:GLU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:SER:N	1:H:173:PRO:CD	2.81	0.43
1:A:172:SER:N	1:A:173:PRO:CD	2.81	0.43
1:B:101:THR:HG22	1:B:104:GLY:H	1.84	0.43
1:C:101:THR:HG22	1:C:104:GLY:H	1.83	0.43
1:J:109:ILE:O	1:J:113:THR:HB	2.18	0.43
1:F:113:THR:HG22	1:F:114:THR:N	2.34	0.43
1:C:101:THR:HG22	1:C:103:GLU:N	2.34	0.43
1:F:168:ASN:ND2	1:F:172:SER:HB3	2.34	0.42
1:E:101:THR:HG22	1:E:104:GLY:H	1.84	0.42
1:E:251:GLN:HE21	1:F:185:ALA:H	1.66	0.42
1:E:139:GLY:O	2:E:300:NAP:H6N	2.19	0.42
1:G:172:SER:N	1:G:173:PRO:CD	2.82	0.42
1:H:162:PHE:HA	1:H:165:GLN:HE21	1.83	0.42
1:B:172:SER:N	1:B:173:PRO:CD	2.82	0.42
1:D:101:THR:HG22	1:D:104:GLY:H	1.84	0.42
1:H:101:THR:HG22	1:H:104:GLY:H	1.85	0.42
1:E:29:HIS:HE1	3:E:2011:HOH:O	2.02	0.42
1:G:101:THR:HG22	1:G:104:GLY:H	1.83	0.42
1:B:247:SER:O	1:B:250:ARG:NH1	2.53	0.41
1:C:156:THR:O	1:C:159:PHE:HB3	2.20	0.41
1:E:92:ALA:HA	1:E:153:TYR:CD1	2.56	0.41
1:E:156:THR:O	1:E:159:PHE:HB3	2.21	0.41
1:B:87:ASN:HD22	1:B:87:ASN:HA	1.71	0.41
1:A:87:ASN:HB2	1:A:137:ASN:HD22	1.85	0.41
1:C:162:PHE:CD1	1:C:162:PHE:C	2.93	0.41
1:C:251:GLN:NE2	1:D:185:ALA:H	2.18	0.41
1:A:101:THR:HG22	1:A:104:GLY:H	1.85	0.41
1:B:156:THR:O	1:B:159:PHE:HB3	2.20	0.40
1:H:156:THR:O	1:H:159:PHE:HB3	2.21	0.40
1:A:11:GLY:O	1:A:17:GLY:HA3	2.22	0.40
1:A:87:ASN:ND2	3:A:2001:HOH:O	2.51	0.40
1:B:103:GLU:CD	1:B:103:GLU:N	2.71	0.40
1:F:156:THR:O	1:F:159:PHE:HB3	2.21	0.40
1:E:126:ARG:HA	1:E:129:GLN:HG2	2.03	0.40
1:I:156:THR:O	1:I:159:PHE:HB3	2.21	0.40
1:F:186:THR:H	2:F:300:NAP:H72N	1.70	0.40
1:I:23:ARG:HD3	1:I:212:ASP:OD1	2.22	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	254/262 (97%)	251 (99%)	3 (1%)	0	100	100
1	B	255/262 (97%)	252 (99%)	3 (1%)	0	100	100
1	C	256/262 (98%)	252 (98%)	4 (2%)	0	100	100
1	D	255/262 (97%)	252 (99%)	3 (1%)	0	100	100
1	E	255/262 (97%)	252 (99%)	3 (1%)	0	100	100
1	F	254/262 (97%)	251 (99%)	3 (1%)	0	100	100
1	G	253/262 (97%)	250 (99%)	3 (1%)	0	100	100
1	H	253/262 (97%)	250 (99%)	3 (1%)	0	100	100
1	I	250/262 (95%)	247 (99%)	3 (1%)	0	100	100
1	J	251/262 (96%)	248 (99%)	3 (1%)	0	100	100
All	All	2536/2620 (97%)	2505 (99%)	31 (1%)	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	191/198 (96%)	183 (96%)	8 (4%)	30	54
1	B	193/198 (98%)	183 (95%)	10 (5%)	23	44
1	C	192/198 (97%)	183 (95%)	9 (5%)	26	49
1	D	192/198 (97%)	186 (97%)	6 (3%)	40	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	193/198 (98%)	183 (95%)	10 (5%)	23 44
1	F	192/198 (97%)	185 (96%)	7 (4%)	35 61
1	G	187/198 (94%)	180 (96%)	7 (4%)	34 60
1	H	184/198 (93%)	177 (96%)	7 (4%)	33 58
1	I	169/198 (85%)	162 (96%)	7 (4%)	30 55
1	J	178/198 (90%)	172 (97%)	6 (3%)	37 63
All	All	1871/1980 (94%)	1794 (96%)	77 (4%)	30 55

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	23	ARG
1	A	34	VAL
1	A	38	LYS
1	A	87	ASN
1	A	99	GLN
1	A	113	THR
1	A	221	ARG
1	B	3	THR
1	B	23	ARG
1	B	34	VAL
1	B	38	LYS
1	B	87	ASN
1	B	99	GLN
1	B	103	GLU
1	B	113	THR
1	B	221	ARG
1	B	259	ARG
1	C	23	ARG
1	C	34	VAL
1	C	38	LYS
1	C	75	ARG
1	C	99	GLN
1	C	113	THR
1	C	221	ARG
1	C	249	ILE
1	C	250	ARG
1	D	23	ARG
1	D	34	VAL

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Mol	Chain	Res	Type
1	D	38	LYS
1	D	99	GLN
1	D	113	THR
1	D	221	ARG
1	E	3	THR
1	E	23	ARG
1	E	34	VAL
1	E	38	LYS
1	E	75	ARG
1	E	99	GLN
1	E	113	THR
1	E	129	GLN
1	E	221	ARG
1	E	259	ARG
1	F	4	LEU
1	F	23	ARG
1	F	34	VAL
1	F	38	LYS
1	F	99	GLN
1	F	113	THR
1	F	221	ARG
1	G	23	ARG
1	G	34	VAL
1	G	38	LYS
1	G	87	ASN
1	G	99	GLN
1	G	113	THR
1	G	221	ARG
1	H	23	ARG
1	H	34	VAL
1	H	38	LYS
1	H	99	GLN
1	H	113	THR
1	H	172	SER
1	H	221	ARG
1	I	23	ARG
1	I	34	VAL
1	I	38	LYS
1	I	99	GLN
1	I	113	THR
1	I	221	ARG
1	I	234	ARG

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Mol	Chain	Res	Type
1	J	23	ARG
1	J	34	VAL
1	J	38	LYS
1	J	99	GLN
1	J	113	THR
1	J	221	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	87	ASN
1	A	137	ASN
1	A	230	HIS
1	A	251	GLN
1	B	29	HIS
1	B	87	ASN
1	B	137	ASN
1	B	230	HIS
1	B	251	GLN
1	C	29	HIS
1	C	60	GLN
1	C	230	HIS
1	C	251	GLN
1	D	29	HIS
1	D	230	HIS
1	E	29	HIS
1	E	129	GLN
1	E	230	HIS
1	E	251	GLN
1	F	29	HIS
1	F	168	ASN
1	F	230	HIS
1	F	251	GLN
1	G	29	HIS
1	G	87	ASN
1	G	137	ASN
1	G	179	GLN
1	G	230	HIS
1	G	251	GLN
1	H	29	HIS
1	H	165	GLN

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Mol	Chain	Res	Type
1	I	29	HIS
1	I	137	ASN
1	J	29	HIS
1	J	137	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
2	NAP	I	300	-	45,52,52	0.86	2 (4%)	56,80,80	1.13	3 (5%)
2	NAP	B	300	-	45,52,52	1.08	3 (6%)	56,80,80	1.53	10 (17%)
2	NAP	G	300	-	45,52,52	0.74	1 (2%)	56,80,80	1.41	7 (12%)
2	NAP	H	300	-	45,52,52	0.88	2 (4%)	56,80,80	1.35	7 (12%)
2	NAP	E	300	-	45,52,52	1.08	3 (6%)	56,80,80	2.08	13 (23%)
2	NAP	C	300	-	45,52,52	1.08	2 (4%)	56,80,80	2.14	9 (16%)
2	NAP	A	300	-	45,52,52	1.04	3 (6%)	56,80,80	1.59	10 (17%)
2	NAP	D	300	-	45,52,52	0.91	2 (4%)	56,80,80	1.24	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAP	J	300	-	45,52,52	0.89	1 (2%)	56,80,80	1.30	8 (14%)
2	NAP	F	300	-	45,52,52	1.05	2 (4%)	56,80,80	1.22	8 (14%)

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	I	300	-	-	10/31/67/67	0/5/5/5
2	NAP	B	300	-	-	7/31/67/67	0/5/5/5
2	NAP	G	300	-	-	4/31/67/67	0/5/5/5
2	NAP	H	300	-	-	8/31/67/67	0/5/5/5
2	NAP	E	300	-	-	9/31/67/67	0/5/5/5
2	NAP	C	300	-	-	9/31/67/67	0/5/5/5
2	NAP	A	300	-	-	6/31/67/67	0/5/5/5
2	NAP	D	300	-	-	8/31/67/67	0/5/5/5
2	NAP	J	300	-	-	9/31/67/67	0/5/5/5
2	NAP	F	300	-	-	7/31/67/67	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	300	NAP	C4A-N3A	-3.94	1.30	1.35
2	C	300	NAP	O7N-C7N	2.97	1.29	1.24
2	A	300	NAP	C3N-C7N	-2.84	1.46	1.50
2	F	300	NAP	C5A-C4A	2.83	1.48	1.40
2	B	300	NAP	O4B-C1B	2.81	1.45	1.41
2	A	300	NAP	O4D-C4D	-2.63	1.39	1.45
2	I	300	NAP	C5A-C4A	2.55	1.47	1.40
2	H	300	NAP	P2B-O2B	2.41	1.63	1.59
2	E	300	NAP	C3N-C7N	2.34	1.54	1.50
2	B	300	NAP	C2A-N1A	-2.33	1.29	1.33
2	J	300	NAP	C5A-C4A	2.23	1.46	1.40
2	D	300	NAP	C5A-C4A	2.19	1.46	1.40
2	H	300	NAP	C5A-C4A	2.17	1.46	1.40
2	E	300	NAP	O4D-C4D	-2.13	1.40	1.45
2	G	300	NAP	C5A-C4A	2.07	1.46	1.40
2	D	300	NAP	P2B-O2B	2.03	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	NAP	C2N-C3N	-2.03	1.35	1.39
2	A	300	NAP	C2D-C1D	-2.02	1.50	1.53
2	E	300	NAP	O7N-C7N	2.02	1.28	1.24
2	B	300	NAP	C3N-C7N	-2.01	1.47	1.50
2	I	300	NAP	O4B-C1B	2.01	1.43	1.41

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	300	NAP	N3A-C2A-N1A	-8.67	115.13	128.68
2	E	300	NAP	N3A-C2A-N1A	-8.53	115.35	128.68
2	A	300	NAP	N3A-C2A-N1A	-6.28	118.86	128.68
2	B	300	NAP	N3A-C2A-N1A	-5.87	119.50	128.68
2	C	300	NAP	C3N-C7N-N7N	-5.71	110.89	117.75
2	E	300	NAP	C1B-N9A-C4A	-5.38	117.20	126.64
2	C	300	NAP	C2A-N1A-C6A	4.74	126.85	118.75
2	C	300	NAP	O2B-P2B-O1X	-4.40	92.39	109.39
2	C	300	NAP	C1B-N9A-C4A	-4.25	119.17	126.64
2	G	300	NAP	C6N-N1N-C2N	-4.13	118.21	121.97
2	D	300	NAP	N3A-C2A-N1A	-3.98	122.46	128.68
2	H	300	NAP	C6N-N1N-C2N	-3.93	118.39	121.97
2	E	300	NAP	O7N-C7N-C3N	3.79	124.17	119.63
2	C	300	NAP	O7N-C7N-C3N	3.74	124.11	119.63
2	E	300	NAP	C2A-N1A-C6A	3.74	125.15	118.75
2	B	300	NAP	C1B-N9A-C4A	-3.67	120.19	126.64
2	E	300	NAP	C6N-N1N-C2N	-3.66	118.64	121.97
2	E	300	NAP	O3X-P2B-O2X	3.54	121.16	107.64
2	G	300	NAP	N3A-C2A-N1A	-3.51	123.19	128.68
2	I	300	NAP	PN-O3-PA	-3.46	120.96	132.83
2	I	300	NAP	N3A-C2A-N1A	-3.46	123.28	128.68
2	E	300	NAP	C3N-C7N-N7N	-3.36	113.71	117.75
2	J	300	NAP	O4D-C1D-C2D	-3.30	102.10	106.93
2	J	300	NAP	N3A-C2A-N1A	-3.19	123.69	128.68
2	C	300	NAP	C6N-C5N-C4N	-3.08	114.96	119.44
2	A	300	NAP	C6N-N1N-C2N	-3.06	119.19	121.97
2	H	300	NAP	N3A-C2A-N1A	-3.04	123.92	128.68
2	A	300	NAP	O4D-C1D-C2D	-2.97	102.59	106.93
2	F	300	NAP	O3X-P2B-O2X	2.89	118.68	107.64
2	E	300	NAP	O2B-P2B-O1X	-2.84	98.45	109.39
2	A	300	NAP	C2A-N1A-C6A	2.83	123.60	118.75
2	B	300	NAP	C2A-N1A-C6A	2.82	123.58	118.75
2	C	300	NAP	O4D-C4D-C3D	2.81	110.68	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	300	NAP	O3B-C3B-C4B	-2.79	102.98	111.05
2	E	300	NAP	C3N-C2N-N1N	2.77	123.14	120.43
2	F	300	NAP	C3N-C7N-N7N	-2.77	114.43	117.75
2	G	300	NAP	C1B-N9A-C4A	-2.75	121.80	126.64
2	E	300	NAP	O2A-PA-O1A	2.72	125.70	112.24
2	F	300	NAP	O2B-P2B-O1X	-2.71	98.92	109.39
2	C	300	NAP	O2N-PN-O5D	2.71	120.33	107.75
2	B	300	NAP	O4B-C4B-C3B	2.70	110.46	105.11
2	A	300	NAP	C5N-C4N-C3N	-2.69	117.16	120.34
2	F	300	NAP	O4D-C1D-C2D	-2.65	103.05	106.93
2	D	300	NAP	C2A-N1A-C6A	2.64	123.27	118.75
2	H	300	NAP	O4D-C1D-C2D	-2.63	103.09	106.93
2	B	300	NAP	O2B-C2B-C1B	2.58	119.38	110.10
2	D	300	NAP	C1B-N9A-C4A	-2.42	122.38	126.64
2	B	300	NAP	C4A-C5A-N7A	-2.39	106.91	109.40
2	G	300	NAP	N6A-C6A-N1A	2.38	123.51	118.57
2	J	300	NAP	C4A-C5A-N7A	-2.35	106.95	109.40
2	J	300	NAP	C6N-N1N-C2N	-2.34	119.84	121.97
2	J	300	NAP	C1B-N9A-C4A	-2.34	122.54	126.64
2	D	300	NAP	O4B-C4B-C3B	2.33	109.72	105.11
2	A	300	NAP	C2N-C3N-C4N	2.31	120.88	118.26
2	J	300	NAP	O3X-P2B-O2X	2.31	116.45	107.64
2	H	300	NAP	O2B-P2B-O1X	-2.29	100.55	109.39
2	E	300	NAP	O2D-C2D-C3D	2.28	119.20	111.82
2	G	300	NAP	O4D-C1D-C2D	-2.26	103.63	106.93
2	F	300	NAP	O4B-C4B-C3B	2.23	109.53	105.11
2	A	300	NAP	C1B-N9A-C4A	-2.23	122.73	126.64
2	H	300	NAP	O3X-P2B-O2X	2.22	116.12	107.64
2	G	300	NAP	O7N-C7N-C3N	2.21	122.28	119.63
2	F	300	NAP	C1B-N9A-C4A	-2.21	122.76	126.64
2	D	300	NAP	O3X-P2B-O2X	2.19	116.00	107.64
2	H	300	NAP	C1B-N9A-C4A	-2.18	122.81	126.64
2	E	300	NAP	O2N-PN-O5D	2.17	117.85	107.75
2	B	300	NAP	C2N-C3N-C4N	2.17	120.72	118.26
2	H	300	NAP	C2N-C3N-C4N	2.16	120.71	118.26
2	B	300	NAP	C6N-C5N-C4N	-2.13	116.34	119.44
2	E	300	NAP	C3B-C2B-C1B	-2.08	98.98	102.89
2	A	300	NAP	C4A-C5A-N7A	-2.08	107.23	109.40
2	B	300	NAP	O2B-P2B-O1X	-2.07	101.42	109.39
2	J	300	NAP	C2A-N1A-C6A	2.07	122.29	118.75
2	J	300	NAP	O2N-PN-O1N	2.06	122.45	112.24
2	G	300	NAP	O2A-PA-O1A	2.06	122.42	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	300	NAP	O2B-C2B-C1B	2.05	117.49	110.10
2	F	300	NAP	O7N-C7N-C3N	2.04	122.08	119.63
2	D	300	NAP	O2B-P2B-O1X	-2.03	101.54	109.39
2	F	300	NAP	N3A-C2A-N1A	-2.03	125.50	128.68
2	I	300	NAP	O2A-PA-O1A	2.02	122.23	112.24
2	B	300	NAP	C5B-C4B-C3B	-2.02	107.61	115.18

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	NAP	PN-O3-PA-O5B
2	A	300	NAP	C5D-O5D-PN-O3
2	B	300	NAP	PN-O3-PA-O5B
2	B	300	NAP	C5D-O5D-PN-O3
2	C	300	NAP	C5D-O5D-PN-O3
2	C	300	NAP	C5D-O5D-PN-O1N
2	C	300	NAP	C5D-O5D-PN-O2N
2	D	300	NAP	C5D-O5D-PN-O3
2	D	300	NAP	C5D-O5D-PN-O2N
2	E	300	NAP	C5D-O5D-PN-O3
2	E	300	NAP	C5D-O5D-PN-O1N
2	E	300	NAP	C5D-O5D-PN-O2N
2	F	300	NAP	C5D-O5D-PN-O3
2	G	300	NAP	C5D-O5D-PN-O3
2	H	300	NAP	PN-O3-PA-O5B
2	H	300	NAP	C2B-O2B-P2B-O1X
2	H	300	NAP	C5D-O5D-PN-O3
2	I	300	NAP	C5B-O5B-PA-O3
2	I	300	NAP	C2B-O2B-P2B-O2X
2	I	300	NAP	C5D-O5D-PN-O2N
2	I	300	NAP	O4D-C1D-N1N-C2N
2	J	300	NAP	C5D-O5D-PN-O3
2	J	300	NAP	O4D-C1D-N1N-C2N
2	C	300	NAP	C3B-C2B-O2B-P2B
2	A	300	NAP	PA-O3-PN-O1N
2	C	300	NAP	PA-O3-PN-O1N
2	J	300	NAP	O4B-C4B-C5B-O5B
2	I	300	NAP	C4B-C5B-O5B-PA
2	C	300	NAP	C1B-C2B-O2B-P2B
2	C	300	NAP	PN-O3-PA-O5B
2	F	300	NAP	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
2	G	300	NAP	PN-O3-PA-O5B
2	D	300	NAP	C2B-O2B-P2B-O1X
2	F	300	NAP	C2B-O2B-P2B-O1X
2	D	300	NAP	C2B-O2B-P2B-O2X
2	E	300	NAP	C2B-O2B-P2B-O2X
2	F	300	NAP	C2B-O2B-P2B-O2X
2	H	300	NAP	C2B-O2B-P2B-O2X
2	J	300	NAP	C2B-O2B-P2B-O2X
2	D	300	NAP	PA-O3-PN-O1N
2	D	300	NAP	PA-O3-PN-O2N
2	E	300	NAP	PA-O3-PN-O2N
2	J	300	NAP	PA-O3-PN-O1N
2	A	300	NAP	C5D-O5D-PN-O1N
2	B	300	NAP	C5D-O5D-PN-O1N
2	D	300	NAP	C5D-O5D-PN-O1N
2	F	300	NAP	C5D-O5D-PN-O1N
2	G	300	NAP	C5D-O5D-PN-O1N
2	H	300	NAP	C5D-O5D-PN-O1N
2	I	300	NAP	C5B-O5B-PA-O1A
2	I	300	NAP	C5B-O5B-PA-O2A
2	I	300	NAP	C5D-O5D-PN-O1N
2	J	300	NAP	C5D-O5D-PN-O1N
2	E	300	NAP	C3B-C2B-O2B-P2B
2	A	300	NAP	PA-O3-PN-O2N
2	C	300	NAP	PA-O3-PN-O2N
2	H	300	NAP	PA-O3-PN-O1N
2	H	300	NAP	PA-O3-PN-O2N
2	J	300	NAP	PA-O3-PN-O2N
2	E	300	NAP	C1B-C2B-O2B-P2B
2	D	300	NAP	O4B-C4B-C5B-O5B
2	F	300	NAP	O4B-C4B-C5B-O5B
2	B	300	NAP	PA-O3-PN-O1N
2	E	300	NAP	PA-O3-PN-O1N
2	B	300	NAP	C1B-C2B-O2B-P2B
2	G	300	NAP	O4B-C4B-C5B-O5B
2	J	300	NAP	C2B-O2B-P2B-O1X
2	J	300	NAP	C3B-C4B-C5B-O5B
2	I	300	NAP	C5D-O5D-PN-O3
2	A	300	NAP	O4B-C4B-C5B-O5B
2	E	300	NAP	O4B-C4B-C5B-O5B
2	B	300	NAP	PA-O3-PN-O2N
2	F	300	NAP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	300	NAP	O4B-C4B-C5B-O5B
2	C	300	NAP	O4B-C4B-C5B-O5B
2	H	300	NAP	O4B-C4B-C5B-O5B
2	I	300	NAP	O4B-C4B-C5B-O5B

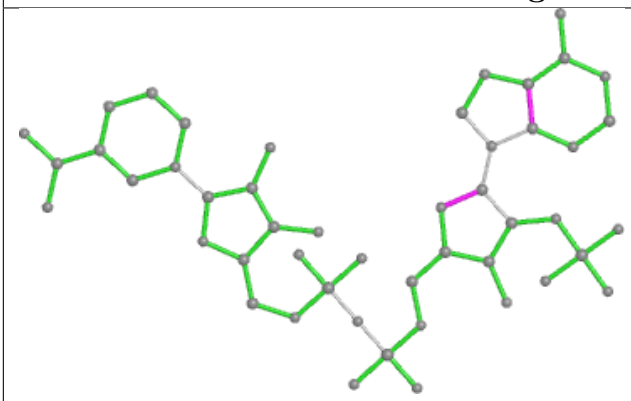
There are no ring outliers.

5 monomers are involved in 7 short contacts:

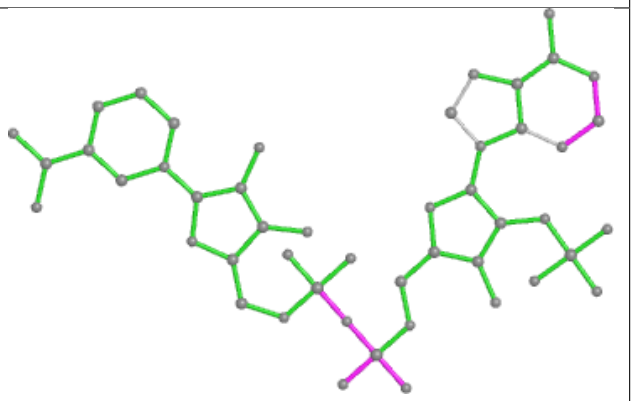
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	300	NAP	1	0
2	B	300	NAP	1	0
2	E	300	NAP	1	0
2	J	300	NAP	1	0
2	F	300	NAP	3	0

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.

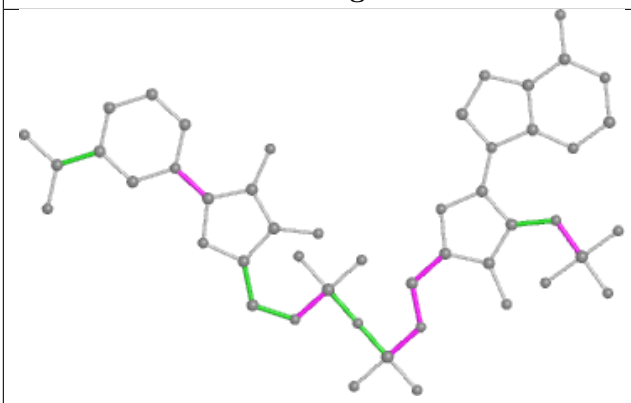
Ligand NAP I 300



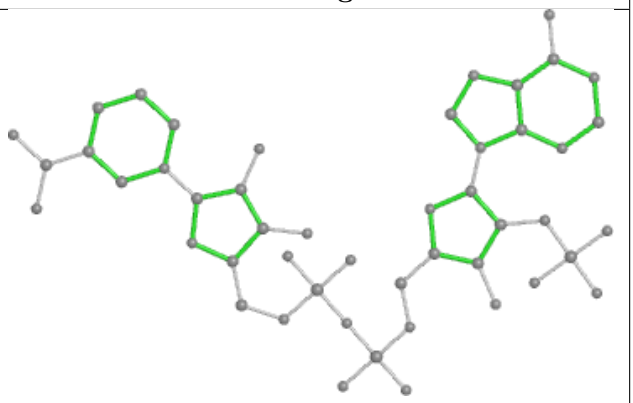
Bond lengths



Bond angles

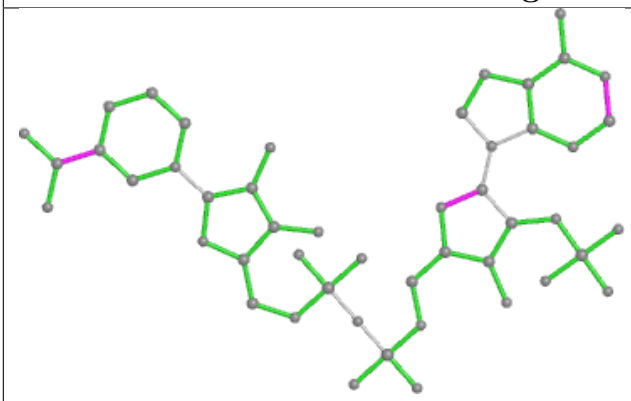


Torsions

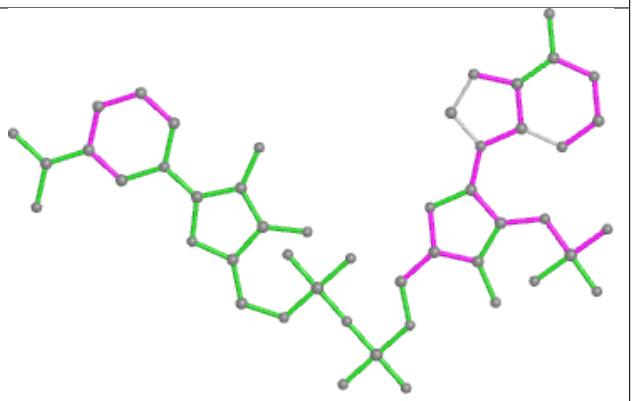


Rings

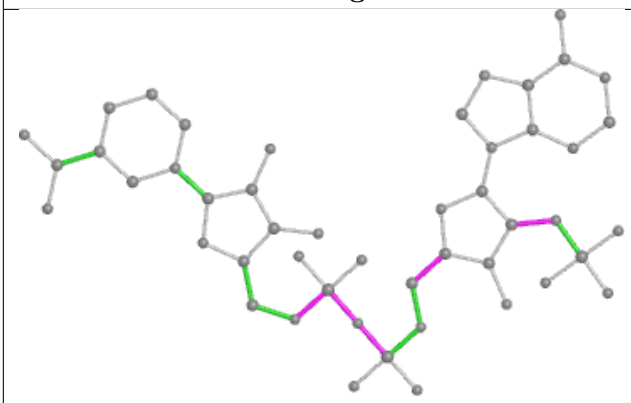
Ligand NAP B 300



Bond lengths



Bond angles



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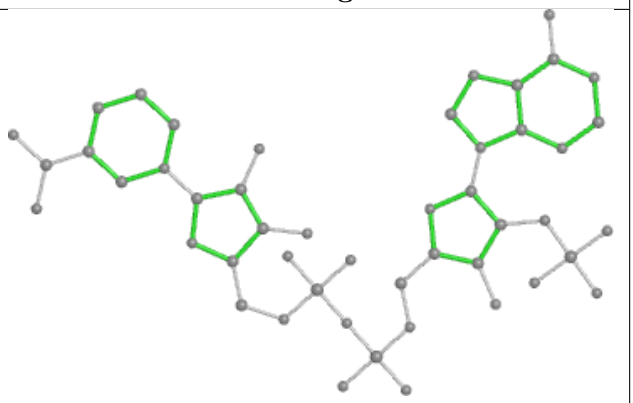
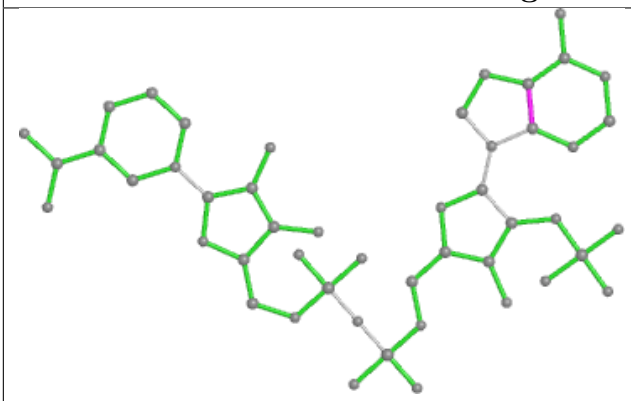
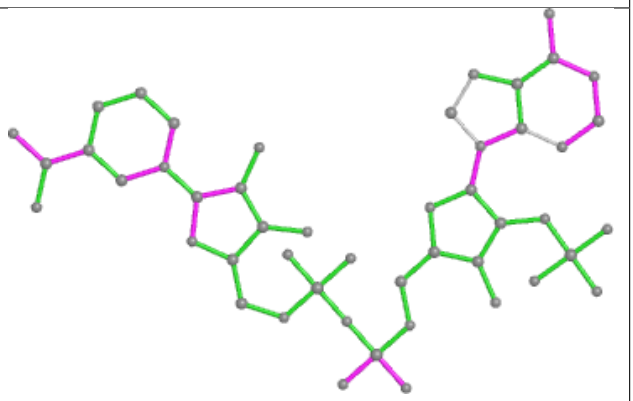


Rings

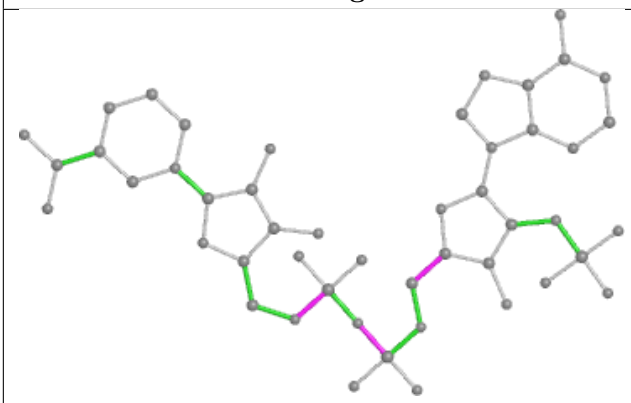
Ligand NAP G 300



Bond lengths



Bond angles



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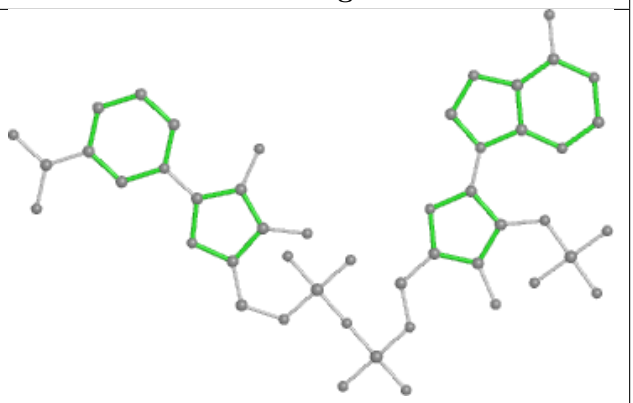
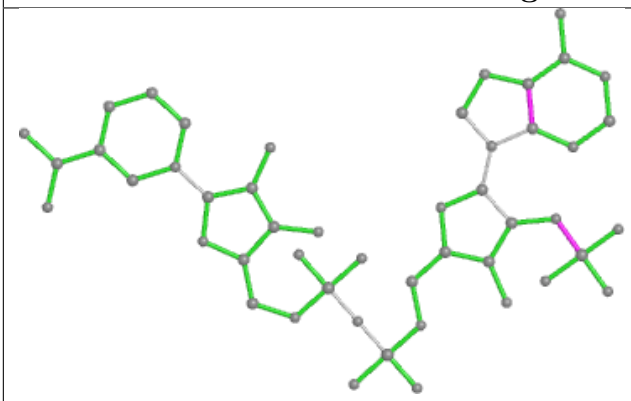
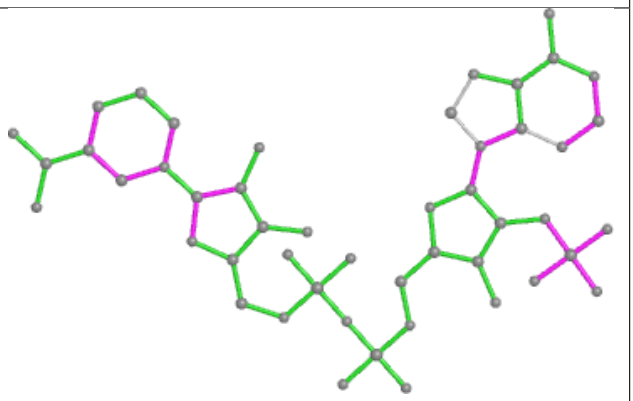


Rings

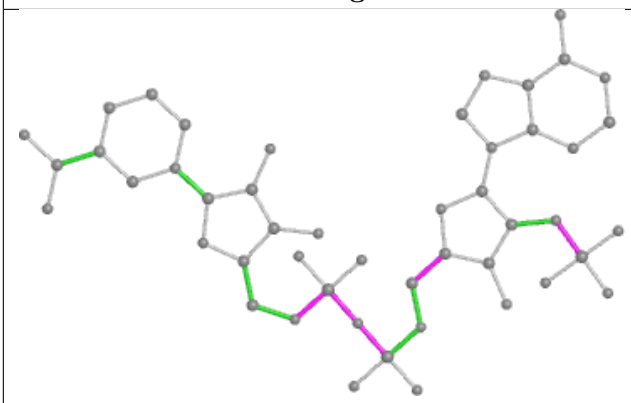
Ligand NAP H 300



Bond lengths



Bond angles



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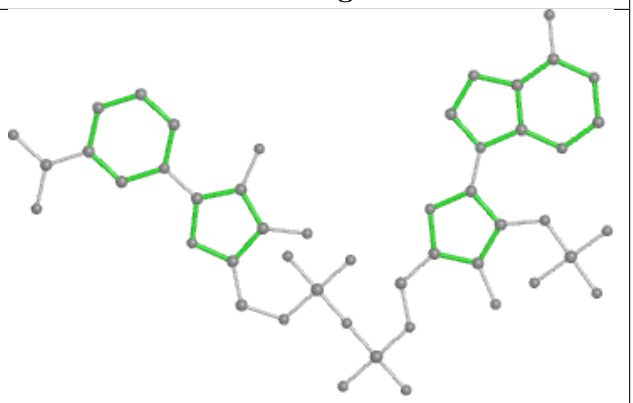
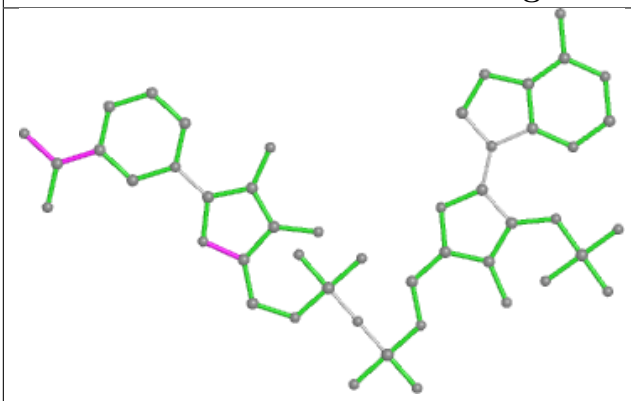
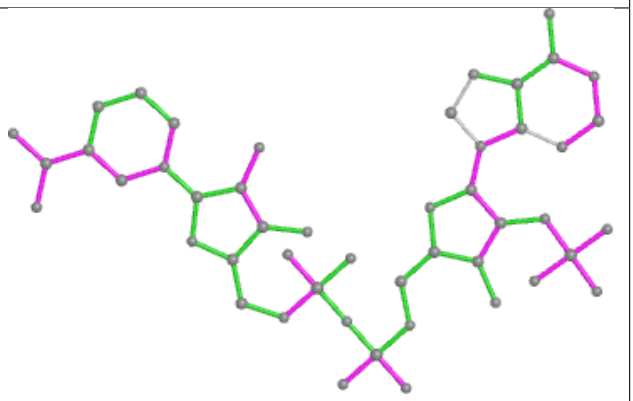


Rings

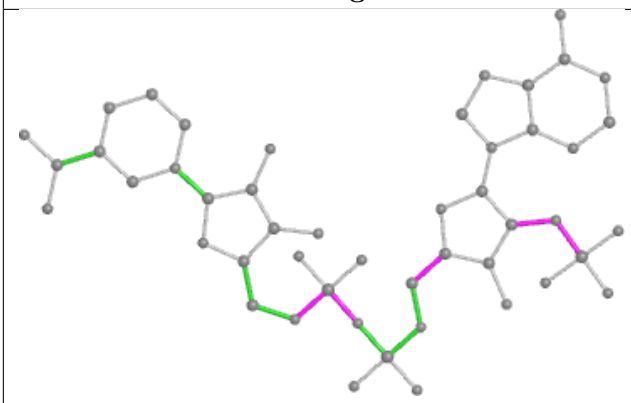
Ligand NAP E 300



Bond lengths



Bond angles



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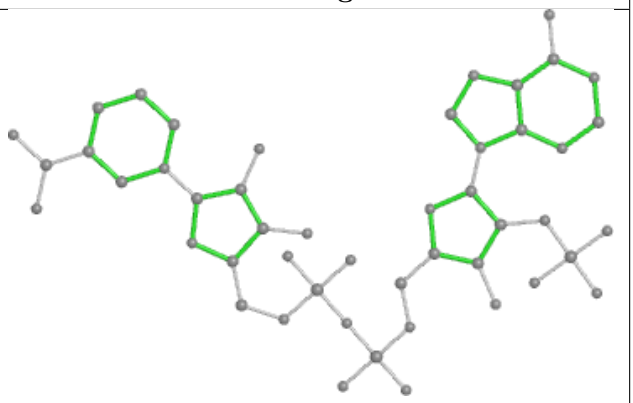
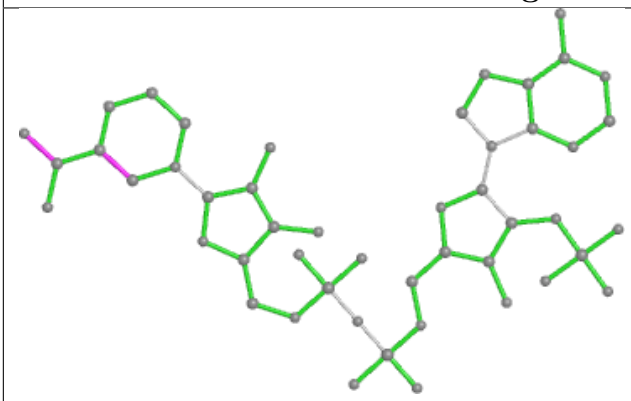
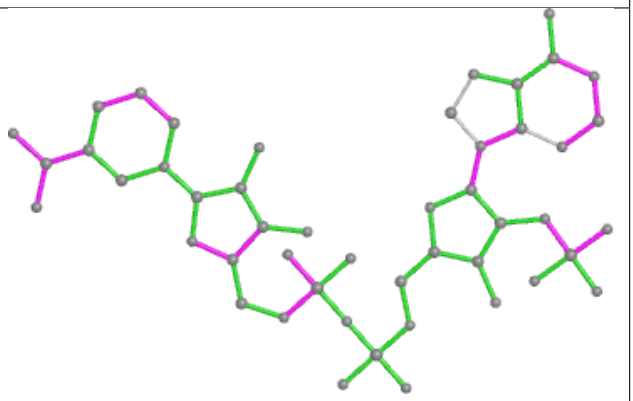


Rings

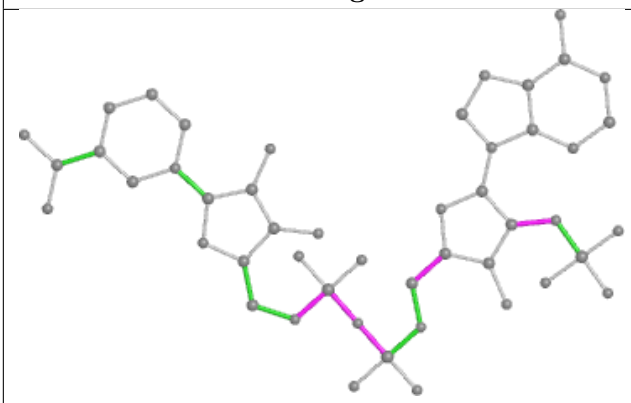
Ligand NAP C 300



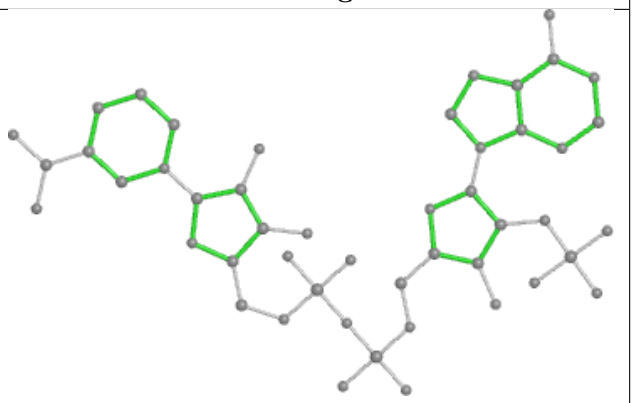
Bond lengths



Bond angles

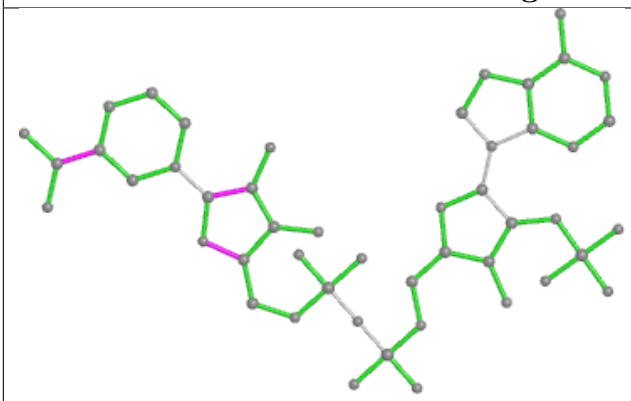


Torsions

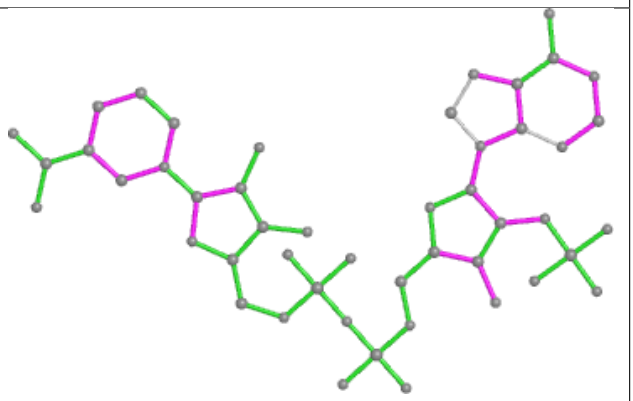


Rings

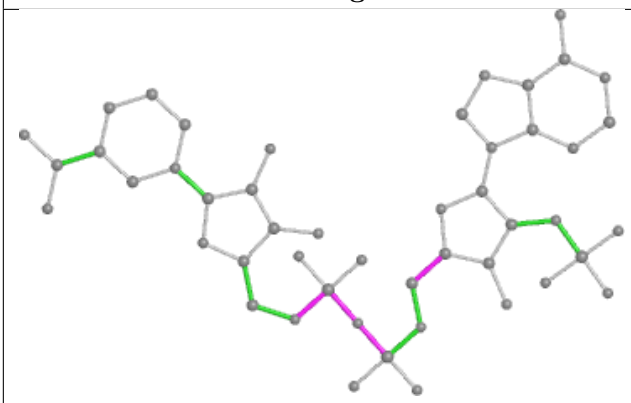
Ligand NAP A 300



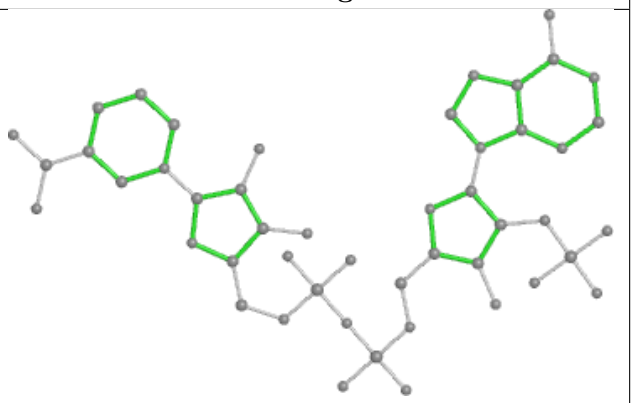
Bond lengths



Bond angles

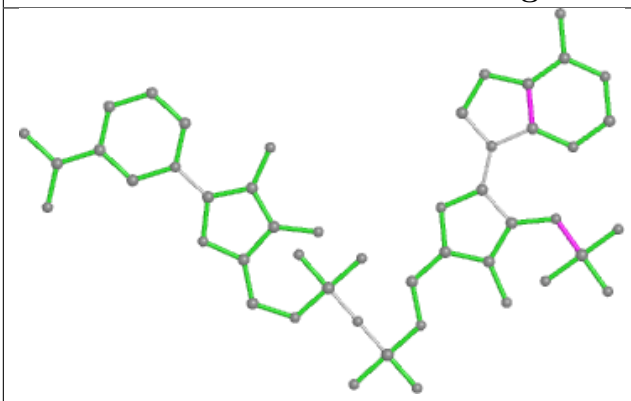


Torsions

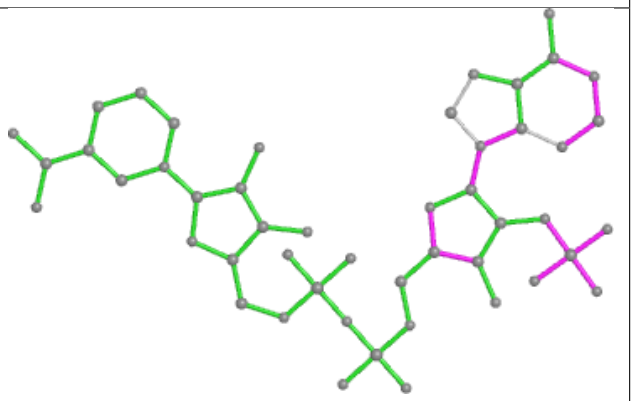


Rings

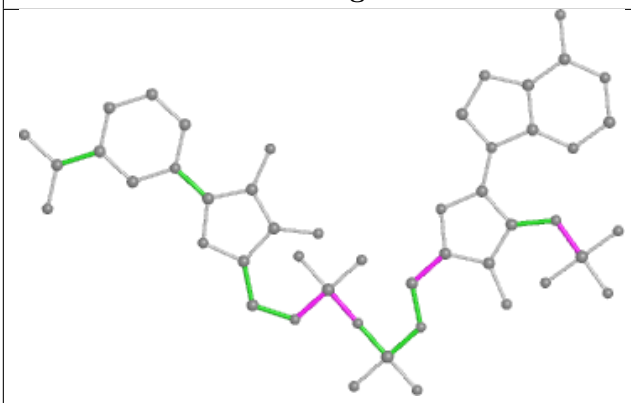
Ligand NAP D 300



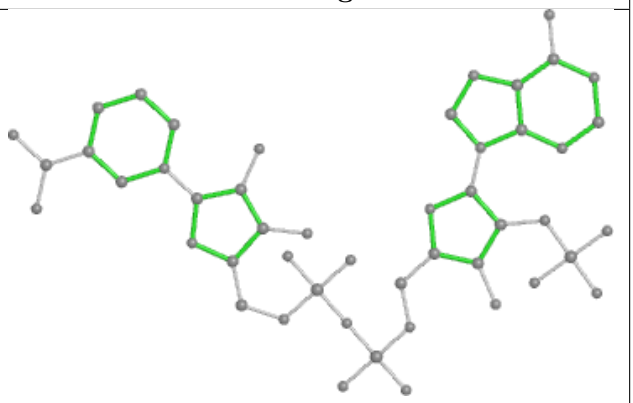
Bond lengths



Bond angles

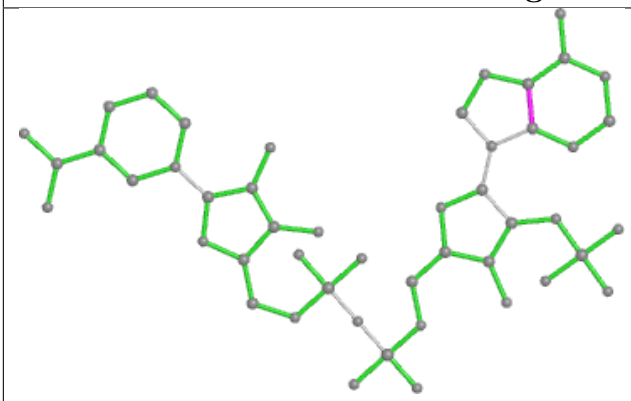


Torsions

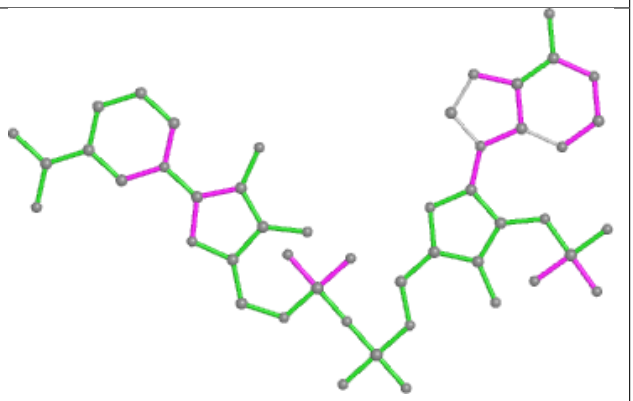


Rings

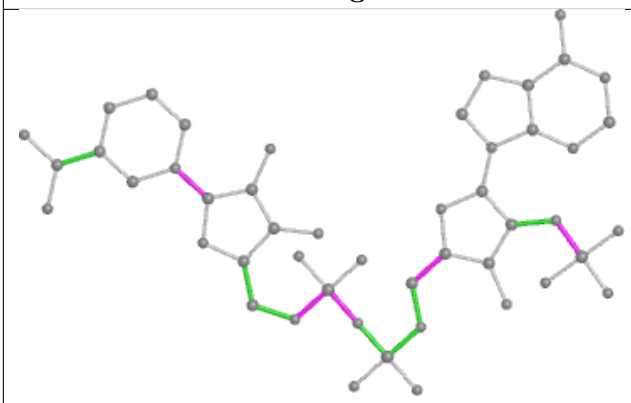
Ligand NAP J 300



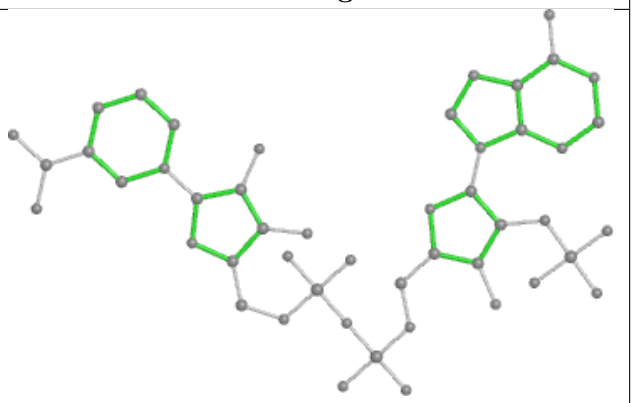
Bond lengths



Bond angles

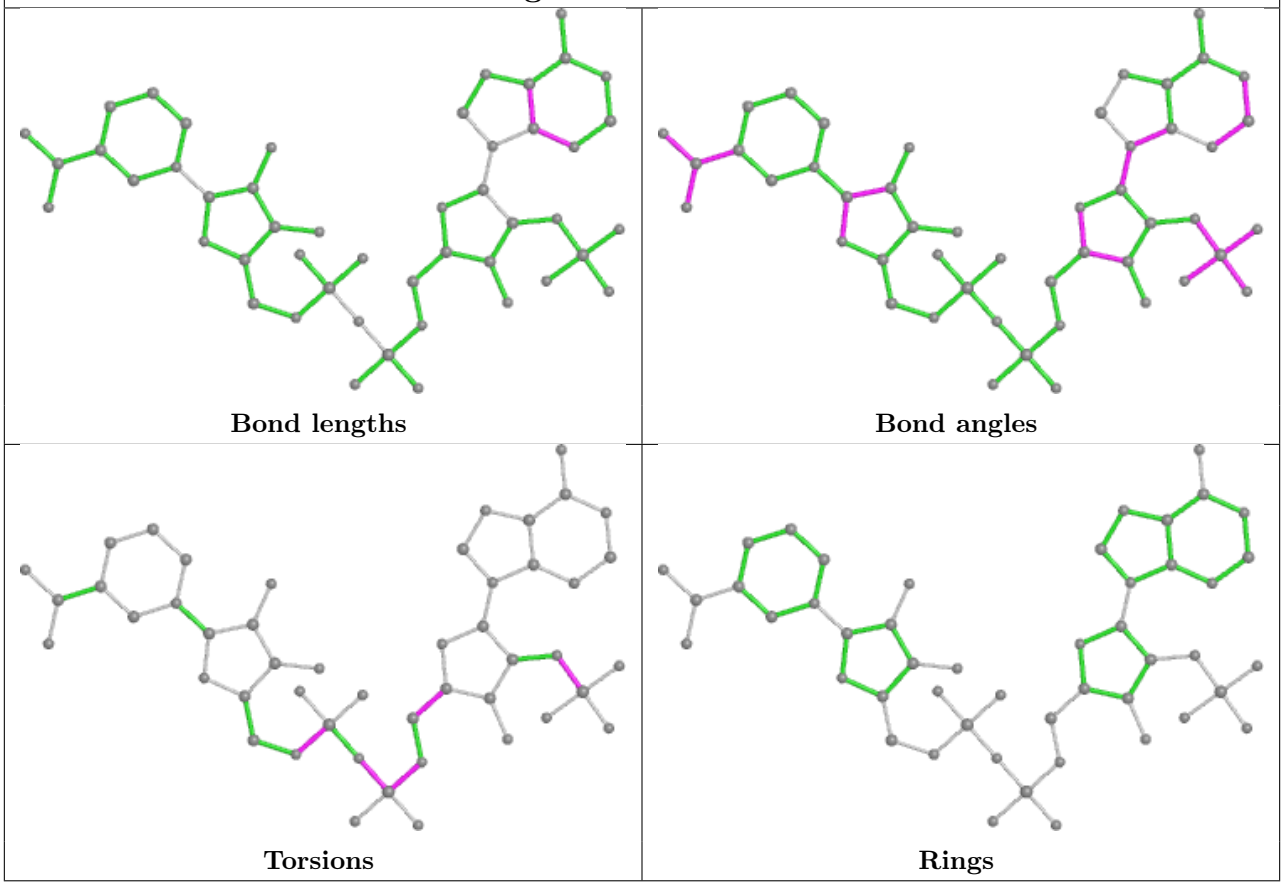


Torsions



Rings

Ligand NAP F 300



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^{th} 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	256/262 (97%)	0.41	0 100 100	14, 23, 36, 53	0
1	B	257/262 (98%)	0.38	0 100 100	15, 23, 37, 65	0
1	C	258/262 (98%)	0.44	0 100 100	14, 22, 35, 58	0
1	D	257/262 (98%)	0.32	0 100 100	15, 29, 45, 58	0
1	E	257/262 (98%)	0.47	0 100 100	13, 22, 34, 53	0
1	F	256/262 (97%)	0.36	0 100 100	14, 28, 43, 57	0
1	G	256/262 (97%)	0.68	15 (5%) 22 23	22, 41, 69, 86	0
1	H	256/262 (97%)	0.63	19 (7%) 14 15	27, 44, 72, 90	0
1	I	254/262 (96%)	1.01	40 (15%) 2 1	37, 59, 77, 90	0
1	J	255/262 (97%)	1.03	37 (14%) 2 2	33, 55, 71, 81	0
All	All	2562/2620 (97%)	0.57	111 (4%) 35 38	13, 32, 67, 90	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	194	ALA	5.3
1	I	128	VAL	4.9
1	G	255	ALA	4.4
1	H	94	SER	4.0
1	I	205	MET	4.0
1	J	50	ASP	3.8
1	J	205	MET	3.7
1	I	204	VAL	3.7
1	I	236	ASP	3.6
1	G	244	GLY	3.5
1	I	130	SER	3.5
1	J	231	VAL	3.4
1	I	174	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	249	ILE	3.3
1	J	230	HIS	3.3
1	H	258	TYR	3.2
1	J	55	ALA	3.2
1	H	240	GLY	3.2
1	I	50	ASP	3.2
1	J	188	THR	3.1
1	H	231	VAL	3.1
1	I	232	ALA	3.1
1	J	235	TRP	3.1
1	J	154	GLY	3.1
1	J	46	ALA	3.1
1	J	94	SER	3.0
1	J	255	ALA	3.0
1	J	54	VAL	3.0
1	G	212	ASP	2.9
1	H	244	GLY	2.9
1	I	94	SER	2.9
1	H	175	GLY	2.9
1	J	218	PHE	2.9
1	J	207	VAL	2.8
1	G	209	GLU	2.8
1	I	60	GLN	2.8
1	I	54	VAL	2.8
1	I	95	GLY	2.8
1	I	5	PRO	2.8
1	I	31	LEU	2.8
1	J	39	VAL	2.8
1	I	235	TRP	2.8
1	G	213	ALA	2.7
1	I	30	ASP	2.7
1	I	188	THR	2.7
1	J	171	LEU	2.7
1	H	233	ALA	2.6
1	H	209	GLU	2.6
1	J	247	SER	2.6
1	I	171	LEU	2.6
1	J	76	LEU	2.6
1	I	218	PHE	2.6
1	I	231	VAL	2.6
1	H	208	ASP	2.6
1	I	10	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	194	ALA	2.5
1	J	196	ILE	2.5
1	G	208	ASP	2.5
1	H	237	ALA	2.5
1	I	71	ALA	2.5
1	H	202	PRO	2.5
1	I	76	LEU	2.5
1	J	81	ARG	2.5
1	I	244	GLY	2.5
1	J	95	GLY	2.5
1	J	174	SER	2.4
1	I	196	ILE	2.4
1	I	45	ALA	2.4
1	I	122	ALA	2.4
1	H	255	ALA	2.4
1	J	132	THR	2.4
1	H	239	ASP	2.4
1	J	130	SER	2.4
1	H	148	PHE	2.4
1	I	38	LYS	2.4
1	J	131	GLY	2.3
1	H	232	ALA	2.3
1	J	71	ALA	2.3
1	G	169	LEU	2.3
1	G	216	VAL	2.3
1	G	247	SER	2.3
1	H	247	SER	2.3
1	I	207	VAL	2.3
1	J	249	ILE	2.3
1	J	127	PHE	2.3
1	I	81	ARG	2.2
1	H	169	LEU	2.2
1	I	172	SER	2.2
1	J	138	ILE	2.2
1	I	245	LEU	2.2
1	I	255	ALA	2.2
1	I	242	ARG	2.2
1	J	200	THR	2.2
1	H	151	SER	2.2
1	G	231	VAL	2.1
1	J	236	ASP	2.1
1	J	31	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	237	ALA	2.1
1	I	131	GLY	2.1
1	G	237	ALA	2.1
1	G	201	LEU	2.1
1	I	149	GLY	2.1
1	G	176	ILE	2.0
1	J	119	LEU	2.0
1	J	208	ASP	2.0
1	J	14	SER	2.0
1	G	166	GLY	2.0
1	I	195	GLY	2.0
1	H	259	ARG	2.0
1	G	258	TYR	2.0
1	I	222	GLU	2.0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	I	300	48/48	0.93	0.21	44,52,60,67	0
2	NAP	J	300	48/48	0.93	0.20	35,45,49,51	0
2	NAP	C	300	48/48	0.95	0.19	13,17,21,24	0
2	NAP	E	300	48/48	0.96	0.18	12,15,18,18	0
2	NAP	G	300	48/48	0.96	0.18	23,29,39,41	0
2	NAP	F	300	48/48	0.97	0.15	18,21,26,32	0
2	NAP	A	300	48/48	0.97	0.17	13,17,21,24	0
2	NAP	H	300	48/48	0.97	0.16	22,26,42,44	0
2	NAP	D	300	48/48	0.97	0.16	20,24,27,30	0

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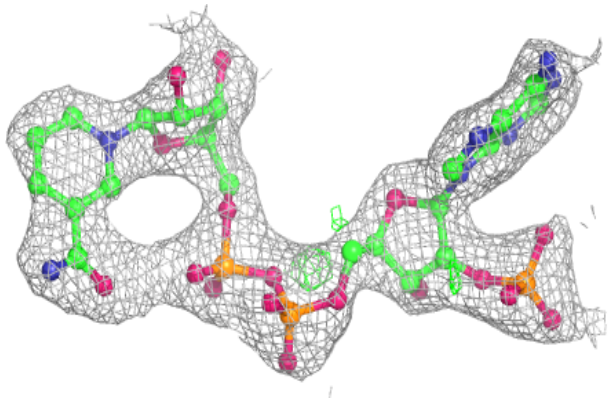
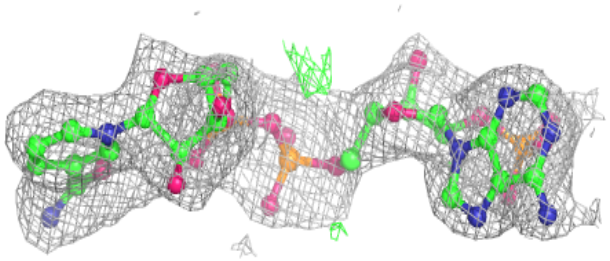
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	B	300	48/48	0.97	0.18	13,18,24,25	0

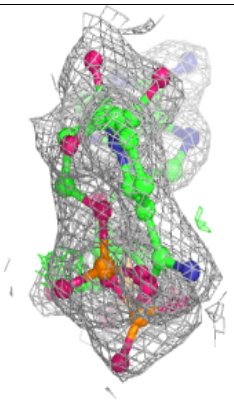
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP I 300:

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

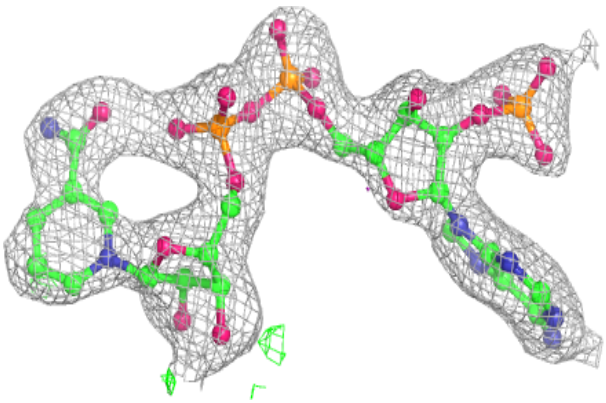


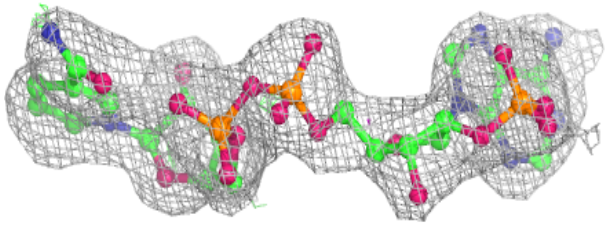


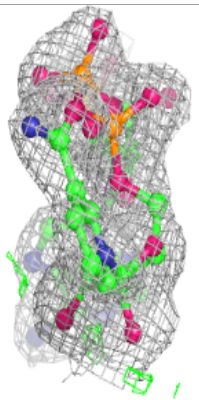


Electron density around NAP J 300:

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

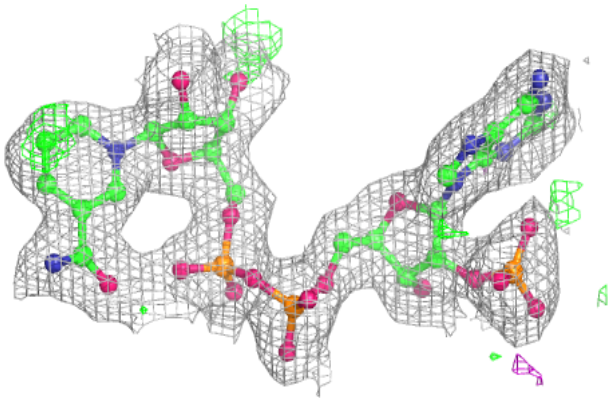


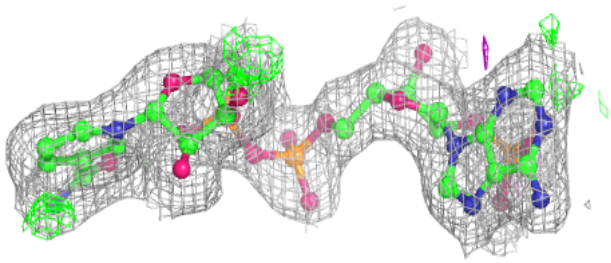


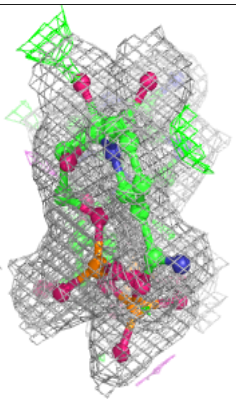


Electron density around NAP C 300:

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

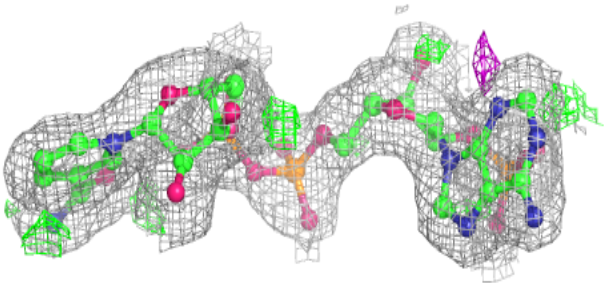


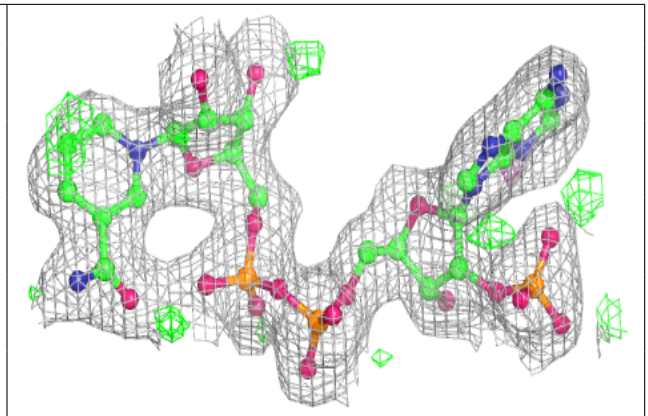


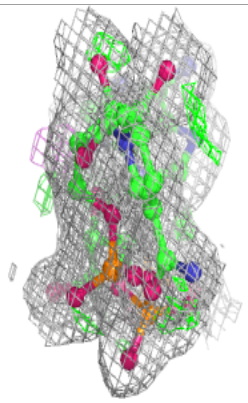


Electron density around NAP E 300:

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

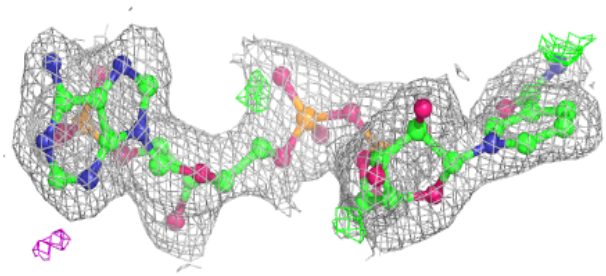


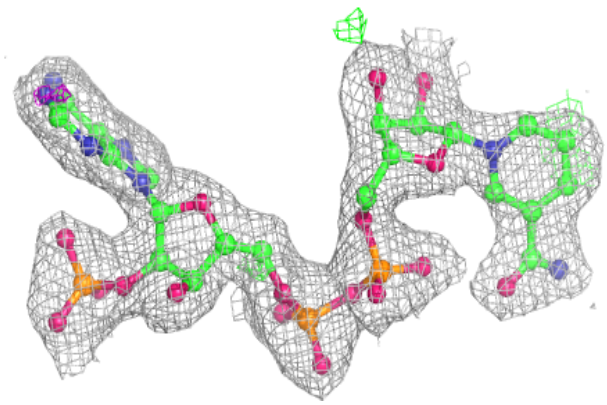


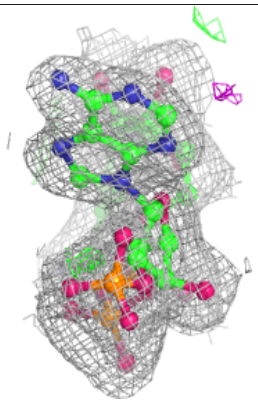


Electron density around NAP G 300:

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

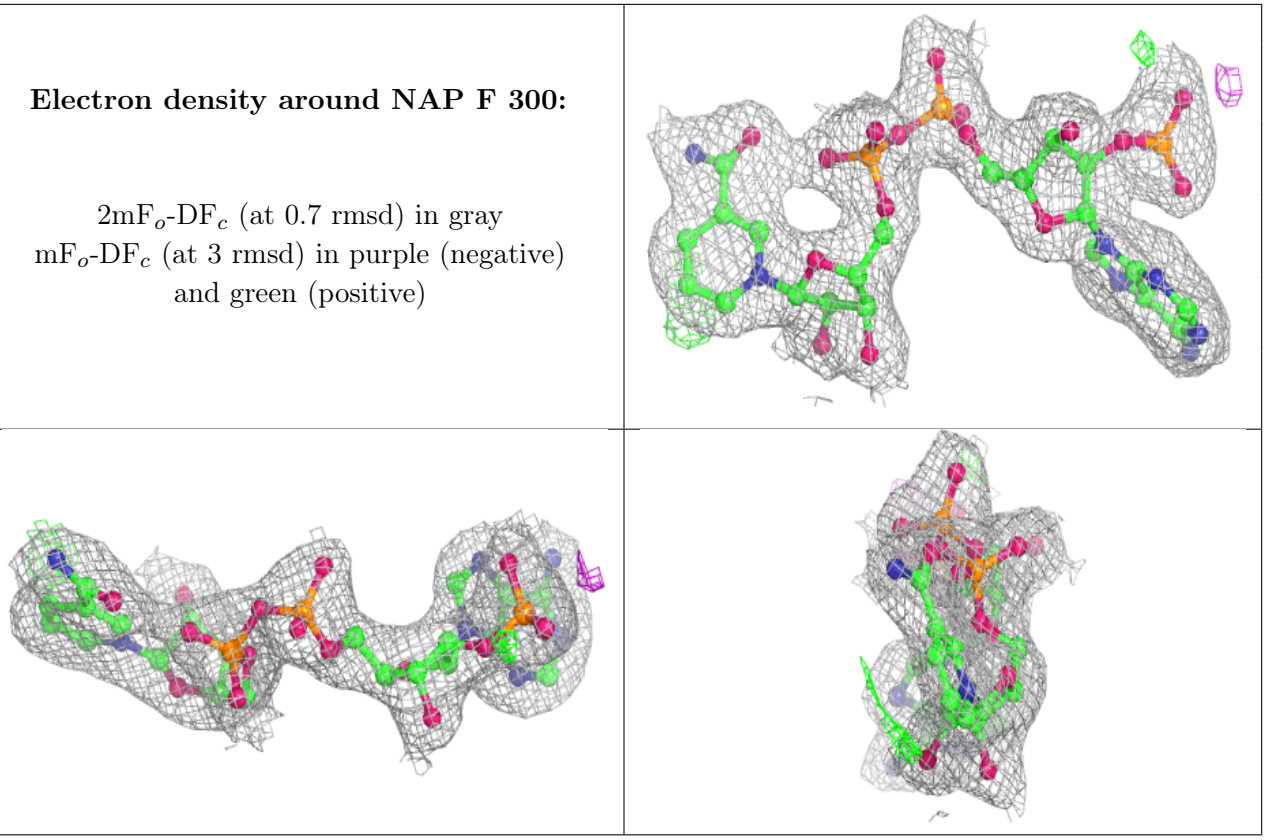






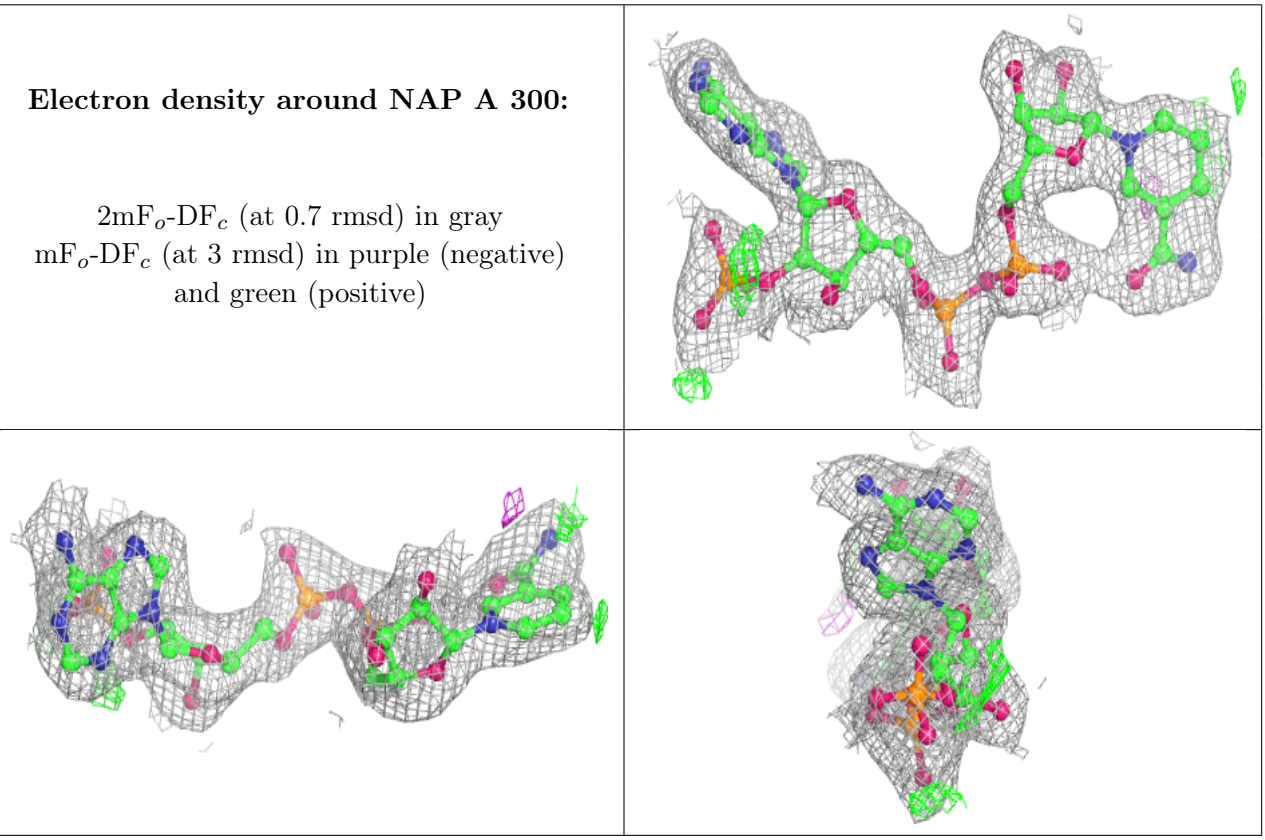
Electron density around NAP F 300:

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



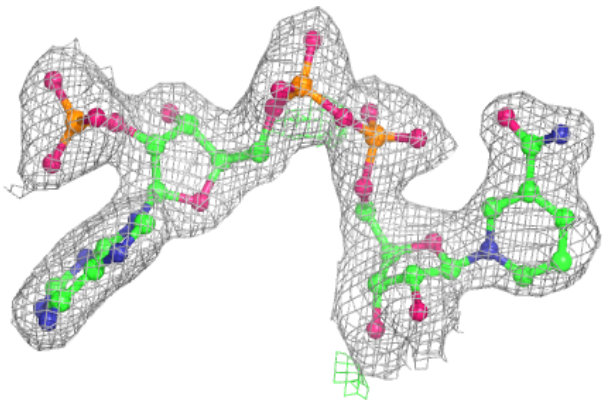
Electron density around NAP A 300:

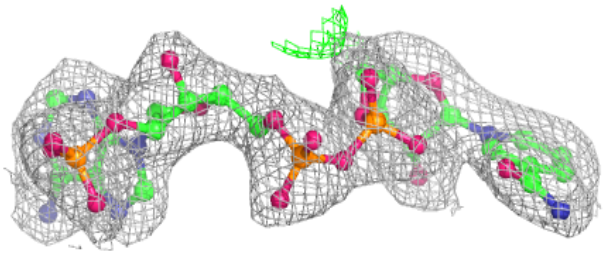
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

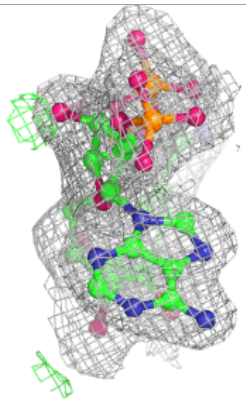


Electron density around NAP H 300:

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

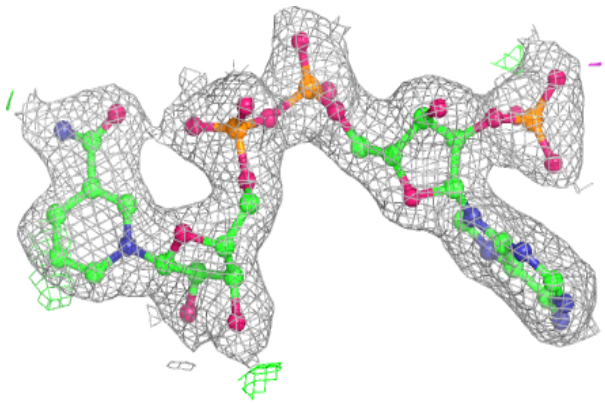


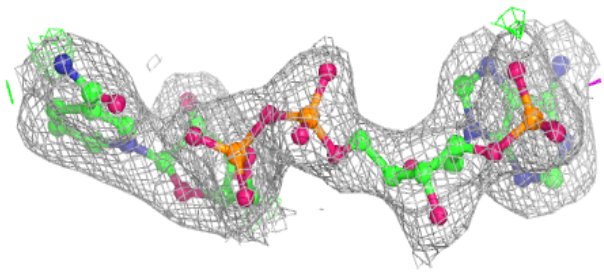


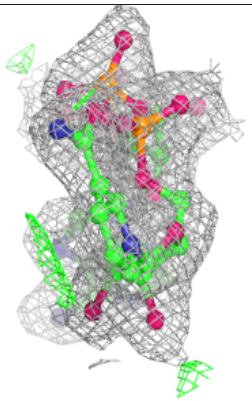


Electron density around NAP D 300:

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

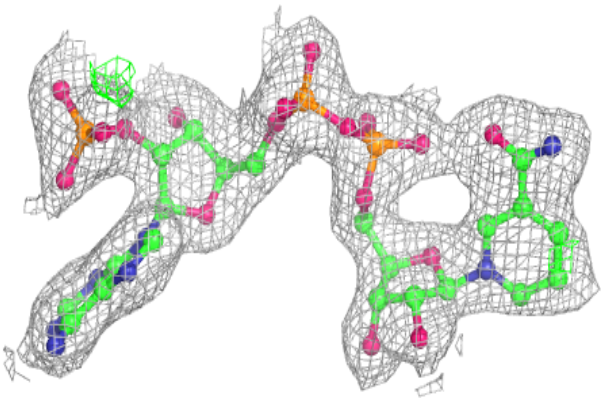


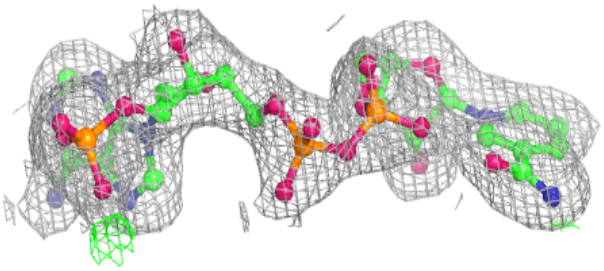


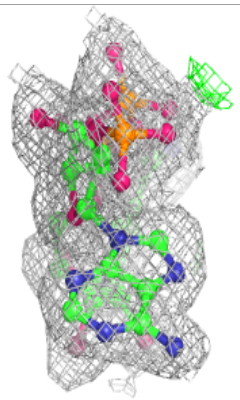


Electron density around NAP B 300:

$2mF_o$-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.