Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 11:27 PM EDT

PDB ID	:	6X0K
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:

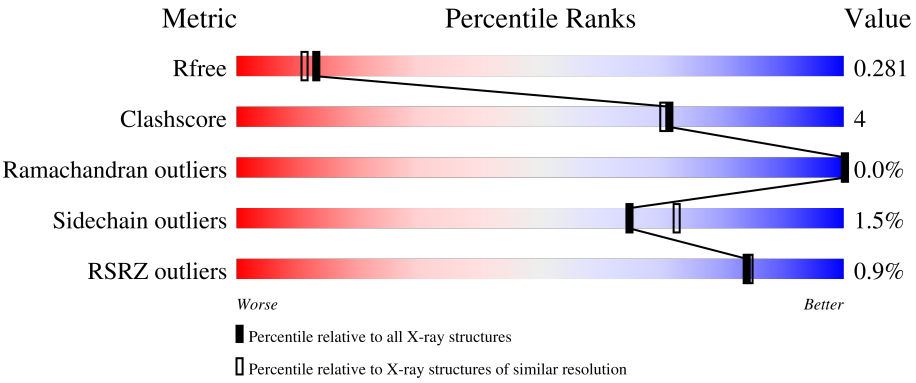
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.23 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}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (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 <=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	81% 8% 11%
1	B	494	83% 6% 11%
1	C	494	.% 80% 7% 12%
1	D	494	.% 81% 9% 11%
1	E	494	78% 11% 11%

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Mol	Chain	Length	Quality of chain
1	F	494	2% 77% 12% 12%
1	G	494	2% 78% 11% 11%
1	H	494	2% 80% 8% 12%

2 Entry composition (i)

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
E	12	HIS	-	expression tag	UNP E9QYP0
E	13	HIS	-	expression tag	UNP E9QYP0
E	14	HIS	-	expression tag	UNP E9QYP0
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
E	21	LEU	-	expression tag	UNP E9QYP0
E	22	VAL	-	expression tag	UNP E9QYP0
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
G	19	SER	-	expression tag	UNP E9QYP0
G	20	GLY	-	expression tag	UNP E9QYP0

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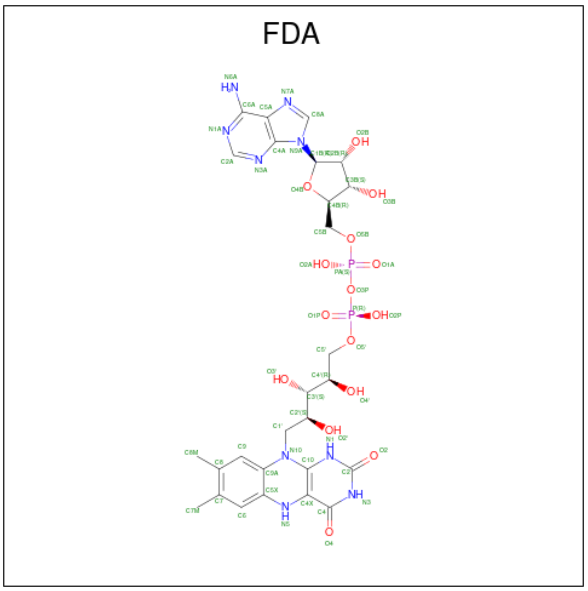
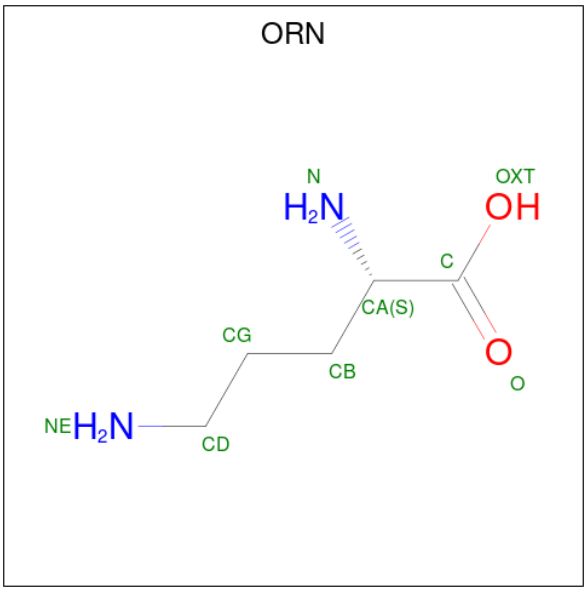
Chain	Residue	Modelled	Actual	Comment	Reference
G	21	LEU	-	expression tag	UNP E9QYP0
G	22	VAL	-	expression tag	UNP E9QYP0
G	23	PRO	-	expression tag	UNP E9QYP0
G	24	ARG	-	expression tag	UNP E9QYP0
G	25	GLY	-	expression tag	UNP E9QYP0
G	26	SER	-	expression tag	UNP E9QYP0
G	27	HIS	-	expression tag	UNP E9QYP0
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 (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

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

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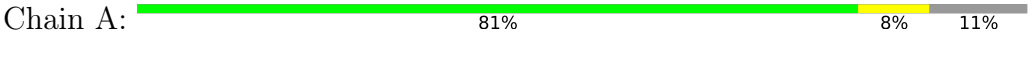
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	29	Total O 29 29	0	0
4	H	33	Total O 33 33	0	0

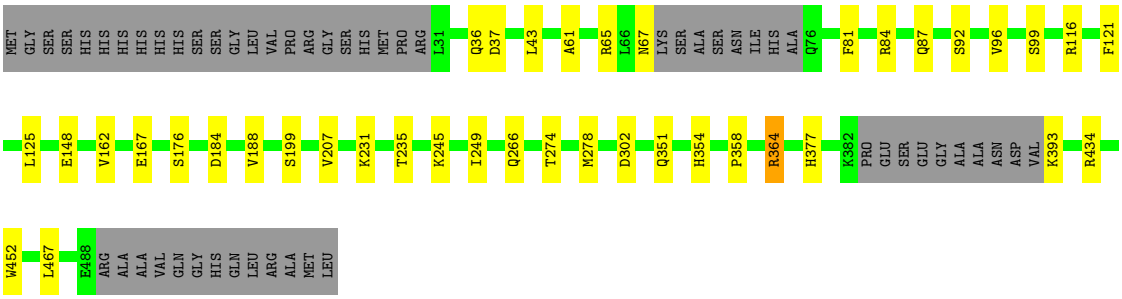
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

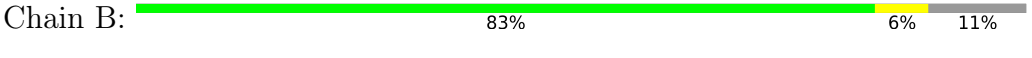
Chain A:

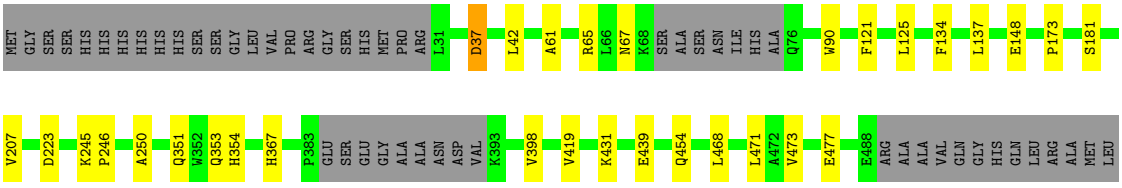




• Molecule 1: L-ornithine N(5)-monooxygenase

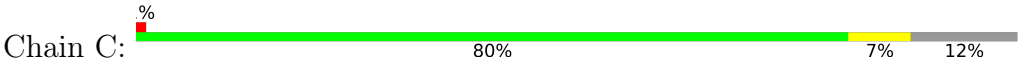
Chain B:

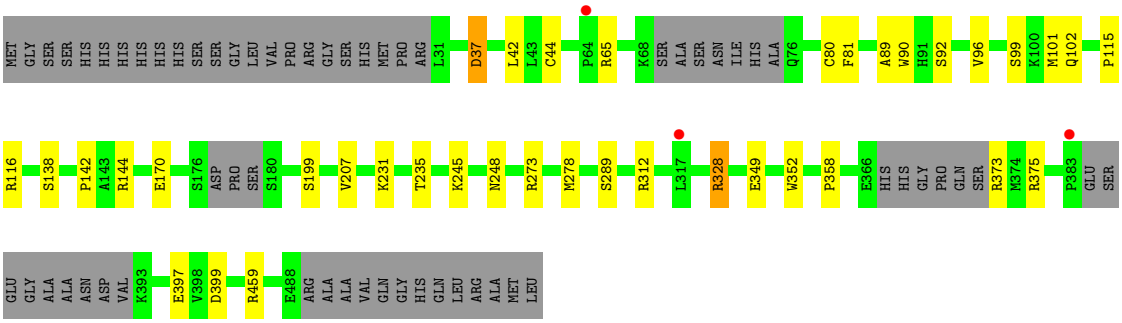




• Molecule 1: L-ornithine N(5)-monooxygenase

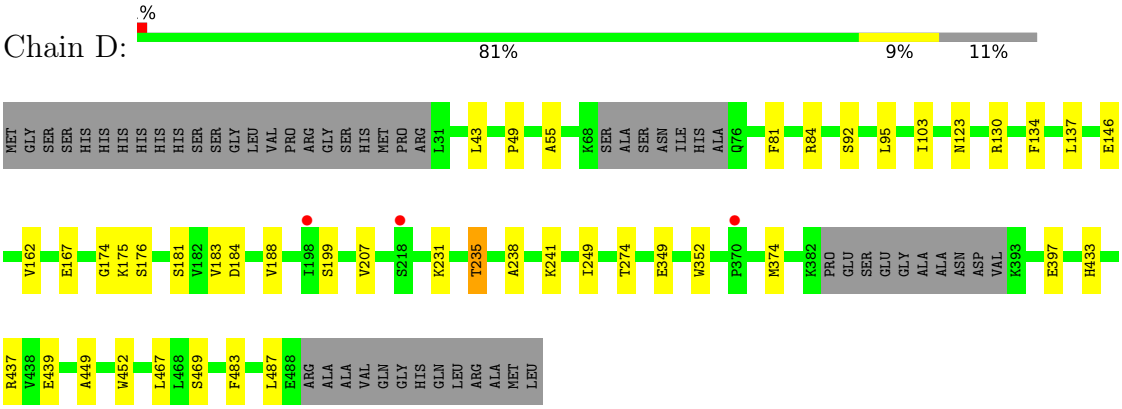
Chain C:





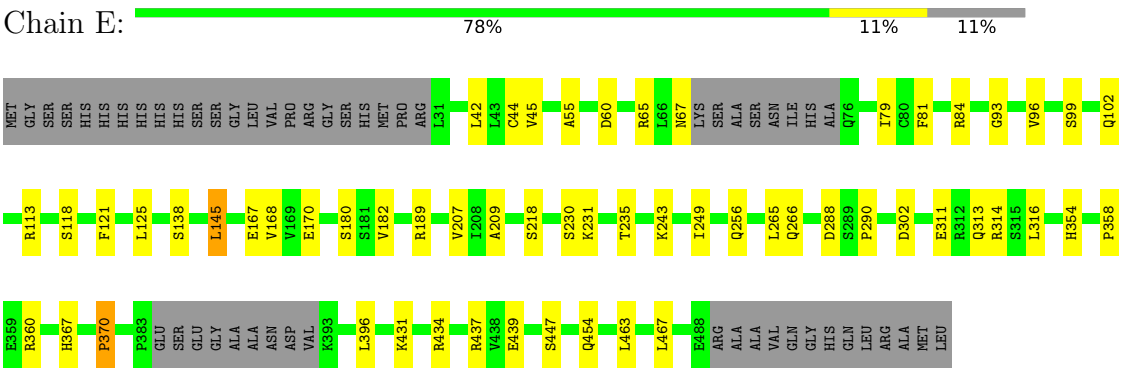
• Molecule 1: L-ornithine N(5)-monooxygenase

Chain D:



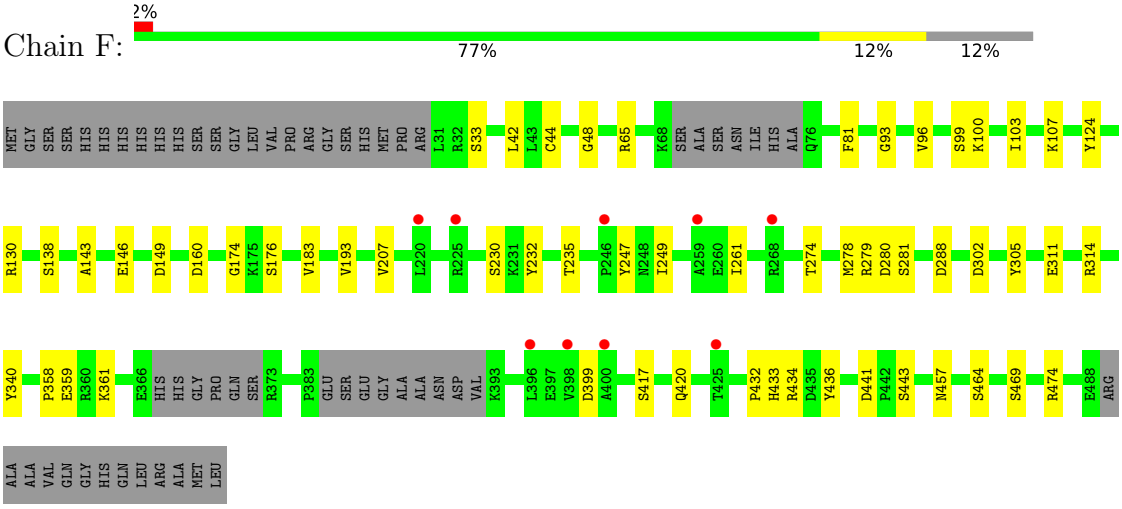
• Molecule 1: L-ornithine N(5)-monooxygenase

Chain E:



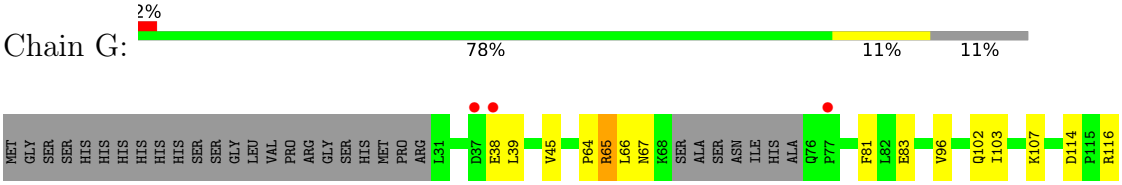
• Molecule 1: L-ornithine N(5)-monooxygenase

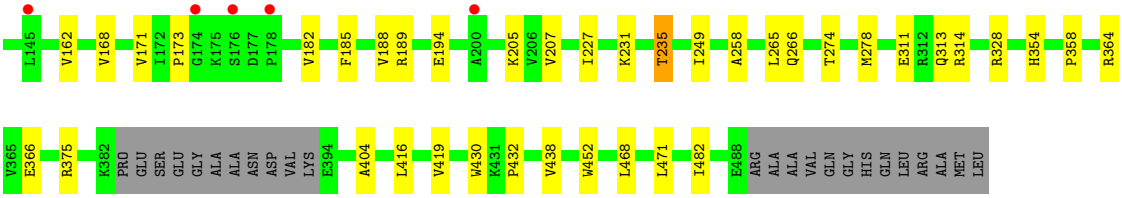
Chain F:



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

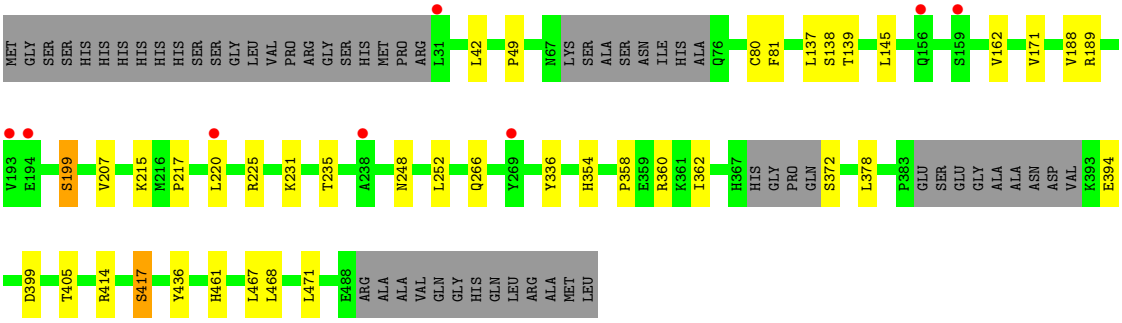
Chain G:





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

Chain H:



4 Data and refinement statistics (i)

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 – 2.23 106.61 – 2.23	Depositor EDS
% Data completeness (in resolution range)	97.0 (68.55-2.23) 97.0 (106.61-2.23)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.231 , 0.281 0.231 , 0.281	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)	0.28 , 21.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ORN, 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	0.48	0/3535	0.65	0/4789
1	B	0.48	0/3557	0.64	0/4816
1	C	0.43	0/3461	0.61	0/4686
1	D	0.40	0/3482	0.60	0/4729
1	E	0.43	0/3526	0.63	2/4783 (0.0%)
1	F	0.37	0/3417	0.54	0/4643
1	G	0.40	0/3493	0.57	0/4739
1	H	0.36	0/3430	0.55	0/4661
All	All	0.42	0/27901	0.60	2/37846 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	396	LEU	CA-CB-CG	6.57	130.40	115.30
1	E	145	LEU	CA-CB-CG	-5.71	102.16	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3460	0	3385	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3481	0	3426	17	0
1	C	3392	0	3314	19	0
1	D	3407	0	3281	25	0
1	E	3450	0	3355	33	0
1	F	3345	0	3213	29	0
1	G	3418	0	3311	30	0
1	H	3357	0	3217	22	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	191	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 (191) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:F:124:TYR:OH	1:F:149:ASP:OD2	2.19	0.58
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:B:90:TRP:HB3	1:B:148:GLU:HG3	1.89	0.55
1:E:45:VAL:HG22	1:E:168:VAL:HG21	1.89	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:175:LYS:NZ	1:D:181:SER:O	2.38	0.50
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: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:G:231:LYS:HB3	1:G:235:THR:HG1	1.76	0.49
1:H:231:LYS:O	1:H:235:THR:OG1	2.25	0.49
1:A:266:GLN:HG2	1:A:354:HIS:CE1	2.47	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:231:LYS:HB3	1:D:235:THR:HG1	1.81	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: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
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:C:373:ARG:HE	1:C:399:ASP:CG	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:E:145:LEU:O	1:E:145:LEU:HG	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:LEU:CD2	1:E:463:LEU:HG	2.50	0.41
1:E:96:VAL:O	1:E:99:SER:OG	2.23	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:E:42:LEU:O	1:E:79:ILE:HA	2.20	0.41
1:A:81:PHE:HB2	1:A:162:VAL:HG22	2.03	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: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:441:ASP:OD1	1:F:443:SER:OG	2.28	0.41
1:A:278:MET:HE2	1:A:278:MET:HB3	1.89	0.40
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: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 (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	434/494 (88%)	420 (97%)	14 (3%)	0	100	100
1	B	436/494 (88%)	425 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	47 53
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	374/433 (86%)	367 (98%)	7 (2%)	57 64
1	B	379/433 (88%)	376 (99%)	3 (1%)	81 87
1	C	364/433 (84%)	356 (98%)	8 (2%)	52 59
1	D	361/433 (83%)	359 (99%)	2 (1%)	86 90
1	E	371/433 (86%)	365 (98%)	6 (2%)	62 70
1	F	352/433 (81%)	347 (99%)	5 (1%)	67 74
1	G	363/433 (84%)	355 (98%)	8 (2%)	52 59
1	H	353/433 (82%)	348 (99%)	5 (1%)	67 74
All	All	2917/3464 (84%)	2873 (98%)	44 (2%)	65 72

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN

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Mol	Chain	Res	Type
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	138	SER
1	C	170	GLU
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	218	SER
1	E	313	GLN
1	E	367	HIS
1	F	138	SER
1	F	176	SER
1	F	193	VAL
1	F	235	THR
1	F	288	ASP
1	G	65	ARG
1	G	96	VAL
1	G	182	VAL
1	G	185	PHE
1	G	189	ARG
1	G	194	GLU
1	G	235	THR
1	G	313	GLN
1	H	80	CYS
1	H	138	SER
1	H	145	LEU
1	H	199	SER

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Mol	Chain	Res	Type
1	H	417	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	263	HIS
1	C	420	GLN
1	D	133	HIS
1	E	102	GLN
1	E	377	HIS
1	F	102	GLN
1	F	337	ASN
1	G	367	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\|>2$
2	FDA	C	601	-	52,58,58	2.75	21 (40%)	60,89,89	1.60	14 (23%)
2	FDA	A	601	-	52,58,58	2.71	21 (40%)	60,89,89	1.55	9 (15%)
2	FDA	E	601	-	52,58,58	2.80	24 (46%)	60,89,89	1.52	9 (15%)
3	ORN	A	602	-	7,8,8	0.91	0	8,9,9	0.77	0
3	ORN	G	602	-	7,8,8	0.78	0	8,9,9	1.14	0
3	ORN	D	602	-	7,8,8	0.73	0	8,9,9	1.21	1 (12%)
3	ORN	B	602	-	7,8,8	1.01	0	8,9,9	1.22	0
2	FDA	G	601	-	52,58,58	2.87	20 (38%)	60,89,89	1.44	7 (11%)
2	FDA	F	601	-	52,58,58	2.75	22 (42%)	60,89,89	1.61	12 (20%)
2	FDA	H	601	-	52,58,58	2.74	22 (42%)	60,89,89	1.62	12 (20%)
3	ORN	H	602	-	7,8,8	0.77	0	8,9,9	1.09	0
2	FDA	D	601	-	52,58,58	2.79	22 (42%)	60,89,89	1.54	11 (18%)
3	ORN	E	602	-	7,8,8	0.67	0	8,9,9	1.17	0
2	FDA	B	601	-	52,58,58	2.71	21 (40%)	60,89,89	1.73	16 (26%)

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	FDA	C	601	-	-	8/30/50/50	0/6/6/6
2	FDA	A	601	-	-	10/30/50/50	0/6/6/6
2	FDA	E	601	-	-	2/30/50/50	0/6/6/6
3	ORN	A	602	-	-	1/8/8/8	-
3	ORN	G	602	-	-	0/8/8/8	-
3	ORN	D	602	-	-	0/8/8/8	-
3	ORN	B	602	-	-	0/8/8/8	-
2	FDA	G	601	-	-	8/30/50/50	0/6/6/6
2	FDA	F	601	-	-	15/30/50/50	0/6/6/6
2	FDA	H	601	-	-	13/30/50/50	0/6/6/6
3	ORN	H	602	-	-	0/8/8/8	-
2	FDA	D	601	-	-	10/30/50/50	0/6/6/6
3	ORN	E	602	-	-	0/8/8/8	-
2	FDA	B	601	-	-	8/30/50/50	0/6/6/6

All (173) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FDA	O4-C4	8.17	1.39	1.23
2	H	601	FDA	O4-C4	8.01	1.38	1.23
2	D	601	FDA	O2-C2	8.00	1.40	1.23
2	F	601	FDA	O4-C4	7.86	1.38	1.23
2	C	601	FDA	O4-C4	7.75	1.38	1.23
2	C	601	FDA	O2-C2	7.73	1.39	1.23
2	D	601	FDA	O4-C4	7.71	1.38	1.23
2	B	601	FDA	O4-C4	7.63	1.38	1.23
2	G	601	FDA	O4-C4	7.50	1.37	1.23
2	E	601	FDA	O4-C4	7.49	1.37	1.23
2	H	601	FDA	O2-C2	7.44	1.39	1.23
2	F	601	FDA	O2-C2	7.40	1.38	1.23
2	G	601	FDA	O2-C2	7.40	1.38	1.23
2	B	601	FDA	O2-C2	7.38	1.38	1.23
2	E	601	FDA	O2-C2	7.22	1.38	1.23
2	A	601	FDA	O2-C2	7.14	1.38	1.23
2	G	601	FDA	C6-C5X	6.72	1.50	1.39
2	E	601	FDA	C6-C5X	6.58	1.49	1.39
2	E	601	FDA	C9-C9A	6.36	1.50	1.39
2	C	601	FDA	C6-C5X	6.29	1.49	1.39
2	F	601	FDA	C9-C9A	6.05	1.49	1.39
2	B	601	FDA	C6-C5X	6.04	1.48	1.39
2	G	601	FDA	C9-C9A	5.98	1.49	1.39
2	D	601	FDA	C9-C9A	5.98	1.49	1.39
2	H	601	FDA	C9-C9A	5.84	1.49	1.39
2	H	601	FDA	C6-C5X	5.78	1.48	1.39
2	F	601	FDA	C6-C5X	5.77	1.48	1.39
2	B	601	FDA	C9-C9A	5.76	1.49	1.39
2	D	601	FDA	C6-C5X	5.63	1.48	1.39
2	C	601	FDA	C9-C9A	5.55	1.48	1.39
2	G	601	FDA	C10-N1	5.47	1.47	1.37
2	A	601	FDA	C9-C9A	5.43	1.48	1.39
2	A	601	FDA	C6-C5X	5.19	1.47	1.39
2	D	601	FDA	C10-N1	5.08	1.46	1.37
2	G	601	FDA	C4X-N5	4.73	1.45	1.35
2	B	601	FDA	C4X-N5	4.66	1.45	1.35
2	F	601	FDA	C10-N1	4.59	1.45	1.37
2	A	601	FDA	C10-N1	4.58	1.45	1.37
2	A	601	FDA	C5X-C9A	-4.57	1.35	1.40
2	G	601	FDA	C2-N1	4.51	1.45	1.37
2	H	601	FDA	C10-N1	4.50	1.45	1.37
2	C	601	FDA	C2-N1	4.45	1.45	1.37
2	H	601	FDA	C4X-N5	4.31	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FDA	C4X-N5	4.30	1.45	1.35
2	A	601	FDA	C4X-N5	4.16	1.44	1.35
2	E	601	FDA	C10-N1	4.11	1.44	1.37
2	F	601	FDA	C2-N1	4.10	1.44	1.37
2	F	601	FDA	C4X-N5	4.09	1.44	1.35
2	B	601	FDA	C10-N1	4.09	1.44	1.37
2	C	601	FDA	C10-N1	4.08	1.44	1.37
2	D	601	FDA	C4X-N5	4.08	1.44	1.35
2	D	601	FDA	C2-N1	3.98	1.44	1.37
2	E	601	FDA	C2A-N3A	3.97	1.38	1.32
2	D	601	FDA	C5X-C9A	-3.95	1.36	1.40
2	E	601	FDA	C2B-C1B	-3.95	1.47	1.53
2	E	601	FDA	C4X-N5	3.94	1.44	1.35
2	A	601	FDA	C2B-C1B	-3.86	1.47	1.53
2	G	601	FDA	C5X-C9A	-3.84	1.36	1.40
2	H	601	FDA	C2-N1	3.78	1.44	1.37
2	H	601	FDA	C5X-C9A	-3.77	1.36	1.40
2	B	601	FDA	C2A-N3A	3.75	1.38	1.32
2	G	601	FDA	C2A-N3A	3.72	1.38	1.32
2	C	601	FDA	C2-N3	3.71	1.43	1.37
2	G	601	FDA	C5X-N5	3.70	1.46	1.39
2	G	601	FDA	C10-N10	3.69	1.45	1.38
2	C	601	FDA	C5X-N5	3.65	1.46	1.39
2	A	601	FDA	C2-N1	3.57	1.43	1.37
2	G	601	FDA	C4X-C4	3.54	1.51	1.42
2	H	601	FDA	C10-N10	3.52	1.44	1.38
2	A	601	FDA	C2A-N3A	3.51	1.37	1.32
2	E	601	FDA	C10-N10	3.50	1.44	1.38
2	A	601	FDA	C4X-C4	3.47	1.51	1.42
2	D	601	FDA	C10-N10	3.43	1.44	1.38
2	B	601	FDA	C10-N10	3.41	1.44	1.38
2	F	601	FDA	C10-N10	3.37	1.44	1.38
2	G	601	FDA	C9A-N10	3.35	1.47	1.41
2	B	601	FDA	C2-N1	3.33	1.43	1.37
2	C	601	FDA	C2B-C1B	-3.32	1.48	1.53
2	F	601	FDA	C2A-N3A	3.31	1.37	1.32
2	A	601	FDA	C10-N10	3.30	1.44	1.38
2	B	601	FDA	C9A-N10	3.28	1.46	1.41
2	E	601	FDA	C5X-N5	3.27	1.45	1.39
2	H	601	FDA	C5X-N5	3.26	1.45	1.39
2	F	601	FDA	C9A-N10	3.20	1.46	1.41
2	E	601	FDA	C2-N1	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	FDA	C4X-C4	3.15	1.50	1.42
2	F	601	FDA	C5X-C9A	-3.15	1.37	1.40
2	D	601	FDA	C9A-N10	3.14	1.46	1.41
2	A	601	FDA	C5X-N5	3.12	1.45	1.39
2	E	601	FDA	C9A-N10	3.11	1.46	1.41
2	D	601	FDA	C2B-C1B	-3.10	1.49	1.53
2	D	601	FDA	C2A-N3A	3.09	1.37	1.32
2	H	601	FDA	C2A-N3A	3.08	1.37	1.32
2	C	601	FDA	C2A-N3A	3.05	1.37	1.32
2	H	601	FDA	C9A-N10	3.05	1.46	1.41
2	D	601	FDA	C6A-N6A	3.04	1.45	1.34
2	F	601	FDA	C2-N3	3.02	1.42	1.37
2	F	601	FDA	C5X-N5	2.99	1.45	1.39
2	F	601	FDA	C6A-N6A	2.99	1.44	1.34
2	C	601	FDA	C4X-C4	2.97	1.50	1.42
2	E	601	FDA	C6A-N6A	2.97	1.44	1.34
2	H	601	FDA	C6A-N6A	2.97	1.44	1.34
2	D	601	FDA	C2-N3	2.95	1.42	1.37
2	E	601	FDA	C5X-C9A	-2.95	1.37	1.40
2	G	601	FDA	C2B-C1B	-2.92	1.49	1.53
2	B	601	FDA	C5X-N5	2.89	1.44	1.39
2	D	601	FDA	C5X-N5	2.89	1.44	1.39
2	B	601	FDA	C4X-C4	2.88	1.49	1.42
2	A	601	FDA	C6A-N6A	2.84	1.44	1.34
2	D	601	FDA	C4X-C4	2.84	1.49	1.42
2	G	601	FDA	C6A-N6A	2.83	1.44	1.34
2	H	601	FDA	C2-N3	2.83	1.42	1.37
2	C	601	FDA	C5X-C9A	-2.81	1.37	1.40
2	C	601	FDA	C9A-N10	2.81	1.46	1.41
2	C	601	FDA	C6A-N6A	2.81	1.44	1.34
2	E	601	FDA	C9-C8	2.81	1.43	1.39
2	A	601	FDA	C2-N3	2.81	1.42	1.37
2	B	601	FDA	C9-C8	2.78	1.43	1.39
2	H	601	FDA	C4X-C4	2.77	1.49	1.42
2	B	601	FDA	C2-N3	2.76	1.42	1.37
2	H	601	FDA	PA-O5B	-2.73	1.48	1.59
2	F	601	FDA	O2'-C2'	-2.73	1.37	1.43
2	A	601	FDA	PA-O5B	-2.71	1.48	1.59
2	C	601	FDA	PA-O5B	-2.70	1.48	1.59
2	F	601	FDA	O3B-C3B	-2.65	1.36	1.43
2	B	601	FDA	C2B-C1B	-2.64	1.49	1.53
2	F	601	FDA	PA-O5B	-2.61	1.48	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	FDA	C2B-C1B	-2.61	1.49	1.53
2	E	601	FDA	PA-O2A	-2.60	1.43	1.55
2	B	601	FDA	C5X-C9A	-2.57	1.37	1.40
2	E	601	FDA	C2-N3	2.52	1.41	1.37
2	E	601	FDA	O3B-C3B	-2.52	1.37	1.43
2	D	601	FDA	PA-O5B	-2.52	1.49	1.59
2	B	601	FDA	C6A-N6A	2.49	1.43	1.34
2	G	601	FDA	PA-O2A	-2.47	1.43	1.55
2	G	601	FDA	PA-O5B	-2.45	1.49	1.59
2	A	601	FDA	O3B-C3B	-2.43	1.37	1.43
2	E	601	FDA	C4X-C4	2.43	1.48	1.42
2	E	601	FDA	PA-O5B	-2.42	1.49	1.59
2	A	601	FDA	PA-O2A	-2.41	1.44	1.55
2	A	601	FDA	O2B-C2B	-2.41	1.37	1.43
2	H	601	FDA	C2B-C1B	-2.40	1.50	1.53
2	H	601	FDA	O3B-C3B	-2.40	1.37	1.43
2	H	601	FDA	P-O1P	2.39	1.59	1.50
2	C	601	FDA	O2'-C2'	-2.37	1.38	1.43
2	G	601	FDA	O3B-C3B	-2.36	1.37	1.43
2	D	601	FDA	O2'-C2'	-2.35	1.38	1.43
2	B	601	FDA	PA-O5B	-2.33	1.49	1.59
2	E	601	FDA	C3B-C4B	-2.31	1.47	1.53
2	D	601	FDA	PA-O2A	-2.30	1.44	1.55
2	B	601	FDA	P-O1P	2.27	1.59	1.50
2	C	601	FDA	P-O1P	2.27	1.58	1.50
2	G	601	FDA	C2-N3	2.25	1.41	1.37
2	F	601	FDA	PA-O2A	-2.24	1.44	1.55
2	D	601	FDA	P-O1P	2.24	1.58	1.50
2	H	601	FDA	O2'-C2'	-2.23	1.38	1.43
2	B	601	FDA	O2'-C2'	-2.21	1.38	1.43
2	H	601	FDA	PA-O2A	-2.19	1.45	1.55
2	C	601	FDA	C10-N10	2.19	1.42	1.38
2	D	601	FDA	O3B-C3B	-2.19	1.37	1.43
2	F	601	FDA	O4B-C4B	-2.19	1.40	1.45
2	D	601	FDA	O2B-C2B	-2.17	1.37	1.43
2	C	601	FDA	PA-O2A	-2.15	1.45	1.55
2	C	601	FDA	O3B-C3B	-2.15	1.37	1.43
2	A	601	FDA	O2'-C2'	-2.15	1.38	1.43
2	E	601	FDA	O4B-C4B	-2.13	1.40	1.45
2	F	601	FDA	P-O1P	2.12	1.58	1.50
2	E	601	FDA	O4B-C1B	-2.11	1.38	1.41
2	E	601	FDA	O2'-C2'	-2.08	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FDA	O3'-C3'	-2.07	1.38	1.43
2	B	601	FDA	O2B-C2B	-2.05	1.38	1.43
2	H	601	FDA	O3'-C3'	-2.04	1.38	1.43
2	G	601	FDA	O2'-C2'	-2.04	1.39	1.43

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	FDA	N3A-C2A-N1A	-5.54	120.02	128.68
2	H	601	FDA	N3A-C2A-N1A	-5.51	120.06	128.68
2	G	601	FDA	N3A-C2A-N1A	-5.40	120.24	128.68
2	F	601	FDA	N3A-C2A-N1A	-5.24	120.48	128.68
2	A	601	FDA	N3A-C2A-N1A	-5.07	120.76	128.68
2	B	601	FDA	N3A-C2A-N1A	-4.71	121.31	128.68
2	B	601	FDA	C4-N3-C2	-4.52	119.82	126.34
2	A	601	FDA	C4-N3-C2	-4.51	119.84	126.34
2	D	601	FDA	N3A-C2A-N1A	-4.48	121.68	128.68
2	E	601	FDA	C4-N3-C2	-4.44	119.94	126.34
2	H	601	FDA	C4-N3-C2	-4.29	120.15	126.34
2	E	601	FDA	N3A-C2A-N1A	-4.28	122.00	128.68
2	D	601	FDA	C4-N3-C2	-4.13	120.38	126.34
2	G	601	FDA	C4-N3-C2	-4.05	120.51	126.34
2	F	601	FDA	C4-N3-C2	-3.99	120.58	126.34
2	D	601	FDA	O4-C4-C4X	-3.97	118.15	127.24
2	B	601	FDA	O4-C4-C4X	-3.95	118.17	127.24
2	C	601	FDA	C4-N3-C2	-3.86	120.78	126.34
2	H	601	FDA	O4-C4-C4X	-3.84	118.43	127.24
2	C	601	FDA	O4-C4-C4X	-3.52	119.17	127.24
2	E	601	FDA	O4-C4-C4X	-3.38	119.49	127.24
2	H	601	FDA	O2A-PA-O5B	-3.29	92.47	107.75
2	B	601	FDA	O4B-C1B-C2B	-3.19	102.27	106.93
2	B	601	FDA	C4A-C5A-N7A	-3.14	106.12	109.40
2	A	601	FDA	N3-C2-N1	3.08	120.75	115.80
2	C	601	FDA	C4A-C5A-N7A	-3.01	106.26	109.40
2	F	601	FDA	O2A-PA-O5B	-2.97	93.96	107.75
2	A	601	FDA	O4-C4-C4X	-2.97	120.44	127.24
2	B	601	FDA	C1'-N10-C9A	2.96	125.44	120.51
2	G	601	FDA	O2A-PA-O5B	-2.95	94.03	107.75
2	F	601	FDA	O4-C4-C4X	-2.84	120.74	127.24
2	B	601	FDA	O2A-PA-O5B	-2.83	94.62	107.75
2	D	601	FDA	O2P-P-O5'	-2.82	94.67	107.75
2	H	601	FDA	O5'-P-O1P	2.78	119.92	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	FDA	C4A-C5A-N7A	-2.77	106.51	109.40
2	D	601	FDA	O5'-P-O1P	2.71	119.65	109.07
2	G	601	FDA	C4X-C4-N3	2.68	120.30	112.31
2	F	601	FDA	N3-C2-N1	2.66	120.08	115.80
2	D	601	FDA	O5B-PA-O1A	2.59	119.20	109.07
2	B	601	FDA	N3-C2-N1	2.59	119.96	115.80
2	H	601	FDA	O2P-P-O5'	-2.58	95.78	107.75
2	G	601	FDA	O4-C4-C4X	-2.57	121.34	127.24
2	D	601	FDA	C4X-C4-N3	2.56	119.94	112.31
2	C	601	FDA	C4'-C3'-C2'	2.54	118.64	113.36
2	B	601	FDA	C4X-C4-N3	2.54	119.86	112.31
2	B	601	FDA	C6-C5X-C9A	2.53	122.34	119.67
2	H	601	FDA	N3-C2-N1	2.53	119.86	115.80
2	C	601	FDA	O2A-PA-O5B	-2.52	96.04	107.75
2	E	601	FDA	N3-C2-N1	2.52	119.84	115.80
2	A	601	FDA	C9A-C5X-N5	2.48	122.88	119.56
2	G	601	FDA	N3-C2-N1	2.47	119.77	115.80
2	E	601	FDA	C4X-C4-N3	2.45	119.62	112.31
2	C	601	FDA	N3-C2-N1	2.45	119.75	115.80
2	H	601	FDA	C1B-N9A-C4A	-2.44	122.35	126.64
2	A	601	FDA	O2A-PA-O5B	-2.42	96.50	107.75
2	F	601	FDA	C4A-C5A-N7A	-2.38	106.92	109.40
2	H	601	FDA	C4X-C4-N3	2.38	119.39	112.31
2	B	601	FDA	O5'-P-O1P	2.36	118.28	109.07
2	B	601	FDA	O2P-P-O5'	-2.34	96.87	107.75
2	F	601	FDA	O5'-P-O1P	2.33	118.18	109.07
2	A	601	FDA	C4X-C4-N3	2.27	119.08	112.31
2	F	601	FDA	C9A-C5X-N5	2.25	122.57	119.56
2	D	601	FDA	O2A-PA-O5B	-2.25	97.32	107.75
2	C	601	FDA	O2-C2-N1	-2.23	117.61	121.82
3	D	602	ORN	CG-CB-CA	-2.23	106.16	113.35
2	F	601	FDA	C4X-C4-N3	2.23	118.94	112.31
2	B	601	FDA	C6-C5X-N5	-2.21	115.84	119.84
2	E	601	FDA	C1B-N9A-C4A	-2.20	122.77	126.64
2	A	601	FDA	O2-C2-N1	-2.19	117.69	121.82
2	F	601	FDA	C5'-C4'-C3'	2.19	116.43	112.20
2	B	601	FDA	O2-C2-N1	-2.19	117.69	121.82
2	D	601	FDA	O2A-PA-O1A	2.18	123.02	112.24
2	F	601	FDA	O5B-PA-O1A	2.17	117.56	109.07
2	C	601	FDA	C1B-N9A-C4A	-2.16	122.85	126.64
2	G	601	FDA	O5B-PA-O1A	2.15	117.46	109.07
2	A	601	FDA	O4B-C1B-C2B	-2.14	103.79	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	FDA	O4B-C1B-C2B	-2.11	103.84	106.93
2	F	601	FDA	C2B-C3B-C4B	2.11	106.75	102.64
2	H	601	FDA	C4A-C5A-N7A	-2.10	107.21	109.40
2	B	601	FDA	O2A-PA-O1A	2.10	122.60	112.24
2	D	601	FDA	C4A-C5A-N7A	-2.07	107.24	109.40
2	E	601	FDA	C9A-C5X-N5	2.07	122.33	119.56
2	C	601	FDA	C4X-C4-N3	2.06	118.45	112.31
2	C	601	FDA	O5'-P-O1P	2.05	117.07	109.07
2	C	601	FDA	C9-C9A-N10	-2.04	119.08	121.84
2	H	601	FDA	C2B-C3B-C4B	2.03	106.59	102.64
2	E	601	FDA	C4'-C3'-C2'	2.02	117.56	113.36
2	C	601	FDA	O4'-C4'-C3'	2.02	114.01	109.10
2	C	601	FDA	O5B-PA-O1A	2.02	116.94	109.07
2	H	601	FDA	O2-C2-N1	-2.01	118.02	121.82
2	B	601	FDA	P-O3P-PA	2.00	139.69	132.83

There are no chirality outliers.

All (75) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	D	601	FDA	C2'-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	E	601	FDA	C3B-C4B-C5B-O5B
2	F	601	FDA	O3'-C3'-C4'-C5'
2	H	601	FDA	O3'-C3'-C4'-C5'
2	F	601	FDA	C2'-C3'-C4'-O4'
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	O4B-C4B-C5B-O5B
2	B	601	FDA	O3'-C3'-C4'-C5'
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	G	601	FDA	O3'-C3'-C4'-O4'
2	B	601	FDA	C2'-C3'-C4'-C5'
2	H	601	FDA	C2'-C3'-C4'-C5'
2	A	601	FDA	C5'-O5'-P-O3P
2	B	601	FDA	C5'-O5'-P-O3P
2	F	601	FDA	P-O3P-PA-O1A
2	A	601	FDA	C2'-C3'-C4'-C5'
2	F	601	FDA	C5'-O5'-P-O2P
2	H	601	FDA	C5'-O5'-P-O1P
2	H	601	FDA	C5'-O5'-P-O2P
2	G	601	FDA	N10-C1'-C2'-O2'
2	H	601	FDA	N10-C1'-C2'-O2'
2	F	601	FDA	O3'-C3'-C4'-O4'
2	A	601	FDA	P-O3P-PA-O2A
2	B	601	FDA	P-O3P-PA-O2A
2	H	601	FDA	PA-O3P-P-O1P
2	A	601	FDA	O3'-C3'-C4'-C5'
2	H	601	FDA	O3'-C3'-C4'-O4'
2	G	601	FDA	C2'-C3'-C4'-O4'
3	A	602	ORN	CA-CB-CG-CD
2	B	601	FDA	PA-O3P-P-O1P
2	C	601	FDA	O3'-C3'-C4'-O4'
2	A	601	FDA	O4'-C4'-C5'-O5'
2	B	601	FDA	O4B-C4B-C5B-O5B
2	D	601	FDA	C5'-O5'-P-O3P
2	F	601	FDA	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
2	H	601	FDA	C5'-O5'-P-O3P
2	A	601	FDA	O4B-C4B-C5B-O5B
2	D	601	FDA	O4B-C4B-C5B-O5B
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	C	601	FDA	C5'-O5'-P-O1P
2	D	601	FDA	C5B-O5B-PA-O1A
2	C	601	FDA	O4B-C4B-C5B-O5B
2	G	601	FDA	O4B-C4B-C5B-O5B
2	H	601	FDA	C3B-C4B-C5B-O5B

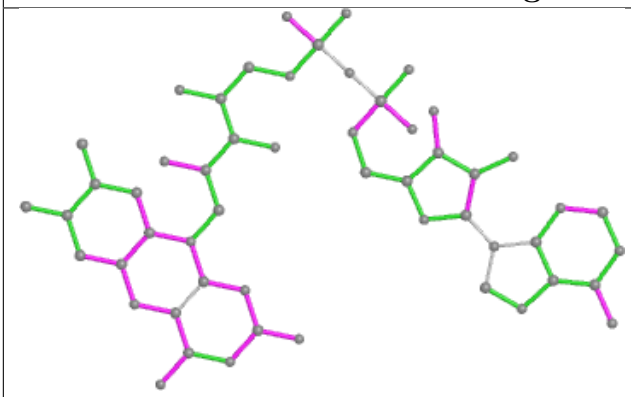
There are no ring outliers.

8 monomers are involved in 9 short contacts:

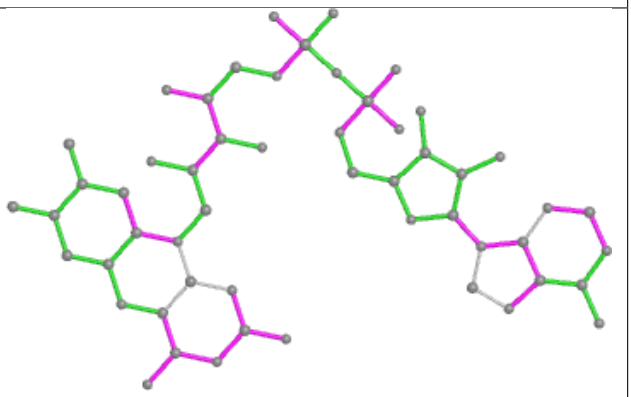
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	ORN	1	0
3	D	602	ORN	1	0
2	G	601	FDA	2	0
2	F	601	FDA	1	0
2	H	601	FDA	1	0
3	H	602	ORN	1	0
2	D	601	FDA	1	0
3	E	602	ORN	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

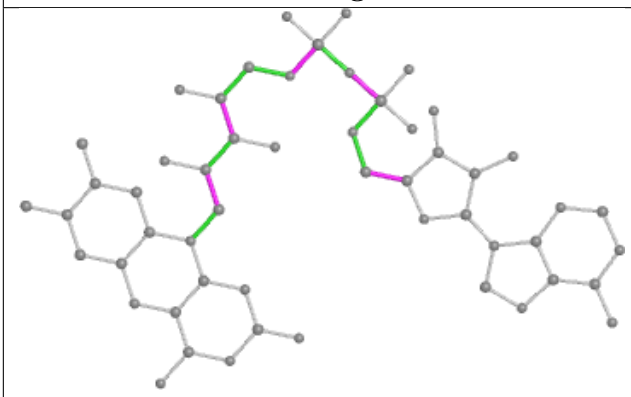
Ligand FDA C 601



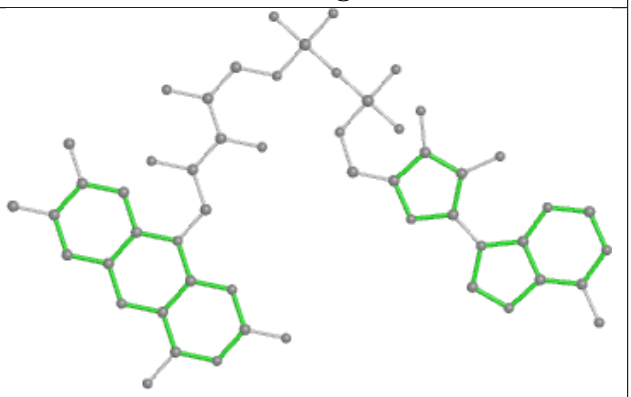
Bond lengths



Bond angles

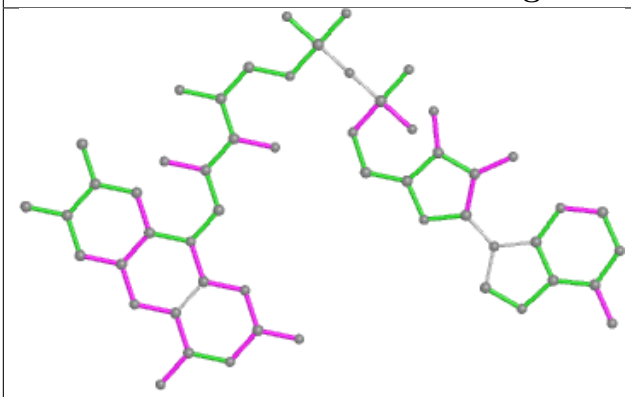


Torsions

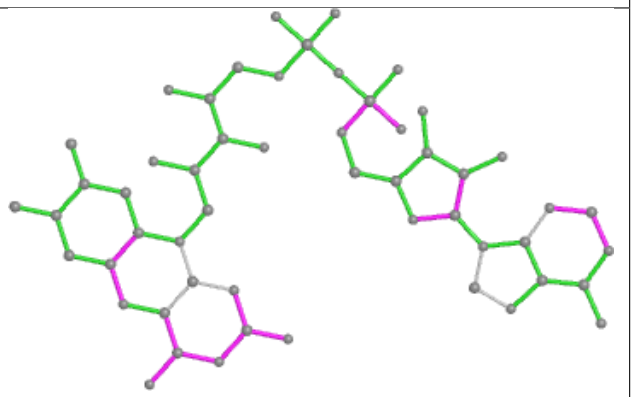


Rings

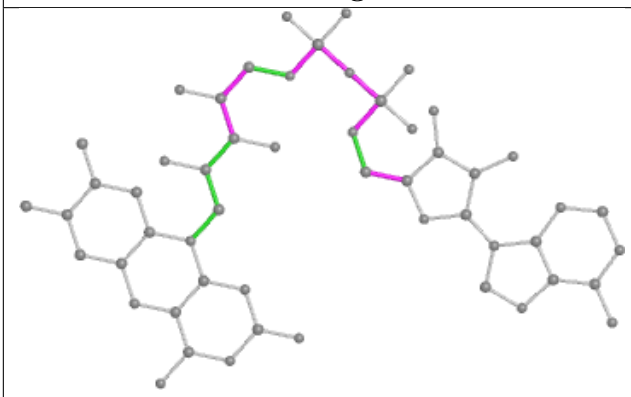
Ligand FDA A 601



Bond lengths



Bond angles



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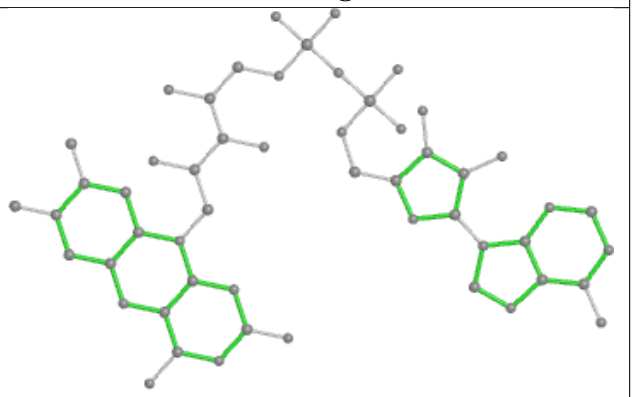
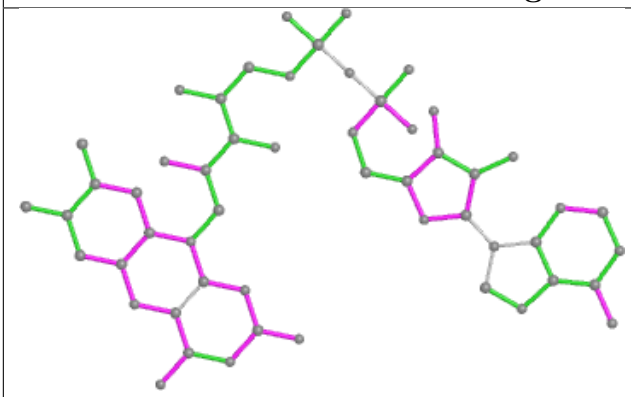
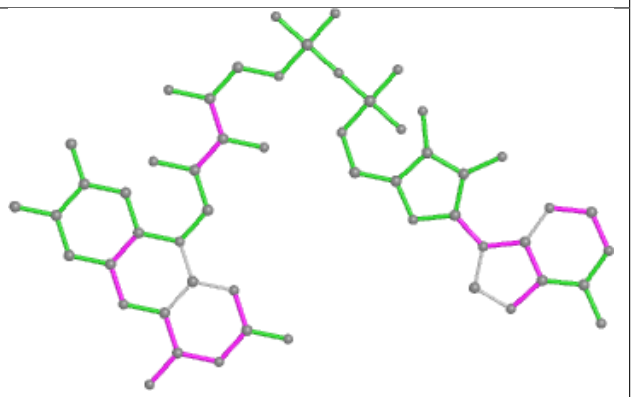


Rings

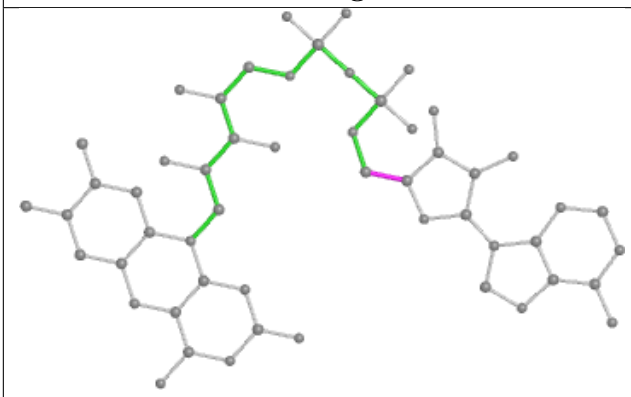
Ligand FDA E 601



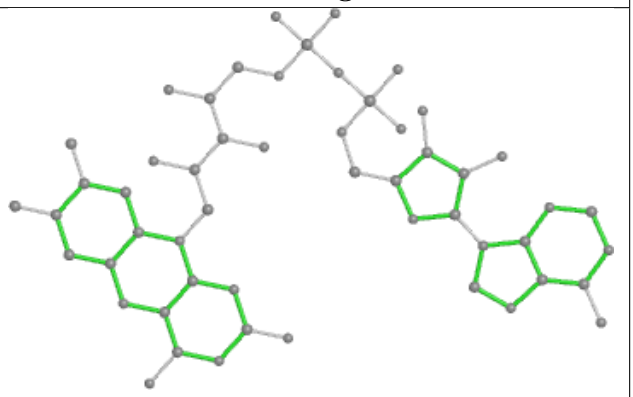
Bond lengths



Bond angles

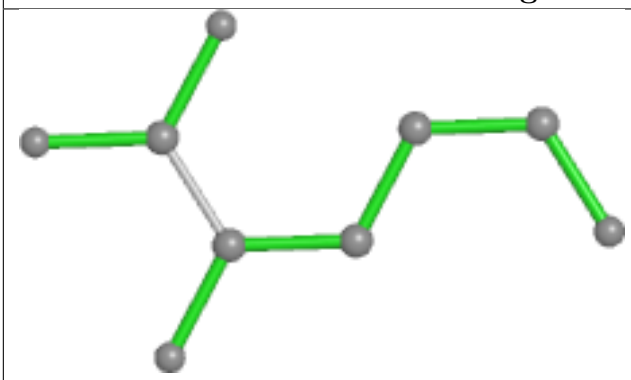


Torsions

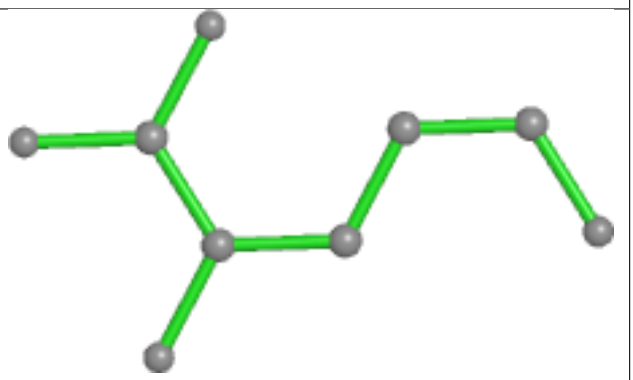


Rings

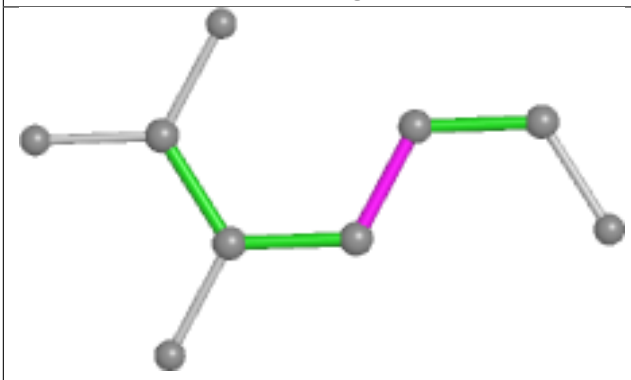
Ligand ORN A 602



Bond lengths



Bond angles



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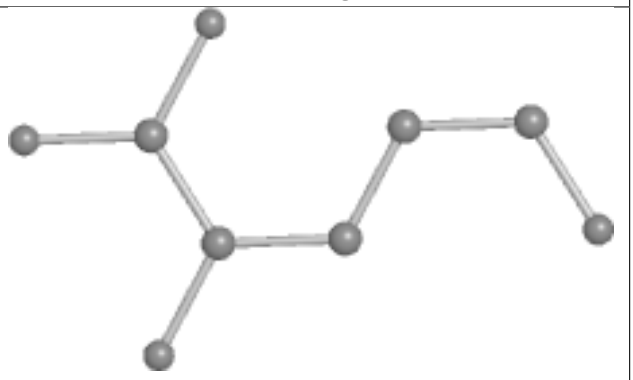
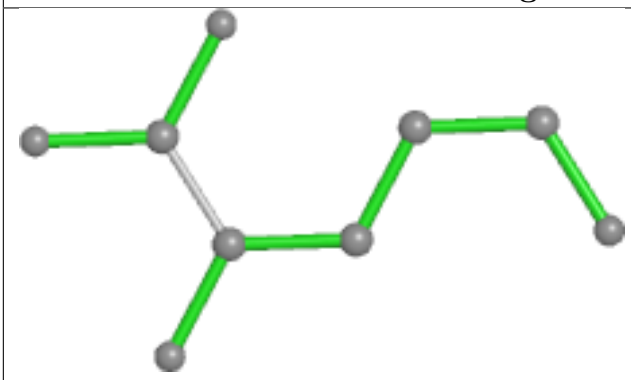
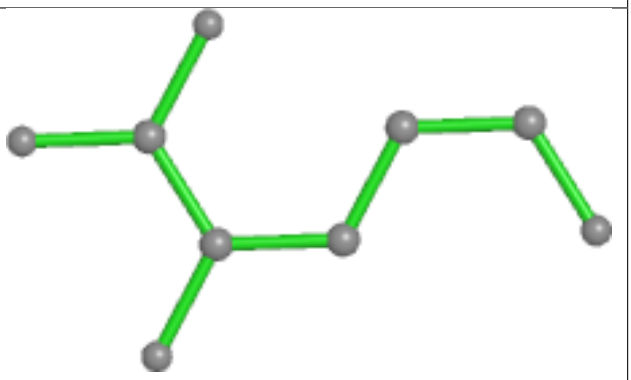


Rings

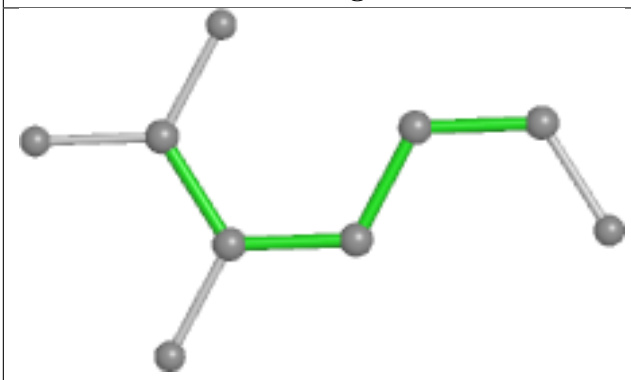
Ligand ORN G 602



Bond lengths



Bond angles



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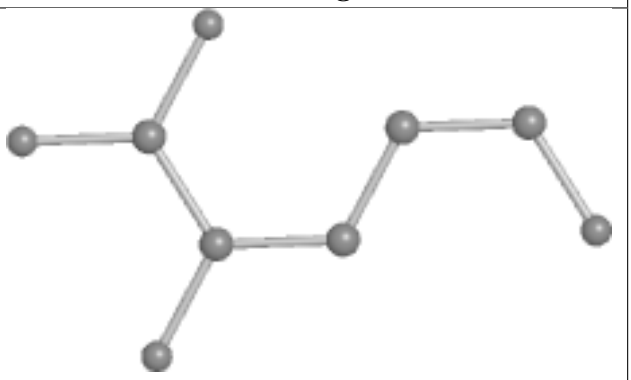
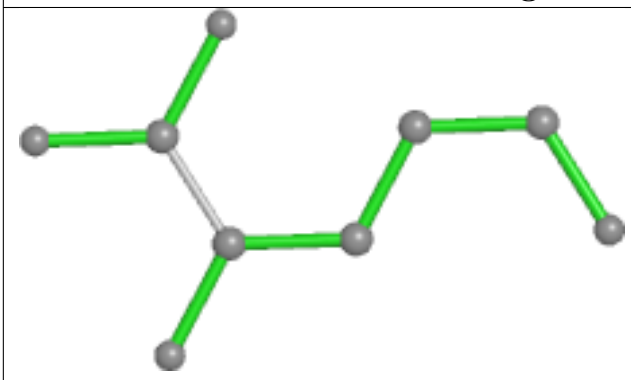
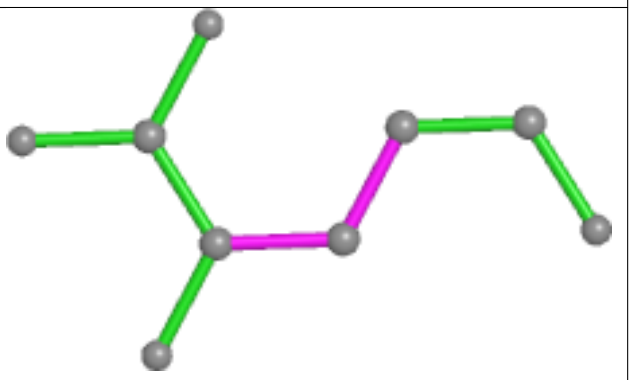


Rings

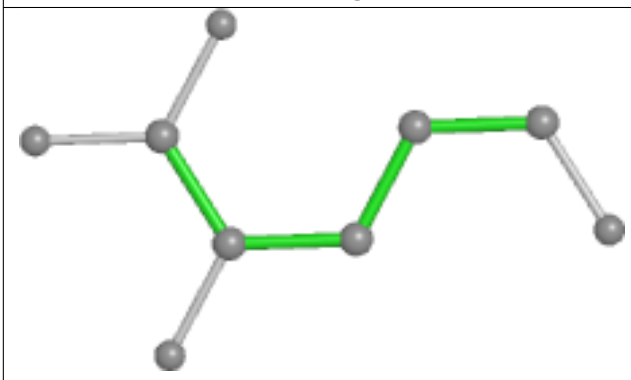
Ligand ORN D 602



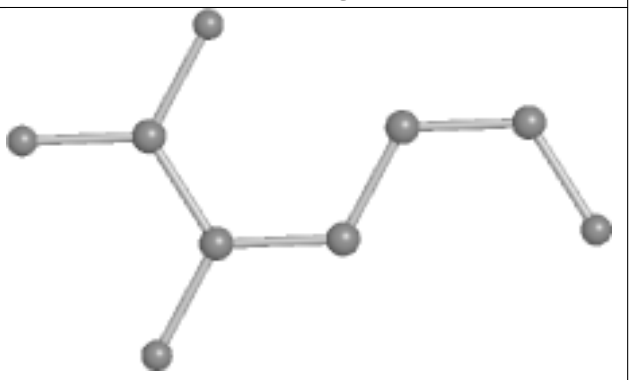
Bond lengths



Bond angles

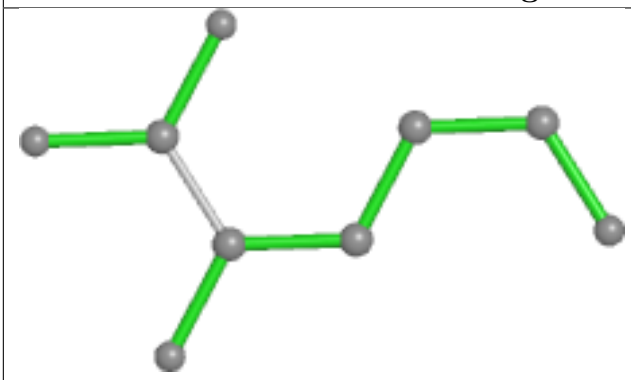


Torsions



Rings

Ligand ORN B 602



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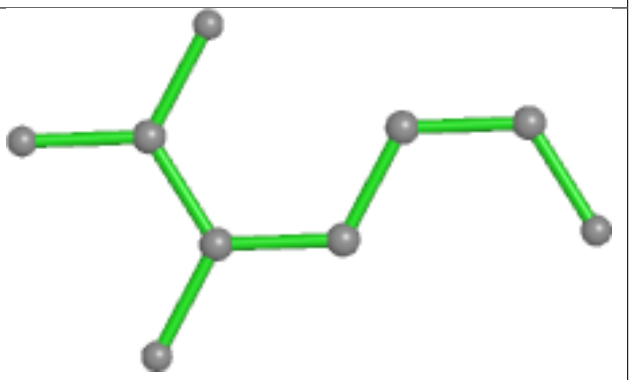
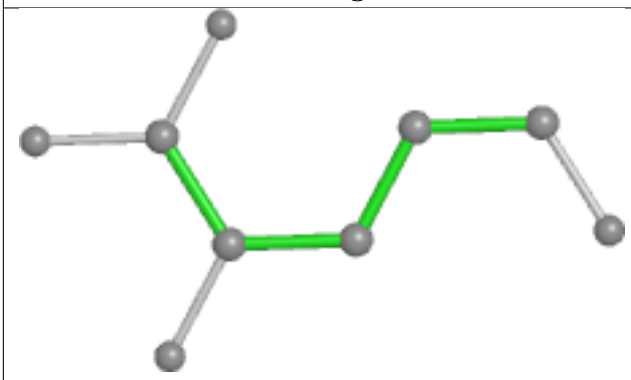
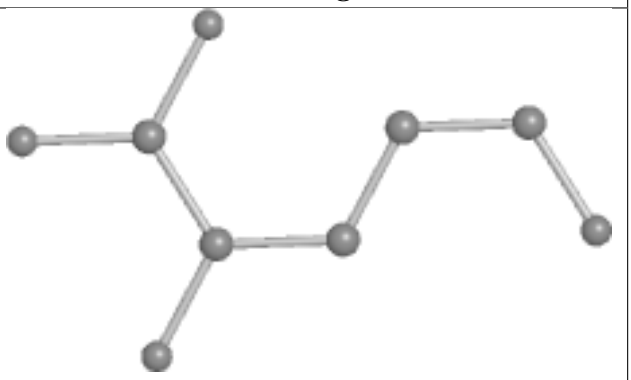


Bond angles

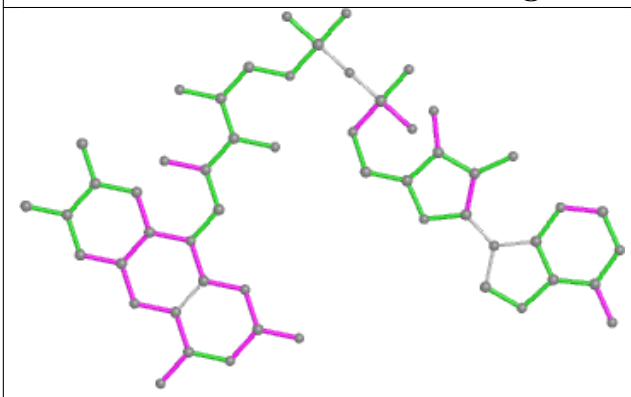


Torsions

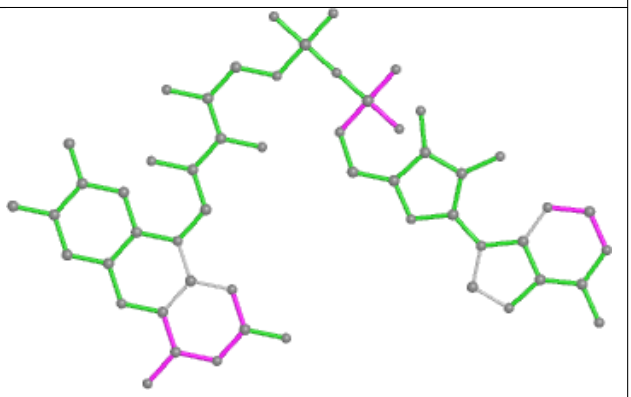


Rings

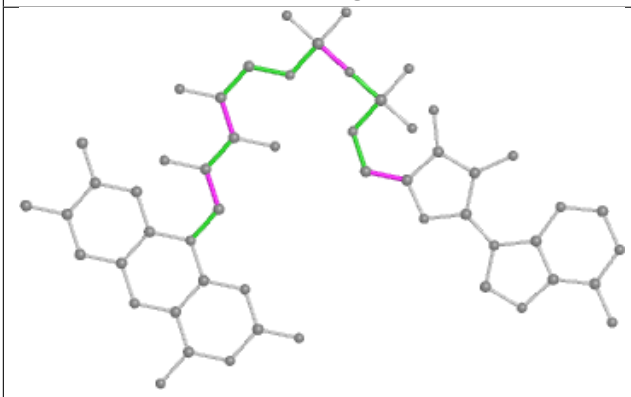
Ligand FDA G 601



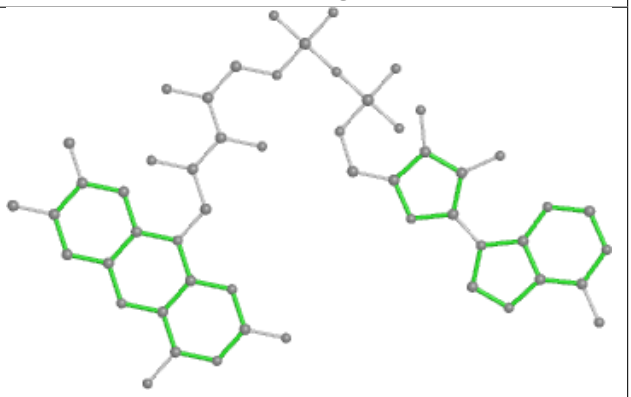
Bond lengths



Bond angles

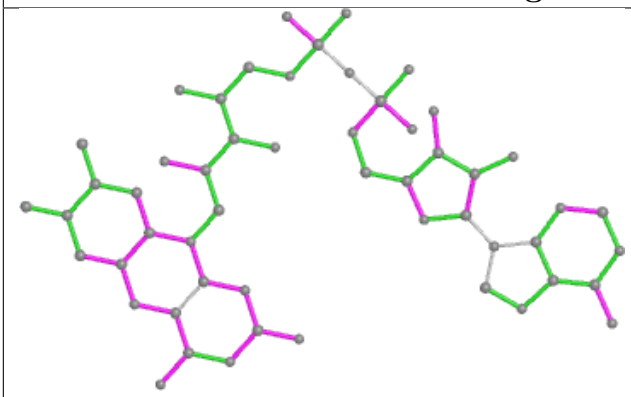


Torsions

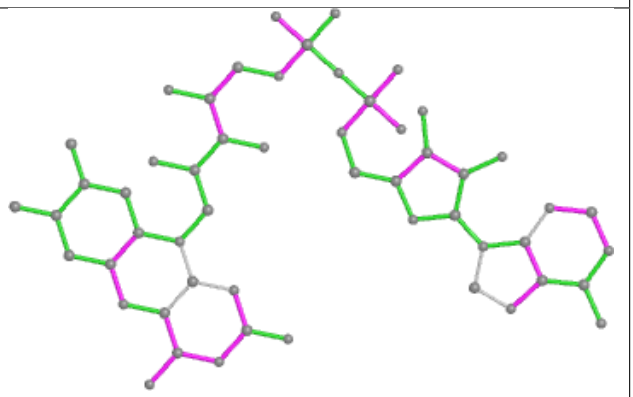


Rings

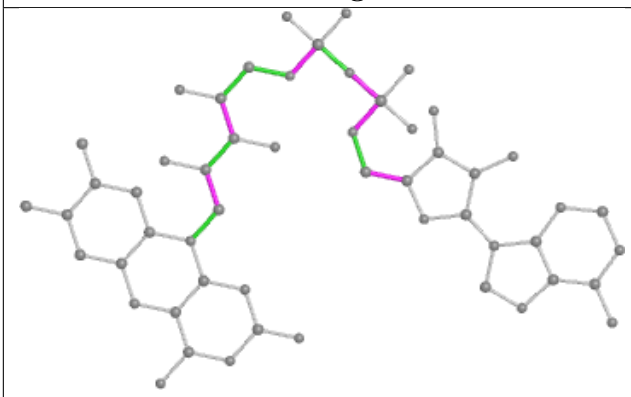
Ligand FDA F 601



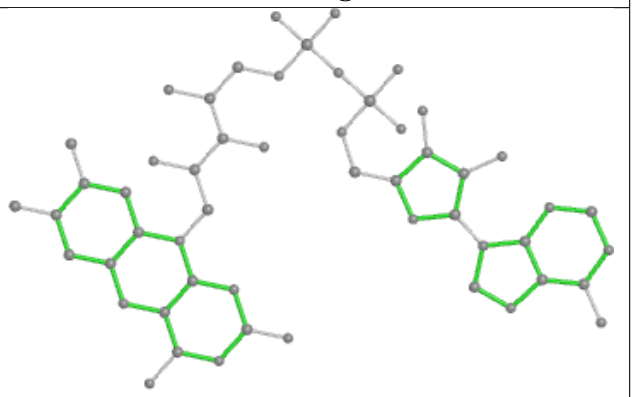
Bond lengths



Bond angles

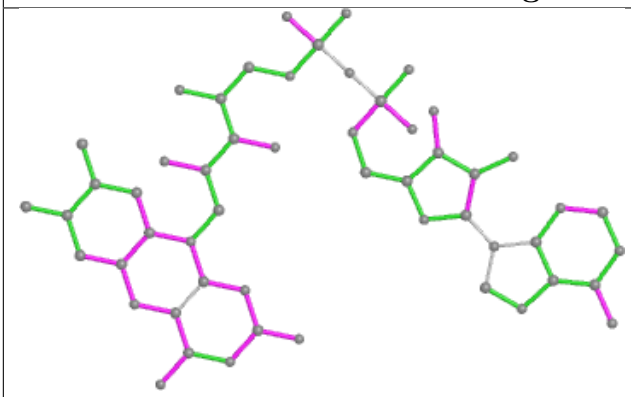


Torsions

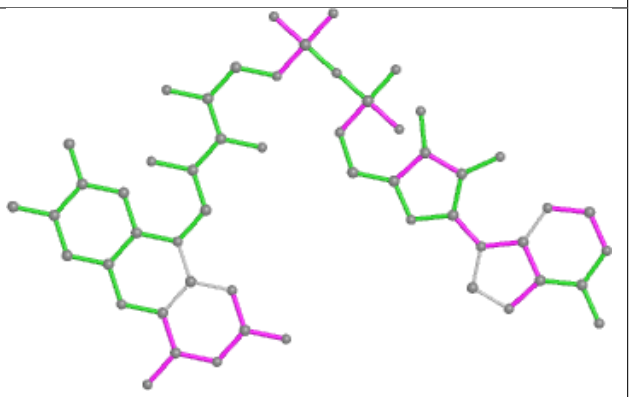


Rings

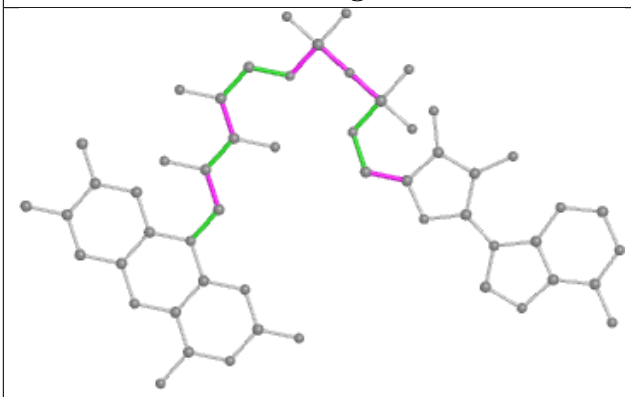
Ligand FDA H 601



Bond lengths



Bond angles



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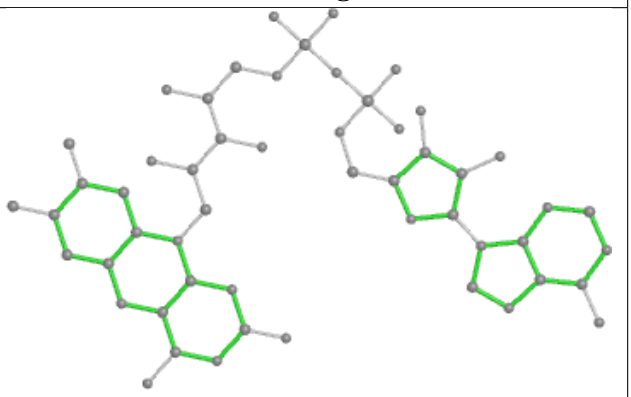
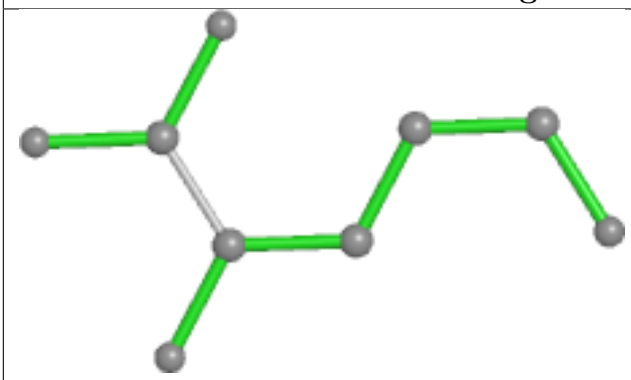
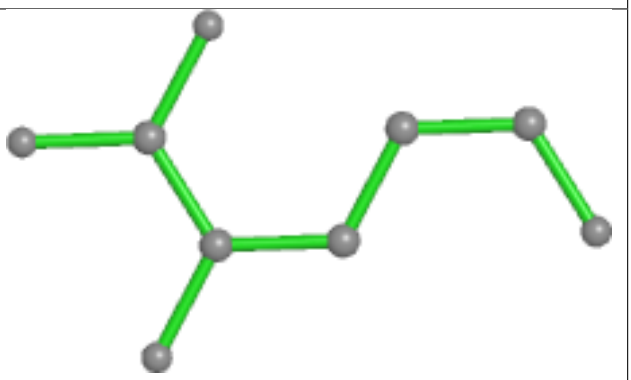


Rings

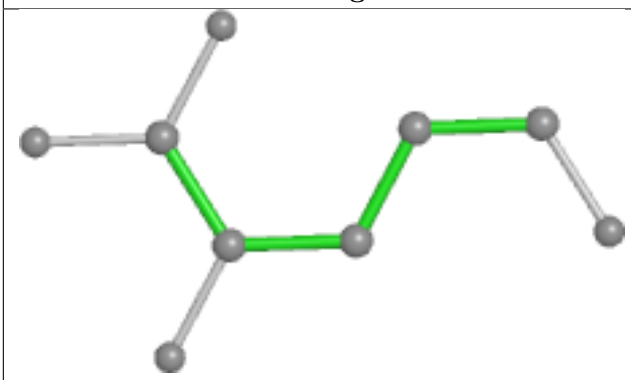
Ligand ORN H 602



Bond lengths



Bond angles



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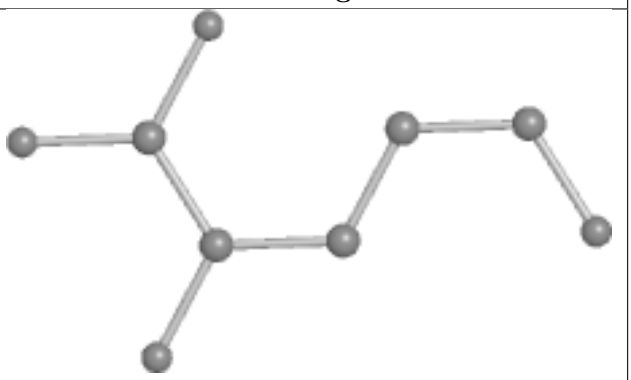
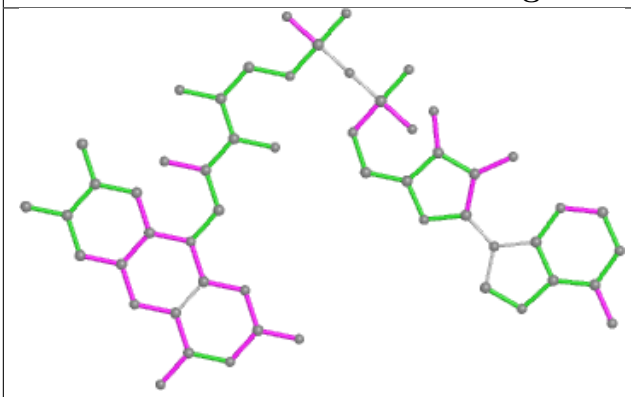
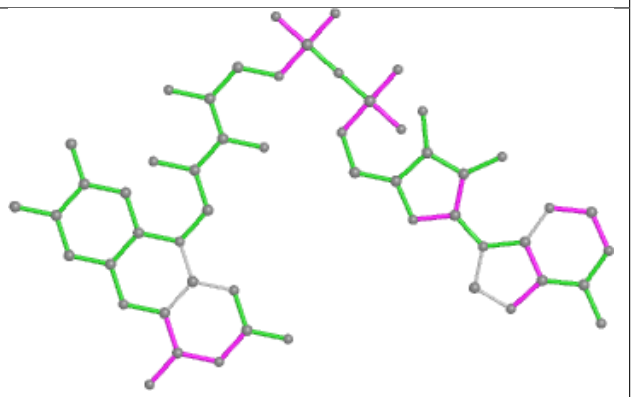


Rings

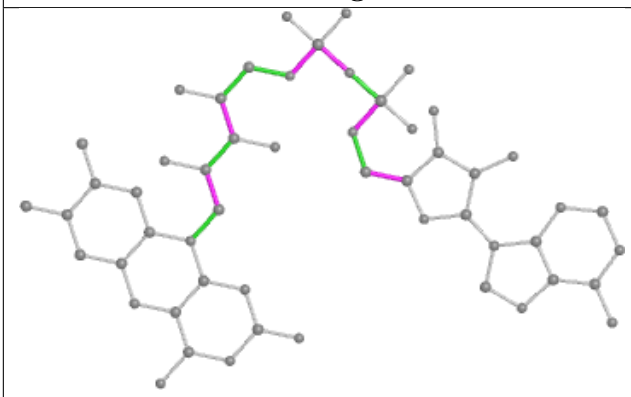
Ligand FDA D 601



Bond lengths



Bond angles



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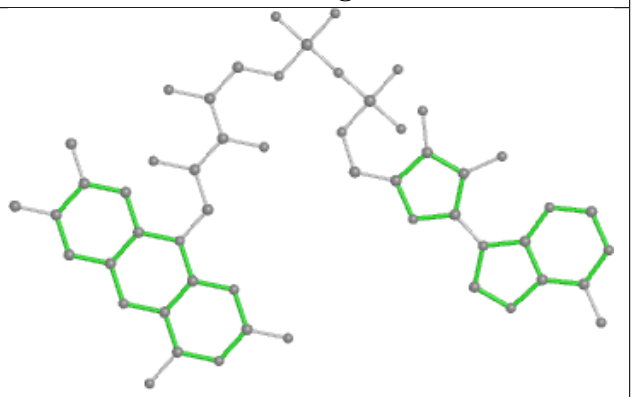
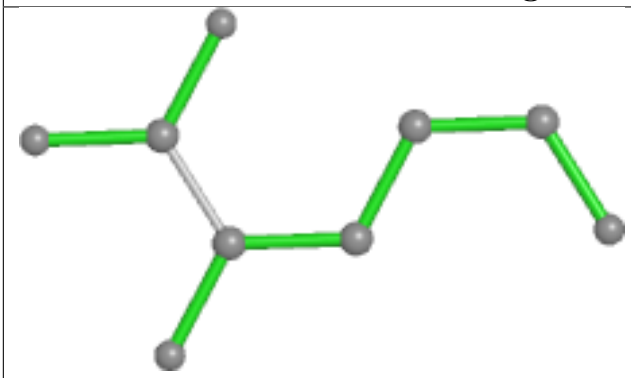


Rings

Ligand ORN E 602



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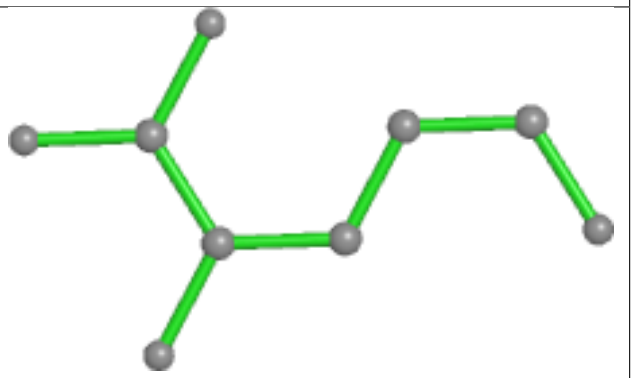
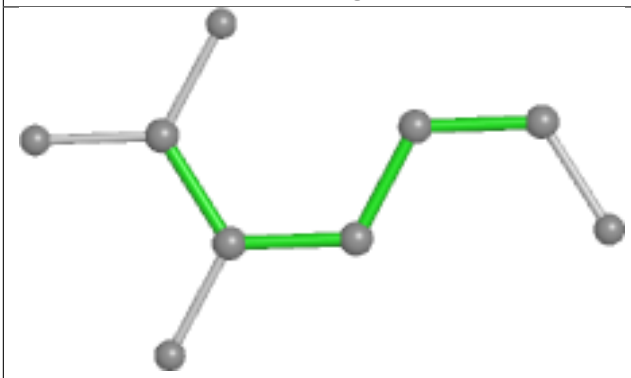


Bond angles



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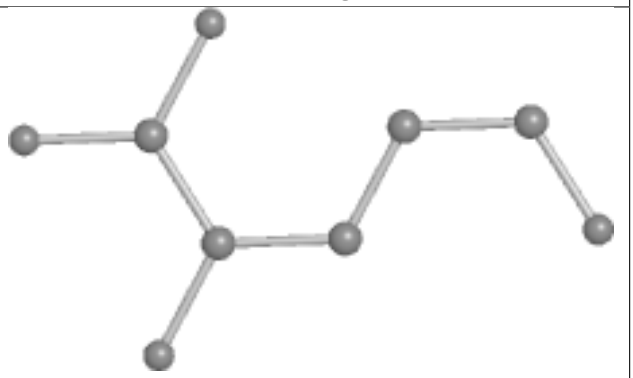
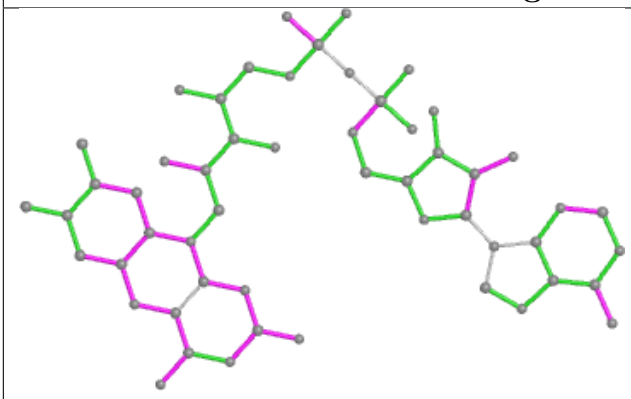
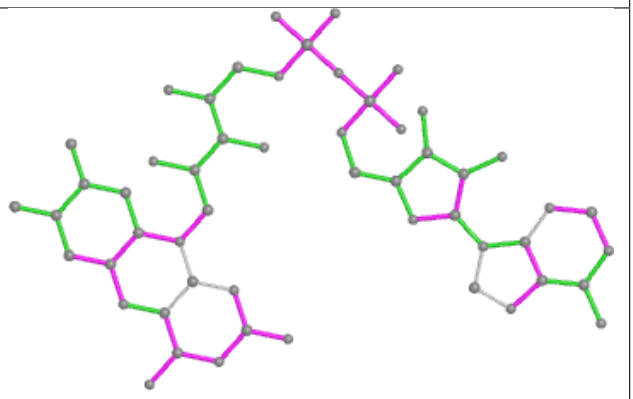


Rings

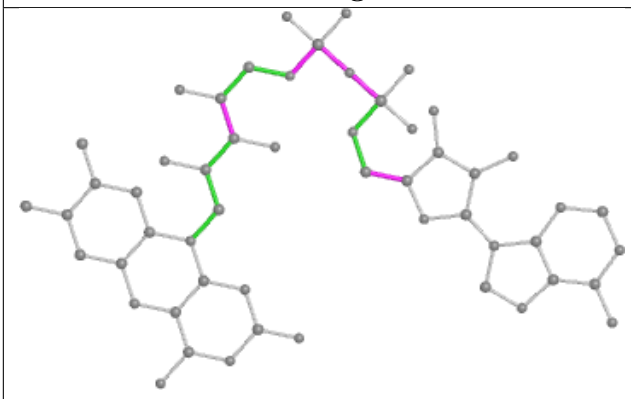
Ligand FDA B 601



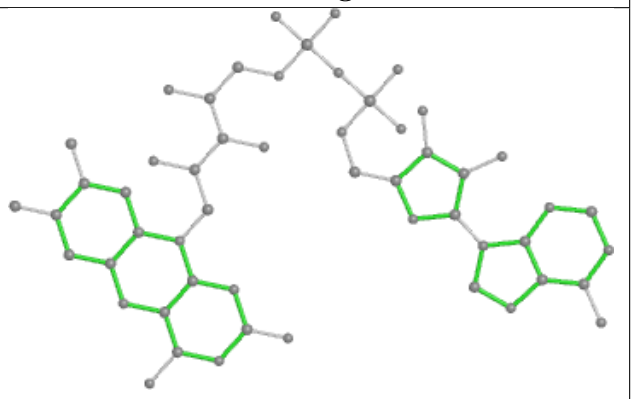
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	440/494 (89%)	-0.36	0 100 100	28, 45, 68, 90	0
1	B	442/494 (89%)	-0.38	0 100 100	28, 46, 70, 100	0
1	C	433/494 (87%)	-0.16	3 (0%) 87 87	31, 53, 85, 107	0
1	D	441/494 (89%)	-0.17	3 (0%) 87 87	32, 54, 81, 112	0
1	E	441/494 (89%)	-0.23	0 100 100	30, 48, 75, 104	0
1	F	436/494 (88%)	0.00	9 (2%) 63 65	41, 69, 97, 111	0
1	G	440/494 (89%)	-0.10	8 (1%) 68 69	37, 64, 105, 153	0
1	H	437/494 (88%)	-0.08	8 (1%) 68 69	42, 65, 99, 115	0
All	All	3510/3952 (88%)	-0.19	31 (0%) 84 84	28, 55, 91, 153	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	383	PRO	4.1
1	G	174	GLY	4.1
1	H	238	ALA	3.9
1	H	220	LEU	3.2
1	F	246	PRO	3.1
1	H	193	VAL	3.1
1	F	400	ALA	3.1
1	D	370	PRO	2.9
1	G	200	ALA	2.9
1	G	178	PRO	2.9
1	F	268	ARG	2.9
1	G	37	ASP	2.8
1	F	425	THR	2.8
1	F	398	VAL	2.6
1	H	159	SER	2.5
1	F	259	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	396	LEU	2.4
1	H	194	GLU	2.3
1	D	218	SER	2.3
1	G	145	LEU	2.2
1	C	317	LEU	2.2
1	F	225	ARG	2.2
1	G	77	PRO	2.2
1	H	156	GLN	2.2
1	H	269	TYR	2.1
1	D	198	ILE	2.1
1	G	176	SER	2.1
1	F	220	LEU	2.1
1	G	38	GLU	2.1
1	H	31	LEU	2.1
1	C	64	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FDA	F	601	53/53	0.92	0.14	47,65,82,85	0
2	FDA	H	601	53/53	0.94	0.12	43,57,70,81	0
3	ORN	D	602	9/9	0.94	0.14	34,43,47,48	0
3	ORN	E	602	9/9	0.94	0.33	27,44,50,52	0
3	ORN	G	602	9/9	0.95	0.12	30,37,44,47	0
3	ORN	H	602	9/9	0.95	0.13	37,44,51,52	0
2	FDA	B	601	53/53	0.96	0.12	29,41,50,54	0
3	ORN	B	602	9/9	0.96	0.13	35,40,46,48	0

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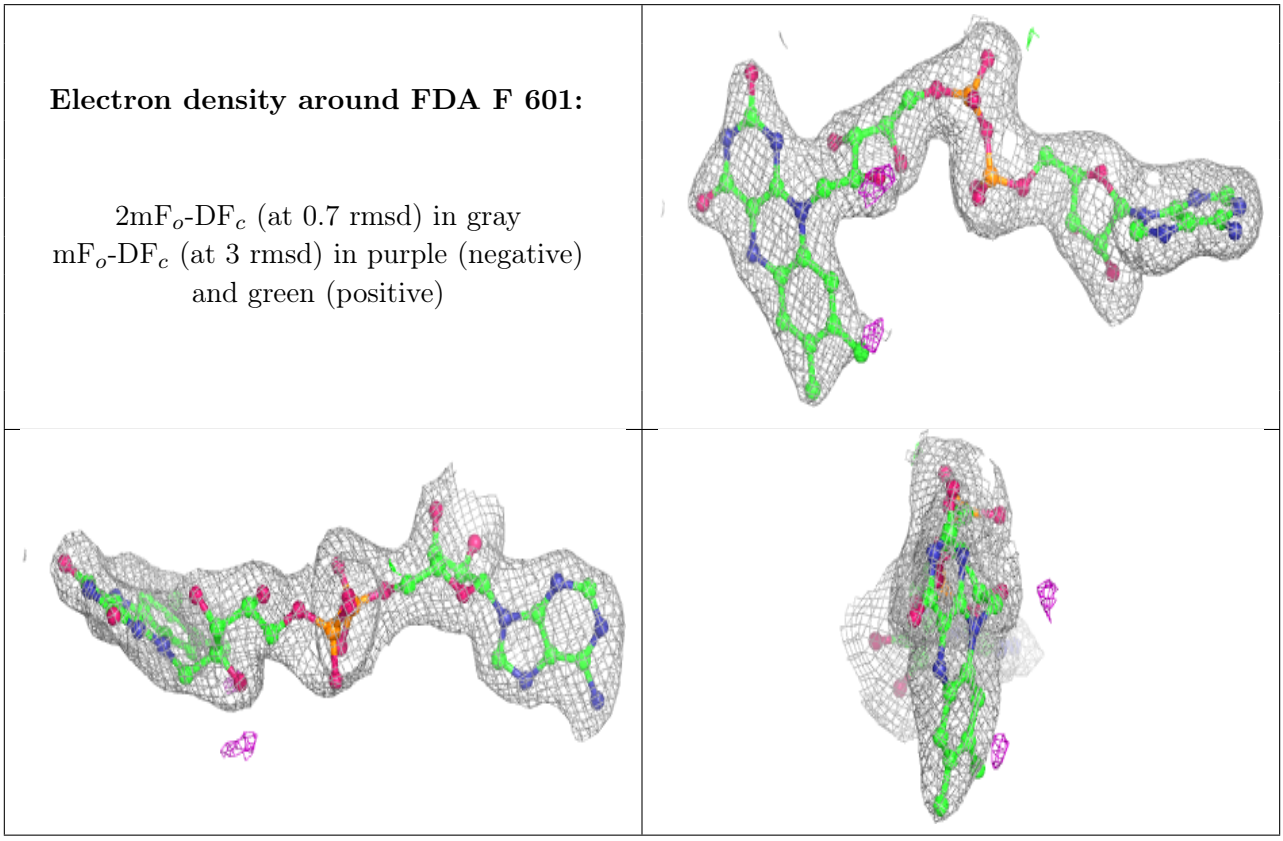
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FDA	D	601	53/53	0.96	0.12	34,48,55,56	0
2	FDA	E	601	53/53	0.96	0.11	21,37,47,60	0
2	FDA	A	601	53/53	0.96	0.12	24,40,53,59	0
2	FDA	G	601	53/53	0.96	0.11	37,54,65,67	0
2	FDA	C	601	53/53	0.97	0.10	22,46,59,60	0
3	ORN	A	602	9/9	0.98	0.10	23,34,40,40	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.

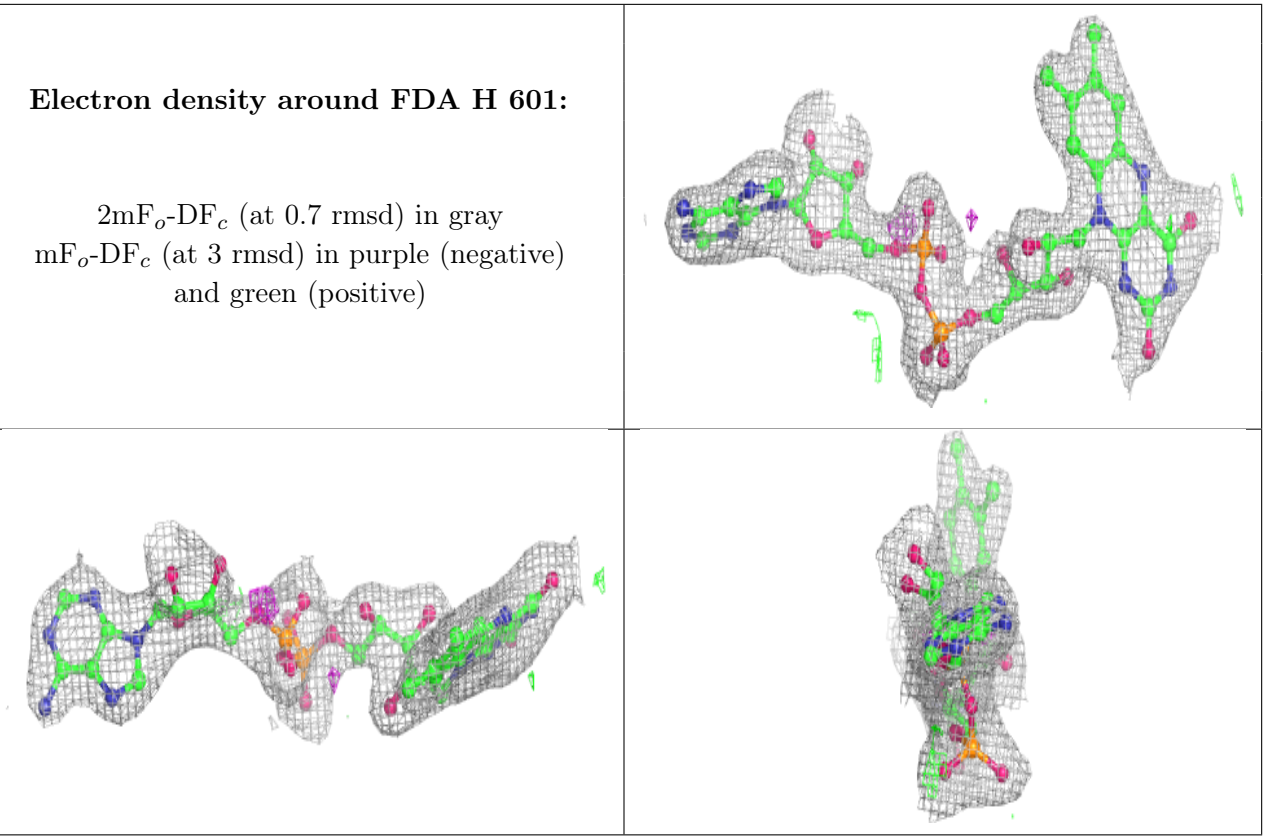
Electron density around FDA F 601:

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



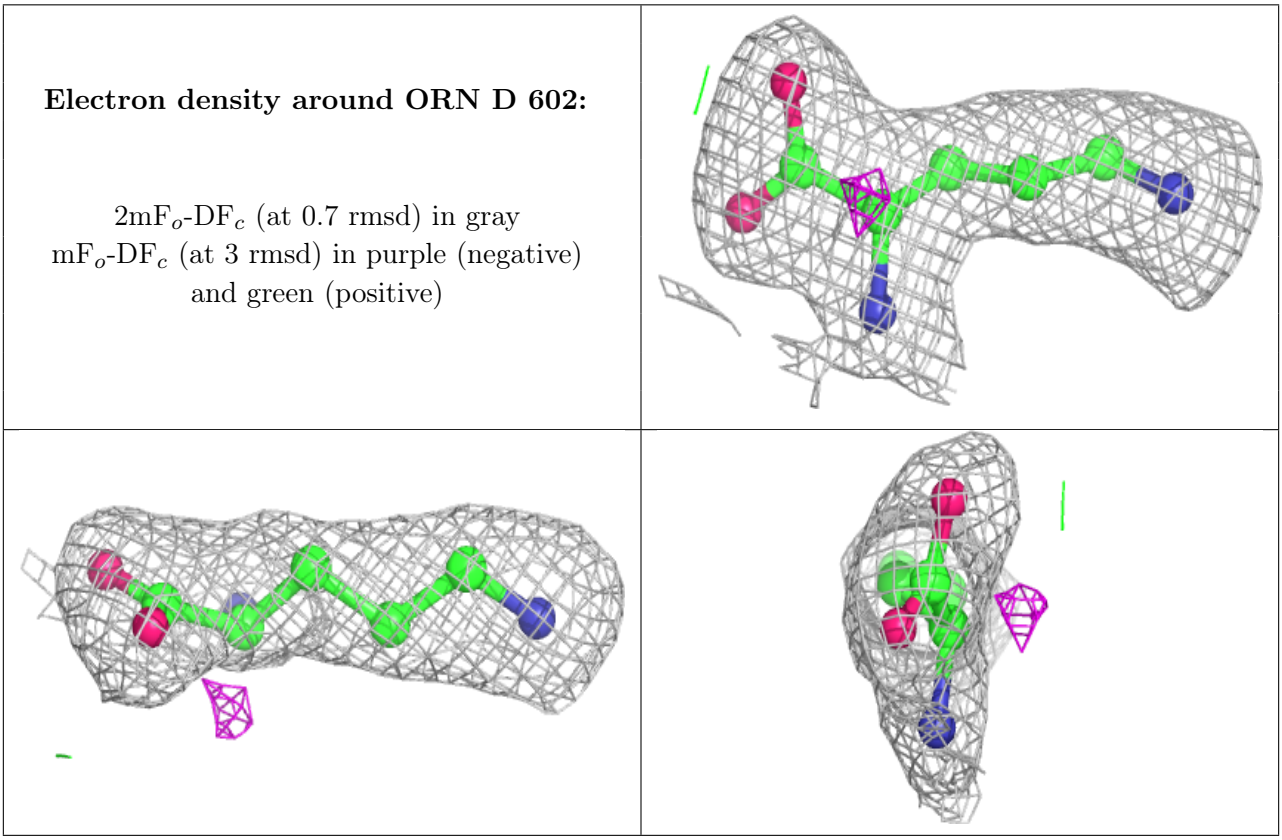
Electron density around FDA H 601:

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



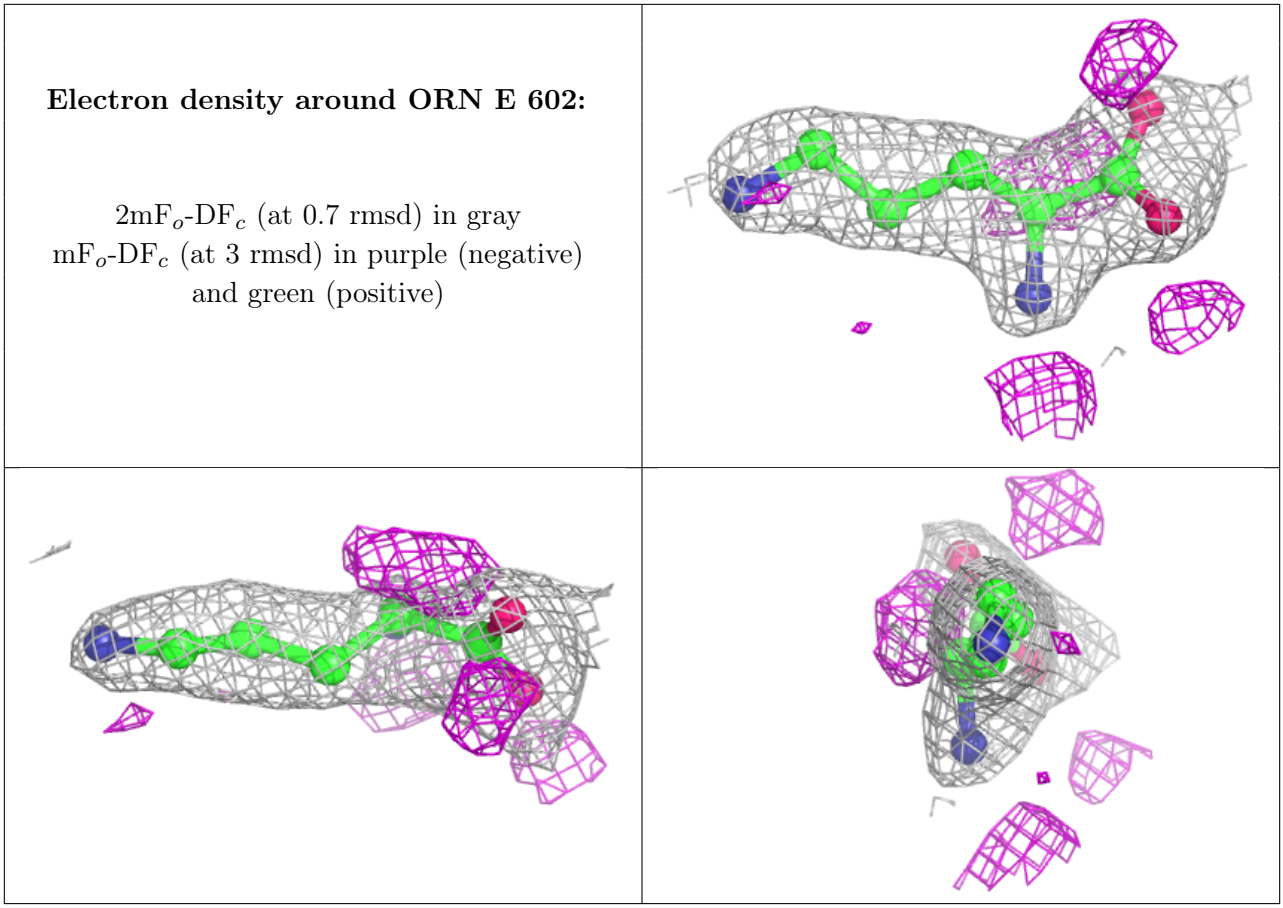
Electron density around ORN D 602:

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



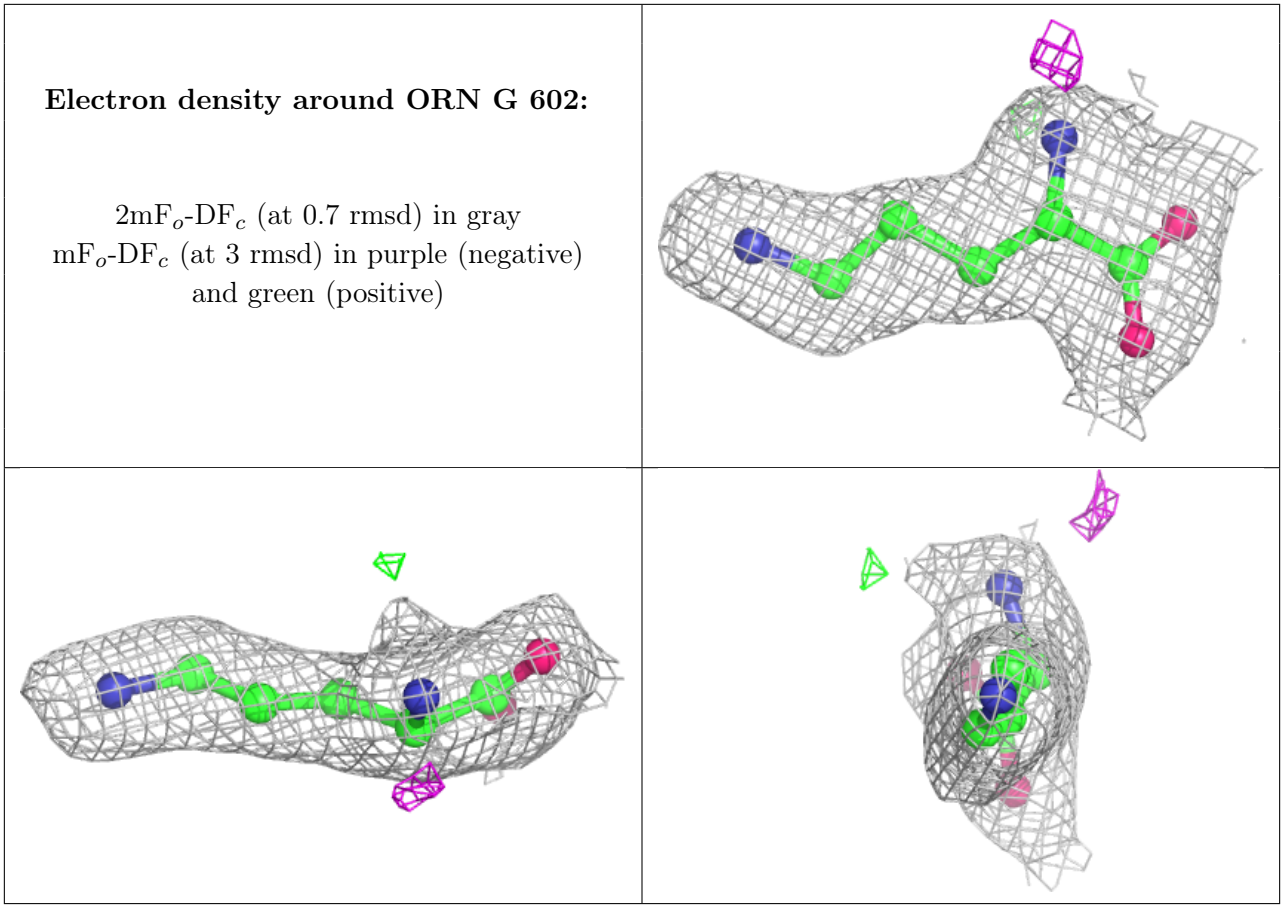
Electron density around ORN E 602:

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



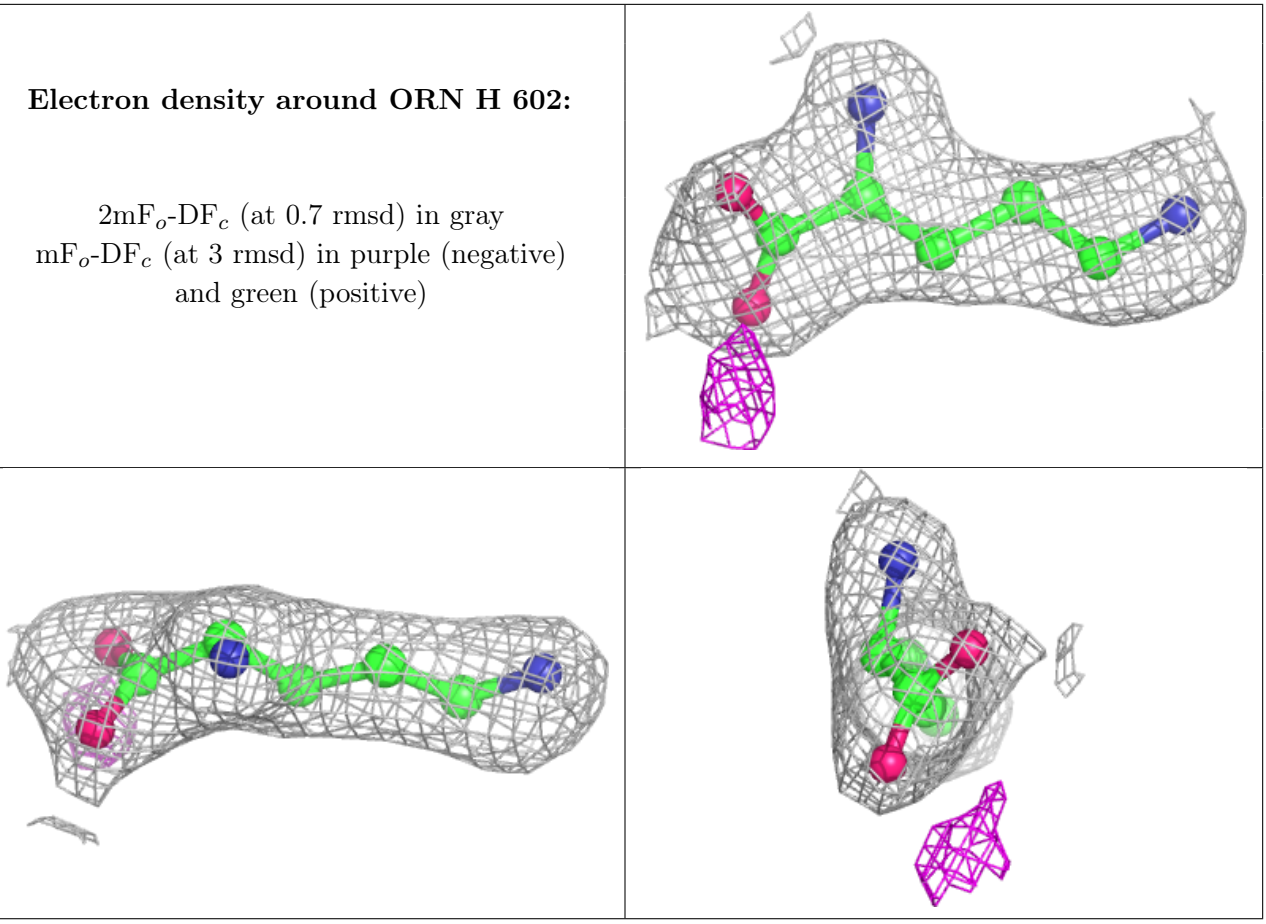
Electron density around ORN G 602:

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



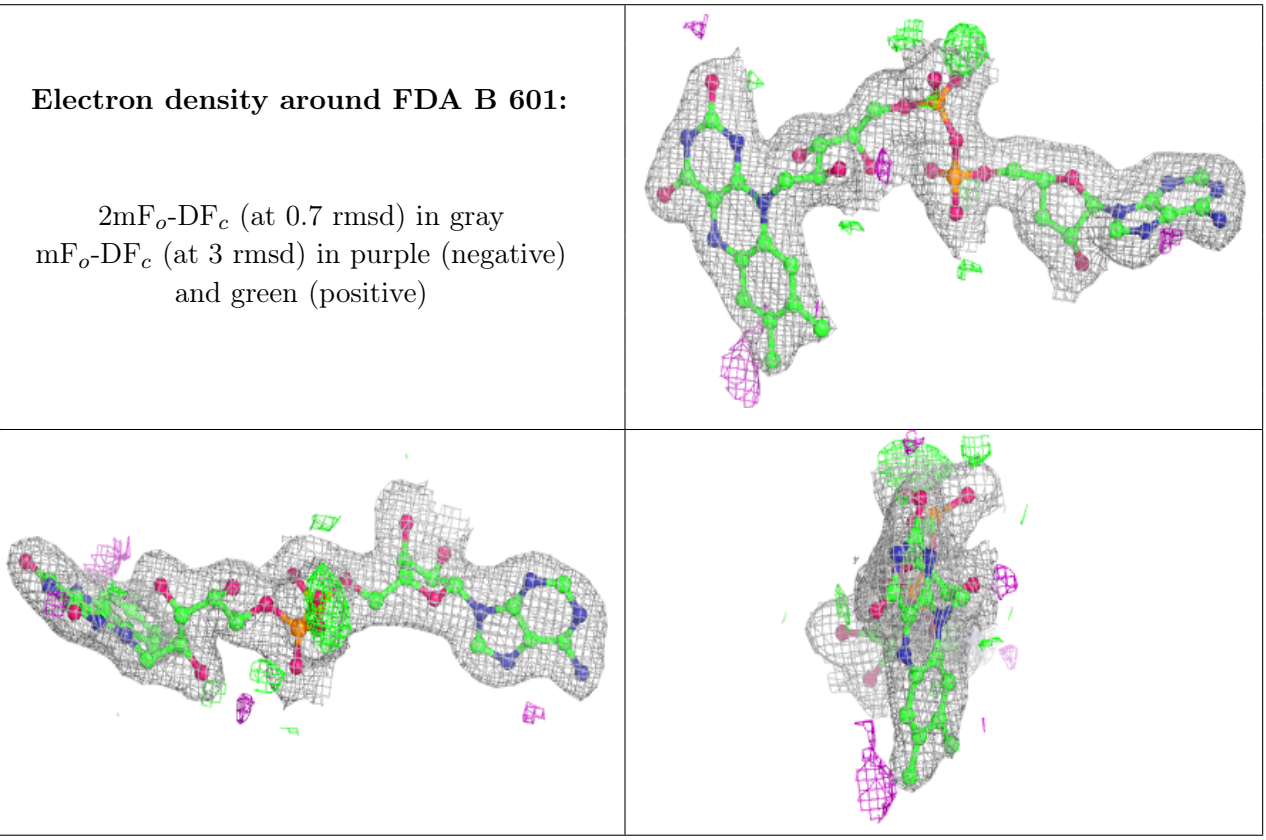
Electron density around ORN H 602:

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



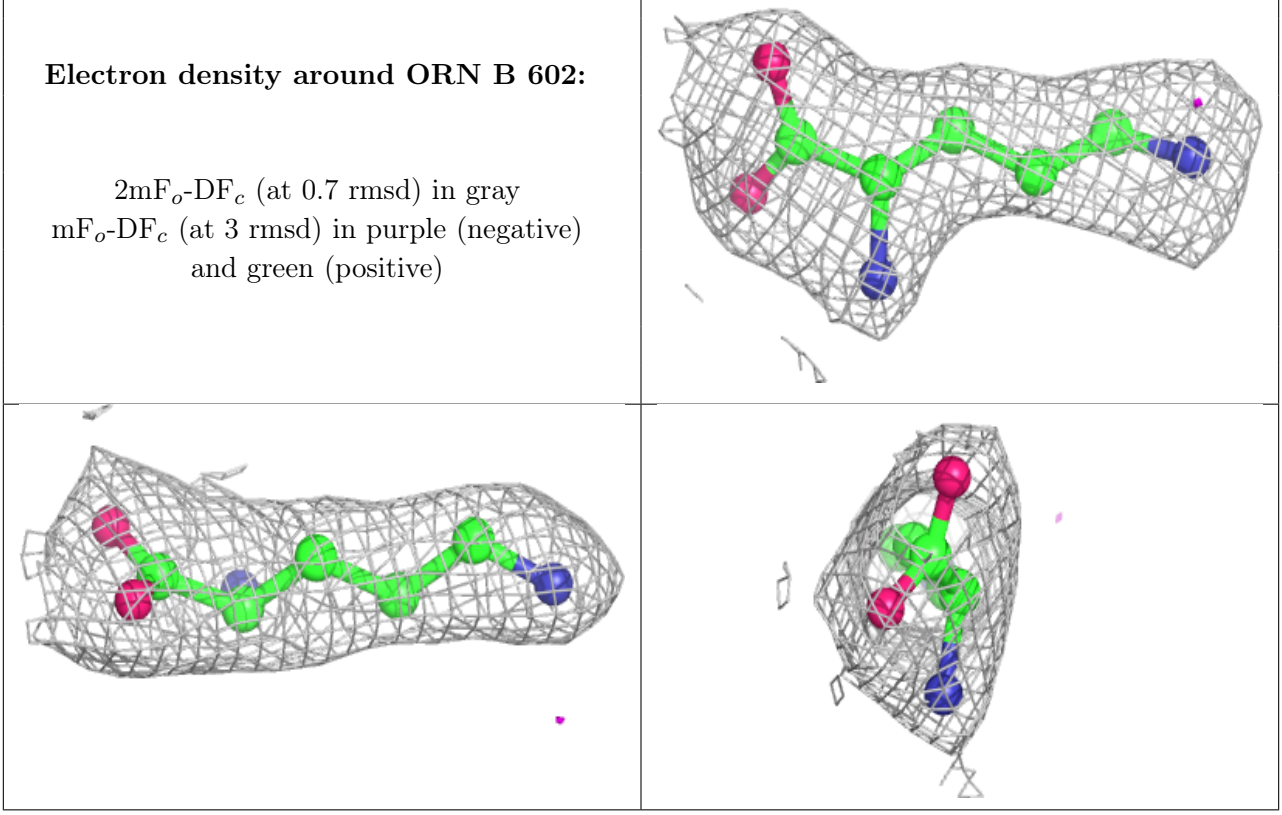
Electron density around FDA B 601:

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



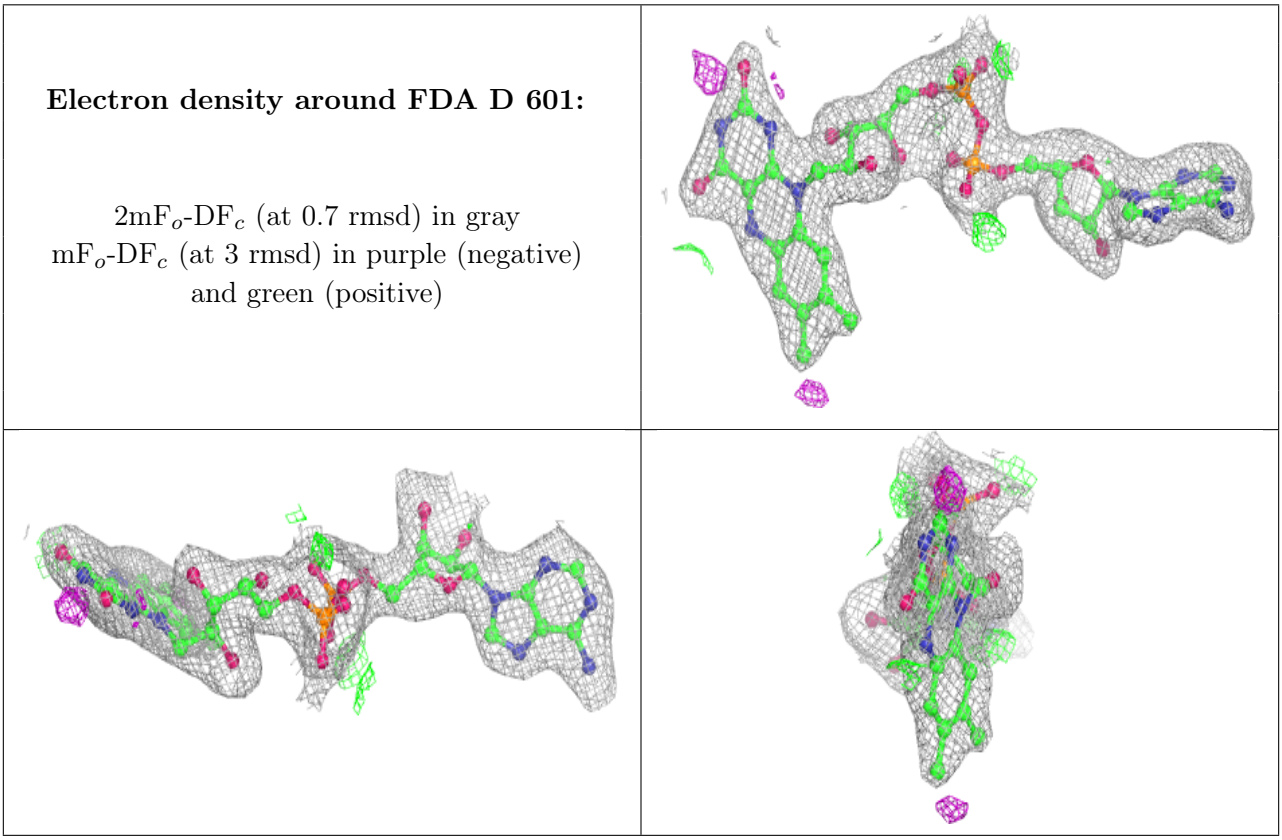
Electron density around ORN B 602:

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



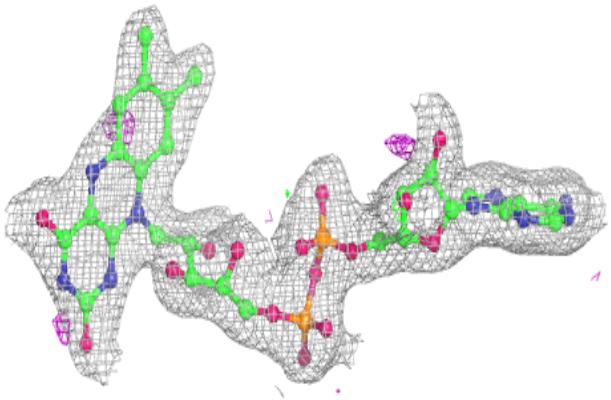
Electron density around FDA D 601:

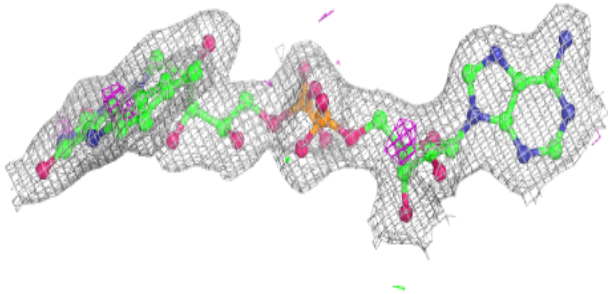
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

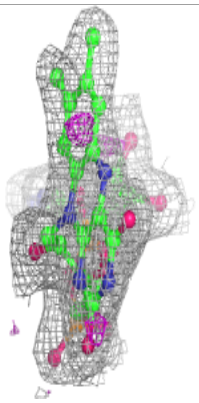


Electron density around FDA E 601:

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

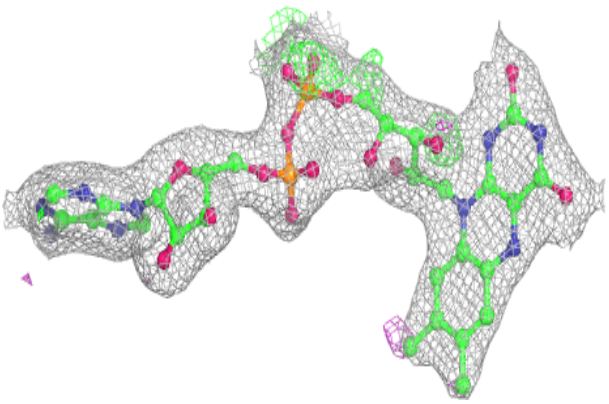


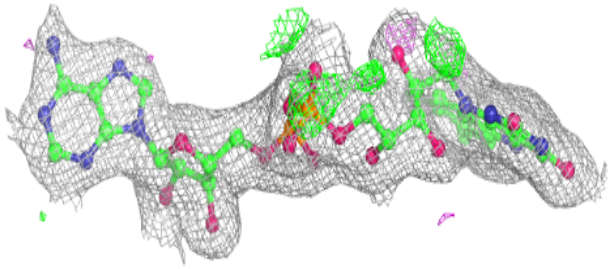


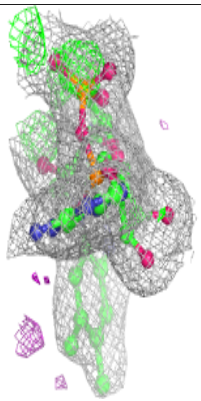


Electron density around FDA A 601:

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

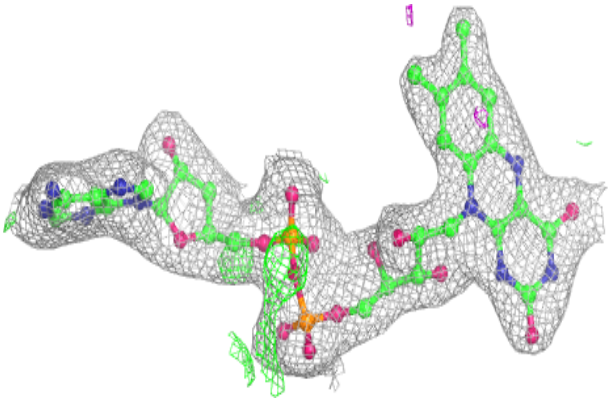


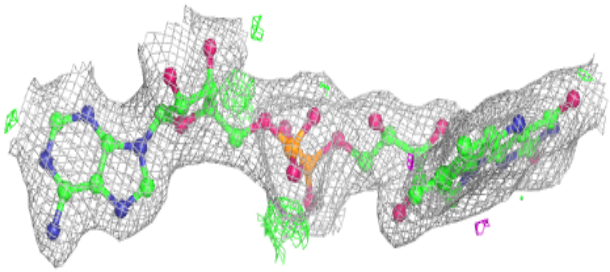


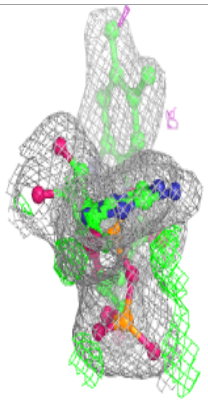


Electron density around FDA G 601:

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

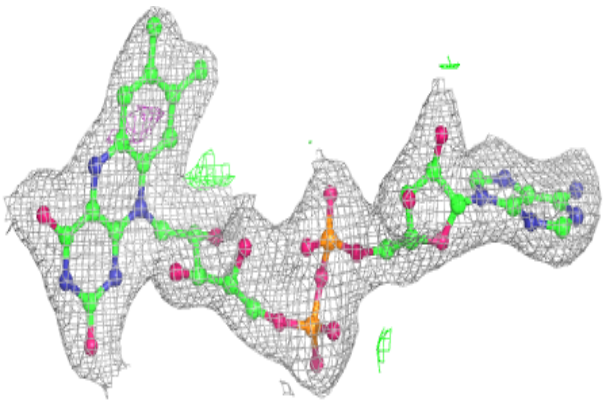


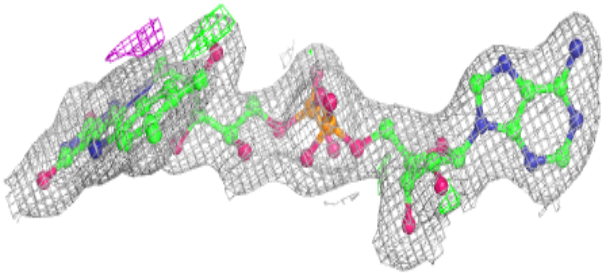


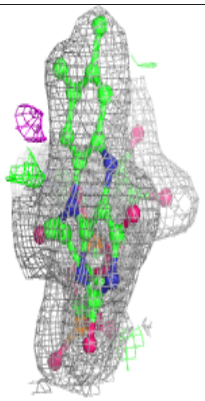


Electron density around FDA C 601:

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

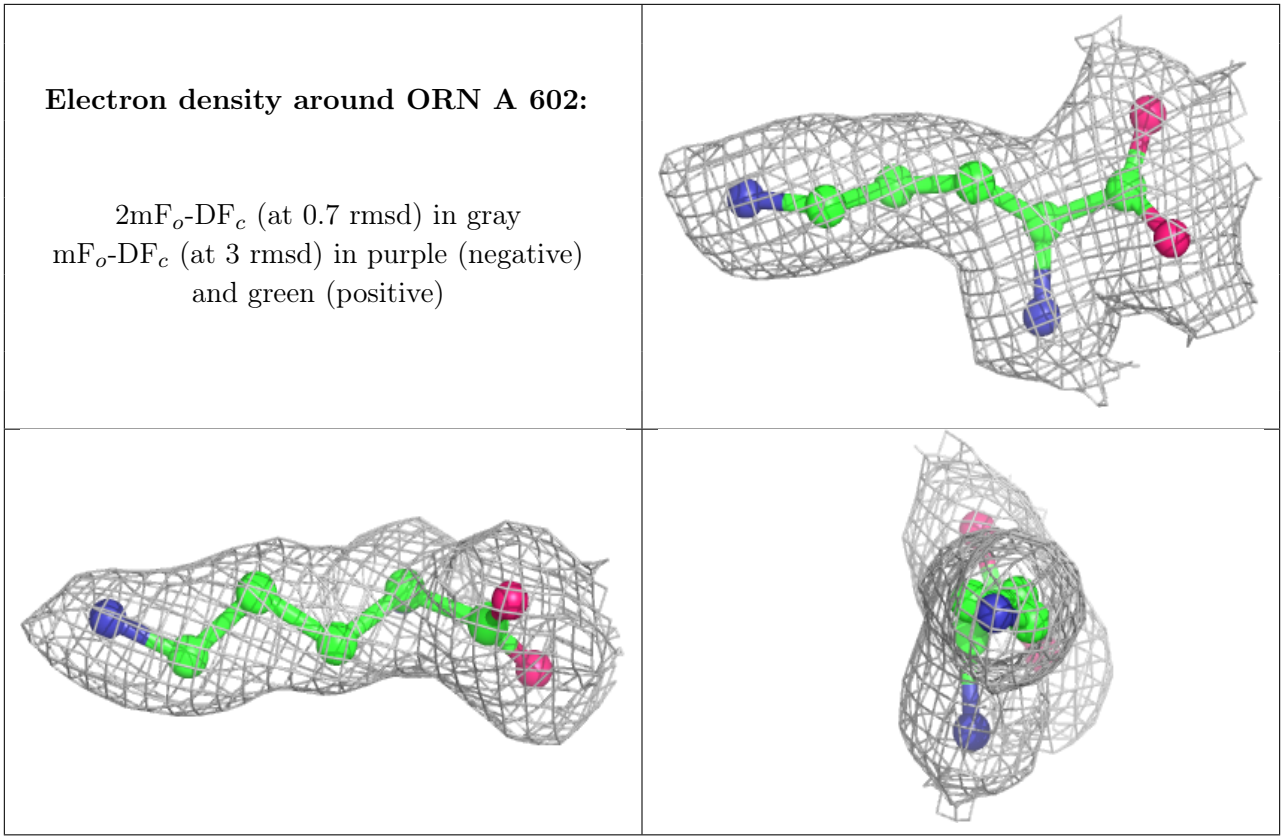






Electron density around ORN A 602:

$2mF_o$-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.