Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 03:44 AM EDT

PDB ID	:	6X0J
Title	:	Structure of reduced SidA ornithine hydroxylase with the FAD "in" and complexed with NADP and L-ornithine
Authors	:	Tanner, J.J.; Campbell, A.C.
Deposited on	:	2020-05-15
Resolution	:	2.33 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:

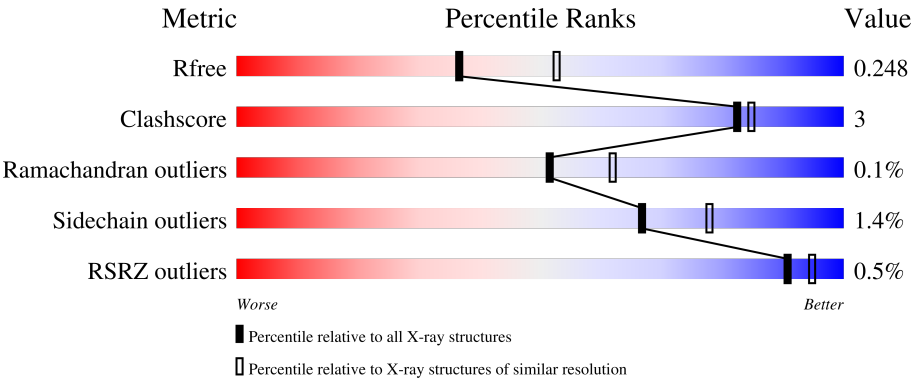
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	494	84% 7% 9%
1	B	494	83% 9% 8%
1	C	494	84% 7% 9%
1	D	494	85% 6% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14802 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 L-ornithine N(5)-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3492	2201	627	648	16			
1	B	455	Total	C	N	O	S	0	0	0
			3511	2207	626	662	16			
1	C	451	Total	C	N	O	S	0	0	0
			3496	2199	626	655	16			
1	D	450	Total	C	N	O	S	0	0	0
			3465	2183	618	648	16			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP E9QYP0
A	9	GLY	-	expression tag	UNP E9QYP0
A	10	SER	-	expression tag	UNP E9QYP0
A	11	SER	-	expression tag	UNP E9QYP0
A	12	HIS	-	expression tag	UNP E9QYP0
A	13	HIS	-	expression tag	UNP E9QYP0
A	14	HIS	-	expression tag	UNP E9QYP0
A	15	HIS	-	expression tag	UNP E9QYP0
A	16	HIS	-	expression tag	UNP E9QYP0
A	17	HIS	-	expression tag	UNP E9QYP0
A	18	SER	-	expression tag	UNP E9QYP0
A	19	SER	-	expression tag	UNP E9QYP0
A	20	GLY	-	expression tag	UNP E9QYP0
A	21	LEU	-	expression tag	UNP E9QYP0
A	22	VAL	-	expression tag	UNP E9QYP0
A	23	PRO	-	expression tag	UNP E9QYP0
A	24	ARG	-	expression tag	UNP E9QYP0
A	25	GLY	-	expression tag	UNP E9QYP0
A	26	SER	-	expression tag	UNP E9QYP0
A	27	HIS	-	expression tag	UNP E9QYP0
A	28	MET	-	expression tag	UNP E9QYP0

Continued on next page...

Continued from previous page...

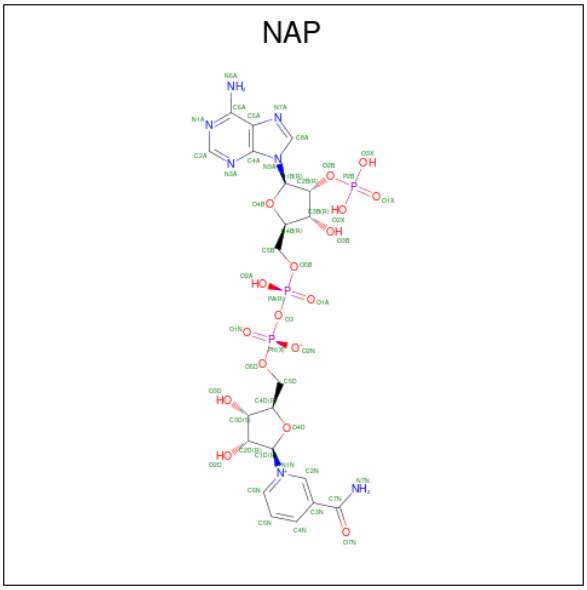
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	initiating methionine	UNP E9QYP0
B	9	GLY	-	expression tag	UNP E9QYP0
B	10	SER	-	expression tag	UNP E9QYP0
B	11	SER	-	expression tag	UNP E9QYP0
B	12	HIS	-	expression tag	UNP E9QYP0
B	13	HIS	-	expression tag	UNP E9QYP0
B	14	HIS	-	expression tag	UNP E9QYP0
B	15	HIS	-	expression tag	UNP E9QYP0
B	16	HIS	-	expression tag	UNP E9QYP0
B	17	HIS	-	expression tag	UNP E9QYP0
B	18	SER	-	expression tag	UNP E9QYP0
B	19	SER	-	expression tag	UNP E9QYP0
B	20	GLY	-	expression tag	UNP E9QYP0
B	21	LEU	-	expression tag	UNP E9QYP0
B	22	VAL	-	expression tag	UNP E9QYP0
B	23	PRO	-	expression tag	UNP E9QYP0
B	24	ARG	-	expression tag	UNP E9QYP0
B	25	GLY	-	expression tag	UNP E9QYP0
B	26	SER	-	expression tag	UNP E9QYP0
B	27	HIS	-	expression tag	UNP E9QYP0
B	28	MET	-	expression tag	UNP E9QYP0
C	8	MET	-	initiating methionine	UNP E9QYP0
C	9	GLY	-	expression tag	UNP E9QYP0
C	10	SER	-	expression tag	UNP E9QYP0
C	11	SER	-	expression tag	UNP E9QYP0
C	12	HIS	-	expression tag	UNP E9QYP0
C	13	HIS	-	expression tag	UNP E9QYP0
C	14	HIS	-	expression tag	UNP E9QYP0
C	15	HIS	-	expression tag	UNP E9QYP0
C	16	HIS	-	expression tag	UNP E9QYP0
C	17	HIS	-	expression tag	UNP E9QYP0
C	18	SER	-	expression tag	UNP E9QYP0
C	19	SER	-	expression tag	UNP E9QYP0
C	20	GLY	-	expression tag	UNP E9QYP0
C	21	LEU	-	expression tag	UNP E9QYP0
C	22	VAL	-	expression tag	UNP E9QYP0
C	23	PRO	-	expression tag	UNP E9QYP0
C	24	ARG	-	expression tag	UNP E9QYP0
C	25	GLY	-	expression tag	UNP E9QYP0
C	26	SER	-	expression tag	UNP E9QYP0
C	27	HIS	-	expression tag	UNP E9QYP0
C	28	MET	-	expression tag	UNP E9QYP0

Continued on next page...

Continued from previous page...

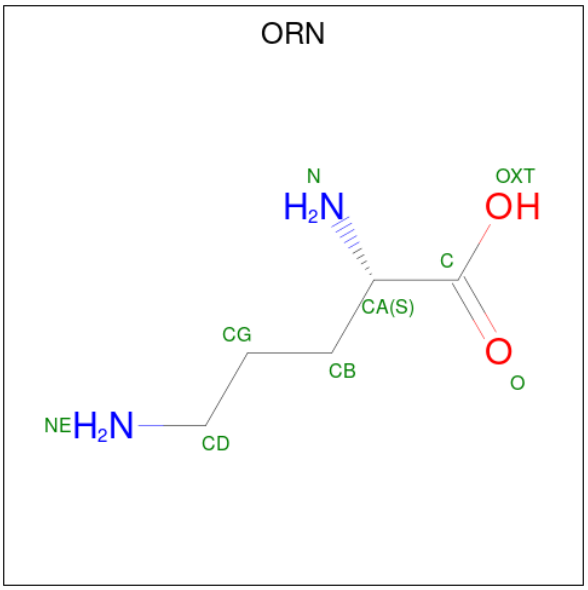
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	MET	-	initiating methionine	UNP E9QYP0
D	9	GLY	-	expression tag	UNP E9QYP0
D	10	SER	-	expression tag	UNP E9QYP0
D	11	SER	-	expression tag	UNP E9QYP0
D	12	HIS	-	expression tag	UNP E9QYP0
D	13	HIS	-	expression tag	UNP E9QYP0
D	14	HIS	-	expression tag	UNP E9QYP0
D	15	HIS	-	expression tag	UNP E9QYP0
D	16	HIS	-	expression tag	UNP E9QYP0
D	17	HIS	-	expression tag	UNP E9QYP0
D	18	SER	-	expression tag	UNP E9QYP0
D	19	SER	-	expression tag	UNP E9QYP0
D	20	GLY	-	expression tag	UNP E9QYP0
D	21	LEU	-	expression tag	UNP E9QYP0
D	22	VAL	-	expression tag	UNP E9QYP0
D	23	PRO	-	expression tag	UNP E9QYP0
D	24	ARG	-	expression tag	UNP E9QYP0
D	25	GLY	-	expression tag	UNP E9QYP0
D	26	SER	-	expression tag	UNP E9QYP0
D	27	HIS	-	expression tag	UNP E9QYP0
D	28	MET	-	expression tag	UNP E9QYP0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



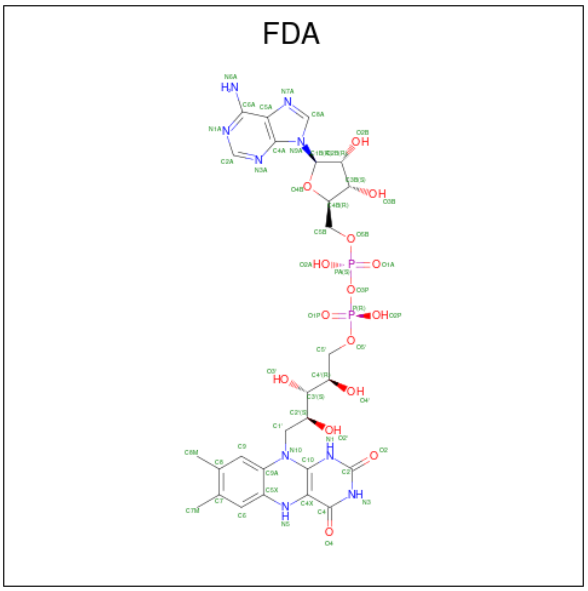
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 48 21 7 17 3	0	0
2	B	1	Total C N O P 48 21 7 17 3	0	0
2	C	1	Total C N O P 48 21 7 17 3	0	0
2	D	1	Total C N O P 48 21 7 17 3	0	0

- Molecule 3 is L-ornithine (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 9 5 2 2	0	0
3	B	1	Total C N O 9 5 2 2	0	0
3	C	1	Total C N O 9 5 2 2	0	0
3	D	1	Total C N O 9 5 2 2	0	0

- Molecule 4 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is water.

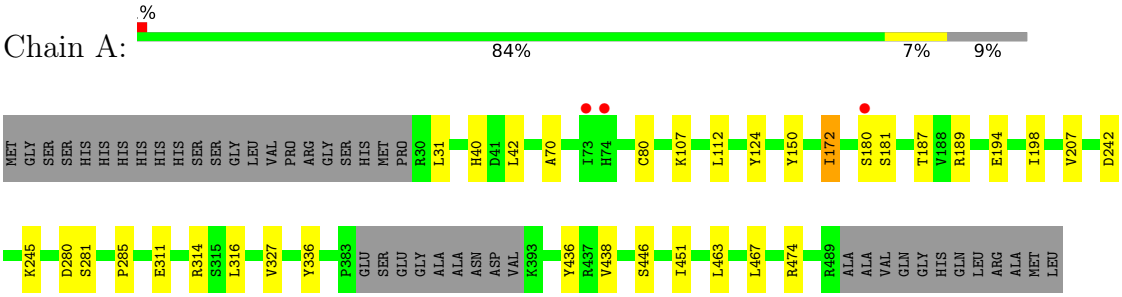
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total	O	0	0
			89	89		
5	B	109	Total	O	0	0
			109	109		
5	C	123	Total	O	0	0
			123	123		
5	D	77	Total	O	0	0
			77	77		

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.

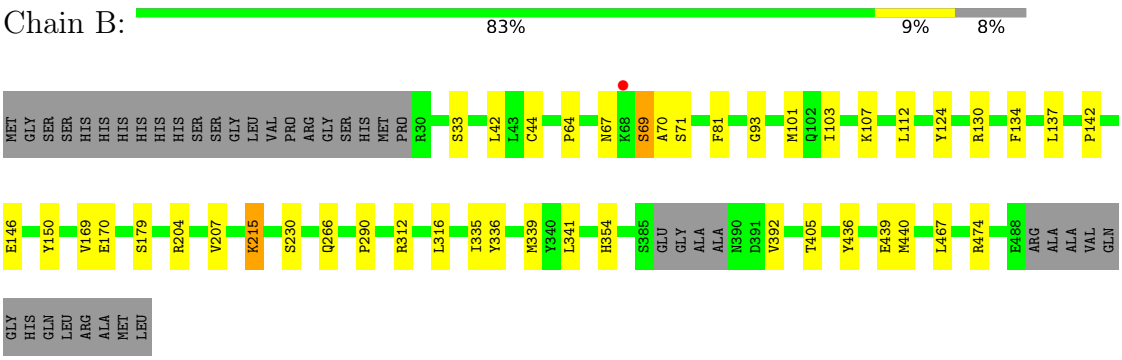
• Molecule 1: L-ornithine N(5)-monooxygenase

Chain A:



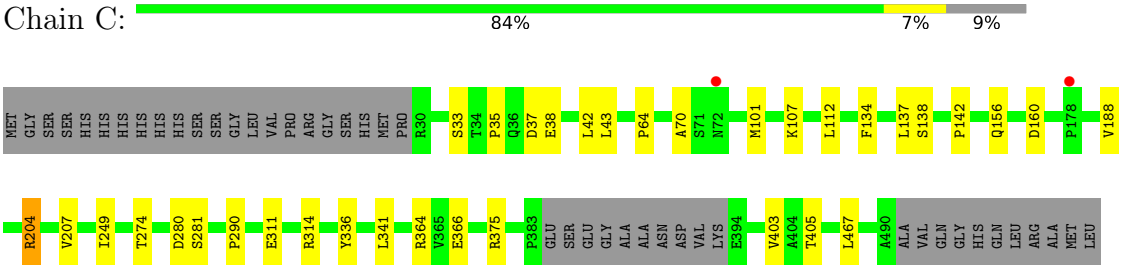
• Molecule 1: L-ornithine N(5)-monooxygenase

Chain B:



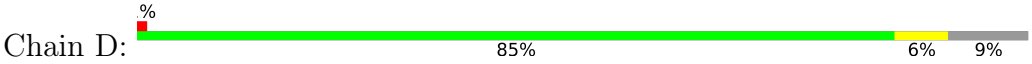
• Molecule 1: L-ornithine N(5)-monooxygenase

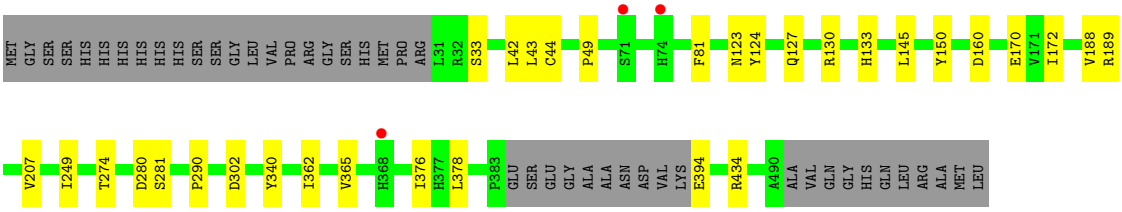
Chain C:



• Molecule 1: L-ornithine N(5)-monooxygenase

Chain D:




MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET PRO ARG L31 R32 S33 L42 L43 C44 P49 S71 H74 F81 N123 Y124 Q127 R130 H133 L145 Y150 D160 E170 V171 I172 V188 R189
V207 I249 T274 D280 S281 P290 D302 Y340 I362 V365 H368 I376 H377 L378 P383 GLU SER GLU GLY ALA ALA ASN ASP VAL LYS E394 R434 A490 ALA VAL GLN GLY HIS GLN LEU ARG ALA MET LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.21Å 153.01Å 91.11Å 90.00° 110.91° 90.00°	Depositor
Resolution (Å)	56.90 – 2.33 85.11 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.3 (56.90-2.33) 98.3 (85.11-2.34)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.183 , 0.249 0.184 , 0.248	Depositor DCC
R_{free} test set	4400 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14802	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

5.1 Standard geometry

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

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	0.41	0/3569	0.57	0/4846
1	B	0.40	0/3588	0.59	0/4876
1	C	0.41	0/3572	0.58	0/4850
1	D	0.39	0/3541	0.58	0/4812
All	All	0.40	0/14270	0.58	0/19384

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3492	0	3377	15	0
1	B	3511	0	3368	23	0
1	C	3496	0	3376	17	0
1	D	3465	0	3342	18	0
2	A	48	0	23	0	0
2	B	48	0	24	0	0
2	C	48	0	24	0	0
2	D	48	0	24	1	0
3	A	9	0	11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	11	0	0
3	C	9	0	11	0	0
3	D	9	0	11	0	0
4	A	53	0	33	1	0
4	B	53	0	32	2	0
4	C	53	0	33	2	0
4	D	53	0	33	1	0
5	A	89	0	0	0	0
5	B	109	0	0	0	0
5	C	123	0	0	0	0
5	D	77	0	0	0	0
All	All	14802	0	13733	71	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 3.

All (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:601:NAP:C1B	2:D:601:NAP:O4B	1.63	1.24
1:A:42:LEU:HD11	1:A:207:VAL:HG23	1.72	0.70
1:C:311:GLU:OE2	1:C:314:ARG:NH2	2.27	0.67
1:C:33:SER:HB3	1:C:160:ASP:O	2.02	0.59
1:D:378:LEU:HB2	1:D:394:GLU:HG3	1.85	0.59
1:C:467:LEU:HB3	4:C:603:FDA:O2	2.04	0.57
1:C:366:GLU:HB2	1:C:375:ARG:HB3	1.87	0.56
1:D:42:LEU:HD11	1:D:207:VAL:HG23	1.88	0.54
1:D:362:ILE:HD13	1:D:378:LEU:HD21	1.88	0.54
1:B:101:MET:SD	1:B:142:PRO:HD2	2.48	0.53
1:C:43:LEU:HD22	1:C:188:VAL:HG21	1.91	0.53
1:A:467:LEU:HB3	4:A:603:FDA:O2	2.09	0.52
1:A:311:GLU:OE1	1:A:314:ARG:NH2	2.44	0.51
1:B:107:LYS:HG2	1:B:112:LEU:HD11	1.94	0.50
1:A:336:TYR:CD2	1:D:290:PRO:HB2	2.46	0.50
1:D:170:GLU:OE2	1:D:189:ARG:HD2	2.13	0.49
1:A:316:LEU:HD22	1:A:463:LEU:HG	1.93	0.49
1:D:33:SER:HB3	1:D:160:ASP:O	2.12	0.49
1:C:134:PHE:O	1:C:137:LEU:HB2	2.14	0.48
1:B:146:GLU:OE2	1:D:340:TYR:OH	2.27	0.48
1:A:438:VAL:HG22	1:A:451:ILE:O	2.14	0.47
1:B:467:LEU:HB3	4:B:603:FDA:O2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ASP:OD1	1:D:281:SER:N	2.39	0.47
1:B:69:SER:O	1:B:71:SER:N	2.47	0.47
1:B:103:ILE:CG2	4:B:603:FDA:HN3	2.28	0.47
1:D:49:PRO:HD2	4:D:603:FDA:O2A	2.15	0.47
1:D:362:ILE:HD13	1:D:378:LEU:CD2	2.44	0.47
1:A:280:ASP:OD1	1:A:281:SER:N	2.47	0.47
1:A:242:ASP:OD2	1:A:245:LYS:HG3	2.14	0.46
1:D:43:LEU:HD22	1:D:188:VAL:HG21	1.98	0.46
1:A:107:LYS:HG2	1:A:112:LEU:HD11	1.98	0.46
1:B:64:PRO:HA	1:B:67:ASN:O	2.16	0.45
1:B:215:LYS:HD2	1:B:405:THR:O	2.17	0.45
1:B:44:CYS:HB2	1:B:81:PHE:CD2	2.52	0.45
1:A:285:PRO:HA	1:A:327:VAL:O	2.17	0.45
1:A:172:ILE:CG1	1:A:187:THR:HB	2.47	0.44
1:C:107:LYS:HG2	1:C:112:LEU:HD11	1.99	0.44
1:B:42:LEU:HD11	1:B:207:VAL:HG23	1.99	0.44
1:B:93:GLY:HA3	1:B:230:SER:O	2.18	0.44
1:B:290:PRO:HB2	1:C:336:TYR:CD1	2.52	0.44
1:C:101:MET:HG2	1:C:142:PRO:O	2.18	0.43
1:A:124:TYR:CE2	1:A:150:TYR:HB2	2.53	0.43
1:A:40:HIS:CD2	1:A:80:CYS:HB2	2.54	0.43
1:C:35:PRO:HB2	1:C:38:GLU:HG3	2.00	0.43
1:C:204:ARG:HE	1:C:204:ARG:HB3	1.36	0.43
1:A:436:TYR:CZ	1:A:474:ARG:HD2	2.54	0.43
1:B:436:TYR:CZ	1:B:474:ARG:HD2	2.54	0.42
1:D:302:ASP:OD1	1:D:434:ARG:NE	2.49	0.42
1:D:123:ASN:O	1:D:127:GLN:HG2	2.19	0.42
1:C:42:LEU:HD11	1:C:207:VAL:HG23	2.00	0.42
1:C:64:PRO:HA	1:C:70:ALA:HB3	2.02	0.42
1:B:169:VAL:HG23	1:B:170:GLU:HG2	2.02	0.42
1:D:130:ARG:HA	1:D:133:HIS:HD2	1.84	0.41
1:A:189:ARG:NH2	1:A:198:ILE:HG21	2.35	0.41
1:D:249:ILE:O	1:D:274:THR:HA	2.20	0.41
1:B:336:TYR:CD1	1:C:290:PRO:HB2	2.55	0.41
1:C:280:ASP:OD1	1:C:281:SER:N	2.50	0.41
4:C:603:FDA:HN1	4:C:603:FDA:H1'2	1.74	0.41
1:B:134:PHE:O	1:B:137:LEU:HB2	2.21	0.41
1:C:249:ILE:O	1:C:274:THR:HA	2.21	0.41
1:C:403:VAL:HG12	1:C:405:THR:OG1	2.20	0.41
1:B:69:SER:C	1:B:71:SER:H	2.24	0.41
1:B:130:ARG:HH11	1:B:130:ARG:HD3	1.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:TYR:CD2	1:B:150:TYR:HB2	2.55	0.41
1:B:335:ILE:O	1:B:339:MET:HG2	2.20	0.41
1:D:124:TYR:CE1	1:D:150:TYR:HA	2.56	0.41
1:B:439:GLU:O	1:B:440:MET:HG2	2.21	0.40
1:D:365:VAL:HG22	1:D:376:ILE:HD12	2.04	0.40
1:B:266:GLN:HG2	1:B:354:HIS:CE1	2.56	0.40
1:B:312:ARG:O	1:B:316:LEU:HG	2.21	0.40
1:D:44:CYS:HB2	1:D:81:PHE:CD2	2.56	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	447/494 (90%)	428 (96%)	18 (4%)	1 (0%)	47	55
1	B	451/494 (91%)	439 (97%)	11 (2%)	1 (0%)	47	55
1	C	447/494 (90%)	431 (96%)	16 (4%)	0	100	100
1	D	446/494 (90%)	432 (97%)	14 (3%)	0	100	100
All	All	1791/1976 (91%)	1730 (97%)	59 (3%)	2 (0%)	51	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	ALA
1	A	70	ALA

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	369/433 (85%)	363 (98%)	6 (2%)	62	74
1	B	373/433 (86%)	366 (98%)	7 (2%)	57	68
1	C	371/433 (86%)	365 (98%)	6 (2%)	62	74
1	D	367/433 (85%)	365 (100%)	2 (0%)	88	93
All	All	1480/1732 (86%)	1459 (99%)	21 (1%)	67	78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	172	ILE
1	A	180	SER
1	A	181	SER
1	A	194	GLU
1	A	446	SER
1	B	33	SER
1	B	69	SER
1	B	179	SER
1	B	204	ARG
1	B	215	LYS
1	B	341	LEU
1	B	392	VAL
1	C	37	ASP
1	C	138	SER
1	C	156	GLN
1	C	204	ARG
1	C	341	LEU
1	C	364	ARG
1	D	145	LEU
1	D	172	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	D	133	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ORN	B	602	-	7,8,8	0.91	0	8,9,9	0.95	0
4	FDA	D	603	-	52,58,58	2.80	23 (44%)	60,89,89	1.67	12 (20%)
4	FDA	B	603	-	52,58,58	2.84	21 (40%)	60,89,89	1.52	9 (15%)
2	NAP	D	601	-	45,52,52	4.50	14 (31%)	56,80,80	1.93	7 (12%)
2	NAP	B	601	-	45,52,52	4.34	14 (31%)	56,80,80	1.85	8 (14%)
3	ORN	C	602	-	7,8,8	0.84	0	8,9,9	1.39	2 (25%)
3	ORN	D	602	-	7,8,8	0.87	0	8,9,9	1.07	1 (12%)
4	FDA	A	603	-	52,58,58	2.87	21 (40%)	60,89,89	1.60	11 (18%)
2	NAP	A	601	-	45,52,52	4.39	15 (33%)	56,80,80	1.81	7 (12%)
4	FDA	C	603	-	52,58,58	2.76	22 (42%)	60,89,89	1.59	11 (18%)
2	NAP	C	601	-	45,52,52	4.37	14 (31%)	56,80,80	2.00	8 (14%)
3	ORN	A	602	-	7,8,8	0.70	0	8,9,9	1.41	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ORN	B	602	-	-	0/8/8/8	-
4	FDA	D	603	-	-	7/30/50/50	0/6/6/6
4	FDA	B	603	-	-	5/30/50/50	0/6/6/6
2	NAP	D	601	-	-	1/31/67/67	0/5/5/5
2	NAP	B	601	-	-	4/31/67/67	0/5/5/5
3	ORN	C	602	-	-	0/8/8/8	-
3	ORN	D	602	-	-	0/8/8/8	-
4	FDA	A	603	-	-	10/30/50/50	0/6/6/6
2	NAP	A	601	-	-	2/31/67/67	0/5/5/5
4	FDA	C	603	-	-	1/30/50/50	0/6/6/6
2	NAP	C	601	-	-	2/31/67/67	0/5/5/5
3	ORN	A	602	-	-	0/8/8/8	-

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAP	O4B-C1B	16.04	1.63	1.41
2	D	601	NAP	O4D-C1D	15.29	1.62	1.41
2	C	601	NAP	O4D-C1D	15.17	1.62	1.41
2	A	601	NAP	O4B-C1B	15.03	1.62	1.41
2	A	601	NAP	O4D-C1D	14.97	1.62	1.41
2	B	601	NAP	O4B-C1B	14.93	1.61	1.41
2	B	601	NAP	O4D-C1D	14.91	1.61	1.41
2	C	601	NAP	O4B-C1B	14.74	1.61	1.41
2	A	601	NAP	C2D-C1D	-14.73	1.31	1.53
2	D	601	NAP	C2D-C1D	-14.72	1.31	1.53
2	C	601	NAP	C2D-C1D	-14.16	1.32	1.53
2	B	601	NAP	C2D-C1D	-14.03	1.32	1.53
4	A	603	FDA	O4-C4	8.83	1.40	1.23
4	B	603	FDA	O4-C4	8.57	1.39	1.23
4	D	603	FDA	O4-C4	8.24	1.39	1.23
4	C	603	FDA	O4-C4	7.53	1.37	1.23
4	A	603	FDA	O2-C2	7.39	1.38	1.23
4	C	603	FDA	O2-C2	7.10	1.38	1.23
4	B	603	FDA	O2-C2	7.09	1.38	1.23
4	D	603	FDA	O2-C2	7.00	1.38	1.23
4	C	603	FDA	C6-C5X	6.99	1.50	1.39
2	C	601	NAP	C7N-N7N	6.87	1.46	1.33
2	D	601	NAP	C7N-N7N	6.65	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAP	C7N-N7N	6.50	1.45	1.33
4	A	603	FDA	C6-C5X	6.46	1.49	1.39
2	A	601	NAP	O4B-C4B	-6.26	1.31	1.45
2	D	601	NAP	O4B-C4B	-6.15	1.31	1.45
2	B	601	NAP	O4D-C4D	-6.11	1.31	1.45
4	D	603	FDA	C9-C9A	6.06	1.49	1.39
4	B	603	FDA	C6-C5X	6.05	1.48	1.39
2	C	601	NAP	O4B-C4B	-6.02	1.31	1.45
2	C	601	NAP	O4D-C4D	-5.98	1.31	1.45
2	A	601	NAP	C7N-N7N	5.94	1.44	1.33
2	B	601	NAP	O4B-C4B	-5.89	1.31	1.45
2	A	601	NAP	O4D-C4D	-5.80	1.32	1.45
4	D	603	FDA	C6-C5X	5.80	1.48	1.39
4	B	603	FDA	C9-C9A	5.79	1.49	1.39
4	A	603	FDA	C9-C9A	5.73	1.49	1.39
2	D	601	NAP	O4D-C4D	-5.71	1.32	1.45
4	D	603	FDA	C10-N1	4.94	1.46	1.37
4	C	603	FDA	C9-C9A	4.92	1.47	1.39
4	B	603	FDA	C10-N1	4.90	1.46	1.37
4	C	603	FDA	C10-N1	4.76	1.45	1.37
4	B	603	FDA	C4X-N5	4.61	1.45	1.35
4	C	603	FDA	C4X-N5	4.61	1.45	1.35
4	A	603	FDA	C10-N1	4.45	1.45	1.37
4	D	603	FDA	C10-N10	4.45	1.46	1.38
4	C	603	FDA	C5X-N5	4.42	1.47	1.39
4	D	603	FDA	C2-N1	4.40	1.45	1.37
4	A	603	FDA	C5X-C9A	-4.17	1.35	1.40
4	B	603	FDA	C5X-C9A	-4.05	1.36	1.40
4	B	603	FDA	C5X-N5	4.00	1.46	1.39
4	A	603	FDA	C2-N1	4.00	1.44	1.37
4	B	603	FDA	C10-N10	3.93	1.45	1.38
4	D	603	FDA	C4X-N5	3.89	1.44	1.35
4	A	603	FDA	C4X-N5	3.75	1.43	1.35
4	B	603	FDA	C4X-C4	3.68	1.51	1.42
4	A	603	FDA	C5X-N5	3.67	1.46	1.39
4	A	603	FDA	C10-N10	3.61	1.44	1.38
4	B	603	FDA	C2-N1	3.59	1.43	1.37
4	D	603	FDA	C9A-N10	3.59	1.47	1.41
4	A	603	FDA	C2-N3	3.57	1.43	1.37
4	A	603	FDA	C2A-N3A	3.49	1.37	1.32
2	C	601	NAP	O2D-C2D	3.43	1.51	1.43
4	D	603	FDA	C5X-C9A	-3.40	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAP	P2B-O2B	3.39	1.65	1.59
4	C	603	FDA	C10-N10	3.39	1.44	1.38
4	A	603	FDA	C4X-C4	3.38	1.51	1.42
4	C	603	FDA	C4X-C4	3.33	1.50	1.42
4	D	603	FDA	C2B-C1B	-3.32	1.48	1.53
4	B	603	FDA	C9A-N10	3.30	1.46	1.41
4	C	603	FDA	C2-N3	3.30	1.43	1.37
2	A	601	NAP	C6A-N6A	3.28	1.46	1.34
4	D	603	FDA	C5X-N5	3.26	1.45	1.39
4	B	603	FDA	C2A-N3A	3.26	1.37	1.32
4	C	603	FDA	C2-N1	3.18	1.43	1.37
4	A	603	FDA	C9A-N10	3.17	1.46	1.41
4	A	603	FDA	C2B-C1B	-3.17	1.49	1.53
4	D	603	FDA	C4X-C4	3.15	1.50	1.42
2	B	601	NAP	O2D-C2D	3.09	1.50	1.43
2	A	601	NAP	O3D-C3D	-3.09	1.35	1.43
2	A	601	NAP	O2D-C2D	3.04	1.50	1.43
2	C	601	NAP	C6A-N6A	3.03	1.45	1.34
2	D	601	NAP	C6A-N6A	3.03	1.45	1.34
4	D	603	FDA	C2A-N3A	3.01	1.37	1.32
4	C	603	FDA	C5X-C9A	-2.98	1.37	1.40
4	C	603	FDA	C2A-N3A	2.97	1.36	1.32
4	A	603	FDA	C6A-N6A	2.97	1.44	1.34
2	B	601	NAP	C6A-N6A	2.96	1.44	1.34
2	D	601	NAP	O2D-C2D	2.94	1.49	1.43
4	C	603	FDA	C9A-N10	2.93	1.46	1.41
4	C	603	FDA	C2B-C1B	-2.91	1.49	1.53
4	B	603	FDA	C6A-N6A	2.85	1.44	1.34
4	B	603	FDA	C2-N3	2.81	1.42	1.37
2	B	601	NAP	C2A-N3A	2.76	1.36	1.32
4	C	603	FDA	C6A-N6A	2.75	1.44	1.34
2	B	601	NAP	O7N-C7N	-2.74	1.18	1.24
4	B	603	FDA	PA-O2A	-2.74	1.42	1.55
4	B	603	FDA	O3B-C3B	-2.73	1.36	1.43
4	D	603	FDA	C2-N3	2.73	1.42	1.37
4	D	603	FDA	PA-O5B	-2.73	1.48	1.59
4	B	603	FDA	PA-O5B	-2.70	1.48	1.59
2	B	601	NAP	O3D-C3D	-2.68	1.36	1.43
2	A	601	NAP	C3N-C7N	2.68	1.54	1.50
4	B	603	FDA	C2B-C1B	-2.67	1.49	1.53
2	D	601	NAP	O3D-C3D	-2.67	1.36	1.43
2	C	601	NAP	C2A-N3A	2.63	1.36	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAP	O3B-C3B	-2.62	1.36	1.43
2	B	601	NAP	P2B-O2B	2.62	1.64	1.59
2	A	601	NAP	O3B-C3B	-2.62	1.36	1.43
2	D	601	NAP	O3B-C3B	-2.60	1.36	1.43
4	C	603	FDA	P-O1P	2.59	1.60	1.50
2	D	601	NAP	O7N-C7N	-2.57	1.19	1.24
4	C	603	FDA	O3B-C3B	-2.52	1.37	1.43
2	D	601	NAP	C5A-C4A	-2.50	1.34	1.40
2	A	601	NAP	C2A-N3A	2.50	1.36	1.32
4	D	603	FDA	PA-O2A	-2.47	1.43	1.55
2	A	601	NAP	O7N-C7N	-2.46	1.19	1.24
2	A	601	NAP	C5A-C4A	-2.45	1.34	1.40
4	B	603	FDA	P-O1P	2.44	1.59	1.50
4	D	603	FDA	C6A-N6A	2.44	1.42	1.34
2	C	601	NAP	O7N-C7N	-2.43	1.19	1.24
4	A	603	FDA	PA-O2A	-2.42	1.44	1.55
4	C	603	FDA	O2'-C2'	-2.37	1.38	1.43
4	A	603	FDA	PA-O5B	-2.36	1.49	1.59
4	D	603	FDA	P-O1P	2.35	1.59	1.50
4	B	603	FDA	O2'-C2'	-2.34	1.38	1.43
2	B	601	NAP	O3B-C3B	-2.33	1.37	1.43
2	D	601	NAP	P2B-O2B	2.32	1.63	1.59
4	C	603	FDA	PA-O2A	-2.30	1.44	1.55
2	C	601	NAP	O3D-C3D	-2.26	1.37	1.43
4	A	603	FDA	O3B-C3B	-2.25	1.37	1.43
4	C	603	FDA	PA-O5B	-2.22	1.50	1.59
4	A	603	FDA	O3'-C3'	-2.21	1.37	1.43
2	B	601	NAP	C5A-C4A	-2.21	1.35	1.40
4	D	603	FDA	C9-C8	2.19	1.42	1.39
2	D	601	NAP	C3N-C7N	2.18	1.53	1.50
2	A	601	NAP	P2B-O2B	2.17	1.63	1.59
4	A	603	FDA	P-O1P	2.13	1.58	1.50
2	C	601	NAP	C5A-C4A	-2.12	1.35	1.40
4	D	603	FDA	O3B-C3B	-2.12	1.38	1.43
4	D	603	FDA	O3'-C3'	-2.11	1.38	1.43
4	C	603	FDA	O2B-C2B	-2.09	1.38	1.43
4	D	603	FDA	O4'-C4'	-2.07	1.39	1.43

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	NAP	C5A-C6A-N6A	9.38	134.61	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	NAP	C5A-C6A-N6A	9.02	134.05	120.35
2	A	601	NAP	C5A-C6A-N6A	7.98	132.47	120.35
2	B	601	NAP	C5A-C6A-N6A	7.63	131.95	120.35
2	C	601	NAP	N6A-C6A-N1A	-6.63	104.81	118.57
2	D	601	NAP	N3A-C2A-N1A	-5.97	119.34	128.68
2	D	601	NAP	N6A-C6A-N1A	-5.91	106.31	118.57
4	D	603	FDA	N3A-C2A-N1A	-5.75	119.70	128.68
4	C	603	FDA	N3A-C2A-N1A	-5.65	119.85	128.68
2	A	601	NAP	N3A-C2A-N1A	-5.63	119.88	128.68
2	A	601	NAP	N6A-C6A-N1A	-5.38	107.40	118.57
4	A	603	FDA	N3A-C2A-N1A	-5.32	120.36	128.68
2	B	601	NAP	N3A-C2A-N1A	-5.17	120.59	128.68
4	B	603	FDA	N3A-C2A-N1A	-5.15	120.64	128.68
2	B	601	NAP	N6A-C6A-N1A	-5.13	107.92	118.57
2	C	601	NAP	N3A-C2A-N1A	-4.90	121.02	128.68
4	D	603	FDA	C4-N3-C2	-4.79	119.44	126.34
4	A	603	FDA	C4-N3-C2	-4.13	120.39	126.34
4	C	603	FDA	C4-N3-C2	-4.08	120.47	126.34
2	B	601	NAP	O4D-C1D-C2D	-3.77	101.41	106.93
4	D	603	FDA	N3-C2-N1	3.65	121.67	115.80
4	D	603	FDA	O4-C4-C4X	-3.43	119.38	127.24
2	C	601	NAP	O4D-C1D-C2D	-3.40	101.96	106.93
4	B	603	FDA	C4-N3-C2	-3.28	121.62	126.34
4	A	603	FDA	N3-C2-N1	3.28	121.07	115.80
2	A	601	NAP	PN-O3-PA	-3.27	121.59	132.83
2	D	601	NAP	C1B-N9A-C4A	-3.20	121.01	126.64
4	B	603	FDA	O2A-PA-O5B	-3.11	93.31	107.75
4	A	603	FDA	O2P-P-O5'	-3.09	93.37	107.75
4	A	603	FDA	O4-C4-C4X	-2.98	120.40	127.24
4	A	603	FDA	C1B-N9A-C4A	-2.96	121.45	126.64
4	C	603	FDA	O4-C4-C4X	-2.95	120.49	127.24
4	B	603	FDA	N3-C2-N1	2.92	120.50	115.80
4	A	603	FDA	O2A-PA-O5B	-2.92	94.17	107.75
2	C	601	NAP	C6N-N1N-C2N	-2.87	119.36	121.97
3	C	602	ORN	OXT-C-O	-2.84	117.65	124.09
2	B	601	NAP	C6N-N1N-C2N	-2.83	119.40	121.97
4	A	603	FDA	O5'-P-O1P	2.82	120.10	109.07
4	D	603	FDA	O5'-P-O1P	2.79	119.98	109.07
2	B	601	NAP	PN-O3-PA	-2.71	123.53	132.83
2	B	601	NAP	C3N-C7N-N7N	2.66	120.94	117.75
4	B	603	FDA	C4A-C5A-N7A	-2.65	106.64	109.40
4	B	603	FDA	O5'-P-O1P	2.63	119.34	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	603	FDA	O2P-P-O5'	-2.60	95.65	107.75
4	C	603	FDA	C1B-N9A-C4A	-2.59	122.09	126.64
4	C	603	FDA	N3-C2-N1	2.54	119.89	115.80
4	D	603	FDA	O2P-P-O5'	-2.51	96.07	107.75
3	C	602	ORN	OXT-C-CA	2.50	121.91	113.38
4	D	603	FDA	C6-C5X-N5	-2.45	115.41	119.84
4	B	603	FDA	O5B-PA-O1A	2.43	118.58	109.07
4	C	603	FDA	O2P-P-O5'	-2.40	96.58	107.75
4	D	603	FDA	O2A-PA-O5B	-2.40	96.60	107.75
4	C	603	FDA	C4X-C4-N3	2.39	119.43	112.31
3	A	602	ORN	OXT-C-CA	2.39	121.52	113.38
2	D	601	NAP	O2B-C2B-C3B	-2.38	103.05	111.68
4	A	603	FDA	O2-C2-N1	-2.37	117.35	121.82
4	C	603	FDA	C4A-C5A-N7A	-2.37	106.93	109.40
2	D	601	NAP	C3D-C2D-C1D	2.35	104.52	100.98
2	B	601	NAP	C2N-C3N-C4N	2.32	120.88	118.26
4	A	603	FDA	C4A-C5A-N7A	-2.31	106.99	109.40
2	A	601	NAP	O7N-C7N-C3N	2.30	122.38	119.63
4	B	603	FDA	C1B-N9A-C4A	-2.28	122.63	126.64
4	D	603	FDA	C6-C5X-C9A	2.28	122.08	119.67
2	C	601	NAP	C2N-C3N-C4N	2.27	120.84	118.26
4	C	603	FDA	C5'-C4'-C3'	2.27	116.59	112.20
4	D	603	FDA	O5B-PA-O1A	2.22	117.76	109.07
4	D	603	FDA	C4X-C4-N3	2.15	118.72	112.31
4	C	603	FDA	O5'-P-O1P	2.12	117.34	109.07
2	D	601	NAP	C6N-N1N-C2N	-2.11	120.05	121.97
4	A	603	FDA	O5B-PA-O1A	2.10	117.27	109.07
2	A	601	NAP	O7N-C7N-N7N	-2.09	119.60	122.58
2	C	601	NAP	PN-O3-PA	-2.09	125.65	132.83
4	D	603	FDA	C9A-C5X-N5	2.09	122.35	119.56
3	D	602	ORN	OXT-C-O	-2.07	119.39	124.09
4	C	603	FDA	O2-C2-N1	-2.05	117.95	121.82
2	C	601	NAP	C5D-C4D-C3D	-2.04	107.53	115.18
2	A	601	NAP	C2N-C3N-C4N	2.02	120.55	118.26

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAP	C2B-O2B-P2B-O1X
2	B	601	NAP	C2B-O2B-P2B-O1X
4	D	603	FDA	N10-C1'-C2'-O2'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	603	FDA	O3'-C3'-C4'-C5'
4	A	603	FDA	C2'-C3'-C4'-C5'
4	A	603	FDA	O3'-C3'-C4'-O4'
4	D	603	FDA	O3'-C3'-C4'-C5'
4	D	603	FDA	C2'-C3'-C4'-C5'
4	A	603	FDA	PA-O3P-P-O5'
4	B	603	FDA	P-O3P-PA-O5B
2	B	601	NAP	C5D-O5D-PN-O3
4	A	603	FDA	C5'-O5'-P-O3P
4	A	603	FDA	P-O3P-PA-O2A
4	B	603	FDA	PA-O3P-P-O1P
4	D	603	FDA	N10-C1'-C2'-C3'
4	A	603	FDA	C2'-C3'-C4'-O4'
4	D	603	FDA	C2'-C3'-C4'-O4'
4	D	603	FDA	O3'-C3'-C4'-O4'
4	B	603	FDA	PA-O3P-P-O2P
4	C	603	FDA	O4B-C4B-C5B-O5B
4	A	603	FDA	P-O3P-PA-O1A
2	B	601	NAP	C2B-O2B-P2B-O3X
2	C	601	NAP	C2B-O2B-P2B-O3X
4	B	603	FDA	C5B-O5B-PA-O3P
2	A	601	NAP	O4B-C4B-C5B-O5B
2	B	601	NAP	O4B-C4B-C5B-O5B
2	C	601	NAP	O4B-C4B-C5B-O5B
2	D	601	NAP	O4B-C4B-C5B-O5B
4	A	603	FDA	O4B-C4B-C5B-O5B
4	B	603	FDA	O4B-C4B-C5B-O5B
4	D	603	FDA	O4B-C4B-C5B-O5B
4	A	603	FDA	C5B-O5B-PA-O1A

There are no ring outliers.

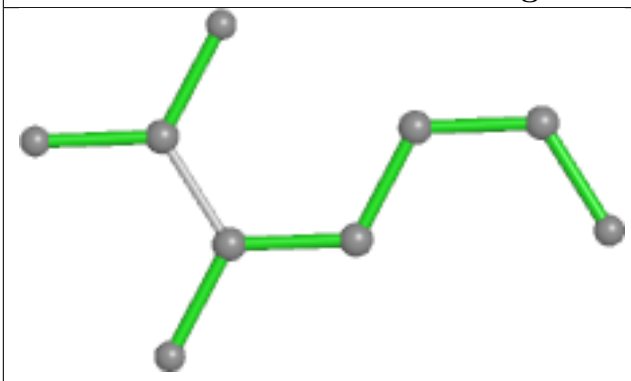
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603	FDA	1	0
4	B	603	FDA	2	0
2	D	601	NAP	1	0
4	A	603	FDA	1	0
4	C	603	FDA	2	0

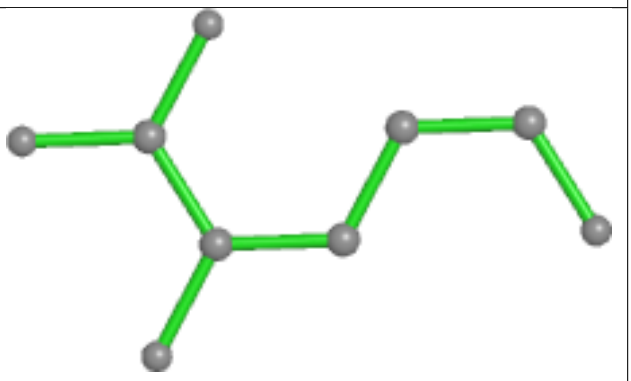
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

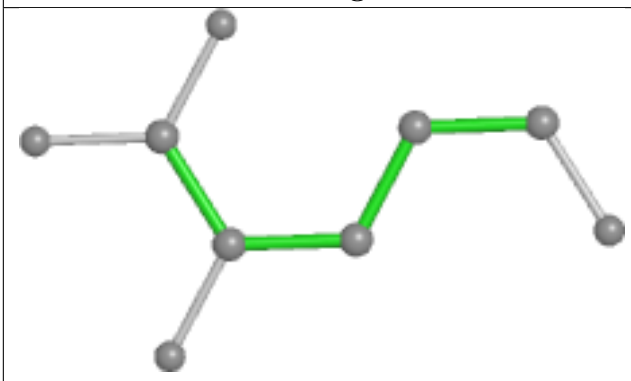
Ligand ORN B 602



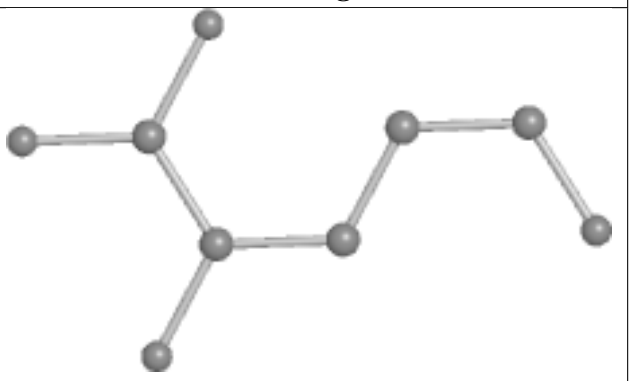
Bond lengths



Bond angles

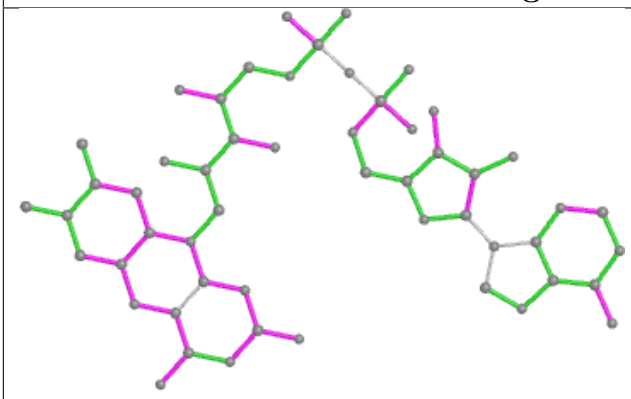


Torsions

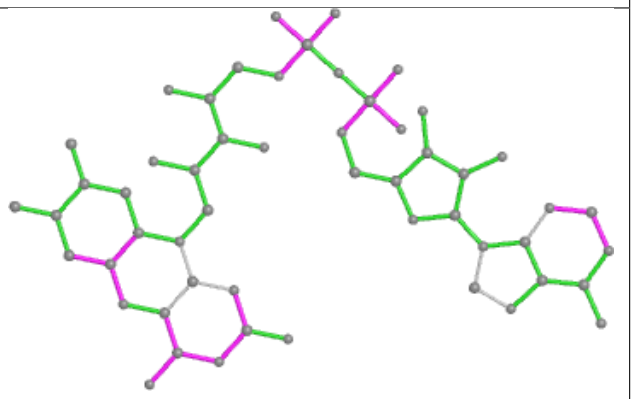


Rings

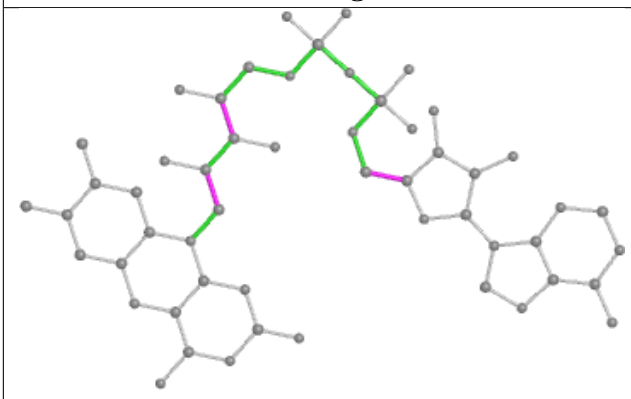
Ligand FDA D 603



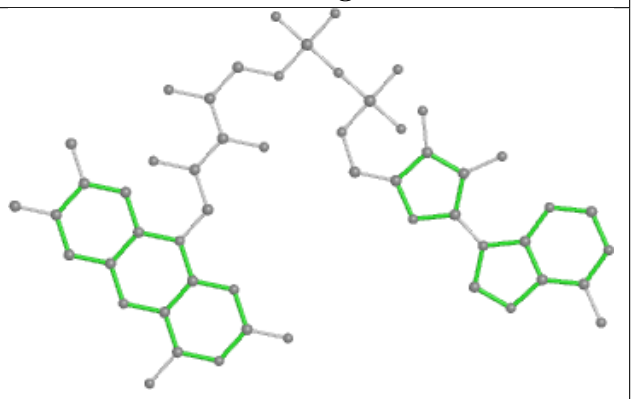
Bond lengths



Bond angles

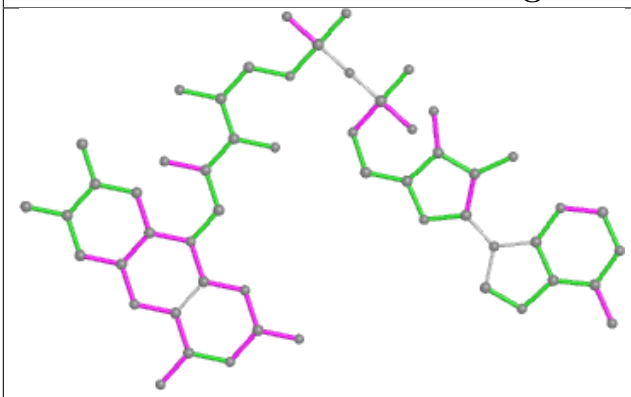


Torsions

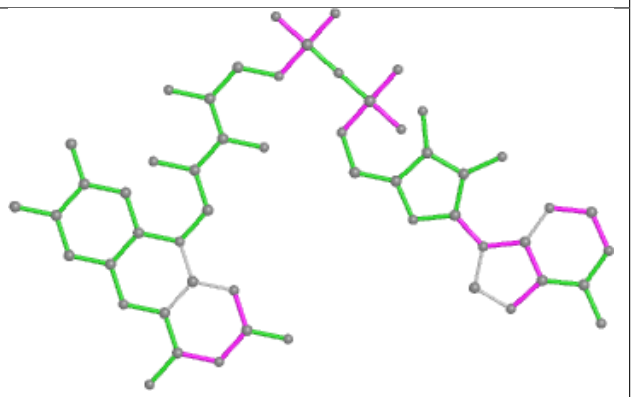


Rings

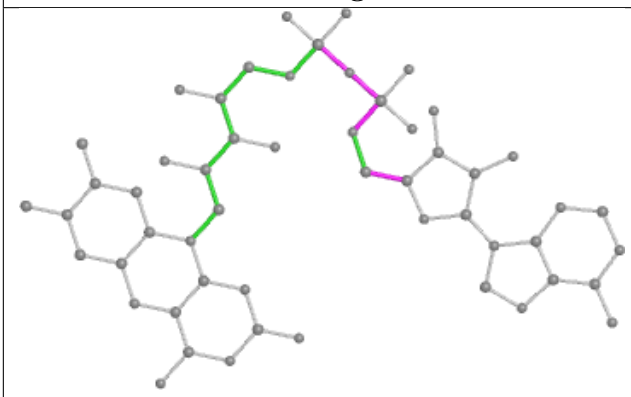
Ligand FDA B 603



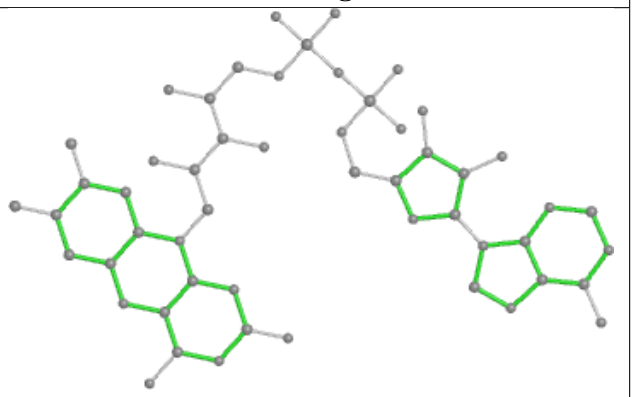
Bond lengths



Bond angles

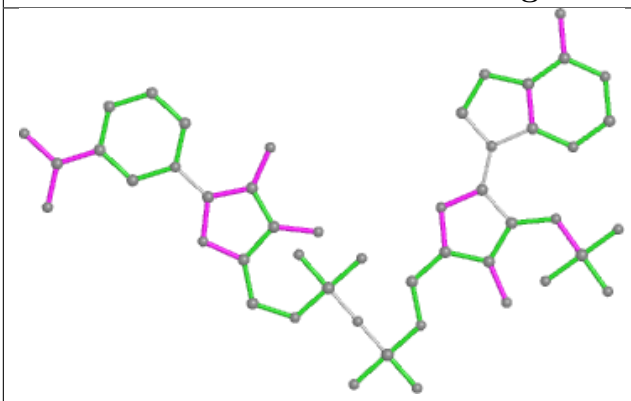


Torsions

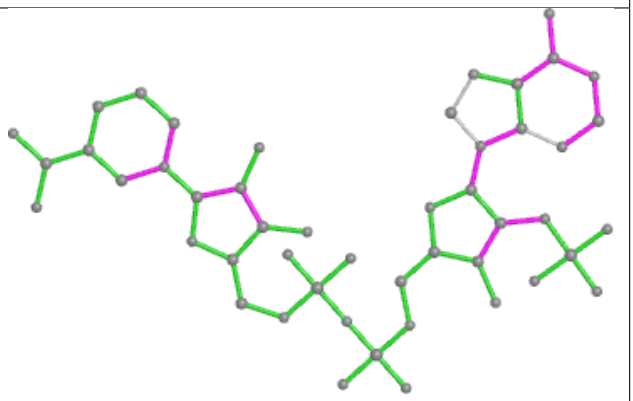


Rings

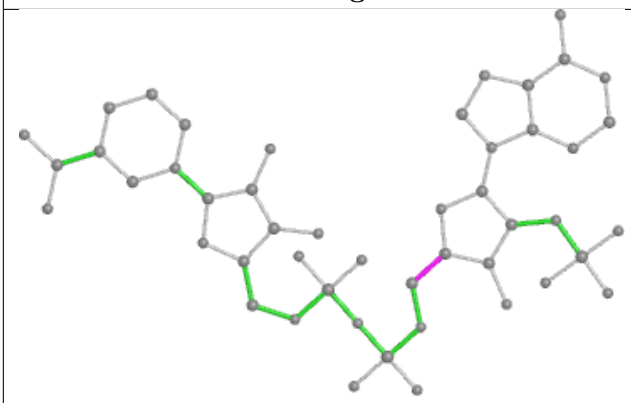
Ligand NAP D 601



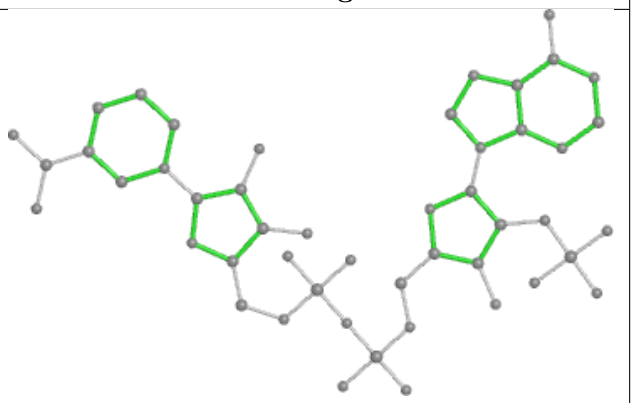
Bond lengths



Bond angles

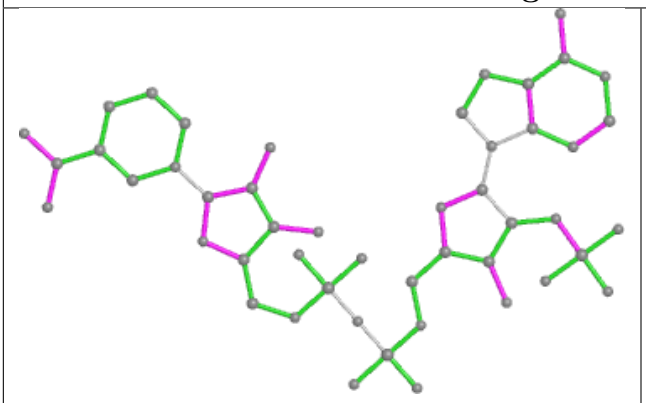


Torsions

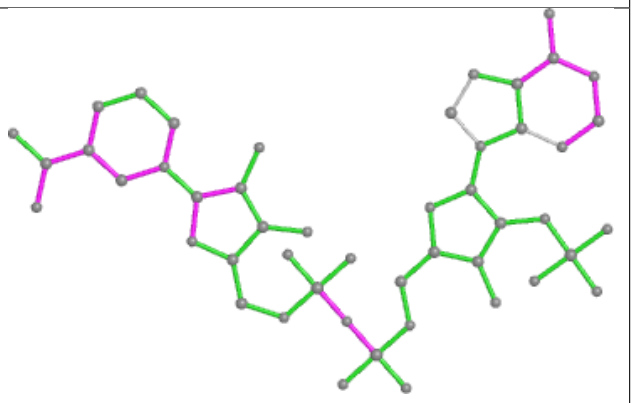


Rings

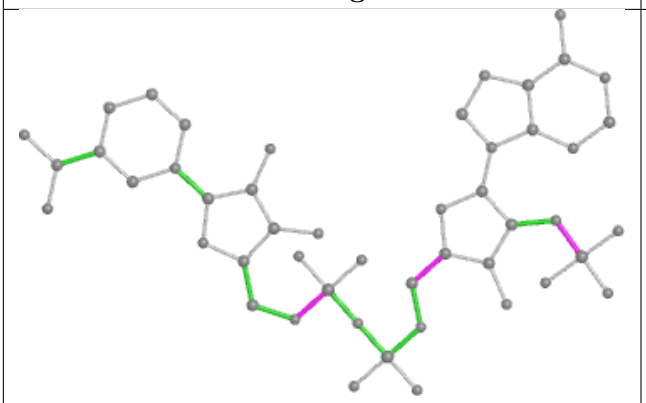
Ligand NAP B 601



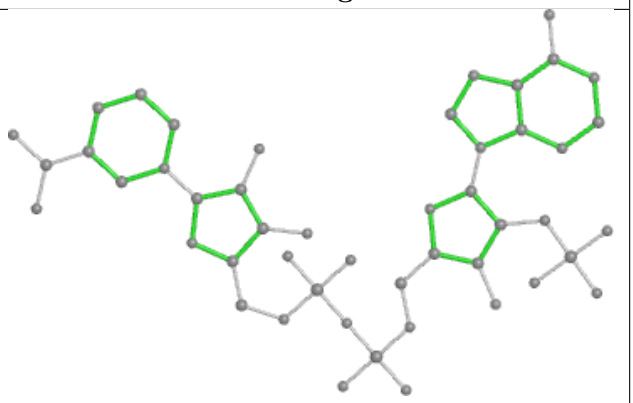
Bond lengths



Bond angles

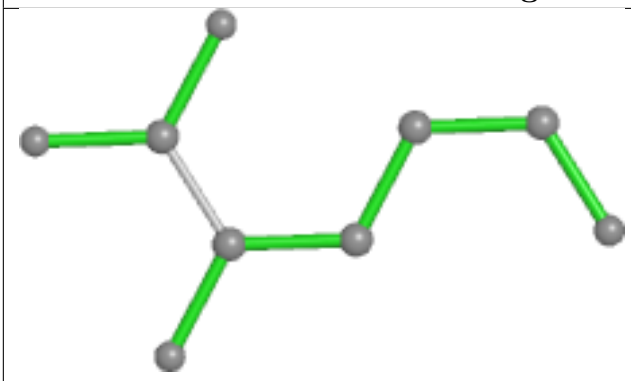


Torsions

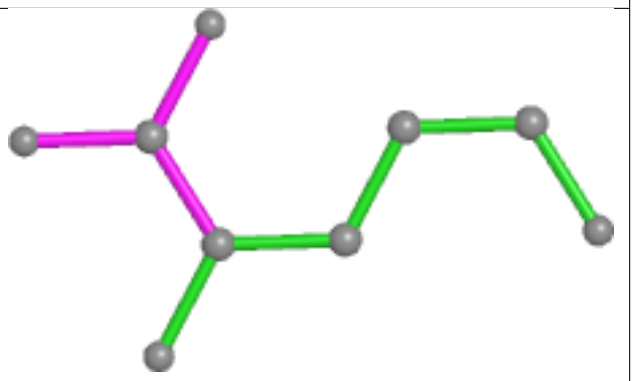


Rings

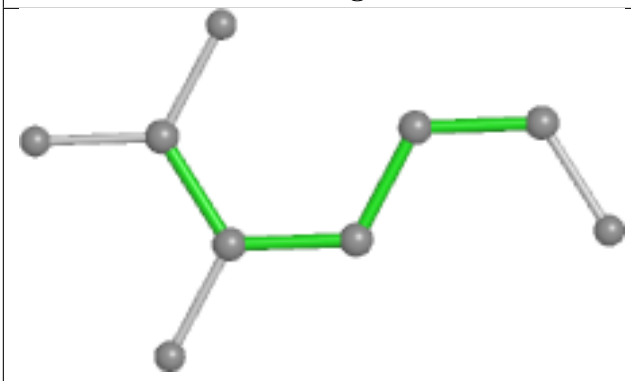
Ligand ORN C 602



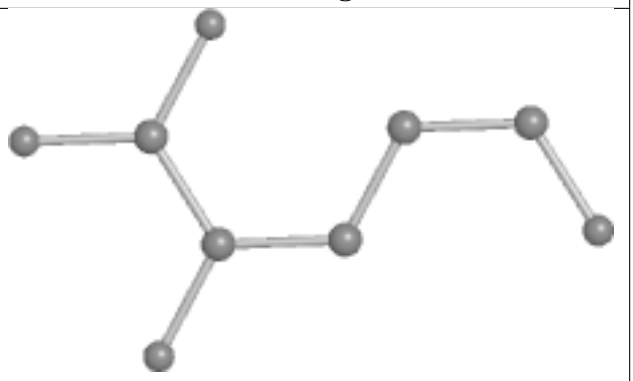
Bond lengths



Bond angles

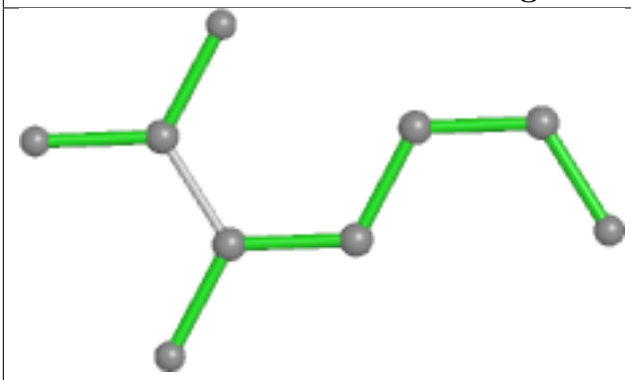


Torsions

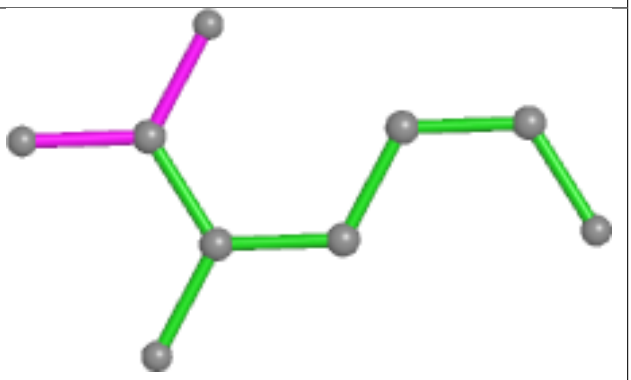


Rings

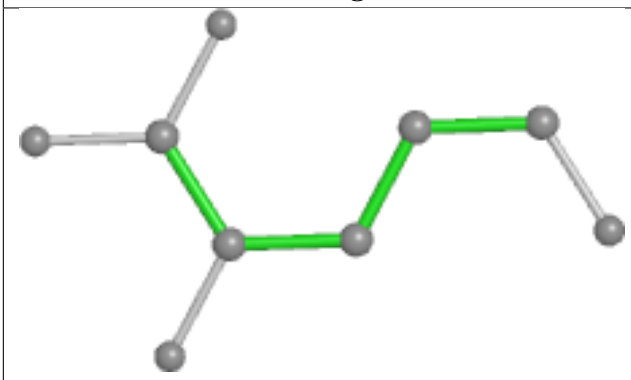
Ligand ORN D 602



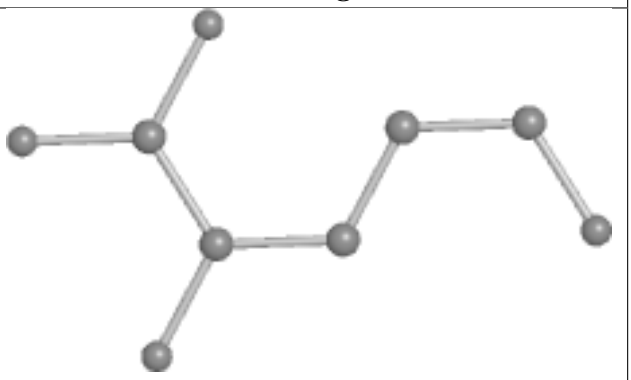
Bond lengths



Bond angles

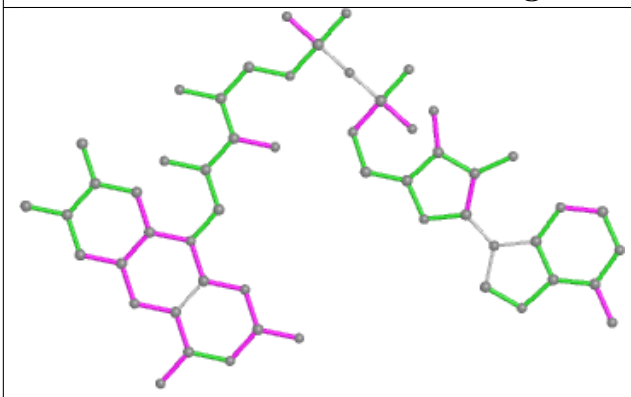


Torsions

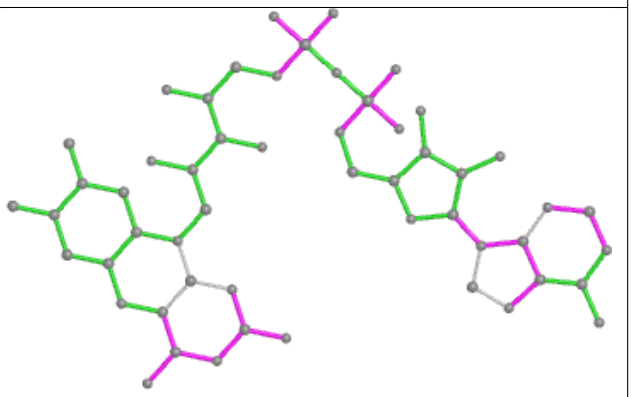


Rings

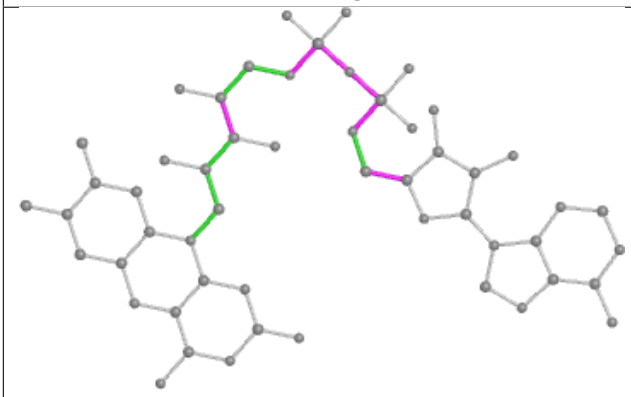
Ligand FDA A 603



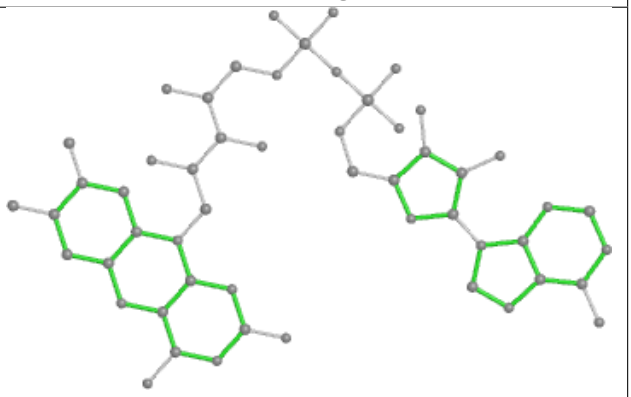
Bond lengths



Bond angles

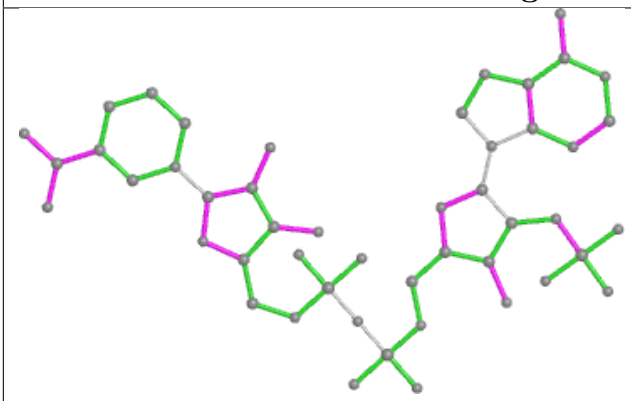


Torsions

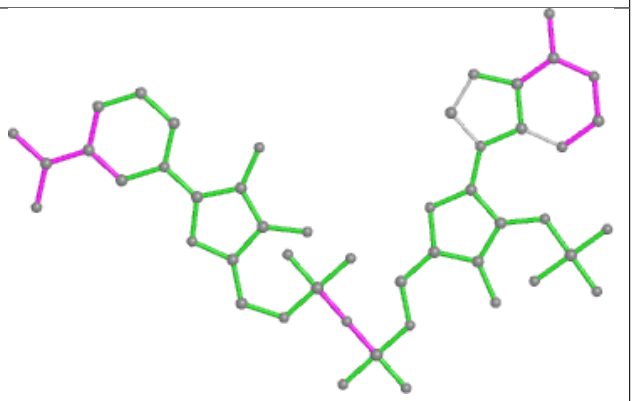


Rings

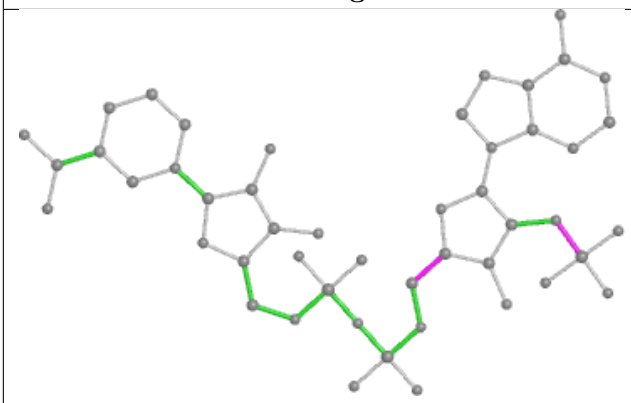
Ligand NAP A 601



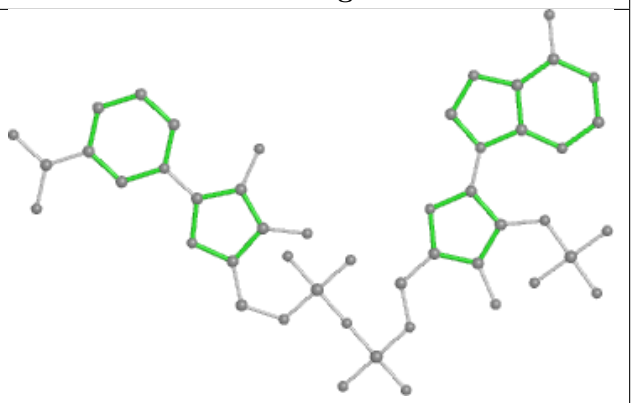
Bond lengths



Bond angles

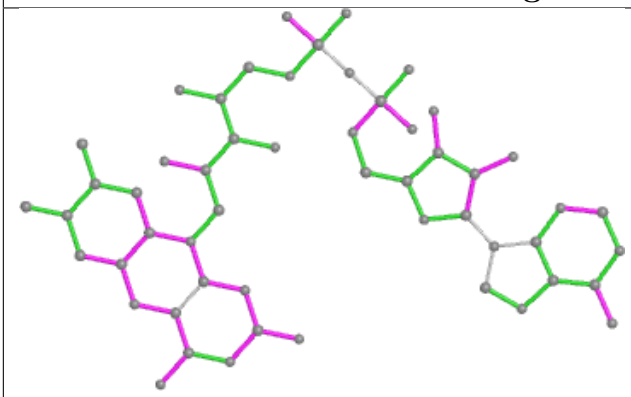


Torsions

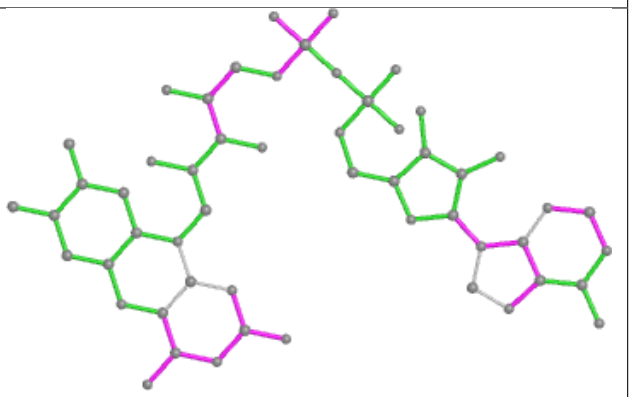


Rings

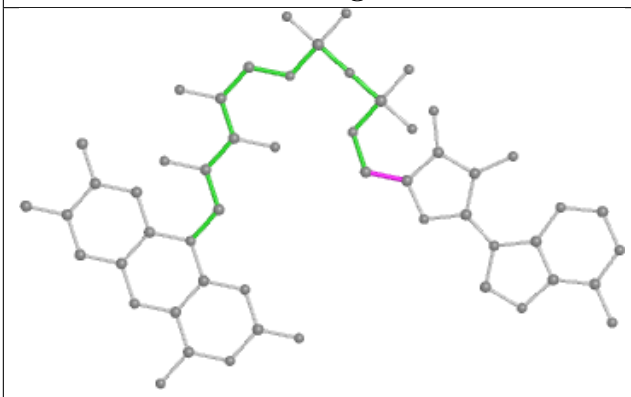
Ligand FDA C 603



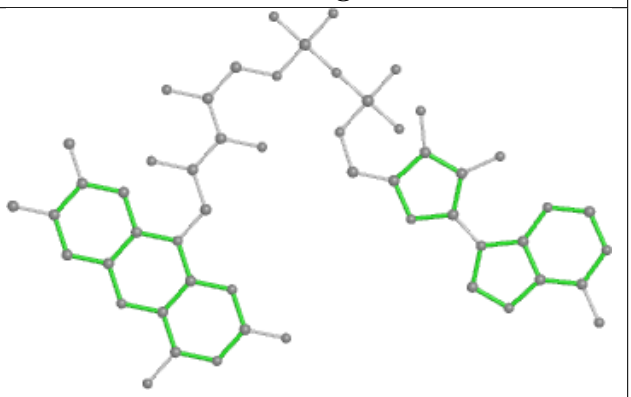
Bond lengths



Bond angles

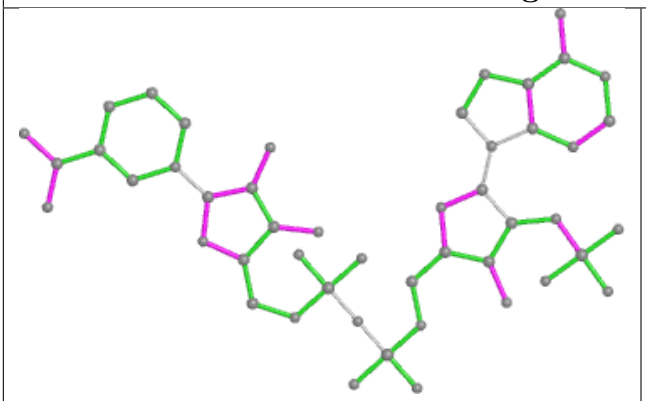


Torsions

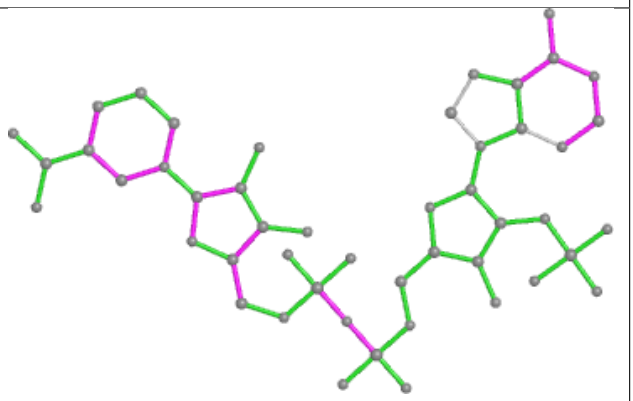


Rings

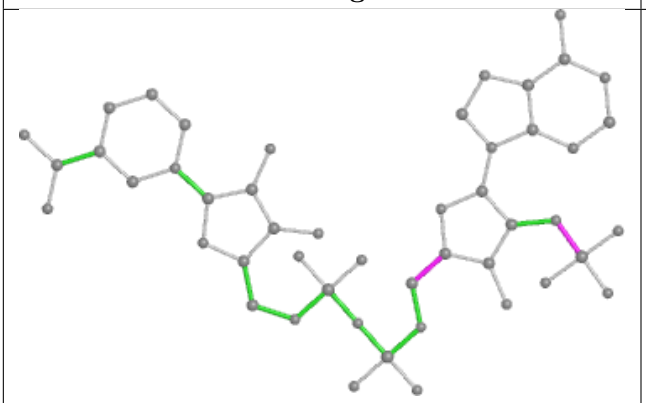
Ligand NAP C 601



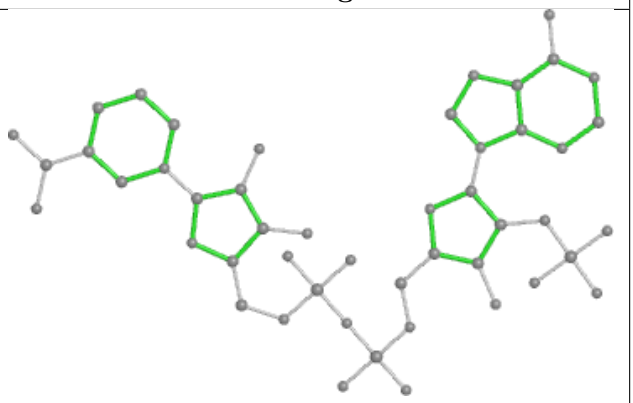
Bond lengths



Bond angles

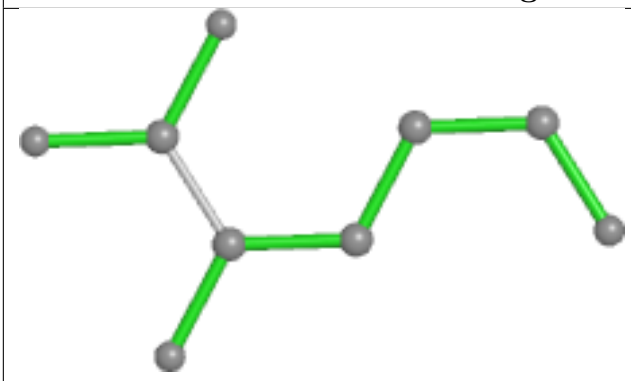


Torsions

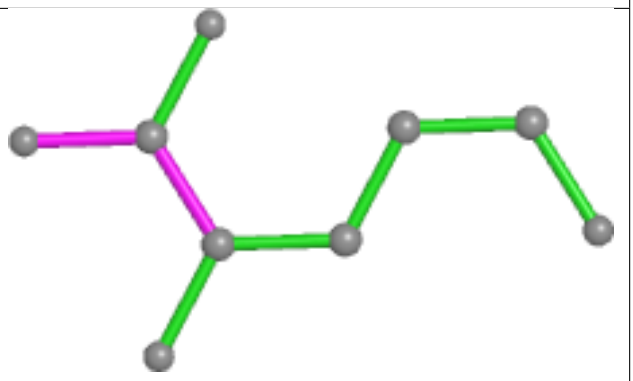


Rings

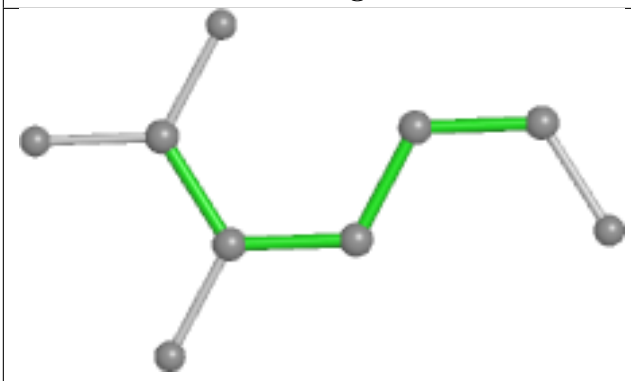
Ligand ORN A 602



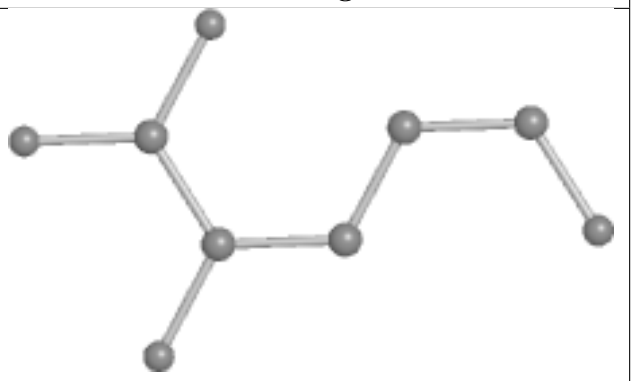
Bond lengths



Bond angles



Torsions



Rings

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	451/494 (91%)	-0.12	3 (0%)	87	92	22, 33, 59, 83	0
1	B	455/494 (92%)	-0.18	1 (0%)	95	97	21, 31, 54, 95	0
1	C	451/494 (91%)	-0.15	2 (0%)	92	96	19, 30, 57, 98	0
1	D	450/494 (91%)	-0.15	3 (0%)	87	92	21, 34, 64, 92	0
All	All	1807/1976 (91%)	-0.15	9 (0%)	91	95	19, 32, 58, 98	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	368	HIS	4.6
1	C	72	ASN	3.1
1	D	74	HIS	2.9
1	B	68	LYS	2.8
1	A	74	HIS	2.3
1	A	180	SER	2.2
1	A	73	ILE	2.2
1	D	71	SER	2.0
1	C	178	PRO	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

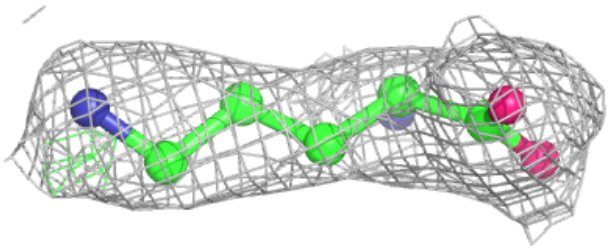
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

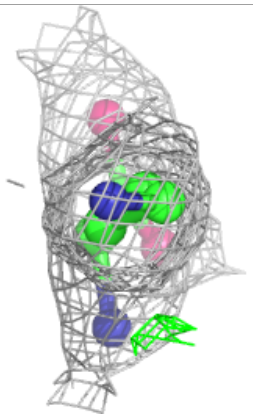
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ORN	A	602	9/9	0.96	0.16	21,29,35,37	0
3	ORN	C	602	9/9	0.96	0.13	15,24,31,31	0
4	FDA	D	603	53/53	0.96	0.12	20,30,39,41	0
2	NAP	B	601	48/48	0.97	0.14	16,31,39,44	0
3	ORN	D	602	9/9	0.97	0.13	20,23,28,29	0
4	FDA	A	603	53/53	0.97	0.12	16,28,33,40	0
4	FDA	B	603	53/53	0.97	0.13	16,27,37,42	0
4	FDA	C	603	53/53	0.97	0.14	18,26,37,44	0
3	ORN	B	602	9/9	0.97	0.11	17,21,31,31	0
2	NAP	D	601	48/48	0.98	0.13	16,31,43,54	0
2	NAP	A	601	48/48	0.98	0.13	14,28,42,52	0
2	NAP	C	601	48/48	0.98	0.13	18,28,37,42	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 ORN A 602:

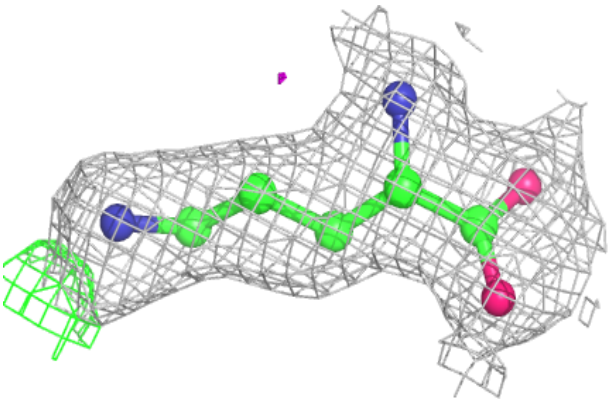
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

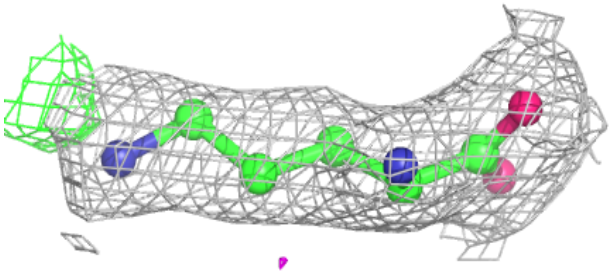


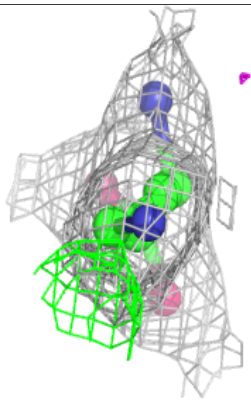


Electron density around ORN C 602:

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

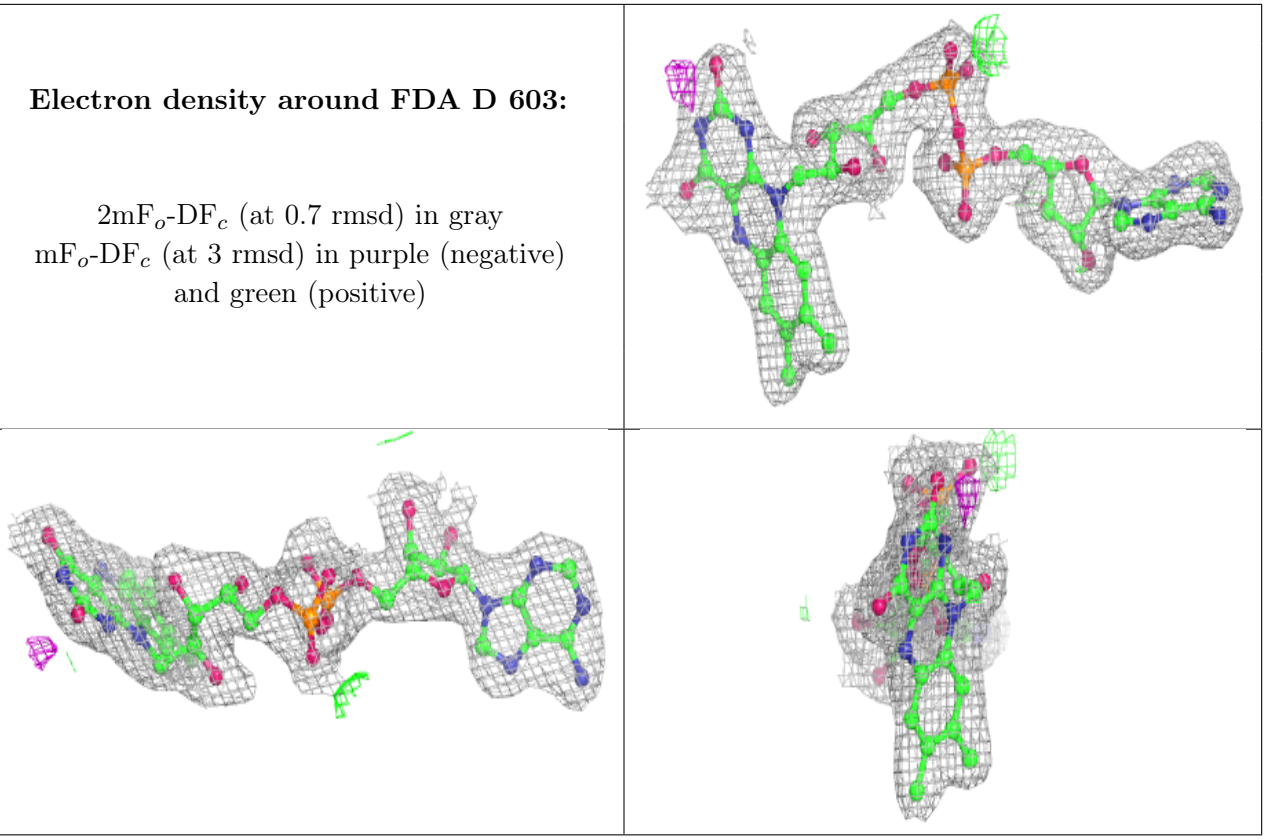






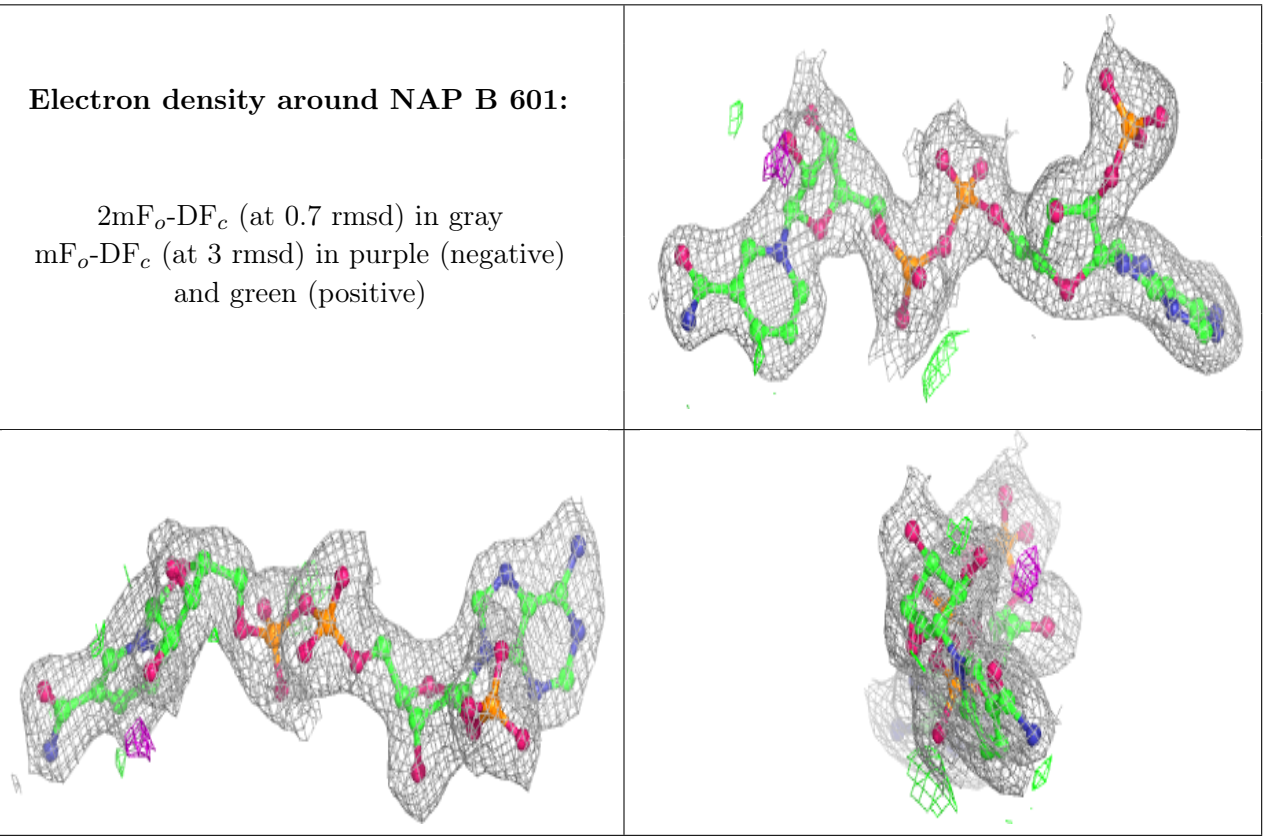
Electron density around FDA D 603:

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



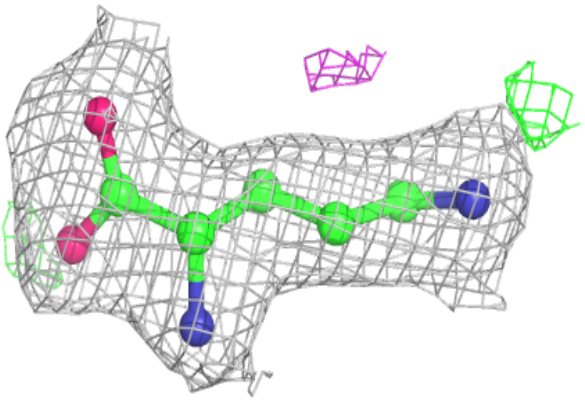
Electron density around NAP B 601:

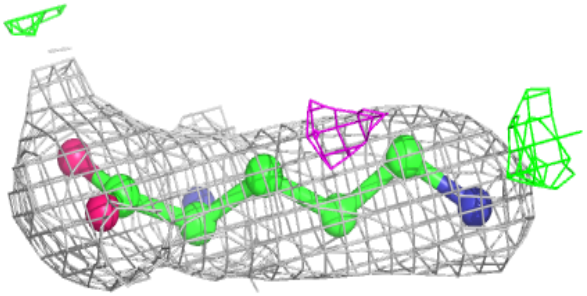
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

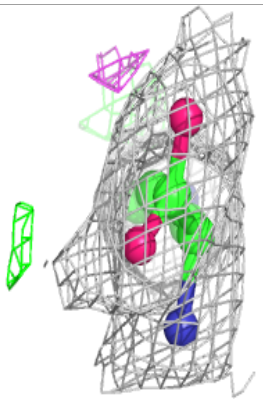


Electron density around ORN D 602:

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

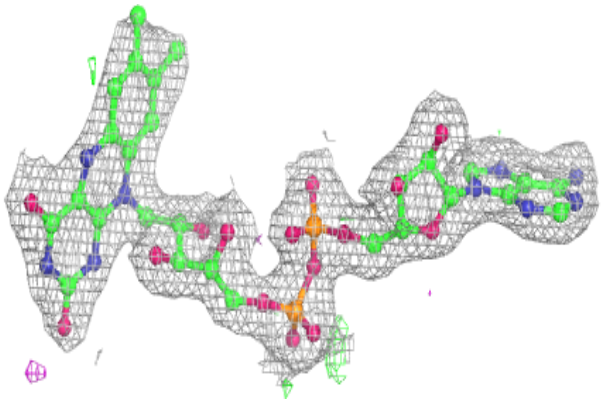


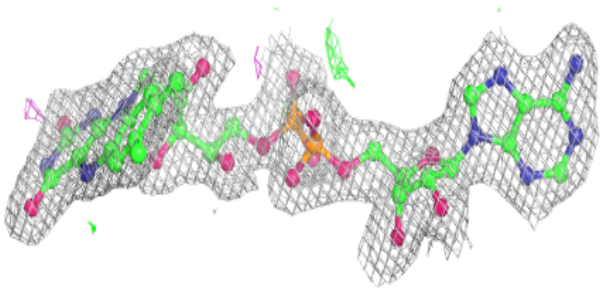


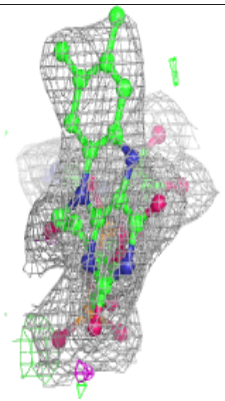


Electron density around FDA A 603:

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

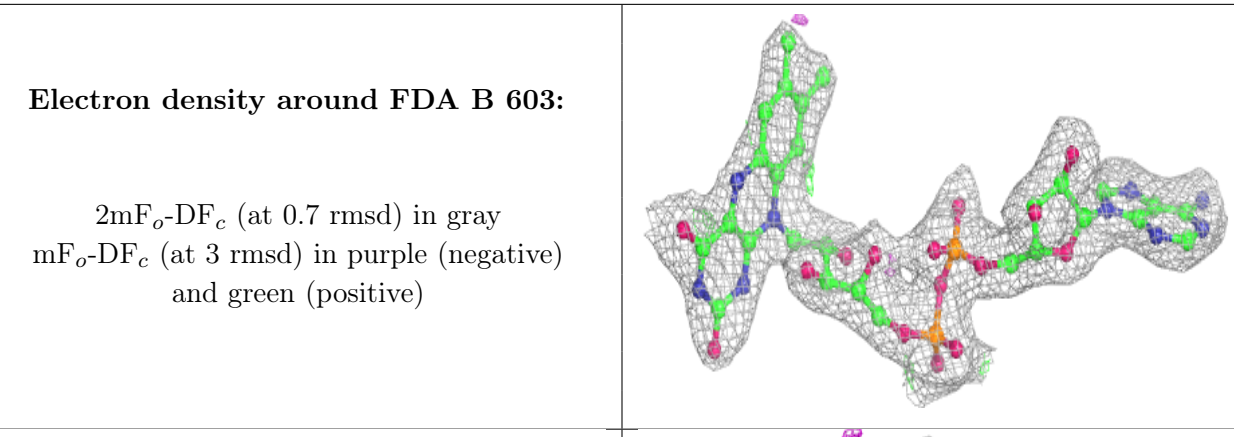






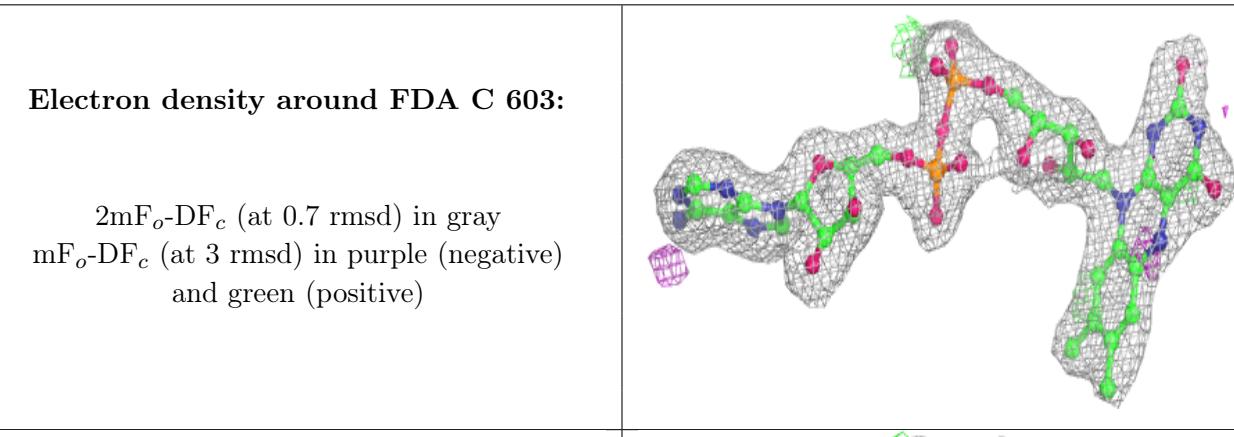
Electron density around FDA B 603:

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



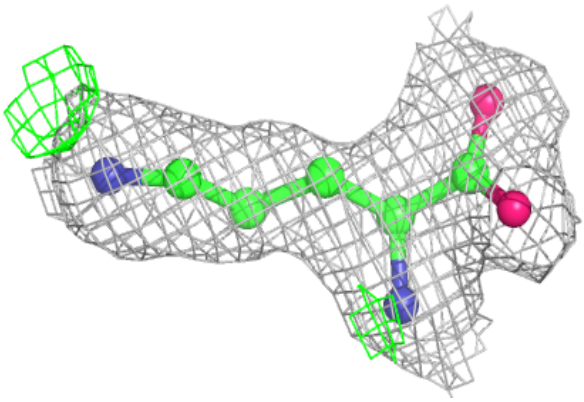
Electron density around FDA C 603:

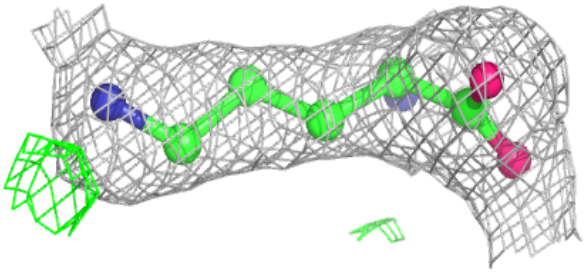
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

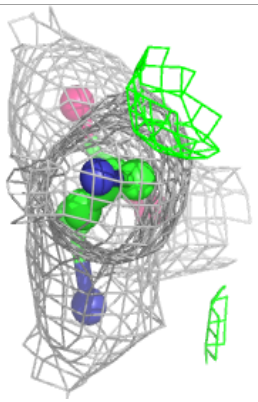


Electron density around ORN B 602:

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

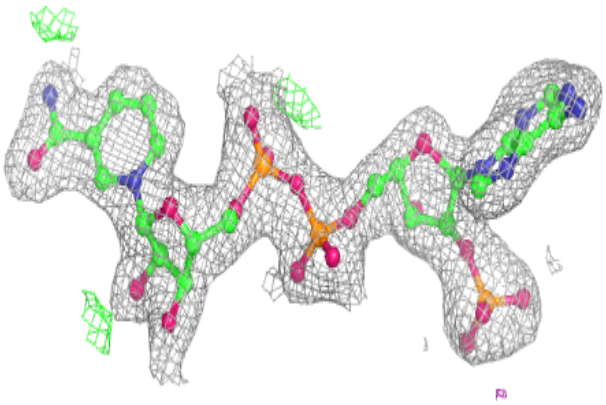


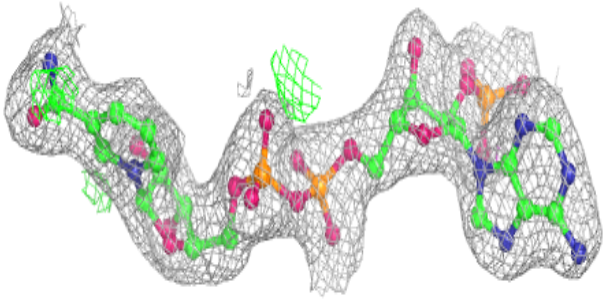


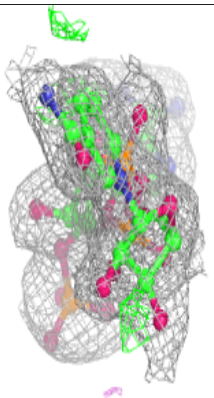


Electron density around NAP D 601:

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

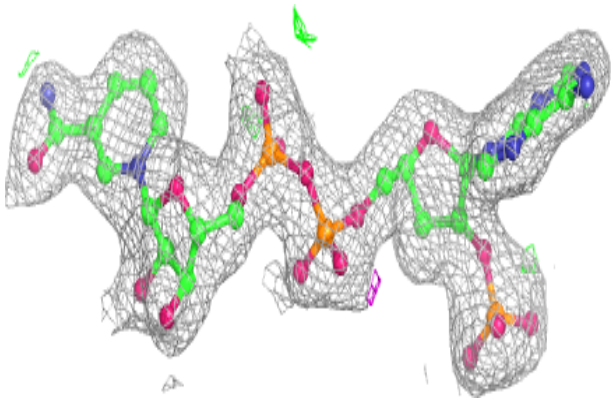


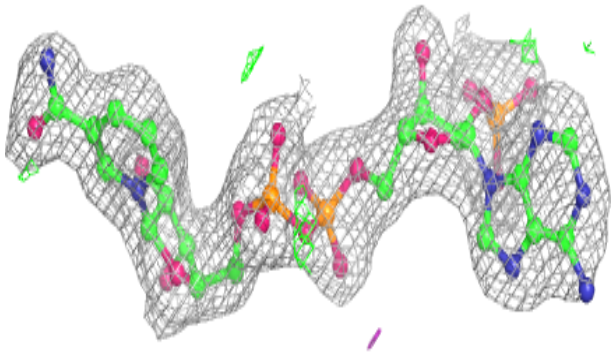


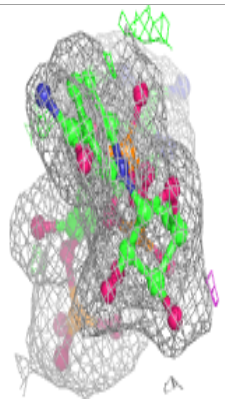


Electron density around NAP A 601:

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

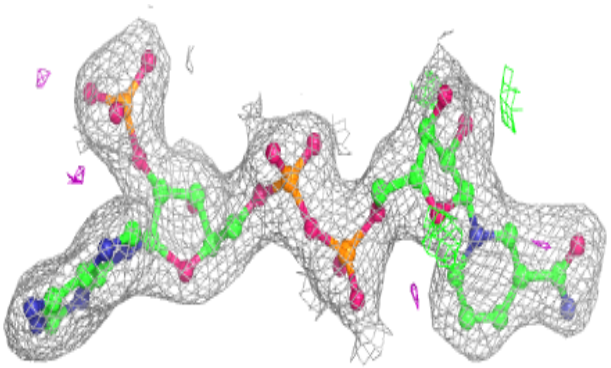


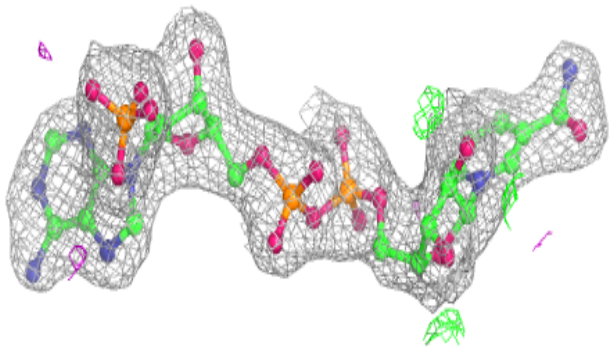


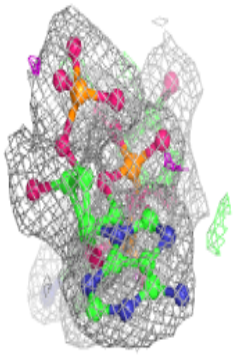


Electron density around NAP C 601:

$2mF_o$-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.