



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:24 PM UTC

PDB ID : 6X0J / pdb_00006x0j
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

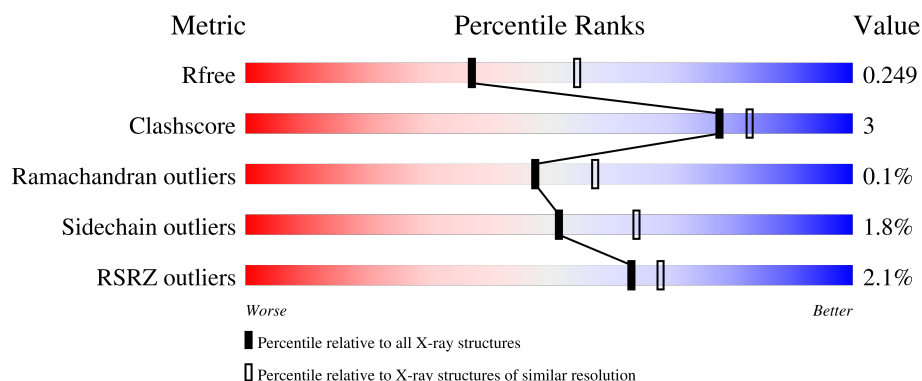
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	494	 2% 83% 8% 9%
1	B	494	 2% 83% 9% 8%
1	C	494	 2% 84% 7% 9%
1	D	494	 2% 84% 7% 9%

2 Entry composition

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

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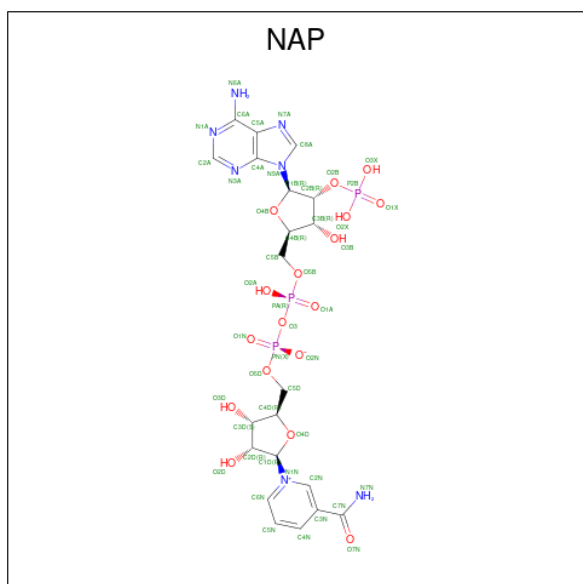
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	initiating methionine	UNP E9QYP0
B	9	GLY	-	expression tag	UNP E9QYP0
B	10	SER	-	expression tag	UNP E9QYP0
B	11	SER	-	expression tag	UNP E9QYP0
B	12	HIS	-	expression tag	UNP E9QYP0
B	13	HIS	-	expression tag	UNP E9QYP0
B	14	HIS	-	expression tag	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

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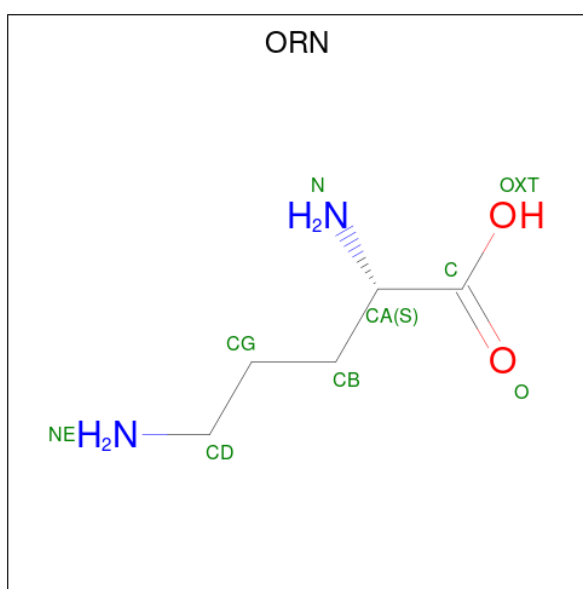
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	MET	-	initiating methionine	UNP E9QYP0
D	9	GLY	-	expression tag	UNP E9QYP0
D	10	SER	-	expression tag	UNP E9QYP0
D	11	SER	-	expression tag	UNP E9QYP0
D	12	HIS	-	expression tag	UNP E9QYP0
D	13	HIS	-	expression tag	UNP E9QYP0
D	14	HIS	-	expression tag	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 (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



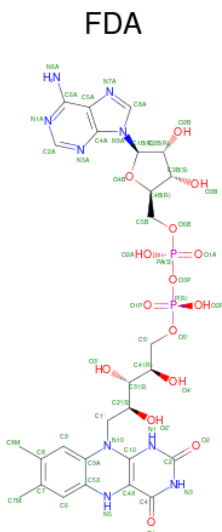
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is L-ornithine (CCD ID: 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	0	0
			9	5	2	2		
3	B	1	Total	C	N	O	0	0
			9	5	2	2		
3	C	1	Total	C	N	O	0	0
			9	5	2	2		
3	D	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 4 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: 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 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

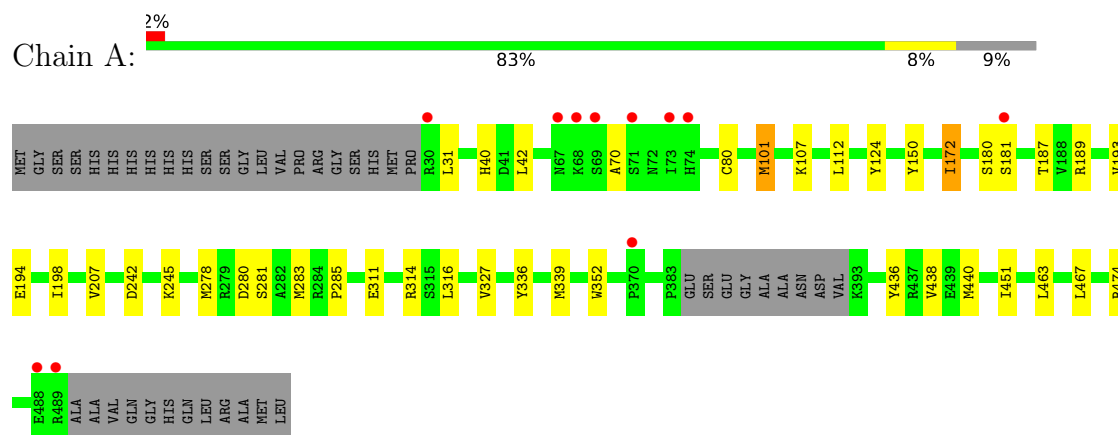
- Molecule 5 is water.

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

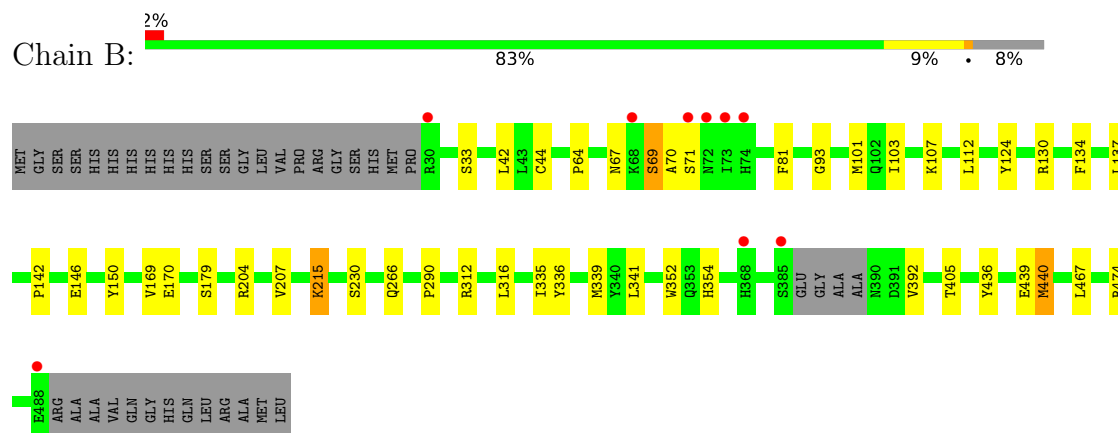
3 Residue-property plots

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.

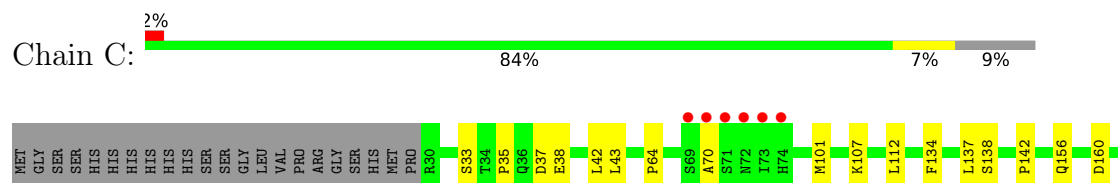
• Molecule 1: L-ornithine N(5)-monooxygenase

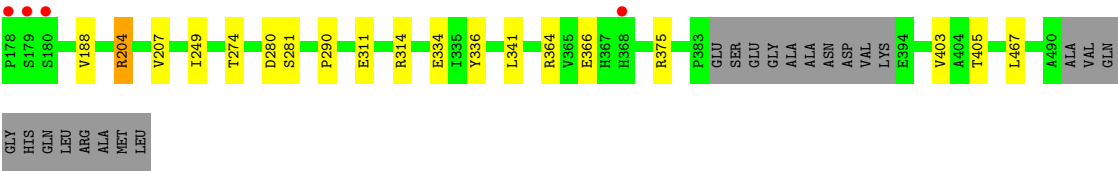


• Molecule 1: L-ornithine N(5)-monooxygenase

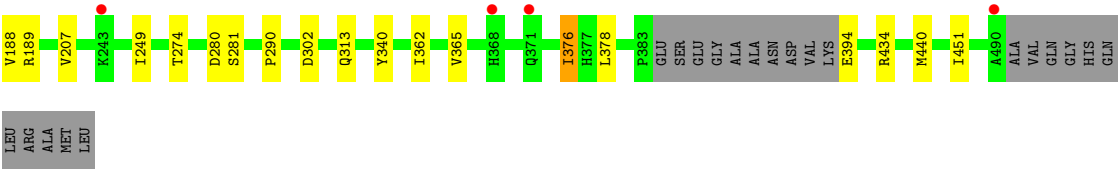
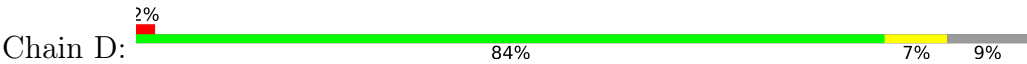


• Molecule 1: L-ornithine N(5)-monooxygenase





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



4 Data and refinement statistics

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 56.90 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.3 (56.90-2.33) 98.2 (56.90-2.33)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.183 , 0.249 0.185 , 0.249	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)	0.35 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/3569	0.53	0/4846
1	B	0.34	0/3588	0.56	0/4876
1	C	0.35	0/3572	0.55	0/4850
1	D	0.33	0/3541	0.54	0/4812
All	All	0.34	0/14270	0.54	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 [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	3492	0	3377	20	0
1	B	3511	0	3368	25	0
1	C	3496	0	3376	17	0
1	D	3465	0	3342	19	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

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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	79	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 (79) 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:D:440:MET:HE1	1:D:451:ILE:HD12	1.77	0.65
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:A:339:MET:HE3	1:A:352:TRP:HZ3	1.74	0.53
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:A:278:MET:HE1	1:A:283:MET:HG3	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:339:MET:HE3	1:B:352:TRP:HZ3	1.79	0.47
1:B:467:LEU:HB3	4:B:603:FDA:O2	2.14	0.47
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:69:SER:C	1:B:71:SER:H	2.24	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:101:MET:HE3	1:A:101:MET:HB3	1.56	0.44
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:A:339:MET:HE3	1:A:352:TRP:CZ3	2.53	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:B:339:MET:HE3	1:B:352:TRP:CZ3	2.54	0.42
1:D:123:ASN:O	1:D:127:GLN:HG2	2.19	0.42
1:A:440:MET:HE1	1:A:451:ILE:HD12	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:130:ARG:HH11	1:B:130:ARG:HD3	1.74	0.41
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%)	43	50
1	B	451/494 (91%)	439 (97%)	11 (2%)	1 (0%)	43	50
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%)	48	57

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/433 (85%)	362 (98%)	7 (2%)	50	63
1	B	373/433 (86%)	365 (98%)	8 (2%)	47	60
1	C	371/433 (86%)	364 (98%)	7 (2%)	50	63
1	D	367/433 (85%)	363 (99%)	4 (1%)	65	77
All	All	1480/1732 (86%)	1454 (98%)	26 (2%)	51	64

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	101	MET
1	A	172	ILE
1	A	180	SER
1	A	181	SER
1	A	193	VAL
1	A	194	GLU
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	B	440	MET
1	C	37	ASP
1	C	138	SER
1	C	156	GLN
1	C	204	ARG
1	C	334	GLU

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Mol	Chain	Res	Type
1	C	341	LEU
1	C	364	ARG
1	D	145	LEU
1	D	172	ILE
1	D	313	GLN
1	D	376	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	408	ASN
1	A	420	GLN
1	B	127	GLN
1	B	133	HIS
1	B	263	HIS
1	B	408	ASN
1	C	91	HIS
1	D	133	HIS
1	D	337	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	NAP	C	601	-	50,52,52	3.69	16 (32%)	71,80,80	1.86	14 (19%)
4	FDA	A	603	-	57,58,58	3.04	25 (43%)	78,89,89	1.89	19 (24%)
2	NAP	A	601	-	50,52,52	3.71	17 (34%)	71,80,80	1.83	13 (18%)
2	NAP	B	601	-	50,52,52	3.66	17 (34%)	71,80,80	1.81	14 (19%)
3	ORN	B	602	-	7,8,8	0.94	0	6,9,9	0.87	0
3	ORN	A	602	-	7,8,8	0.72	0	6,9,9	1.17	0
4	FDA	D	603	-	57,58,58	3.03	23 (40%)	78,89,89	1.92	19 (24%)
4	FDA	B	603	-	57,58,58	3.12	23 (40%)	78,89,89	1.88	17 (21%)
3	ORN	C	602	-	7,8,8	0.86	0	6,9,9	1.22	1 (16%)
2	NAP	D	601	-	50,52,52	3.73	18 (36%)	71,80,80	1.75	14 (19%)
3	ORN	D	602	-	7,8,8	0.90	0	6,9,9	1.06	1 (16%)
4	FDA	C	603	-	57,58,58	2.99	23 (40%)	78,89,89	1.94	20 (25%)

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	C	601	-	-	0/35/67/67	0/5/5/5
4	FDA	A	603	-	-	9/34/50/50	0/6/6/6
2	NAP	A	601	-	-	1/35/67/67	0/5/5/5
2	NAP	B	601	-	-	2/35/67/67	0/5/5/5
3	ORN	B	602	-	-	0/8/8/8	-
3	ORN	A	602	-	-	0/8/8/8	-
4	FDA	D	603	-	-	6/34/50/50	0/6/6/6
4	FDA	B	603	-	-	3/34/50/50	0/6/6/6
3	ORN	C	602	-	-	0/8/8/8	-
2	NAP	D	601	-	-	1/35/67/67	0/5/5/5
3	ORN	D	602	-	-	0/8/8/8	-
4	FDA	C	603	-	-	1/34/50/50	0/6/6/6

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAP	O4D-C1D	16.40	1.62	1.40
2	C	601	NAP	O4D-C1D	16.27	1.62	1.40
2	A	601	NAP	O4D-C1D	16.05	1.62	1.40
2	B	601	NAP	O4D-C1D	15.99	1.61	1.40
4	D	603	FDA	PA-O3P	-9.38	1.49	1.59
2	D	601	NAP	O4B-C1B	9.29	1.63	1.42
2	A	601	NAP	C2B-C1B	-9.22	1.30	1.53
2	D	601	NAP	C2B-C1B	-9.00	1.31	1.53
4	A	603	FDA	O4-C4	8.86	1.40	1.23
4	B	603	FDA	PA-O3P	-8.86	1.49	1.59
2	B	601	NAP	C2B-C1B	-8.75	1.31	1.53
2	A	601	NAP	O4B-C1B	8.67	1.62	1.42
2	B	601	NAP	O4B-C1B	8.62	1.61	1.42
4	B	603	FDA	O4-C4	8.61	1.39	1.23
2	C	601	NAP	C2B-C1B	-8.53	1.32	1.53
2	C	601	NAP	O4B-C1B	8.50	1.61	1.42
4	A	603	FDA	PA-O3P	-8.34	1.50	1.59
4	D	603	FDA	O4-C4	8.27	1.39	1.23
4	C	603	FDA	PA-O3P	-7.59	1.51	1.59
4	C	603	FDA	O4-C4	7.56	1.37	1.23
4	A	603	FDA	O2-C2	7.30	1.38	1.23
2	C	601	NAP	C7N-N7N	7.12	1.46	1.33
4	C	603	FDA	O2-C2	7.02	1.38	1.23
4	B	603	FDA	O2-C2	7.01	1.38	1.23
4	D	603	FDA	O2-C2	6.92	1.38	1.23
4	C	603	FDA	C6-C5X	6.91	1.50	1.39
2	D	601	NAP	C7N-N7N	6.90	1.45	1.33
2	B	601	NAP	C7N-N7N	6.74	1.45	1.33
4	C	603	FDA	P-O3P	6.69	1.66	1.59
4	A	603	FDA	C6-C5X	6.38	1.49	1.39
2	A	601	NAP	O4B-C4B	-6.29	1.31	1.45
4	B	603	FDA	P-O3P	6.23	1.66	1.59
2	D	601	NAP	O4B-C4B	-6.18	1.31	1.45
2	A	601	NAP	C7N-N7N	6.16	1.44	1.33
2	B	601	NAP	O4D-C4D	-6.14	1.31	1.45
4	D	603	FDA	C9-C9A	6.10	1.49	1.39
2	C	601	NAP	O4B-C4B	-6.05	1.31	1.45
2	C	601	NAP	O4D-C4D	-6.01	1.31	1.45
4	B	603	FDA	C6-C5X	5.98	1.48	1.39
2	B	601	NAP	O4B-C4B	-5.92	1.31	1.45
2	A	601	NAP	O4D-C4D	-5.83	1.32	1.45
4	B	603	FDA	C9-C9A	5.82	1.49	1.39
4	A	603	FDA	C9-C9A	5.76	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAP	O4D-C4D	-5.74	1.32	1.45
4	D	603	FDA	C6-C5X	5.73	1.48	1.39
2	C	601	NAP	PN-O3	5.36	1.65	1.59
2	A	601	NAP	PA-O3	5.34	1.65	1.59
4	D	603	FDA	C10-N1	5.10	1.46	1.37
4	B	603	FDA	C10-N1	5.07	1.46	1.37
4	B	603	FDA	C4X-N5	4.95	1.45	1.35
4	C	603	FDA	C4X-N5	4.95	1.45	1.35
4	C	603	FDA	C9-C9A	4.95	1.47	1.39
4	C	603	FDA	C10-N1	4.92	1.45	1.37
2	D	601	NAP	PA-O3	4.78	1.64	1.59
4	D	603	FDA	C10-N10	4.66	1.46	1.38
2	A	601	NAP	C6A-N6A	4.62	1.46	1.34
4	A	603	FDA	C10-N1	4.61	1.45	1.37
4	D	603	FDA	C2-N1	4.59	1.45	1.37
2	A	601	NAP	PN-O3	4.57	1.64	1.59
2	B	601	NAP	PA-O3	4.54	1.64	1.59
4	D	603	FDA	P-O3P	4.52	1.64	1.59
4	C	603	FDA	C5X-N5	4.45	1.47	1.39
2	C	601	NAP	C6A-N6A	4.27	1.45	1.34
2	D	601	NAP	C6A-N6A	4.26	1.45	1.34
4	A	603	FDA	C5X-C9A	-4.26	1.35	1.40
2	B	601	NAP	PN-O3	4.21	1.64	1.59
4	A	603	FDA	C2-N1	4.18	1.44	1.37
4	D	603	FDA	C4X-N5	4.18	1.44	1.35
4	A	603	FDA	C6A-N6A	4.17	1.44	1.34
2	B	601	NAP	C6A-N6A	4.16	1.44	1.34
4	B	603	FDA	C5X-C9A	-4.14	1.36	1.40
4	B	603	FDA	C10-N10	4.10	1.45	1.38
4	B	603	FDA	C5X-N5	4.03	1.46	1.39
4	A	603	FDA	C4X-N5	4.02	1.43	1.35
4	B	603	FDA	C6A-N6A	4.01	1.44	1.34
2	C	601	NAP	PA-O3	3.87	1.63	1.59
4	C	603	FDA	C6A-N6A	3.85	1.44	1.34
4	A	603	FDA	C10-N10	3.76	1.44	1.38
4	B	603	FDA	C2-N1	3.76	1.43	1.37
4	A	603	FDA	C2-N3	3.74	1.43	1.37
4	A	603	FDA	C5X-N5	3.69	1.46	1.39
4	D	603	FDA	C9A-N10	3.63	1.47	1.41
4	A	603	FDA	P-O3P	3.56	1.63	1.59
2	C	601	NAP	P2B-O2B	3.53	1.65	1.59
4	C	603	FDA	C10-N10	3.52	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	FDA	C5X-C9A	-3.48	1.36	1.40
4	C	603	FDA	C2-N3	3.45	1.43	1.37
2	D	601	NAP	PN-O3	3.42	1.63	1.59
4	D	603	FDA	C6A-N6A	3.41	1.42	1.34
4	B	603	FDA	C9A-N10	3.34	1.46	1.41
4	C	603	FDA	C2-N1	3.33	1.43	1.37
4	B	603	FDA	C4X-C4	3.32	1.51	1.41
4	D	603	FDA	C5X-N5	3.28	1.45	1.39
2	C	601	NAP	O2D-C2D	3.27	1.51	1.43
4	A	603	FDA	C9A-N10	3.21	1.46	1.41
2	B	601	NAP	C5A-N7A	-3.13	1.33	1.39
4	A	603	FDA	C4X-C4	3.06	1.51	1.41
4	C	603	FDA	C5X-C9A	-3.04	1.37	1.40
4	C	603	FDA	C4X-C4	3.02	1.50	1.41
4	C	603	FDA	C9A-N10	2.96	1.46	1.41
2	B	601	NAP	O2D-C2D	2.95	1.50	1.43
4	B	603	FDA	C2-N3	2.94	1.42	1.37
2	A	601	NAP	O3D-C3D	-2.93	1.35	1.43
2	A	601	NAP	O2D-C2D	2.90	1.50	1.43
4	D	603	FDA	C4X-C4	2.86	1.50	1.41
4	D	603	FDA	C2-N3	2.86	1.42	1.37
4	D	603	FDA	PA-O5B	-2.84	1.48	1.59
4	A	603	FDA	C5A-C4A	2.84	1.44	1.39
4	B	603	FDA	PA-O5B	-2.82	1.48	1.59
2	B	601	NAP	O7N-C7N	-2.81	1.18	1.24
2	D	601	NAP	O2D-C2D	2.81	1.49	1.43
4	B	603	FDA	PA-O2A	-2.78	1.42	1.55
2	B	601	NAP	P2B-O2B	2.70	1.64	1.59
2	A	601	NAP	C3N-C7N	2.69	1.54	1.50
2	D	601	NAP	C5A-C4A	-2.68	1.34	1.39
4	C	603	FDA	P-O1P	2.67	1.60	1.50
2	D	601	NAP	O7N-C7N	-2.63	1.19	1.24
2	A	601	NAP	C5A-C4A	-2.60	1.34	1.39
4	B	603	FDA	O3B-C3B	-2.59	1.36	1.43
2	B	601	NAP	O3D-C3D	-2.54	1.36	1.43
2	D	601	NAP	O3D-C3D	-2.53	1.36	1.43
4	B	603	FDA	P-O1P	2.52	1.59	1.50
2	A	601	NAP	O7N-C7N	-2.52	1.19	1.24
4	D	603	FDA	PA-O2A	-2.51	1.43	1.55
2	A	601	NAP	C5A-N7A	-2.50	1.34	1.39
2	C	601	NAP	O7N-C7N	-2.49	1.19	1.24
2	C	601	NAP	O3B-C3B	-2.49	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAP	O3B-C3B	-2.48	1.36	1.43
4	A	603	FDA	PA-O5B	-2.47	1.49	1.59
4	B	603	FDA	C4A-N9A	2.47	1.42	1.37
4	C	603	FDA	C4A-N9A	2.47	1.42	1.37
2	D	601	NAP	C5A-N7A	-2.46	1.34	1.39
2	D	601	NAP	O3B-C3B	-2.46	1.36	1.43
4	A	603	FDA	PA-O2A	-2.46	1.44	1.55
4	D	603	FDA	P-O1P	2.43	1.59	1.50
4	C	603	FDA	O3B-C3B	-2.39	1.37	1.43
4	C	603	FDA	O2'-C2'	-2.38	1.38	1.43
2	D	601	NAP	P2B-O2B	2.38	1.63	1.59
4	B	603	FDA	O2'-C2'	-2.35	1.38	1.43
4	B	603	FDA	C5A-C4A	2.35	1.43	1.39
4	D	603	FDA	C5A-C4A	2.35	1.43	1.39
2	C	601	NAP	C5A-N7A	-2.34	1.34	1.39
4	C	603	FDA	PA-O2A	-2.33	1.44	1.55
4	D	603	FDA	C9-C8	2.33	1.42	1.39
4	C	603	FDA	PA-O5B	-2.31	1.50	1.59
2	B	601	NAP	C8A-N9A	-2.27	1.33	1.37
2	B	601	NAP	C5A-C4A	-2.25	1.35	1.39
4	A	603	FDA	C4A-N9A	2.24	1.42	1.37
2	A	601	NAP	P2B-O2B	2.22	1.63	1.59
4	A	603	FDA	P-O1P	2.21	1.58	1.50
2	B	601	NAP	O3B-C3B	-2.20	1.37	1.43
2	D	601	NAP	C3N-C7N	2.18	1.53	1.50
4	C	603	FDA	C5A-C4A	2.17	1.43	1.39
2	C	601	NAP	O3D-C3D	-2.14	1.37	1.43
2	D	601	NAP	C4N-C3N	-2.14	1.36	1.39
4	A	603	FDA	O3B-C3B	-2.13	1.37	1.43
4	A	603	FDA	C2A-N3A	2.13	1.37	1.33
2	C	601	NAP	C5A-C4A	-2.11	1.35	1.39
4	A	603	FDA	C9-C8	2.11	1.42	1.39
4	A	603	FDA	O3'-C3'	-2.10	1.37	1.43
4	D	603	FDA	O4'-C4'	-2.08	1.39	1.43
4	D	603	FDA	O3B-C3B	-2.01	1.38	1.43

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NAP	N3A-C2A-N1A	-6.10	119.34	128.58
2	C	601	NAP	N6A-C6A-N1A	-6.09	104.81	118.38
4	D	603	FDA	N3A-C2A-N1A	-5.87	119.70	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	FDA	N3A-C2A-N1A	-5.77	119.85	128.58
2	B	601	NAP	C5A-C4A-N3A	-5.76	118.79	126.72
2	A	601	NAP	N3A-C2A-N1A	-5.75	119.88	128.58
2	A	601	NAP	C5A-C4A-N3A	-5.63	118.97	126.72
4	B	603	FDA	C5A-C4A-N3A	-5.63	118.97	126.72
4	C	603	FDA	C5A-C4A-N3A	-5.57	119.05	126.72
2	C	601	NAP	C5A-C4A-N3A	-5.49	119.16	126.72
4	A	603	FDA	N3A-C2A-N1A	-5.43	120.36	128.58
2	D	601	NAP	N6A-C6A-N1A	-5.42	106.31	118.38
2	B	601	NAP	N3A-C2A-N1A	-5.28	120.59	128.58
4	B	603	FDA	N3A-C2A-N1A	-5.25	120.64	128.58
4	D	603	FDA	N3A-C4A-N9A	5.12	135.87	127.17
4	D	603	FDA	C4-N3-C2	-5.04	119.44	126.37
4	D	603	FDA	C5A-C4A-N3A	-5.03	119.79	126.72
4	A	603	FDA	C5A-C4A-N3A	-5.00	119.84	126.72
2	C	601	NAP	N3A-C2A-N1A	-5.00	121.02	128.58
2	A	601	NAP	N6A-C6A-N1A	-4.93	107.40	118.38
4	C	603	FDA	N3A-C4A-N9A	4.72	135.19	127.17
2	B	601	NAP	N6A-C6A-N1A	-4.70	107.92	118.38
4	B	603	FDA	N3A-C4A-N9A	4.69	135.14	127.17
2	C	601	NAP	C5A-C6A-N6A	4.57	134.61	123.29
4	A	603	FDA	N3A-C4A-N9A	4.38	134.62	127.17
2	D	601	NAP	C5A-C6A-N6A	4.35	134.05	123.29
4	A	603	FDA	C4-N3-C2	-4.34	120.39	126.37
4	C	603	FDA	C4-N3-C2	-4.29	120.47	126.37
4	B	603	FDA	C5A-N7A-C8A	4.26	110.15	103.45
4	C	603	FDA	C5A-N7A-C8A	4.22	110.08	103.45
2	D	601	NAP	C5A-C4A-N3A	-4.19	120.95	126.72
2	D	601	NAP	N9A-C8A-N7A	-4.11	108.11	113.94
2	B	601	NAP	N3A-C4A-N9A	4.06	134.07	127.17
4	C	603	FDA	C2A-N3A-C4A	3.99	121.56	111.83
4	A	603	FDA	C5A-N7A-C8A	3.98	109.70	103.45
4	B	603	FDA	O2A-PA-O3P	-3.79	97.04	107.27
4	D	603	FDA	N3-C2-N1	3.77	121.67	115.74
2	A	601	NAP	N3A-C4A-N9A	3.72	133.50	127.17
2	A	601	NAP	N9A-C8A-N7A	-3.72	108.66	113.94
2	A	601	NAP	C5A-C6A-N6A	3.71	132.47	123.29
2	A	601	NAP	C2A-N3A-C4A	3.70	120.86	111.83
4	D	603	FDA	C2A-N3A-C4A	3.69	120.83	111.83
2	C	601	NAP	N9A-C8A-N7A	-3.63	108.78	113.94
4	B	603	FDA	C2A-N3A-C4A	3.63	120.70	111.83
4	A	603	FDA	C2A-N3A-C4A	3.60	120.63	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	NAP	C4D-O4D-C1D	-3.59	106.63	109.92
2	B	601	NAP	C5A-C6A-N6A	3.50	131.95	123.29
2	C	601	NAP	C2A-N3A-C4A	3.46	120.27	111.83
4	B	603	FDA	C4-N3-C2	-3.45	121.62	126.37
4	B	603	FDA	C4A-C5A-N7A	-3.45	106.64	110.58
4	C	603	FDA	N9A-C8A-N7A	-3.43	109.07	113.94
2	C	601	NAP	N3A-C4A-N9A	3.40	132.95	127.17
2	A	601	NAP	C4D-O4D-C1D	-3.40	106.81	109.92
4	A	603	FDA	N3-C2-N1	3.39	121.07	115.74
2	B	601	NAP	C2A-N3A-C4A	3.38	120.10	111.83
2	B	601	NAP	N9A-C8A-N7A	-3.32	109.23	113.94
4	B	603	FDA	N9A-C8A-N7A	-3.29	109.27	113.94
4	D	603	FDA	O4-C4-C4X	-3.27	119.38	127.26
4	A	603	FDA	N9A-C8A-N7A	-3.27	109.30	113.94
2	D	601	NAP	C2A-N3A-C4A	3.25	119.77	111.83
4	D	603	FDA	C5A-N7A-C8A	3.24	108.55	103.45
4	C	603	FDA	C4A-C5A-N7A	-3.19	106.93	110.58
4	B	603	FDA	O2A-PA-O5B	-3.15	93.31	107.57
4	A	603	FDA	C4A-C5A-N7A	-3.14	106.99	110.58
4	A	603	FDA	O2P-P-O5'	-3.13	93.37	107.57
4	B	603	FDA	N3-C2-N1	3.03	120.50	115.74
2	C	601	NAP	C6N-N1N-C2N	-2.96	119.36	121.88
4	A	603	FDA	O2A-PA-O5B	-2.95	94.17	107.57
2	B	601	NAP	C6N-N1N-C2N	-2.91	119.40	121.88
2	B	601	NAP	C6A-C5A-C4A	2.89	121.13	117.18
4	A	603	FDA	O2P-P-O3P	-2.89	99.46	107.27
2	C	601	NAP	C5A-N7A-C8A	2.89	107.99	103.45
2	A	601	NAP	C2B-C1B-N9A	-2.89	109.00	113.75
4	A	603	FDA	O4-C4-C4X	-2.85	120.40	127.26
3	C	602	ORN	OXT-C-O	-2.84	117.65	124.08
4	A	603	FDA	O5'-P-O1P	2.82	120.10	108.94
4	C	603	FDA	O4-C4-C4X	-2.81	120.49	127.26
4	D	603	FDA	N9A-C8A-N7A	-2.81	109.96	113.94
4	D	603	FDA	O5'-P-O1P	2.79	119.98	108.94
2	B	601	NAP	C4D-O4D-C1D	-2.77	107.39	109.92
2	D	601	NAP	C5A-N7A-C8A	2.76	107.79	103.45
4	A	603	FDA	O3P-P-O1P	2.73	118.91	110.70
2	A	601	NAP	C5A-N7A-C8A	2.71	107.71	103.45
4	D	603	FDA	C4A-N9A-C8A	2.71	108.58	105.74
2	B	601	NAP	C5A-N7A-C8A	2.70	107.69	103.45
4	C	603	FDA	C4X-C4-N3	2.66	119.43	112.13
4	C	603	FDA	N3-C2-N1	2.64	119.89	115.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	FDA	O2P-P-O5'	-2.63	95.65	107.57
4	B	603	FDA	O5'-P-O1P	2.63	119.34	108.94
2	B	601	NAP	C3N-C7N-N7N	2.60	120.94	117.74
4	A	603	FDA	C4A-N9A-C8A	2.60	108.46	105.74
4	A	603	FDA	O2-C2-N1	-2.54	117.35	121.86
4	D	603	FDA	O2P-P-O5'	-2.54	96.07	107.57
4	D	603	FDA	C6-C5X-N5	-2.51	115.41	119.76
2	D	601	NAP	C4D-O4D-C1D	-2.47	107.66	109.92
2	D	601	NAP	N3A-C4A-N9A	2.46	131.35	127.17
4	C	603	FDA	O2A-PA-O3P	-2.46	100.62	107.27
4	C	603	FDA	O3P-PA-O1A	2.46	118.10	110.70
2	C	601	NAP	C4A-C5A-N7A	-2.45	107.78	110.58
4	D	603	FDA	C9A-C5X-N5	2.44	122.35	119.37
4	B	603	FDA	O5B-PA-O1A	2.43	118.58	108.94
4	C	603	FDA	O2P-P-O5'	-2.43	96.58	107.57
4	D	603	FDA	O2A-PA-O5B	-2.42	96.60	107.57
2	D	601	NAP	O2B-C2B-C3B	-2.40	103.05	111.68
2	D	601	NAP	C4A-N9A-C1B	-2.40	121.01	126.63
4	D	603	FDA	C4X-C4-N3	2.40	118.72	112.13
2	A	601	NAP	C6A-C5A-C4A	2.39	120.44	117.18
4	C	603	FDA	C5'-C4'-C3'	2.32	116.59	112.22
4	C	603	FDA	C4A-N9A-C8A	2.32	108.17	105.74
2	A	601	NAP	O7N-C7N-C3N	2.28	122.38	119.60
4	C	603	FDA	C4'-C3'-C2'	2.28	117.36	113.57
2	B	601	NAP	C2N-C3N-C4N	2.26	120.88	118.26
2	C	601	NAP	P2B-O2B-C2B	-2.25	117.43	123.43
2	D	601	NAP	C4A-N9A-C8A	2.23	108.08	105.74
4	D	603	FDA	O5B-PA-O1A	2.23	117.76	108.94
4	A	603	FDA	C4A-N9A-C1B	-2.22	121.45	126.63
2	C	601	NAP	C2N-C3N-C4N	2.22	120.84	118.26
4	C	603	FDA	O2-C2-N1	-2.20	117.95	121.86
4	B	603	FDA	C4A-N9A-C8A	2.20	108.05	105.74
4	D	603	FDA	O3P-PA-O1A	2.16	117.19	110.70
2	D	601	NAP	C6N-N1N-C2N	-2.14	120.05	121.88
2	C	601	NAP	C5D-C4D-C3D	-2.13	107.53	115.21
4	C	603	FDA	O5'-P-O1P	2.12	117.34	108.94
4	B	603	FDA	O3P-PA-O1A	2.11	117.06	110.70
4	A	603	FDA	O5B-PA-O1A	2.10	117.27	108.94
2	A	601	NAP	O7N-C7N-N7N	-2.09	119.60	122.62
4	D	603	FDA	C6-C5X-C9A	2.08	122.08	119.80
3	D	602	ORN	OXT-C-O	-2.07	119.39	124.08
4	B	603	FDA	C4X-C4-N3	2.05	117.76	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NAP	C5B-C4B-C3B	-2.02	107.92	115.21
4	C	603	FDA	O3'-C3'-C4'	-2.02	104.33	108.93
2	B	601	NAP	C5D-C4D-C3D	-2.01	107.98	115.21

There are no chirality outliers.

All (23) torsion outliers are listed below:

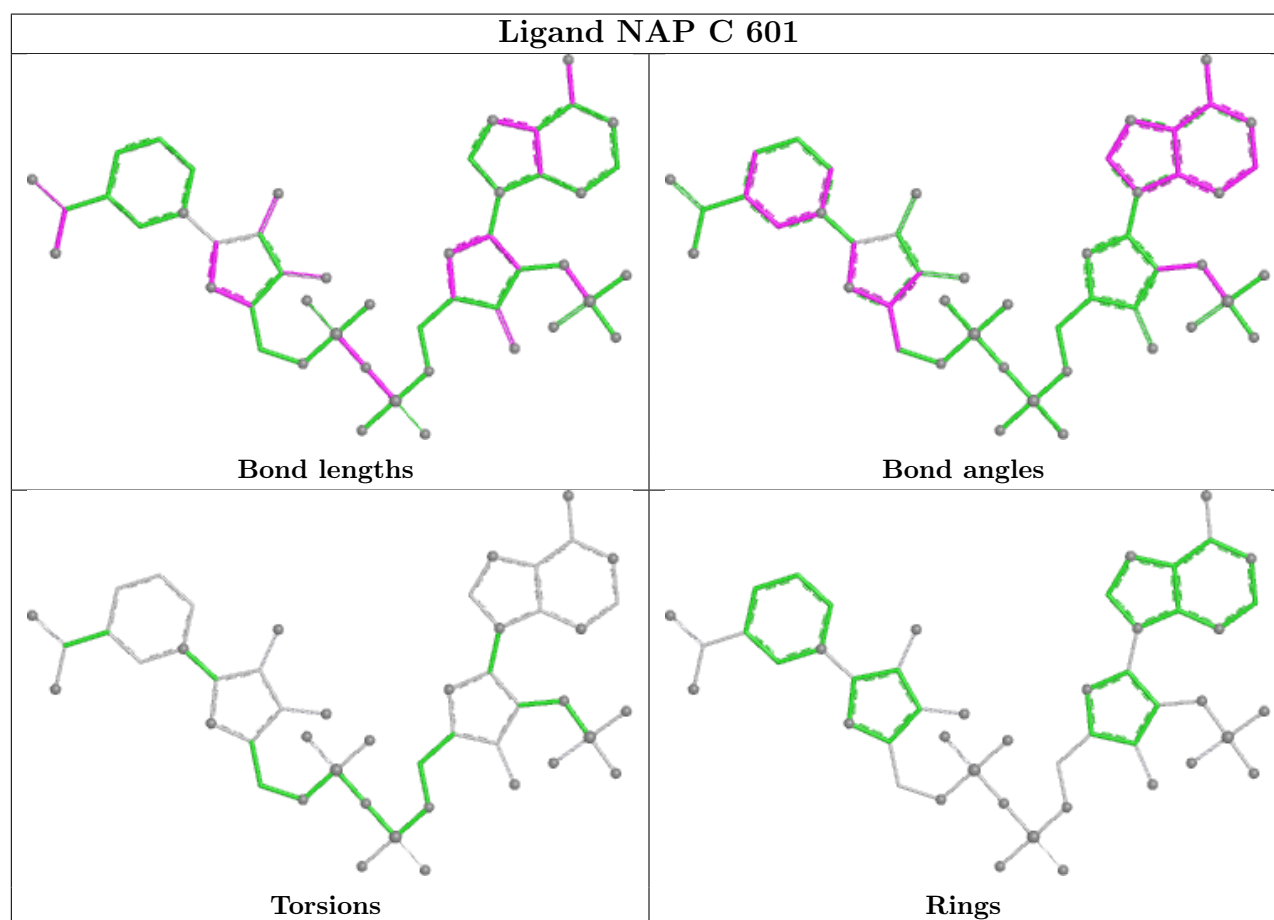
Mol	Chain	Res	Type	Atoms
4	A	603	FDA	C5'-O5'-P-O3P
4	D	603	FDA	N10-C1'-C2'-O2'
4	A	603	FDA	O3'-C3'-C4'-C5'
4	A	603	FDA	C2'-C3'-C4'-C5'
4	A	603	FDA	O3'-C3'-C4'-O4'
4	D	603	FDA	C2'-C3'-C4'-C5'
4	D	603	FDA	O3'-C3'-C4'-C5'
4	A	603	FDA	PA-O3P-P-O5'
4	B	603	FDA	P-O3P-PA-O5B
4	A	603	FDA	C2'-C3'-C4'-O4'
4	D	603	FDA	C2'-C3'-C4'-O4'
4	A	603	FDA	P-O3P-PA-O2A
4	B	603	FDA	PA-O3P-P-O1P
4	D	603	FDA	N10-C1'-C2'-C3'
2	B	601	NAP	C5D-O5D-PN-O3
4	A	603	FDA	C5B-O5B-PA-O1A
4	B	603	FDA	PA-O3P-P-O2P
4	D	603	FDA	O3'-C3'-C4'-O4'
4	A	603	FDA	P-O3P-PA-O1A
4	C	603	FDA	O4B-C4B-C5B-O5B
2	A	601	NAP	C2B-O2B-P2B-O1X
2	B	601	NAP	C2B-O2B-P2B-O1X
2	D	601	NAP	PN-O3-PA-O2A

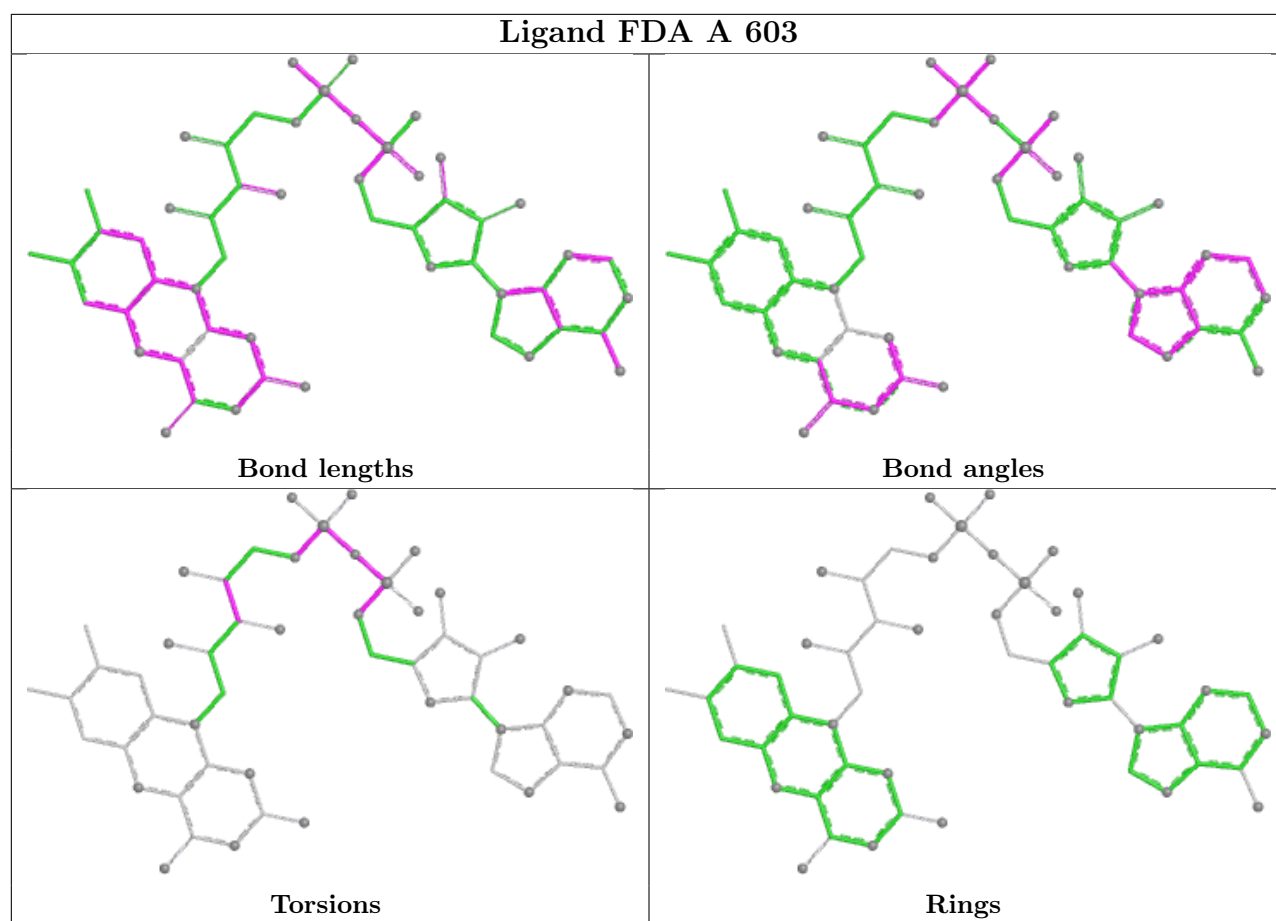
There are no ring outliers.

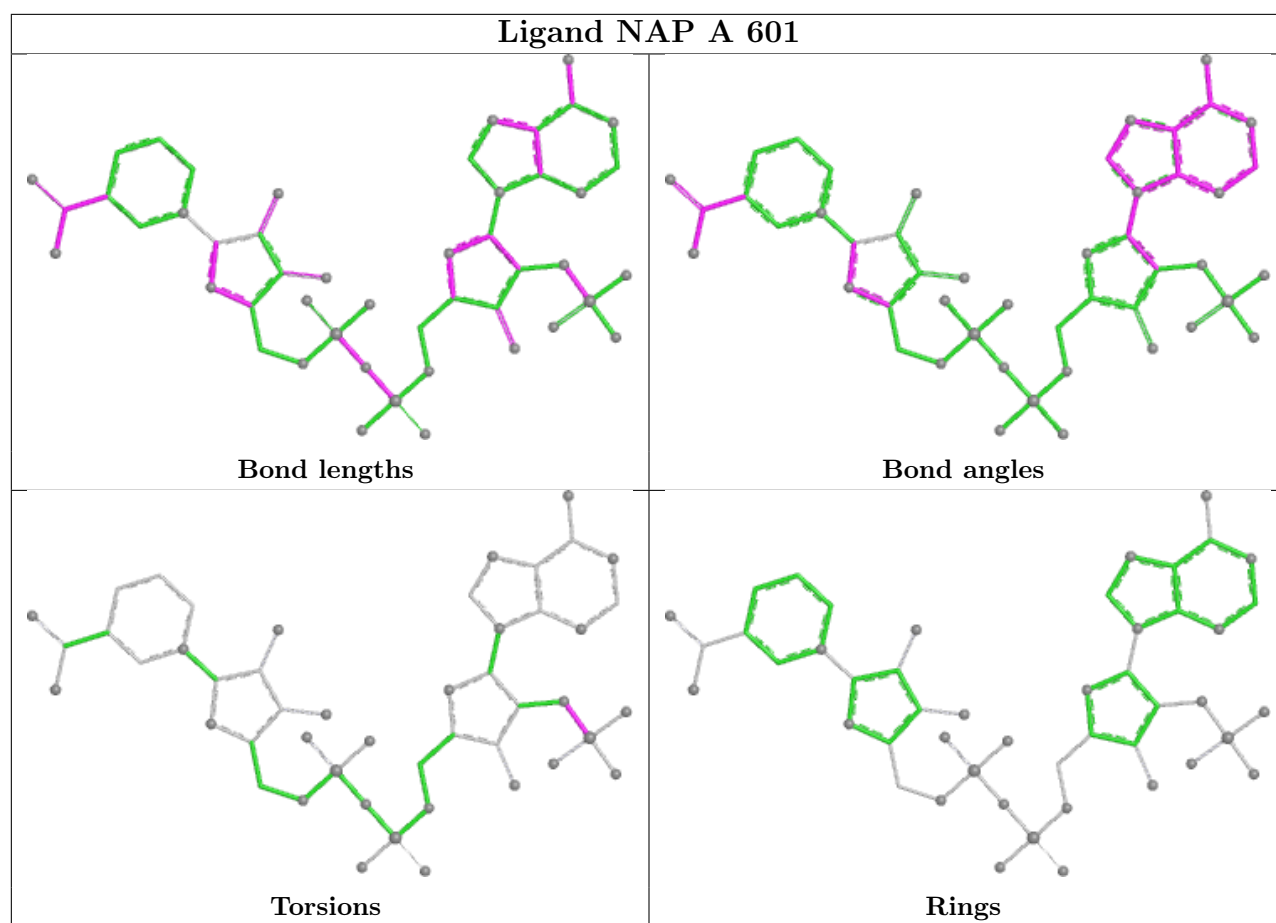
5 monomers are involved in 7 short contacts:

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

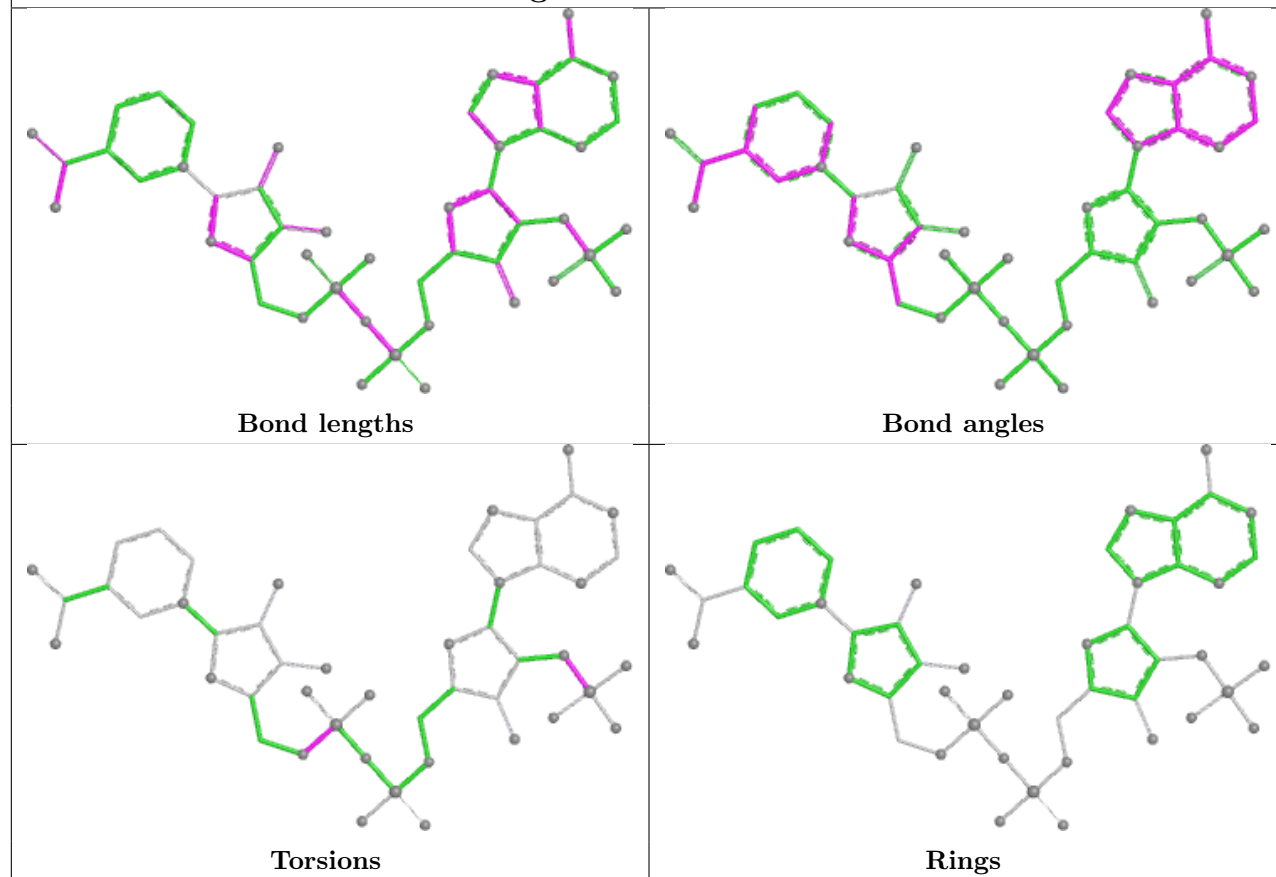
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



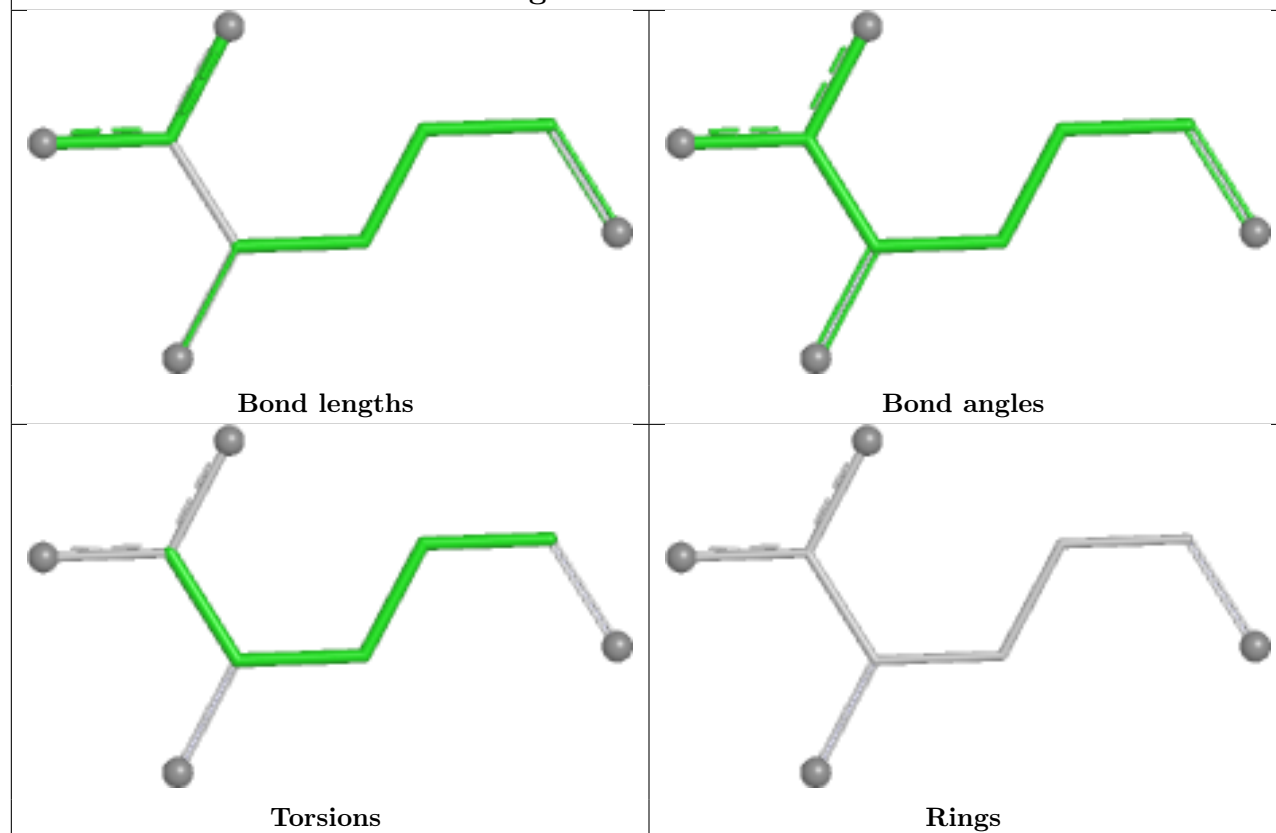


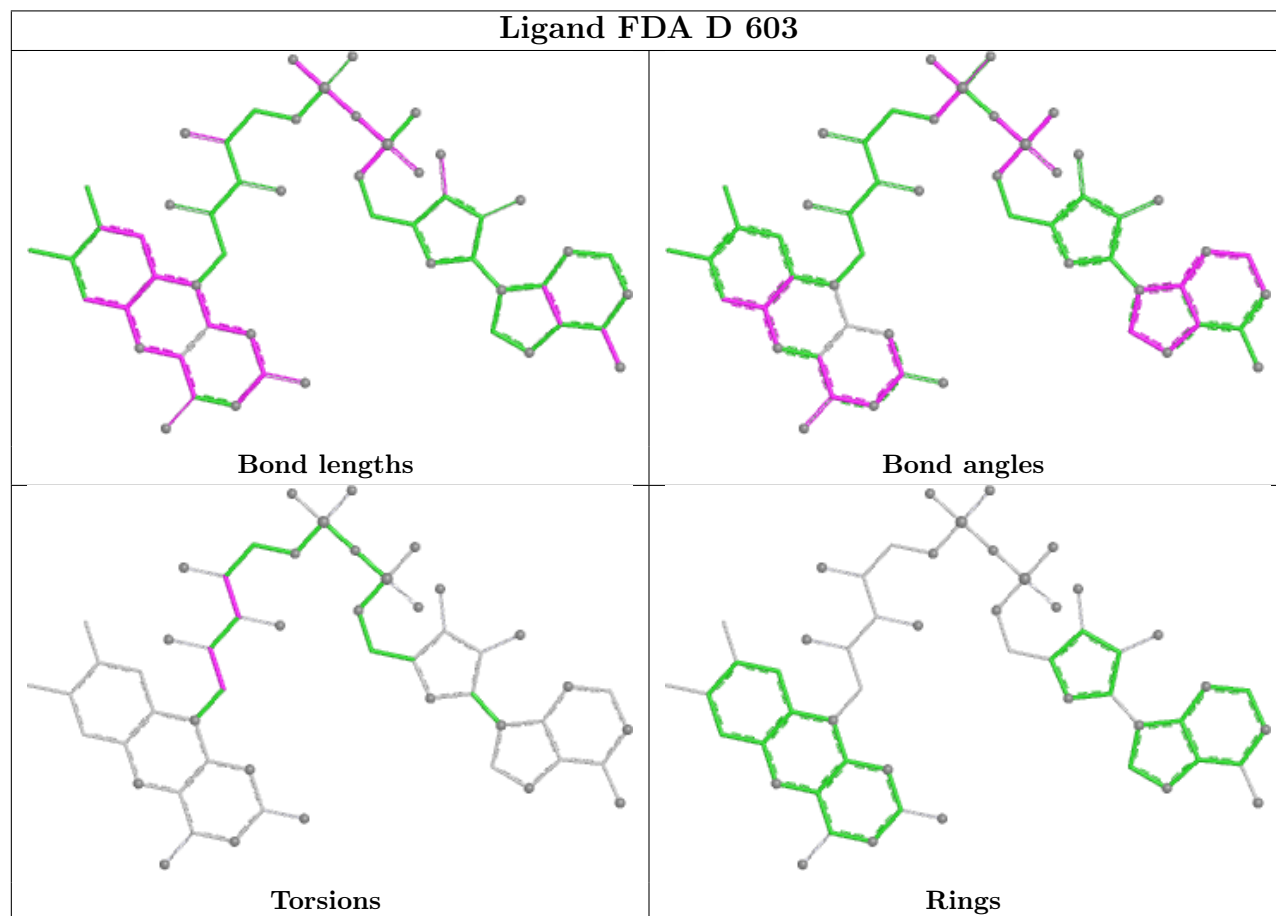
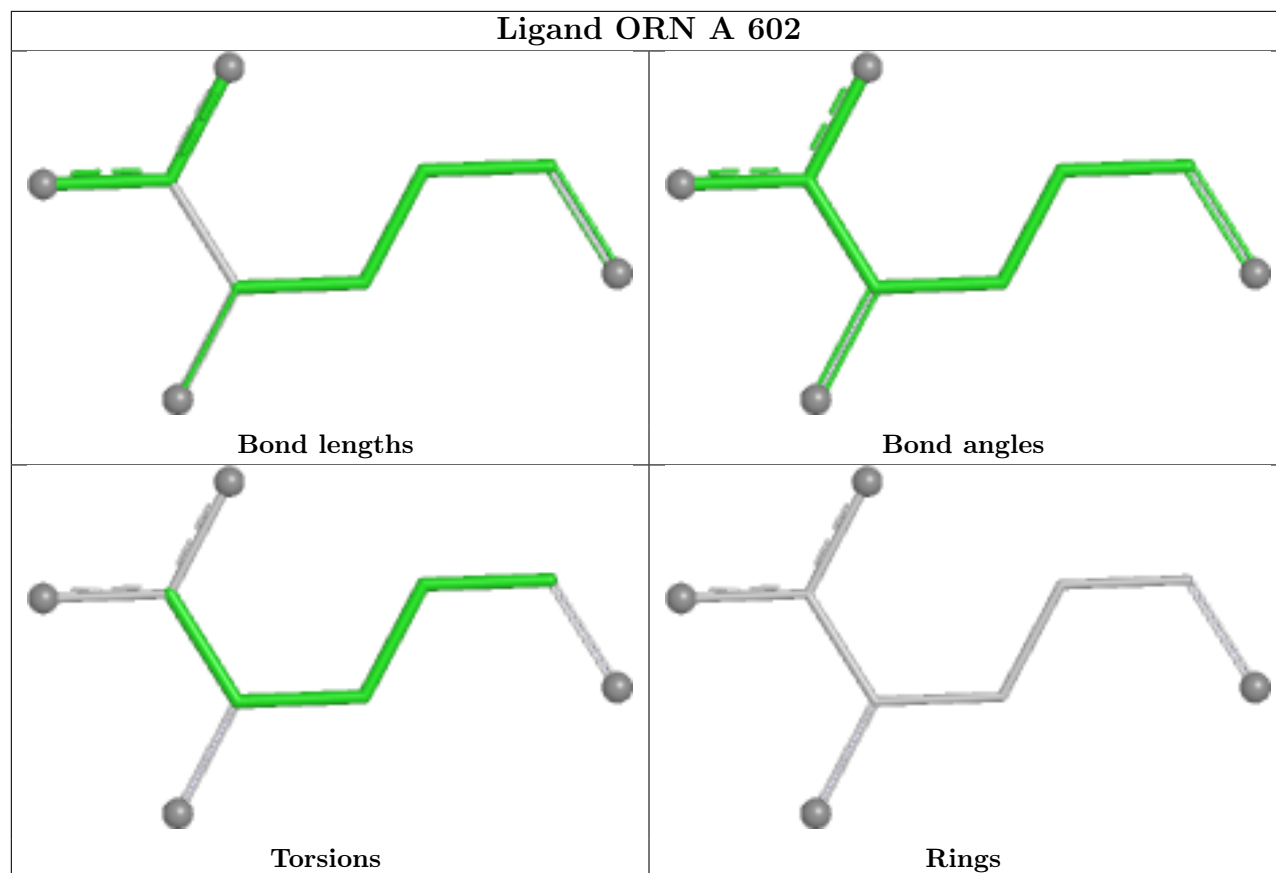


Ligand NAP B 601

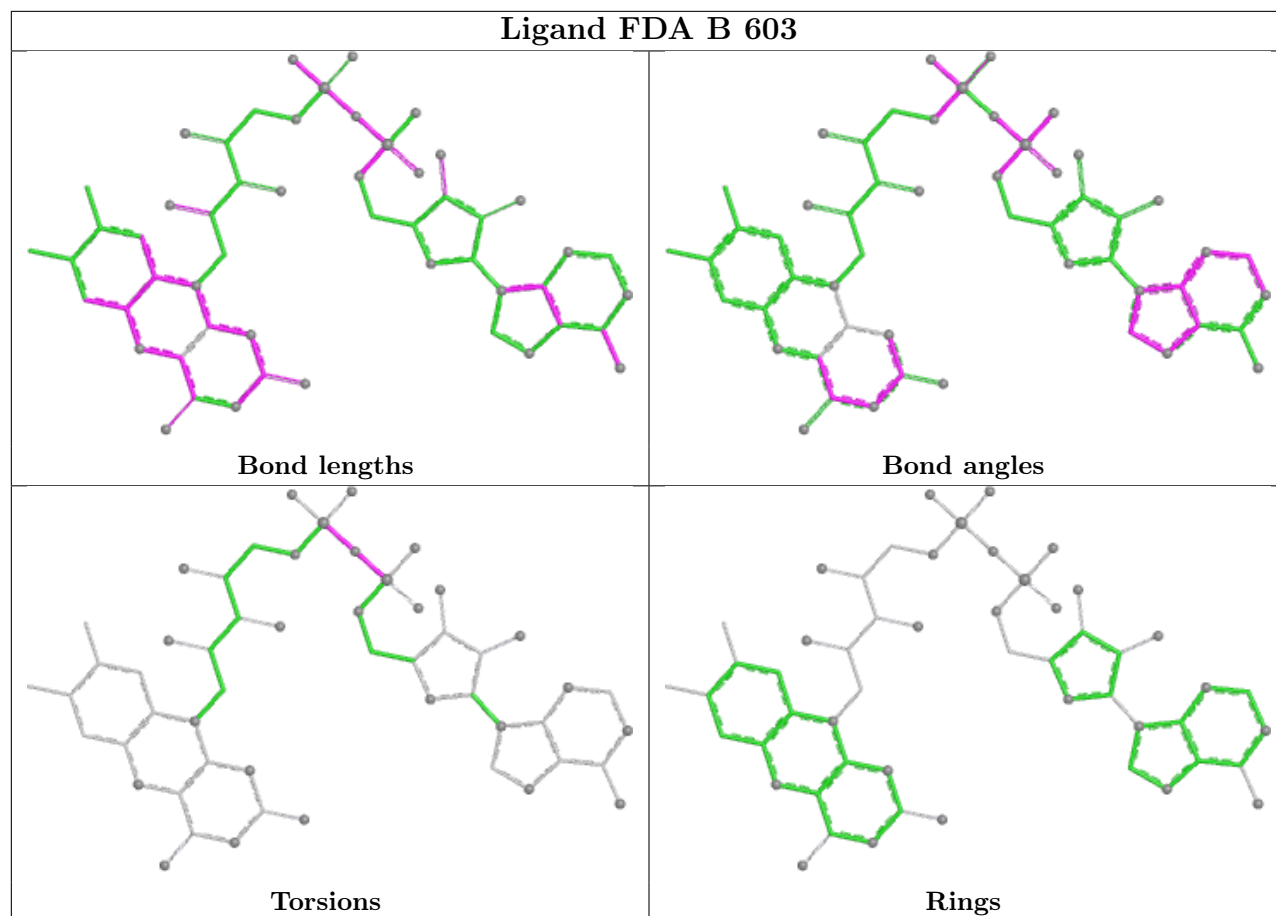


Ligand ORN B 602

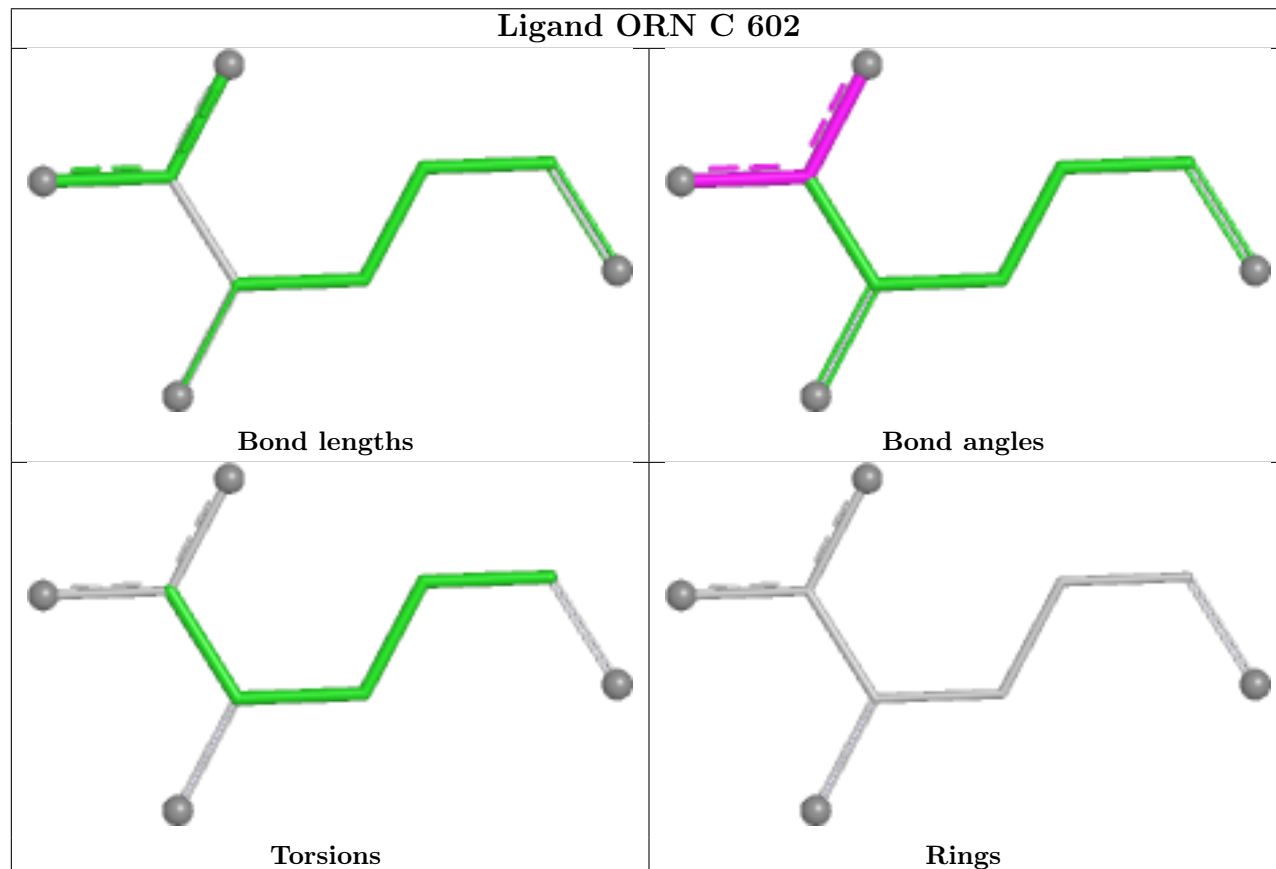


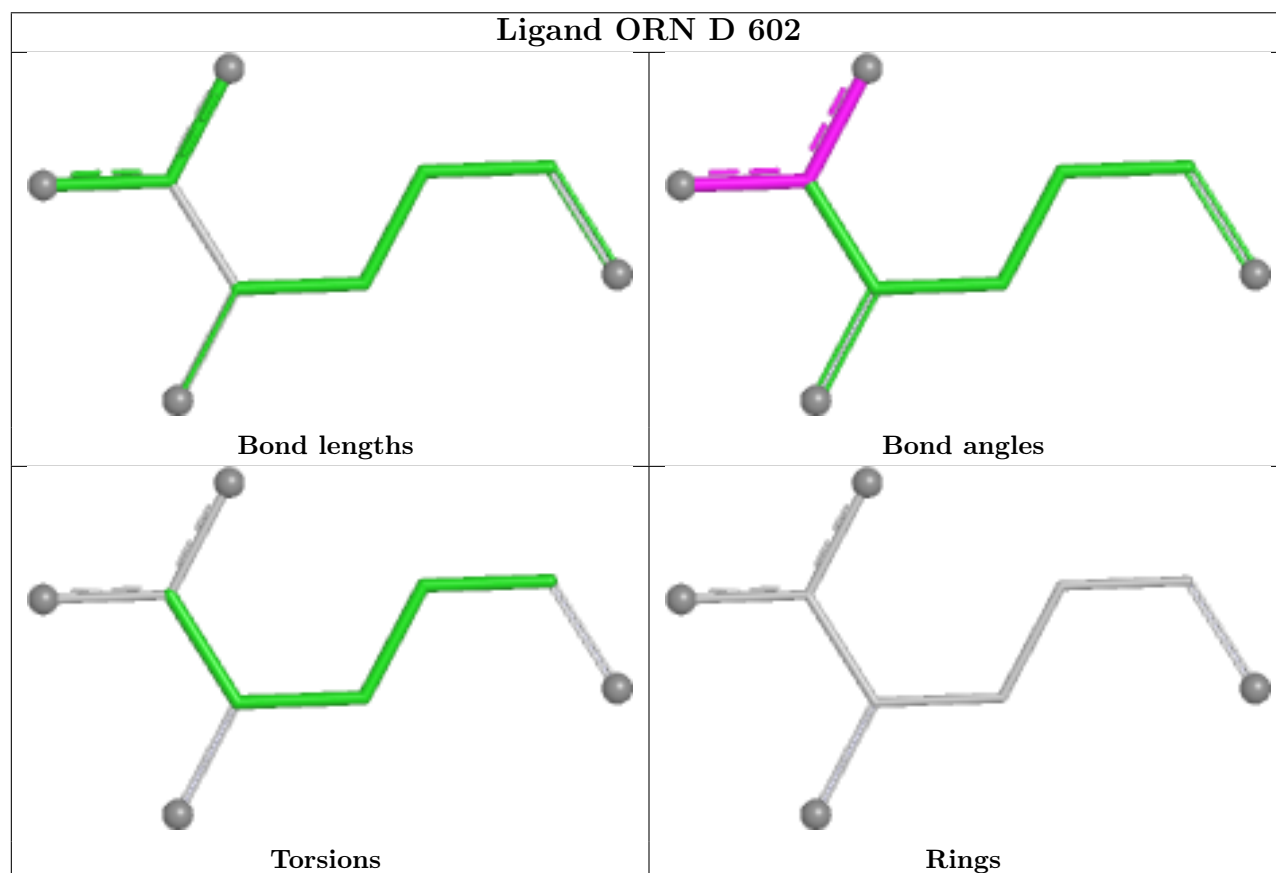
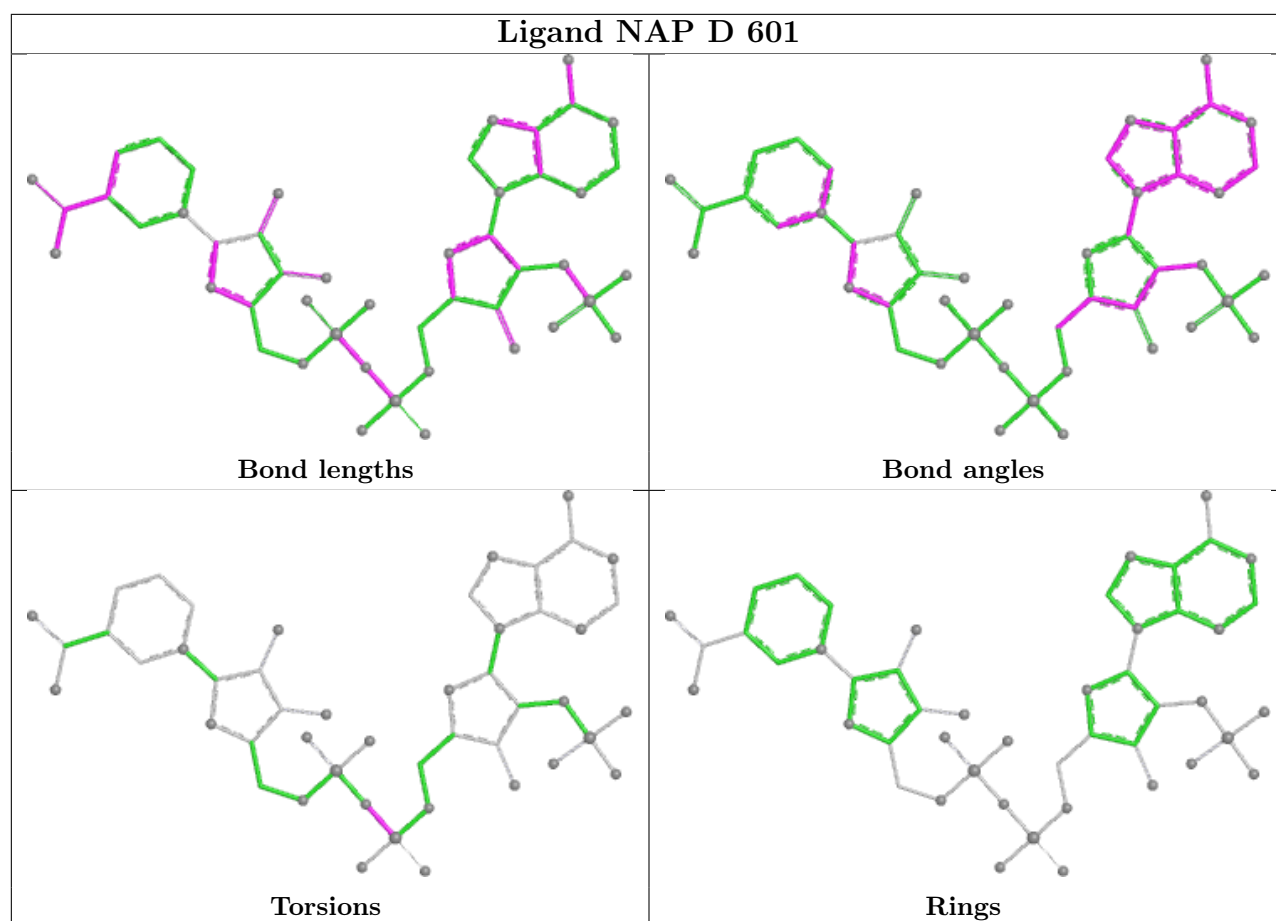


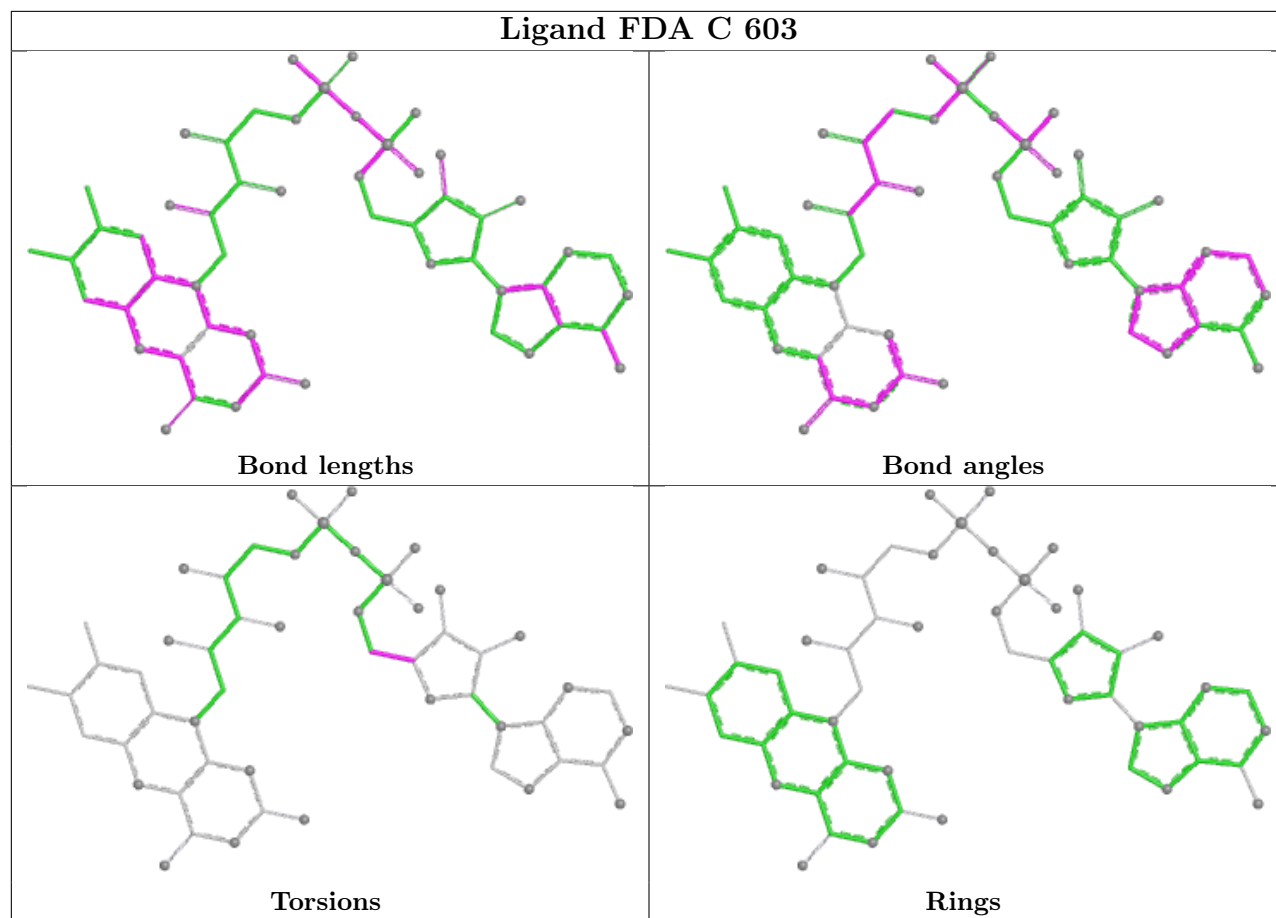
Ligand FDA B 603



Ligand ORN C 602







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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	451/494 (91%)	-0.17	11 (2%) 59 65	22, 33, 59, 83	0
1	B	455/494 (92%)	-0.27	9 (1%) 65 70	21, 31, 54, 95	0
1	C	451/494 (91%)	-0.27	10 (2%) 62 67	19, 30, 57, 98	0
1	D	450/494 (91%)	-0.15	8 (1%) 67 72	21, 34, 64, 92	0
All	All	1807/1976 (91%)	-0.21	38 (2%) 63 68	19, 32, 58, 98	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	368	HIS	4.1
1	B	73	ILE	4.1
1	A	30	ARG	4.0
1	C	72	ASN	3.9
1	C	178	PRO	3.5
1	D	371	GLN	3.4
1	C	179	SER	3.4
1	B	74	HIS	3.3
1	C	368	HIS	3.2
1	D	74	HIS	3.1
1	A	489	ARG	3.0
1	B	71	SER	3.0
1	A	74	HIS	2.9
1	A	370	PRO	2.9
1	B	30	ARG	2.8
1	A	68	LYS	2.8
1	D	72	ASN	2.8
1	C	74	HIS	2.8
1	A	71	SER	2.8
1	B	68	LYS	2.7
1	B	488	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	70	ALA	2.6
1	D	71	SER	2.6
1	C	73	ILE	2.5
1	A	69	SER	2.4
1	C	180	SER	2.4
1	A	488	GLU	2.4
1	B	72	ASN	2.3
1	C	71	SER	2.3
1	B	368	HIS	2.3
1	C	70	ALA	2.2
1	A	67	ASN	2.2
1	B	385	SER	2.1
1	A	181	SER	2.1
1	A	73	ILE	2.1
1	D	243	LYS	2.0
1	C	69	SER	2.0
1	D	490	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

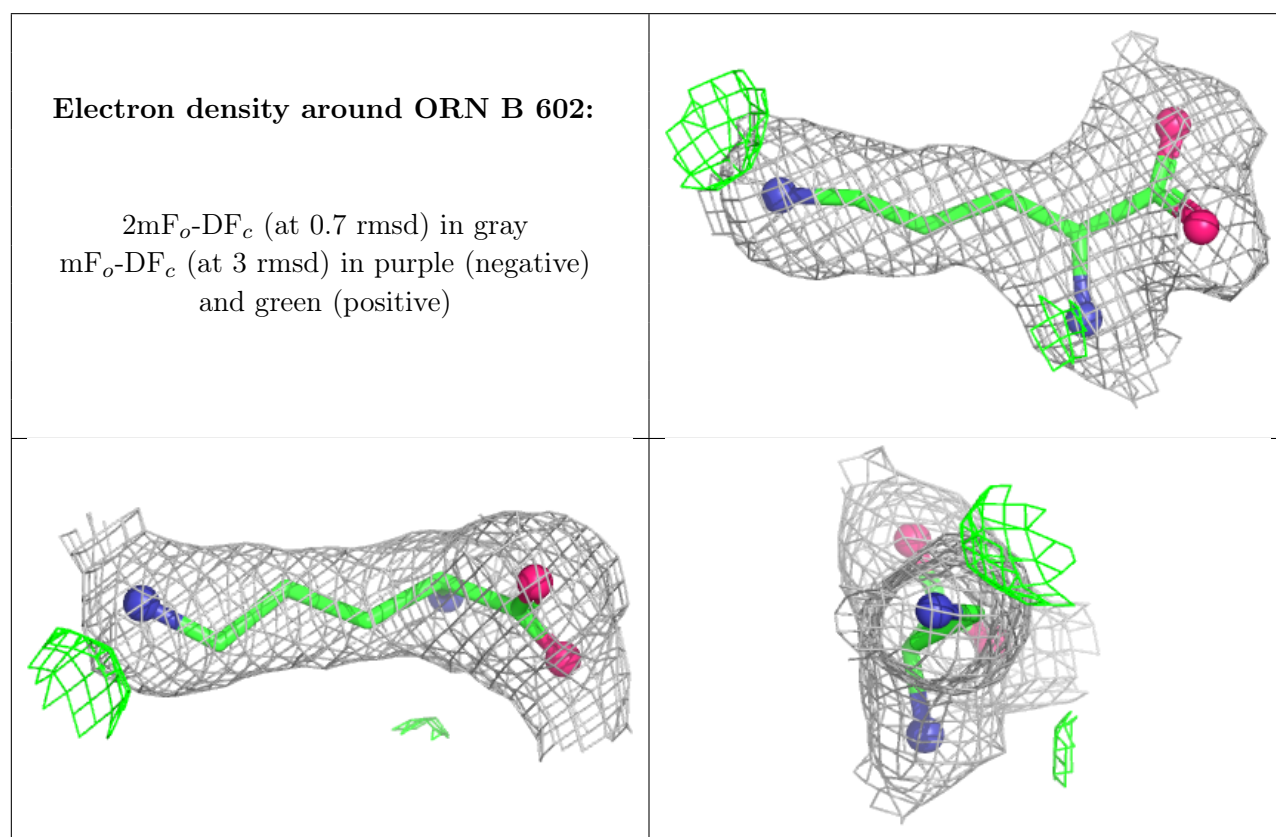
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ORN	B	602	9/9	0.96	0.06	17,21,31,31	0
4	FDA	D	603	53/53	0.96	0.06	20,30,39,41	0
3	ORN	A	602	9/9	0.97	0.06	21,29,35,37	0
2	NAP	B	601	48/48	0.97	0.07	16,31,39,44	0
3	ORN	C	602	9/9	0.97	0.06	15,24,31,31	0
3	ORN	D	602	9/9	0.97	0.05	20,23,28,29	0

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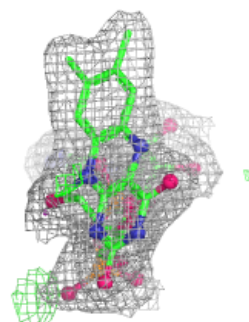
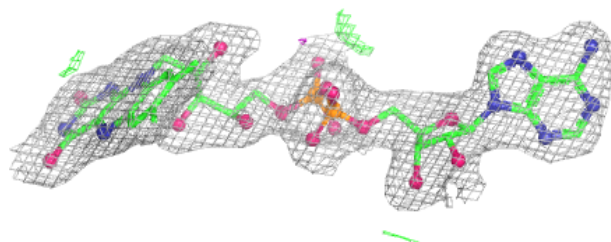
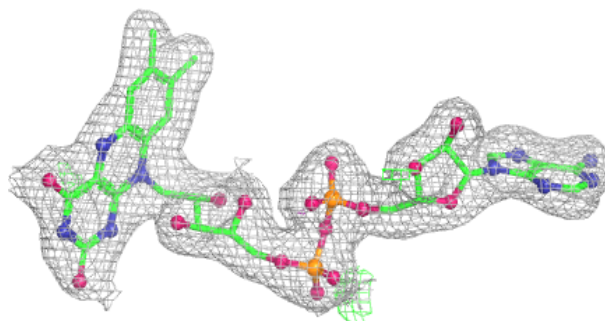
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FDA	B	603	53/53	0.97	0.06	16,27,37,42	0
2	NAP	D	601	48/48	0.97	0.06	16,31,43,54	0
4	FDA	A	603	53/53	0.98	0.05	16,28,33,40	0
2	NAP	C	601	48/48	0.98	0.06	18,28,37,42	0
4	FDA	C	603	53/53	0.98	0.05	18,26,37,44	0
2	NAP	A	601	48/48	0.98	0.06	14,28,42,52	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.

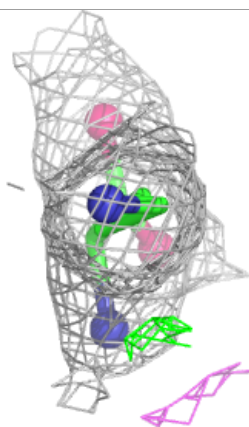
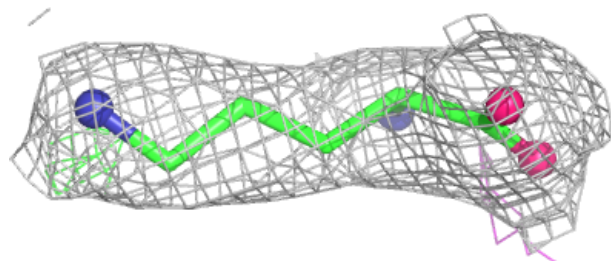
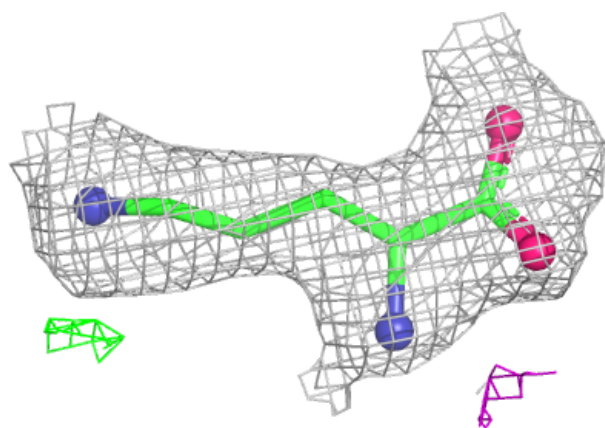


Electron density around FDA D 603:

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

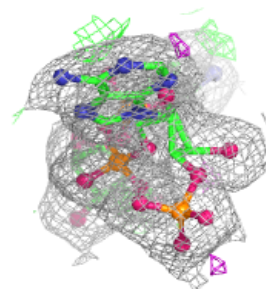
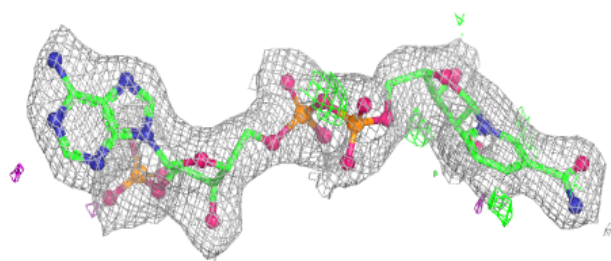
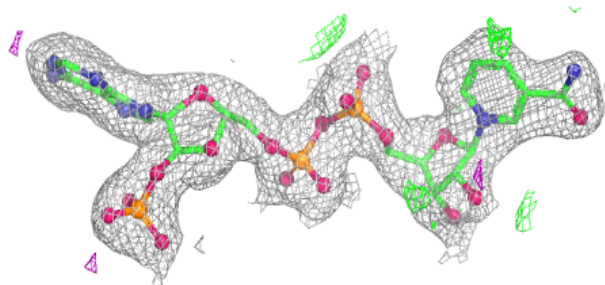
**Electron density around ORN A 602:**

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

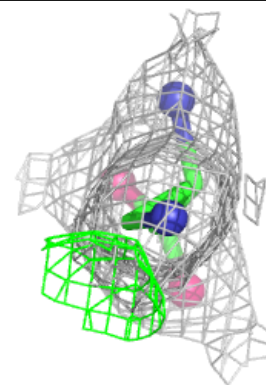
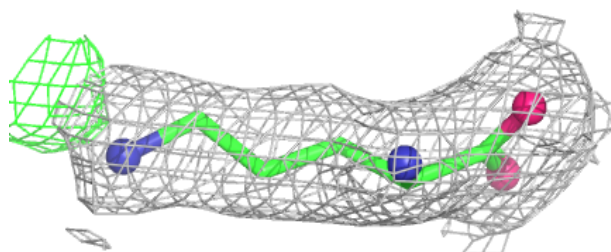
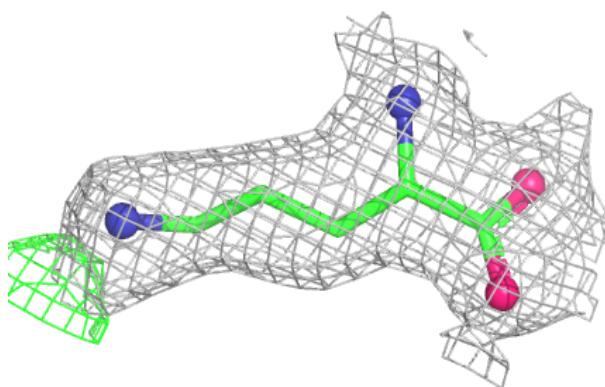


Electron density around NAP B 601:

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

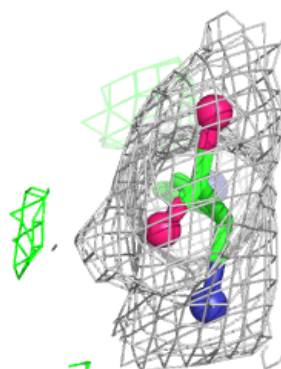
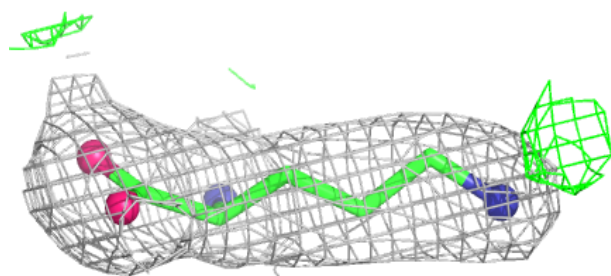
**Electron density around ORN C 602:**

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

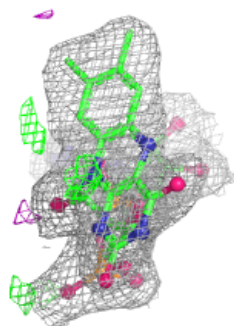
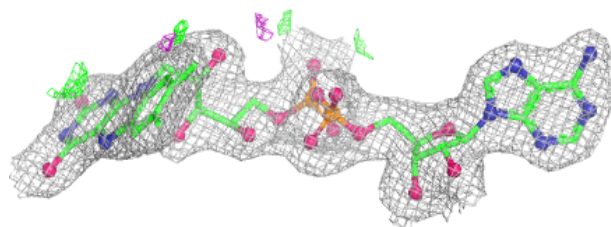
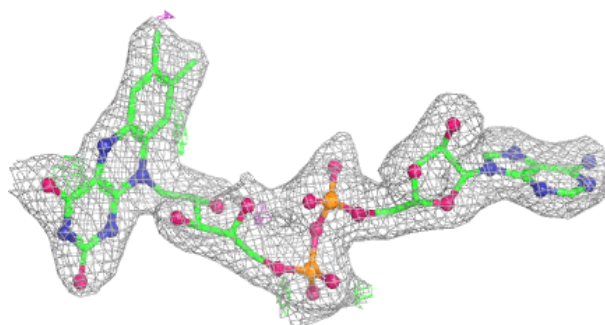


Electron density around ORN D 602:

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

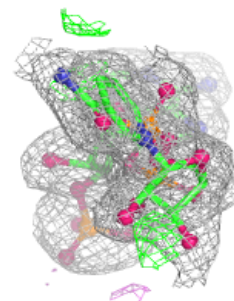
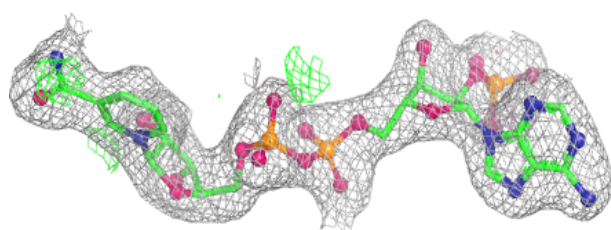
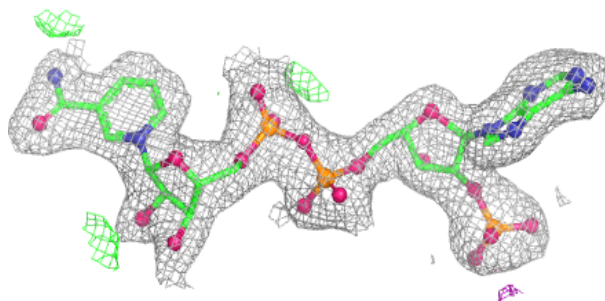
**Electron density around FDA B 603:**

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

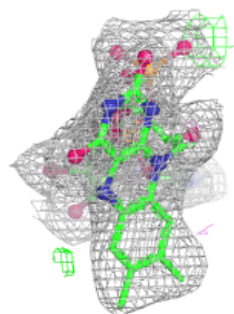
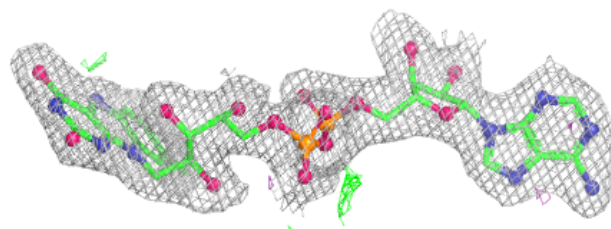
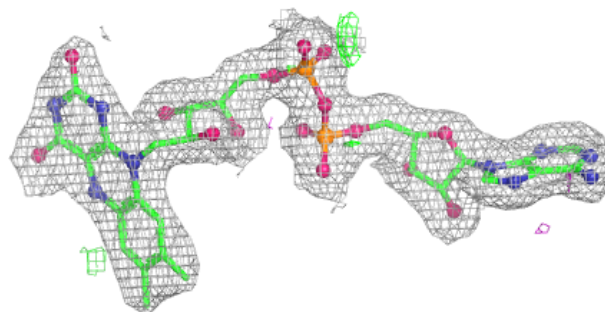


Electron density around NAP D 601:

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

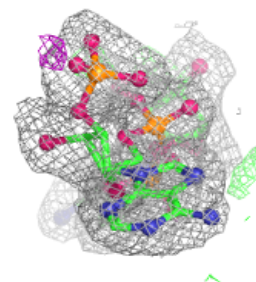
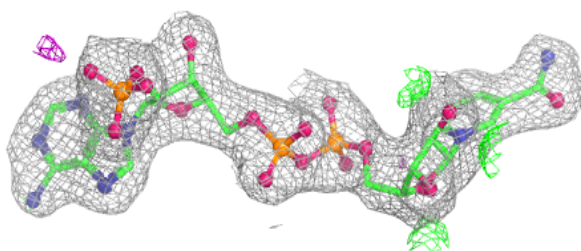
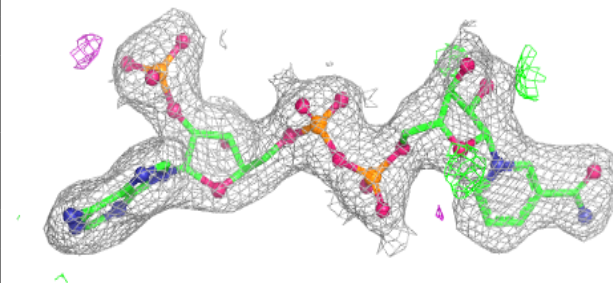
**Electron density around FDA A 603:**

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

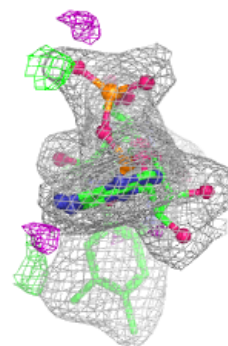
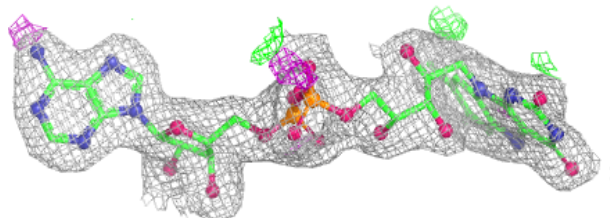
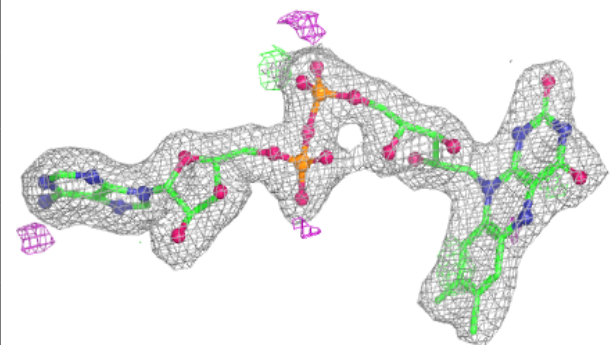


Electron density around NAP C 601:

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

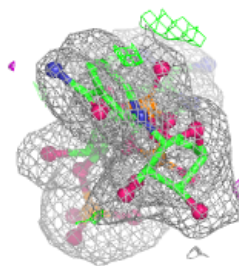
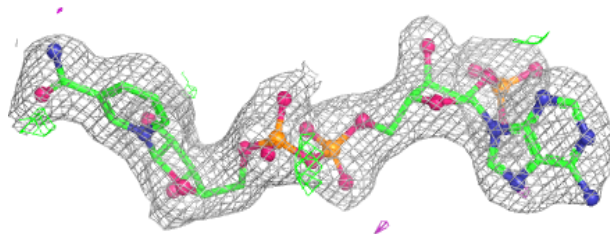
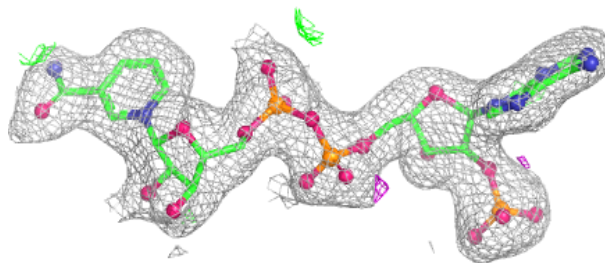
**Electron density around FDA C 603:**

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.