



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:46 PM UTC

PDB ID : 6X0K / pdb_00006x0k
Title : Structure of dithionite-reduced SidA ornithine hydroxylase with the FAD "in" and complexed with L-ornithine
Authors : Tanner, J.J.; Campbell, A.C.
Deposited on : 2020-05-15
Resolution : 2.23 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

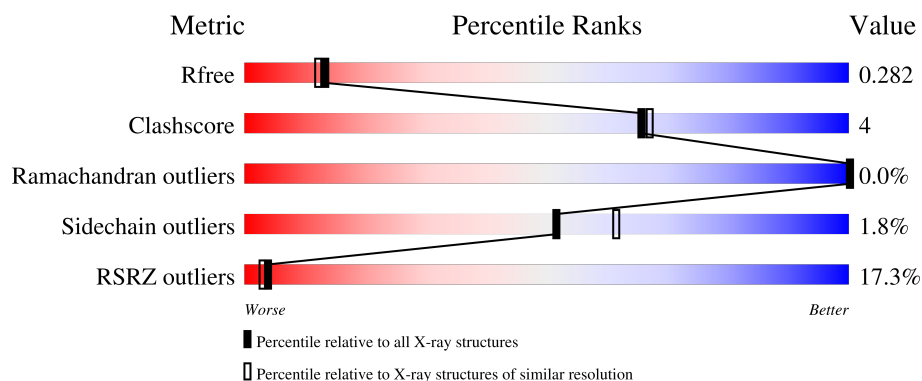
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	6% 81% 8% 11%
1	B	494	5% 83% 7% 11%
1	C	494	13% 78% 9% 12%
1	D	494	16% 80% 10% 11%
1	E	494	9% 77% 12% 11%

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Mol	Chain	Length	Quality of chain
1	F	494	28% 76% 12% 12%
1	G	494	25% 77% 11% 11%
1	H	494	21% 79% 9% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28171 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	440	Total	C	N	O	S	0	0	0
			3460	2178	624	642	16			
1	B	442	Total	C	N	O	S	0	0	0
			3481	2193	627	645	16			
1	C	433	Total	C	N	O	S	0	0	0
			3392	2139	606	631	16			
1	D	441	Total	C	N	O	S	0	0	0
			3407	2149	607	635	16			
1	E	441	Total	C	N	O	S	0	0	0
			3450	2173	619	642	16			
1	F	436	Total	C	N	O	S	0	0	0
			3345	2116	589	625	15			
1	G	440	Total	C	N	O	S	0	0	0
			3418	2158	610	634	16			
1	H	437	Total	C	N	O	S	0	0	0
			3357	2119	597	625	16			

There are 168 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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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
E	8	MET	-	initiating methionine	UNP E9QYP0
E	9	GLY	-	expression tag	UNP E9QYP0
E	10	SER	-	expression tag	UNP E9QYP0
E	11	SER	-	expression tag	UNP E9QYP0
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E	15	HIS	-	expression tag	UNP E9QYP0
E	16	HIS	-	expression tag	UNP E9QYP0
E	17	HIS	-	expression tag	UNP E9QYP0
E	18	SER	-	expression tag	UNP E9QYP0
E	19	SER	-	expression tag	UNP E9QYP0
E	20	GLY	-	expression tag	UNP E9QYP0

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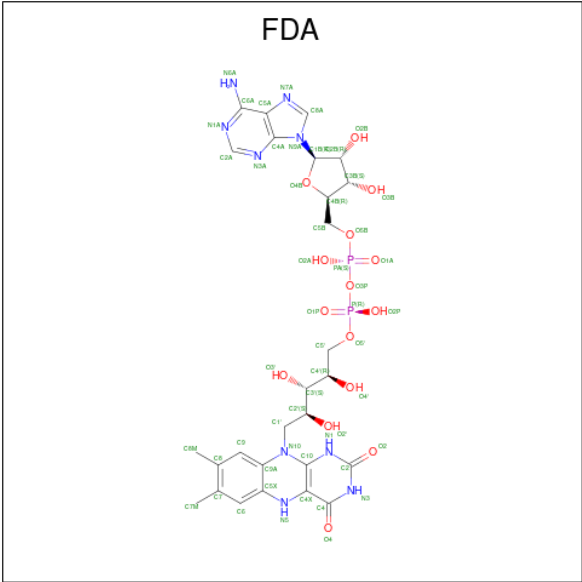
Chain	Residue	Modelled	Actual	Comment	Reference
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E	23	PRO	-	expression tag	UNP E9QYP0
E	24	ARG	-	expression tag	UNP E9QYP0
E	25	GLY	-	expression tag	UNP E9QYP0
E	26	SER	-	expression tag	UNP E9QYP0
E	27	HIS	-	expression tag	UNP E9QYP0
E	28	MET	-	expression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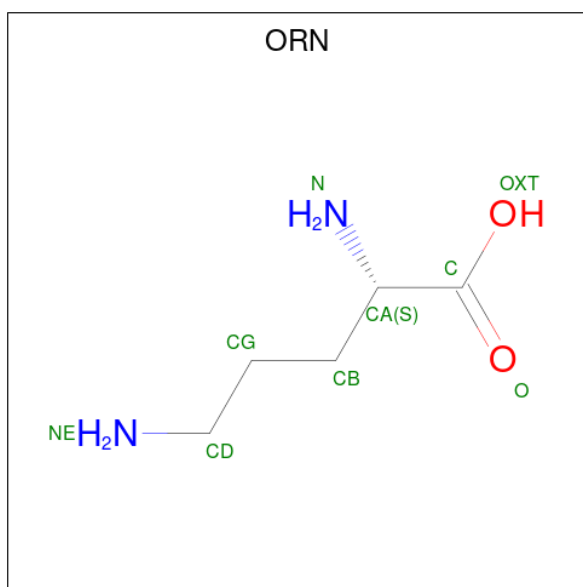
Chain	Residue	Modelled	Actual	Comment	Reference
G	21	LEU	-	expression tag	UNP E9QYP0
G	22	VAL	-	expression tag	UNP E9QYP0
G	23	PRO	-	expression tag	UNP E9QYP0
G	24	ARG	-	expression tag	UNP E9QYP0
G	25	GLY	-	expression tag	UNP E9QYP0
G	26	SER	-	expression tag	UNP E9QYP0
G	27	HIS	-	expression tag	UNP E9QYP0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

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is L-ornithine (CCD ID: ORN) (formula: C₅H₁₂N₂O₂) (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	D	1	Total	C	N	O	0	0
			9	5	2	2		
3	E	1	Total	C	N	O	0	0
			9	5	2	2		
3	G	1	Total	C	N	O	0	0
			9	5	2	2		
3	H	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	77	Total	O	0	0
			77	77		
4	C	43	Total	O	0	0
			43	43		
4	D	41	Total	O	0	0
			41	41		
4	E	54	Total	O	0	0
			54	54		
4	F	15	Total	O	0	0
			15	15		

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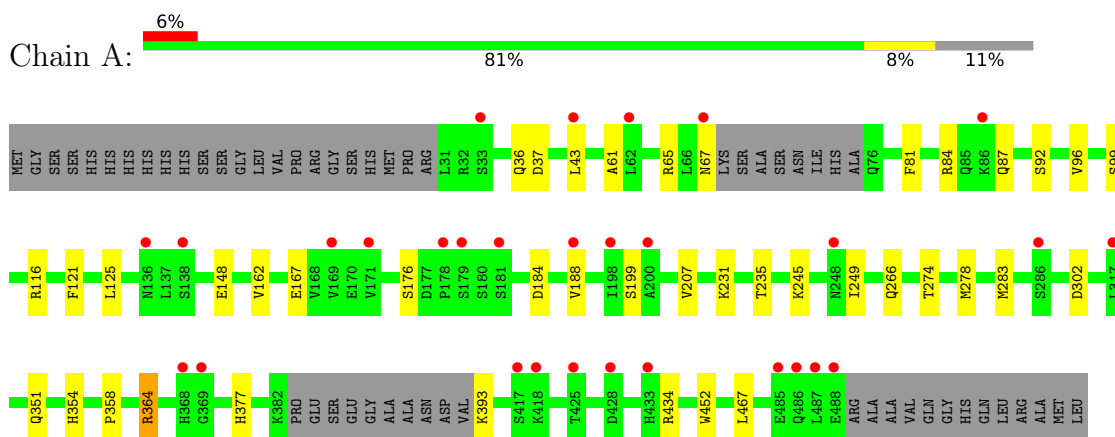
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	29	Total	O	0	0
			29	29		
4	H	33	Total	O	0	0
			33	33		

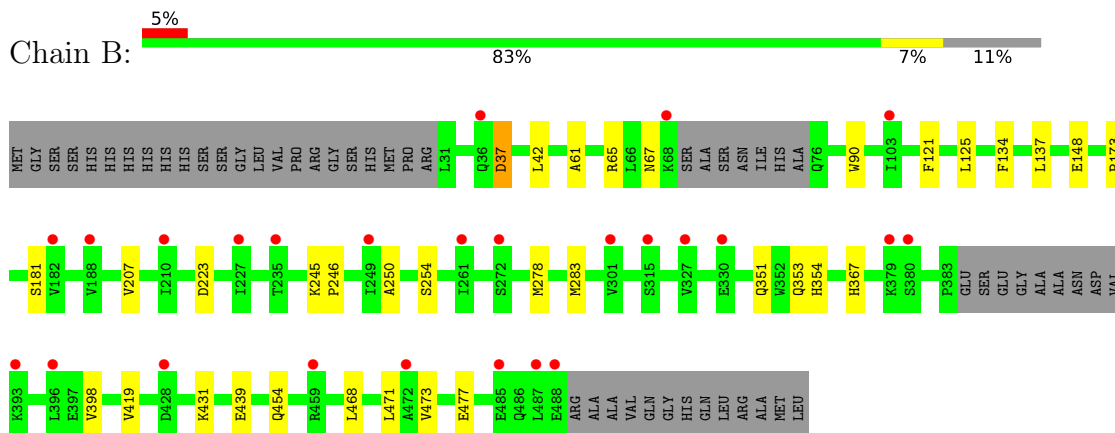
3 Residue-property plots [i](#)

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.

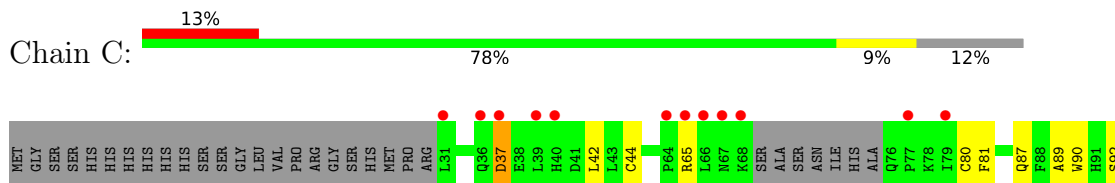
- Molecule 1: L-ornithine N(5)-monooxygenase

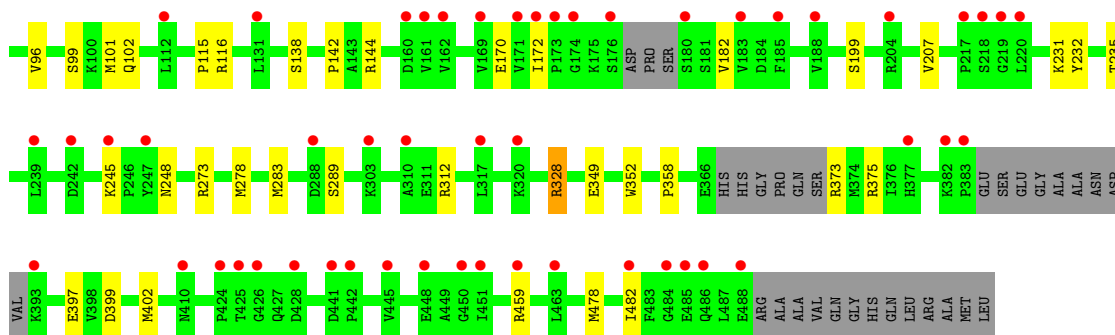


- Molecule 1: L-ornithine N(5)-monooxygenase

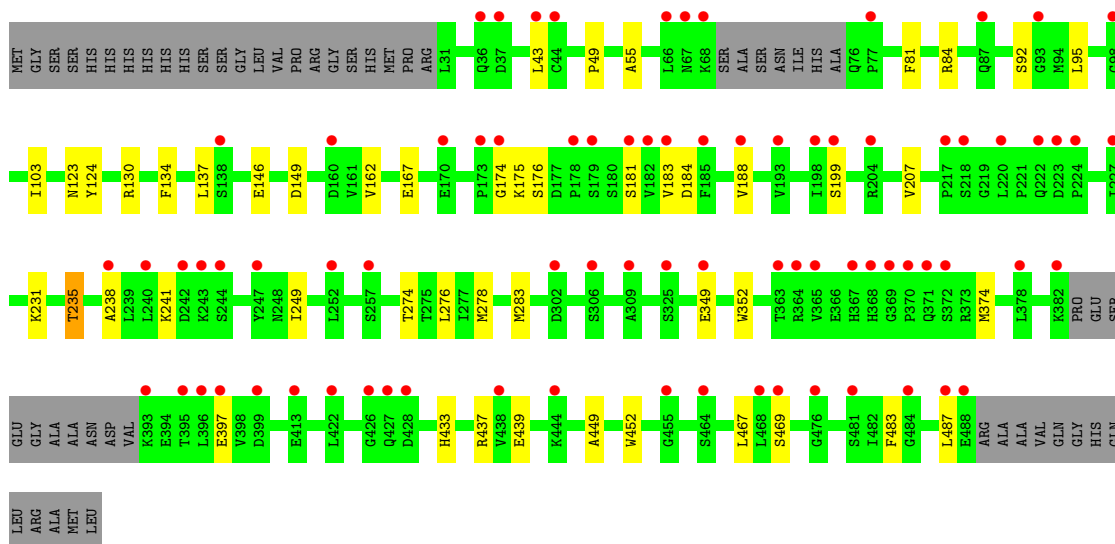
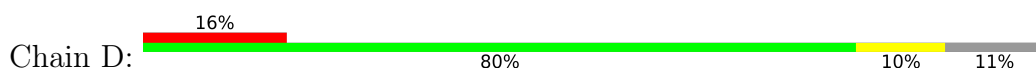


- Molecule 1: L-ornithine N(5)-monooxygenase

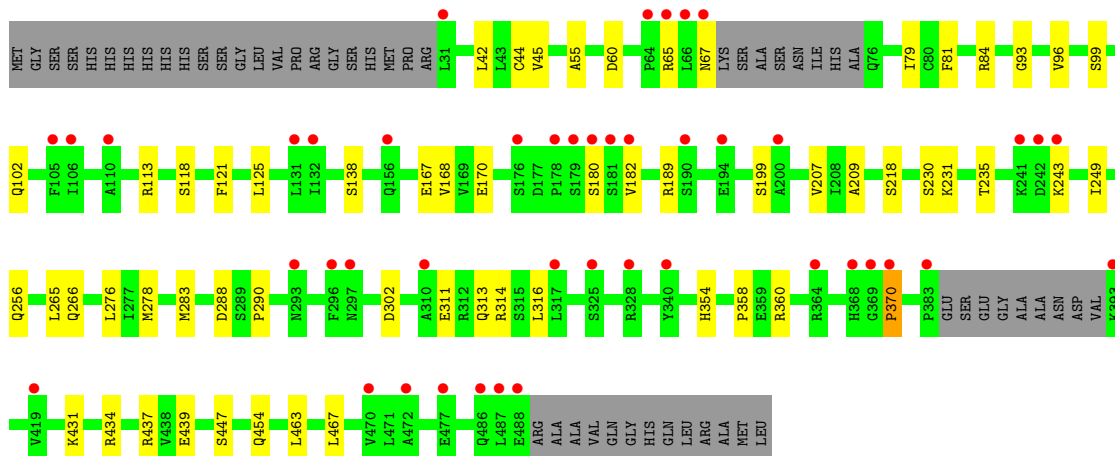
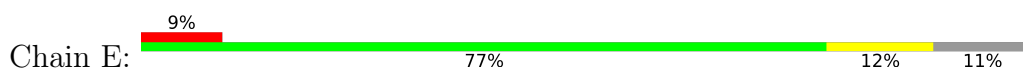




• Molecule 1: L-ornithine N(5)-monooxygenase

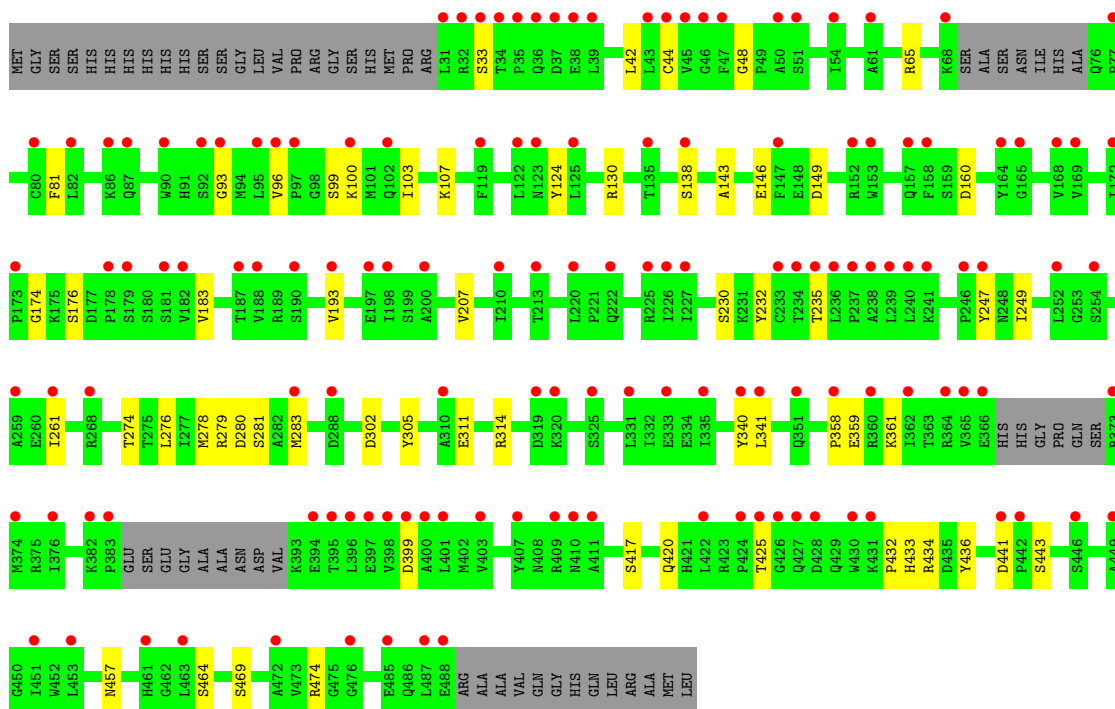


• Molecule 1: L-ornithine N(5)-monooxygenase



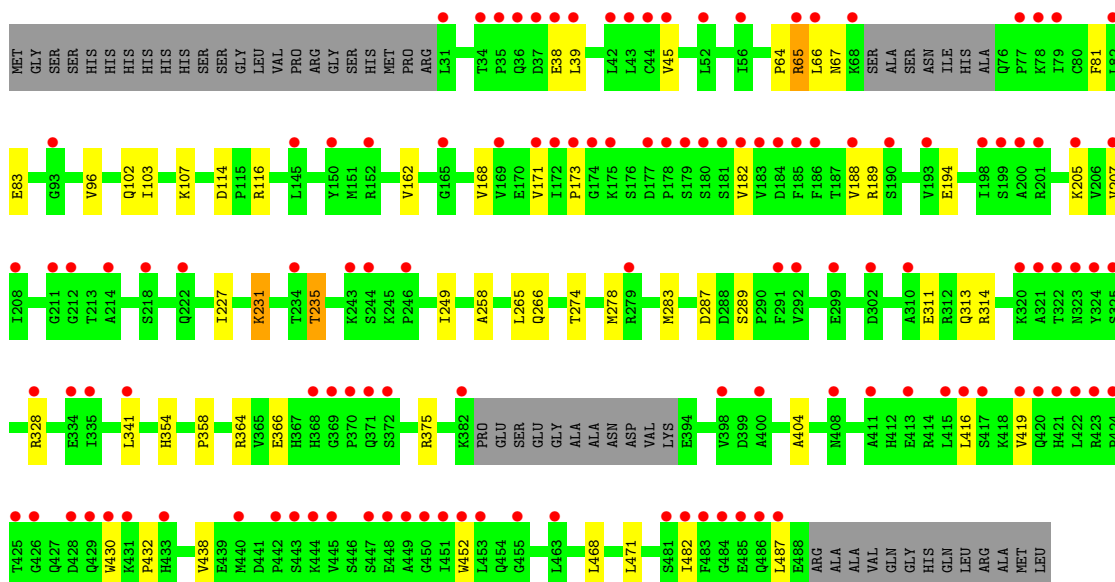
• Molecule 1: L-ornithine N(5)-monooxygenase

Chain F: 



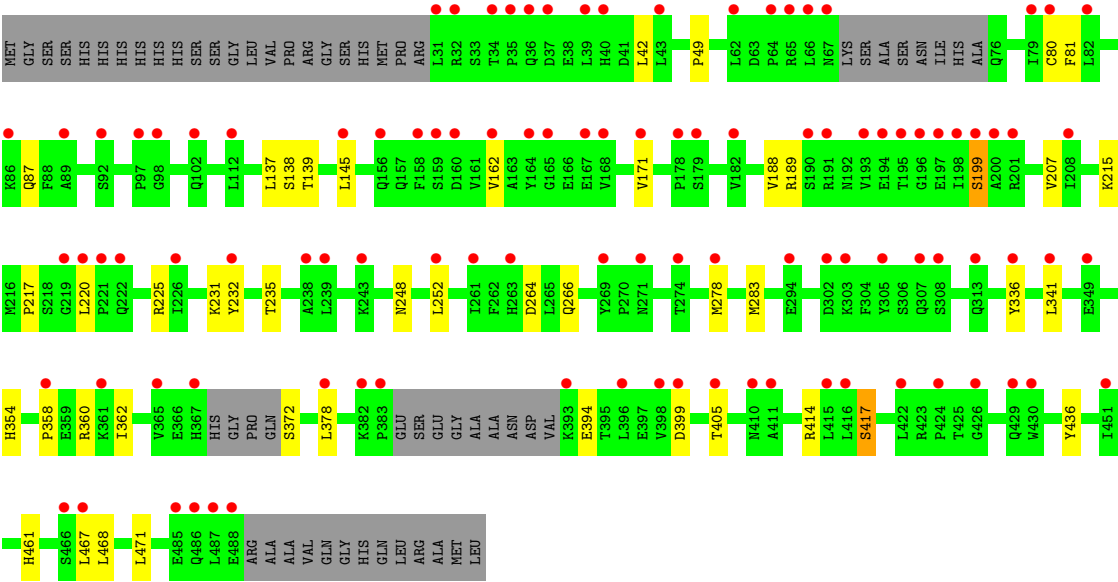
• Molecule 1: L-ornithine N(5)-monooxygenase

Chain G: 



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

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.90Å 155.04Å 146.85Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	68.55 – 2.23 68.55 – 2.23	Depositor EDS
% Data completeness (in resolution range)	97.0 (68.55-2.23) 97.0 (68.55-2.23)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.231 , 0.281 0.233 , 0.282	Depositor DCC
R_{free} test set	11102 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28171	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: 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	0.44	0/3535	0.64	0/4789
1	B	0.43	0/3557	0.61	0/4816
1	C	0.38	0/3461	0.57	0/4686
1	D	0.36	0/3482	0.56	0/4729
1	E	0.38	0/3526	0.61	0/4783
1	F	0.30	0/3417	0.51	0/4643
1	G	0.32	0/3493	0.53	0/4739
1	H	0.30	0/3430	0.52	0/4661
All	All	0.37	0/27901	0.57	0/37846

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	3460	0	3385	23	0
1	B	3481	0	3426	19	0
1	C	3392	0	3314	22	0
1	D	3407	0	3281	27	0
1	E	3450	0	3355	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3345	0	3213	31	0
1	G	3418	0	3311	32	0
1	H	3357	0	3217	24	0
2	A	53	0	33	0	0
2	B	53	0	33	0	0
2	C	53	0	33	0	0
2	D	53	0	33	1	0
2	E	53	0	33	0	0
2	F	53	0	32	1	0
2	G	53	0	33	2	0
2	H	53	0	33	1	0
3	A	9	0	11	1	0
3	B	9	0	11	0	0
3	D	9	0	11	1	0
3	E	9	0	11	1	0
3	G	9	0	11	0	0
3	H	9	0	11	1	0
4	A	91	0	0	1	0
4	B	77	0	0	1	0
4	C	43	0	0	0	0
4	D	41	0	0	0	0
4	E	54	0	0	0	0
4	F	15	0	0	0	0
4	G	29	0	0	0	0
4	H	33	0	0	0	0
All	All	28171	0	26831	206	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:LEU:HD13	3:A:602:ORN:HG3	1.56	0.88
1:B:278:MET:HE1	1:B:283:MET:HG3	1.58	0.84
1:D:467:LEU:HD13	3:D:602:ORN:HG3	1.64	0.80
1:F:103:ILE:HD11	1:F:107:LYS:HD2	1.64	0.79
1:C:278:MET:HG3	1:C:358:PRO:HA	1.68	0.74
1:A:84:ARG:HD3	1:A:167:GLU:HG3	1.68	0.74
1:H:360:ARG:NE	1:H:394:GLU:OE2	2.23	0.70
1:B:37:ASP:N	1:B:37:ASP:OD1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ASP:N	1:C:37:ASP:OD1	2.25	0.69
1:B:61:ALA:O	1:B:67:ASN:ND2	2.22	0.69
1:D:130:ARG:NH2	1:D:146:GLU:OE2	2.21	0.68
1:H:215:LYS:O	1:H:405:THR:OG1	2.12	0.68
1:F:311:GLU:OE1	1:F:314:ARG:NH2	2.28	0.65
1:H:278:MET:HE1	1:H:283:MET:HG3	1.80	0.64
1:G:231:LYS:HB3	1:G:235:THR:OG1	1.98	0.64
1:G:103:ILE:HD11	1:G:107:LYS:HD2	1.80	0.64
1:H:225:ARG:NH1	1:H:372:SER:O	2.31	0.63
1:D:231:LYS:HB3	1:D:235:THR:OG1	2.01	0.61
1:E:209:ALA:HB2	1:E:454:GLN:HB2	1.84	0.60
1:A:121:PHE:CE2	1:A:125:LEU:HD11	2.37	0.59
1:E:467:LEU:HD13	3:E:602:ORN:HD2	1.83	0.59
1:F:33:SER:HB3	1:F:160:ASP:O	2.01	0.59
1:G:364:ARG:NH2	1:G:366:GLU:OE2	2.35	0.59
1:G:311:GLU:OE1	1:G:314:ARG:NH2	2.36	0.58
1:D:437:ARG:NH2	1:D:449:ALA:O	2.37	0.57
1:H:42:LEU:HD11	1:H:207:VAL:HG23	1.87	0.57
1:A:207:VAL:HG22	1:A:452:TRP:HB2	1.87	0.56
1:H:248:ASN:O	1:H:399:ASP:N	2.35	0.56
1:H:266:GLN:HG2	1:H:354:HIS:CE1	2.41	0.56
1:C:65:ARG:NH2	1:C:116:ARG:O	2.31	0.55
1:G:278:MET:HE1	1:G:283:MET:HG3	1.87	0.55
1:B:90:TRP:HB3	1:B:148:GLU:HG3	1.89	0.55
1:H:231:LYS:O	1:H:235:THR:OG1	2.25	0.55
1:D:276:LEU:HG	1:D:278:MET:HE3	1.89	0.54
1:E:45:VAL:HG22	1:E:168:VAL:HG21	1.89	0.54
1:F:124:TYR:OH	1:F:149:ASP:OD2	2.19	0.54
1:E:60:ASP:OD2	1:E:113:ARG:NH2	2.33	0.54
1:G:65:ARG:HG2	1:G:66:LEU:HG	1.90	0.54
1:G:81:PHE:HB2	1:G:162:VAL:HG22	1.90	0.54
1:G:278:MET:HG3	1:G:358:PRO:HA	1.89	0.53
1:E:102:GLN:HE22	1:E:256:GLN:HG2	1.73	0.53
1:H:378:LEU:HB2	1:H:394:GLU:HG3	1.90	0.53
1:E:311:GLU:OE1	1:E:314:ARG:NH1	2.41	0.53
1:H:81:PHE:HB2	1:H:162:VAL:HG22	1.91	0.53
1:A:61:ALA:O	1:A:67:ASN:ND2	2.41	0.52
1:A:43:LEU:HD22	1:A:188:VAL:HG21	1.92	0.52
1:A:278:MET:HE1	1:A:283:MET:HG3	1.92	0.52
1:F:302:ASP:OD1	1:F:434:ARG:NE	2.34	0.52
1:B:42:LEU:HD11	1:B:207:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:366:GLU:HB2	1:G:375:ARG:HB3	1.91	0.52
1:D:374:MET:O	1:D:397:GLU:HA	2.09	0.52
1:A:65:ARG:HD3	1:B:65:ARG:CB	2.40	0.51
1:B:468:LEU:HA	1:B:471:LEU:HG	1.92	0.51
1:F:48:GLY:HA3	2:F:601:FDA:H52A	1.92	0.51
1:C:96:VAL:HG22	1:C:99:SER:HB3	1.91	0.51
1:B:245:LYS:HG3	1:B:246:PRO:HD2	1.91	0.51
1:F:278:MET:HE1	1:F:283:MET:HG3	1.93	0.51
1:A:176:SER:OG	1:A:184:ASP:OD2	2.22	0.51
1:D:81:PHE:HB2	1:D:162:VAL:HG22	1.92	0.51
1:C:349:GLU:HA	1:C:352:TRP:CE2	2.46	0.51
1:F:174:GLY:O	1:F:183:VAL:HG13	2.11	0.50
1:H:252:LEU:HD22	1:H:362:ILE:HD12	1.93	0.50
1:C:115:PRO:HG2	1:D:123:ASN:HA	1.94	0.50
1:B:223:ASP:OD2	1:B:367:HIS:HB2	2.12	0.50
1:E:42:LEU:HD11	1:E:207:VAL:HG23	1.94	0.50
1:F:249:ILE:O	1:F:274:THR:HA	2.12	0.50
1:G:45:VAL:HG22	1:G:168:VAL:HG21	1.94	0.50
1:G:83:GLU:OE2	2:G:601:FDA:O2B	2.26	0.50
1:D:49:PRO:HD2	2:D:601:FDA:O2A	2.12	0.50
1:A:278:MET:HG3	1:A:358:PRO:HA	1.93	0.49
1:F:93:GLY:HA3	1:F:230:SER:O	2.11	0.49
1:E:96:VAL:O	1:E:99:SER:OG	2.23	0.49
1:B:121:PHE:CE2	1:B:125:LEU:HD11	2.48	0.49
1:E:42:LEU:HD23	1:E:79:ILE:HD12	1.93	0.49
1:C:373:ARG:HE	1:C:399:ASP:CG	2.20	0.49
1:G:231:LYS:HB3	1:G:235:THR:HG1	1.76	0.49
1:D:278:MET:HE1	1:D:283:MET:HG3	1.94	0.49
1:A:266:GLN:HG2	1:A:354:HIS:CE1	2.47	0.48
1:F:441:ASP:OD1	1:F:443:SER:OG	2.28	0.48
1:H:217:PRO:HD2	1:H:220:LEU:HD12	1.95	0.48
1:A:364:ARG:HG2	1:A:377:HIS:CD2	2.48	0.48
1:G:65:ARG:NH2	1:G:116:ARG:O	2.40	0.48
1:E:170:GLU:OE1	1:E:189:ARG:NH1	2.46	0.48
1:F:432:PRO:HG3	1:F:457:ASN:ND2	2.29	0.48
1:G:207:VAL:HG22	1:G:452:TRP:HB2	1.95	0.48
1:H:468:LEU:HA	1:H:471:LEU:HG	1.96	0.48
1:A:96:VAL:CG2	1:A:99:SER:HB3	2.44	0.48
1:E:290:PRO:HB2	1:H:336:TYR:CD1	2.49	0.48
1:D:174:GLY:O	1:D:183:VAL:HG13	2.14	0.47
1:F:361:LYS:HE3	1:F:361:LYS:HB2	1.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:GLN:HA	1:G:328:ARG:HH11	1.78	0.47
1:C:65:ARG:HH12	1:C:116:ARG:HB3	1.78	0.47
1:D:84:ARG:HD3	1:D:167:GLU:HG3	1.95	0.47
1:A:302:ASP:OD1	1:A:434:ARG:NE	2.46	0.47
1:E:102:GLN:NE2	1:E:256:GLN:HG2	2.29	0.47
1:B:173:PRO:HD3	1:B:419:VAL:HG12	1.96	0.47
1:G:227:ILE:HG23	1:G:231:LYS:HE2	1.96	0.47
1:E:266:GLN:HG2	1:E:354:HIS:CE1	2.50	0.47
1:F:436:TYR:CZ	1:F:474:ARG:HD2	2.50	0.47
1:G:416:LEU:HB3	1:G:430:TRP:CZ2	2.49	0.47
1:A:231:LYS:O	1:A:235:THR:HB	2.15	0.47
1:H:137:LEU:HB3	1:H:139:THR:HG22	1.96	0.47
1:C:248:ASN:OD1	1:C:273:ARG:HB2	2.15	0.47
1:F:100:LYS:HD3	1:F:143:ALA:HA	1.96	0.47
1:G:432:PRO:HA	1:G:438:VAL:HA	1.96	0.47
1:D:238:ALA:O	1:D:241:LYS:NZ	2.35	0.46
1:D:176:SER:HB3	1:D:184:ASP:OD2	2.15	0.46
1:F:305:TYR:OH	1:F:433:HIS:HA	2.15	0.46
1:D:433:HIS:CE1	1:D:439:GLU:HG2	2.50	0.46
1:E:249:ILE:HD13	1:E:265:LEU:HD22	1.97	0.46
1:B:431:LYS:HD3	1:B:439:GLU:OE2	2.14	0.46
1:D:349:GLU:HA	1:D:352:TRP:CE2	2.50	0.46
1:G:249:ILE:O	1:G:274:THR:HA	2.16	0.46
1:H:49:PRO:HD2	2:H:601:FDA:O2A	2.16	0.46
1:G:266:GLN:HG2	1:G:354:HIS:CE1	2.49	0.46
1:A:249:ILE:O	1:A:274:THR:HA	2.16	0.46
1:E:180:SER:OG	1:E:182:VAL:HG23	2.15	0.46
1:H:171:VAL:HG22	1:H:188:VAL:HG22	1.97	0.46
1:F:464:SER:HB2	1:F:469:SER:HB2	1.98	0.46
1:D:55:ALA:HB2	1:D:81:PHE:CZ	2.51	0.46
1:G:231:LYS:HE2	1:G:231:LYS:HB2	1.54	0.46
1:G:258:ALA:HB2	1:G:404:ALA:HB3	1.98	0.46
1:B:250:ALA:HB2	1:B:398:VAL:HG11	1.98	0.45
1:F:42:LEU:HD11	1:F:207:VAL:HG23	1.98	0.45
1:D:483:PHE:O	1:D:487:LEU:HG	2.17	0.45
1:A:148:GLU:O	1:A:148:GLU:HG2	2.15	0.45
1:E:276:LEU:HG	1:E:278:MET:HE3	1.99	0.45
1:E:316:LEU:HD22	1:E:463:LEU:HG	1.99	0.45
1:C:101:MET:HG2	1:C:142:PRO:O	2.18	0.44
1:D:92:SER:HA	1:D:95:LEU:HG	1.99	0.44
1:E:121:PHE:CE2	1:E:125:LEU:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:MET:HE1	1:E:283:MET:HG3	1.98	0.44
1:F:417:SER:O	1:F:420:GLN:HG2	2.17	0.44
1:C:90:TRP:CZ3	1:C:144:ARG:HD2	2.52	0.44
1:D:134:PHE:O	1:D:137:LEU:HB2	2.17	0.44
1:F:96:VAL:HG23	1:F:99:SER:HB3	2.00	0.44
1:E:231:LYS:O	1:E:235:THR:HB	2.17	0.44
1:F:279:ARG:O	1:F:359:GLU:HA	2.17	0.44
1:B:468:LEU:HD23	1:B:471:LEU:HD12	2.00	0.44
1:G:205:LYS:HD3	1:G:482:ILE:HG23	2.00	0.44
1:E:288:ASP:OD1	1:E:288:ASP:N	2.51	0.44
1:G:102:GLN:N	2:G:601:FDA:O4	2.41	0.44
1:D:249:ILE:O	1:D:274:THR:HA	2.17	0.44
1:A:92:SER:HB2	1:E:370:PRO:HG3	1.99	0.44
1:G:38:GLU:HG2	1:G:39:LEU:N	2.33	0.44
1:B:473:VAL:O	1:B:477:GLU:HG3	2.18	0.44
1:F:278:MET:HG3	1:F:358:PRO:HA	2.00	0.44
1:G:249:ILE:HD13	1:G:265:LEU:HD22	2.00	0.44
1:B:254:SER:CB	1:B:278:MET:HE2	2.48	0.43
1:E:93:GLY:HA3	1:E:230:SER:O	2.18	0.43
1:E:302:ASP:OD1	1:E:434:ARG:NE	2.49	0.43
1:H:189:ARG:HA	1:H:199:SER:O	2.18	0.43
1:C:102:GLN:HG2	1:C:328:ARG:HD2	2.00	0.43
1:E:84:ARG:HD3	1:E:167:GLU:HG3	2.00	0.43
1:F:130:ARG:NH2	1:F:146:GLU:OE2	2.45	0.43
1:G:468:LEU:HA	1:G:471:LEU:HG	2.00	0.43
1:E:243:LYS:HB3	1:E:243:LYS:HE3	1.80	0.43
1:G:171:VAL:HG22	1:G:188:VAL:HG22	1.99	0.43
1:G:64:PRO:HA	1:G:67:ASN:O	2.18	0.43
1:F:247:TYR:HA	1:F:399:ASP:OD2	2.19	0.43
1:H:436:TYR:CE1	1:H:461:HIS:CD2	3.06	0.43
1:A:65:ARG:HH22	1:A:116:ARG:HB3	1.84	0.43
1:C:231:LYS:O	1:C:235:THR:HB	2.19	0.43
1:H:358:PRO:O	1:H:360:ARG:NH1	2.50	0.43
1:D:175:LYS:NZ	1:D:181:SER:O	2.38	0.42
1:E:55:ALA:HB2	1:E:81:PHE:CZ	2.54	0.42
1:G:173:PRO:HG3	1:G:419:VAL:HG12	2.00	0.42
1:C:89:ALA:HB1	1:C:92:SER:OG	2.19	0.42
1:E:65:ARG:HD3	1:F:65:ARG:CB	2.49	0.42
1:C:44:CYS:HB2	1:C:81:PHE:CD2	2.54	0.42
1:D:43:LEU:HD22	1:D:188:VAL:HG21	2.01	0.42
1:F:232:TYR:CE1	1:F:261:ILE:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ARG:HD2	1:C:459:ARG:O	2.18	0.42
1:C:373:ARG:NH2	1:C:399:ASP:OD2	2.48	0.42
1:D:134:PHE:CD1	1:D:137:LEU:HD12	2.55	0.42
1:D:207:VAL:HG22	1:D:452:TRP:HB2	2.02	0.42
1:F:276:LEU:HG	1:F:278:MET:HE3	2.02	0.42
1:F:340:TYR:CD2	1:H:137:LEU:HD11	2.55	0.42
1:H:467:LEU:HD13	3:H:602:ORN:HD2	2.02	0.42
1:C:232:TYR:CD1	1:C:402:MET:HE2	2.55	0.41
1:D:124:TYR:OH	1:D:149:ASP:OD2	2.28	0.41
1:E:316:LEU:CD2	1:E:463:LEU:HG	2.50	0.41
1:F:280:ASP:OD1	1:F:281:SER:N	2.53	0.41
1:B:134:PHE:O	1:B:137:LEU:HB2	2.20	0.41
1:C:42:LEU:HD11	1:C:207:VAL:HG23	2.03	0.41
1:A:96:VAL:HG23	1:A:99:SER:HB3	2.02	0.41
1:C:478:MET:HE3	1:C:482:ILE:HD11	2.01	0.41
1:E:42:LEU:O	1:E:79:ILE:HA	2.20	0.41
1:G:287:ASP:OD1	1:G:289:SER:OG	2.33	0.41
1:A:81:PHE:HB2	1:A:162:VAL:HG22	2.03	0.41
1:H:232:TYR:OH	1:H:264:ASP:OD2	2.28	0.41
1:E:358:PRO:O	1:E:360:ARG:HD3	2.20	0.41
1:F:103:ILE:CD1	1:F:107:LYS:HD2	2.43	0.41
1:A:278:MET:HB3	1:A:278:MET:HE2	1.84	0.41
1:D:103:ILE:HD11	1:D:469:SER:HA	2.03	0.41
1:B:454:GLN:HA	4:B:733:HOH:O	2.21	0.41
1:F:44:CYS:HB2	1:F:81:PHE:CD2	2.56	0.40
1:A:351:GLN:HG3	4:A:768:HOH:O	2.21	0.40
1:H:414:ARG:O	1:H:417:SER:OG	2.32	0.40
1:B:353:GLN:HG2	1:B:354:HIS:CE1	2.55	0.40
1:E:431:LYS:O	1:E:439:GLU:HG3	2.22	0.40
1:E:437:ARG:NH2	1:E:447:SER:O	2.55	0.40
1:G:114:ASP:OD2	1:G:116:ARG:NH2	2.40	0.40
1:C:278:MET:HE1	1:C:283:MET:HG3	2.04	0.40
1:C:375:ARG:NE	1:C:397:GLU:OE2	2.54	0.40
1:E:44:CYS:HB2	1:E:81:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	434/494 (88%)	420 (97%)	14 (3%)	0	100	100
1	B	436/494 (88%)	425 (98%)	11 (2%)	0	100	100
1	C	423/494 (86%)	413 (98%)	10 (2%)	0	100	100
1	D	435/494 (88%)	423 (97%)	12 (3%)	0	100	100
1	E	435/494 (88%)	422 (97%)	12 (3%)	1 (0%)	43	48
1	F	428/494 (87%)	417 (97%)	11 (3%)	0	100	100
1	G	434/494 (88%)	424 (98%)	10 (2%)	0	100	100
1	H	429/494 (87%)	419 (98%)	10 (2%)	0	100	100
All	All	3454/3952 (87%)	3363 (97%)	90 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	370	PRO

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	374/433 (86%)	367 (98%)	7 (2%)	50	59
1	B	379/433 (88%)	376 (99%)	3 (1%)	73	80
1	C	364/433 (84%)	353 (97%)	11 (3%)	36	43
1	D	361/433 (83%)	359 (99%)	2 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	371/433 (86%)	365 (98%)	6 (2%)	55	65
1	F	352/433 (81%)	346 (98%)	6 (2%)	53	63
1	G	363/433 (84%)	353 (97%)	10 (3%)	38	45
1	H	353/433 (82%)	346 (98%)	7 (2%)	48	58
All	All	2917/3464 (84%)	2865 (98%)	52 (2%)	51	61

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	37	ASP
1	A	87	GLN
1	A	199	SER
1	A	245	LYS
1	A	364	ARG
1	A	393	LYS
1	B	37	ASP
1	B	181	SER
1	B	351	GLN
1	C	37	ASP
1	C	80	CYS
1	C	87	GLN
1	C	138	SER
1	C	170	GLU
1	C	172	ILE
1	C	182	VAL
1	C	199	SER
1	C	245	LYS
1	C	289	SER
1	C	328	ARG
1	D	199	SER
1	D	235	THR
1	E	67	ASN
1	E	118	SER
1	E	138	SER
1	E	199	SER
1	E	218	SER
1	E	313	GLN
1	F	138	SER
1	F	176	SER
1	F	193	VAL

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Mol	Chain	Res	Type
1	F	235	THR
1	F	341	LEU
1	F	425	THR
1	G	65	ARG
1	G	96	VAL
1	G	182	VAL
1	G	189	ARG
1	G	194	GLU
1	G	231	LYS
1	G	235	THR
1	G	313	GLN
1	G	341	LEU
1	G	487	LEU
1	H	80	CYS
1	H	87	GLN
1	H	138	SER
1	H	145	LEU
1	H	199	SER
1	H	341	LEU
1	H	417	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	HIS
1	A	337	ASN
1	A	367	HIS
1	A	410	ASN
1	C	40	HIS
1	C	293	ASN
1	C	351	GLN
1	C	420	GLN
1	D	133	HIS
1	D	337	ASN
1	D	480	GLN
1	E	40	HIS
1	E	102	GLN
1	E	126	HIS
1	E	367	HIS
1	E	377	HIS
1	F	40	HIS
1	F	102	GLN

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Mol	Chain	Res	Type
1	F	293	ASN
1	F	433	HIS
1	F	457	ASN
1	G	40	HIS
1	G	351	GLN
1	H	102	GLN
1	H	337	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ORN	B	602	-	7,8,8	1.05	0	6,9,9	1.10	0
3	ORN	H	602	-	7,8,8	0.80	0	6,9,9	1.01	0
2	FDA	G	601	-	57,58,58	3.10	24 (42%)	78,89,89	1.94	18 (23%)
3	ORN	D	602	-	7,8,8	0.75	0	6,9,9	1.17	1 (16%)
2	FDA	A	601	-	57,58,58	2.90	23 (40%)	78,89,89	2.06	18 (23%)
3	ORN	E	602	-	7,8,8	0.69	0	6,9,9	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ORN	A	602	-	7,8,8	0.94	0	6,9,9	0.74	0
3	ORN	G	602	-	7,8,8	0.80	0	6,9,9	1.16	0
2	FDA	D	601	-	57,58,58	3.11	23 (40%)	78,89,89	2.17	21 (26%)
2	FDA	C	601	-	57,58,58	2.96	23 (40%)	78,89,89	2.03	23 (29%)
2	FDA	E	601	-	57,58,58	3.06	26 (45%)	78,89,89	2.01	20 (25%)
2	FDA	H	601	-	57,58,58	2.97	22 (38%)	78,89,89	2.02	20 (25%)
2	FDA	F	601	-	57,58,58	3.05	24 (42%)	78,89,89	2.19	24 (30%)
2	FDA	B	601	-	57,58,58	2.97	23 (40%)	78,89,89	2.09	24 (30%)

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	-
3	ORN	H	602	-	-	0/8/8/8	-
2	FDA	G	601	-	-	7/34/50/50	0/6/6/6
3	ORN	D	602	-	-	0/8/8/8	-
2	FDA	A	601	-	-	8/34/50/50	0/6/6/6
3	ORN	E	602	-	-	0/8/8/8	-
3	ORN	A	602	-	-	1/8/8/8	-
3	ORN	G	602	-	-	1/8/8/8	-
2	FDA	D	601	-	-	10/34/50/50	0/6/6/6
2	FDA	C	601	-	-	7/34/50/50	0/6/6/6
2	FDA	E	601	-	-	2/34/50/50	0/6/6/6
2	FDA	H	601	-	-	12/34/50/50	0/6/6/6
2	FDA	F	601	-	-	15/34/50/50	0/6/6/6
2	FDA	B	601	-	-	8/34/50/50	0/6/6/6

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FDA	PA-O3P	-11.38	1.47	1.59
2	F	601	FDA	PA-O3P	-10.23	1.48	1.59
2	B	601	FDA	PA-O3P	-9.95	1.48	1.59
2	H	601	FDA	PA-O3P	-9.60	1.49	1.59
2	E	601	FDA	PA-O3P	-9.46	1.49	1.59
2	C	601	FDA	PA-O3P	-8.87	1.49	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	FDA	PA-O3P	-8.72	1.50	1.59
2	A	601	FDA	PA-O3P	-8.27	1.50	1.59
2	A	601	FDA	O4-C4	8.20	1.39	1.23
2	H	601	FDA	O4-C4	8.05	1.38	1.23
2	D	601	FDA	O2-C2	7.90	1.40	1.23
2	F	601	FDA	O4-C4	7.89	1.38	1.23
2	C	601	FDA	O4-C4	7.78	1.38	1.23
2	D	601	FDA	O4-C4	7.74	1.38	1.23
2	B	601	FDA	O4-C4	7.66	1.38	1.23
2	C	601	FDA	O2-C2	7.64	1.39	1.23
2	G	601	FDA	O4-C4	7.53	1.37	1.23
2	E	601	FDA	O4-C4	7.52	1.37	1.23
2	H	601	FDA	O2-C2	7.35	1.39	1.23
2	F	601	FDA	O2-C2	7.32	1.38	1.23
2	G	601	FDA	O2-C2	7.32	1.38	1.23
2	B	601	FDA	O2-C2	7.30	1.38	1.23
2	E	601	FDA	O2-C2	7.14	1.38	1.23
2	A	601	FDA	O2-C2	7.06	1.38	1.23
2	G	601	FDA	C6-C5X	6.64	1.50	1.39
2	E	601	FDA	C6-C5X	6.51	1.49	1.39
2	E	601	FDA	C9-C9A	6.39	1.50	1.39
2	C	601	FDA	C6-C5X	6.22	1.49	1.39
2	F	601	FDA	C9-C9A	6.09	1.49	1.39
2	G	601	FDA	C9-C9A	6.02	1.49	1.39
2	D	601	FDA	C9-C9A	6.01	1.49	1.39
2	B	601	FDA	C6-C5X	5.97	1.48	1.39
2	H	601	FDA	C9-C9A	5.88	1.49	1.39
2	B	601	FDA	C9-C9A	5.79	1.49	1.39
2	H	601	FDA	C6-C5X	5.71	1.48	1.39
2	F	601	FDA	C6-C5X	5.70	1.48	1.39
2	G	601	FDA	C10-N1	5.65	1.47	1.37
2	C	601	FDA	C9-C9A	5.58	1.48	1.39
2	D	601	FDA	C6-C5X	5.57	1.48	1.39
2	A	601	FDA	C9-C9A	5.46	1.48	1.39
2	D	601	FDA	C10-N1	5.26	1.46	1.37
2	A	601	FDA	P-O3P	5.20	1.65	1.59
2	A	601	FDA	C6-C5X	5.12	1.47	1.39
2	G	601	FDA	P-O3P	5.09	1.65	1.59
2	G	601	FDA	C4X-N5	5.08	1.45	1.35
2	E	601	FDA	P-O3P	5.07	1.65	1.59
2	B	601	FDA	C4X-N5	5.00	1.45	1.35
2	F	601	FDA	C10-N1	4.75	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FDA	C10-N1	4.73	1.45	1.37
2	G	601	FDA	C2-N1	4.71	1.45	1.37
2	A	601	FDA	C5X-C9A	-4.68	1.35	1.40
2	H	601	FDA	C10-N1	4.65	1.45	1.37
2	C	601	FDA	C2-N1	4.65	1.45	1.37
2	H	601	FDA	C4X-N5	4.62	1.45	1.35
2	C	601	FDA	C4X-N5	4.62	1.45	1.35
2	A	601	FDA	C4X-N5	4.46	1.44	1.35
2	F	601	FDA	C4X-N5	4.39	1.44	1.35
2	D	601	FDA	C4X-N5	4.38	1.44	1.35
2	F	601	FDA	C2-N1	4.28	1.44	1.37
2	D	601	FDA	C6A-N6A	4.28	1.45	1.34
2	E	601	FDA	C10-N1	4.26	1.44	1.37
2	E	601	FDA	C4X-N5	4.23	1.44	1.35
2	B	601	FDA	C10-N1	4.23	1.44	1.37
2	C	601	FDA	C10-N1	4.23	1.44	1.37
2	F	601	FDA	C6A-N6A	4.20	1.44	1.34
2	E	601	FDA	C6A-N6A	4.17	1.44	1.34
2	H	601	FDA	C6A-N6A	4.17	1.44	1.34
2	D	601	FDA	C2-N1	4.16	1.44	1.37
2	D	601	FDA	C5X-C9A	-4.04	1.36	1.40
2	A	601	FDA	C6A-N6A	3.99	1.44	1.34
2	G	601	FDA	C6A-N6A	3.98	1.44	1.34
2	H	601	FDA	C2-N1	3.95	1.44	1.37
2	C	601	FDA	C6A-N6A	3.95	1.44	1.34
2	G	601	FDA	C5X-C9A	-3.93	1.36	1.40
2	C	601	FDA	C2-N3	3.88	1.43	1.37
2	H	601	FDA	C5X-C9A	-3.86	1.36	1.40
2	G	601	FDA	C10-N10	3.85	1.45	1.38
2	F	601	FDA	P-O3P	3.78	1.63	1.59
2	A	601	FDA	C2-N1	3.74	1.43	1.37
2	C	601	FDA	P-O3P	3.72	1.63	1.59
2	G	601	FDA	C5X-N5	3.72	1.46	1.39
2	C	601	FDA	C5X-N5	3.67	1.46	1.39
2	H	601	FDA	C10-N10	3.66	1.44	1.38
2	E	601	FDA	C10-N10	3.64	1.44	1.38
2	D	601	FDA	C10-N10	3.57	1.44	1.38
2	B	601	FDA	C10-N10	3.55	1.44	1.38
2	B	601	FDA	P-O3P	3.53	1.63	1.59
2	F	601	FDA	C10-N10	3.51	1.44	1.38
2	B	601	FDA	C2-N1	3.49	1.43	1.37
2	B	601	FDA	C6A-N6A	3.49	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FDA	C10-N10	3.42	1.44	1.38
2	G	601	FDA	C9A-N10	3.39	1.47	1.41
2	E	601	FDA	C2-N1	3.32	1.42	1.37
2	B	601	FDA	C9A-N10	3.32	1.46	1.41
2	E	601	FDA	C5X-N5	3.29	1.45	1.39
2	H	601	FDA	C5X-N5	3.28	1.45	1.39
2	F	601	FDA	C9A-N10	3.24	1.46	1.41
2	F	601	FDA	C5X-C9A	-3.21	1.37	1.40
2	G	601	FDA	C4X-C4	3.20	1.51	1.41
2	D	601	FDA	C9A-N10	3.18	1.46	1.41
2	F	601	FDA	C2-N3	3.16	1.42	1.37
2	E	601	FDA	C9A-N10	3.15	1.46	1.41
2	A	601	FDA	C4X-C4	3.14	1.51	1.41
2	A	601	FDA	C5X-N5	3.14	1.45	1.39
2	D	601	FDA	C2-N3	3.09	1.42	1.37
2	H	601	FDA	C9A-N10	3.09	1.46	1.41
2	F	601	FDA	C5X-N5	3.01	1.45	1.39
2	E	601	FDA	C5X-C9A	-3.01	1.37	1.40
2	E	601	FDA	C9-C8	3.00	1.43	1.39
2	H	601	FDA	C2-N3	2.96	1.42	1.37
2	B	601	FDA	C9-C8	2.96	1.43	1.39
2	A	601	FDA	C2-N3	2.94	1.42	1.37
2	G	601	FDA	C4A-N9A	2.92	1.43	1.37
2	B	601	FDA	C5X-N5	2.91	1.44	1.39
2	D	601	FDA	C5X-N5	2.91	1.44	1.39
2	B	601	FDA	C2-N3	2.89	1.42	1.37
2	C	601	FDA	C5X-C9A	-2.87	1.37	1.40
2	F	601	FDA	C4X-C4	2.87	1.50	1.41
2	H	601	FDA	PA-O5B	-2.85	1.48	1.59
2	C	601	FDA	C9A-N10	2.85	1.46	1.41
2	E	601	FDA	C5A-C4A	2.84	1.44	1.39
2	A	601	FDA	PA-O5B	-2.82	1.48	1.59
2	C	601	FDA	PA-O5B	-2.82	1.48	1.59
2	D	601	FDA	C4A-N9A	2.81	1.43	1.37
2	E	601	FDA	C4A-N9A	2.79	1.43	1.37
2	F	601	FDA	O2'-C2'	-2.75	1.37	1.43
2	H	601	FDA	P-O3P	2.73	1.62	1.59
2	F	601	FDA	PA-O5B	-2.72	1.48	1.59
2	C	601	FDA	C4X-C4	2.71	1.50	1.41
2	G	601	FDA	C5A-C4A	2.67	1.43	1.39
2	D	601	FDA	C5A-C4A	2.65	1.43	1.39
2	E	601	FDA	PA-O2A	-2.64	1.43	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	FDA	C2-N3	2.64	1.41	1.37
2	B	601	FDA	C4X-C4	2.64	1.49	1.41
2	D	601	FDA	PA-O5B	-2.62	1.49	1.59
2	B	601	FDA	C5X-C9A	-2.62	1.37	1.40
2	C	601	FDA	C4A-N9A	2.61	1.43	1.37
2	F	601	FDA	C5A-C4A	2.61	1.43	1.39
2	D	601	FDA	C4X-C4	2.60	1.49	1.41
2	F	601	FDA	C4A-N9A	2.59	1.43	1.37
2	E	601	FDA	C2A-N3A	2.57	1.38	1.33
2	G	601	FDA	PA-O5B	-2.56	1.49	1.59
2	H	601	FDA	C4X-C4	2.54	1.49	1.41
2	E	601	FDA	PA-O5B	-2.52	1.49	1.59
2	G	601	FDA	PA-O2A	-2.51	1.43	1.55
2	B	601	FDA	C4A-N9A	2.51	1.42	1.37
2	F	601	FDA	O3B-C3B	-2.51	1.36	1.43
2	H	601	FDA	P-O1P	2.47	1.59	1.50
2	A	601	FDA	PA-O2A	-2.44	1.44	1.55
2	B	601	FDA	PA-O5B	-2.43	1.49	1.59
2	A	601	FDA	C5A-C4A	2.39	1.43	1.39
2	C	601	FDA	O2'-C2'	-2.39	1.38	1.43
2	E	601	FDA	O3B-C3B	-2.38	1.37	1.43
2	D	601	FDA	O2'-C2'	-2.37	1.38	1.43
2	B	601	FDA	C2A-N3A	2.37	1.38	1.33
2	G	601	FDA	C2-N3	2.36	1.41	1.37
2	B	601	FDA	P-O1P	2.35	1.59	1.50
2	B	601	FDA	C5A-C4A	2.35	1.43	1.39
2	C	601	FDA	P-O1P	2.35	1.58	1.50
2	G	601	FDA	C2A-N3A	2.34	1.38	1.33
2	D	601	FDA	PA-O2A	-2.34	1.44	1.55
2	E	601	FDA	C3B-C4B	-2.33	1.47	1.53
2	D	601	FDA	P-O1P	2.31	1.58	1.50
2	A	601	FDA	O3B-C3B	-2.30	1.37	1.43
2	A	601	FDA	O2B-C2B	-2.28	1.37	1.43
2	C	601	FDA	C5A-C4A	2.28	1.43	1.39
2	F	601	FDA	PA-O2A	-2.27	1.44	1.55
2	H	601	FDA	O3B-C3B	-2.27	1.37	1.43
2	C	601	FDA	C10-N10	2.25	1.42	1.38
2	H	601	FDA	O2'-C2'	-2.25	1.38	1.43
2	E	601	FDA	C4X-C4	2.24	1.48	1.41
2	G	601	FDA	O3B-C3B	-2.23	1.37	1.43
2	B	601	FDA	O2'-C2'	-2.23	1.38	1.43
2	H	601	FDA	PA-O2A	-2.23	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	FDA	O4B-C4B	-2.20	1.40	1.45
2	F	601	FDA	P-O1P	2.19	1.58	1.50
2	C	601	FDA	PA-O2A	-2.18	1.45	1.55
2	A	601	FDA	O2'-C2'	-2.16	1.38	1.43
2	A	601	FDA	C2A-N3A	2.15	1.37	1.33
2	E	601	FDA	O4B-C4B	-2.14	1.40	1.45
2	E	601	FDA	O2'-C2'	-2.10	1.38	1.43
2	D	601	FDA	O3B-C3B	-2.07	1.37	1.43
2	A	601	FDA	PA-O1A	2.07	1.58	1.50
2	G	601	FDA	O2'-C2'	-2.05	1.39	1.43
2	D	601	FDA	O2B-C2B	-2.05	1.37	1.43
2	C	601	FDA	O3B-C3B	-2.03	1.37	1.43
2	G	601	FDA	P-O1P	2.02	1.57	1.50
2	H	601	FDA	C2B-C3B	-2.00	1.47	1.53

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FDA	O2P-P-O3P	-7.78	86.25	107.27
2	B	601	FDA	C5A-C4A-N3A	-6.73	117.45	126.72
2	D	601	FDA	C5A-C4A-N3A	-6.61	117.61	126.72
2	F	601	FDA	O2P-P-O3P	-6.45	89.84	107.27
2	G	601	FDA	C5A-C4A-N3A	-6.13	118.27	126.72
2	A	601	FDA	C5A-C4A-N3A	-5.92	118.56	126.72
2	C	601	FDA	C5A-C4A-N3A	-5.87	118.64	126.72
2	E	601	FDA	C5A-C4A-N3A	-5.73	118.83	126.72
2	C	601	FDA	N3A-C2A-N1A	-5.65	120.02	128.58
2	A	601	FDA	N3A-C4A-N9A	5.63	136.75	127.17
2	D	601	FDA	N3A-C4A-N9A	5.63	136.74	127.17
2	H	601	FDA	N3A-C2A-N1A	-5.63	120.06	128.58
2	G	601	FDA	N3A-C4A-N9A	5.58	136.66	127.17
2	F	601	FDA	C5A-C4A-N3A	-5.57	119.05	126.72
2	A	601	FDA	O2P-P-O3P	-5.55	92.27	107.27
2	G	601	FDA	N3A-C2A-N1A	-5.51	120.24	128.58
2	F	601	FDA	N3A-C2A-N1A	-5.35	120.48	128.58
2	B	601	FDA	N3A-C4A-N9A	5.26	136.11	127.17
2	A	601	FDA	N3A-C2A-N1A	-5.17	120.76	128.58
2	F	601	FDA	O2A-PA-O3P	-5.09	93.52	107.27
2	F	601	FDA	N3A-C4A-N9A	4.91	135.52	127.17
2	H	601	FDA	C5A-C4A-N3A	-4.89	119.98	126.72
2	B	601	FDA	N3A-C2A-N1A	-4.80	121.31	128.58
2	B	601	FDA	C4-N3-C2	-4.76	119.82	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	FDA	N3A-C4A-N9A	4.75	135.25	127.17
2	A	601	FDA	C4-N3-C2	-4.74	119.84	126.37
2	E	601	FDA	N3A-C4A-N9A	4.71	135.18	127.17
2	B	601	FDA	C5A-N7A-C8A	4.69	110.83	103.45
2	E	601	FDA	C4-N3-C2	-4.67	119.94	126.37
2	C	601	FDA	N3A-C4A-N9A	4.66	135.09	127.17
2	D	601	FDA	N3A-C2A-N1A	-4.56	121.68	128.58
2	H	601	FDA	C4-N3-C2	-4.51	120.15	126.37
2	C	601	FDA	C5A-N7A-C8A	4.44	110.43	103.45
2	E	601	FDA	C5A-N7A-C8A	4.42	110.39	103.45
2	E	601	FDA	N3A-C2A-N1A	-4.35	122.00	128.58
2	D	601	FDA	C4-N3-C2	-4.35	120.38	126.37
2	F	601	FDA	C5A-N7A-C8A	4.31	110.22	103.45
2	H	601	FDA	C5A-N7A-C8A	4.27	110.16	103.45
2	G	601	FDA	C4-N3-C2	-4.26	120.51	126.37
2	E	601	FDA	O3P-P-O1P	4.23	123.44	110.70
2	F	601	FDA	C4-N3-C2	-4.20	120.58	126.37
2	G	601	FDA	C5A-N7A-C8A	4.20	110.05	103.45
2	B	601	FDA	C2A-N3A-C4A	4.11	121.86	111.83
2	C	601	FDA	C4-N3-C2	-4.06	120.78	126.37
2	A	601	FDA	C5A-N7A-C8A	4.05	109.81	103.45
2	C	601	FDA	C2A-N3A-C4A	4.01	121.63	111.83
2	F	601	FDA	O3P-P-O1P	3.98	122.68	110.70
2	H	601	FDA	N9A-C8A-N7A	-3.93	108.36	113.94
2	D	601	FDA	C5A-N7A-C8A	3.92	109.61	103.45
2	D	601	FDA	O3P-P-O1P	3.91	122.48	110.70
2	G	601	FDA	C2A-N3A-C4A	3.91	121.39	111.83
2	B	601	FDA	C4A-C5A-N7A	-3.90	106.12	110.58
2	E	601	FDA	O2A-PA-O3P	-3.84	96.89	107.27
2	H	601	FDA	O2P-P-O3P	-3.81	96.97	107.27
2	A	601	FDA	O3P-P-O1P	3.79	122.11	110.70
2	D	601	FDA	O4-C4-C4X	-3.78	118.15	127.26
2	C	601	FDA	C4A-C5A-N7A	-3.78	106.26	110.58
2	B	601	FDA	O4-C4-C4X	-3.77	118.17	127.26
2	E	601	FDA	O3P-PA-O1A	3.76	122.02	110.70
2	D	601	FDA	C2A-N3A-C4A	3.70	120.87	111.83
2	H	601	FDA	O4-C4-C4X	-3.66	118.43	127.26
2	F	601	FDA	C2A-N3A-C4A	3.66	120.76	111.83
2	G	601	FDA	O2P-P-O3P	-3.66	97.39	107.27
2	A	601	FDA	C2A-N3A-C4A	3.64	120.73	111.83
2	H	601	FDA	C4A-N9A-C8A	3.58	109.49	105.74
2	E	601	FDA	C4A-C5A-N7A	-3.56	106.51	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FDA	O2P-P-O3P	-3.55	97.69	107.27
2	H	601	FDA	C2A-N3A-C4A	3.54	120.48	111.83
2	B	601	FDA	N9A-C8A-N7A	-3.50	108.97	113.94
2	H	601	FDA	O3P-PA-O1A	3.47	121.14	110.70
2	F	601	FDA	N9A-C8A-N7A	-3.39	109.13	113.94
2	F	601	FDA	O3P-PA-O1A	3.38	120.88	110.70
2	C	601	FDA	O4-C4-C4X	-3.36	119.17	127.26
2	H	601	FDA	O2A-PA-O5B	-3.33	92.47	107.57
2	E	601	FDA	C2A-N3A-C4A	3.32	119.94	111.83
2	E	601	FDA	N9A-C8A-N7A	-3.28	109.28	113.94
2	C	601	FDA	O3P-P-O1P	3.28	120.56	110.70
2	G	601	FDA	N9A-C8A-N7A	-3.27	109.30	113.94
2	C	601	FDA	N9A-C8A-N7A	-3.23	109.35	113.94
2	C	601	FDA	O2A-PA-O3P	-3.23	98.53	107.27
2	E	601	FDA	O4-C4-C4X	-3.22	119.49	127.26
2	F	601	FDA	C4A-C5A-N7A	-3.20	106.92	110.58
2	A	601	FDA	N9A-C8A-N7A	-3.20	109.39	113.94
2	A	601	FDA	N3-C2-N1	3.19	120.75	115.74
2	B	601	FDA	O3P-P-O1P	3.06	119.91	110.70
2	C	601	FDA	C4'-C3'-C2'	3.04	118.64	113.57
2	B	601	FDA	O2P-P-O3P	-3.04	99.05	107.27
2	F	601	FDA	O2A-PA-O5B	-3.00	93.96	107.57
2	G	601	FDA	O2A-PA-O5B	-2.99	94.03	107.57
2	G	601	FDA	C4X-C4-N3	2.97	120.30	112.13
2	H	601	FDA	C4A-C5A-N7A	-2.95	107.21	110.58
2	D	601	FDA	C4A-C5A-N7A	-2.93	107.24	110.58
2	H	601	FDA	O3P-P-O1P	2.91	119.47	110.70
2	A	601	FDA	C9A-C5X-N5	2.88	122.88	119.37
2	E	601	FDA	O2P-P-O3P	-2.88	99.50	107.27
2	B	601	FDA	O2A-PA-O5B	-2.86	94.62	107.57
2	D	601	FDA	O2A-PA-O3P	-2.85	99.58	107.27
2	D	601	FDA	O2P-P-O5'	-2.85	94.67	107.57
2	D	601	FDA	C4X-C4-N3	2.85	119.94	112.13
2	G	601	FDA	C4A-C5A-N7A	-2.84	107.34	110.58
2	A	601	FDA	O4-C4-C4X	-2.83	120.44	127.26
2	B	601	FDA	C4X-C4-N3	2.81	119.86	112.13
2	D	601	FDA	O3P-PA-O1A	2.77	119.05	110.70
2	H	601	FDA	O5'-P-O1P	2.77	119.92	108.94
2	F	601	FDA	N3-C2-N1	2.76	120.08	115.74
2	E	601	FDA	C4X-C4-N3	2.73	119.62	112.13
2	D	601	FDA	O5'-P-O1P	2.70	119.65	108.94
2	F	601	FDA	O4-C4-C4X	-2.70	120.74	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FDA	N3-C2-N1	2.69	119.96	115.74
2	D	601	FDA	N9A-C8A-N7A	-2.66	110.16	113.94
2	H	601	FDA	C4X-C4-N3	2.64	119.39	112.13
2	F	601	FDA	C9A-C5X-N5	2.62	122.57	119.37
2	H	601	FDA	N3-C2-N1	2.62	119.86	115.74
2	E	601	FDA	N3-C2-N1	2.61	119.84	115.74
2	H	601	FDA	O2P-P-O5'	-2.60	95.78	107.57
2	D	601	FDA	O5B-PA-O1A	2.59	119.20	108.94
2	G	601	FDA	N3-C2-N1	2.56	119.77	115.74
2	C	601	FDA	N3-C2-N1	2.55	119.75	115.74
2	C	601	FDA	O2A-PA-O5B	-2.54	96.04	107.57
2	A	601	FDA	C4X-C4-N3	2.53	119.08	112.13
2	G	601	FDA	O2A-PA-O3P	-2.50	100.50	107.27
2	A	601	FDA	O3P-PA-O1A	2.50	118.22	110.70
2	C	601	FDA	C5X-C9A-N10	2.49	120.83	118.01
2	F	601	FDA	C4X-C4-N3	2.48	118.94	112.13
2	B	601	FDA	C1'-N10-C9A	2.47	125.44	120.63
2	G	601	FDA	O4-C4-C4X	-2.46	121.34	127.26
2	F	601	FDA	C4A-N9A-C8A	2.44	108.30	105.74
2	A	601	FDA	O2A-PA-O5B	-2.44	96.50	107.57
2	E	601	FDA	C9A-C5X-N5	2.43	122.33	119.37
2	E	601	FDA	C4'-C3'-C2'	2.40	117.56	113.57
2	C	601	FDA	O2-C2-N1	-2.40	117.61	121.86
2	G	601	FDA	C4A-N9A-C8A	2.39	108.25	105.74
2	B	601	FDA	O2P-P-O5'	-2.36	96.87	107.57
2	B	601	FDA	O5'-P-O1P	2.36	118.28	108.94
2	A	601	FDA	O2-C2-N1	-2.35	117.69	121.86
2	B	601	FDA	O2-C2-N1	-2.35	117.69	121.86
2	A	601	FDA	C4A-C5A-N7A	-2.34	107.91	110.58
2	F	601	FDA	O5'-P-O1P	2.33	118.18	108.94
2	B	601	FDA	C6-C5X-C9A	2.33	122.34	119.80
2	A	601	FDA	C4A-N9A-C8A	2.32	108.17	105.74
2	C	601	FDA	C4X-C4-N3	2.30	118.45	112.13
2	B	601	FDA	O3P-PA-O1A	2.30	117.62	110.70
2	G	601	FDA	C5X-C9A-N10	2.29	120.60	118.01
2	D	601	FDA	O2A-PA-O1A	2.27	123.02	112.44
2	D	601	FDA	O2A-PA-O5B	-2.26	97.32	107.57
2	G	601	FDA	O3P-P-O1P	2.26	117.49	110.70
2	B	601	FDA	C6-C5X-N5	-2.25	115.84	119.76
2	E	601	FDA	O2B-C2B-C1B	2.25	117.84	110.10
2	F	601	FDA	C5'-C4'-C3'	2.23	116.43	112.22
3	D	602	ORN	CG-CB-CA	-2.19	106.16	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FDA	O2A-PA-O1A	2.18	122.60	112.44
2	C	601	FDA	O3P-PA-O1A	2.18	117.27	110.70
2	F	601	FDA	O5B-PA-O1A	2.18	117.56	108.94
2	H	601	FDA	O2-C2-N1	-2.16	118.02	121.86
2	G	601	FDA	O5B-PA-O1A	2.15	117.46	108.94
2	F	601	FDA	C2B-C3B-C4B	2.14	106.75	102.61
2	B	601	FDA	C4'-C3'-C2'	2.13	117.12	113.57
2	E	601	FDA	C1'-C2'-C3'	2.08	115.30	109.66
2	C	601	FDA	C9-C9A-N10	-2.07	119.08	121.85
2	D	601	FDA	N3-C2-N1	2.06	118.98	115.74
2	H	601	FDA	C2B-C3B-C4B	2.06	106.59	102.61
2	C	601	FDA	O5'-P-O1P	2.05	117.07	108.94
2	C	601	FDA	O4'-C4'-C3'	2.03	114.01	109.25
2	B	601	FDA	O4B-C1B-C2B	-2.03	102.27	106.62
2	C	601	FDA	O5B-PA-O1A	2.02	116.94	108.94
2	F	601	FDA	C6-C5X-N5	-2.01	116.26	119.76
2	D	601	FDA	C6A-C5A-C4A	2.01	119.92	117.18
2	E	601	FDA	C5'-C4'-C3'	2.01	116.01	112.22
2	F	601	FDA	O2P-P-O5'	-2.01	98.48	107.57

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FDA	C5B-O5B-PA-O1A
2	A	601	FDA	C5'-O5'-P-O3P
2	B	601	FDA	C5'-O5'-P-O3P
2	C	601	FDA	N10-C1'-C2'-O2'
2	C	601	FDA	N10-C1'-C2'-C3'
2	D	601	FDA	N10-C1'-C2'-O2'
2	D	601	FDA	N10-C1'-C2'-C3'
2	D	601	FDA	C5'-O5'-P-O3P
2	D	601	FDA	PA-O3P-P-O5'
2	F	601	FDA	C5B-O5B-PA-O1A
2	F	601	FDA	C5B-O5B-PA-O2A
2	F	601	FDA	N10-C1'-C2'-O2'
2	F	601	FDA	N10-C1'-C2'-C3'
2	F	601	FDA	C5'-O5'-P-O1P
2	F	601	FDA	C5'-O5'-P-O3P
2	G	601	FDA	N10-C1'-C2'-C3'
2	G	601	FDA	PA-O3P-P-O5'
2	H	601	FDA	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
2	H	601	FDA	C5'-O5'-P-O1P
2	H	601	FDA	C5'-O5'-P-O3P
2	H	601	FDA	PA-O3P-P-O5'
2	D	601	FDA	O3'-C3'-C4'-C5'
2	D	601	FDA	C2'-C3'-C4'-C5'
2	F	601	FDA	O4B-C4B-C5B-O5B
2	F	601	FDA	C3B-C4B-C5B-O5B
2	D	601	FDA	C2'-C3'-C4'-O4'
2	D	601	FDA	O3'-C3'-C4'-O4'
2	F	601	FDA	C2'-C3'-C4'-C5'
2	C	601	FDA	O3'-C3'-C4'-C5'
2	G	601	FDA	O3'-C3'-C4'-C5'
2	F	601	FDA	C2'-C3'-C4'-O4'
2	E	601	FDA	O4B-C4B-C5B-O5B
2	F	601	FDA	O3'-C3'-C4'-C5'
2	C	601	FDA	C2'-C3'-C4'-C5'
2	G	601	FDA	C2'-C3'-C4'-C5'
2	A	601	FDA	PA-O3P-P-O1P
2	H	601	FDA	O3'-C3'-C4'-C5'
2	E	601	FDA	C3B-C4B-C5B-O5B
2	A	601	FDA	PA-O3P-P-O5'
2	B	601	FDA	PA-O3P-P-O5'
2	C	601	FDA	P-O3P-PA-O5B
2	H	601	FDA	C2'-C3'-C4'-C5'
2	F	601	FDA	P-O3P-PA-O1A
2	G	601	FDA	O3'-C3'-C4'-O4'
2	G	601	FDA	N10-C1'-C2'-O2'
2	H	601	FDA	N10-C1'-C2'-O2'
2	B	601	FDA	C2'-C3'-C4'-C5'
2	C	601	FDA	C5'-O5'-P-O1P
2	D	601	FDA	C5B-O5B-PA-O1A
2	F	601	FDA	C5B-O5B-PA-O3P
2	F	601	FDA	C5'-O5'-P-O2P
2	H	601	FDA	C5'-O5'-P-O2P
2	G	601	FDA	C2'-C3'-C4'-O4'
2	A	601	FDA	C2'-C3'-C4'-C5'
2	H	601	FDA	O4B-C4B-C5B-O5B
2	F	601	FDA	O3'-C3'-C4'-O4'
2	B	601	FDA	O3'-C3'-C4'-C5'
2	A	601	FDA	P-O3P-PA-O2A
2	B	601	FDA	P-O3P-PA-O2A
2	H	601	FDA	PA-O3P-P-O1P

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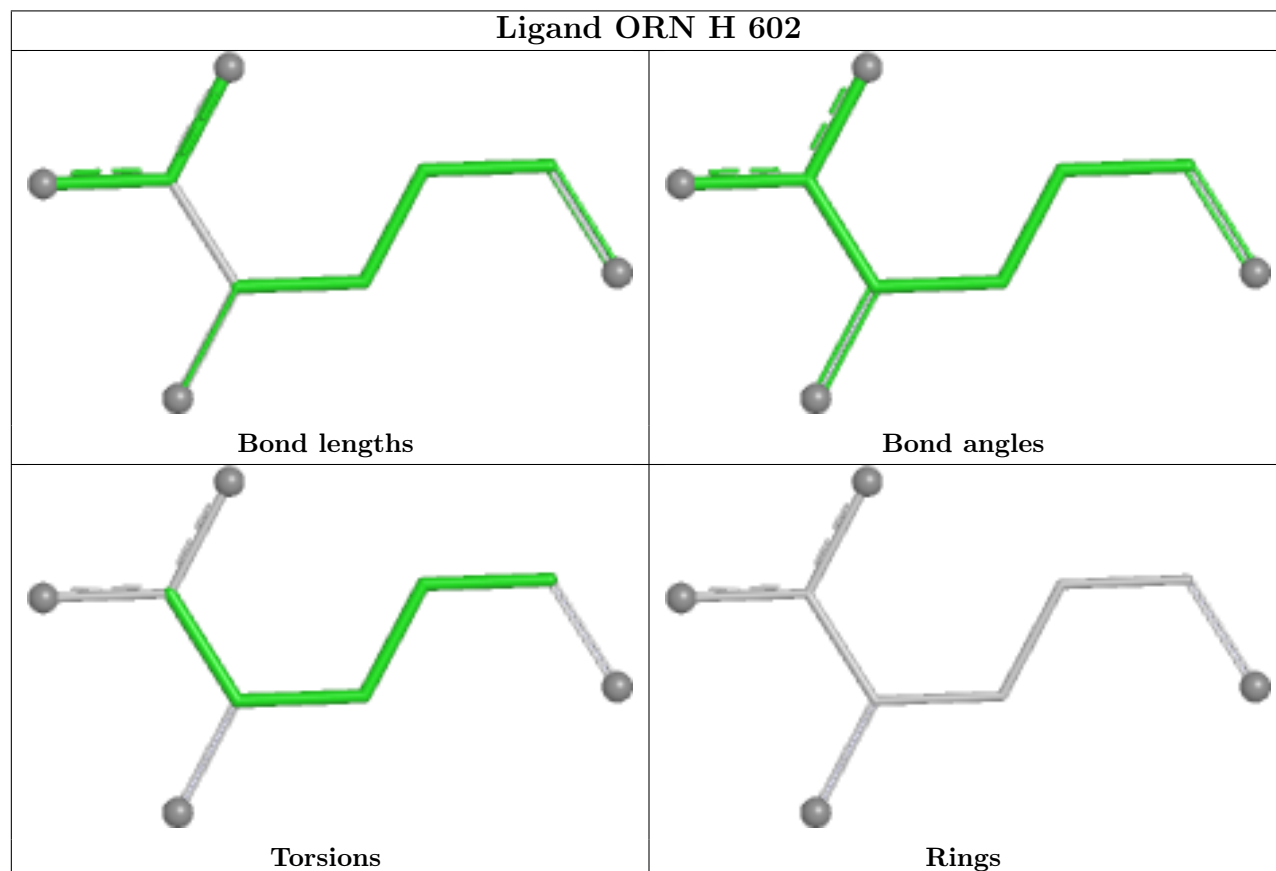
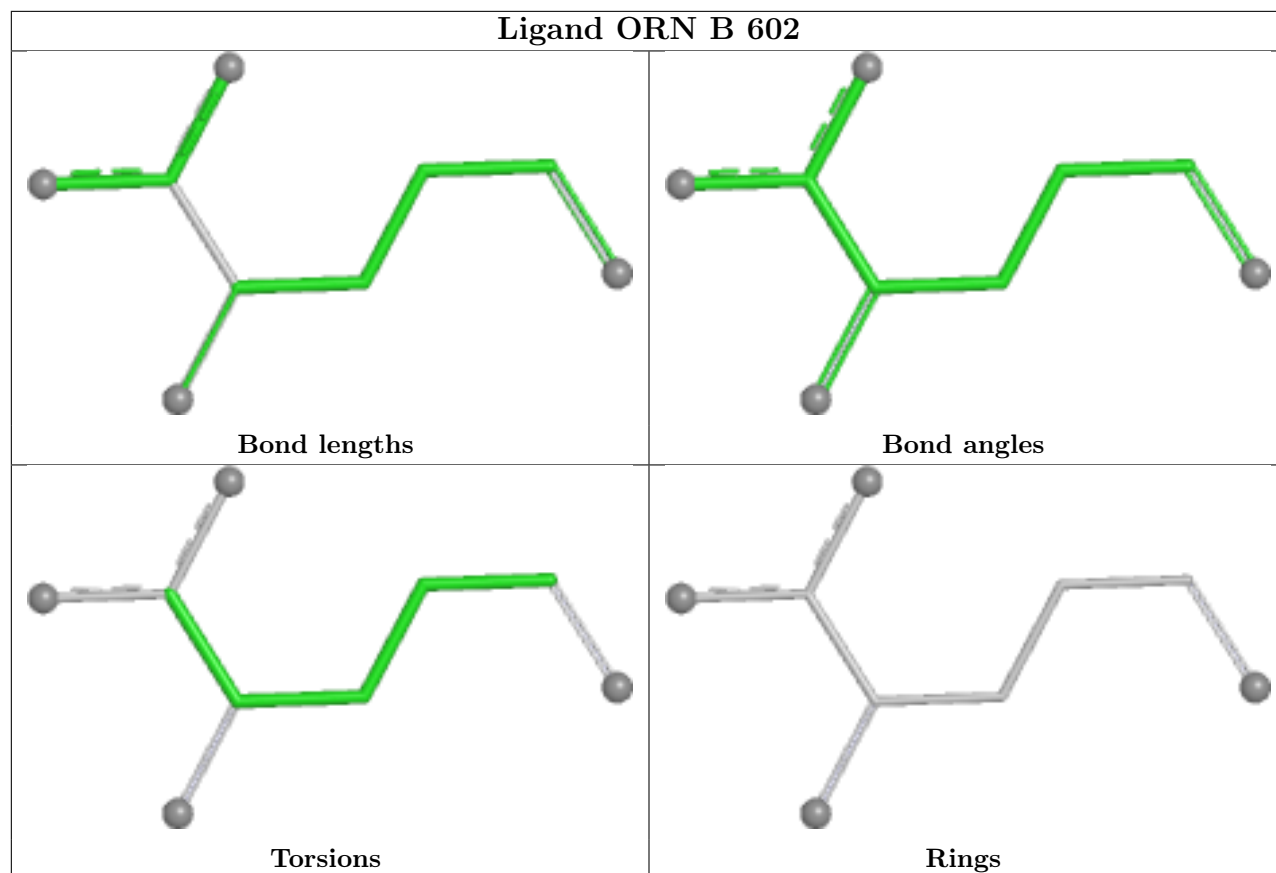
Mol	Chain	Res	Type	Atoms
2	B	601	FDA	PA-O3P-P-O1P
2	H	601	FDA	O3'-C3'-C4'-O4'
2	C	601	FDA	O3'-C3'-C4'-O4'
3	A	602	ORN	CA-CB-CG-CD
2	A	601	FDA	P-O3P-PA-O1A
2	B	601	FDA	P-O3P-PA-O1A
2	H	601	FDA	P-O3P-PA-O1A
2	A	601	FDA	O4'-C4'-C5'-O5'
3	G	602	ORN	O-C-CA-CB
2	D	601	FDA	PA-O3P-P-O2P
2	B	601	FDA	O4B-C4B-C5B-O5B

There are no ring outliers.

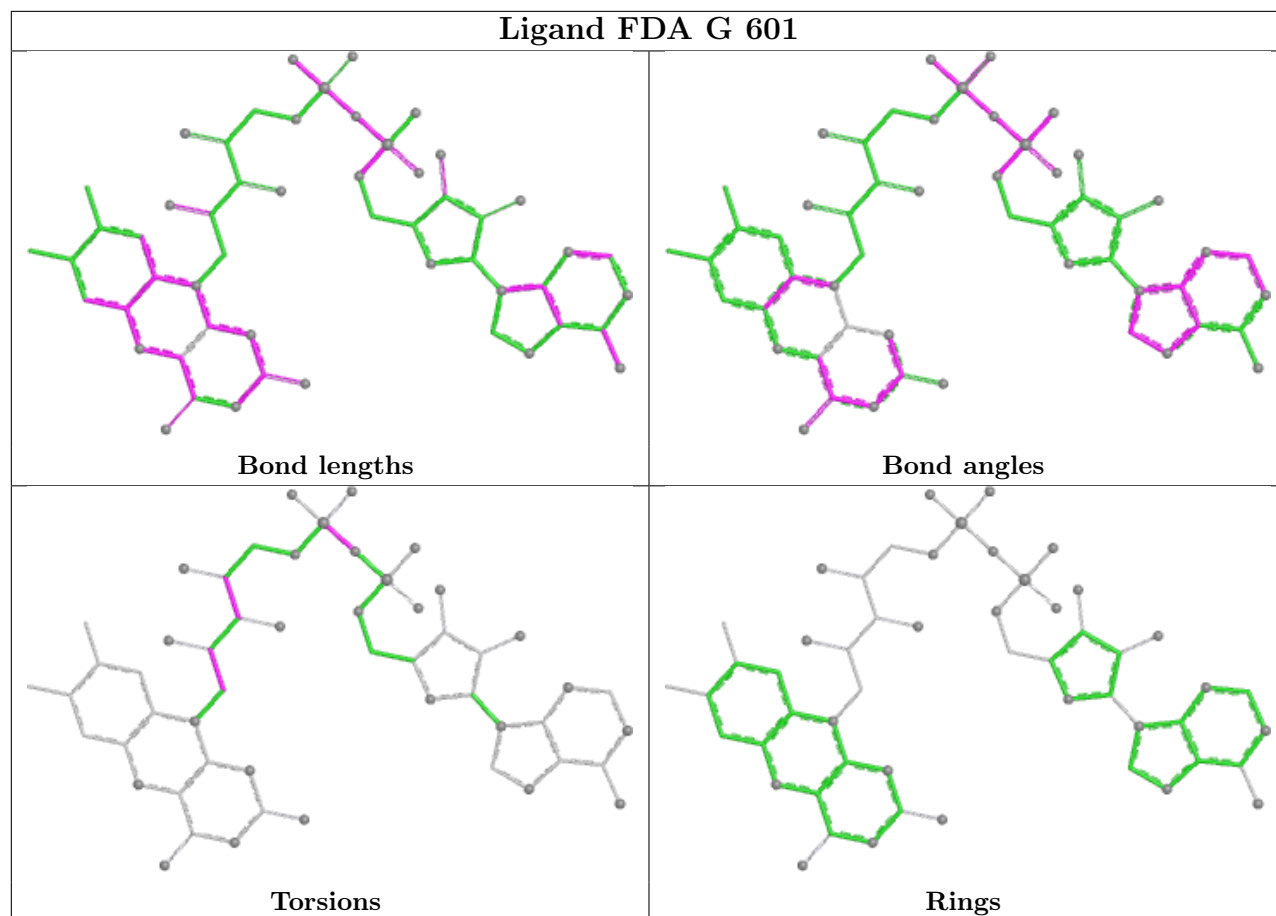
8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	602	ORN	1	0
2	G	601	FDA	2	0
3	D	602	ORN	1	0
3	E	602	ORN	1	0
3	A	602	ORN	1	0
2	D	601	FDA	1	0
2	H	601	FDA	1	0
2	F	601	FDA	1	0

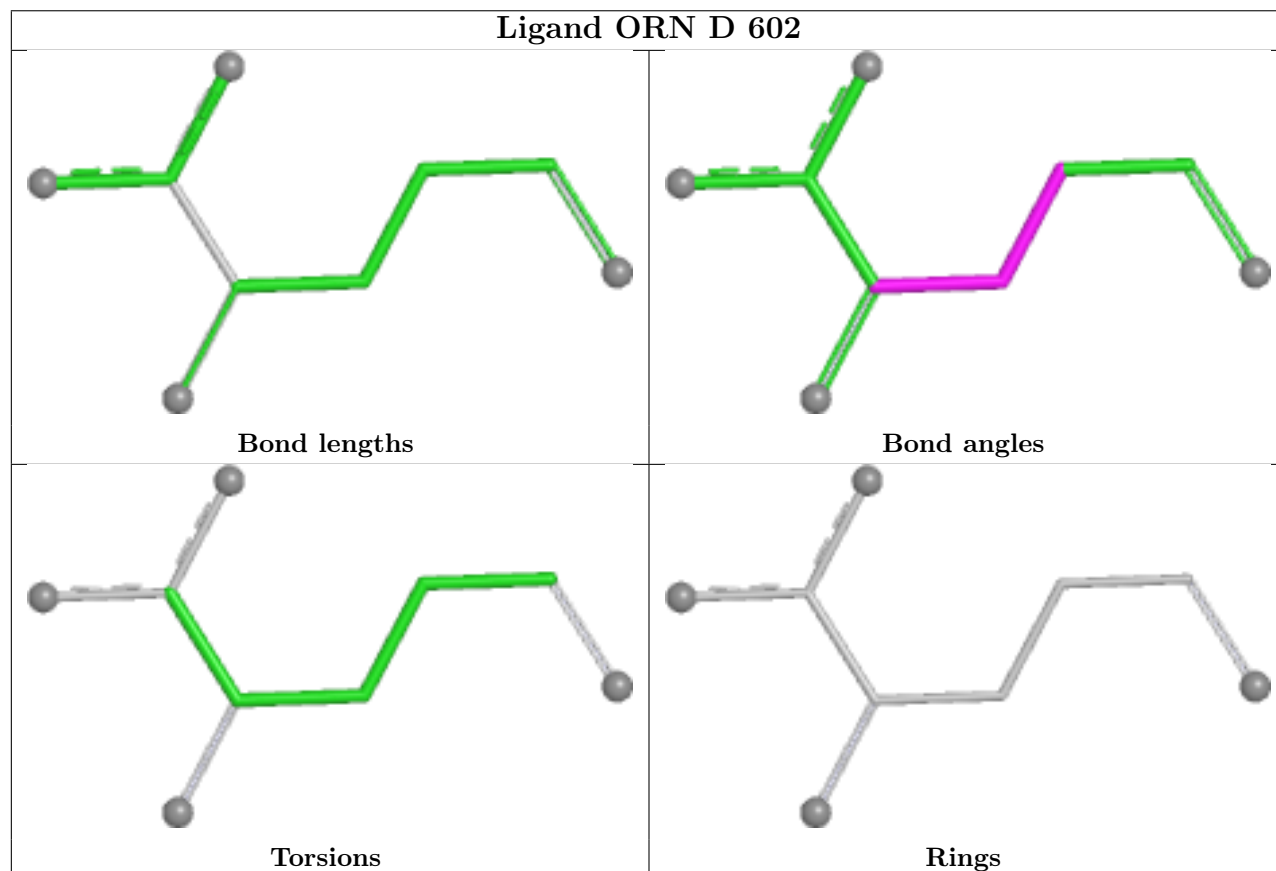
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



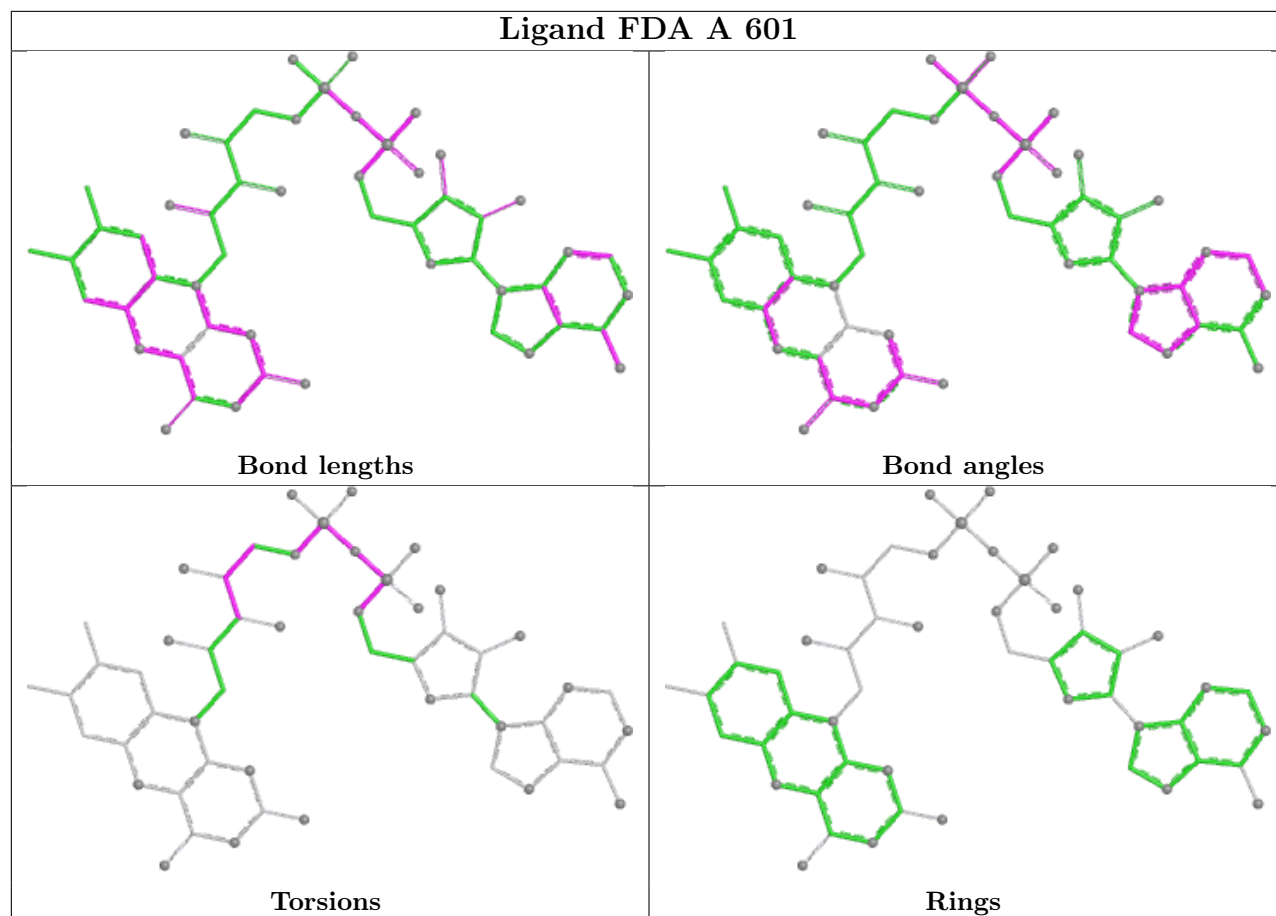
Ligand FDA G 601



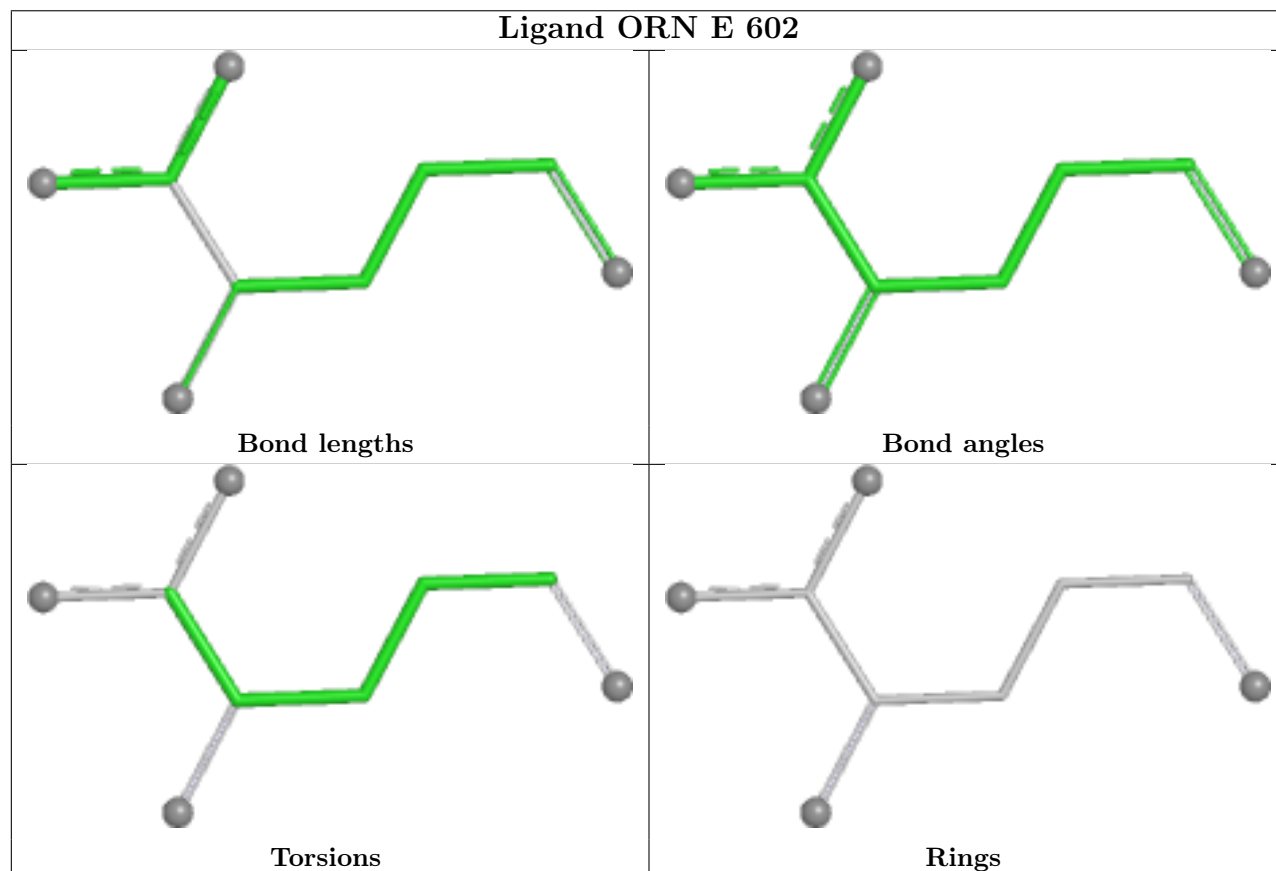
Ligand ORN D 602

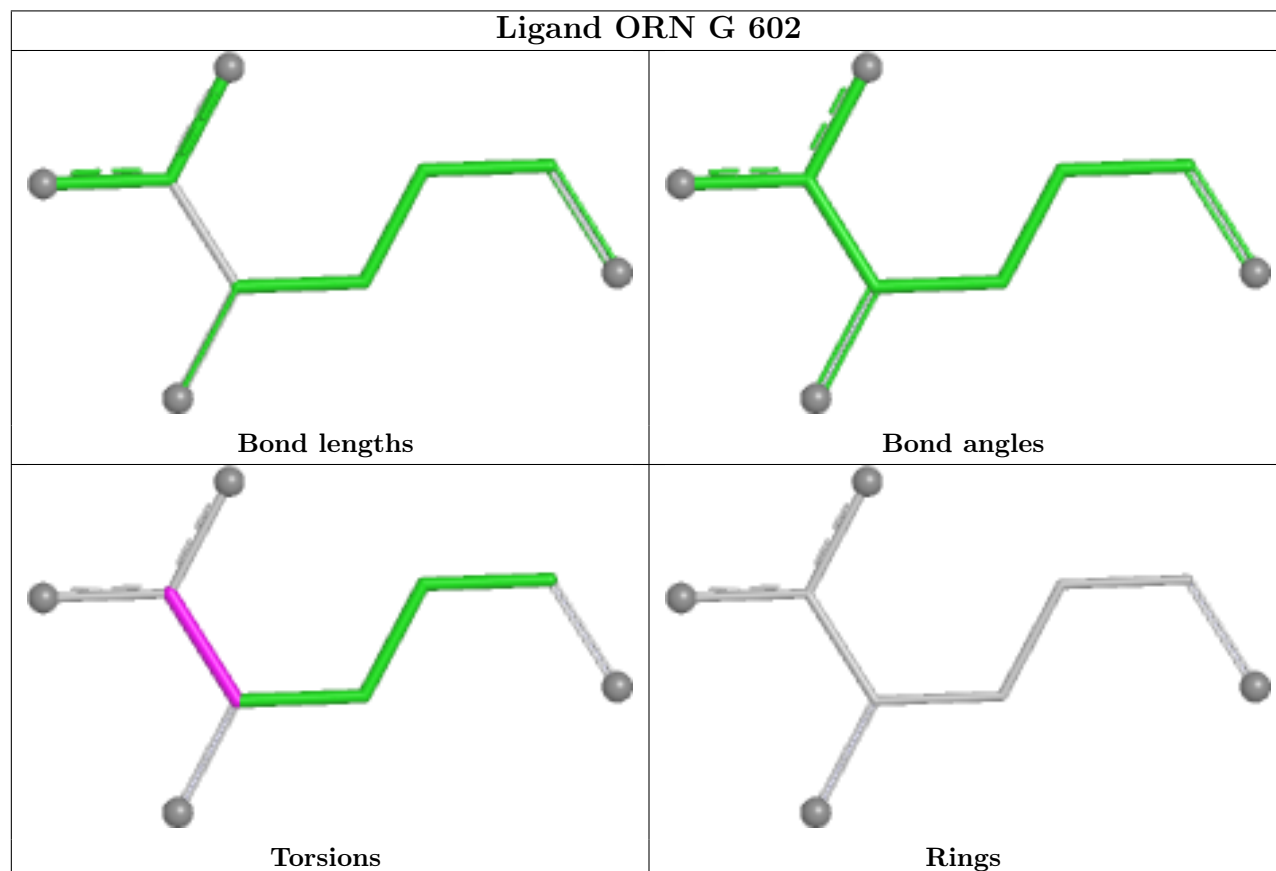
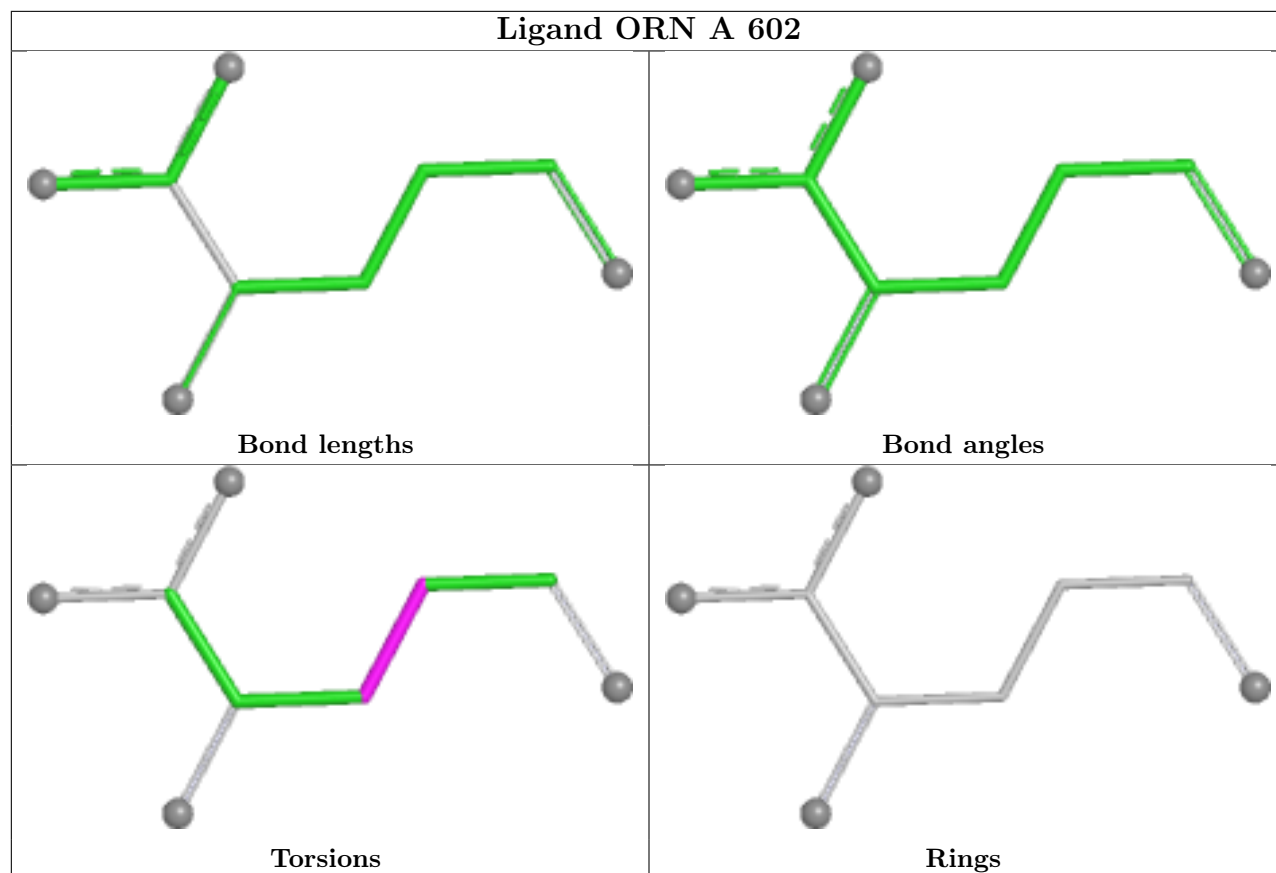


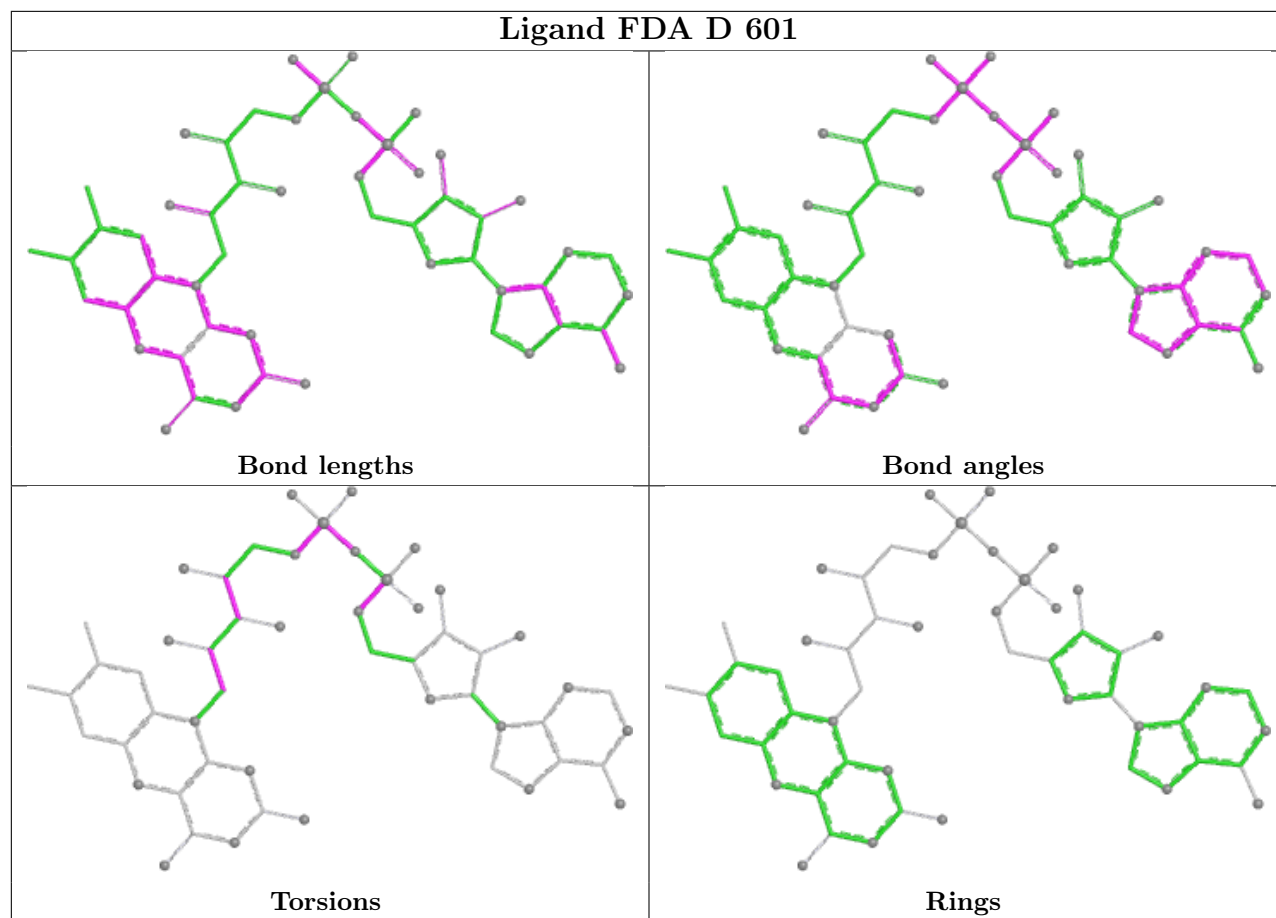
Ligand FDA A 601

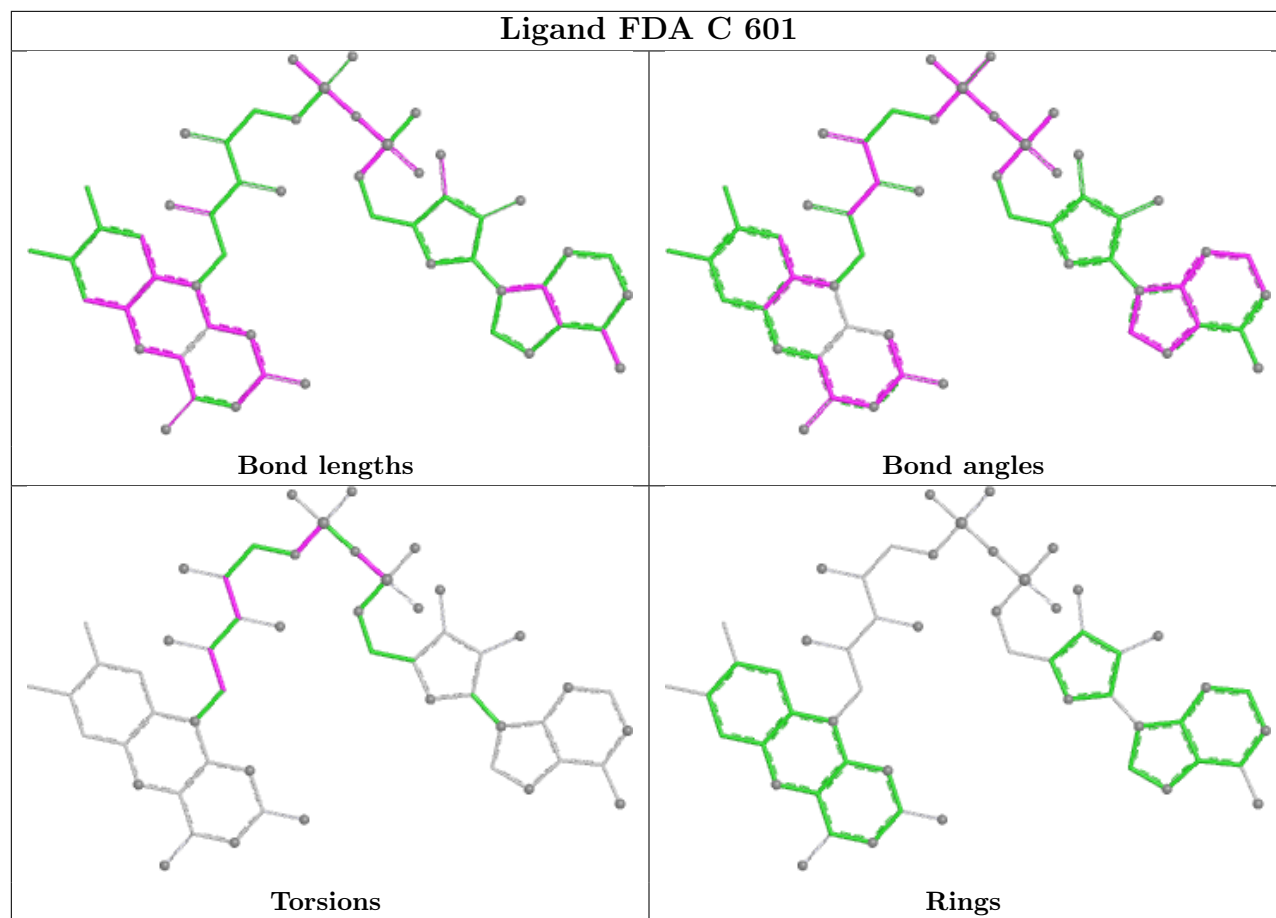


Ligand ORN E 602

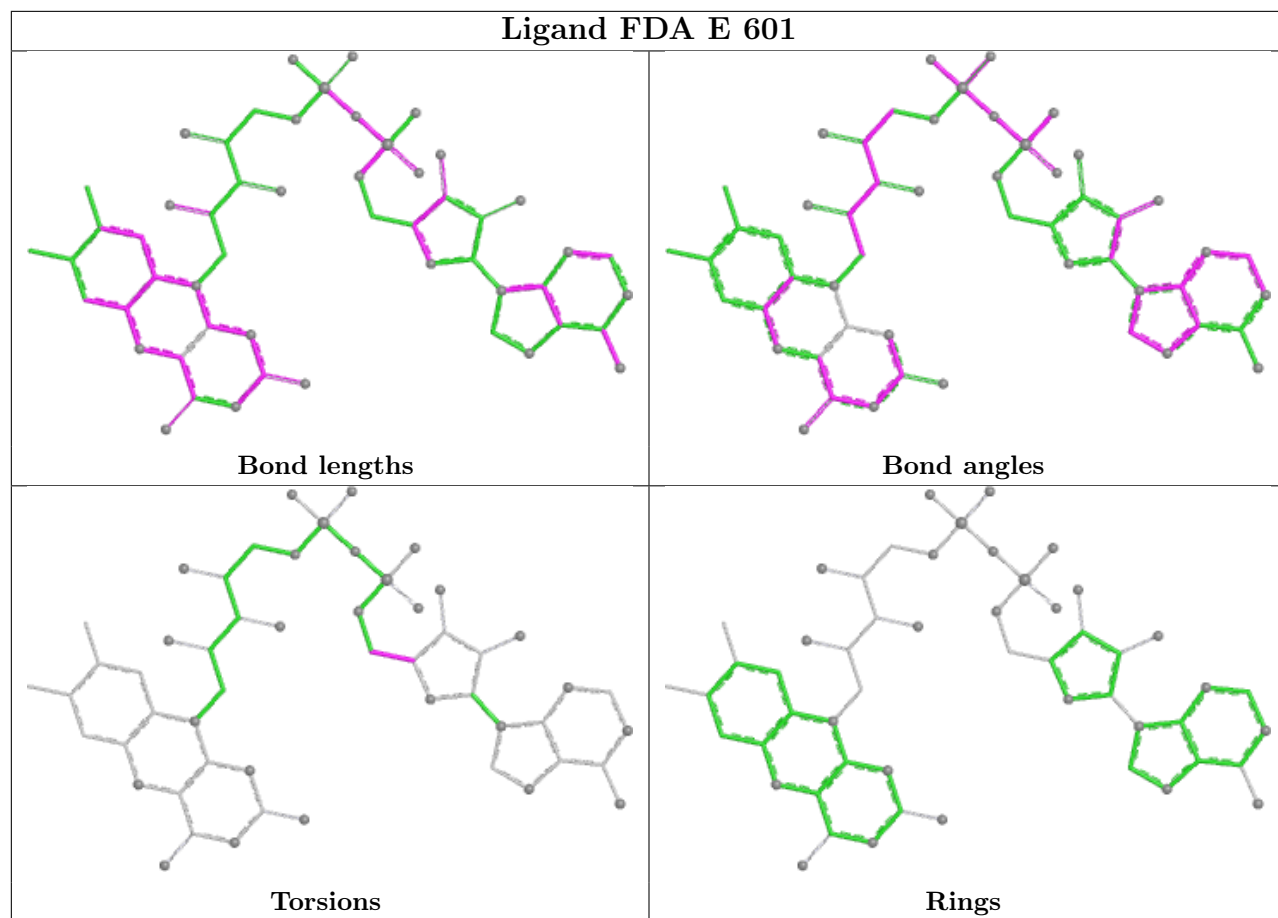


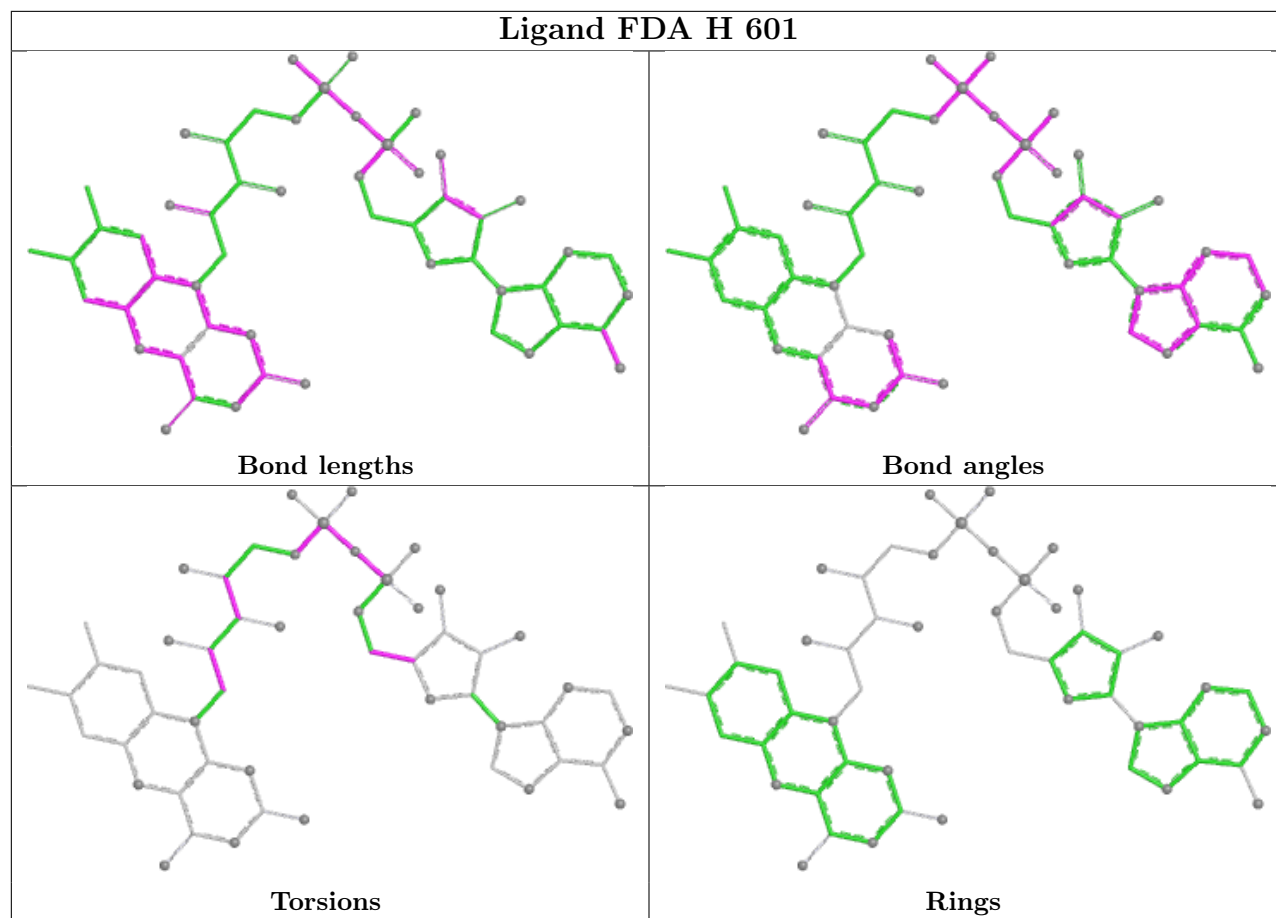


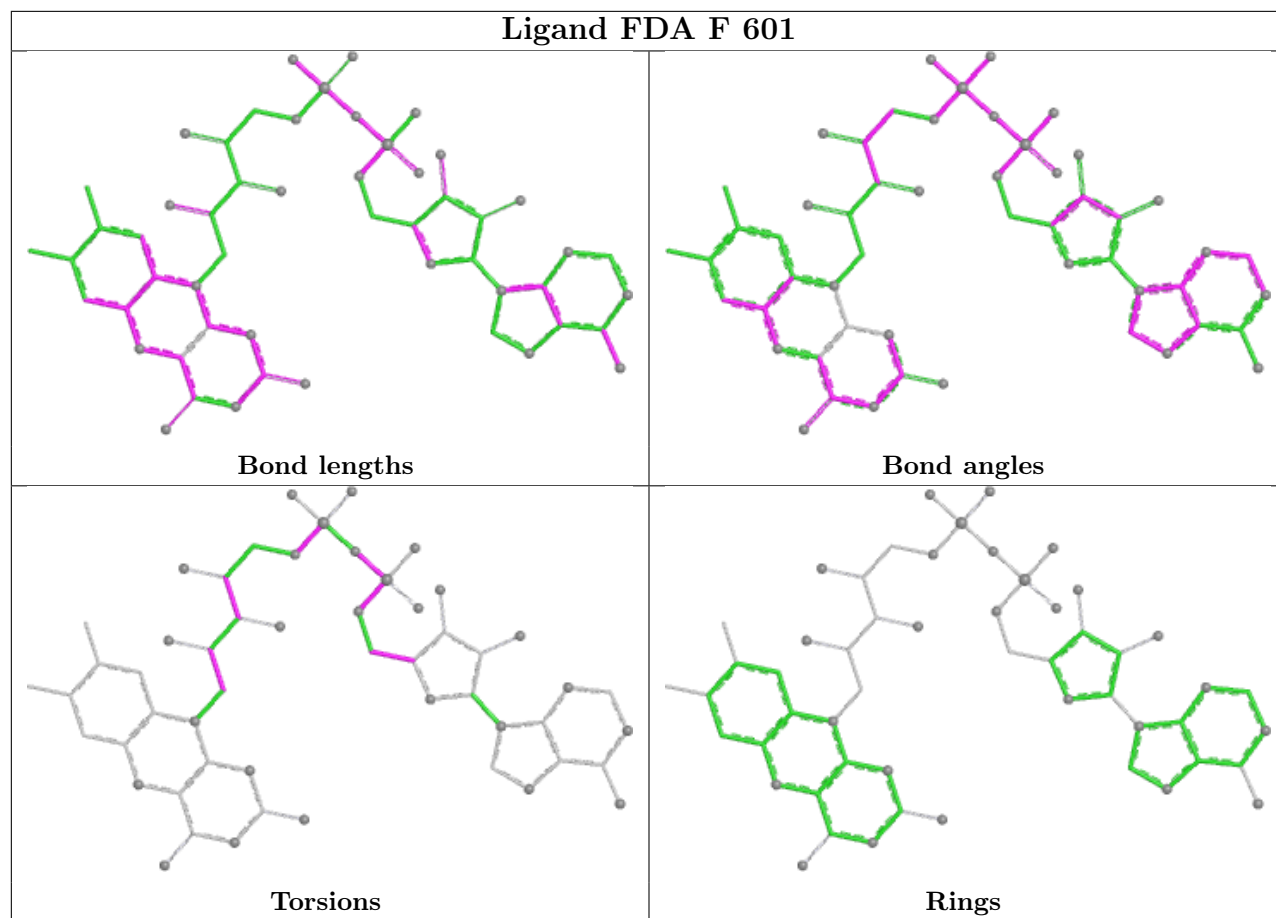


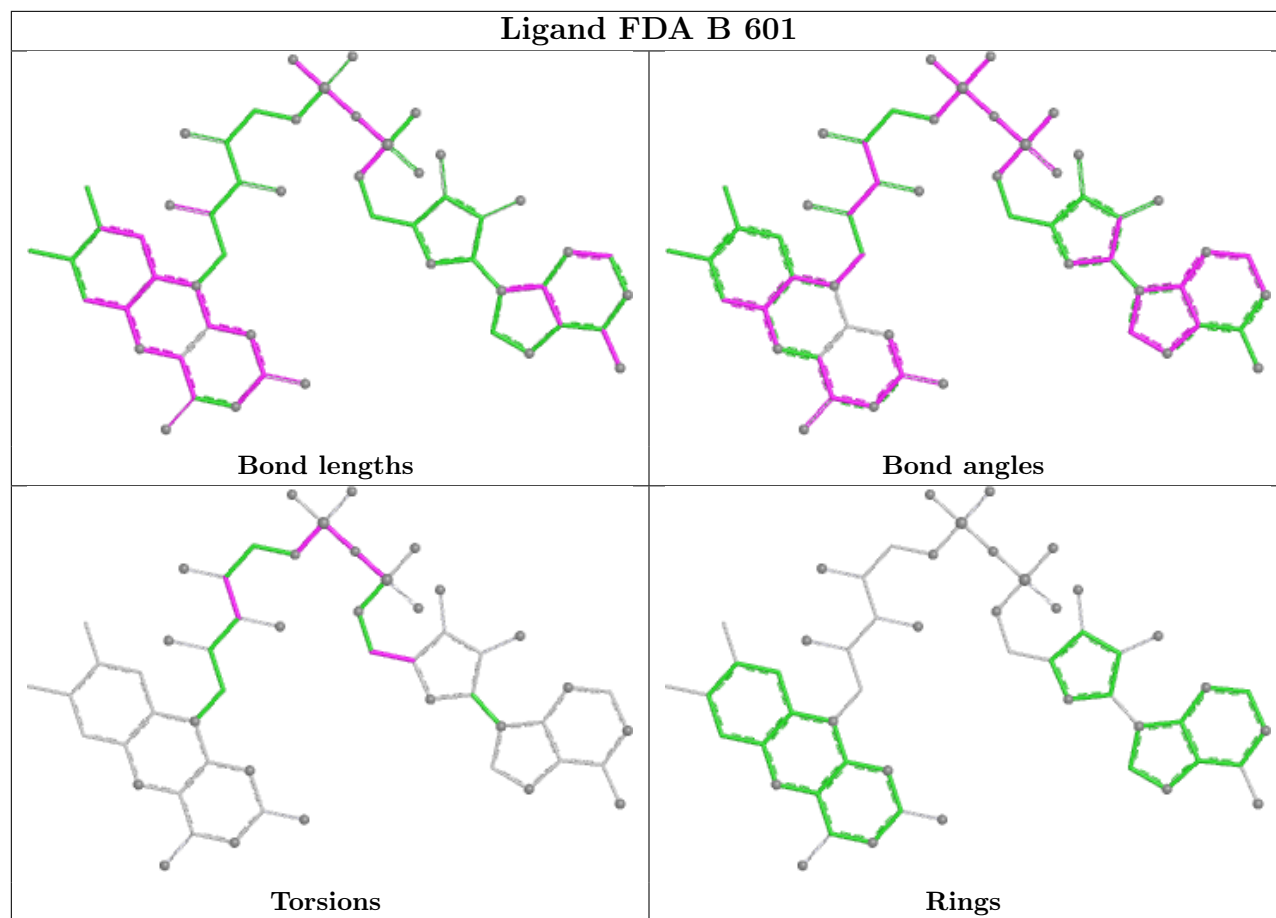


Ligand FDA E 601









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	440/494 (89%)	0.74	29 (6%) 24 22	28, 45, 68, 90	0
1	B	442/494 (89%)	0.77	25 (5%) 29 27	28, 46, 70, 100	0
1	C	433/494 (87%)	1.13	63 (14%) 6 5	31, 53, 85, 107	0
1	D	441/494 (89%)	1.27	79 (17%) 3 3	32, 54, 81, 112	0
1	E	441/494 (89%)	1.03	44 (9%) 12 11	30, 48, 75, 104	0
1	F	436/494 (88%)	1.74	140 (32%) 1 1	41, 69, 97, 111	0
1	G	440/494 (89%)	1.56	124 (28%) 1 1	37, 64, 105, 153	0
1	H	437/494 (88%)	1.51	104 (23%) 2 1	42, 65, 99, 115	0
All	All	3510/3952 (88%)	1.22	608 (17%) 4 3	28, 55, 91, 153	0

All (608) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	200	ALA	7.0
1	H	194	GLU	5.3
1	G	429	GLN	5.3
1	G	425	THR	5.1
1	D	488	GLU	5.0
1	G	183	VAL	5.0
1	G	174	GLY	5.0
1	E	393	LYS	5.0
1	F	488	GLU	4.8
1	E	181	SER	4.8
1	G	182	VAL	4.8
1	D	67	ASN	4.7
1	B	488	GLU	4.7
1	H	238	ALA	4.6
1	F	45	VAL	4.5
1	G	169	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	68	LYS	4.5
1	F	240	LEU	4.5
1	F	246	PRO	4.5
1	G	38	GLU	4.5
1	H	193	VAL	4.4
1	F	398	VAL	4.4
1	F	400	ALA	4.4
1	G	430	TRP	4.4
1	G	419	VAL	4.3
1	E	66	LEU	4.3
1	E	370	PRO	4.3
1	G	39	LEU	4.3
1	D	370	PRO	4.2
1	A	487	LEU	4.2
1	G	185	PHE	4.2
1	E	383	PRO	4.2
1	G	178	PRO	4.2
1	F	82	LEU	4.2
1	C	488	GLU	4.2
1	F	425	THR	4.1
1	F	268	ARG	4.1
1	F	430	TRP	4.1
1	F	32	ARG	4.1
1	D	363	THR	4.0
1	F	397	GLU	4.0
1	G	485	GLU	4.0
1	F	68	LYS	3.8
1	G	450	GLY	3.8
1	F	96	VAL	3.8
1	F	247	TYR	3.8
1	G	77	PRO	3.8
1	C	183	VAL	3.8
1	D	37	ASP	3.7
1	G	145	LEU	3.7
1	D	427	GLN	3.7
1	H	429	GLN	3.7
1	C	64	PRO	3.7
1	F	409	ARG	3.7
1	E	132	ILE	3.7
1	H	485	GLU	3.7
1	F	428	ASP	3.7
1	H	67	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	369	GLY	3.7
1	F	235	THR	3.7
1	B	393	LYS	3.7
1	A	62	LEU	3.6
1	G	35	PRO	3.6
1	G	180	SER	3.6
1	G	372	SER	3.6
1	G	417	SER	3.6
1	H	159	SER	3.6
1	H	178	PRO	3.6
1	A	138	SER	3.6
1	G	37	ASP	3.6
1	D	222	GLN	3.6
1	E	31	LEU	3.6
1	G	370	PRO	3.6
1	B	487	LEU	3.5
1	G	324	TYR	3.5
1	D	367	HIS	3.5
1	F	411	ALA	3.5
1	F	441	ASP	3.5
1	H	341	LEU	3.5
1	F	173	PRO	3.5
1	F	424	PRO	3.5
1	F	259	ALA	3.5
1	G	68	LYS	3.5
1	H	488	GLU	3.5
1	F	147	PHE	3.5
1	F	383	PRO	3.4
1	C	393	LYS	3.4
1	D	481	SER	3.4
1	G	447	SER	3.4
1	F	93	GLY	3.4
1	D	138	SER	3.4
1	F	238	ALA	3.4
1	C	67	ASN	3.4
1	D	371	GLN	3.4
1	H	66	LEU	3.4
1	D	244	SER	3.4
1	D	428	ASP	3.4
1	C	428	ASP	3.4
1	D	242	ASP	3.4
1	G	416	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	488	GLU	3.3
1	G	193	VAL	3.3
1	F	226	ILE	3.3
1	F	325	SER	3.3
1	G	486	GLN	3.3
1	F	125	LEU	3.3
1	F	401	LEU	3.3
1	H	383	PRO	3.3
1	H	40	HIS	3.3
1	E	179	SER	3.3
1	G	420	GLN	3.3
1	G	428	ASP	3.3
1	H	396	LEU	3.3
1	G	234	THR	3.3
1	C	180	SER	3.3
1	F	92	SER	3.3
1	H	164	TYR	3.3
1	H	199	SER	3.3
1	H	269	TYR	3.3
1	F	403	VAL	3.3
1	H	411	ALA	3.2
1	C	219	GLY	3.2
1	F	396	LEU	3.2
1	G	186	PHE	3.2
1	G	483	PHE	3.2
1	D	382	LYS	3.2
1	E	178	PRO	3.2
1	G	171	VAL	3.2
1	E	67	ASN	3.2
1	E	297	ASN	3.2
1	F	95	LEU	3.2
1	C	383	PRO	3.2
1	H	156	GLN	3.2
1	A	169	VAL	3.2
1	G	426	GLY	3.2
1	E	293	ASN	3.2
1	F	427	GLN	3.2
1	F	179	SER	3.1
1	F	341	LEU	3.1
1	G	222	GLN	3.1
1	G	369	GLY	3.1
1	H	307	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	451	ILE	3.1
1	E	180	SER	3.1
1	C	410	ASN	3.1
1	G	398	VAL	3.1
1	F	442	PRO	3.1
1	H	145	LEU	3.1
1	G	452	TRP	3.1
1	A	368	HIS	3.1
1	F	351	GLN	3.1
1	B	188	VAL	3.1
1	H	64	PRO	3.1
1	D	487	LEU	3.1
1	H	430	TRP	3.0
1	H	179	SER	3.0
1	F	158	PHE	3.0
1	H	98	GLY	3.0
1	H	196	GLY	3.0
1	H	200	ALA	3.0
1	D	217	PRO	3.0
1	A	317	LEU	3.0
1	B	68	LYS	3.0
1	F	178	PRO	3.0
1	H	31	LEU	3.0
1	C	79	ILE	3.0
1	F	164	TYR	3.0
1	F	90	TRP	3.0
1	H	165	GLY	3.0
1	F	44	CYS	3.0
1	E	182	VAL	3.0
1	H	82	LEU	3.0
1	F	54	ILE	3.0
1	C	204	ARG	3.0
1	A	67	ASN	3.0
1	C	288	ASP	3.0
1	G	440	MET	3.0
1	G	449	ALA	2.9
1	G	45	VAL	2.9
1	G	445	VAL	2.9
1	D	87	GLN	2.9
1	H	36	GLN	2.9
1	G	172	ILE	2.9
1	C	450	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	261	ILE	2.9
1	D	181	SER	2.9
1	B	182	VAL	2.9
1	D	199	SER	2.9
1	G	56	ILE	2.9
1	G	211	GLY	2.8
1	C	173	PRO	2.8
1	C	112	LEU	2.8
1	G	487	LEU	2.8
1	E	105	PHE	2.8
1	G	400	ALA	2.8
1	A	485	GLU	2.8
1	F	80	CYS	2.8
1	H	198	ILE	2.8
1	H	451	ILE	2.8
1	D	243	LYS	2.8
1	F	288	ASP	2.8
1	D	204	ARG	2.8
1	F	476	GLY	2.8
1	H	219	GLY	2.8
1	B	330	GLU	2.8
1	H	294	GLU	2.8
1	F	100	LYS	2.8
1	G	79	ILE	2.8
1	D	93	GLY	2.8
1	H	102	GLN	2.8
1	H	486	GLN	2.8
1	C	66	LEU	2.8
1	D	43	LEU	2.8
1	G	411	ALA	2.8
1	G	188	VAL	2.8
1	F	461	HIS	2.8
1	D	174	GLY	2.8
1	G	218	SER	2.8
1	H	313	GLN	2.8
1	G	448	GLU	2.8
1	D	378	LEU	2.8
1	F	252	LEU	2.8
1	H	220	LEU	2.8
1	A	86	LYS	2.8
1	F	119	PHE	2.8
1	F	365	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	37	ASP	2.7
1	F	376	ILE	2.7
1	C	174	GLY	2.7
1	H	190	SER	2.7
1	D	178	PRO	2.7
1	F	485	GLU	2.7
1	G	422	LEU	2.7
1	H	378	LEU	2.7
1	F	193	VAL	2.7
1	G	198	ILE	2.7
1	H	410	ASN	2.7
1	H	197	GLU	2.7
1	E	328	ARG	2.7
1	F	39	LEU	2.7
1	G	321	ALA	2.7
1	B	301	VAL	2.7
1	G	292	VAL	2.7
1	A	418	LYS	2.7
1	F	233	CYS	2.7
1	H	239	LEU	2.7
1	F	200	ALA	2.7
1	F	340	TYR	2.7
1	E	470	VAL	2.7
1	G	382	LYS	2.7
1	G	481	SER	2.7
1	G	453	LEU	2.7
1	G	36	GLN	2.6
1	D	393	LYS	2.6
1	G	78	LYS	2.6
1	G	431	LYS	2.6
1	G	177	ASP	2.6
1	H	171	VAL	2.6
1	G	34	THR	2.6
1	H	201	ARG	2.6
1	E	176	SER	2.6
1	B	396	LEU	2.6
1	G	31	LEU	2.6
1	G	82	LEU	2.6
1	H	39	LEU	2.6
1	H	252	LEU	2.6
1	H	416	LEU	2.6
1	E	310	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	413	GLU	2.6
1	F	225	ARG	2.6
1	C	425	THR	2.6
1	D	193	VAL	2.6
1	A	33	SER	2.6
1	C	172	ILE	2.6
1	C	451	ILE	2.6
1	G	368	HIS	2.6
1	F	236	LEU	2.6
1	G	415	LEU	2.6
1	H	222	GLN	2.6
1	H	415	LEU	2.6
1	H	86	LYS	2.6
1	E	477	GLU	2.6
1	E	200	ALA	2.6
1	G	279	ARG	2.6
1	C	161	VAL	2.6
1	C	217	PRO	2.6
1	D	77	PRO	2.6
1	H	232	TYR	2.6
1	F	198	ILE	2.6
1	G	179	SER	2.6
1	D	368	HIS	2.6
1	G	371	GLN	2.6
1	H	382	LYS	2.6
1	C	448	GLU	2.6
1	F	38	GLU	2.6
1	F	366	GLU	2.6
1	D	44	CYS	2.6
1	D	183	VAL	2.6
1	D	224	PRO	2.6
1	G	173	PRO	2.6
1	H	221	PRO	2.6
1	H	365	VAL	2.6
1	B	272	SER	2.6
1	C	247	TYR	2.6
1	G	325	SER	2.6
1	H	367	HIS	2.6
1	G	444	LYS	2.6
1	G	328	ARG	2.5
1	D	238	ALA	2.5
1	F	472	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	242	ASP	2.5
1	G	323	ASN	2.5
1	D	426	GLY	2.5
1	H	426	GLY	2.5
1	D	185	PHE	2.5
1	G	421	HIS	2.5
1	H	208	ILE	2.5
1	H	308	SER	2.5
1	F	333	GLU	2.5
1	F	463	LEU	2.5
1	H	43	LEU	2.5
1	B	472	ALA	2.5
1	D	223	ASP	2.5
1	C	424	PRO	2.5
1	C	484	GLY	2.5
1	G	175	LYS	2.5
1	F	135	THR	2.5
1	D	218	SER	2.5
1	F	102	GLN	2.5
1	C	65	ARG	2.5
1	C	245	LYS	2.5
1	H	271	ASN	2.5
1	H	302	ASP	2.5
1	D	98	GLY	2.5
1	G	484	GLY	2.5
1	D	257	SER	2.5
1	D	365	VAL	2.5
1	A	43	LEU	2.5
1	G	52	LEU	2.5
1	D	444	LYS	2.5
1	C	160	ASP	2.5
1	D	399	ASP	2.5
1	F	50	ALA	2.5
1	E	64	PRO	2.5
1	G	442	PRO	2.5
1	H	80	CYS	2.4
1	E	419	VAL	2.4
1	G	291	PHE	2.4
1	D	247	TYR	2.4
1	F	374	MET	2.4
1	F	123	ASN	2.4
1	G	302	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	160	ASP	2.4
1	A	178	PRO	2.4
1	H	349	GLU	2.4
1	H	424	PRO	2.4
1	H	226	ILE	2.4
1	F	382	LYS	2.4
1	G	320	LYS	2.4
1	C	220	LEU	2.4
1	F	220	LEU	2.4
1	C	242	ASP	2.4
1	E	156	GLN	2.4
1	G	184	ASP	2.4
1	H	32	ARG	2.4
1	D	369	GLY	2.4
1	F	172	ILE	2.4
1	G	208	ILE	2.4
1	H	168	VAL	2.4
1	F	283	MET	2.4
1	H	278	MET	2.4
1	D	66	LEU	2.4
1	D	422	LEU	2.4
1	G	341	LEU	2.4
1	G	433	HIS	2.4
1	F	364	ARG	2.4
1	G	65	ARG	2.4
1	H	336	TYR	2.4
1	D	160	ASP	2.4
1	H	37	ASP	2.4
1	F	426	GLY	2.4
1	C	382	LYS	2.4
1	H	34	THR	2.4
1	E	190	SER	2.4
1	C	185	PHE	2.4
1	C	188	VAL	2.4
1	H	182	VAL	2.4
1	C	39	LEU	2.4
1	C	463	LEU	2.4
1	F	422	LEU	2.4
1	G	43	LEU	2.4
1	H	112	LEU	2.4
1	E	368	HIS	2.4
1	A	488	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	485	GLU	2.4
1	F	394	GLU	2.4
1	G	334	GLU	2.4
1	A	428	ASP	2.3
1	G	424	PRO	2.3
1	H	97	PRO	2.3
1	H	358	PRO	2.3
1	C	320	LYS	2.3
1	F	449	ALA	2.3
1	F	234	THR	2.3
1	B	380	SER	2.3
1	D	198	ILE	2.3
1	F	47	PHE	2.3
1	F	182	VAL	2.3
1	G	152	ARG	2.3
1	H	263	HIS	2.3
1	F	487	LEU	2.3
1	F	86	LYS	2.3
1	F	241	LYS	2.3
1	H	243	LYS	2.3
1	D	455	GLY	2.3
1	G	165	GLY	2.3
1	G	214	ALA	2.3
1	H	89	ALA	2.3
1	F	190	SER	2.3
1	D	227	ILE	2.3
1	F	227	ILE	2.3
1	F	335	ILE	2.3
1	H	79	ILE	2.3
1	C	486	GLN	2.3
1	D	349	GLU	2.3
1	E	296	PHE	2.3
1	F	169	VAL	2.3
1	H	398	VAL	2.3
1	D	252	LEU	2.3
1	A	369	GLY	2.3
1	D	484	GLY	2.3
1	E	472	ALA	2.3
1	B	235	THR	2.3
1	F	33	SER	2.3
1	F	446	SER	2.3
1	B	227	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	210	ILE	2.3
1	D	182	VAL	2.3
1	F	168	VAL	2.3
1	H	162	VAL	2.3
1	H	487	LEU	2.3
1	D	173	PRO	2.3
1	F	165	GLY	2.3
1	G	150	TYR	2.3
1	F	34	THR	2.3
1	A	179	SER	2.3
1	G	190	SER	2.3
1	F	36	GLN	2.3
1	F	87	GLN	2.3
1	F	197	GLU	2.3
1	F	222	GLN	2.3
1	G	243	LYS	2.3
1	G	482	ILE	2.3
1	F	331	LEU	2.2
1	G	463	LEU	2.2
1	F	358	PRO	2.2
1	C	426	GLY	2.2
1	G	201	ARG	2.2
1	F	61	ALA	2.2
1	A	486	GLN	2.2
1	D	36	GLN	2.2
1	H	195	THR	2.2
1	G	181	SER	2.2
1	G	199	SER	2.2
1	G	443	SER	2.2
1	E	243	LYS	2.2
1	B	261	ILE	2.2
1	F	362	ILE	2.2
1	C	171	VAL	2.2
1	C	317	LEU	2.2
1	D	438	VAL	2.2
1	E	487	LEU	2.2
1	F	188	VAL	2.2
1	C	37	ASP	2.2
1	G	299	GLU	2.2
1	H	167	GLU	2.2
1	D	309	ALA	2.2
1	E	241	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	310	ALA	2.2
1	D	469	SER	2.2
1	F	407	TYR	2.2
1	H	466	SER	2.2
1	C	131	LEU	2.2
1	A	171	VAL	2.2
1	C	445	VAL	2.2
1	F	373	ARG	2.2
1	C	77	PRO	2.2
1	F	77	PRO	2.2
1	F	97	PRO	2.2
1	F	46	GLY	2.2
1	G	44	CYS	2.2
1	C	40	HIS	2.2
1	C	485	GLU	2.2
1	A	286	SER	2.2
1	D	372	SER	2.2
1	F	187	THR	2.2
1	F	310	ALA	2.2
1	B	210	ILE	2.2
1	D	220	LEU	2.2
1	E	106	ILE	2.2
1	E	65	ARG	2.2
1	H	422	LEU	2.2
1	F	319	ASP	2.2
1	D	397	GLU	2.2
1	E	486	GLN	2.2
1	G	93	GLY	2.2
1	B	315	SER	2.2
1	C	176	SER	2.2
1	C	218	SER	2.2
1	D	464	SER	2.2
1	E	325	SER	2.2
1	F	138	SER	2.2
1	F	254	SER	2.2
1	F	395	THR	2.2
1	E	340	TYR	2.1
1	F	122	LEU	2.1
1	G	66	LEU	2.1
1	H	62	LEU	2.1
1	H	261	ILE	2.1
1	C	162	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	169	VAL	2.1
1	C	441	ASP	2.1
1	F	410	ASN	2.1
1	G	207	VAL	2.1
1	B	379	LYS	2.1
1	C	68	LYS	2.1
1	D	170	GLU	2.1
1	F	237	PRO	2.1
1	C	377	HIS	2.1
1	A	425	THR	2.1
1	D	325	SER	2.1
1	H	274	THR	2.1
1	H	191	ARG	2.1
1	B	249	ILE	2.1
1	C	239	LEU	2.1
1	F	431	LYS	2.1
1	G	42	LEU	2.1
1	G	451	ILE	2.1
1	A	136	ASN	2.1
1	F	399	ASP	2.1
1	H	399	ASP	2.1
1	A	188	VAL	2.1
1	B	36	GLN	2.1
1	F	35	PRO	2.1
1	H	35	PRO	2.1
1	C	459	ARG	2.1
1	D	364	ARG	2.1
1	D	395	THR	2.1
1	E	364	ARG	2.1
1	G	423	ARG	2.1
1	A	200	ALA	2.1
1	C	310	ALA	2.1
1	D	179	SER	2.1
1	F	51	SER	2.1
1	F	181	SER	2.1
1	H	361	LYS	2.1
1	E	131	LEU	2.1
1	H	467	LEU	2.1
1	B	428	ASP	2.1
1	G	408	ASN	2.1
1	C	36	GLN	2.1
1	F	157	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	188	VAL	2.1
1	G	246	PRO	2.1
1	H	158	PHE	2.1
1	A	181	SER	2.1
1	A	417	SER	2.1
1	F	213	THR	2.1
1	G	322	THR	2.1
1	E	194	GLU	2.1
1	A	433	HIS	2.1
1	C	31	LEU	2.1
1	E	317	LEU	2.1
1	F	43	LEU	2.1
1	D	302	ASP	2.1
1	H	305	TYR	2.1
1	G	212	GLY	2.1
1	F	153	TRP	2.1
1	F	360	ARG	2.1
1	D	306	SER	2.0
1	E	110	ALA	2.0
1	A	248	ASN	2.0
1	D	240	LEU	2.0
1	D	396	LEU	2.0
1	D	468	LEU	2.0
1	F	239	LEU	2.0
1	F	453	LEU	2.0
1	C	482	ILE	2.0
1	G	335	ILE	2.0
1	C	442	PRO	2.0
1	B	327	VAL	2.0
1	B	459	ARG	2.0
1	D	476	GLY	2.0
1	G	455	GLY	2.0
1	H	393	LYS	2.0
1	D	413	GLU	2.0
1	G	244	SER	2.0
1	H	92	SER	2.0
1	H	405	THR	2.0
1	F	31	LEU	2.0
1	A	198	ILE	2.0
1	B	103	ILE	2.0
1	F	152	ARG	2.0
1	H	65	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	303	LYS	2.0
1	F	320	LYS	2.0
1	G	205	LYS	2.0
1	H	303	LYS	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](#)

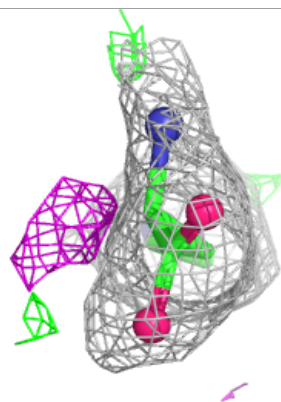
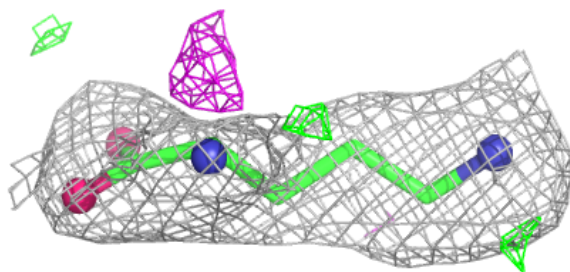
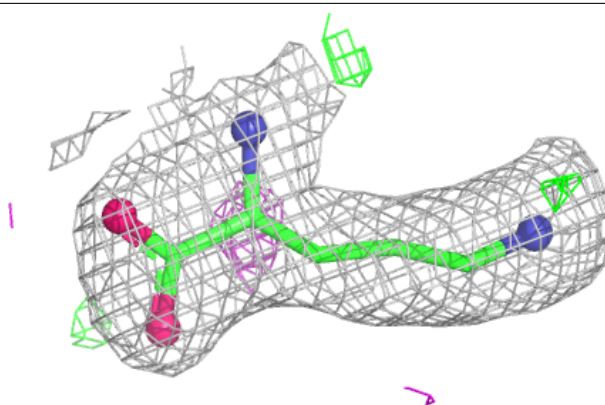
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D	602	9/9	0.88	0.15	34,43,47,48	0
2	FDA	H	601	53/53	0.89	0.13	43,57,70,81	0
2	FDA	F	601	53/53	0.89	0.14	47,65,82,85	0
3	ORN	E	602	9/9	0.91	0.11	27,44,50,52	0
3	ORN	G	602	9/9	0.91	0.10	30,37,44,47	0
3	ORN	B	602	9/9	0.92	0.12	35,40,46,48	0
2	FDA	D	601	53/53	0.92	0.11	34,48,55,56	0
2	FDA	E	601	53/53	0.93	0.10	21,37,47,60	0
2	FDA	C	601	53/53	0.93	0.10	22,46,59,60	0
2	FDA	G	601	53/53	0.93	0.11	37,54,65,67	0
2	FDA	B	601	53/53	0.93	0.10	29,41,50,54	0
3	ORN	H	602	9/9	0.93	0.09	37,44,51,52	0
2	FDA	A	601	53/53	0.94	0.10	24,40,53,59	0
3	ORN	A	602	9/9	0.96	0.07	23,34,40,40	0

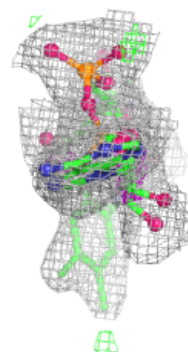
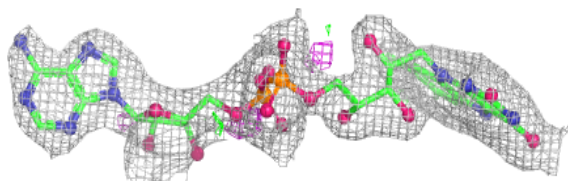
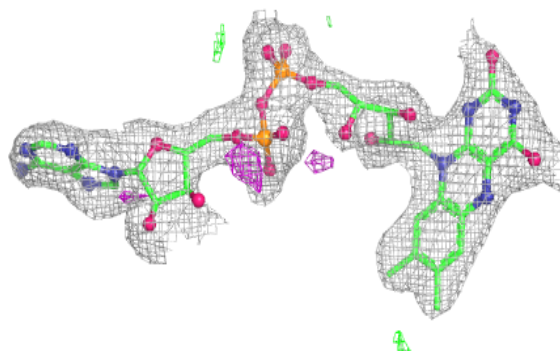
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ORN 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)

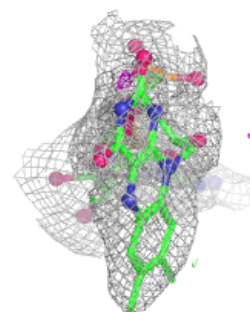
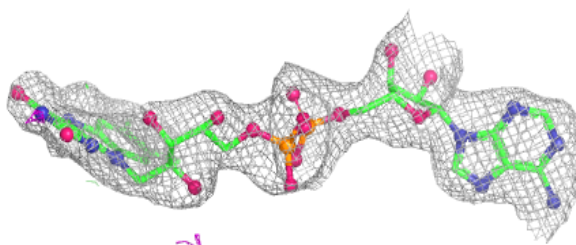
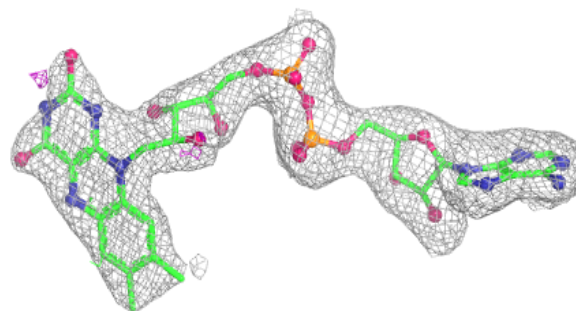
**Electron density around FDA H 601:**

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

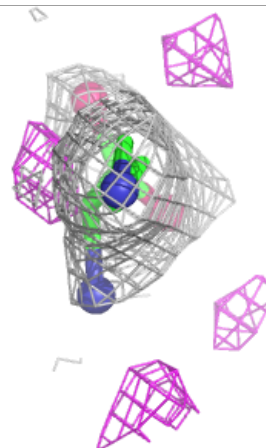
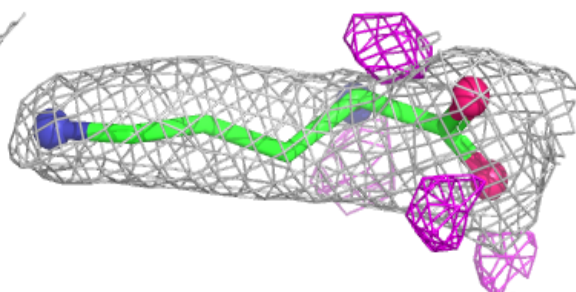
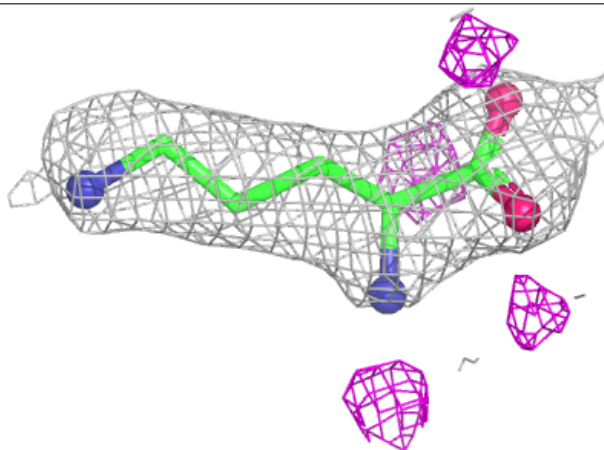


Electron density around FDA F 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

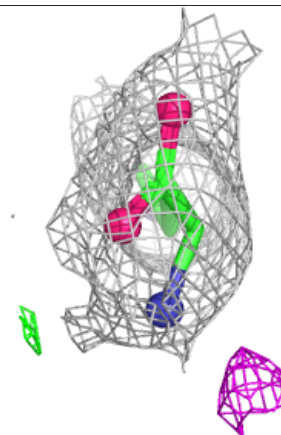
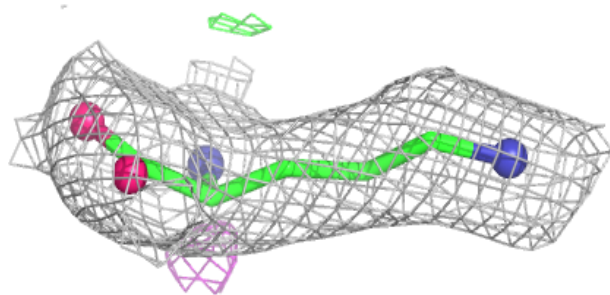
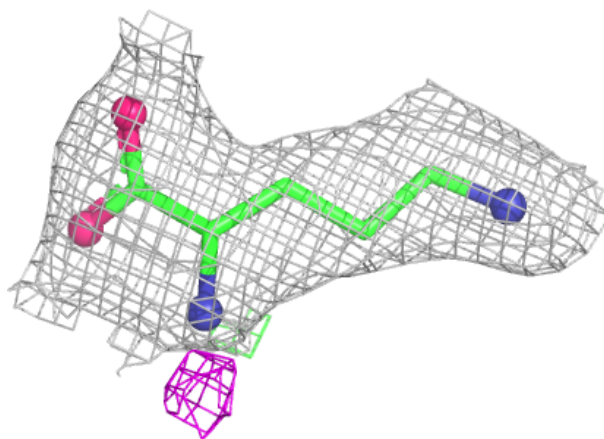
**Electron density around ORN E 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

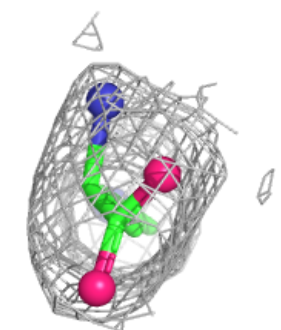
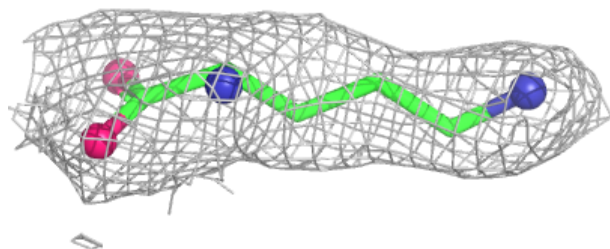
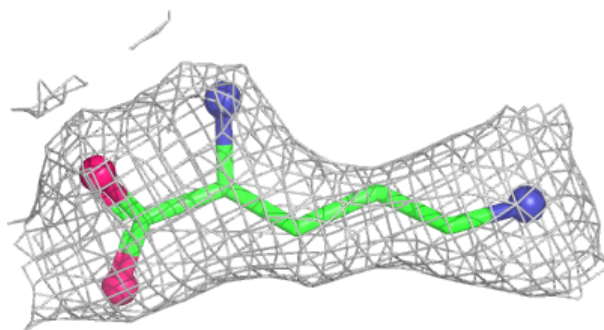


Electron density around ORN G 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

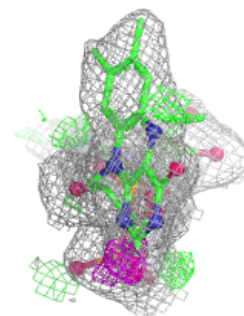
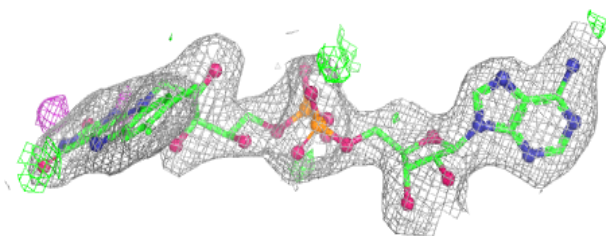
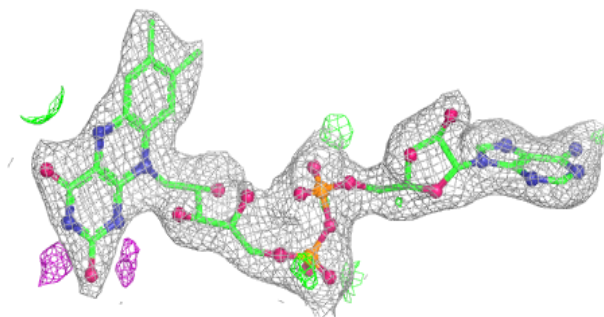
**Electron density around ORN B 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

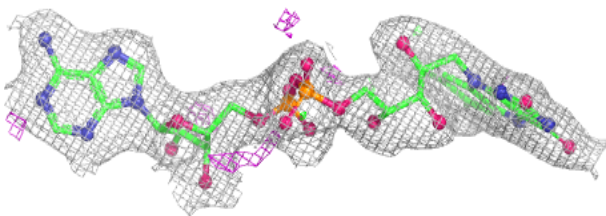
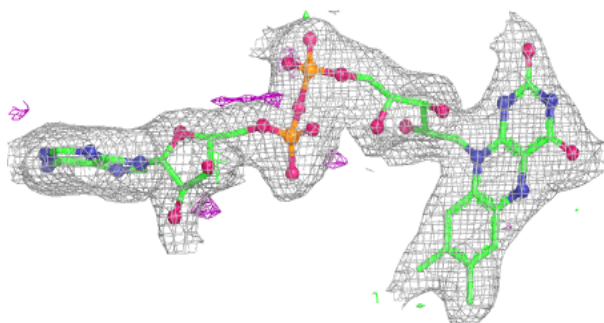


Electron density around FDA D 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

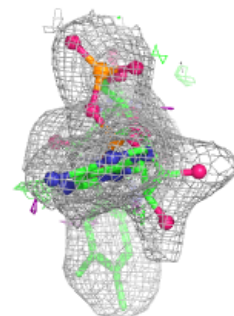
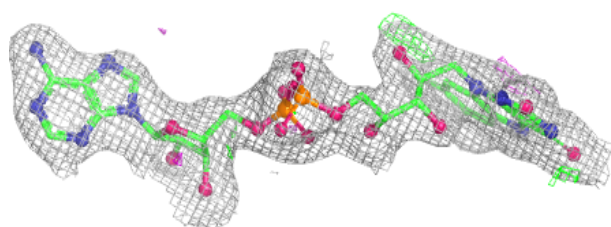
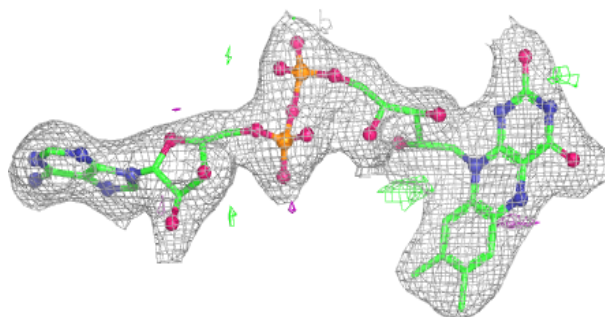
**Electron density around FDA E 601:**

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

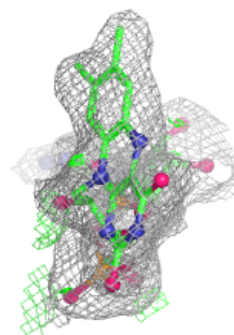
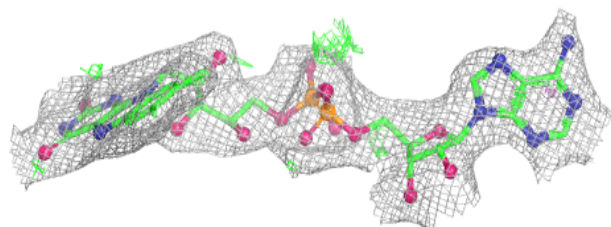
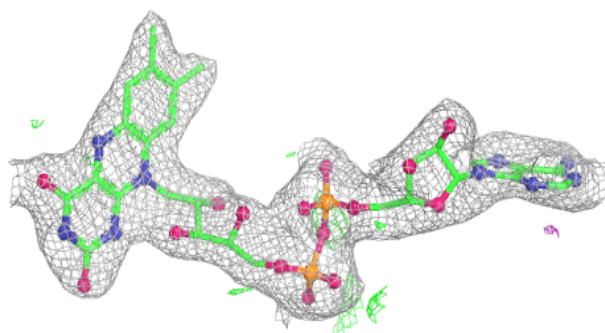


Electron density around FDA C 601:

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

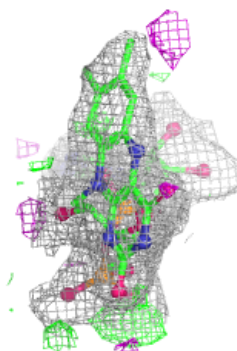
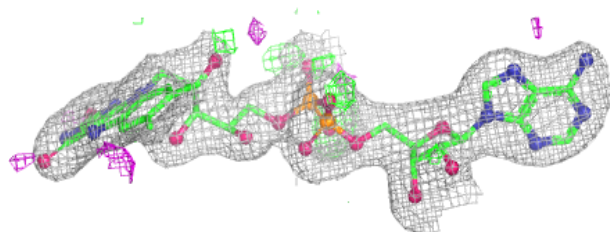
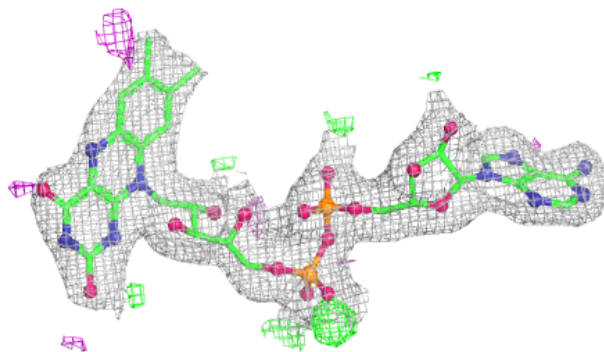
**Electron density around FDA G 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

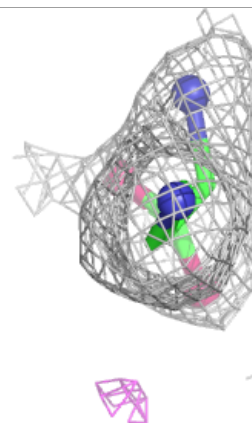
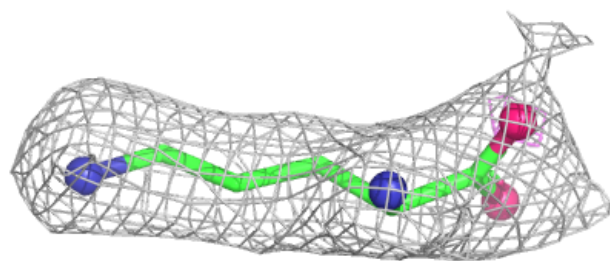
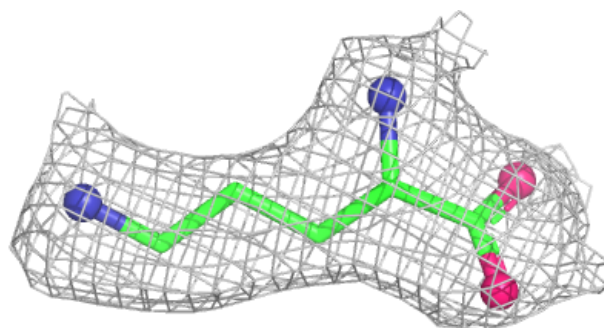


Electron density around FDA B 601:

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

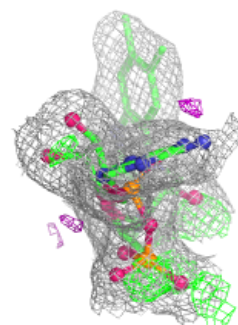
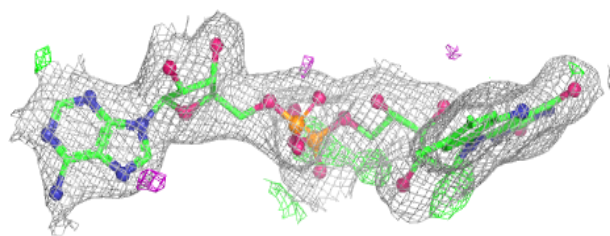
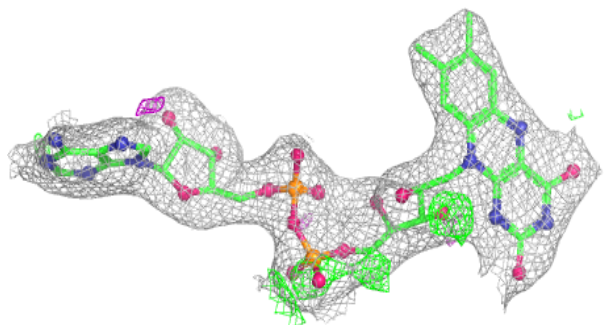
**Electron density around ORN H 602:**

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

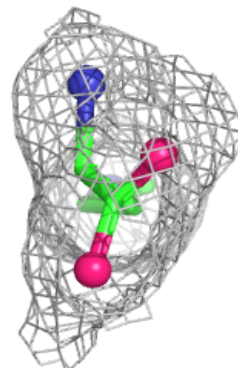
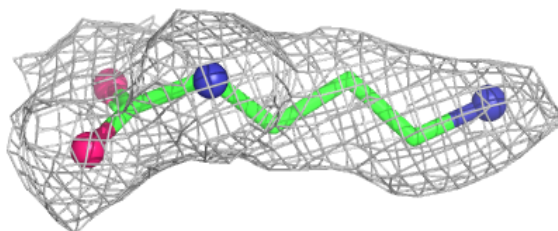
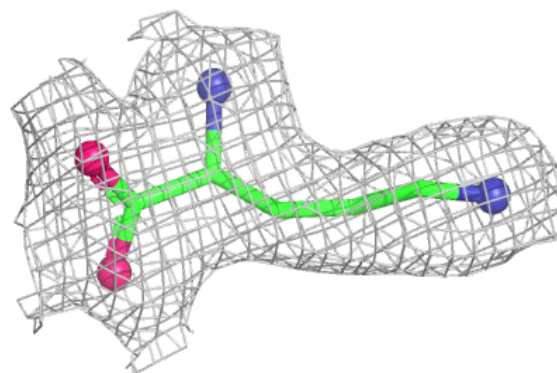


Electron density around FDA A 601:

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

**Electron density around ORN 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.