Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 06:04 PM EDT

PDB ID	:	5MR6
Title	:	XiaF from Streptomyces sp. in complex with FADH2 and Glycerol
Authors	:	Kugel, S.; Baunach, M.; Baer, P.; Ishida-Ito, M.; Sundaram, S.; Xu, Z.; Groll, M.; Hertweck, C.
Deposited on	:	2016-12-21
Resolution	:	2.40 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:

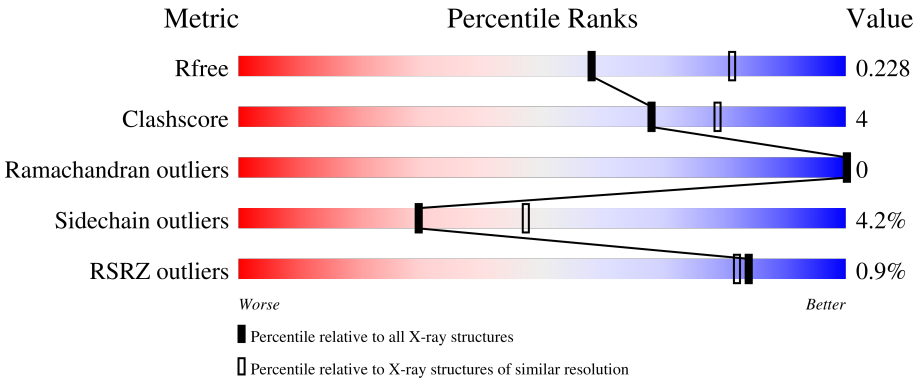
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	413	87% 8%
1	B	413	86% 8%
1	C	413	86% 8%
1	D	413	87% 8%
1	E	413	86% 8%

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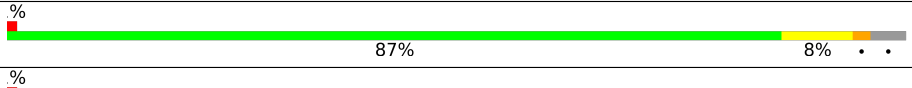
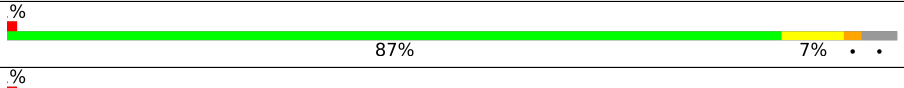
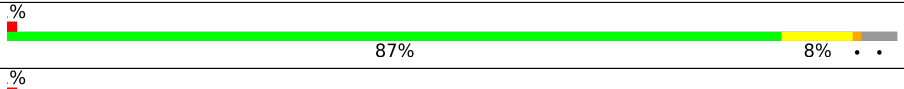
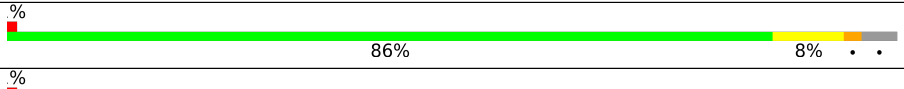
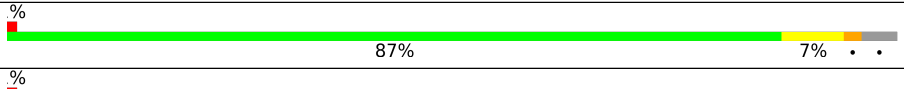
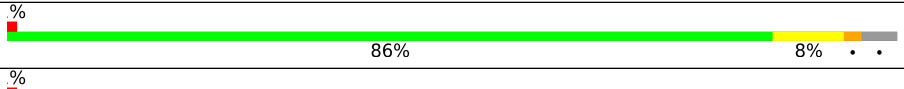
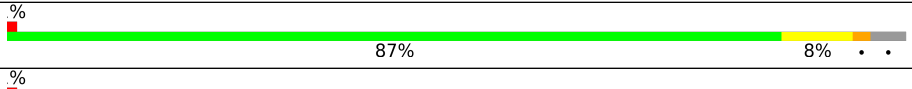
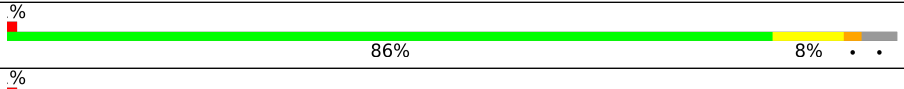
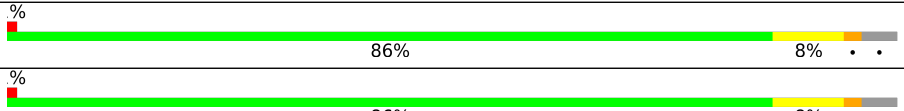
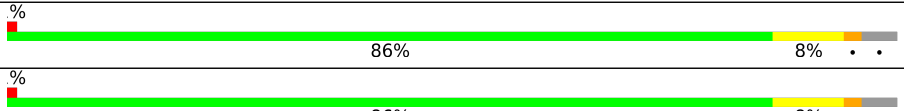
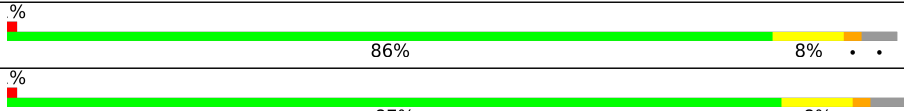
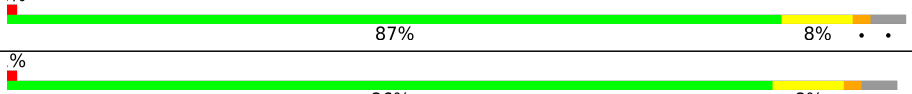
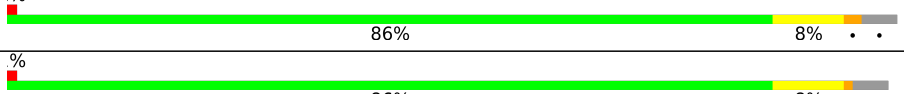
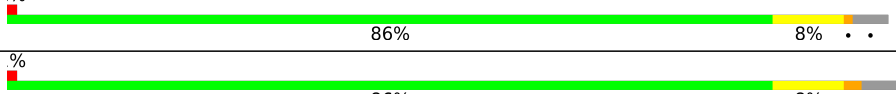
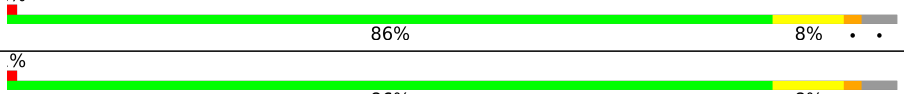
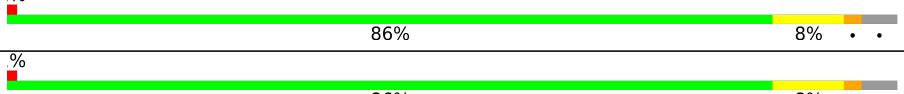
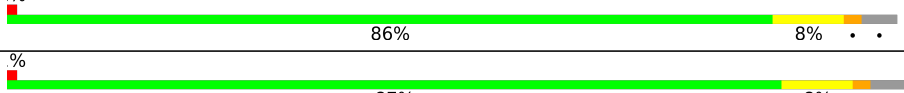
Mol	Chain	Length	Quality of chain
1	F	413	
1	G	413	
1	H	413	
1	I	413	
1	J	413	
1	K	413	
1	L	413	
1	M	413	
1	N	413	
1	O	413	
1	P	413	
1	Q	413	
1	R	413	
1	S	413	
1	T	413	
1	U	413	
1	V	413	
1	W	413	
1	X	413	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 77543 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 XiaF protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	B	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	C	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	D	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	E	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	F	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	G	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	H	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	I	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	J	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	K	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	L	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	M	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	N	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	O	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	P	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	R	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	S	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	T	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	U	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	V	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	W	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			
1	X	396	Total	C	N	O	S	0	0	0
			2977	1863	536	569	9			

There are 384 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP I7IIA9
A	-14	HIS	-	expression tag	UNP I7IIA9
A	-13	HIS	-	expression tag	UNP I7IIA9
A	-12	HIS	-	expression tag	UNP I7IIA9
A	-11	HIS	-	expression tag	UNP I7IIA9
A	-10	HIS	-	expression tag	UNP I7IIA9
A	-9	SER	-	expression tag	UNP I7IIA9
A	-8	SER	-	expression tag	UNP I7IIA9
A	-7	GLY	-	expression tag	UNP I7IIA9
A	-6	LEU	-	expression tag	UNP I7IIA9
A	-5	VAL	-	expression tag	UNP I7IIA9
A	-4	PRO	-	expression tag	UNP I7IIA9
A	-3	ARG	-	expression tag	UNP I7IIA9
A	-2	GLY	-	expression tag	UNP I7IIA9
A	-1	SER	-	expression tag	UNP I7IIA9
A	0	HIS	-	expression tag	UNP I7IIA9
B	-15	HIS	-	expression tag	UNP I7IIA9
B	-14	HIS	-	expression tag	UNP I7IIA9
B	-13	HIS	-	expression tag	UNP I7IIA9
B	-12	HIS	-	expression tag	UNP I7IIA9
B	-11	HIS	-	expression tag	UNP I7IIA9
B	-10	HIS	-	expression tag	UNP I7IIA9
B	-9	SER	-	expression tag	UNP I7IIA9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	SER	-	expression tag	UNP I7IIA9
B	-7	GLY	-	expression tag	UNP I7IIA9
B	-6	LEU	-	expression tag	UNP I7IIA9
B	-5	VAL	-	expression tag	UNP I7IIA9
B	-4	PRO	-	expression tag	UNP I7IIA9
B	-3	ARG	-	expression tag	UNP I7IIA9
B	-2	GLY	-	expression tag	UNP I7IIA9
B	-1	SER	-	expression tag	UNP I7IIA9
B	0	HIS	-	expression tag	UNP I7IIA9
C	-15	HIS	-	expression tag	UNP I7IIA9
C	-14	HIS	-	expression tag	UNP I7IIA9
C	-13	HIS	-	expression tag	UNP I7IIA9
C	-12	HIS	-	expression tag	UNP I7IIA9
C	-11	HIS	-	expression tag	UNP I7IIA9
C	-10	HIS	-	expression tag	UNP I7IIA9
C	-9	SER	-	expression tag	UNP I7IIA9
C	-8	SER	-	expression tag	UNP I7IIA9
C	-7	GLY	-	expression tag	UNP I7IIA9
C	-6	LEU	-	expression tag	UNP I7IIA9
C	-5	VAL	-	expression tag	UNP I7IIA9
C	-4	PRO	-	expression tag	UNP I7IIA9
C	-3	ARG	-	expression tag	UNP I7IIA9
C	-2	GLY	-	expression tag	UNP I7IIA9
C	-1	SER	-	expression tag	UNP I7IIA9
C	0	HIS	-	expression tag	UNP I7IIA9
D	-15	HIS	-	expression tag	UNP I7IIA9
D	-14	HIS	-	expression tag	UNP I7IIA9
D	-13	HIS	-	expression tag	UNP I7IIA9
D	-12	HIS	-	expression tag	UNP I7IIA9
D	-11	HIS	-	expression tag	UNP I7IIA9
D	-10	HIS	-	expression tag	UNP I7IIA9
D	-9	SER	-	expression tag	UNP I7IIA9
D	-8	SER	-	expression tag	UNP I7IIA9
D	-7	GLY	-	expression tag	UNP I7IIA9
D	-6	LEU	-	expression tag	UNP I7IIA9
D	-5	VAL	-	expression tag	UNP I7IIA9
D	-4	PRO	-	expression tag	UNP I7IIA9
D	-3	ARG	-	expression tag	UNP I7IIA9
D	-2	GLY	-	expression tag	UNP I7IIA9
D	-1	SER	-	expression tag	UNP I7IIA9
D	0	HIS	-	expression tag	UNP I7IIA9
E	-15	HIS	-	expression tag	UNP I7IIA9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	HIS	-	expression tag	UNP I7IIA9
E	-13	HIS	-	expression tag	UNP I7IIA9
E	-12	HIS	-	expression tag	UNP I7IIA9
E	-11	HIS	-	expression tag	UNP I7IIA9
E	-10	HIS	-	expression tag	UNP I7IIA9
E	-9	SER	-	expression tag	UNP I7IIA9
E	-8	SER	-	expression tag	UNP I7IIA9
E	-7	GLY	-	expression tag	UNP I7IIA9
E	-6	LEU	-	expression tag	UNP I7IIA9
E	-5	VAL	-	expression tag	UNP I7IIA9
E	-4	PRO	-	expression tag	UNP I7IIA9
E	-3	ARG	-	expression tag	UNP I7IIA9
E	-2	GLY	-	expression tag	UNP I7IIA9
E	-1	SER	-	expression tag	UNP I7IIA9
E	0	HIS	-	expression tag	UNP I7IIA9
F	-15	HIS	-	expression tag	UNP I7IIA9
F	-14	HIS	-	expression tag	UNP I7IIA9
F	-13	HIS	-	expression tag	UNP I7IIA9
F	-12	HIS	-	expression tag	UNP I7IIA9
F	-11	HIS	-	expression tag	UNP I7IIA9
F	-10	HIS	-	expression tag	UNP I7IIA9
F	-9	SER	-	expression tag	UNP I7IIA9
F	-8	SER	-	expression tag	UNP I7IIA9
F	-7	GLY	-	expression tag	UNP I7IIA9
F	-6	LEU	-	expression tag	UNP I7IIA9
F	-5	VAL	-	expression tag	UNP I7IIA9
F	-4	PRO	-	expression tag	UNP I7IIA9
F	-3	ARG	-	expression tag	UNP I7IIA9
F	-2	GLY	-	expression tag	UNP I7IIA9
F	-1	SER	-	expression tag	UNP I7IIA9
F	0	HIS	-	expression tag	UNP I7IIA9
G	-15	HIS	-	expression tag	UNP I7IIA9
G	-14	HIS	-	expression tag	UNP I7IIA9
G	-13	HIS	-	expression tag	UNP I7IIA9
G	-12	HIS	-	expression tag	UNP I7IIA9
G	-11	HIS	-	expression tag	UNP I7IIA9
G	-10	HIS	-	expression tag	UNP I7IIA9
G	-9	SER	-	expression tag	UNP I7IIA9
G	-8	SER	-	expression tag	UNP I7IIA9
G	-7	GLY	-	expression tag	UNP I7IIA9
G	-6	LEU	-	expression tag	UNP I7IIA9
G	-5	VAL	-	expression tag	UNP I7IIA9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	PRO	-	expression tag	UNP I7IIA9
G	-3	ARG	-	expression tag	UNP I7IIA9
G	-2	GLY	-	expression tag	UNP I7IIA9
G	-1	SER	-	expression tag	UNP I7IIA9
G	0	HIS	-	expression tag	UNP I7IIA9
H	-15	HIS	-	expression tag	UNP I7IIA9
H	-14	HIS	-	expression tag	UNP I7IIA9
H	-13	HIS	-	expression tag	UNP I7IIA9
H	-12	HIS	-	expression tag	UNP I7IIA9
H	-11	HIS	-	expression tag	UNP I7IIA9
H	-10	HIS	-	expression tag	UNP I7IIA9
H	-9	SER	-	expression tag	UNP I7IIA9
H	-8	SER	-	expression tag	UNP I7IIA9
H	-7	GLY	-	expression tag	UNP I7IIA9
H	-6	LEU	-	expression tag	UNP I7IIA9
H	-5	VAL	-	expression tag	UNP I7IIA9
H	-4	PRO	-	expression tag	UNP I7IIA9
H	-3	ARG	-	expression tag	UNP I7IIA9
H	-2	GLY	-	expression tag	UNP I7IIA9
H	-1	SER	-	expression tag	UNP I7IIA9
H	0	HIS	-	expression tag	UNP I7IIA9
I	-15	HIS	-	expression tag	UNP I7IIA9
I	-14	HIS	-	expression tag	UNP I7IIA9
I	-13	HIS	-	expression tag	UNP I7IIA9
I	-12	HIS	-	expression tag	UNP I7IIA9
I	-11	HIS	-	expression tag	UNP I7IIA9
I	-10	HIS	-	expression tag	UNP I7IIA9
I	-9	SER	-	expression tag	UNP I7IIA9
I	-8	SER	-	expression tag	UNP I7IIA9
I	-7	GLY	-	expression tag	UNP I7IIA9
I	-6	LEU	-	expression tag	UNP I7IIA9
I	-5	VAL	-	expression tag	UNP I7IIA9
I	-4	PRO	-	expression tag	UNP I7IIA9
I	-3	ARG	-	expression tag	UNP I7IIA9
I	-2	GLY	-	expression tag	UNP I7IIA9
I	-1	SER	-	expression tag	UNP I7IIA9
I	0	HIS	-	expression tag	UNP I7IIA9
J	-15	HIS	-	expression tag	UNP I7IIA9
J	-14	HIS	-	expression tag	UNP I7IIA9
J	-13	HIS	-	expression tag	UNP I7IIA9
J	-12	HIS	-	expression tag	UNP I7IIA9
J	-11	HIS	-	expression tag	UNP I7IIA9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-10	HIS	-	expression tag	UNP I7IIA9
J	-9	SER	-	expression tag	UNP I7IIA9
J	-8	SER	-	expression tag	UNP I7IIA9
J	-7	GLY	-	expression tag	UNP I7IIA9
J	-6	LEU	-	expression tag	UNP I7IIA9
J	-5	VAL	-	expression tag	UNP I7IIA9
J	-4	PRO	-	expression tag	UNP I7IIA9
J	-3	ARG	-	expression tag	UNP I7IIA9
J	-2	GLY	-	expression tag	UNP I7IIA9
J	-1	SER	-	expression tag	UNP I7IIA9
J	0	HIS	-	expression tag	UNP I7IIA9
K	-15	HIS	-	expression tag	UNP I7IIA9
K	-14	HIS	-	expression tag	UNP I7IIA9
K	-13	HIS	-	expression tag	UNP I7IIA9
K	-12	HIS	-	expression tag	UNP I7IIA9
K	-11	HIS	-	expression tag	UNP I7IIA9
K	-10	HIS	-	expression tag	UNP I7IIA9
K	-9	SER	-	expression tag	UNP I7IIA9
K	-8	SER	-	expression tag	UNP I7IIA9
K	-7	GLY	-	expression tag	UNP I7IIA9
K	-6	LEU	-	expression tag	UNP I7IIA9
K	-5	VAL	-	expression tag	UNP I7IIA9
K	-4	PRO	-	expression tag	UNP I7IIA9
K	-3	ARG	-	expression tag	UNP I7IIA9
K	-2	GLY	-	expression tag	UNP I7IIA9
K	-1	SER	-	expression tag	UNP I7IIA9
K	0	HIS	-	expression tag	UNP I7IIA9
L	-15	HIS	-	expression tag	UNP I7IIA9
L	-14	HIS	-	expression tag	UNP I7IIA9
L	-13	HIS	-	expression tag	UNP I7IIA9
L	-12	HIS	-	expression tag	UNP I7IIA9
L	-11	HIS	-	expression tag	UNP I7IIA9
L	-10	HIS	-	expression tag	UNP I7IIA9
L	-9	SER	-	expression tag	UNP I7IIA9
L	-8	SER	-	expression tag	UNP I7IIA9
L	-7	GLY	-	expression tag	UNP I7IIA9
L	-6	LEU	-	expression tag	UNP I7IIA9
L	-5	VAL	-	expression tag	UNP I7IIA9
L	-4	PRO	-	expression tag	UNP I7IIA9
L	-3	ARG	-	expression tag	UNP I7IIA9
L	-2	GLY	-	expression tag	UNP I7IIA9
L	-1	SER	-	expression tag	UNP I7IIA9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	0	HIS	-	expression tag	UNP I7IIA9
M	-15	HIS	-	expression tag	UNP I7IIA9
M	-14	HIS	-	expression tag	UNP I7IIA9
M	-13	HIS	-	expression tag	UNP I7IIA9
M	-12	HIS	-	expression tag	UNP I7IIA9
M	-11	HIS	-	expression tag	UNP I7IIA9
M	-10	HIS	-	expression tag	UNP I7IIA9
M	-9	SER	-	expression tag	UNP I7IIA9
M	-8	SER	-	expression tag	UNP I7IIA9
M	-7	GLY	-	expression tag	UNP I7IIA9
M	-6	LEU	-	expression tag	UNP I7IIA9
M	-5	VAL	-	expression tag	UNP I7IIA9
M	-4	PRO	-	expression tag	UNP I7IIA9
M	-3	ARG	-	expression tag	UNP I7IIA9
M	-2	GLY	-	expression tag	UNP I7IIA9
M	-1	SER	-	expression tag	UNP I7IIA9
M	0	HIS	-	expression tag	UNP I7IIA9
N	-15	HIS	-	expression tag	UNP I7IIA9
N	-14	HIS	-	expression tag	UNP I7IIA9
N	-13	HIS	-	expression tag	UNP I7IIA9
N	-12	HIS	-	expression tag	UNP I7IIA9
N	-11	HIS	-	expression tag	UNP I7IIA9
N	-10	HIS	-	expression tag	UNP I7IIA9
N	-9	SER	-	expression tag	UNP I7IIA9
N	-8	SER	-	expression tag	UNP I7IIA9
N	-7	GLY	-	expression tag	UNP I7IIA9
N	-6	LEU	-	expression tag	UNP I7IIA9
N	-5	VAL	-	expression tag	UNP I7IIA9
N	-4	PRO	-	expression tag	UNP I7IIA9
N	-3	ARG	-	expression tag	UNP I7IIA9
N	-2	GLY	-	expression tag	UNP I7IIA9
N	-1	SER	-	expression tag	UNP I7IIA9
N	0	HIS	-	expression tag	UNP I7IIA9
O	-15	HIS	-	expression tag	UNP I7IIA9
O	-14	HIS	-	expression tag	UNP I7IIA9
O	-13	HIS	-	expression tag	UNP I7IIA9
O	-12	HIS	-	expression tag	UNP I7IIA9
O	-11	HIS	-	expression tag	UNP I7IIA9
O	-10	HIS	-	expression tag	UNP I7IIA9
O	-9	SER	-	expression tag	UNP I7IIA9
O	-8	SER	-	expression tag	UNP I7IIA9
O	-7	GLY	-	expression tag	UNP I7IIA9

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-6	LEU	-	expression tag	UNP I7IIA9
O	-5	VAL	-	expression tag	UNP I7IIA9
O	-4	PRO	-	expression tag	UNP I7IIA9
O	-3	ARG	-	expression tag	UNP I7IIA9
O	-2	GLY	-	expression tag	UNP I7IIA9
O	-1	SER	-	expression tag	UNP I7IIA9
O	0	HIS	-	expression tag	UNP I7IIA9
P	-15	HIS	-	expression tag	UNP I7IIA9
P	-14	HIS	-	expression tag	UNP I7IIA9
P	-13	HIS	-	expression tag	UNP I7IIA9
P	-12	HIS	-	expression tag	UNP I7IIA9
P	-11	HIS	-	expression tag	UNP I7IIA9
P	-10	HIS	-	expression tag	UNP I7IIA9
P	-9	SER	-	expression tag	UNP I7IIA9
P	-8	SER	-	expression tag	UNP I7IIA9
P	-7	GLY	-	expression tag	UNP I7IIA9
P	-6	LEU	-	expression tag	UNP I7IIA9
P	-5	VAL	-	expression tag	UNP I7IIA9
P	-4	PRO	-	expression tag	UNP I7IIA9
P	-3	ARG	-	expression tag	UNP I7IIA9
P	-2	GLY	-	expression tag	UNP I7IIA9
P	-1	SER	-	expression tag	UNP I7IIA9
P	0	HIS	-	expression tag	UNP I7IIA9
Q	-15	HIS	-	expression tag	UNP I7IIA9
Q	-14	HIS	-	expression tag	UNP I7IIA9
Q	-13	HIS	-	expression tag	UNP I7IIA9
Q	-12	HIS	-	expression tag	UNP I7IIA9
Q	-11	HIS	-	expression tag	UNP I7IIA9
Q	-10	HIS	-	expression tag	UNP I7IIA9
Q	-9	SER	-	expression tag	UNP I7IIA9
Q	-8	SER	-	expression tag	UNP I7IIA9
Q	-7	GLY	-	expression tag	UNP I7IIA9
Q	-6	LEU	-	expression tag	UNP I7IIA9
Q	-5	VAL	-	expression tag	UNP I7IIA9
Q	-4	PRO	-	expression tag	UNP I7IIA9
Q	-3	ARG	-	expression tag	UNP I7IIA9
Q	-2	GLY	-	expression tag	UNP I7IIA9
Q	-1	SER	-	expression tag	UNP I7IIA9
Q	0	HIS	-	expression tag	UNP I7IIA9
R	-15	HIS	-	expression tag	UNP I7IIA9
R	-14	HIS	-	expression tag	UNP I7IIA9
R	-13	HIS	-	expression tag	UNP I7IIA9

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-12	HIS	-	expression tag	UNP I7IIA9
R	-11	HIS	-	expression tag	UNP I7IIA9
R	-10	HIS	-	expression tag	UNP I7IIA9
R	-9	SER	-	expression tag	UNP I7IIA9
R	-8	SER	-	expression tag	UNP I7IIA9
R	-7	GLY	-	expression tag	UNP I7IIA9
R	-6	LEU	-	expression tag	UNP I7IIA9
R	-5	VAL	-	expression tag	UNP I7IIA9
R	-4	PRO	-	expression tag	UNP I7IIA9
R	-3	ARG	-	expression tag	UNP I7IIA9
R	-2	GLY	-	expression tag	UNP I7IIA9
R	-1	SER	-	expression tag	UNP I7IIA9
R	0	HIS	-	expression tag	UNP I7IIA9
S	-15	HIS	-	expression tag	UNP I7IIA9
S	-14	HIS	-	expression tag	UNP I7IIA9
S	-13	HIS	-	expression tag	UNP I7IIA9
S	-12	HIS	-	expression tag	UNP I7IIA9
S	-11	HIS	-	expression tag	UNP I7IIA9
S	-10	HIS	-	expression tag	UNP I7IIA9
S	-9	SER	-	expression tag	UNP I7IIA9
S	-8	SER	-	expression tag	UNP I7IIA9
S	-7	GLY	-	expression tag	UNP I7IIA9
S	-6	LEU	-	expression tag	UNP I7IIA9
S	-5	VAL	-	expression tag	UNP I7IIA9
S	-4	PRO	-	expression tag	UNP I7IIA9
S	-3	ARG	-	expression tag	UNP I7IIA9
S	-2	GLY	-	expression tag	UNP I7IIA9
S	-1	SER	-	expression tag	UNP I7IIA9
S	0	HIS	-	expression tag	UNP I7IIA9
T	-15	HIS	-	expression tag	UNP I7IIA9
T	-14	HIS	-	expression tag	UNP I7IIA9
T	-13	HIS	-	expression tag	UNP I7IIA9
T	-12	HIS	-	expression tag	UNP I7IIA9
T	-11	HIS	-	expression tag	UNP I7IIA9
T	-10	HIS	-	expression tag	UNP I7IIA9
T	-9	SER	-	expression tag	UNP I7IIA9
T	-8	SER	-	expression tag	UNP I7IIA9
T	-7	GLY	-	expression tag	UNP I7IIA9
T	-6	LEU	-	expression tag	UNP I7IIA9
T	-5	VAL	-	expression tag	UNP I7IIA9
T	-4	PRO	-	expression tag	UNP I7IIA9
T	-3	ARG	-	expression tag	UNP I7IIA9

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-2	GLY	-	expression tag	UNP I7IIA9
T	-1	SER	-	expression tag	UNP I7IIA9
T	0	HIS	-	expression tag	UNP I7IIA9
U	-15	HIS	-	expression tag	UNP I7IIA9
U	-14	HIS	-	expression tag	UNP I7IIA9
U	-13	HIS	-	expression tag	UNP I7IIA9
U	-12	HIS	-	expression tag	UNP I7IIA9
U	-11	HIS	-	expression tag	UNP I7IIA9
U	-10	HIS	-	expression tag	UNP I7IIA9
U	-9	SER	-	expression tag	UNP I7IIA9
U	-8	SER	-	expression tag	UNP I7IIA9
U	-7	GLY	-	expression tag	UNP I7IIA9
U	-6	LEU	-	expression tag	UNP I7IIA9
U	-5	VAL	-	expression tag	UNP I7IIA9
U	-4	PRO	-	expression tag	UNP I7IIA9
U	-3	ARG	-	expression tag	UNP I7IIA9
U	-2	GLY	-	expression tag	UNP I7IIA9
U	-1	SER	-	expression tag	UNP I7IIA9
U	0	HIS	-	expression tag	UNP I7IIA9
V	-15	HIS	-	expression tag	UNP I7IIA9
V	-14	HIS	-	expression tag	UNP I7IIA9
V	-13	HIS	-	expression tag	UNP I7IIA9
V	-12	HIS	-	expression tag	UNP I7IIA9
V	-11	HIS	-	expression tag	UNP I7IIA9
V	-10	HIS	-	expression tag	UNP I7IIA9
V	-9	SER	-	expression tag	UNP I7IIA9
V	-8	SER	-	expression tag	UNP I7IIA9
V	-7	GLY	-	expression tag	UNP I7IIA9
V	-6	LEU	-	expression tag	UNP I7IIA9
V	-5	VAL	-	expression tag	UNP I7IIA9
V	-4	PRO	-	expression tag	UNP I7IIA9
V	-3	ARG	-	expression tag	UNP I7IIA9
V	-2	GLY	-	expression tag	UNP I7IIA9
V	-1	SER	-	expression tag	UNP I7IIA9
V	0	HIS	-	expression tag	UNP I7IIA9
W	-15	HIS	-	expression tag	UNP I7IIA9
W	-14	HIS	-	expression tag	UNP I7IIA9
W	-13	HIS	-	expression tag	UNP I7IIA9
W	-12	HIS	-	expression tag	UNP I7IIA9
W	-11	HIS	-	expression tag	UNP I7IIA9
W	-10	HIS	-	expression tag	UNP I7IIA9
W	-9	SER	-	expression tag	UNP I7IIA9

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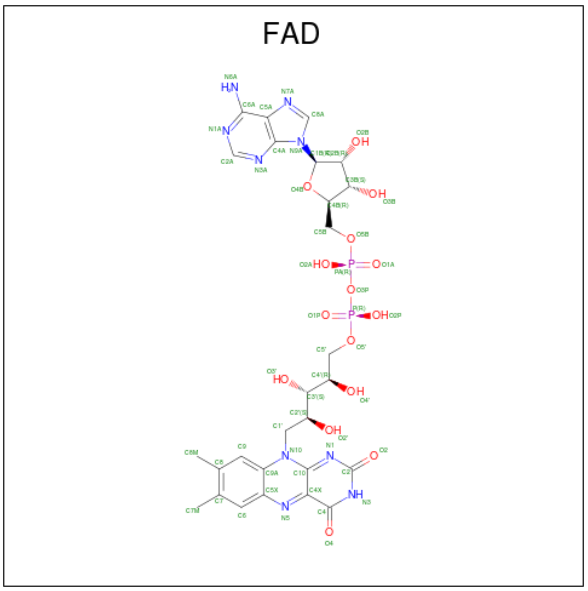
Chain	Residue	Modelled	Actual	Comment	Reference
W	-8	SER	-	expression tag	UNP I7IIA9
W	-7	GLY	-	expression tag	UNP I7IIA9
W	-6	LEU	-	expression tag	UNP I7IIA9
W	-5	VAL	-	expression tag	UNP I7IIA9
W	-4	PRO	-	expression tag	UNP I7IIA9
W	-3	ARG	-	expression tag	UNP I7IIA9
W	-2	GLY	-	expression tag	UNP I7IIA9
W	-1	SER	-	expression tag	UNP I7IIA9
W	0	HIS	-	expression tag	UNP I7IIA9
X	-15	HIS	-	expression tag	UNP I7IIA9
X	-14	HIS	-	expression tag	UNP I7IIA9
X	-13	HIS	-	expression tag	UNP I7IIA9
X	-12	HIS	-	expression tag	UNP I7IIA9
X	-11	HIS	-	expression tag	UNP I7IIA9
X	-10	HIS	-	expression tag	UNP I7IIA9
X	-9	SER	-	expression tag	UNP I7IIA9
X	-8	SER	-	expression tag	UNP I7IIA9
X	-7	GLY	-	expression tag	UNP I7IIA9
X	-6	LEU	-	expression tag	UNP I7IIA9
X	-5	VAL	-	expression tag	UNP I7IIA9
X	-4	PRO	-	expression tag	UNP I7IIA9
X	-3	ARG	-	expression tag	UNP I7IIA9
X	-2	GLY	-	expression tag	UNP I7IIA9
X	-1	SER	-	expression tag	UNP I7IIA9
X	0	HIS	-	expression tag	UNP I7IIA9

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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		
2	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	J	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	L	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	N	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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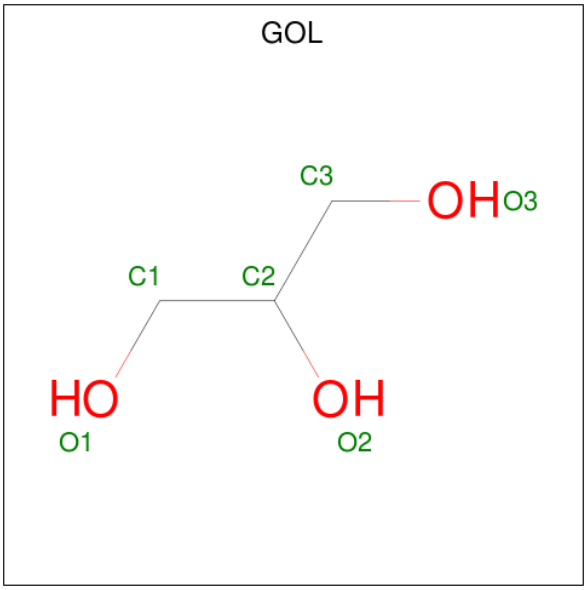
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	P	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	Q	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	R	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	S	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	T	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	U	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	V	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	W	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	X	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	N	1	Total	C	O	0	0
			6	3	3		
3	O	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		
3	Q	1	Total	C	O	0	0
			6	3	3		
3	R	1	Total	C	O	0	0
			6	3	3		
3	S	1	Total	C	O	0	0
			6	3	3		
3	T	1	Total	C	O	0	0
			6	3	3		
3	U	1	Total	C	O	0	0
			6	3	3		
3	V	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	W	1	Total C O 6 3 3	0	0
3	X	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	198	Total O 198 198	0	0
4	B	229	Total O 229 229	0	0
4	C	218	Total O 218 218	0	0
4	D	199	Total O 199 199	0	0
4	E	197	Total O 197 197	0	0
4	F	199	Total O 199 199	0	0
4	G	170	Total O 170 170	0	0
4	H	228	Total O 228 228	0	0
4	I	180	Total O 180 180	0	0
4	J	179	Total O 179 179	0	0
4	K	175	Total O 175 175	0	0
4	L	201	Total O 201 201	0	0
4	M	188	Total O 188 188	0	0
4	N	207	Total O 207 207	0	0
4	O	214	Total O 214 214	0	0
4	P	184	Total O 184 184	0	0
4	Q	218	Total O 218 218	0	0

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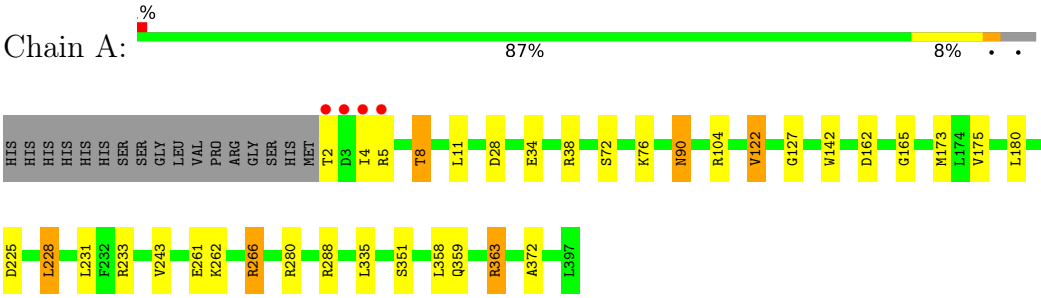
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	R	190	Total O 190 190	0	0
4	S	186	Total O 186 186	0	0
4	T	204	Total O 204 204	0	0
4	U	180	Total O 180 180	0	0
4	V	191	Total O 191 191	0	0
4	W	176	Total O 176 176	0	0
4	X	168	Total O 168 168	0	0

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.

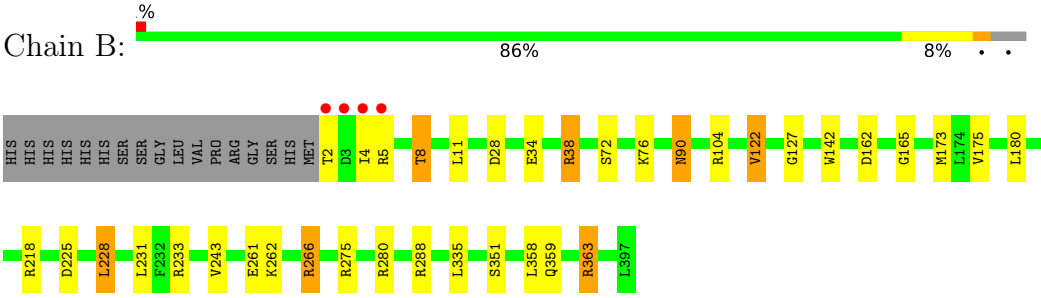
- Molecule 1: XiaF protein

Chain A:



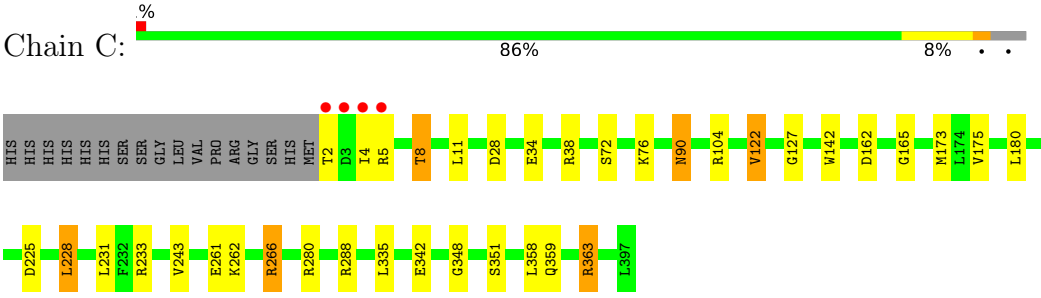
- Molecule 1: XiaF protein

Chain B:



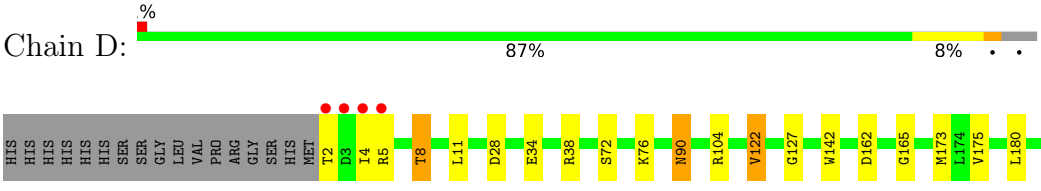
- Molecule 1: XiaF protein

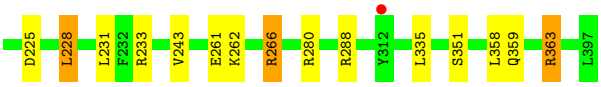
Chain C:



- Molecule 1: XiaF protein

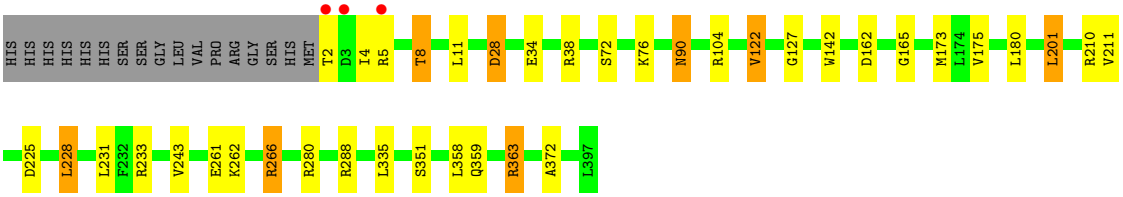
Chain D:





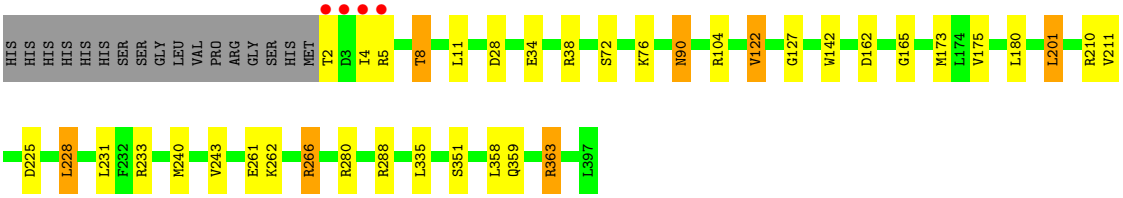
• Molecule 1: XiaF protein

Chain E:



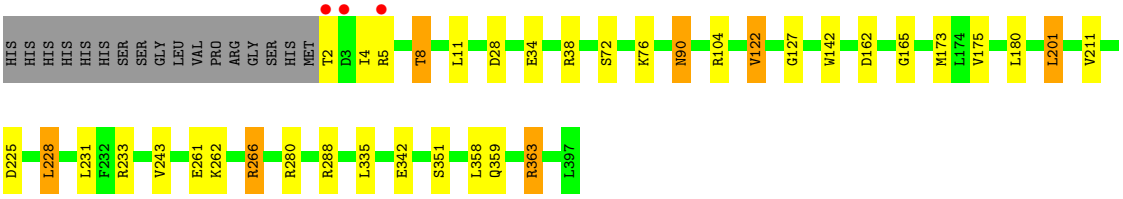
• Molecule 1: XiaF protein

Chain F:



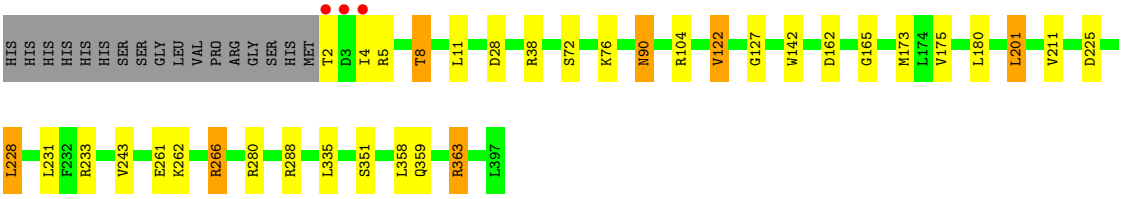
• Molecule 1: XiaF protein

Chain G:



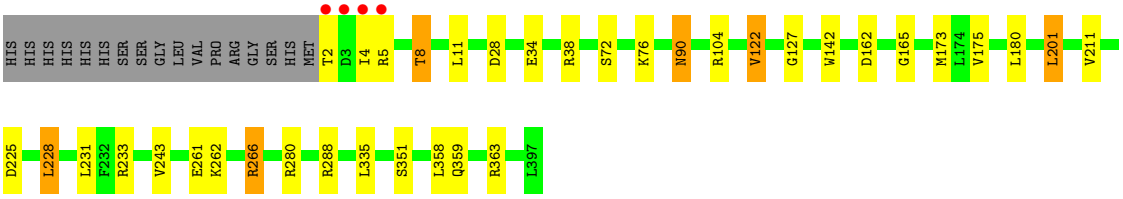
• Molecule 1: XiaF protein

Chain H:



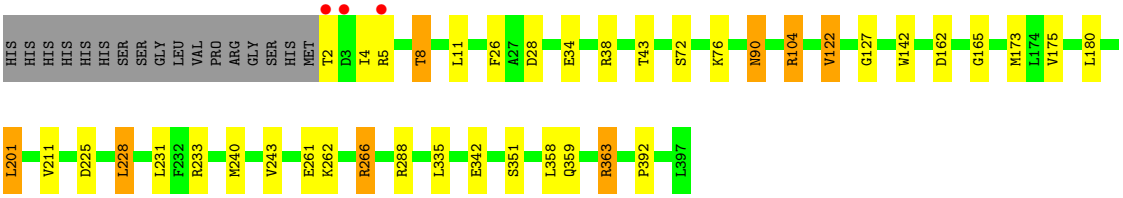
• Molecule 1: XiaF protein

Chain I:



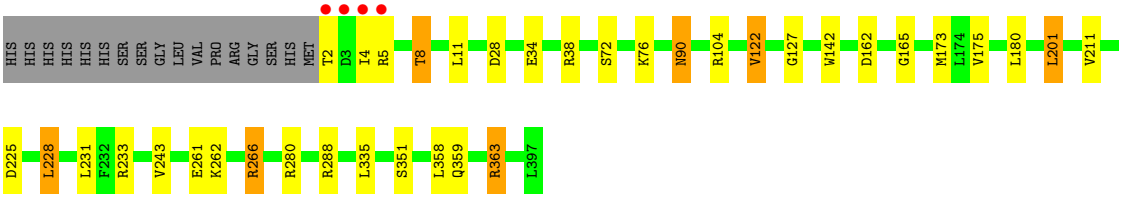
• Molecule 1: XiaF protein

Chain J:



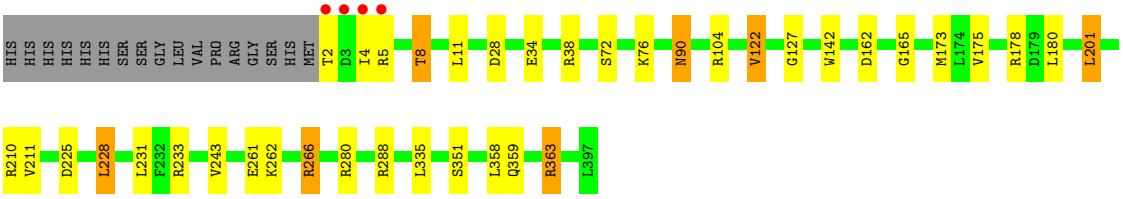
• Molecule 1: XiaF protein

Chain K:



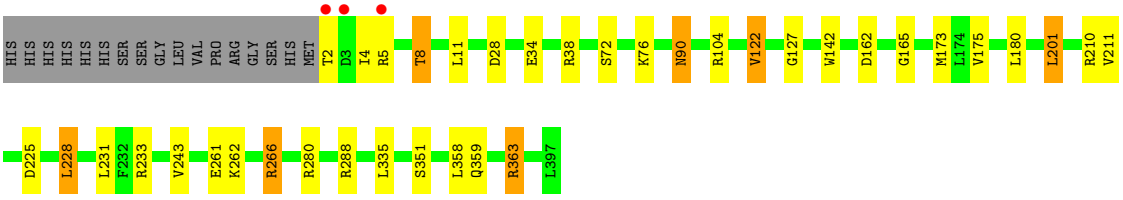
• Molecule 1: XiaF protein

Chain L:



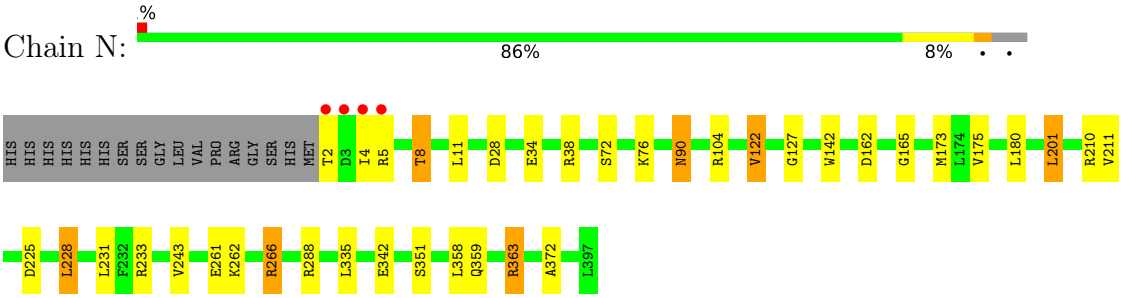
• Molecule 1: XiaF protein

Chain M:



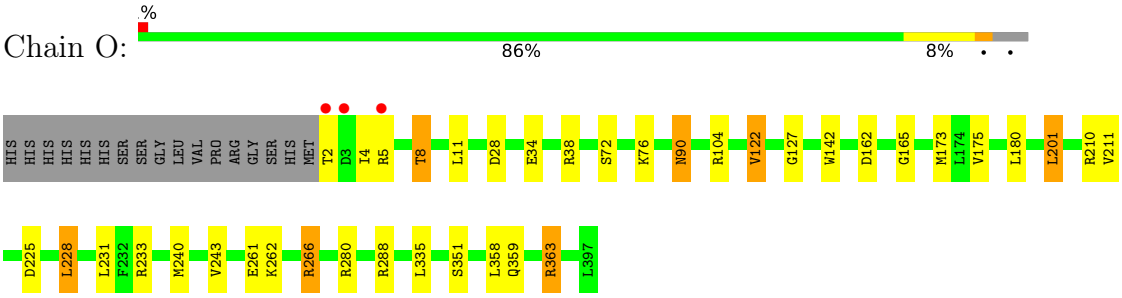
• Molecule 1: XiaF protein

Chain N:



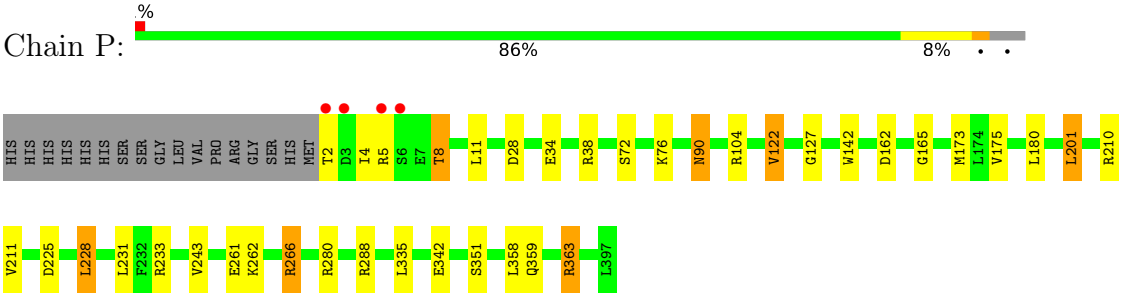
• Molecule 1: XiaF protein

Chain O:



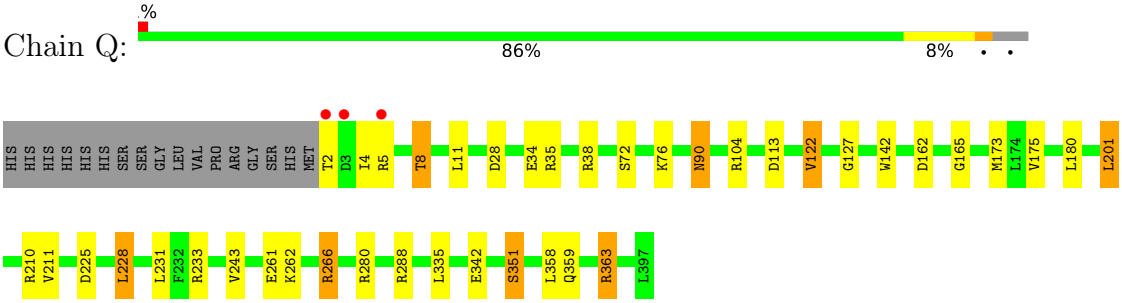
• Molecule 1: XiaF protein

Chain P:



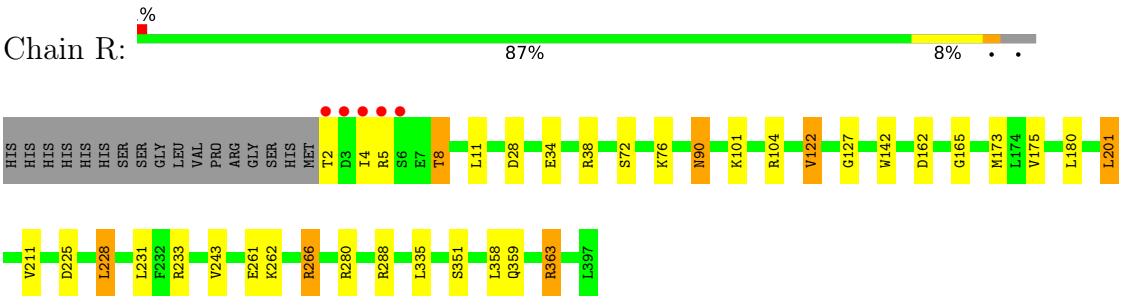
• Molecule 1: XiaF protein

Chain Q:



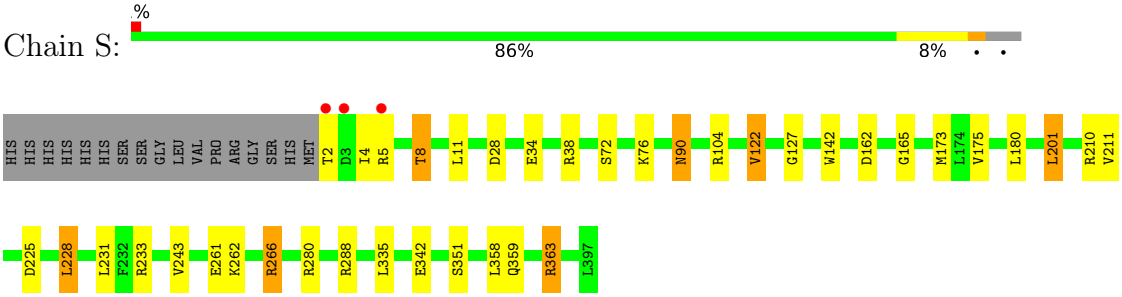
• Molecule 1: XiaF protein

Chain R:



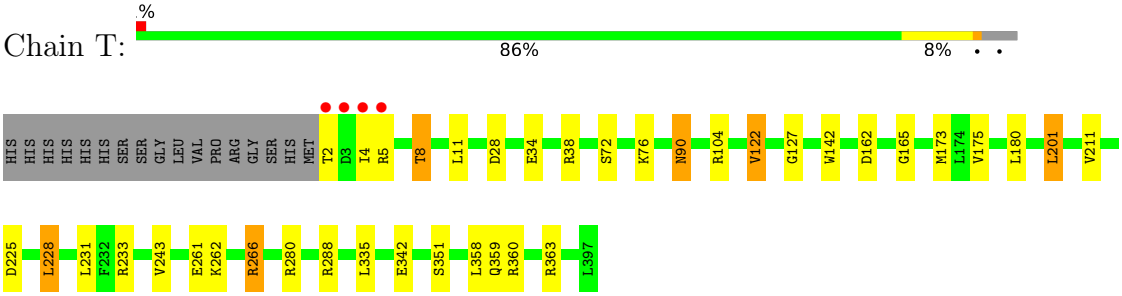
• Molecule 1: XiaF protein

Chain S:



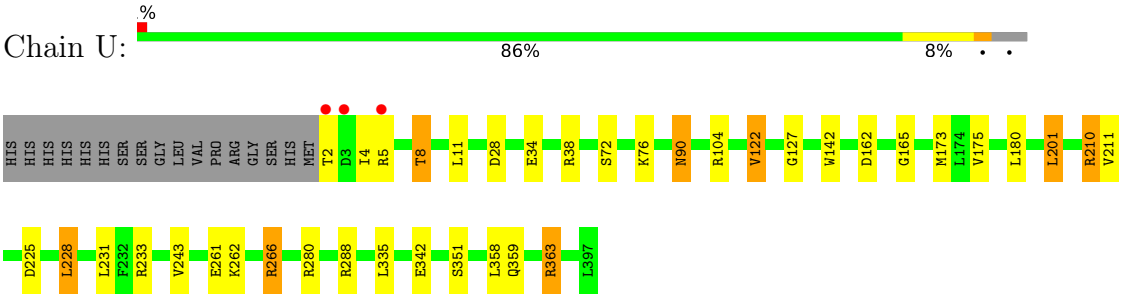
• Molecule 1: XiaF protein

Chain T:



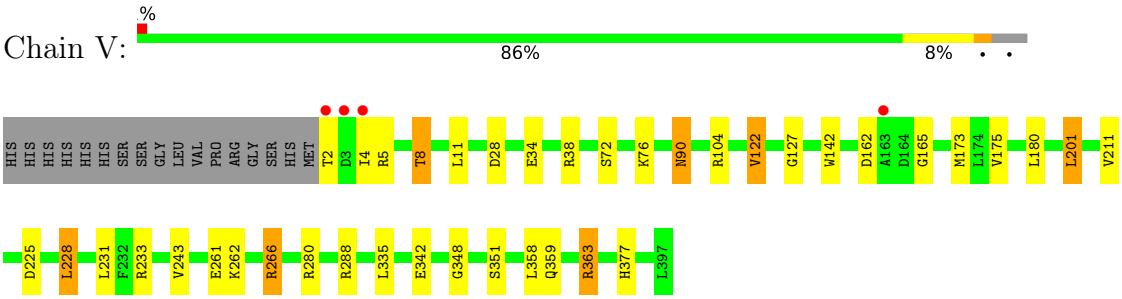
• Molecule 1: XiaF protein

Chain U:



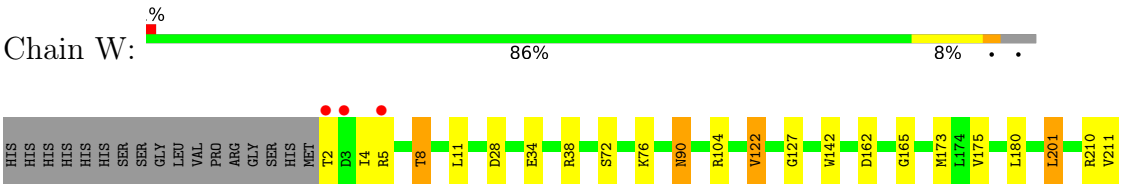
• Molecule 1: XiaF protein

Chain V:

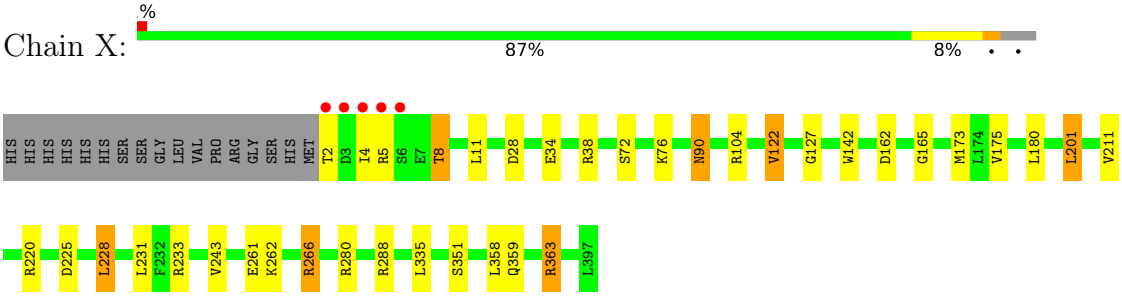


• Molecule 1: XiaF protein

Chain W:



• Molecule 1: XiaF protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	166.93Å 167.09Å 200.94Å 89.96° 90.18° 119.82°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (15.00-2.40) 94.5 (15.00-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.198 , 0.229 0.199 , 0.228	Depositor DCC
R_{free} test set	35038 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 16.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.58$, $< L^2 > = 0.42$	Xtriage
Estimated twinning fraction	0.025 for -k,h+k,l 0.025 for h+k,-h,l 0.019 for -h-k,h,l 0.019 for k,-h-k,l 0.017 for h,-h-k,-l 0.419 for -h-k,k,-l 0.025 for -h,-k,l 0.026 for -k,-h,-l 0.026 for k,h,-l 0.025 for -h,h+k,-l 0.025 for h+k,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	77543	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0361e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, GOL

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	0.63	0/3038	0.80	4/4141 (0.1%)
1	B	0.62	0/3038	0.80	6/4141 (0.1%)
1	C	0.63	0/3038	0.80	4/4141 (0.1%)
1	D	0.61	0/3038	0.80	5/4141 (0.1%)
1	E	0.63	0/3038	0.81	5/4141 (0.1%)
1	F	0.62	0/3038	0.80	5/4141 (0.1%)
1	G	0.64	0/3038	0.80	5/4141 (0.1%)
1	H	0.62	0/3038	0.80	5/4141 (0.1%)
1	I	0.61	0/3038	0.79	3/4141 (0.1%)
1	J	0.61	0/3038	0.79	4/4141 (0.1%)
1	K	0.61	0/3038	0.79	5/4141 (0.1%)
1	L	0.61	0/3038	0.80	4/4141 (0.1%)
1	M	0.61	0/3038	0.79	5/4141 (0.1%)
1	N	0.62	0/3038	0.79	4/4141 (0.1%)
1	O	0.62	0/3038	0.80	4/4141 (0.1%)
1	P	0.61	0/3038	0.79	5/4141 (0.1%)
1	Q	0.63	1/3038 (0.0%)	0.80	5/4141 (0.1%)
1	R	0.61	0/3038	0.79	4/4141 (0.1%)
1	S	0.62	0/3038	0.79	5/4141 (0.1%)
1	T	0.61	0/3038	0.79	3/4141 (0.1%)
1	U	0.61	0/3038	0.80	6/4141 (0.1%)
1	V	0.62	0/3038	0.79	5/4141 (0.1%)
1	W	0.61	0/3038	0.79	5/4141 (0.1%)
1	X	0.61	0/3038	0.79	5/4141 (0.1%)
All	All	0.62	1/72912 (0.0%)	0.80	111/99384 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	351	SER	CB-OG	-5.26	1.35	1.42

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	288	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	U	288	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	N	288	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	W	288	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	A	288	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	O	288	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	Q	288	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	R	288	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	X	288	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	M	288	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	H	288	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	E	288	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	B	288	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	S	288	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	G	288	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	T	288	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	F	288	ARG	NE-CZ-NH2	6.71	123.65	120.30
1	K	288	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	P	288	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	C	288	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	V	288	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	J	127	GLY	N-CA-C	-6.34	97.24	113.10
1	X	127	GLY	N-CA-C	-6.33	97.27	113.10
1	T	127	GLY	N-CA-C	-6.31	97.32	113.10
1	I	288	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	D	288	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	B	127	GLY	N-CA-C	-6.29	97.39	113.10
1	K	127	GLY	N-CA-C	-6.28	97.41	113.10
1	H	127	GLY	N-CA-C	-6.28	97.41	113.10
1	O	127	GLY	N-CA-C	-6.25	97.47	113.10
1	L	288	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	W	127	GLY	N-CA-C	-6.24	97.51	113.10
1	M	127	GLY	N-CA-C	-6.23	97.53	113.10
1	H	288	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	R	127	GLY	N-CA-C	-6.22	97.56	113.10
1	D	127	GLY	N-CA-C	-6.21	97.58	113.10
1	N	127	GLY	N-CA-C	-6.20	97.59	113.10
1	E	127	GLY	N-CA-C	-6.19	97.62	113.10
1	F	127	GLY	N-CA-C	-6.18	97.64	113.10
1	P	127	GLY	N-CA-C	-6.18	97.64	113.10
1	I	127	GLY	N-CA-C	-6.18	97.65	113.10
1	A	127	GLY	N-CA-C	-6.17	97.67	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	127	GLY	N-CA-C	-6.15	97.72	113.10
1	U	127	GLY	N-CA-C	-6.15	97.72	113.10
1	Q	127	GLY	N-CA-C	-6.14	97.74	113.10
1	N	288	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	C	127	GLY	N-CA-C	-6.13	97.77	113.10
1	G	127	GLY	N-CA-C	-6.10	97.84	113.10
1	J	288	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	V	127	GLY	N-CA-C	-6.09	97.87	113.10
1	L	127	GLY	N-CA-C	-6.04	97.99	113.10
1	S	288	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	288	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	S	363	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	X	288	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	O	288	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	R	288	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	U	363	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	U	288	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	S	363	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	M	288	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	T	288	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	F	288	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	W	363	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	W	288	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	E	288	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	C	288	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	F	363	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	D	363	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	I	288	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	B	288	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	V	363	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	G	288	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	J	363	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	O	363	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	W	363	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	M	363	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	G	363	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	U	363	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	N	363	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	363	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	K	288	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	P	288	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	H	363	ARG	NE-CZ-NH1	-5.47	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	363	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	Q	363	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	M	363	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	E	363	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	X	363	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	L	288	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	K	363	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	D	210	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	Q	288	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	V	363	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	B	363	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	X	363	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	J	288	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	H	363	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	C	363	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	P	363	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	B	210	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	L	363	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	B	363	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	R	363	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	Q	363	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	K	363	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	F	210	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	E	210	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	P	363	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	U	210	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	V	288	ARG	NE-CZ-NH1	-5.01	117.79	120.30

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	2977	0	2939	21	0
1	B	2977	0	2939	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2977	0	2939	22	0
1	D	2977	0	2939	20	0
1	E	2977	0	2939	23	0
1	F	2977	0	2939	23	0
1	G	2977	0	2939	21	0
1	H	2977	0	2939	19	0
1	I	2977	0	2939	20	0
1	J	2977	0	2939	23	0
1	K	2977	0	2939	18	0
1	L	2977	0	2939	21	0
1	M	2977	0	2939	21	0
1	N	2977	0	2939	22	0
1	O	2977	0	2939	21	0
1	P	2977	0	2939	22	0
1	Q	2977	0	2939	23	0
1	R	2977	0	2939	21	0
1	S	2977	0	2939	23	0
1	T	2977	0	2939	22	0
1	U	2977	0	2939	21	0
1	V	2977	0	2939	23	0
1	W	2977	0	2939	22	0
1	X	2977	0	2939	21	0
2	A	53	0	31	3	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	3	0
2	E	53	0	31	2	0
2	F	53	0	31	2	0
2	G	53	0	31	0	0
2	H	53	0	31	0	0
2	I	53	0	31	1	0
2	J	53	0	31	1	0
2	K	53	0	31	2	0
2	L	53	0	31	2	0
2	M	53	0	31	0	0
2	N	53	0	31	2	0
2	O	53	0	31	2	0
2	P	53	0	31	1	0
2	Q	53	0	31	1	0
2	R	53	0	31	0	0
2	S	53	0	31	1	0
2	T	53	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	U	53	0	31	1	0
2	V	53	0	31	1	0
2	W	53	0	31	2	0
2	X	53	0	31	2	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	1	0
3	G	6	0	8	1	0
3	H	6	0	8	0	0
3	I	6	0	8	0	0
3	J	6	0	8	0	0
3	K	6	0	8	1	0
3	L	6	0	8	1	0
3	M	6	0	8	0	0
3	N	6	0	8	0	0
3	O	6	0	8	0	0
3	P	6	0	8	0	0
3	Q	6	0	8	0	0
3	R	6	0	8	0	0
3	S	6	0	8	0	0
3	T	6	0	8	1	0
3	U	6	0	8	1	0
3	V	6	0	8	0	0
3	W	6	0	8	1	0
3	X	6	0	8	1	0
4	A	198	0	0	0	0
4	B	229	0	0	4	0
4	C	218	0	0	1	0
4	D	199	0	0	1	0
4	E	197	0	0	1	0
4	F	199	0	0	4	0
4	G	170	0	0	1	0
4	H	228	0	0	0	0
4	I	180	0	0	1	0
4	J	179	0	0	3	0
4	K	175	0	0	2	0
4	L	201	0	0	3	0
4	M	188	0	0	3	0
4	N	207	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	214	0	0	4	0
4	P	184	0	0	2	0
4	Q	218	0	0	2	0
4	R	190	0	0	2	0
4	S	186	0	0	1	0
4	T	204	0	0	2	0
4	U	180	0	0	2	0
4	V	191	0	0	2	0
4	W	176	0	0	3	0
4	X	168	0	0	2	0
All	All	77543	0	71472	547	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 (547) 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)
3:K:602:GOL:O3	4:K:701:HOH:O	1.60	1.18
2:L:601:FAD:H52A	2:L:601:FAD:H8A	1.15	1.08
2:L:601:FAD:H52A	2:L:601:FAD:C8A	1.90	1.02
1:W:90:ASN:OD1	1:W:243:VAL:HG23	1.64	0.98
1:N:90:ASN:OD1	1:N:243:VAL:HG23	1.64	0.98
1:S:90:ASN:OD1	1:S:243:VAL:HG23	1.64	0.98
1:J:90:ASN:OD1	1:J:243:VAL:HG23	1.64	0.98
1:D:90:ASN:OD1	1:D:243:VAL:HG23	1.64	0.97
1:P:90:ASN:OD1	1:P:243:VAL:HG23	1.64	0.97
1:B:90:ASN:OD1	1:B:243:VAL:HG23	1.63	0.97
1:F:90:ASN:OD1	1:F:243:VAL:HG23	1.63	0.97
1:L:90:ASN:OD1	1:L:243:VAL:HG23	1.64	0.97
1:H:90:ASN:OD1	1:H:243:VAL:HG23	1.65	0.97
1:U:90:ASN:OD1	1:U:243:VAL:HG23	1.64	0.97
1:A:90:ASN:OD1	1:A:243:VAL:HG23	1.64	0.97
1:Q:90:ASN:OD1	1:Q:243:VAL:HG23	1.64	0.97
1:E:90:ASN:OD1	1:E:243:VAL:HG23	1.65	0.96
1:R:90:ASN:OD1	1:R:243:VAL:HG23	1.64	0.96
1:V:90:ASN:OD1	1:V:243:VAL:HG23	1.65	0.96
1:I:90:ASN:OD1	1:I:243:VAL:HG23	1.64	0.96
1:M:90:ASN:OD1	1:M:243:VAL:HG23	1.63	0.96
1:K:90:ASN:OD1	1:K:243:VAL:HG23	1.65	0.96
1:G:90:ASN:OD1	1:G:243:VAL:HG23	1.64	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:90:ASN:OD1	1:O:243:VAL:HG23	1.65	0.95
1:T:90:ASN:OD1	1:T:243:VAL:HG23	1.64	0.95
1:C:90:ASN:OD1	1:C:243:VAL:HG23	1.64	0.95
1:X:90:ASN:OD1	1:X:243:VAL:HG23	1.64	0.95
1:R:4:ILE:O	1:R:8:THR:HG22	1.71	0.91
1:S:4:ILE:O	1:S:8:THR:HG22	1.71	0.90
1:V:4:ILE:O	1:V:8:THR:HG22	1.71	0.90
1:D:4:ILE:O	1:D:8:THR:HG22	1.71	0.90
1:E:4:ILE:O	1:E:8:THR:HG22	1.72	0.90
1:M:4:ILE:O	1:M:8:THR:HG22	1.71	0.90
1:H:4:ILE:O	1:H:8:THR:HG22	1.72	0.90
1:A:4:ILE:O	1:A:8:THR:HG22	1.72	0.90
1:O:4:ILE:O	1:O:8:THR:HG22	1.71	0.90
1:W:4:ILE:O	1:W:8:THR:HG22	1.72	0.90
1:I:4:ILE:O	1:I:8:THR:HG22	1.72	0.90
1:P:4:ILE:O	1:P:8:THR:HG22	1.71	0.90
1:N:4:ILE:O	1:N:8:THR:HG22	1.71	0.90
1:Q:4:ILE:O	1:Q:8:THR:HG22	1.71	0.89
1:L:4:ILE:O	1:L:8:THR:HG22	1.72	0.89
1:G:4:ILE:O	1:G:8:THR:HG22	1.71	0.89
1:F:4:ILE:O	1:F:8:THR:HG22	1.71	0.89
1:C:4:ILE:O	1:C:8:THR:HG22	1.72	0.89
1:B:4:ILE:O	1:B:8:THR:HG22	1.72	0.89
1:K:4:ILE:O	1:K:8:THR:HG22	1.73	0.89
1:U:4:ILE:O	1:U:8:THR:HG22	1.72	0.88
1:T:4:ILE:O	1:T:8:THR:HG22	1.72	0.88
1:J:4:ILE:O	1:J:8:THR:HG22	1.73	0.88
1:X:4:ILE:O	1:X:8:THR:HG22	1.72	0.88
3:L:602:GOL:O1	4:L:701:HOH:O	2.03	0.76
2:F:601:FAD:N6A	3:F:602:GOL:O2	2.20	0.75
1:F:240:MET:SD	4:F:826:HOH:O	2.48	0.71
2:T:601:FAD:N6A	3:T:602:GOL:O2	2.24	0.70
3:U:602:GOL:O1	4:U:701:HOH:O	2.10	0.69
1:K:359:GLN:OE1	1:K:363:ARG:NH2	2.26	0.67
1:C:359:GLN:OE1	1:C:363:ARG:NH2	2.27	0.67
1:I:359:GLN:OE1	1:I:363:ARG:NH2	2.27	0.67
1:X:359:GLN:OE1	1:X:363:ARG:NH2	2.27	0.67
1:J:359:GLN:OE1	1:J:363:ARG:NH2	2.27	0.66
1:I:280:ARG:HD3	4:I:702:HOH:O	1.93	0.66
1:H:359:GLN:OE1	1:H:363:ARG:NH2	2.28	0.66
1:E:28:ASP:OD1	4:E:701:HOH:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:359:GLN:OE1	1:N:363:ARG:NH2	2.28	0.66
1:A:359:GLN:OE1	1:A:363:ARG:NH2	2.28	0.66
1:D:359:GLN:OE1	1:D:363:ARG:NH2	2.28	0.66
1:E:359:GLN:OE1	1:E:363:ARG:NH2	2.28	0.66
1:M:359:GLN:OE1	1:M:363:ARG:NH2	2.28	0.66
1:O:359:GLN:OE1	1:O:363:ARG:NH2	2.28	0.66
1:L:359:GLN:OE1	1:L:363:ARG:NH2	2.28	0.65
1:S:359:GLN:OE1	1:S:363:ARG:NH2	2.29	0.65
2:O:601:FAD:O1A	4:O:701:HOH:O	2.14	0.65
1:Q:359:GLN:OE1	1:Q:363:ARG:NH2	2.28	0.65
1:U:359:GLN:OE1	1:U:363:ARG:NH2	2.28	0.65
1:T:359:GLN:OE1	1:T:363:ARG:NH2	2.28	0.65
1:V:359:GLN:OE1	1:V:363:ARG:NH2	2.29	0.65
1:R:359:GLN:OE1	1:R:363:ARG:NH2	2.29	0.65
1:G:359:GLN:OE1	1:G:363:ARG:NH2	2.29	0.64
1:B:359:GLN:OE1	1:B:363:ARG:NH2	2.28	0.64
1:F:359:GLN:OE1	1:F:363:ARG:NH2	2.29	0.64
1:W:359:GLN:OE1	1:W:363:ARG:NH2	2.30	0.64
1:P:359:GLN:OE1	1:P:363:ARG:NH2	2.30	0.64
1:E:28:ASP:OD1	1:Q:35:ARG:NH1	2.32	0.62
1:O:240:MET:SD	4:O:829:HOH:O	2.56	0.60
1:L:122:VAL:HG21	1:L:142:TRP:HB3	1.84	0.60
1:T:122:VAL:HG21	1:T:142:TRP:HB3	1.84	0.60
4:B:885:HOH:O	1:C:342:GLU:HG2	2.01	0.59
1:N:122:VAL:HG21	1:N:142:TRP:HB3	1.84	0.59
1:X:122:VAL:HG21	1:X:142:TRP:HB3	1.84	0.59
1:C:122:VAL:HG21	1:C:142:TRP:HB3	1.85	0.59
1:P:122:VAL:HG21	1:P:142:TRP:HB3	1.85	0.59
1:H:122:VAL:HG21	1:H:142:TRP:HB3	1.84	0.59
1:J:122:VAL:HG21	1:J:142:TRP:HB3	1.85	0.59
1:B:122:VAL:HG21	1:B:142:TRP:HB3	1.85	0.59
1:D:122:VAL:HG21	1:D:142:TRP:HB3	1.85	0.59
1:G:122:VAL:HG21	1:G:142:TRP:HB3	1.85	0.59
1:S:122:VAL:HG21	1:S:142:TRP:HB3	1.85	0.58
1:E:122:VAL:HG21	1:E:142:TRP:HB3	1.84	0.58
1:U:122:VAL:HG21	1:U:142:TRP:HB3	1.85	0.58
1:W:122:VAL:HG21	1:W:142:TRP:HB3	1.85	0.58
1:O:122:VAL:HG21	1:O:142:TRP:HB3	1.84	0.58
1:K:122:VAL:HG21	1:K:142:TRP:HB3	1.85	0.58
1:Q:122:VAL:HG21	1:Q:142:TRP:HB3	1.86	0.58
1:V:122:VAL:HG21	1:V:142:TRP:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:VAL:HG21	1:I:142:TRP:HB3	1.85	0.58
1:R:122:VAL:HG21	1:R:142:TRP:HB3	1.85	0.58
1:A:122:VAL:HG21	1:A:142:TRP:HB3	1.85	0.58
1:M:122:VAL:HG21	1:M:142:TRP:HB3	1.85	0.57
1:F:122:VAL:HG21	1:F:142:TRP:HB3	1.87	0.57
1:P:280:ARG:NH2	4:P:701:HOH:O	2.35	0.56
4:F:857:HOH:O	1:G:342:GLU:HG2	2.04	0.56
1:A:372:ALA:HB2	2:A:601:FAD:H3'	1.88	0.56
4:Q:878:HOH:O	1:T:342:GLU:HG2	2.04	0.56
2:D:601:FAD:O1P	4:D:701:HOH:O	2.18	0.55
1:S:175:VAL:CG2	1:S:180:LEU:HD21	2.38	0.55
1:C:210:ARG:NH1	4:C:701:HOH:O	2.40	0.54
1:A:175:VAL:CG2	1:A:180:LEU:HD21	2.38	0.54
1:G:175:VAL:CG2	1:G:180:LEU:HD21	2.38	0.54
1:E:175:VAL:CG2	1:E:180:LEU:HD21	2.38	0.54
1:C:175:VAL:CG2	1:C:180:LEU:HD21	2.38	0.54
1:M:175:VAL:CG2	1:M:180:LEU:HD21	2.38	0.54
1:V:175:VAL:CG2	1:V:180:LEU:HD21	2.38	0.54
1:G:175:VAL:HG22	1:G:180:LEU:HD21	1.90	0.53
1:A:175:VAL:HG22	1:A:180:LEU:HD21	1.90	0.53
1:Q:175:VAL:CG2	1:Q:180:LEU:HD21	2.38	0.53
1:T:175:VAL:CG2	1:T:180:LEU:HD21	2.39	0.53
1:C:175:VAL:HG22	1:C:180:LEU:HD21	1.91	0.53
1:D:175:VAL:CG2	1:D:180:LEU:HD21	2.39	0.53
1:J:175:VAL:CG2	1:J:180:LEU:HD21	2.38	0.53
1:K:175:VAL:CG2	1:K:180:LEU:HD21	2.38	0.53
1:L:280:ARG:NH2	4:L:702:HOH:O	2.42	0.53
1:U:175:VAL:CG2	1:U:180:LEU:HD21	2.39	0.53
1:O:175:VAL:CG2	1:O:180:LEU:HD21	2.39	0.53
1:S:175:VAL:HG22	1:S:180:LEU:HD21	1.91	0.53
1:X:175:VAL:CG2	1:X:180:LEU:HD21	2.39	0.53
1:H:175:VAL:CG2	1:H:180:LEU:HD21	2.39	0.53
1:F:175:VAL:CG2	1:F:180:LEU:HD21	2.39	0.53
1:P:175:VAL:CG2	1:P:180:LEU:HD21	2.39	0.52
1:E:175:VAL:HG22	1:E:180:LEU:HD21	1.91	0.52
1:J:175:VAL:HG22	1:J:180:LEU:HD21	1.91	0.52
1:P:175:VAL:HG22	1:P:180:LEU:HD21	1.92	0.52
1:B:175:VAL:CG2	1:B:180:LEU:HD21	2.40	0.52
1:D:175:VAL:HG22	1:D:180:LEU:HD21	1.92	0.52
1:N:175:VAL:CG2	1:N:180:LEU:HD21	2.39	0.52
1:R:175:VAL:CG2	1:R:180:LEU:HD21	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:175:VAL:CG2	1:W:180:LEU:HD21	2.40	0.52
1:L:175:VAL:CG2	1:L:180:LEU:HD21	2.40	0.52
1:I:175:VAL:CG2	1:I:180:LEU:HD21	2.40	0.51
1:T:175:VAL:HG22	1:T:180:LEU:HD21	1.92	0.51
1:N:175:VAL:HG22	1:N:180:LEU:HD21	1.92	0.51
1:U:175:VAL:HG22	1:U:180:LEU:HD21	1.91	0.51
1:V:175:VAL:HG22	1:V:180:LEU:HD21	1.93	0.51
1:H:175:VAL:HG22	1:H:180:LEU:HD21	1.93	0.51
1:L:175:VAL:HG22	1:L:180:LEU:HD21	1.93	0.51
1:X:175:VAL:HG22	1:X:180:LEU:HD21	1.93	0.51
1:F:175:VAL:HG22	1:F:180:LEU:HD21	1.92	0.51
1:K:175:VAL:HG22	1:K:180:LEU:HD21	1.92	0.51
1:D:351:SER:HB3	1:D:358:LEU:HD23	1.93	0.51
1:J:342:GLU:HG2	4:K:841:HOH:O	2.10	0.51
1:W:210:ARG:NH1	4:W:706:HOH:O	2.44	0.51
1:M:175:VAL:HG22	1:M:180:LEU:HD21	1.92	0.51
1:M:210:ARG:NH1	4:M:706:HOH:O	2.44	0.51
1:W:175:VAL:HG22	1:W:180:LEU:HD21	1.93	0.50
1:H:351:SER:HB3	1:H:358:LEU:HD23	1.93	0.50
1:Q:342:GLU:HG2	4:T:861:HOH:O	2.11	0.50
1:K:351:SER:HB3	1:K:358:LEU:HD23	1.94	0.50
4:R:849:HOH:O	1:S:342:GLU:HG2	2.11	0.50
1:I:175:VAL:HG22	1:I:180:LEU:HD21	1.93	0.50
1:R:175:VAL:HG22	1:R:180:LEU:HD21	1.94	0.50
1:Q:175:VAL:HG22	1:Q:180:LEU:HD21	1.93	0.50
1:B:175:VAL:HG22	1:B:180:LEU:HD21	1.93	0.49
4:M:857:HOH:O	1:P:342:GLU:HG2	2.11	0.49
1:N:351:SER:HB3	1:N:358:LEU:HD23	1.94	0.49
1:O:351:SER:HB3	1:O:358:LEU:HD23	1.94	0.49
1:O:175:VAL:HG22	1:O:180:LEU:HD21	1.93	0.49
1:R:351:SER:HB3	1:R:358:LEU:HD23	1.95	0.49
1:A:351:SER:HB3	1:A:358:LEU:HD23	1.95	0.49
1:E:351:SER:HB3	1:E:358:LEU:HD23	1.95	0.49
1:T:351:SER:HB3	1:T:358:LEU:HD23	1.94	0.49
1:M:351:SER:HB3	1:M:358:LEU:HD23	1.95	0.48
2:S:601:FAD:H9	2:S:601:FAD:H1'2	1.69	0.48
1:U:210:ARG:NH1	4:U:708:HOH:O	2.46	0.48
1:V:351:SER:HB3	1:V:358:LEU:HD23	1.96	0.48
1:J:351:SER:HB3	1:J:358:LEU:HD23	1.95	0.48
2:X:601:FAD:N6A	3:X:602:GOL:O2	2.47	0.48
1:U:351:SER:HB3	1:U:358:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:351:SER:HB3	1:X:358:LEU:HD23	1.95	0.48
1:N:342:GLU:HG2	4:O:866:HOH:O	2.12	0.48
1:S:351:SER:HB3	1:S:358:LEU:HD23	1.96	0.48
1:I:351:SER:HB3	1:I:358:LEU:HD23	1.96	0.48
1:V:342:GLU:HG2	4:W:852:HOH:O	2.14	0.47
1:F:351:SER:HB3	1:F:358:LEU:HD23	1.96	0.47
1:P:351:SER:HB3	1:P:358:LEU:HD23	1.96	0.47
1:Q:351:SER:HB3	1:Q:358:LEU:HD23	1.96	0.47
1:R:280:ARG:HD2	1:R:280:ARG:HA	1.70	0.47
1:W:351:SER:HB3	1:W:358:LEU:HD23	1.97	0.47
1:B:351:SER:HB3	1:B:358:LEU:HD23	1.96	0.47
1:U:342:GLU:HG2	4:X:826:HOH:O	2.13	0.47
1:B:218:ARG:NH2	4:B:701:HOH:O	2.21	0.47
1:G:72:SER:O	1:G:76:LYS:HG3	2.15	0.47
1:I:34:GLU:OE1	1:I:363:ARG:NH1	2.48	0.47
1:L:351:SER:HB3	1:L:358:LEU:HD23	1.96	0.47
1:U:228:LEU:O	1:U:233:ARG:NH1	2.48	0.47
1:C:351:SER:HB3	1:C:358:LEU:HD23	1.96	0.47
1:Q:228:LEU:O	1:Q:233:ARG:NH1	2.49	0.47
1:S:228:LEU:O	1:S:233:ARG:NH1	2.48	0.47
1:I:228:LEU:O	1:I:233:ARG:NH1	2.48	0.46
2:T:601:FAD:H1'2	2:T:601:FAD:H4'	1.72	0.46
1:M:228:LEU:O	1:M:233:ARG:NH1	2.48	0.46
1:G:351:SER:HB3	1:G:358:LEU:HD23	1.97	0.46
1:O:72:SER:O	1:O:76:LYS:HG3	2.16	0.46
1:T:72:SER:O	1:T:76:LYS:HG3	2.16	0.46
1:T:228:LEU:O	1:T:233:ARG:NH1	2.48	0.46
2:A:601:FAD:H9	2:A:601:FAD:H1'2	1.79	0.46
1:B:72:SER:O	1:B:76:LYS:HG3	2.15	0.46
1:S:210:ARG:NH1	4:S:706:HOH:O	2.49	0.46
1:A:72:SER:O	1:A:76:LYS:HG3	2.15	0.46
1:C:72:SER:O	1:C:76:LYS:HG3	2.16	0.46
1:I:72:SER:O	1:I:76:LYS:HG3	2.16	0.46
2:U:601:FAD:H9	2:U:601:FAD:H1'2	1.68	0.46
1:L:228:LEU:O	1:L:233:ARG:NH1	2.49	0.46
1:J:228:LEU:O	1:J:233:ARG:NH1	2.49	0.45
1:N:2:THR:HG23	1:N:5:ARG:HB3	1.98	0.45
1:D:72:SER:O	1:D:76:LYS:HG3	2.16	0.45
1:F:34:GLU:OE1	1:F:363:ARG:NH1	2.48	0.45
1:P:228:LEU:O	1:P:233:ARG:NH1	2.50	0.45
1:W:72:SER:O	1:W:76:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:O	1:B:233:ARG:NH1	2.50	0.45
1:C:280:ARG:HA	1:C:280:ARG:HD2	1.68	0.45
1:J:392:PRO:HA	4:J:826:HOH:O	2.15	0.45
1:K:72:SER:O	1:K:76:LYS:HG3	2.16	0.45
1:N:72:SER:O	1:N:76:LYS:HG3	2.16	0.45
1:N:228:LEU:O	1:N:233:ARG:NH1	2.50	0.45
1:Q:280:ARG:HD2	1:Q:280:ARG:HA	1.67	0.45
1:R:101:LYS:NZ	4:R:708:HOH:O	2.49	0.45
1:V:34:GLU:OE1	1:V:363:ARG:NH1	2.49	0.45
1:W:228:LEU:O	1:W:233:ARG:NH1	2.49	0.45
1:B:275:ARG:HD3	4:B:801:HOH:O	2.15	0.45
1:F:228:LEU:O	1:F:233:ARG:NH1	2.50	0.45
1:S:72:SER:O	1:S:76:LYS:HG3	2.16	0.45
1:B:280:ARG:HA	1:B:280:ARG:HD2	1.69	0.45
1:D:2:THR:HG23	1:D:5:ARG:HB3	1.98	0.45
1:F:72:SER:O	1:F:76:LYS:HG3	2.16	0.45
1:H:72:SER:O	1:H:76:LYS:HG3	2.16	0.45
1:M:72:SER:O	1:M:76:LYS:HG3	2.16	0.45
1:R:228:LEU:O	1:R:233:ARG:NH1	2.49	0.45
2:Q:601:FAD:H9	2:Q:601:FAD:H1'2	1.68	0.45
1:V:228:LEU:O	1:V:233:ARG:NH1	2.49	0.45
1:C:228:LEU:O	1:C:233:ARG:NH1	2.50	0.45
1:R:72:SER:O	1:R:76:LYS:HG3	2.16	0.45
1:E:228:LEU:O	1:E:233:ARG:NH1	2.50	0.45
1:L:210:ARG:NH1	4:L:705:HOH:O	2.50	0.45
1:N:180:LEU:HD23	1:N:201:LEU:HD11	1.99	0.45
1:P:72:SER:O	1:P:76:LYS:HG3	2.17	0.45
4:V:2256:HOH:O	1:W:342:GLU:HG2	2.16	0.45
2:W:601:FAD:H9	2:W:601:FAD:H1'2	1.74	0.45
1:H:2:THR:HG23	1:H:5:ARG:HB3	1.99	0.45
1:M:180:LEU:HD23	1:M:201:LEU:HD11	1.99	0.45
1:T:180:LEU:HD23	1:T:201:LEU:HD11	1.99	0.45
1:B:38:ARG:HD2	4:B:851:HOH:O	2.17	0.45
1:J:2:THR:HG23	1:J:5:ARG:HB3	1.99	0.45
1:Q:72:SER:O	1:Q:76:LYS:HG3	2.17	0.45
1:V:72:SER:O	1:V:76:LYS:HG3	2.16	0.45
1:D:34:GLU:OE1	1:D:363:ARG:NH1	2.49	0.44
1:F:2:THR:HG23	1:F:5:ARG:HB3	1.98	0.44
1:G:162:ASP:OD1	1:G:165:GLY:N	2.50	0.44
1:O:210:ARG:NH1	4:O:705:HOH:O	2.51	0.44
1:P:2:THR:HG23	1:P:5:ARG:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ASP:OD1	1:C:165:GLY:N	2.50	0.44
1:E:72:SER:O	1:E:76:LYS:HG3	2.17	0.44
1:E:280:ARG:HD2	1:E:280:ARG:HA	1.68	0.44
2:E:601:FAD:H9	2:E:601:FAD:H1'2	1.75	0.44
1:F:240:MET:HB2	4:F:826:HOH:O	2.18	0.44
1:I:180:LEU:HD23	1:I:201:LEU:HD11	2.00	0.44
1:S:2:THR:HG23	1:S:5:ARG:HB3	1.99	0.44
1:U:72:SER:O	1:U:76:LYS:HG3	2.17	0.44
1:X:72:SER:O	1:X:76:LYS:HG3	2.18	0.44
1:A:280:ARG:HD2	1:A:280:ARG:HA	1.68	0.44
1:G:228:LEU:O	1:G:233:ARG:NH1	2.50	0.44
1:J:72:SER:O	1:J:76:LYS:HG3	2.17	0.44
1:L:2:THR:HG23	1:L:5:ARG:HB3	1.99	0.44
1:L:72:SER:O	1:L:76:LYS:HG3	2.17	0.44
1:P:210:ARG:NH1	4:P:706:HOH:O	2.50	0.44
1:T:34:GLU:OE1	1:T:363:ARG:NH1	2.50	0.44
1:L:34:GLU:OE1	1:L:363:ARG:NH1	2.49	0.44
1:T:280:ARG:HA	1:T:280:ARG:HD2	1.68	0.44
1:U:280:ARG:HA	1:U:280:ARG:HD2	1.68	0.44
1:F:280:ARG:HA	1:F:280:ARG:HD2	1.70	0.44
1:K:180:LEU:HD23	1:K:201:LEU:HD11	2.00	0.44
1:L:180:LEU:HD23	1:L:201:LEU:HD11	2.00	0.44
1:P:262:LYS:O	1:P:266:ARG:HG2	2.17	0.44
1:Q:162:ASP:OD1	1:Q:165:GLY:N	2.51	0.44
1:X:34:GLU:OE1	1:X:363:ARG:NH1	2.50	0.44
1:X:162:ASP:OD1	1:X:165:GLY:N	2.51	0.44
1:X:280:ARG:HA	1:X:280:ARG:HD2	1.69	0.44
1:A:228:LEU:O	1:A:233:ARG:NH1	2.51	0.44
1:K:228:LEU:O	1:K:233:ARG:NH1	2.50	0.44
1:P:180:LEU:HD23	1:P:201:LEU:HD11	2.00	0.44
1:U:162:ASP:OD1	1:U:165:GLY:N	2.51	0.44
1:X:228:LEU:O	1:X:233:ARG:NH1	2.50	0.44
1:H:225:ASP:O	1:H:233:ARG:HD3	2.18	0.44
1:L:262:LYS:O	1:L:266:ARG:HG2	2.18	0.44
2:O:601:FAD:H1'2	2:O:601:FAD:H9	1.67	0.44
1:T:162:ASP:OD1	1:T:165:GLY:N	2.51	0.44
1:B:162:ASP:OD1	1:B:165:GLY:N	2.51	0.44
1:C:262:LYS:O	1:C:266:ARG:HG2	2.18	0.44
1:X:180:LEU:HD23	1:X:201:LEU:HD11	2.00	0.44
1:B:262:LYS:O	1:B:266:ARG:HG2	2.18	0.44
1:P:34:GLU:OE1	1:P:363:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:225:ASP:O	1:S:233:ARG:HD3	2.18	0.44
1:V:162:ASP:OD1	1:V:165:GLY:N	2.50	0.44
1:C:34:GLU:OE1	1:C:363:ARG:NH1	2.50	0.43
1:C:180:LEU:HD23	1:C:201:LEU:HD11	2.00	0.43
1:G:180:LEU:HD23	1:G:201:LEU:HD11	2.00	0.43
1:H:228:LEU:O	1:H:233:ARG:NH1	2.51	0.43
1:I:162:ASP:OD1	1:I:165:GLY:N	2.51	0.43
1:K:34:GLU:OE1	1:K:363:ARG:NH1	2.51	0.43
1:K:162:ASP:OD1	1:K:165:GLY:N	2.51	0.43
1:O:228:LEU:O	1:O:233:ARG:NH1	2.50	0.43
2:P:601:FAD:H4'	2:P:601:FAD:H1'2	1.77	0.43
1:S:280:ARG:HA	1:S:280:ARG:HD2	1.68	0.43
1:W:34:GLU:OE1	1:W:363:ARG:NH1	2.51	0.43
1:A:162:ASP:OD1	1:A:165:GLY:N	2.51	0.43
1:B:225:ASP:O	1:B:233:ARG:HD3	2.18	0.43
1:F:90:ASN:OD1	1:F:243:VAL:CG2	2.52	0.43
1:F:162:ASP:OD1	1:F:165:GLY:N	2.51	0.43
1:F:180:LEU:HD23	1:F:201:LEU:HD11	2.00	0.43
1:J:180:LEU:HD23	1:J:201:LEU:HD11	2.00	0.43
1:R:162:ASP:OD1	1:R:165:GLY:N	2.51	0.43
1:S:180:LEU:HD23	1:S:201:LEU:HD11	2.00	0.43
1:T:2:THR:CG2	1:T:5:ARG:HB3	2.48	0.43
1:F:2:THR:CG2	1:F:5:ARG:HB3	2.49	0.43
1:O:162:ASP:OD1	1:O:165:GLY:N	2.51	0.43
1:O:225:ASP:O	1:O:233:ARG:HD3	2.18	0.43
1:V:2:THR:HG23	1:V:5:ARG:HB3	1.99	0.43
1:W:280:ARG:HD2	1:W:280:ARG:HA	1.68	0.43
1:X:2:THR:HG23	1:X:5:ARG:HB3	1.99	0.43
1:B:90:ASN:OD1	1:B:243:VAL:CG2	2.52	0.43
1:E:162:ASP:OD1	1:E:165:GLY:N	2.51	0.43
1:L:173:MET:HG2	1:L:211:VAL:HG22	2.01	0.43
1:M:225:ASP:O	1:M:233:ARG:HD3	2.18	0.43
1:N:2:THR:CG2	1:N:5:ARG:HB3	2.48	0.43
1:Q:180:LEU:HD23	1:Q:201:LEU:HD11	2.01	0.43
1:U:180:LEU:HD23	1:U:201:LEU:HD11	2.01	0.43
1:X:225:ASP:O	1:X:233:ARG:HD3	2.18	0.43
1:B:2:THR:HG23	1:B:5:ARG:HB3	1.99	0.43
1:D:225:ASP:O	1:D:233:ARG:HD3	2.19	0.43
1:J:173:MET:HG2	1:J:211:VAL:HG22	2.00	0.43
1:M:162:ASP:OD1	1:M:165:GLY:N	2.51	0.43
1:N:372:ALA:HB2	2:N:601:FAD:H3'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:2:THR:HG23	1:T:5:ARG:HB3	1.99	0.43
1:T:262:LYS:O	1:T:266:ARG:HG2	2.18	0.43
1:A:180:LEU:HD23	1:A:201:LEU:HD11	2.01	0.43
1:A:225:ASP:O	1:A:233:ARG:HD3	2.18	0.43
1:D:228:LEU:O	1:D:233:ARG:NH1	2.51	0.43
1:F:262:LYS:O	1:F:266:ARG:HG2	2.18	0.43
1:H:2:THR:CG2	1:H:5:ARG:HB3	2.48	0.43
1:J:262:LYS:O	1:J:266:ARG:HG2	2.18	0.43
1:K:2:THR:HG23	1:K:5:ARG:HB3	2.00	0.43
1:M:2:THR:HG23	1:M:5:ARG:HB3	2.00	0.43
1:N:262:LYS:O	1:N:266:ARG:HG2	2.19	0.43
1:O:2:THR:HG23	1:O:5:ARG:HB3	2.00	0.43
1:P:173:MET:HG2	1:P:211:VAL:HG22	2.01	0.43
1:V:180:LEU:HD23	1:V:201:LEU:HD11	2.01	0.43
1:X:220:ARG:NH2	4:X:704:HOH:O	2.49	0.43
1:B:180:LEU:HD23	1:B:201:LEU:HD11	2.01	0.43
1:E:180:LEU:HD23	1:E:201:LEU:HD11	2.01	0.43
1:H:180:LEU:HD23	1:H:201:LEU:HD11	2.01	0.43
1:O:262:LYS:O	1:O:266:ARG:HG2	2.18	0.43
1:Q:262:LYS:O	1:Q:266:ARG:HG2	2.18	0.43
1:U:2:THR:CG2	1:U:5:ARG:HB3	2.49	0.43
1:X:262:LYS:O	1:X:266:ARG:HG2	2.19	0.43
1:B:2:THR:CG2	1:B:5:ARG:HB3	2.49	0.43
1:G:2:THR:HG23	1:G:5:ARG:HB3	2.00	0.43
1:H:280:ARG:HD2	1:H:280:ARG:HA	1.69	0.43
1:I:262:LYS:O	1:I:266:ARG:HG2	2.18	0.43
1:J:2:THR:CG2	1:J:5:ARG:HB3	2.49	0.43
1:O:180:LEU:HD23	1:O:201:LEU:HD11	2.01	0.43
1:P:2:THR:CG2	1:P:5:ARG:HB3	2.49	0.43
1:R:225:ASP:O	1:R:233:ARG:HD3	2.19	0.43
1:S:2:THR:CG2	1:S:5:ARG:HB3	2.48	0.43
1:U:2:THR:HG23	1:U:5:ARG:HB3	2.00	0.43
1:W:2:THR:HG23	1:W:5:ARG:HB3	2.00	0.43
1:X:2:THR:CG2	1:X:5:ARG:HB3	2.49	0.43
1:A:2:THR:HG23	1:A:5:ARG:HB3	2.00	0.43
1:D:180:LEU:HD23	1:D:201:LEU:HD11	2.01	0.43
1:F:280:ARG:NH2	4:F:703:HOH:O	2.51	0.43
1:G:2:THR:CG2	1:G:5:ARG:HB3	2.49	0.43
1:H:262:LYS:O	1:H:266:ARG:HG2	2.18	0.43
1:K:2:THR:CG2	1:K:5:ARG:HB3	2.48	0.43
1:V:262:LYS:O	1:V:266:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:THR:O	1:D:2:THR:HG22	2.19	0.43
1:G:262:LYS:O	1:G:266:ARG:HG2	2.19	0.43
3:G:602:GOL:H12	4:G:764:HOH:O	2.19	0.43
1:I:2:THR:HG23	1:I:5:ARG:HB3	2.00	0.43
1:M:34:GLU:OE1	1:M:363:ARG:NH1	2.52	0.43
1:T:225:ASP:O	1:T:233:ARG:HD3	2.19	0.43
1:B:173:MET:HG2	1:B:211:VAL:HG22	2.01	0.42
1:C:2:THR:CG2	1:C:5:ARG:HB3	2.49	0.42
1:E:225:ASP:O	1:E:233:ARG:HD3	2.19	0.42
1:E:262:LYS:O	1:E:266:ARG:HG2	2.18	0.42
1:G:225:ASP:O	1:G:233:ARG:HD3	2.19	0.42
1:I:225:ASP:O	1:I:233:ARG:HD3	2.19	0.42
1:J:225:ASP:O	1:J:233:ARG:HD3	2.18	0.42
1:M:2:THR:CG2	1:M:5:ARG:HB3	2.49	0.42
1:N:34:GLU:OE1	1:N:363:ARG:NH1	2.52	0.42
1:R:262:LYS:O	1:R:266:ARG:HG2	2.18	0.42
1:U:34:GLU:OE1	1:U:363:ARG:NH1	2.51	0.42
1:V:2:THR:CG2	1:V:5:ARG:HB3	2.49	0.42
1:V:225:ASP:O	1:V:233:ARG:HD3	2.19	0.42
1:D:2:THR:CG2	1:D:5:ARG:HB3	2.49	0.42
1:F:225:ASP:O	1:F:233:ARG:HD3	2.19	0.42
1:K:225:ASP:O	1:K:233:ARG:HD3	2.19	0.42
1:N:210:ARG:NH1	4:N:710:HOH:O	2.52	0.42
1:O:34:GLU:OE1	1:O:363:ARG:NH1	2.52	0.42
1:P:225:ASP:O	1:P:233:ARG:HD3	2.19	0.42
1:Q:2:THR:CG2	1:Q:5:ARG:HB3	2.49	0.42
1:U:262:LYS:O	1:U:266:ARG:HG2	2.19	0.42
1:F:2:THR:HG22	1:F:2:THR:O	2.20	0.42
2:K:601:FAD:H1'2	2:K:601:FAD:H9	1.67	0.42
1:L:2:THR:CG2	1:L:5:ARG:HB3	2.49	0.42
1:O:280:ARG:HD2	1:O:280:ARG:HA	1.69	0.42
1:Q:225:ASP:O	1:Q:233:ARG:HD3	2.19	0.42
1:R:180:LEU:HD23	1:R:201:LEU:HD11	2.01	0.42
1:E:2:THR:CG2	1:E:5:ARG:HB3	2.49	0.42
1:E:2:THR:HG23	1:E:5:ARG:HB3	2.00	0.42
1:G:280:ARG:HA	1:G:280:ARG:HD2	1.70	0.42
1:J:240:MET:HB2	4:J:794:HOH:O	2.19	0.42
1:L:162:ASP:OD1	1:L:165:GLY:N	2.50	0.42
1:Q:173:MET:HG2	1:Q:211:VAL:HG22	2.01	0.42
1:R:2:THR:HG23	1:R:5:ARG:HB3	2.00	0.42
1:W:225:ASP:O	1:W:233:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:262:LYS:O	1:W:266:ARG:HG2	2.19	0.42
1:L:280:ARG:HA	1:L:280:ARG:HD2	1.67	0.42
1:M:2:THR:HG22	1:M:2:THR:O	2.19	0.42
1:Q:2:THR:HG23	1:Q:5:ARG:HB3	2.00	0.42
1:A:2:THR:CG2	1:A:5:ARG:HB3	2.49	0.42
1:B:34:GLU:OE1	1:B:363:ARG:NH1	2.52	0.42
1:C:2:THR:HG23	1:C:5:ARG:HB3	2.00	0.42
1:M:280:ARG:NH2	4:M:711:HOH:O	2.53	0.42
1:R:2:THR:CG2	1:R:5:ARG:HB3	2.49	0.42
1:A:2:THR:HG22	1:A:2:THR:O	2.20	0.42
1:A:262:LYS:O	1:A:266:ARG:HG2	2.19	0.42
1:C:348:GLY:O	1:C:351:SER:OG	2.35	0.42
1:D:262:LYS:O	1:D:266:ARG:HG2	2.19	0.42
1:M:173:MET:HG2	1:M:211:VAL:HG22	2.00	0.42
1:O:2:THR:CG2	1:O:5:ARG:HB3	2.49	0.42
1:T:2:THR:HG22	1:T:2:THR:O	2.19	0.42
1:V:280:ARG:HD2	1:V:280:ARG:HA	1.70	0.42
1:W:180:LEU:HD23	1:W:201:LEU:HD11	2.01	0.42
1:C:225:ASP:O	1:C:233:ARG:HD3	2.20	0.42
1:E:173:MET:HG2	1:E:211:VAL:HG22	2.00	0.42
1:F:173:MET:HG2	1:F:211:VAL:HG22	2.02	0.42
1:G:34:GLU:OE1	1:G:363:ARG:NH1	2.52	0.42
1:N:173:MET:HG2	1:N:211:VAL:HG22	2.02	0.42
1:N:225:ASP:O	1:N:233:ARG:HD3	2.19	0.42
1:P:2:THR:O	1:P:2:THR:HG22	2.20	0.42
1:E:34:GLU:OE1	1:E:363:ARG:NH1	2.53	0.42
2:F:601:FAD:H4'	2:F:601:FAD:H1'2	1.69	0.42
1:I:2:THR:CG2	1:I:5:ARG:HB3	2.50	0.42
1:J:34:GLU:OE1	1:J:363:ARG:NH1	2.52	0.42
1:P:162:ASP:OD1	1:P:165:GLY:N	2.50	0.42
1:Q:2:THR:HG22	1:Q:2:THR:O	2.20	0.42
1:S:262:LYS:O	1:S:266:ARG:HG2	2.19	0.42
1:W:2:THR:HG22	1:W:2:THR:O	2.20	0.42
1:M:280:ARG:HD2	1:M:280:ARG:HA	1.69	0.42
1:T:122:VAL:CG2	1:T:142:TRP:HB3	2.50	0.42
1:U:225:ASP:O	1:U:233:ARG:HD3	2.20	0.42
1:W:2:THR:CG2	1:W:5:ARG:HB3	2.50	0.42
1:W:173:MET:HG2	1:W:211:VAL:HG22	2.01	0.42
1:E:2:THR:HG22	1:E:2:THR:O	2.20	0.41
1:E:122:VAL:CG2	1:E:142:TRP:HB3	2.50	0.41
1:M:262:LYS:O	1:M:266:ARG:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:34:GLU:OE1	1:R:363:ARG:NH1	2.53	0.41
1:U:173:MET:HG2	1:U:211:VAL:HG22	2.02	0.41
1:A:34:GLU:OE1	1:A:363:ARG:NH1	2.53	0.41
2:D:601:FAD:H9	2:D:601:FAD:H1'2	1.63	0.41
1:V:122:VAL:CG2	1:V:142:TRP:HB3	2.50	0.41
1:A:122:VAL:CG2	1:A:142:TRP:HB3	2.50	0.41
1:D:280:ARG:HA	1:D:280:ARG:HD2	1.71	0.41
1:J:104:ARG:HG3	4:J:873:HOH:O	2.19	0.41
1:K:262:LYS:O	1:K:266:ARG:HG2	2.19	0.41
1:L:225:ASP:O	1:L:233:ARG:HD3	2.20	0.41
1:Q:34:GLU:OE1	1:Q:363:ARG:NH1	2.52	0.41
1:V:173:MET:HG2	1:V:211:VAL:HG22	2.01	0.41
2:V:601:FAD:H4'	2:V:601:FAD:H1'2	1.72	0.41
1:H:2:THR:HG22	1:H:2:THR:O	2.21	0.41
1:Q:210:ARG:NH1	4:Q:710:HOH:O	2.54	0.41
1:N:2:THR:O	1:N:2:THR:HG22	2.20	0.41
1:O:2:THR:HG22	1:O:2:THR:O	2.20	0.41
2:W:601:FAD:H1'2	2:W:601:FAD:H4'	1.78	0.41
2:A:601:FAD:H1'2	2:A:601:FAD:H4'	1.73	0.41
1:C:173:MET:HG2	1:C:211:VAL:HG22	2.02	0.41
1:G:2:THR:HG22	1:G:2:THR:O	2.20	0.41
1:I:280:ARG:HD2	1:I:280:ARG:HA	1.68	0.41
1:J:162:ASP:OD1	1:J:165:GLY:N	2.51	0.41
1:S:2:THR:HG22	1:S:2:THR:O	2.21	0.41
1:B:2:THR:O	1:B:2:THR:HG22	2.21	0.41
1:C:122:VAL:CG2	1:C:142:TRP:HB3	2.50	0.41
1:D:122:VAL:CG2	1:D:142:TRP:HB3	2.50	0.41
1:H:173:MET:HG2	1:H:211:VAL:HG22	2.02	0.41
1:K:280:ARG:HD2	1:K:280:ARG:HA	1.70	0.41
1:X:122:VAL:CG2	1:X:142:TRP:HB3	2.50	0.41
1:G:173:MET:HG2	1:G:211:VAL:HG22	2.03	0.41
1:S:34:GLU:OE1	1:S:363:ARG:NH1	2.53	0.41
1:T:360:ARG:HB3	4:T:799:HOH:O	2.19	0.41
2:X:601:FAD:H9	2:X:601:FAD:H1'2	1.65	0.41
1:G:122:VAL:CG2	1:G:142:TRP:HB3	2.50	0.41
2:K:601:FAD:H1'2	2:K:601:FAD:H4'	1.77	0.41
1:L:178:ARG:NH2	1:Q:113:ASP:OD2	2.53	0.41
1:N:162:ASP:OD1	1:N:165:GLY:N	2.51	0.41
1:R:2:THR:HG22	1:R:2:THR:O	2.21	0.41
1:R:122:VAL:CG2	1:R:142:TRP:HB3	2.51	0.41
1:S:90:ASN:OD1	1:S:243:VAL:CG2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:2:THR:HG22	1:V:2:THR:O	2.21	0.41
1:X:173:MET:HG2	1:X:211:VAL:HG22	2.03	0.41
1:D:173:MET:HG2	1:D:211:VAL:HG22	2.02	0.41
2:D:601:FAD:N7A	2:D:601:FAD:O2'	2.49	0.41
1:H:162:ASP:OD1	1:H:165:GLY:N	2.51	0.41
1:I:2:THR:HG22	1:I:2:THR:O	2.21	0.41
1:J:2:THR:O	1:J:2:THR:HG22	2.21	0.41
1:N:372:ALA:H	2:N:601:FAD:H2'	1.86	0.41
1:S:173:MET:HG2	1:S:211:VAL:HG22	2.02	0.41
1:U:2:THR:O	1:U:2:THR:HG22	2.21	0.41
1:H:122:VAL:CG2	1:H:142:TRP:HB3	2.50	0.40
1:I:173:MET:HG2	1:I:211:VAL:HG22	2.02	0.40
2:J:601:FAD:H9	2:J:601:FAD:H1'2	1.69	0.40
1:S:122:VAL:CG2	1:S:142:TRP:HB3	2.51	0.40
1:V:348:GLY:O	1:V:351:SER:OG	2.35	0.40
1:V:377:HIS:CD2	4:V:2214:HOH:O	2.74	0.40
3:W:602:GOL:H12	4:W:795:HOH:O	2.21	0.40
1:D:162:ASP:OD1	1:D:165:GLY:N	2.51	0.40
1:P:280:ARG:HA	1:P:280:ARG:HD2	1.69	0.40
1:S:162:ASP:OD1	1:S:165:GLY:N	2.51	0.40
2:T:601:FAD:H1'2	2:T:601:FAD:H9	1.65	0.40
1:W:162:ASP:OD1	1:W:165:GLY:N	2.50	0.40
1:A:173:MET:HG2	1:A:211:VAL:HG22	2.02	0.40
1:O:173:MET:HG2	1:O:211:VAL:HG22	2.02	0.40
1:W:122:VAL:CG2	1:W:142:TRP:HB3	2.51	0.40
1:X:2:THR:HG22	1:X:2:THR:O	2.21	0.40
1:J:26:PHE:CD1	1:J:43:THR:HG23	2.56	0.40
1:K:173:MET:HG2	1:K:211:VAL:HG22	2.02	0.40
1:R:173:MET:HG2	1:R:211:VAL:HG22	2.02	0.40
1:T:173:MET:HG2	1:T:211:VAL:HG22	2.03	0.40
1:E:372:ALA:HB2	2:E:601:FAD:H3'	2.03	0.40
2:I:601:FAD:H4'	2:I:601:FAD:H1'2	1.79	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	394/413 (95%)	390 (99%)	4 (1%)	0	100	100
1	B	394/413 (95%)	390 (99%)	4 (1%)	0	100	100
1	C	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	D	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	E	394/413 (95%)	390 (99%)	4 (1%)	0	100	100
1	F	394/413 (95%)	390 (99%)	4 (1%)	0	100	100
1	G	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	H	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	I	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	J	394/413 (95%)	390 (99%)	4 (1%)	0	100	100
1	K	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	L	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	M	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	N	394/413 (95%)	391 (99%)	3 (1%)	0	100	100
1	O	394/413 (95%)	390 (99%)	4 (1%)	0	100	100
1	P	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	Q	394/413 (95%)	390 (99%)	4 (1%)	0	100	100
1	R	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	S	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	T	394/413 (95%)	390 (99%)	4 (1%)	0	100	100
1	U	394/413 (95%)	391 (99%)	3 (1%)	0	100	100
1	V	394/413 (95%)	389 (99%)	5 (1%)	0	100	100
1	W	394/413 (95%)	390 (99%)	4 (1%)	0	100	100
1	X	394/413 (95%)	391 (99%)	3 (1%)	0	100	100
All	All	9456/9912 (95%)	9351 (99%)	105 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	B	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	C	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	D	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	E	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	F	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	G	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	H	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	I	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	J	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	K	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	L	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	M	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	N	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	O	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	P	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	Q	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	R	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	S	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	T	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	U	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	V	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	W	306/321 (95%)	293 (96%)	13 (4%)	30	47
1	X	306/321 (95%)	293 (96%)	13 (4%)	30	47
All	All	7344/7704 (95%)	7032 (96%)	312 (4%)	30	47

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	11	LEU
1	A	28	ASP
1	A	38	ARG
1	A	90	ASN
1	A	104	ARG
1	A	122	VAL
1	A	201	LEU
1	A	228	LEU
1	A	231	LEU
1	A	261	GLU
1	A	266	ARG
1	A	335	LEU
1	B	8	THR
1	B	11	LEU
1	B	28	ASP
1	B	38	ARG
1	B	90	ASN
1	B	104	ARG
1	B	122	VAL
1	B	201	LEU
1	B	228	LEU
1	B	231	LEU
1	B	261	GLU
1	B	266	ARG
1	B	335	LEU
1	C	8	THR
1	C	11	LEU
1	C	28	ASP
1	C	38	ARG
1	C	90	ASN
1	C	104	ARG
1	C	122	VAL
1	C	201	LEU
1	C	228	LEU
1	C	231	LEU
1	C	261	GLU
1	C	266	ARG
1	C	335	LEU
1	D	8	THR
1	D	11	LEU
1	D	28	ASP
1	D	38	ARG

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Mol	Chain	Res	Type
1	D	90	ASN
1	D	104	ARG
1	D	122	VAL
1	D	201	LEU
1	D	228	LEU
1	D	231	LEU
1	D	261	GLU
1	D	266	ARG
1	D	335	LEU
1	E	8	THR
1	E	11	LEU
1	E	28	ASP
1	E	38	ARG
1	E	90	ASN
1	E	104	ARG
1	E	122	VAL
1	E	201	LEU
1	E	228	LEU
1	E	231	LEU
1	E	261	GLU
1	E	266	ARG
1	E	335	LEU
1	F	8	THR
1	F	11	LEU
1	F	28	ASP
1	F	38	ARG
1	F	90	ASN
1	F	104	ARG
1	F	122	VAL
1	F	201	LEU
1	F	228	LEU
1	F	231	LEU
1	F	261	GLU
1	F	266	ARG
1	F	335	LEU
1	G	8	THR
1	G	11	LEU
1	G	28	ASP
1	G	38	ARG
1	G	90	ASN
1	G	104	ARG
1	G	122	VAL

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Mol	Chain	Res	Type
1	G	201	LEU
1	G	228	LEU
1	G	231	LEU
1	G	261	GLU
1	G	266	ARG
1	G	335	LEU
1	H	8	THR
1	H	11	LEU
1	H	28	ASP
1	H	38	ARG
1	H	90	ASN
1	H	104	ARG
1	H	122	VAL
1	H	201	LEU
1	H	228	LEU
1	H	231	LEU
1	H	261	GLU
1	H	266	ARG
1	H	335	LEU
1	I	8	THR
1	I	11	LEU
1	I	28	ASP
1	I	38	ARG
1	I	90	ASN
1	I	104	ARG
1	I	122	VAL
1	I	201	LEU
1	I	228	LEU
1	I	231	LEU
1	I	261	GLU
1	I	266	ARG
1	I	335	LEU
1	J	8	THR
1	J	11	LEU
1	J	28	ASP
1	J	38	ARG
1	J	90	ASN
1	J	104	ARG
1	J	122	VAL
1	J	201	LEU
1	J	228	LEU
1	J	231	LEU

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Mol	Chain	Res	Type
1	J	261	GLU
1	J	266	ARG
1	J	335	LEU
1	K	8	THR
1	K	11	LEU
1	K	28	ASP
1	K	38	ARG
1	K	90	ASN
1	K	104	ARG
1	K	122	VAL
1	K	201	LEU
1	K	228	LEU
1	K	231	LEU
1	K	261	GLU
1	K	266	ARG
1	K	335	LEU
1	L	8	THR
1	L	11	LEU
1	L	28	ASP
1	L	38	ARG
1	L	90	ASN
1	L	104	ARG
1	L	122	VAL
1	L	201	LEU
1	L	228	LEU
1	L	231	LEU
1	L	261	GLU
1	L	266	ARG
1	L	335	LEU
1	M	8	THR
1	M	11	LEU
1	M	28	ASP
1	M	38	ARG
1	M	90	ASN
1	M	104	ARG
1	M	122	VAL
1	M	201	LEU
1	M	228	LEU
1	M	231	LEU
1	M	261	GLU
1	M	266	ARG
1	M	335	LEU

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Mol	Chain	Res	Type
1	N	8	THR
1	N	11	LEU
1	N	28	ASP
1	N	38	ARG
1	N	90	ASN
1	N	104	ARG
1	N	122	VAL
1	N	201	LEU
1	N	228	LEU
1	N	231	LEU
1	N	261	GLU
1	N	266	ARG
1	N	335	LEU
1	O	8	THR
1	O	11	LEU
1	O	28	ASP
1	O	38	ARG
1	O	90	ASN
1	O	104	ARG
1	O	122	VAL
1	O	201	LEU
1	O	228	LEU
1	O	231	LEU
1	O	261	GLU
1	O	266	ARG
1	O	335	LEU
1	P	8	THR
1	P	11	LEU
1	P	28	ASP
1	P	38	ARG
1	P	90	ASN
1	P	104	ARG
1	P	122	VAL
1	P	201	LEU
1	P	228	LEU
1	P	231	LEU
1	P	261	GLU
1	P	266	ARG
1	P	335	LEU
1	Q	8	THR
1	Q	11	LEU
1	Q	28	ASP

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Mol	Chain	Res	Type
1	Q	38	ARG
1	Q	90	ASN
1	Q	104	ARG
1	Q	122	VAL
1	Q	201	LEU
1	Q	228	LEU
1	Q	231	LEU
1	Q	261	GLU
1	Q	266	ARG
1	Q	335	LEU
1	R	8	THR
1	R	11	LEU
1	R	28	ASP
1	R	38	ARG
1	R	90	ASN
1	R	104	ARG
1	R	122	VAL
1	R	201	LEU
1	R	228	LEU
1	R	231	LEU
1	R	261	GLU
1	R	266	ARG
1	R	335	LEU
1	S	8	THR
1	S	11	LEU
1	S	28	ASP
1	S	38	ARG
1	S	90	ASN
1	S	104	ARG
1	S	122	VAL
1	S	201	LEU
1	S	228	LEU
1	S	231	LEU
1	S	261	GLU
1	S	266	ARG
1	S	335	LEU
1	T	8	THR
1	T	11	LEU
1	T	28	ASP
1	T	38	ARG
1	T	90	ASN
1	T	104	ARG

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Mol	Chain	Res	Type
1	T	122	VAL
1	T	201	LEU
1	T	228	LEU
1	T	231	LEU
1	T	261	GLU
1	T	266	ARG
1	T	335	LEU
1	U	8	THR
1	U	11	LEU
1	U	28	ASP
1	U	38	ARG
1	U	90	ASN
1	U	104	ARG
1	U	122	VAL
1	U	201	LEU
1	U	228	LEU
1	U	231	LEU
1	U	261	GLU
1	U	266	ARG
1	U	335	LEU
1	V	8	THR
1	V	11	LEU
1	V	28	ASP
1	V	38	ARG
1	V	90	ASN
1	V	104	ARG
1	V	122	VAL
1	V	201	LEU
1	V	228	LEU
1	V	231	LEU
1	V	261	GLU
1	V	266	ARG
1	V	335	LEU
1	W	8	THR
1	W	11	LEU
1	W	28	ASP
1	W	38	ARG
1	W	90	ASN
1	W	104	ARG
1	W	122	VAL
1	W	201	LEU
1	W	228	LEU

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Mol	Chain	Res	Type
1	W	231	LEU
1	W	261	GLU
1	W	266	ARG
1	W	335	LEU
1	X	8	THR
1	X	11	LEU
1	X	28	ASP
1	X	38	ARG
1	X	90	ASN
1	X	104	ARG
1	X	122	VAL
1	X	201	LEU
1	X	228	LEU
1	X	231	LEU
1	X	261	GLU
1	X	266	ARG
1	X	335	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	80	HIS
1	D	80	HIS
1	I	80	HIS
1	Q	80	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)

48 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	FAD	U	601	-	53,58,58	1.69	12 (22%)	68,89,89	1.32	10 (14%)
2	FAD	I	601	-	53,58,58	1.73	13 (24%)	68,89,89	1.54	14 (20%)
3	GOL	S	602	-	5,5,5	0.45	0	5,5,5	0.41	0
3	GOL	R	602	-	5,5,5	0.37	0	5,5,5	0.47	0
3	GOL	D	602	-	5,5,5	0.33	0	5,5,5	0.60	0
2	FAD	X	601	-	53,58,58	1.75	13 (24%)	68,89,89	1.43	14 (20%)
2	FAD	T	601	-	53,58,58	1.80	13 (24%)	68,89,89	1.45	13 (19%)
3	GOL	H	602	-	5,5,5	0.30	0	5,5,5	0.52	0
3	GOL	W	602	-	5,5,5	0.46	0	5,5,5	0.38	0
2	FAD	M	601	-	53,58,58	1.72	13 (24%)	68,89,89	1.45	14 (20%)
3	GOL	M	602	-	5,5,5	0.21	0	5,5,5	0.43	0
3	GOL	V	602	-	5,5,5	0.47	0	5,5,5	0.55	0
2	FAD	D	601	-	53,58,58	1.72	9 (16%)	68,89,89	1.49	13 (19%)
3	GOL	X	602	-	5,5,5	0.36	0	5,5,5	1.05	0
3	GOL	B	602	-	5,5,5	0.38	0	5,5,5	0.88	0
2	FAD	Q	601	-	53,58,58	1.70	12 (22%)	68,89,89	1.44	12 (17%)
3	GOL	L	602	-	5,5,5	0.31	0	5,5,5	0.53	0
2	FAD	G	601	-	53,58,58	1.73	13 (24%)	68,89,89	1.57	16 (23%)
2	FAD	W	601	-	53,58,58	1.74	15 (28%)	68,89,89	1.43	13 (19%)
3	GOL	K	602	-	5,5,5	0.24	0	5,5,5	0.96	0
2	FAD	V	601	-	53,58,58	1.72	12 (22%)	68,89,89	1.53	14 (20%)
2	FAD	S	601	-	53,58,58	1.72	13 (24%)	68,89,89	1.56	15 (22%)
2	FAD	B	601	-	53,58,58	1.74	11 (20%)	68,89,89	1.48	15 (22%)
3	GOL	A	602	-	5,5,5	0.34	0	5,5,5	0.96	0
3	GOL	O	602	-	5,5,5	0.37	0	5,5,5	0.53	0
2	FAD	L	601	-	53,58,58	1.67	8 (15%)	68,89,89	1.64	18 (26%)
2	FAD	J	601	-	53,58,58	1.69	11 (20%)	68,89,89	1.39	10 (14%)
2	FAD	K	601	-	53,58,58	1.68	10 (18%)	68,89,89	1.49	12 (17%)
3	GOL	P	602	-	5,5,5	0.39	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FAD	N	601	-	53,58,58	1.76	14 (26%)	68,89,89	1.45	9 (13%)
2	FAD	C	601	-	53,58,58	1.70	15 (28%)	68,89,89	1.46	11 (16%)
3	GOL	G	602	-	5,5,5	0.41	0	5,5,5	0.60	0
3	GOL	F	602	-	5,5,5	0.18	0	5,5,5	0.65	0
2	FAD	E	601	-	53,58,58	1.74	10 (18%)	68,89,89	1.45	15 (22%)
3	GOL	C	602	-	5,5,5	0.35	0	5,5,5	0.82	0
3	GOL	E	602	-	5,5,5	0.45	0	5,5,5	0.60	0
2	FAD	A	601	-	53,58,58	1.73	13 (24%)	68,89,89	1.45	12 (17%)
2	FAD	P	601	-	53,58,58	1.65	10 (18%)	68,89,89	1.52	13 (19%)
2	FAD	H	601	-	53,58,58	1.80	13 (24%)	68,89,89	1.51	12 (17%)
3	GOL	N	602	-	5,5,5	0.32	0	5,5,5	0.91	0
3	GOL	J	602	-	5,5,5	0.21	0	5,5,5	0.54	0
3	GOL	Q	602	-	5,5,5	0.39	0	5,5,5	0.50	0
2	FAD	O	601	-	53,58,58	1.72	13 (24%)	68,89,89	1.47	15 (22%)
3	GOL	U	602	-	5,5,5	0.49	0	5,5,5	0.55	0
2	FAD	F	601	-	53,58,58	1.66	7 (13%)	68,89,89	1.50	16 (23%)
3	GOL	I	602	-	5,5,5	0.26	0	5,5,5	0.42	0
2	FAD	R	601	-	53,58,58	1.70	11 (20%)	68,89,89	1.57	14 (20%)
3	GOL	T	602	-	5,5,5	0.46	0	5,5,5	0.87	0

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	FAD	U	601	-	-	5/30/50/50	0/6/6/6
2	FAD	I	601	-	-	6/30/50/50	0/6/6/6
3	GOL	S	602	-	-	3/4/4/4	-
3	GOL	R	602	-	-	3/4/4/4	-
3	GOL	D	602	-	-	3/4/4/4	-
2	FAD	X	601	-	-	6/30/50/50	0/6/6/6
2	FAD	T	601	-	-	6/30/50/50	0/6/6/6
3	GOL	H	602	-	-	2/4/4/4	-
3	GOL	W	602	-	-	4/4/4/4	-
2	FAD	M	601	-	-	6/30/50/50	0/6/6/6
3	GOL	M	602	-	-	0/4/4/4	-
3	GOL	V	602	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	601	-	-	6/30/50/50	0/6/6/6
3	GOL	X	602	-	-	2/4/4/4	-
3	GOL	B	602	-	-	4/4/4/4	-
2	FAD	Q	601	-	-	6/30/50/50	0/6/6/6
3	GOL	L	602	-	-	1/4/4/4	-
2	FAD	G	601	-	-	6/30/50/50	0/6/6/6
2	FAD	W	601	-	-	5/30/50/50	0/6/6/6
3	GOL	K	602	-	-	4/4/4/4	-
2	FAD	V	601	-	-	6/30/50/50	0/6/6/6
2	FAD	S	601	-	-	3/30/50/50	0/6/6/6
2	FAD	B	601	-	-	1/30/50/50	0/6/6/6
3	GOL	A	602	-	-	3/4/4/4	-
3	GOL	O	602	-	-	4/4/4/4	-
2	FAD	L	601	-	-	3/30/50/50	0/6/6/6
2	FAD	J	601	-	-	4/30/50/50	0/6/6/6
2	FAD	K	601	-	-	2/30/50/50	0/6/6/6
3	GOL	P	602	-	-	3/4/4/4	-
2	FAD	N	601	-	-	4/30/50/50	0/6/6/6
2	FAD	C	601	-	-	6/30/50/50	0/6/6/6
3	GOL	G	602	-	-	0/4/4/4	-
3	GOL	F	602	-	-	2/4/4/4	-
2	FAD	E	601	-	-	6/30/50/50	0/6/6/6
3	GOL	C	602	-	-	4/4/4/4	-
3	GOL	E	602	-	-	3/4/4/4	-
2	FAD	A	601	-	-	0/30/50/50	0/6/6/6
2	FAD	P	601	-	-	5/30/50/50	0/6/6/6
2	FAD	H	601	-	-	3/30/50/50	0/6/6/6
3	GOL	N	602	-	-	2/4/4/4	-
3	GOL	J	602	-	-	0/4/4/4	-
3	GOL	Q	602	-	-	2/4/4/4	-
2	FAD	O	601	-	-	5/30/50/50	0/6/6/6
3	GOL	U	602	-	-	3/4/4/4	-
2	FAD	F	601	-	-	0/30/50/50	0/6/6/6
3	GOL	I	602	-	-	2/4/4/4	-
2	FAD	R	601	-	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	T	602	-	-	2/4/4/4	-

All (284) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	601	FAD	C4-N3	-5.15	1.29	1.38
2	T	601	FAD	C4-N3	-4.99	1.29	1.38
2	D	601	FAD	C4-N3	-4.81	1.29	1.38
2	R	601	FAD	C4-N3	-4.80	1.29	1.38
2	H	601	FAD	C5X-N5	-4.68	1.30	1.39
2	N	601	FAD	C4-N3	-4.66	1.30	1.38
2	K	601	FAD	C4-N3	-4.64	1.30	1.38
2	F	601	FAD	C4-N3	-4.59	1.30	1.38
2	E	601	FAD	C9A-C5X	4.56	1.48	1.41
2	E	601	FAD	C4-N3	-4.56	1.30	1.38
2	H	601	FAD	C4-N3	-4.55	1.30	1.38
2	C	601	FAD	C5X-N5	-4.53	1.30	1.39
2	A	601	FAD	C4-N3	-4.48	1.30	1.38
2	W	601	FAD	C4-N3	-4.42	1.30	1.38
2	M	601	FAD	C4-N3	-4.41	1.30	1.38
2	B	601	FAD	C4-N3	-4.39	1.30	1.38
2	U	601	FAD	C9A-C5X	4.36	1.48	1.41
2	J	601	FAD	C4-N3	-4.34	1.30	1.38
2	N	601	FAD	C9A-C5X	4.30	1.48	1.41
2	O	601	FAD	C4-N3	-4.29	1.30	1.38
2	I	601	FAD	C9A-C5X	4.29	1.48	1.41
2	V	601	FAD	C4-N3	-4.27	1.30	1.38
2	Q	601	FAD	C9A-C5X	4.26	1.48	1.41
2	P	601	FAD	C4-N3	-4.23	1.31	1.38
2	O	601	FAD	C5X-N5	-4.20	1.31	1.39
2	P	601	FAD	C5X-N5	-4.18	1.31	1.39
2	J	601	FAD	C9A-C5X	4.14	1.48	1.41
2	M	601	FAD	C9A-C5X	4.14	1.48	1.41
2	B	601	FAD	C2-N3	-4.14	1.29	1.39
2	A	601	FAD	C9A-C5X	4.12	1.48	1.41
2	D	601	FAD	C2-N3	-4.12	1.29	1.39
2	K	601	FAD	C5X-N5	-4.10	1.31	1.39
2	R	601	FAD	C5X-N5	-4.10	1.31	1.39
2	H	601	FAD	C2-N3	-4.04	1.29	1.39
2	P	601	FAD	C9A-C5X	4.04	1.47	1.41
2	Q	601	FAD	C4-N3	-4.04	1.31	1.38
2	F	601	FAD	C9A-C5X	4.03	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	601	FAD	C5X-N5	-4.01	1.31	1.39
2	C	601	FAD	C9A-C5X	4.01	1.47	1.41
2	V	601	FAD	C2-N3	-4.01	1.29	1.39
2	D	601	FAD	C5X-N5	-4.01	1.31	1.39
2	R	601	FAD	C2-N3	-3.99	1.29	1.39
2	U	601	FAD	C4-N3	-3.98	1.31	1.38
2	S	601	FAD	C5X-N5	-3.98	1.31	1.39
2	G	601	FAD	C5X-N5	-3.98	1.31	1.39
2	W	601	FAD	C9A-C5X	3.97	1.47	1.41
2	T	601	FAD	C5X-N5	-3.97	1.31	1.39
2	S	601	FAD	C4-N3	-3.97	1.31	1.38
2	T	601	FAD	C2-N3	-3.94	1.29	1.39
2	L	601	FAD	C4-N3	-3.91	1.31	1.38
2	X	601	FAD	C2-N3	-3.90	1.29	1.39
2	S	601	FAD	C9A-C5X	3.89	1.47	1.41
2	X	601	FAD	C5X-N5	-3.88	1.32	1.39
2	V	601	FAD	C5X-N5	-3.86	1.32	1.39
2	I	601	FAD	C5X-N5	-3.83	1.32	1.39
2	L	601	FAD	C5X-N5	-3.81	1.32	1.39
2	F	601	FAD	C2-N3	-3.79	1.30	1.39
2	N	601	FAD	C2-N3	-3.76	1.30	1.39
2	E	601	FAD	C5X-N5	-3.74	1.32	1.39
2	G	601	FAD	C9A-C5X	3.74	1.47	1.41
2	A	601	FAD	C2-N3	-3.72	1.30	1.39
2	A	601	FAD	C5X-N5	-3.71	1.32	1.39
2	G	601	FAD	C4-N3	-3.70	1.32	1.38
2	L	601	FAD	C9A-C5X	3.70	1.47	1.41
2	W	601	FAD	C5X-N5	-3.67	1.32	1.39
2	E	601	FAD	C2-N3	-3.67	1.30	1.39
2	M	601	FAD	C2-N3	-3.64	1.30	1.39
2	M	601	FAD	C5X-N5	-3.59	1.32	1.39
2	J	601	FAD	C5X-N5	-3.57	1.32	1.39
2	B	601	FAD	C5X-N5	-3.57	1.32	1.39
2	O	601	FAD	C2-N3	-3.56	1.30	1.39
2	U	601	FAD	C5X-N5	-3.55	1.32	1.39
2	I	601	FAD	C4-N3	-3.53	1.32	1.38
2	K	601	FAD	C2-N3	-3.53	1.30	1.39
2	C	601	FAD	C4-N3	-3.52	1.32	1.38
2	T	601	FAD	C9A-C5X	3.47	1.47	1.41
2	J	601	FAD	C2-N3	-3.44	1.31	1.39
2	P	601	FAD	C2-N3	-3.44	1.31	1.39
2	N	601	FAD	C5X-N5	-3.43	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	601	FAD	C2-N3	-3.41	1.31	1.39
2	U	601	FAD	C2-N3	-3.41	1.31	1.39
2	I	601	FAD	C2-N3	-3.39	1.31	1.39
2	L	601	FAD	C2-N3	-3.37	1.31	1.39
2	B	601	FAD	C9A-C5X	3.35	1.46	1.41
2	G	601	FAD	C1'-C2'	-3.33	1.48	1.52
2	V	601	FAD	C9A-C5X	3.32	1.46	1.41
2	H	601	FAD	C9-C8	-3.31	1.34	1.39
2	S	601	FAD	C2-N3	-3.27	1.31	1.39
2	G	601	FAD	C2-N3	-3.24	1.31	1.39
2	T	601	FAD	C9-C8	-3.20	1.34	1.39
2	X	601	FAD	C9A-C5X	3.18	1.46	1.41
2	D	601	FAD	C9A-C5X	3.17	1.46	1.41
2	O	601	FAD	C9A-C5X	3.15	1.46	1.41
2	F	601	FAD	C5X-N5	-3.13	1.33	1.39
2	C	601	FAD	C2-N3	-3.08	1.31	1.39
2	W	601	FAD	C6-C7	-3.08	1.35	1.39
2	R	601	FAD	C9A-C5X	3.07	1.46	1.41
2	D	601	FAD	C9-C8	-3.01	1.35	1.39
2	E	601	FAD	C8-C7	3.01	1.48	1.40
2	C	601	FAD	C8-C7	3.01	1.48	1.40
2	X	601	FAD	C9-C8	-2.96	1.35	1.39
2	A	601	FAD	C8-C7	2.94	1.48	1.40
2	H	601	FAD	C8-C7	2.93	1.48	1.40
2	V	601	FAD	C9-C8	-2.93	1.35	1.39
2	S	601	FAD	C6-C7	-2.91	1.35	1.39
2	Q	601	FAD	C8-C7	2.88	1.48	1.40
2	W	601	FAD	C8-C7	2.87	1.48	1.40
2	Q	601	FAD	C6-C7	-2.87	1.35	1.39
2	Q	601	FAD	C2-N3	-2.84	1.32	1.39
2	L	601	FAD	C8-C7	2.77	1.47	1.40
2	V	601	FAD	C1'-C2'	-2.76	1.48	1.52
2	I	601	FAD	C6-C7	-2.72	1.35	1.39
2	I	601	FAD	C8-C7	2.72	1.47	1.40
2	S	601	FAD	O4B-C4B	-2.71	1.38	1.45
2	J	601	FAD	C8-C7	2.71	1.47	1.40
2	N	601	FAD	C6-C7	-2.69	1.35	1.39
2	B	601	FAD	C9-C8	-2.69	1.35	1.39
2	T	601	FAD	C1'-C2'	-2.68	1.48	1.52
2	B	601	FAD	O2-C2	-2.67	1.19	1.24
2	P	601	FAD	C8-C7	2.67	1.47	1.40
2	K	601	FAD	C9A-C5X	2.66	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	601	FAD	C8-C7	2.65	1.47	1.40
2	O	601	FAD	C6-C7	-2.65	1.35	1.39
2	M	601	FAD	C6-C7	-2.64	1.35	1.39
2	J	601	FAD	C1'-C2'	-2.61	1.49	1.52
2	H	601	FAD	C9A-C5X	2.61	1.45	1.41
2	F	601	FAD	C9-C8	-2.59	1.35	1.39
2	I	601	FAD	C2B-C1B	-2.59	1.49	1.53
2	U	601	FAD	C8-C7	2.58	1.47	1.40
2	C	601	FAD	C5A-N7A	-2.58	1.30	1.39
2	U	601	FAD	C6-C7	-2.58	1.35	1.39
2	X	601	FAD	C1'-C2'	-2.57	1.49	1.52
2	I	601	FAD	C9-C8	-2.57	1.35	1.39
2	G	601	FAD	O4'-C4'	-2.56	1.37	1.43
2	M	601	FAD	C1'-C2'	-2.56	1.49	1.52
2	G	601	FAD	C5A-N7A	-2.56	1.30	1.39
2	D	601	FAD	C8-C7	2.56	1.47	1.40
2	N	601	FAD	C8-C7	2.55	1.47	1.40
2	K	601	FAD	C2B-C1B	-2.55	1.49	1.53
2	I	601	FAD	C1'-C2'	-2.52	1.49	1.52
2	K	601	FAD	C6-C5X	-2.51	1.36	1.40
2	O	601	FAD	C9-C8	-2.51	1.35	1.39
2	H	601	FAD	C6-C5X	-2.48	1.36	1.40
2	K	601	FAD	C6-C7	-2.48	1.35	1.39
2	N	601	FAD	C1'-C2'	-2.47	1.49	1.52
2	B	601	FAD	C6-C7	-2.47	1.36	1.39
2	P	601	FAD	C4A-N3A	-2.47	1.32	1.35
2	C	601	FAD	C1'-C2'	-2.46	1.49	1.52
2	H	601	FAD	O2-C2	-2.46	1.19	1.24
2	F	601	FAD	C2B-C1B	-2.46	1.50	1.53
2	V	601	FAD	O2-C2	-2.45	1.19	1.24
2	B	601	FAD	C2B-C1B	-2.45	1.50	1.53
2	T	601	FAD	C6-C7	-2.44	1.36	1.39
2	L	601	FAD	C6-C7	-2.43	1.36	1.39
2	G	601	FAD	O2'-C2'	-2.43	1.38	1.43
2	R	601	FAD	C9-C8	-2.42	1.36	1.39
2	K	601	FAD	C9-C8	-2.41	1.36	1.39
2	U	601	FAD	O2-C2	-2.40	1.19	1.24
2	T	601	FAD	C8-C7	2.40	1.46	1.40
2	G	601	FAD	C8-C7	2.39	1.46	1.40
2	R	601	FAD	C6-C7	-2.39	1.36	1.39
2	S	601	FAD	C1'-C2'	-2.39	1.49	1.52
2	A	601	FAD	C6-C7	-2.39	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	601	FAD	C9-C8	-2.37	1.36	1.39
2	A	601	FAD	C2-N1	-2.37	1.31	1.36
2	G	601	FAD	C2B-C1B	-2.36	1.50	1.53
2	E	601	FAD	PA-O2A	-2.36	1.44	1.55
2	A	601	FAD	C5A-N7A	-2.36	1.31	1.39
2	T	601	FAD	C2B-C1B	-2.36	1.50	1.53
2	W	601	FAD	O4B-C4B	-2.36	1.39	1.45
2	Q	601	FAD	PA-O2A	-2.36	1.44	1.55
2	Q	601	FAD	C5A-N7A	-2.36	1.31	1.39
2	S	601	FAD	C5A-N7A	-2.35	1.31	1.39
2	O	601	FAD	C6-C5X	-2.34	1.36	1.40
2	R	601	FAD	C2B-C1B	-2.34	1.50	1.53
2	Q	601	FAD	O4-C4	-2.34	1.19	1.23
2	U	601	FAD	C1'-C2'	-2.34	1.49	1.52
2	B	601	FAD	C1'-C2'	-2.33	1.49	1.52
2	F	601	FAD	C8-C7	2.32	1.46	1.40
2	Q	601	FAD	O2-C2	-2.31	1.20	1.24
2	G	601	FAD	P-O2P	-2.31	1.44	1.55
2	W	601	FAD	C5A-N7A	-2.31	1.31	1.39
2	R	601	FAD	O2-C2	-2.31	1.20	1.24
2	M	601	FAD	C5A-N7A	-2.30	1.31	1.39
2	K	601	FAD	C1'-C2'	-2.29	1.49	1.52
2	P	601	FAD	C6-C7	-2.29	1.36	1.39
2	E	601	FAD	C6-C7	-2.29	1.36	1.39
2	B	601	FAD	C8-C7	2.28	1.46	1.40
2	U	601	FAD	PA-O2A	-2.26	1.44	1.55
2	W	601	FAD	C1'-C2'	-2.25	1.49	1.52
2	L	601	FAD	O4B-C4B	-2.25	1.40	1.45
2	N	601	FAD	O2'-C2'	-2.25	1.38	1.43
2	V	601	FAD	C2B-C1B	-2.25	1.50	1.53
2	C	601	FAD	P-O2P	-2.24	1.44	1.55
2	R	601	FAD	C1'-C2'	-2.24	1.49	1.52
2	S	601	FAD	O2'-C2'	-2.23	1.38	1.43
2	M	601	FAD	C9-C8	-2.23	1.36	1.39
2	E	601	FAD	P-O2P	-2.22	1.44	1.55
2	J	601	FAD	PA-O2A	-2.22	1.44	1.55
2	C	601	FAD	O2'-C2'	-2.22	1.38	1.43
2	A	601	FAD	C6-C5X	-2.21	1.36	1.40
2	V	601	FAD	PA-O2A	-2.21	1.44	1.55
2	W	601	FAD	P-O2P	-2.21	1.45	1.55
2	N	601	FAD	PA-O2A	-2.21	1.45	1.55
2	N	601	FAD	C6-C5X	-2.20	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	601	FAD	C5A-N7A	-2.20	1.31	1.39
2	W	601	FAD	C2B-C1B	-2.19	1.50	1.53
2	G	601	FAD	C6-C7	-2.19	1.36	1.39
2	P	601	FAD	C2B-C1B	-2.19	1.50	1.53
2	M	601	FAD	O2'-C2'	-2.19	1.38	1.43
2	J	601	FAD	C9-C8	-2.19	1.36	1.39
2	D	601	FAD	PA-O2A	-2.18	1.45	1.55
2	M	601	FAD	C2B-C1B	-2.18	1.50	1.53
2	O	601	FAD	C5A-N7A	-2.18	1.31	1.39
2	O	601	FAD	C2-N1	-2.18	1.31	1.36
2	J	601	FAD	C5A-N7A	-2.17	1.31	1.39
2	C	601	FAD	C6-C7	-2.17	1.36	1.39
2	I	601	FAD	C5A-N7A	-2.17	1.31	1.39
2	O	601	FAD	C2B-C1B	-2.17	1.50	1.53
2	X	601	FAD	PA-O2A	-2.17	1.45	1.55
2	N	601	FAD	P-O2P	-2.17	1.45	1.55
2	O	601	FAD	PA-O2A	-2.17	1.45	1.55
2	C	601	FAD	C2B-C1B	-2.17	1.50	1.53
2	V	601	FAD	C5A-N7A	-2.17	1.31	1.39
2	D	601	FAD	O2-C2	-2.17	1.20	1.24
2	T	601	FAD	C5A-N7A	-2.17	1.31	1.39
2	M	601	FAD	PA-O2A	-2.17	1.45	1.55
2	M	601	FAD	P-O2P	-2.15	1.45	1.55
2	C	601	FAD	C1'-N10	-2.15	1.42	1.48
2	A	601	FAD	C4A-N3A	-2.14	1.32	1.35
2	X	601	FAD	C8-C7	2.14	1.46	1.40
2	M	601	FAD	C8-C7	2.14	1.46	1.40
2	H	601	FAD	PA-O2A	-2.13	1.45	1.55
2	B	601	FAD	C5A-N7A	-2.13	1.32	1.39
2	S	601	FAD	C9-C8	-2.13	1.36	1.39
2	J	601	FAD	C6-C7	-2.13	1.36	1.39
2	R	601	FAD	P-O1P	-2.12	1.43	1.50
2	V	601	FAD	C6-C7	-2.12	1.36	1.39
2	A	601	FAD	PA-O2A	-2.12	1.45	1.55
2	O	601	FAD	O2-C2	-2.12	1.20	1.24
2	N	601	FAD	C5A-N7A	-2.12	1.32	1.39
2	I	601	FAD	P-O2P	-2.12	1.45	1.55
2	P	601	FAD	O4B-C4B	-2.11	1.40	1.45
2	L	601	FAD	O2-C2	-2.11	1.20	1.24
2	R	601	FAD	C5A-N7A	-2.11	1.32	1.39
2	U	601	FAD	C4A-N3A	-2.11	1.32	1.35
2	C	601	FAD	O4'-C4'	-2.11	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	601	FAD	O2'-C2'	-2.11	1.38	1.43
2	Q	601	FAD	C1'-C2'	-2.11	1.49	1.52
2	D	601	FAD	C5A-N7A	-2.11	1.32	1.39
2	W	601	FAD	C9-C8	-2.10	1.36	1.39
2	A	601	FAD	C1'-C2'	-2.10	1.49	1.52
2	E	601	FAD	C5A-N7A	-2.10	1.32	1.39
2	T	601	FAD	O2'-C2'	-2.10	1.38	1.43
2	H	601	FAD	C6-C7	-2.09	1.36	1.39
2	I	601	FAD	O2-C2	-2.09	1.20	1.24
2	H	601	FAD	C2-N1	-2.09	1.31	1.36
2	X	601	FAD	C2B-C1B	-2.08	1.50	1.53
2	N	601	FAD	O4-C4	-2.08	1.19	1.23
2	X	601	FAD	O2-C2	-2.08	1.20	1.24
2	H	601	FAD	C5A-N7A	-2.07	1.32	1.39
2	A	601	FAD	O2-C2	-2.07	1.20	1.24
2	X	601	FAD	C6-C7	-2.07	1.36	1.39
2	T	601	FAD	PA-O2A	-2.06	1.45	1.55
2	P	601	FAD	O4'-C4'	-2.06	1.39	1.43
2	G	601	FAD	PA-O2A	-2.05	1.45	1.55
2	S	601	FAD	P-O2P	-2.05	1.45	1.55
2	W	601	FAD	PA-O2A	-2.05	1.45	1.55
2	Q	601	FAD	P-O2P	-2.05	1.45	1.55
2	U	601	FAD	C6-C5X	-2.05	1.36	1.40
2	O	601	FAD	C1'-C2'	-2.05	1.49	1.52
2	H	601	FAD	O4'-C4'	-2.04	1.39	1.43
2	S	601	FAD	P-O1P	-2.03	1.43	1.50
2	X	601	FAD	O2'-C2'	-2.03	1.39	1.43
2	U	601	FAD	C5A-N7A	-2.02	1.32	1.39
2	C	601	FAD	PA-O2A	-2.02	1.45	1.55
2	V	601	FAD	P-O2P	-2.02	1.45	1.55
2	W	601	FAD	P-O1P	-2.01	1.43	1.50
2	E	601	FAD	O2'-C2'	-2.01	1.39	1.43
2	T	601	FAD	P-O1P	-2.01	1.43	1.50
2	J	601	FAD	O4B-C4B	-2.01	1.40	1.45
2	K	601	FAD	O4'-C4'	-2.00	1.39	1.43
2	W	601	FAD	O2'-C2'	-2.00	1.39	1.43
2	C	601	FAD	C4A-N3A	-2.00	1.32	1.35

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	FAD	C4A-C5A-N7A	-3.90	105.33	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	FAD	C4-C4X-N5	3.89	123.77	118.23
2	F	601	FAD	C4A-C5A-N7A	-3.84	105.39	109.40
2	S	601	FAD	C4A-C5A-N7A	-3.74	105.50	109.40
2	H	601	FAD	C4A-C5A-N7A	-3.73	105.51	109.40
2	X	601	FAD	C4A-C5A-N7A	-3.71	105.53	109.40
2	I	601	FAD	C5'-C4'-C3'	3.65	119.26	112.20
2	E	601	FAD	N3A-C2A-N1A	-3.65	122.98	128.68
2	D	601	FAD	C4X-C10-N1	-3.64	116.29	124.73
2	G	601	FAD	C5'-C4'-C3'	3.57	119.10	112.20
2	L	601	FAD	C4X-C10-N1	-3.56	116.46	124.73
2	F	601	FAD	C4-C4X-N5	3.54	123.27	118.23
2	P	601	FAD	C4X-C10-N1	-3.53	116.55	124.73
2	V	601	FAD	C4A-C5A-N7A	-3.52	105.73	109.40
2	N	601	FAD	C4X-C10-N1	-3.49	116.64	124.73
2	S	601	FAD	C5'-C4'-C3'	3.48	118.92	112.20
2	E	601	FAD	O3B-C3B-C4B	-3.44	101.09	111.05
2	F	601	FAD	C4X-C10-N10	3.41	121.47	116.48
2	R	601	FAD	C4X-C10-N1	-3.40	116.84	124.73
2	M	601	FAD	C4A-C5A-N7A	-3.37	105.88	109.40
2	I	601	FAD	O2-C2-N1	-3.35	116.28	121.83
2	N	601	FAD	C4A-C5A-N7A	-3.34	105.91	109.40
2	C	601	FAD	O3B-C3B-C4B	-3.34	101.39	111.05
2	V	601	FAD	C4-N3-C2	-3.30	119.54	125.64
2	V	601	FAD	N3-C2-N1	3.30	125.87	119.38
2	R	601	FAD	C4A-C5A-N7A	-3.30	105.96	109.40
2	S	601	FAD	C4X-C10-N1	-3.29	117.09	124.73
2	G	601	FAD	C4X-C10-N1	-3.27	117.14	124.73
2	A	601	FAD	C4-C4X-N5	3.27	122.88	118.23
2	M	601	FAD	C4X-C10-N1	-3.26	117.16	124.73
2	R	601	FAD	N3-C2-N1	3.25	125.76	119.38
2	W	601	FAD	C5'-C4'-C3'	3.24	118.47	112.20
2	Q	601	FAD	C4X-C10-N1	-3.24	117.21	124.73
2	F	601	FAD	C4X-C10-N1	-3.24	117.22	124.73
2	I	601	FAD	C4A-C5A-N7A	-3.23	106.03	109.40
2	N	601	FAD	N3A-C2A-N1A	-3.22	123.64	128.68
2	K	601	FAD	C4X-C10-N1	-3.21	117.29	124.73
2	P	601	FAD	C4A-C5A-N7A	-3.20	106.06	109.40
2	R	601	FAD	O5B-C5B-C4B	3.20	120.01	108.99
2	W	601	FAD	C4X-C10-N1	-3.20	117.30	124.73
2	O	601	FAD	C4X-C10-N1	-3.18	117.34	124.73
2	W	601	FAD	C4A-C5A-N7A	-3.17	106.09	109.40
2	L	601	FAD	N3A-C2A-N1A	-3.17	123.73	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	601	FAD	C10-N1-C2	3.16	123.22	116.90
2	T	601	FAD	N3A-C2A-N1A	-3.15	123.75	128.68
2	B	601	FAD	C4X-C10-N1	-3.15	117.43	124.73
2	C	601	FAD	C4X-C10-N1	-3.14	117.44	124.73
2	B	601	FAD	C4X-C10-N10	3.14	121.07	116.48
2	X	601	FAD	C4X-C10-N1	-3.13	117.46	124.73
2	V	601	FAD	C4X-C10-N1	-3.11	117.52	124.73
2	C	601	FAD	O4B-C1B-C2B	-3.10	102.39	106.93
2	T	601	FAD	C4A-C5A-N7A	-3.10	106.17	109.40
2	D	601	FAD	C4-N3-C2	-3.10	119.92	125.64
2	G	601	FAD	C3B-C2B-C1B	3.10	105.64	100.98
2	S	601	FAD	C10-N1-C2	3.09	123.08	116.90
2	A	601	FAD	C5'-C4'-C3'	3.07	118.13	112.20
2	J	601	FAD	C4A-C5A-N7A	-3.07	106.20	109.40
2	T	601	FAD	C4X-C10-N1	-3.06	117.62	124.73
2	R	601	FAD	C4-N3-C2	-3.05	120.01	125.64
2	H	601	FAD	C4-N3-C2	-3.04	120.02	125.64
2	R	601	FAD	N3A-C2A-N1A	-3.02	123.96	128.68
2	N	601	FAD	C4-C4X-N5	3.02	122.52	118.23
2	P	601	FAD	N3A-C2A-N1A	-2.99	124.00	128.68
2	I	601	FAD	C4X-C10-N10	2.99	120.85	116.48
2	J	601	FAD	C4X-C10-N1	-2.98	117.82	124.73
2	H	601	FAD	C4X-C10-N1	-2.97	117.83	124.73
2	Q	601	FAD	C10-N1-C2	2.96	122.82	116.90
2	G	601	FAD	C10-N1-C2	2.96	122.81	116.90
2	E	601	FAD	C4X-C10-N1	-2.95	117.87	124.73
2	L	601	FAD	C4A-C5A-N7A	-2.95	106.33	109.40
2	L	601	FAD	C4-C4X-N5	2.93	122.40	118.23
2	D	601	FAD	C4-C4X-N5	2.90	122.36	118.23
2	U	601	FAD	C4-C4X-N5	2.90	122.36	118.23
2	V	601	FAD	C4-C4X-N5	2.90	122.36	118.23
2	F	601	FAD	C10-N1-C2	2.90	122.70	116.90
2	L	601	FAD	C10-N1-C2	2.90	122.70	116.90
2	X	601	FAD	N3A-C2A-N1A	-2.90	124.15	128.68
2	M	601	FAD	C5'-C4'-C3'	2.87	117.74	112.20
2	K	601	FAD	N3A-C2A-N1A	-2.87	124.20	128.68
2	M	601	FAD	C4X-C10-N10	2.86	120.67	116.48
2	D	601	FAD	C10-N1-C2	2.86	122.62	116.90
2	J	601	FAD	N3A-C2A-N1A	-2.86	124.21	128.68
2	O	601	FAD	C4-C4X-N5	2.86	122.30	118.23
2	G	601	FAD	C4A-C5A-N7A	-2.86	106.42	109.40
2	V	601	FAD	N3A-C2A-N1A	-2.85	124.22	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	601	FAD	O5B-PA-O1A	-2.85	97.94	109.07
2	I	601	FAD	C4X-C10-N1	-2.84	118.14	124.73
2	W	601	FAD	N3A-C2A-N1A	-2.84	124.24	128.68
2	S	601	FAD	O2A-PA-O5B	-2.84	94.58	107.75
2	E	601	FAD	C5'-C4'-C3'	2.83	117.67	112.20
2	J	601	FAD	C10-N1-C2	2.83	122.56	116.90
2	K	601	FAD	O3B-C3B-C4B	-2.83	102.87	111.05
2	G	601	FAD	C4-C4X-N5	2.82	122.24	118.23
2	U	601	FAD	C4A-C5A-N7A	-2.81	106.47	109.40
2	W	601	FAD	C4X-C10-N10	2.80	120.58	116.48
2	I	601	FAD	C4-C4X-N5	2.80	122.22	118.23
2	G	601	FAD	O4B-C1B-C2B	-2.80	102.83	106.93
2	K	601	FAD	O5B-C5B-C4B	2.79	118.60	108.99
2	P	601	FAD	C10-N1-C2	2.79	122.48	116.90
2	T	601	FAD	C2A-N1A-C6A	2.79	123.53	118.75
2	D	601	FAD	C4A-C5A-N7A	-2.78	106.50	109.40
2	N	601	FAD	C4X-C4-N3	2.78	120.26	113.19
2	L	601	FAD	C4X-C10-N10	2.78	120.54	116.48
2	X	601	FAD	C4-N3-C2	-2.77	120.52	125.64
2	B	601	FAD	C10-N1-C2	2.77	122.44	116.90
2	A	601	FAD	N3A-C2A-N1A	-2.77	124.35	128.68
2	K	601	FAD	C10-N1-C2	2.76	122.43	116.90
2	Q	601	FAD	C4X-C4-N3	2.76	120.20	113.19
2	Q	601	FAD	C4A-C5A-N7A	-2.75	106.53	109.40
2	L	601	FAD	C4-N3-C2	-2.74	120.57	125.64
2	D	601	FAD	C4X-C4-N3	2.74	120.15	113.19
2	Q	601	FAD	O4-C4-C4X	-2.73	119.36	126.60
2	O	601	FAD	O2-C2-N1	-2.73	117.31	121.83
2	A	601	FAD	O2A-PA-O1A	2.72	125.71	112.24
2	O	601	FAD	O3B-C3B-C4B	-2.71	103.21	111.05
2	M	601	FAD	C4-C4X-N5	2.70	122.08	118.23
2	S	601	FAD	N3A-C2A-N1A	-2.70	124.45	128.68
2	P	601	FAD	C4X-C10-N10	2.69	120.42	116.48
2	U	601	FAD	C4X-C10-N1	-2.68	118.50	124.73
2	E	601	FAD	C4X-C10-N10	2.68	120.40	116.48
2	C	601	FAD	C10-N1-C2	2.68	122.26	116.90
2	Q	601	FAD	C4-N3-C2	-2.67	120.70	125.64
2	L	601	FAD	O5B-C5B-C4B	2.67	118.19	108.99
2	G	601	FAD	N3A-C2A-N1A	-2.67	124.50	128.68
2	S	601	FAD	C4-C4X-N5	2.66	122.02	118.23
2	O	601	FAD	C10-N1-C2	2.64	122.18	116.90
2	J	601	FAD	C4X-C4-N3	2.64	119.89	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	601	FAD	C4-C4X-N5	2.64	121.99	118.23
2	S	601	FAD	C4-N3-C2	-2.64	120.77	125.64
2	J	601	FAD	O4-C4-C4X	-2.64	119.61	126.60
2	O	601	FAD	N3A-C2A-N1A	-2.62	124.58	128.68
2	M	601	FAD	N3A-C2A-N1A	-2.62	124.58	128.68
2	L	601	FAD	C5'-C4'-C3'	2.62	117.26	112.20
2	I	601	FAD	C10-N1-C2	2.62	122.14	116.90
2	V	601	FAD	C4X-C4-N3	2.61	119.82	113.19
2	H	601	FAD	C4X-C4-N3	2.61	119.82	113.19
2	M	601	FAD	C10-N1-C2	2.60	122.11	116.90
2	N	601	FAD	C4-N3-C2	-2.60	120.84	125.64
2	J	601	FAD	C1'-C2'-C3'	-2.60	102.52	109.79
2	D	601	FAD	O3'-C3'-C4'	-2.60	102.53	108.81
2	B	601	FAD	N3A-C2A-N1A	-2.59	124.62	128.68
2	C	601	FAD	C3B-C2B-C1B	2.59	104.88	100.98
2	A	601	FAD	C4X-C10-N1	-2.59	118.73	124.73
2	W	601	FAD	C4-C4X-N5	2.58	121.91	118.23
2	U	601	FAD	O2P-P-O1P	2.58	125.01	112.24
2	P	601	FAD	C4-N3-C2	-2.58	120.87	125.64
2	C	601	FAD	N3A-C2A-N1A	-2.57	124.66	128.68
2	W	601	FAD	C10-N1-C2	2.57	122.04	116.90
2	U	601	FAD	O4B-C1B-C2B	-2.57	103.17	106.93
2	H	601	FAD	O4-C4-C4X	-2.56	119.80	126.60
2	F	601	FAD	C3B-C2B-C1B	2.56	104.84	100.98
2	X	601	FAD	N3-C2-N1	2.56	124.41	119.38
2	K	601	FAD	C4-N3-C2	-2.54	120.94	125.64
2	T	601	FAD	C4-N3-C2	-2.54	120.94	125.64
2	K	601	FAD	C4X-C4-N3	2.54	119.64	113.19
2	H	601	FAD	N3-C2-N1	2.54	124.36	119.38
2	O	601	FAD	C4X-C10-N10	2.53	120.19	116.48
2	O	601	FAD	C4A-C5A-N7A	-2.53	106.76	109.40
2	A	601	FAD	O3B-C3B-C4B	-2.52	103.77	111.05
2	X	601	FAD	C4X-C4-N3	2.51	119.58	113.19
2	K	601	FAD	C4A-C5A-N7A	-2.51	106.78	109.40
2	O	601	FAD	C4-N3-C2	-2.51	121.00	125.64
2	M	601	FAD	C9A-N10-C10	-2.51	116.86	120.77
2	T	601	FAD	C4X-C4-N3	2.51	119.56	113.19
2	D	601	FAD	N3-C2-N1	2.50	124.29	119.38
2	N	601	FAD	C4X-C10-N10	2.50	120.13	116.48
2	U	601	FAD	C4X-C4-N3	2.49	119.52	113.19
2	W	601	FAD	C4-N3-C2	-2.49	121.04	125.64
2	S	601	FAD	C4X-C4-N3	2.49	119.51	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	601	FAD	C2A-N1A-C6A	2.49	123.01	118.75
2	V	601	FAD	C1'-C2'-C3'	-2.49	102.84	109.79
2	P	601	FAD	C1'-C2'-C3'	-2.48	102.86	109.79
2	F	601	FAD	N3A-C2A-N1A	-2.47	124.81	128.68
2	K	601	FAD	C5'-C4'-C3'	2.47	116.98	112.20
2	X	601	FAD	C4-C4X-N5	2.47	121.74	118.23
2	U	601	FAD	C10-N1-C2	2.46	121.81	116.90
2	N	601	FAD	C1'-C2'-C3'	-2.46	102.92	109.79
2	T	601	FAD	N3-C2-N1	2.46	124.20	119.38
2	J	601	FAD	C4-C4X-N5	2.45	121.72	118.23
2	L	601	FAD	O2-C2-N1	-2.45	117.77	121.83
2	Q	601	FAD	N3A-C2A-N1A	-2.44	124.86	128.68
2	S	601	FAD	O2-C2-N1	-2.44	117.79	121.83
2	W	601	FAD	O2-C2-N1	-2.43	117.81	121.83
2	L	601	FAD	C5B-C4B-C3B	-2.42	106.10	115.18
2	L	601	FAD	O5'-C5'-C4'	2.42	115.82	109.36
2	E	601	FAD	C4-C4X-N5	2.41	121.67	118.23
2	G	601	FAD	O3B-C3B-C4B	-2.39	104.13	111.05
2	D	601	FAD	C1'-C2'-C3'	-2.39	103.11	109.79
2	T	601	FAD	O4'-C4'-C5'	-2.39	104.55	109.92
2	E	601	FAD	C10-N1-C2	2.39	121.68	116.90
2	W	601	FAD	N3-C2-N1	2.39	124.07	119.38
2	I	601	FAD	C9A-N10-C10	-2.39	117.05	120.77
2	I	601	FAD	N3A-C2A-N1A	-2.39	124.95	128.68
2	G	601	FAD	O4'-C4'-C3'	-2.39	103.30	109.10
2	A	601	FAD	O2'-C2'-C3'	-2.39	103.30	109.10
2	G	601	FAD	C4X-C4-N3	2.38	119.25	113.19
2	G	601	FAD	C4-N3-C2	-2.38	121.24	125.64
2	U	601	FAD	O4-C4-C4X	-2.38	120.29	126.60
2	H	601	FAD	C3B-C2B-C1B	2.37	104.55	100.98
2	B	601	FAD	C4-N3-C2	-2.37	121.27	125.64
2	G	601	FAD	C5X-N5-C4X	2.37	122.01	118.07
2	H	601	FAD	C1'-C2'-C3'	-2.37	103.17	109.79
2	K	601	FAD	O4-C4-C4X	-2.37	120.33	126.60
2	R	601	FAD	C1'-C2'-C3'	-2.36	103.18	109.79
2	L	601	FAD	N3-C2-N1	2.36	124.01	119.38
2	O	601	FAD	N3-C2-N1	2.36	124.01	119.38
2	D	601	FAD	C4X-C10-N10	2.35	119.92	116.48
2	E	601	FAD	O4B-C1B-C2B	-2.35	103.49	106.93
2	R	601	FAD	C4-C4X-N5	2.35	121.58	118.23
2	R	601	FAD	C4X-C4-N3	2.34	119.14	113.19
2	E	601	FAD	N3-C2-N1	2.34	123.98	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	C4X-C10-N10	2.34	119.90	116.48
2	K	601	FAD	C4-C4X-N5	2.34	121.56	118.23
2	S	601	FAD	C4X-C10-N10	2.34	119.89	116.48
2	Q	601	FAD	C4-C4X-N5	2.33	121.55	118.23
2	O	601	FAD	O3'-C3'-C4'	-2.33	103.17	108.81
2	J	601	FAD	C4-N3-C2	-2.33	121.34	125.64
2	A	601	FAD	C10-N1-C2	2.33	121.56	116.90
2	H	601	FAD	C10-N1-C2	2.33	121.56	116.90
2	B	601	FAD	O2P-P-O1P	2.33	123.75	112.24
2	D	601	FAD	N3A-C2A-N1A	-2.32	125.06	128.68
2	S	601	FAD	C9A-N10-C10	-2.32	117.16	120.77
2	P	601	FAD	C9A-N10-C10	-2.31	117.17	120.77
2	P	601	FAD	N3-C2-N1	2.31	123.92	119.38
2	M	601	FAD	N3-C2-N1	2.31	123.91	119.38
2	C	601	FAD	O4-C4-C4X	-2.31	120.48	126.60
2	U	601	FAD	C1'-C2'-C3'	-2.31	103.34	109.79
2	C	601	FAD	C4-N3-C2	-2.30	121.39	125.64
2	O	601	FAD	C9A-N10-C10	-2.30	117.18	120.77
2	V	601	FAD	O4-C4-C4X	-2.29	120.52	126.60
2	B	601	FAD	C4X-C4-N3	2.29	119.00	113.19
2	P	601	FAD	C4-C4X-N5	2.28	121.47	118.23
2	F	601	FAD	C1'-C2'-C3'	-2.28	103.42	109.79
2	M	601	FAD	O2A-PA-O1A	2.28	123.50	112.24
2	Q	601	FAD	C5'-C4'-C3'	2.27	116.60	112.20
2	M	601	FAD	C4-N3-C2	-2.27	121.44	125.64
2	B	601	FAD	N3-C2-N1	2.27	123.84	119.38
2	X	601	FAD	C10-N1-C2	2.27	121.44	116.90
2	A	601	FAD	N6A-C6A-N1A	2.26	123.28	118.57
2	X	601	FAD	O4-C4-C4X	-2.26	120.61	126.60
2	I	601	FAD	O4-C4-C4X	-2.25	120.64	126.60
2	R	601	FAD	O2-C2-N1	-2.24	118.11	121.83
2	L	601	FAD	C5X-N5-C4X	2.24	121.80	118.07
2	M	601	FAD	O2-C2-N1	-2.24	118.12	121.83
2	L	601	FAD	C10-C4X-N5	-2.23	120.11	124.86
2	G	601	FAD	O2A-PA-O1A	2.23	123.28	112.24
2	V	601	FAD	O2'-C2'-C1'	-2.23	104.40	109.80
2	T	601	FAD	C4-C4X-N5	2.23	121.41	118.23
2	I	601	FAD	C4-N3-C2	-2.23	121.52	125.64
2	H	601	FAD	N3A-C2A-N1A	-2.22	125.20	128.68
2	E	601	FAD	C4-N3-C2	-2.22	121.53	125.64
2	F	601	FAD	C9A-N10-C10	-2.22	117.31	120.77
2	Q	601	FAD	O4'-C4'-C5'	2.22	114.90	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	601	FAD	O5B-C5B-C4B	2.21	116.61	108.99
2	O	601	FAD	C4X-C4-N3	2.21	118.80	113.19
2	T	601	FAD	C4X-C10-N10	2.21	119.70	116.48
2	L	601	FAD	O2P-P-O1P	2.20	123.14	112.24
2	A	601	FAD	O2P-P-O1P	2.20	123.11	112.24
2	L	601	FAD	C4X-C4-N3	2.20	118.77	113.19
2	B	601	FAD	C10-C4X-N5	-2.18	120.22	124.86
2	V	601	FAD	C2A-N1A-C6A	2.18	122.49	118.75
2	D	601	FAD	C3B-C2B-C1B	2.18	104.26	100.98
2	F	601	FAD	C4X-C4-N3	2.18	118.72	113.19
2	M	601	FAD	O3B-C3B-C4B	-2.18	104.75	111.05
2	F	601	FAD	C5A-C6A-N6A	2.18	123.66	120.35
2	E	601	FAD	C9A-N10-C10	-2.17	117.38	120.77
2	O	601	FAD	C1'-C2'-C3'	-2.17	103.71	109.79
2	P	601	FAD	C4X-C4-N3	2.17	118.70	113.19
2	G	601	FAD	O4-C4-C4X	-2.17	120.86	126.60
2	I	601	FAD	C4X-C4-N3	2.15	118.66	113.19
2	E	601	FAD	O5'-C5'-C4'	2.15	115.11	109.36
2	E	601	FAD	N6A-C6A-N1A	2.15	123.04	118.57
2	B	601	FAD	C1'-C2'-C3'	-2.15	103.78	109.79
2	V	601	FAD	O2-C2-N1	-2.14	118.27	121.83
2	U	601	FAD	N3A-C2A-N1A	-2.14	125.33	128.68
2	R	601	FAD	O3'-C3'-C4'	-2.14	103.64	108.81
2	F	601	FAD	C4-N3-C2	-2.14	121.69	125.64
2	Q	601	FAD	O4B-C1B-C2B	-2.14	103.80	106.93
2	H	601	FAD	C4X-C10-N10	2.14	119.60	116.48
2	K	601	FAD	C1'-C2'-C3'	-2.13	103.82	109.79
2	F	601	FAD	C10-C4X-N5	-2.13	120.33	124.86
2	B	601	FAD	O2-C2-N1	-2.13	118.30	121.83
2	W	601	FAD	C4X-C4-N3	2.13	118.60	113.19
2	X	601	FAD	C2A-N1A-C6A	2.13	122.39	118.75
2	F	601	FAD	O2-C2-N1	-2.13	118.30	121.83
2	C	601	FAD	O5'-C5'-C4'	2.13	115.04	109.36
2	L	601	FAD	C1'-C2'-C3'	-2.12	103.85	109.79
2	I	601	FAD	O2A-PA-O1A	2.12	122.74	112.24
2	M	601	FAD	C4X-C4-N3	2.11	118.56	113.19
2	X	601	FAD	C4X-C10-N10	2.11	119.56	116.48
2	S	601	FAD	O4-C4-C4X	-2.11	121.00	126.60
2	C	601	FAD	C4X-C4-N3	2.11	118.54	113.19
2	P	601	FAD	O2'-C2'-C1'	2.10	114.88	109.80
2	T	601	FAD	C10-N1-C2	2.10	121.09	116.90
2	B	601	FAD	O4B-C1B-C2B	-2.09	103.87	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	FAD	C1'-C2'-C3'	-2.09	103.94	109.79
2	R	601	FAD	C4X-C10-N10	2.09	119.53	116.48
2	X	601	FAD	C1'-C2'-C3'	-2.08	103.96	109.79
2	S	601	FAD	O2P-P-O1P	2.08	122.52	112.24
2	E	601	FAD	C4X-C4-N3	2.08	118.47	113.19
2	J	601	FAD	C9A-C5X-N5	-2.07	120.19	122.43
2	W	601	FAD	C1'-C2'-C3'	-2.06	104.02	109.79
2	A	601	FAD	N3-C2-N1	2.06	123.44	119.38
2	V	601	FAD	O3'-C3'-C4'	-2.06	103.83	108.81
2	T	601	FAD	C9A-N10-C10	-2.06	117.55	120.77
2	R	601	FAD	C5A-C6A-N6A	2.06	123.49	120.35
2	D	601	FAD	C5X-N5-C4X	2.05	121.48	118.07
2	F	601	FAD	O3B-C3B-C4B	-2.03	105.17	111.05
2	E	601	FAD	C1'-C2'-C3'	-2.03	104.11	109.79
2	W	601	FAD	O4-C4-C4X	-2.03	121.22	126.60
2	X	601	FAD	C9A-C5X-N5	-2.03	120.23	122.43
2	Q	601	FAD	N10-C10-N1	2.02	124.16	118.35
2	F	601	FAD	O5B-C5B-C4B	2.02	115.95	108.99
2	B	601	FAD	C3B-C2B-C1B	2.02	104.02	100.98
2	P	601	FAD	O2P-P-O1P	2.01	122.19	112.24
2	X	601	FAD	C5A-C6A-N6A	2.01	123.41	120.35
2	I	601	FAD	C4'-C3'-C2'	-2.01	109.17	113.36
2	G	601	FAD	O2P-P-O1P	2.00	122.15	112.24
2	V	601	FAD	C10-N1-C2	2.00	120.91	116.90
2	T	601	FAD	C5A-C6A-N1A	-2.00	115.81	120.35

There are no chirality outliers.

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	FAD	C5'-O5'-P-O2P
2	D	601	FAD	C5'-O5'-P-O1P
2	D	601	FAD	C5'-O5'-P-O2P
2	E	601	FAD	C5B-O5B-PA-O2A
2	E	601	FAD	C5B-O5B-PA-O3P
2	E	601	FAD	C5'-O5'-P-O2P
2	G	601	FAD	C5'-O5'-P-O2P
2	H	601	FAD	C5B-O5B-PA-O1A
2	I	601	FAD	C5'-O5'-P-O1P
2	I	601	FAD	C5'-O5'-P-O2P
2	J	601	FAD	C5B-O5B-PA-O1A
2	J	601	FAD	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
2	L	601	FAD	C3B-C4B-C5B-O5B
2	M	601	FAD	C5'-O5'-P-O1P
2	M	601	FAD	C5'-O5'-P-O2P
2	N	601	FAD	C5'-O5'-P-O2P
2	P	601	FAD	C5B-O5B-PA-O1A
2	P	601	FAD	C5'-O5'-P-O2P
2	Q	601	FAD	C5B-O5B-PA-O1A
2	Q	601	FAD	C5'-O5'-P-O2P
2	R	601	FAD	C5B-O5B-PA-O1A
2	T	601	FAD	C5'-O5'-P-O2P
2	V	601	FAD	C5B-O5B-PA-O1A
2	V	601	FAD	C5'-O5'-P-O1P
2	V	601	FAD	C5'-O5'-P-O2P
2	W	601	FAD	C5B-O5B-PA-O1A
2	W	601	FAD	C5'-O5'-P-O2P
2	X	601	FAD	C5'-O5'-P-O2P
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O1-C1-C2-C3
3	B	602	GOL	C1-C2-C3-O3
3	C	602	GOL	O1-C1-C2-C3
3	C	602	GOL	C1-C2-C3-O3
3	D	602	GOL	C1-C2-C3-O3
3	F	602	GOL	C1-C2-C3-O3
3	H	602	GOL	C1-C2-C3-O3
3	I	602	GOL	C1-C2-C3-O3
3	O	602	GOL	O1-C1-C2-C3
3	P	602	GOL	O1-C1-C2-C3
3	Q	602	GOL	C1-C2-C3-O3
3	T	602	GOL	C1-C2-C3-O3
3	U	602	GOL	C1-C2-C3-O3
3	V	602	GOL	O1-C1-C2-C3
3	V	602	GOL	C1-C2-C3-O3
3	W	602	GOL	C1-C2-C3-O3
3	A	602	GOL	O2-C2-C3-O3
3	I	602	GOL	O2-C2-C3-O3
2	L	601	FAD	O4B-C4B-C5B-O5B
3	E	602	GOL	C1-C2-C3-O3
3	K	602	GOL	C1-C2-C3-O3
3	O	602	GOL	C1-C2-C3-O3
3	R	602	GOL	C1-C2-C3-O3
3	S	602	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	W	602	GOL	O1-C1-C2-C3
3	X	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3
3	C	602	GOL	O2-C2-C3-O3
3	D	602	GOL	O2-C2-C3-O3
3	F	602	GOL	O2-C2-C3-O3
3	O	602	GOL	O1-C1-C2-O2
3	Q	602	GOL	O2-C2-C3-O3
3	R	602	GOL	O2-C2-C3-O3
3	T	602	GOL	O2-C2-C3-O3
3	V	602	GOL	O2-C2-C3-O3
2	X	601	FAD	C3B-C4B-C5B-O5B
2	M	601	FAD	O4B-C4B-C5B-O5B
2	O	601	FAD	O4B-C4B-C5B-O5B
2	T	601	FAD	O4B-C4B-C5B-O5B
2	X	601	FAD	O4B-C4B-C5B-O5B
3	E	602	GOL	O2-C2-C3-O3
3	H	602	GOL	O2-C2-C3-O3
3	O	602	GOL	O2-C2-C3-O3
3	U	602	GOL	O2-C2-C3-O3
3	W	602	GOL	O2-C2-C3-O3
2	O	601	FAD	C3B-C4B-C5B-O5B
2	I	601	FAD	O4B-C4B-C5B-O5B
2	T	601	FAD	C3B-C4B-C5B-O5B
2	U	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	C2'-C1'-N10-C10
2	K	601	FAD	C2'-C1'-N10-C10
2	Q	601	FAD	C2'-C1'-N10-C10
2	T	601	FAD	C2'-C1'-N10-C10
2	U	601	FAD	C2'-C1'-N10-C10
2	X	601	FAD	C2'-C1'-N10-C10
3	K	602	GOL	O2-C2-C3-O3
3	S	602	GOL	O2-C2-C3-O3
3	X	602	GOL	O2-C2-C3-O3
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C5'-O5'-P-O3P
2	D	601	FAD	C5'-O5'-P-O3P
2	E	601	FAD	C5'-O5'-P-O3P
2	G	601	FAD	C5'-O5'-P-O3P
2	J	601	FAD	C5'-O5'-P-O3P
2	N	601	FAD	C5'-O5'-P-O3P
2	O	601	FAD	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
2	P	601	FAD	C5'-O5'-P-O3P
2	Q	601	FAD	C5B-O5B-PA-O3P
2	T	601	FAD	C5'-O5'-P-O3P
2	W	601	FAD	C5'-O5'-P-O3P
2	X	601	FAD	C5'-O5'-P-O3P
3	K	602	GOL	O1-C1-C2-O2
3	N	602	GOL	O2-C2-C3-O3
2	M	601	FAD	C3B-C4B-C5B-O5B
3	N	602	GOL	C1-C2-C3-O3
3	U	602	GOL	O1-C1-C2-C3
2	E	601	FAD	C5B-O5B-PA-O1A
2	E	601	FAD	C5'-O5'-P-O1P
2	N	601	FAD	C5'-O5'-P-O1P
2	P	601	FAD	C5'-O5'-P-O1P
2	Q	601	FAD	C5'-O5'-P-O1P
2	T	601	FAD	C5'-O5'-P-O1P
2	W	601	FAD	C5'-O5'-P-O1P
2	X	601	FAD	C5'-O5'-P-O1P
2	I	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	C2'-C1'-N10-C10
2	H	601	FAD	C2'-C1'-N10-C10
2	O	601	FAD	C2'-C1'-N10-C10
2	R	601	FAD	C2'-C1'-N10-C10
2	S	601	FAD	C2'-C1'-N10-C10
2	V	601	FAD	C2'-C1'-N10-C10
2	I	601	FAD	C3'-C4'-C5'-O5'
2	U	601	FAD	C3B-C4B-C5B-O5B
3	E	602	GOL	O1-C1-C2-C3
3	B	602	GOL	O1-C1-C2-O2
3	C	602	GOL	O1-C1-C2-O2
3	P	602	GOL	O1-C1-C2-O2
2	B	601	FAD	O4'-C4'-C5'-O5'
2	D	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	C3B-C4B-C5B-O5B
2	G	601	FAD	O4B-C4B-C5B-O5B
2	H	601	FAD	C5B-O5B-PA-O3P
2	I	601	FAD	C5'-O5'-P-O3P
2	M	601	FAD	C5'-O5'-P-O3P
2	P	601	FAD	C5B-O5B-PA-O3P
2	Q	601	FAD	C5'-O5'-P-O3P
2	R	601	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
2	S	601	FAD	C5B-O5B-PA-O3P
2	U	601	FAD	C5B-O5B-PA-O3P
2	V	601	FAD	C5B-O5B-PA-O3P
2	V	601	FAD	C5'-O5'-P-O3P
2	W	601	FAD	C5B-O5B-PA-O3P
3	W	602	GOL	O1-C1-C2-O2
2	L	601	FAD	C4B-C5B-O5B-PA
3	D	602	GOL	O1-C1-C2-C3
3	K	602	GOL	O1-C1-C2-C3
3	L	602	GOL	O1-C1-C2-C3
3	R	602	GOL	O1-C1-C2-C3
3	S	602	GOL	O1-C1-C2-C3
2	C	601	FAD	C5'-O5'-P-O1P
2	G	601	FAD	C5B-O5B-PA-O1A
2	G	601	FAD	C5'-O5'-P-O1P
2	J	601	FAD	C5'-O5'-P-O1P
2	K	601	FAD	C5B-O5B-PA-O1A
2	M	601	FAD	C5B-O5B-PA-O1A
2	N	601	FAD	C5B-O5B-PA-O1A
2	O	601	FAD	C5'-O5'-P-O1P
2	S	601	FAD	C5B-O5B-PA-O1A
2	U	601	FAD	C5B-O5B-PA-O1A
2	G	601	FAD	C3B-C4B-C5B-O5B
3	P	602	GOL	O2-C2-C3-O3

There are no ring outliers.

26 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	U	601	FAD	1	0
2	I	601	FAD	1	0
2	X	601	FAD	2	0
2	T	601	FAD	3	0
3	W	602	GOL	1	0
2	D	601	FAD	3	0
3	X	602	GOL	1	0
2	Q	601	FAD	1	0
3	L	602	GOL	1	0
2	W	601	FAD	2	0
3	K	602	GOL	1	0
2	V	601	FAD	1	0
2	S	601	FAD	1	0

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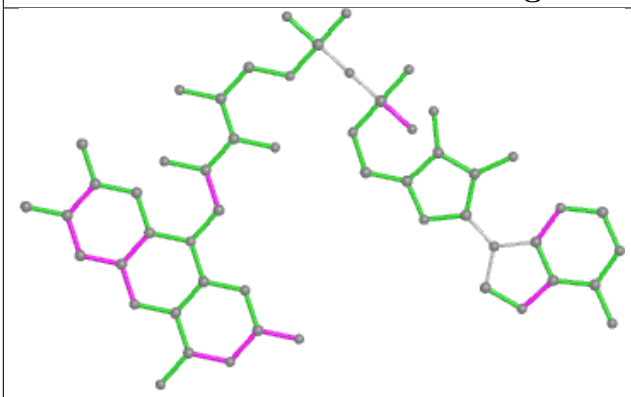
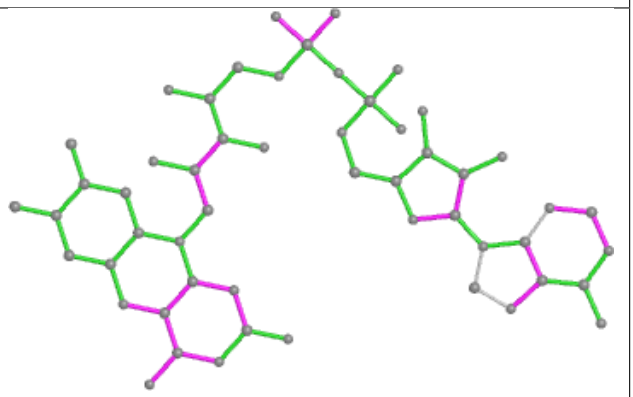
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	601	FAD	2	0
2	J	601	FAD	1	0
2	K	601	FAD	2	0
2	N	601	FAD	2	0
3	G	602	GOL	1	0
3	F	602	GOL	1	0
2	E	601	FAD	2	0
2	A	601	FAD	3	0
2	P	601	FAD	1	0
2	O	601	FAD	2	0
3	U	602	GOL	1	0
2	F	601	FAD	2	0
3	T	602	GOL	1	0

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.

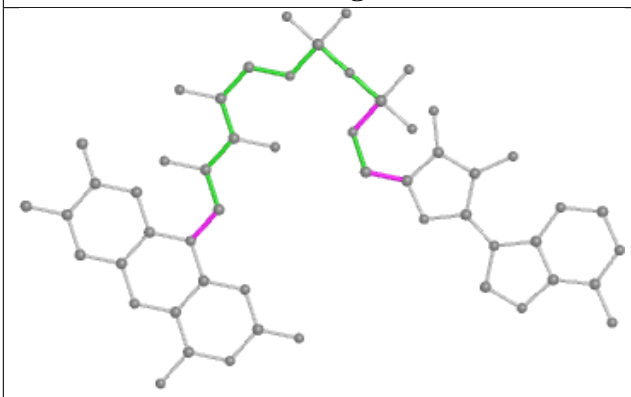
Ligand FAD U 601



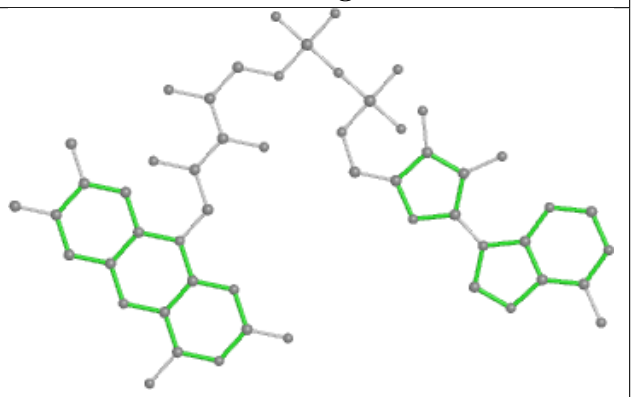
Bond lengths



Bond angles

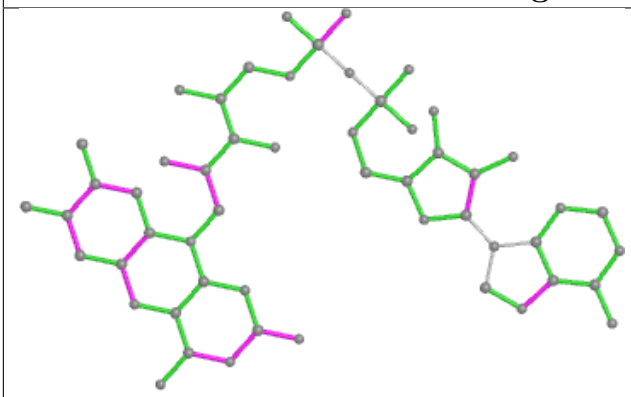


Torsions

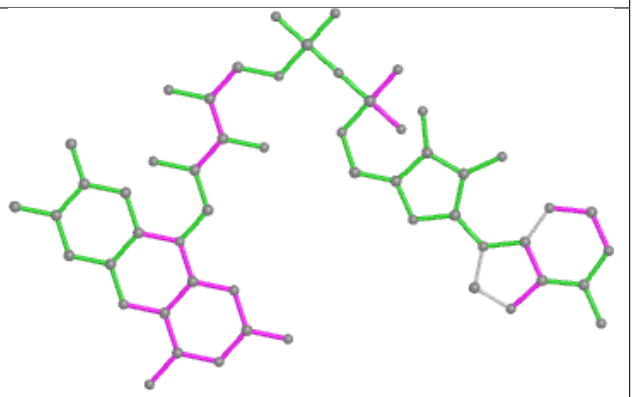


Rings

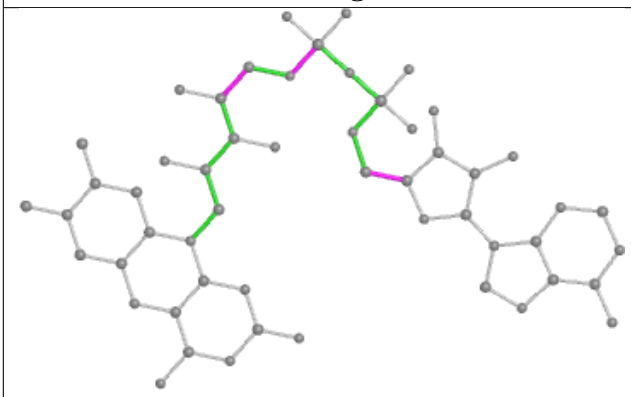
Ligand FAD I 601



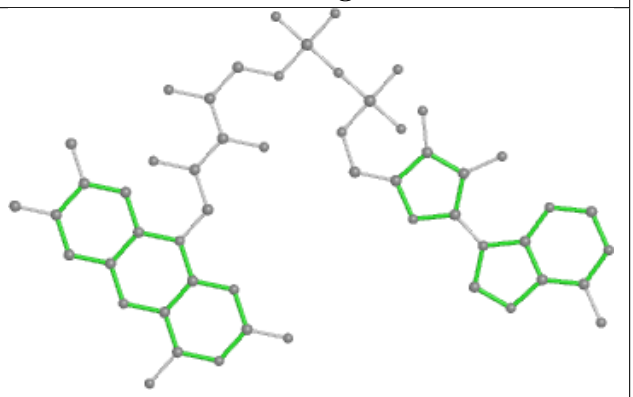
Bond lengths



Bond angles

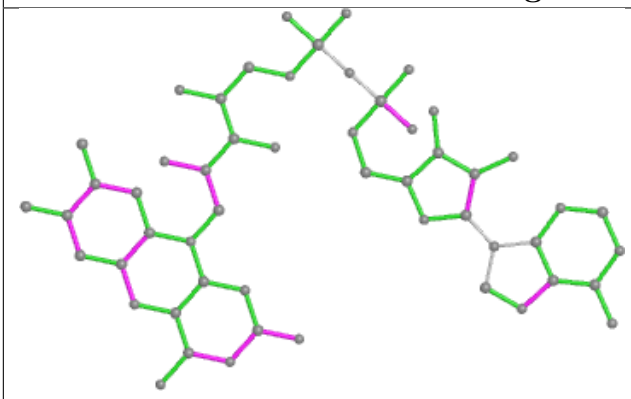


Torsions

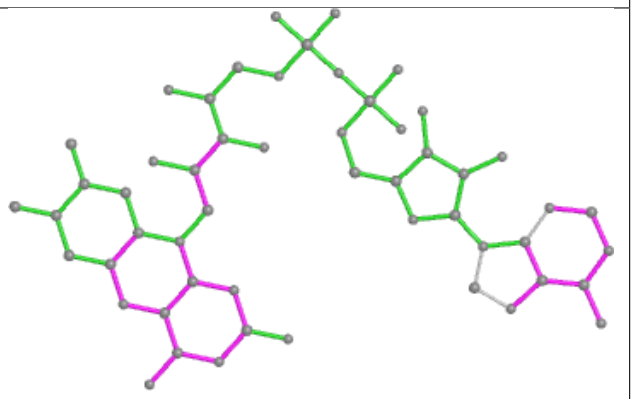


Rings

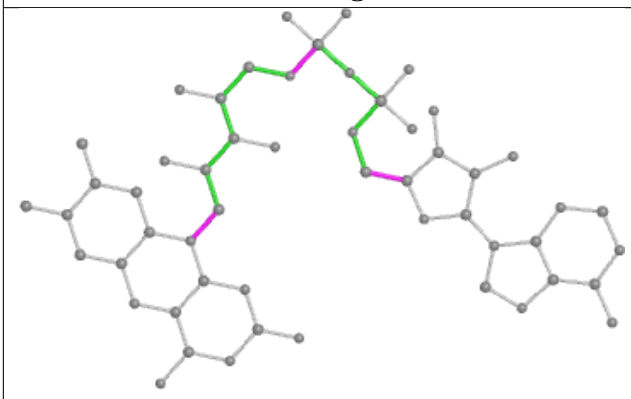
Ligand FAD X 601



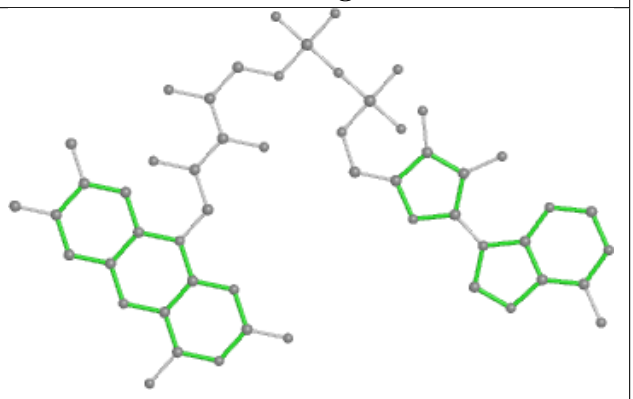
Bond lengths



Bond angles

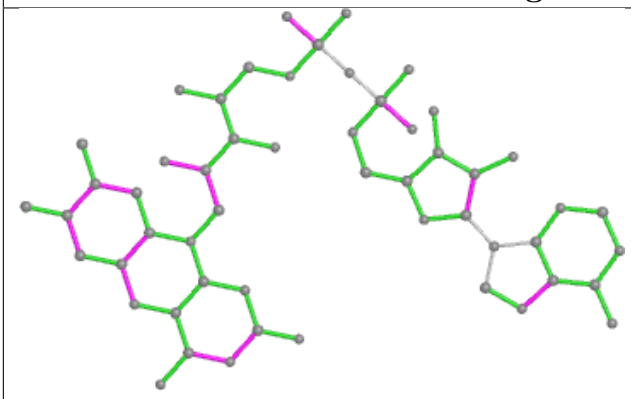


Torsions

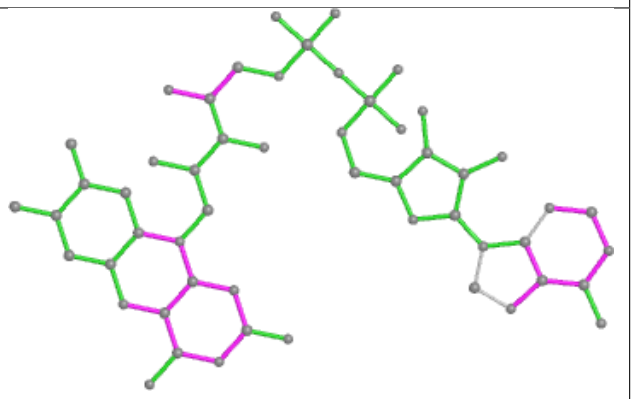


Rings

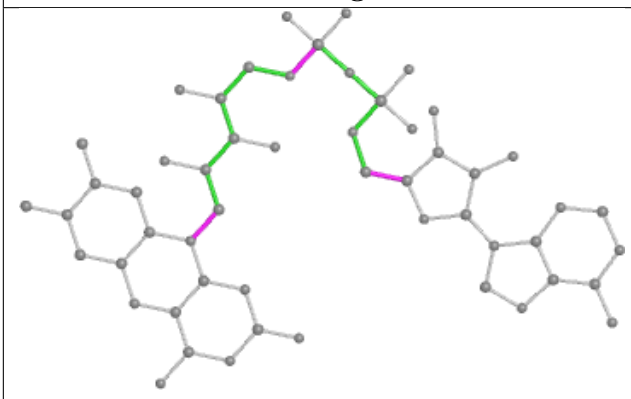
Ligand FAD T 601



Bond lengths



Bond angles



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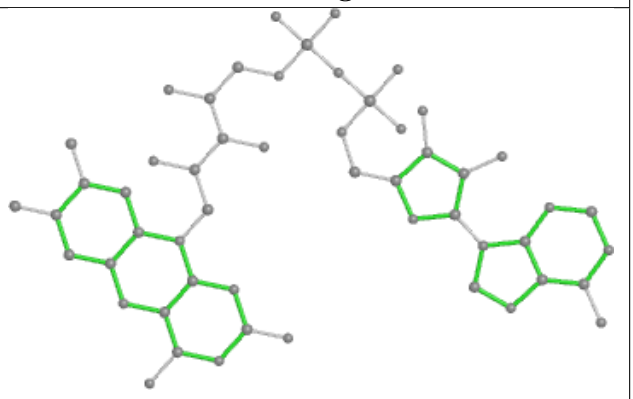
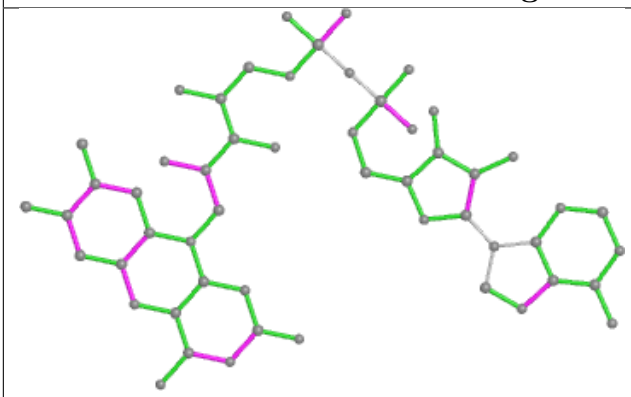


Rings

Ligand FAD M 601



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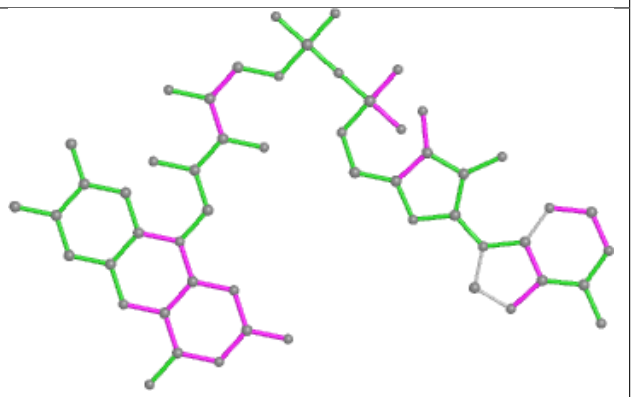
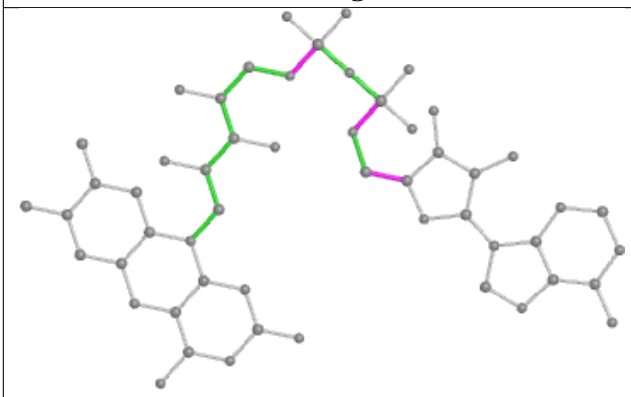


Bond angles



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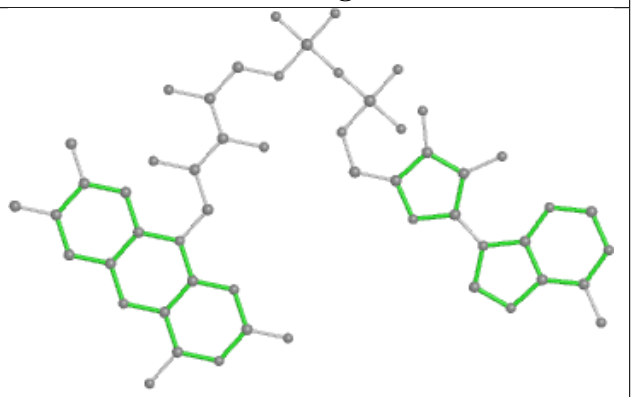
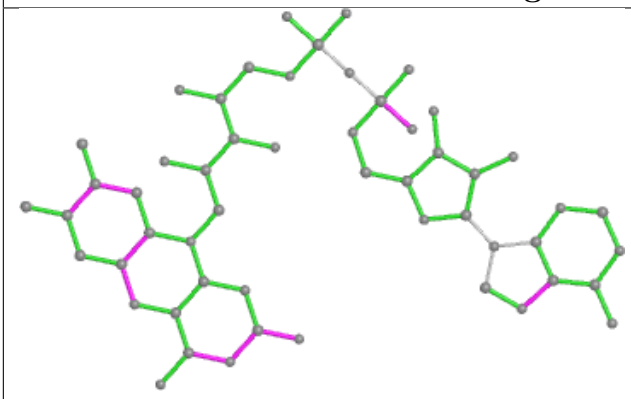
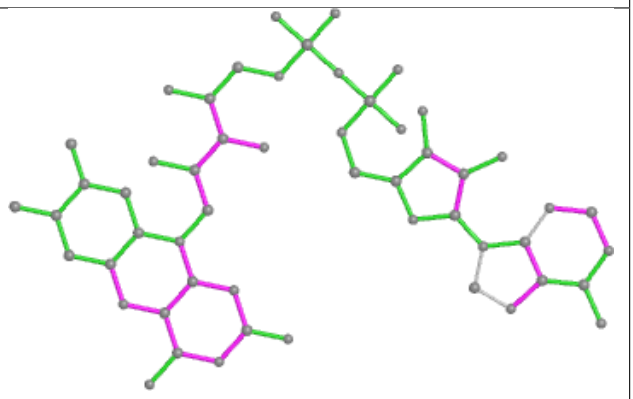


Rings

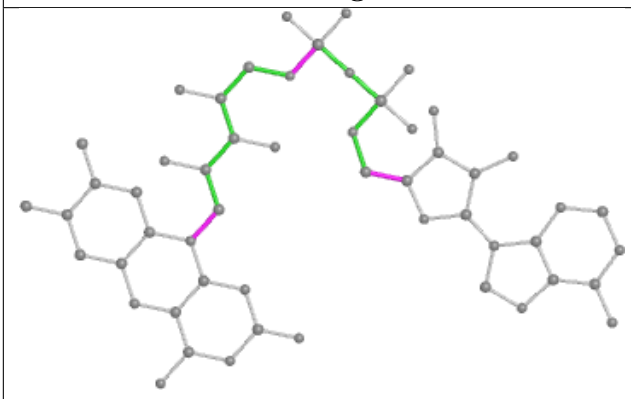
Ligand FAD D 601



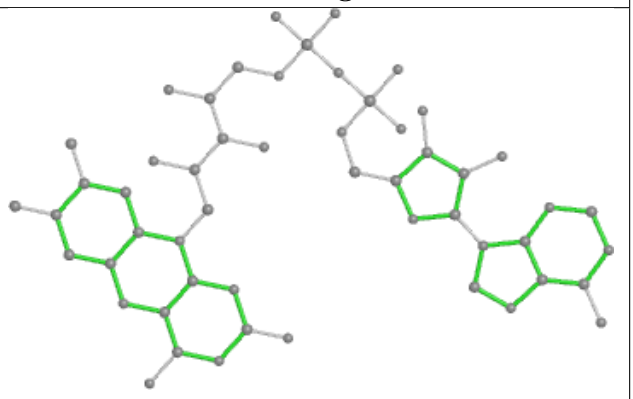
Bond lengths



Bond angles

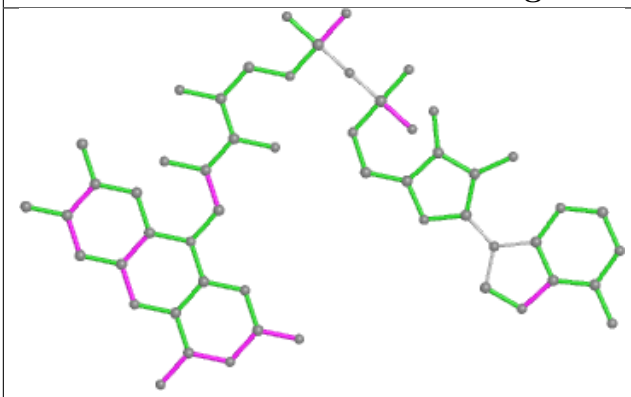


Torsions

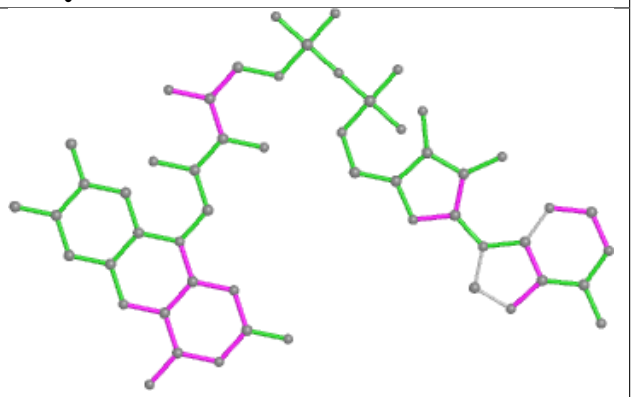


Rings

Ligand FAD Q 601



Bond lengths



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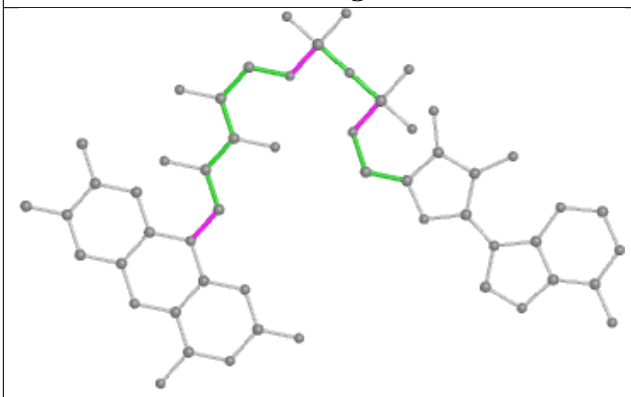
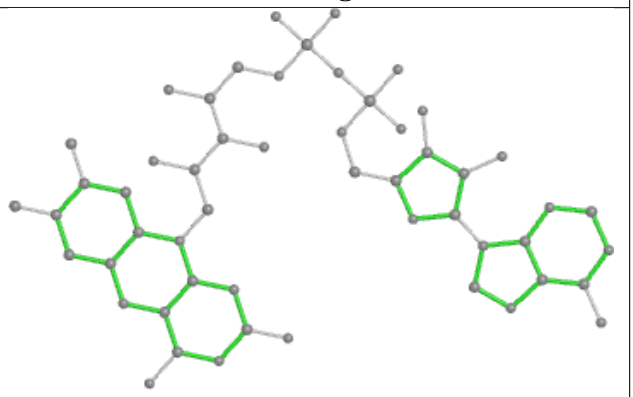


Torsions



Rings

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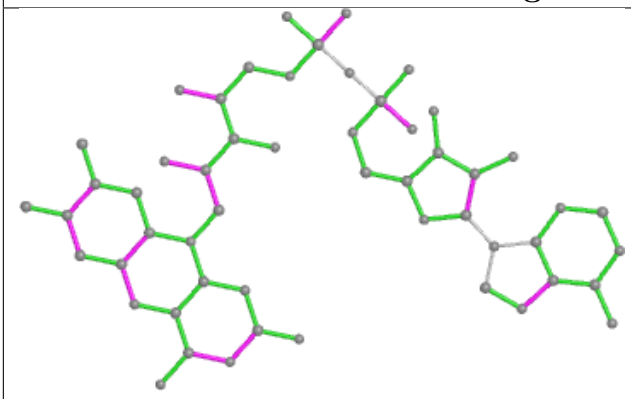

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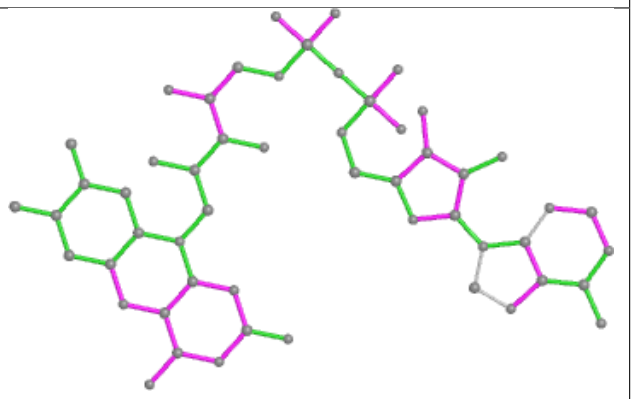

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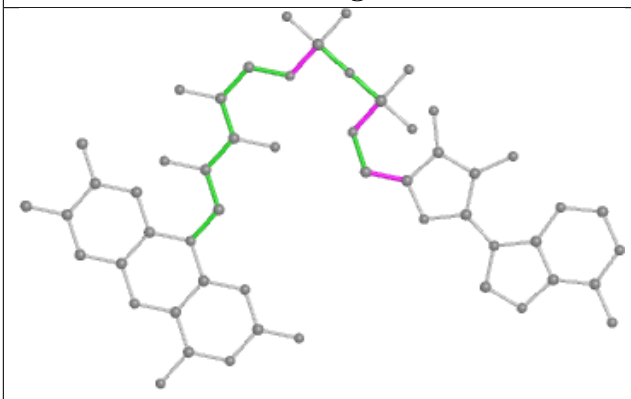

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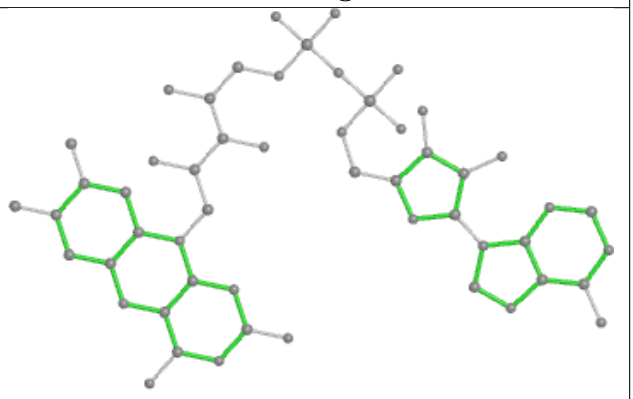

Rings

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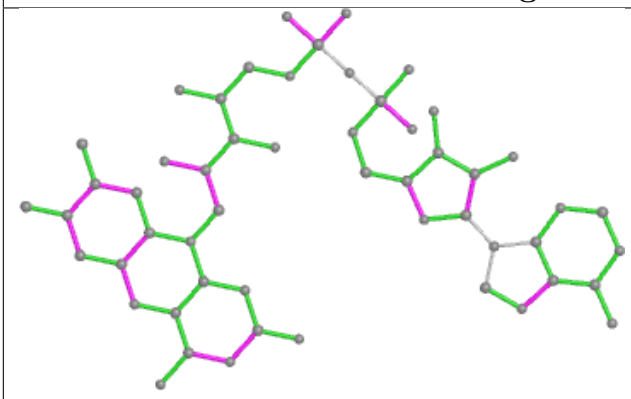

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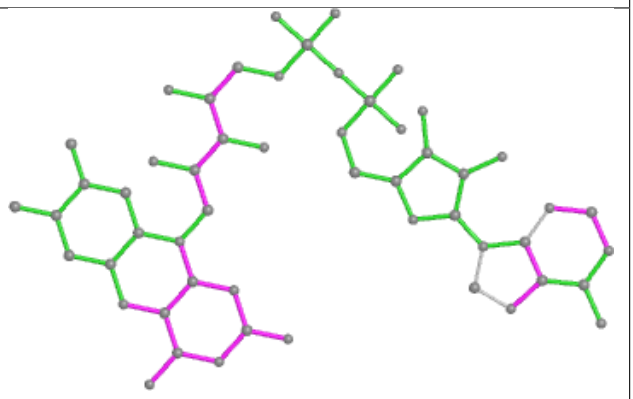

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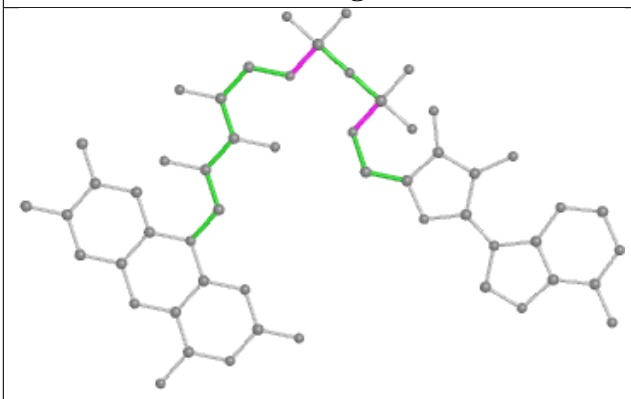

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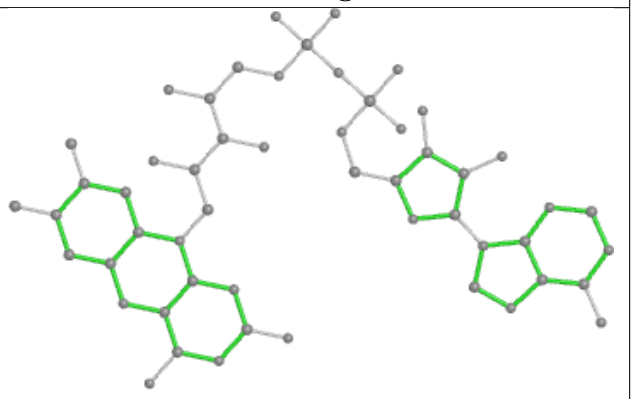

Rings

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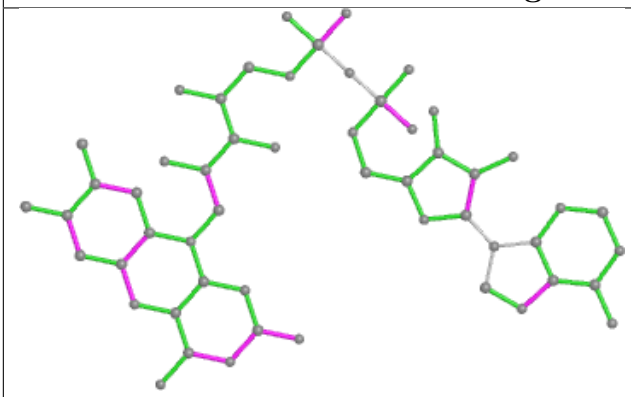

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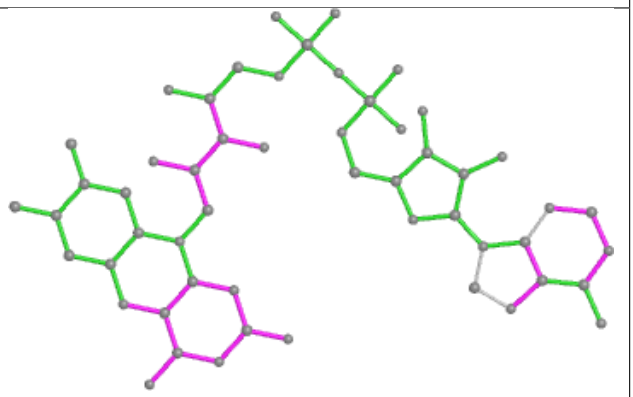

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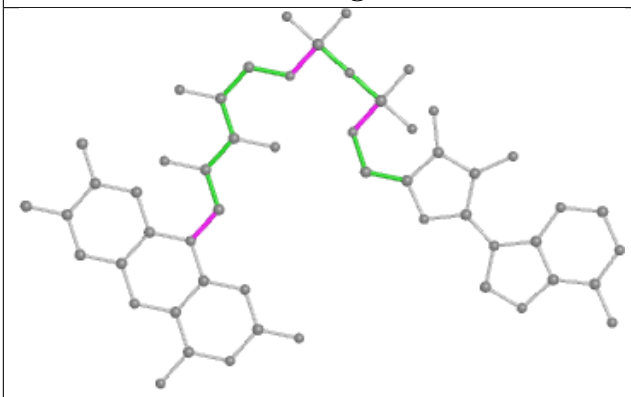

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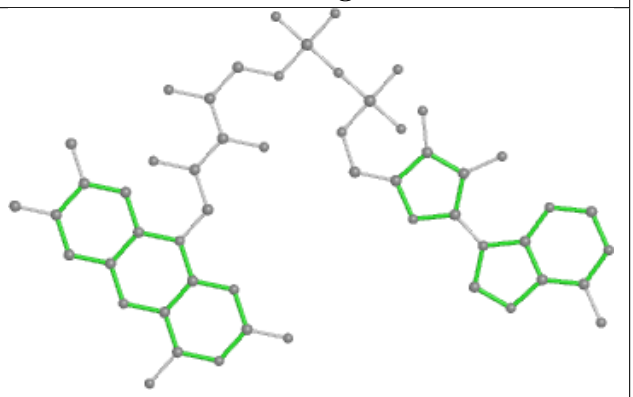

Rings

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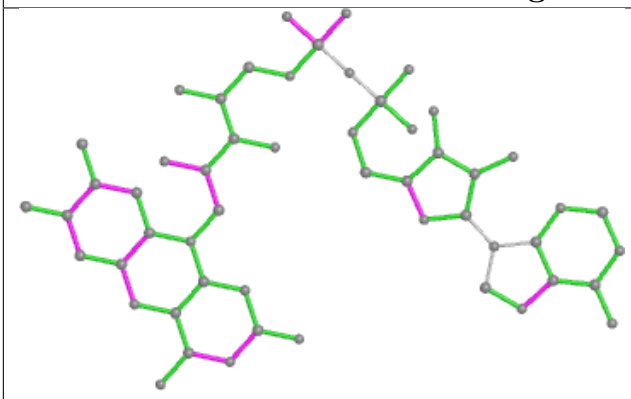

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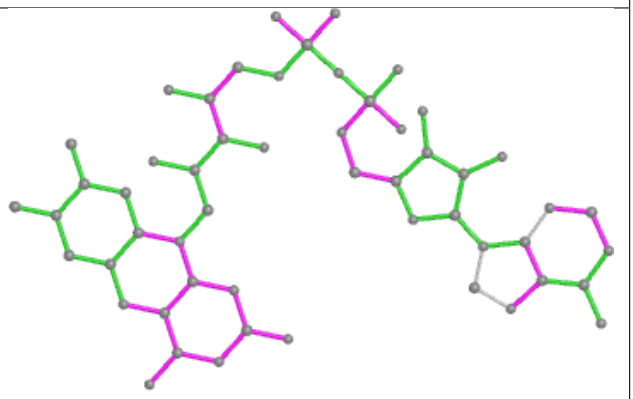

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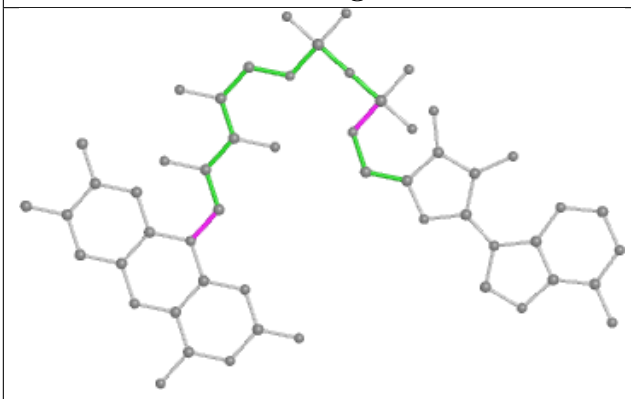

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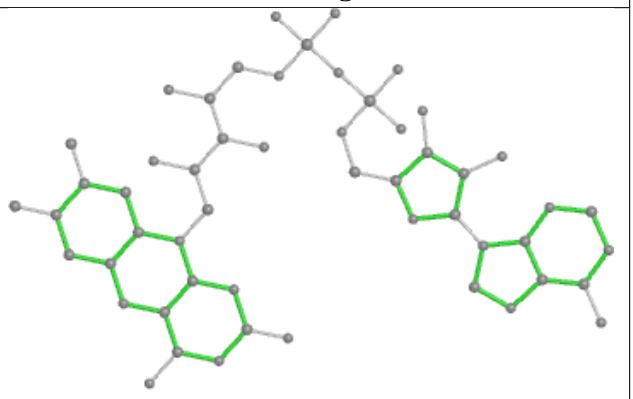

Rings

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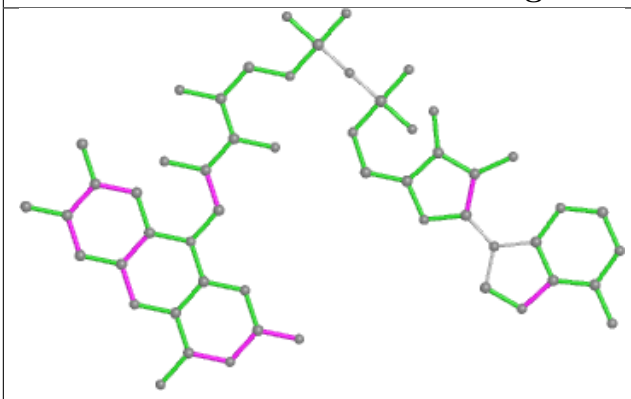

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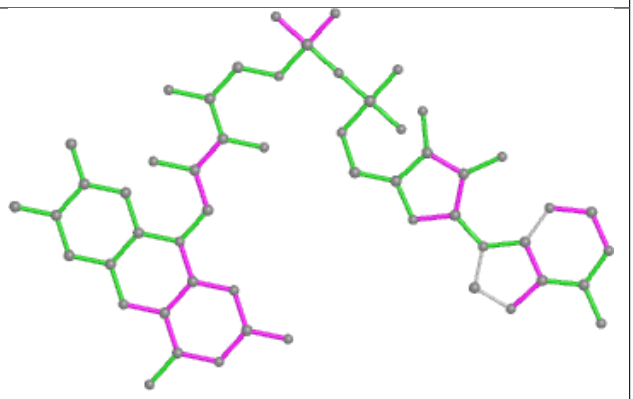

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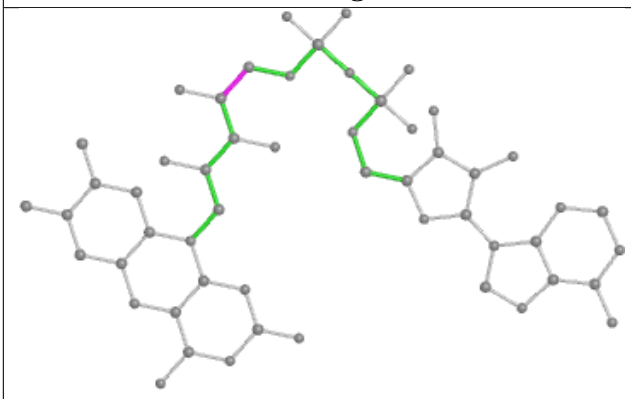

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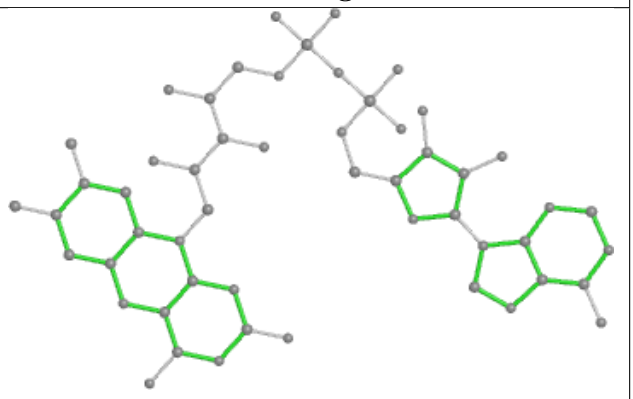

Rings

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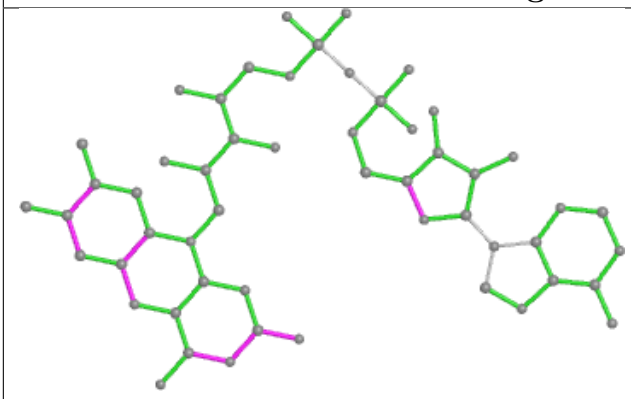

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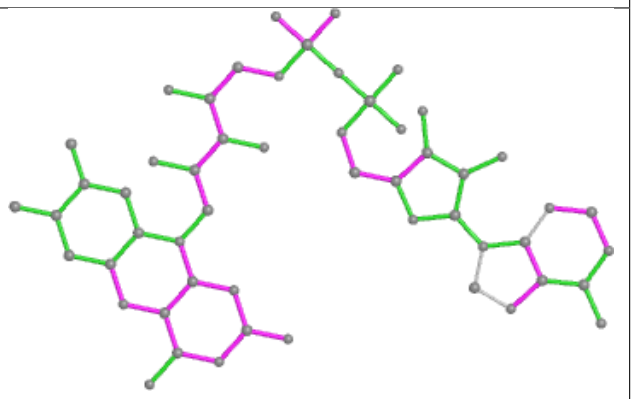

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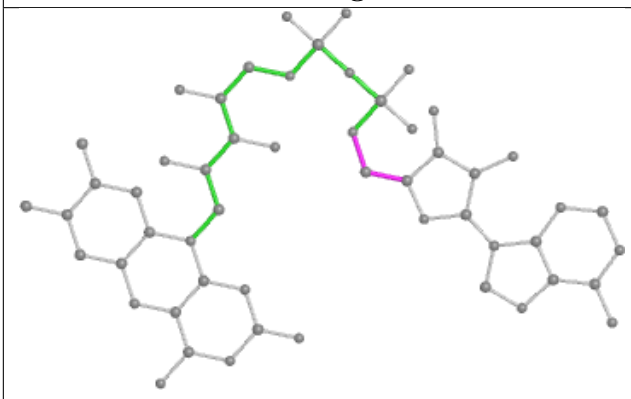

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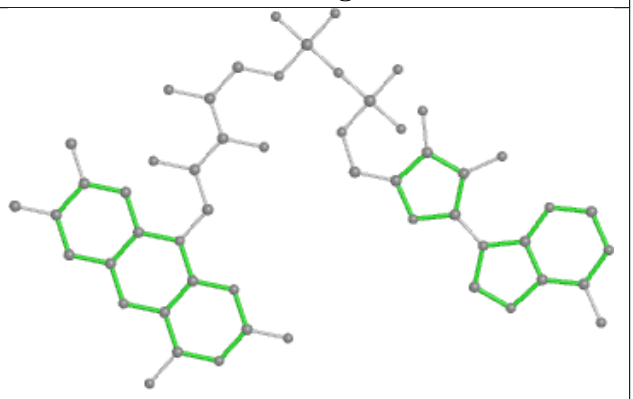

Rings

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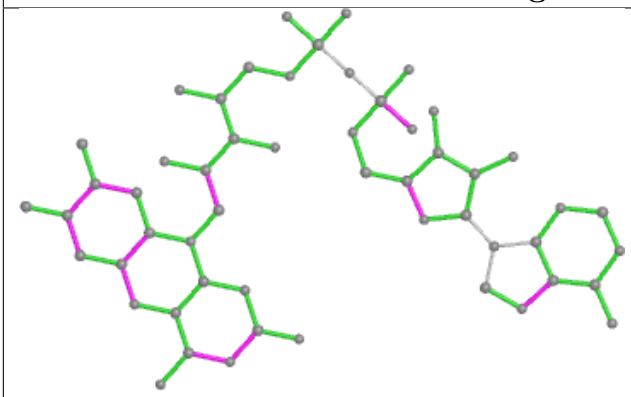

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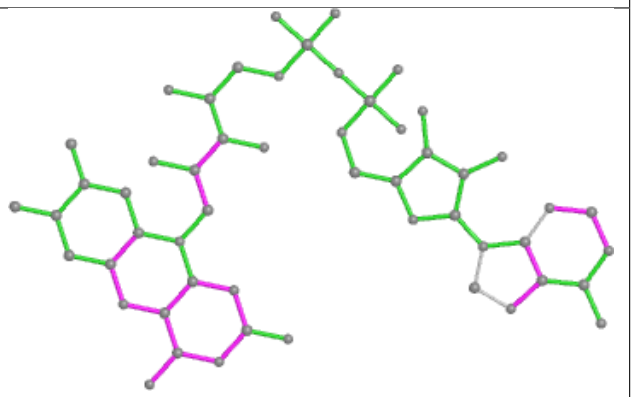

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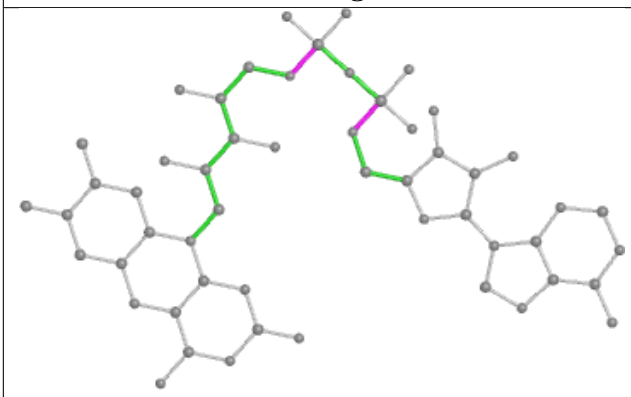

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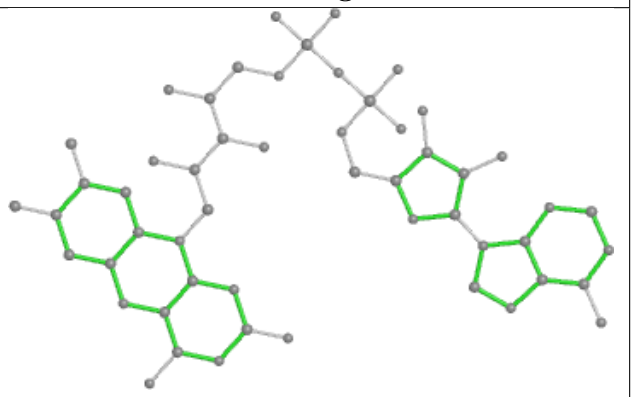

Rings

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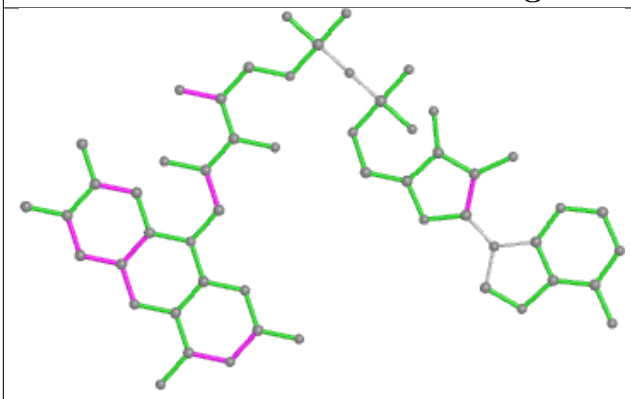

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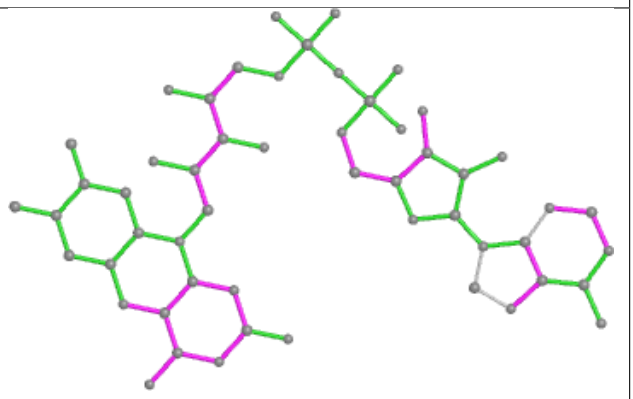

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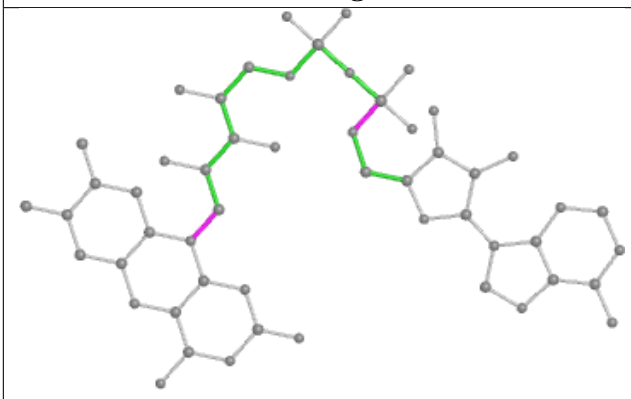

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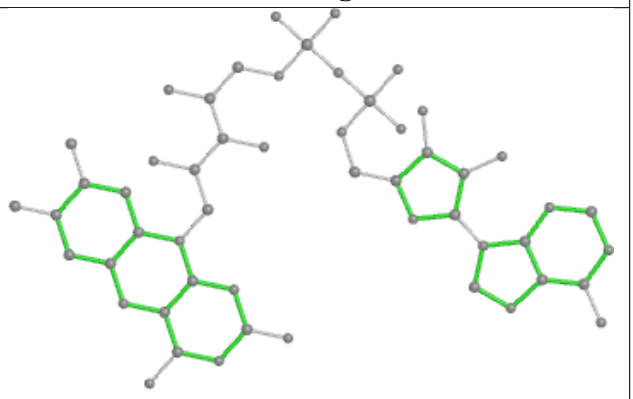

Rings

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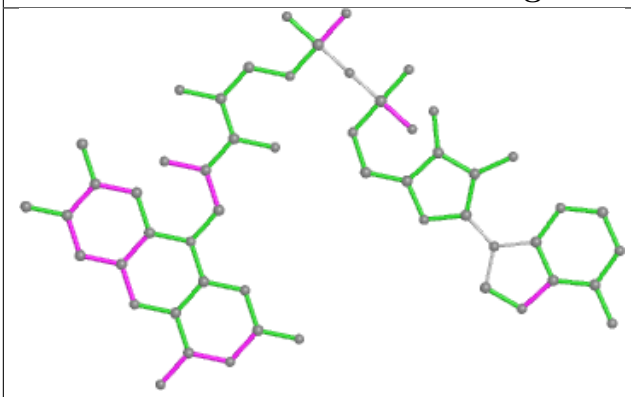

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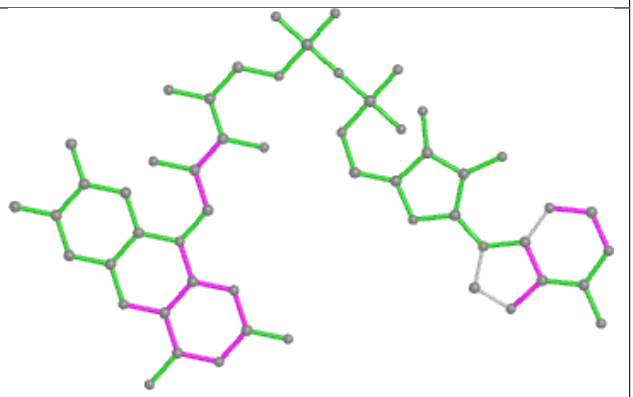

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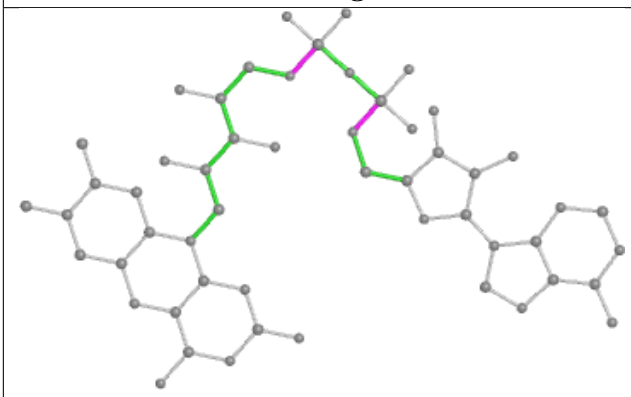

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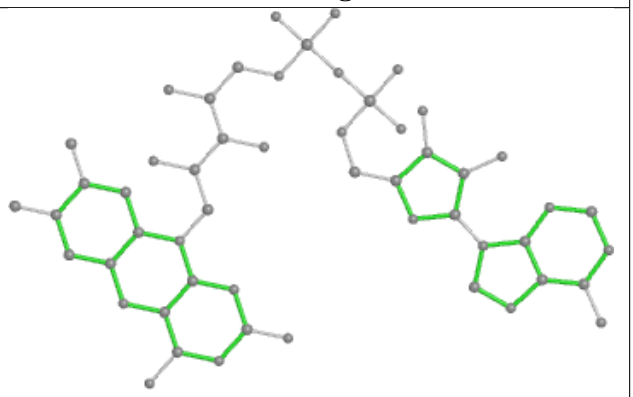

Rings

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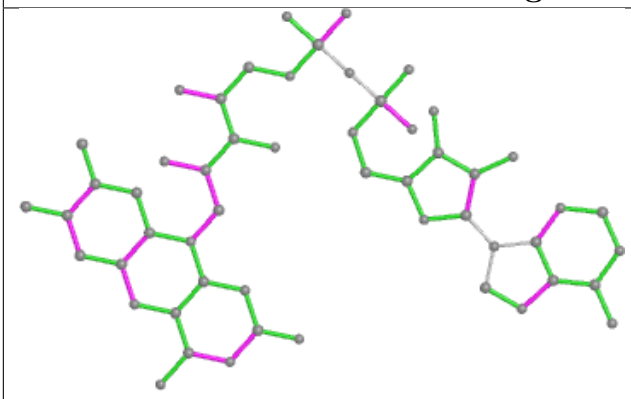

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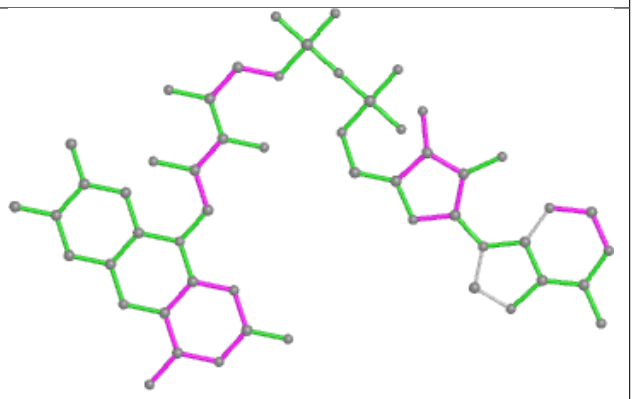

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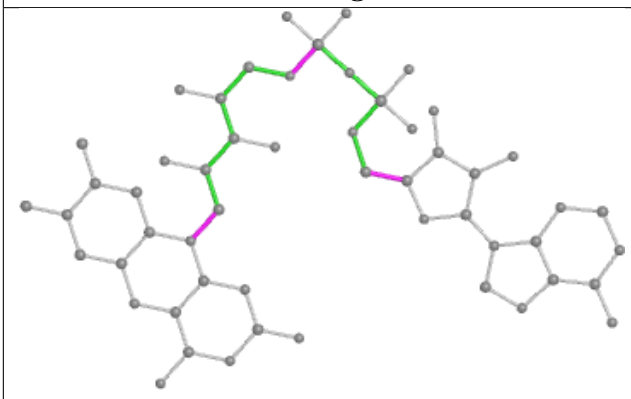

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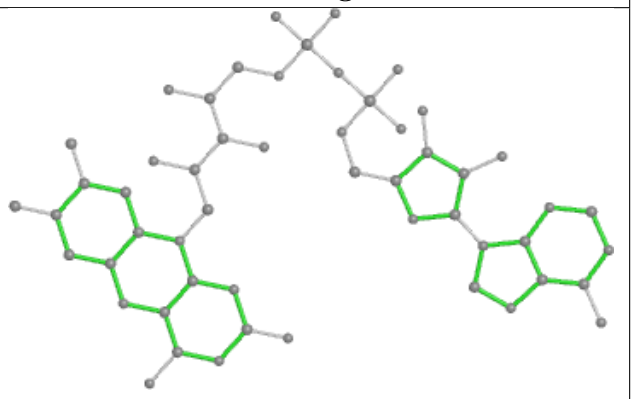

Rings

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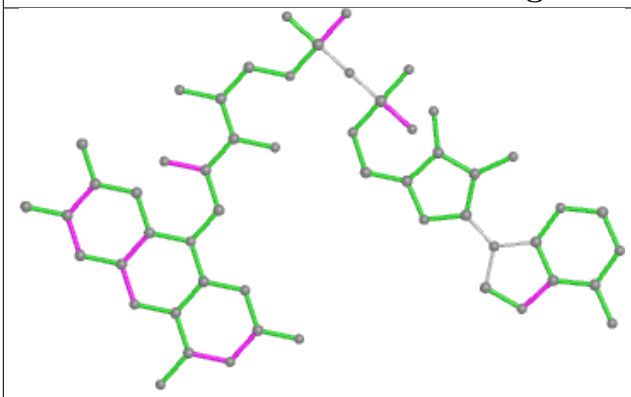

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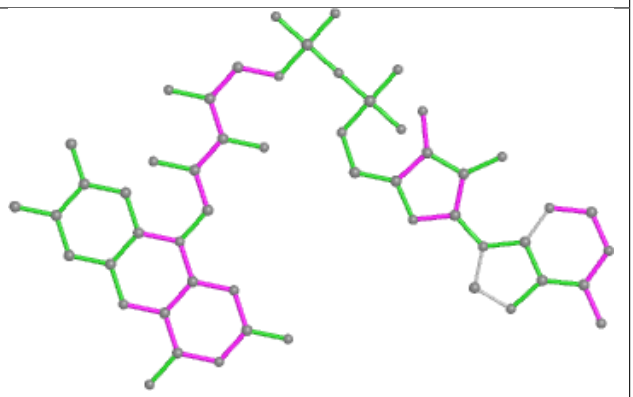

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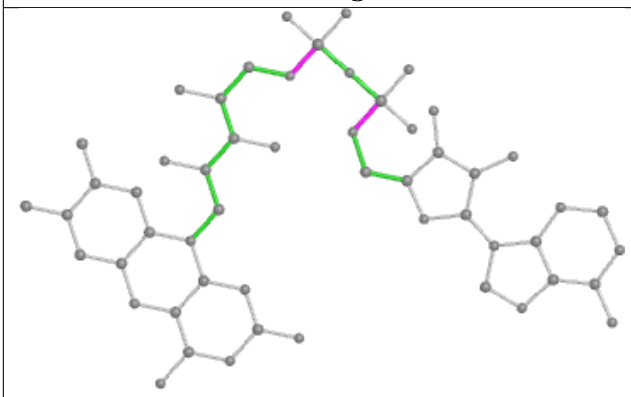

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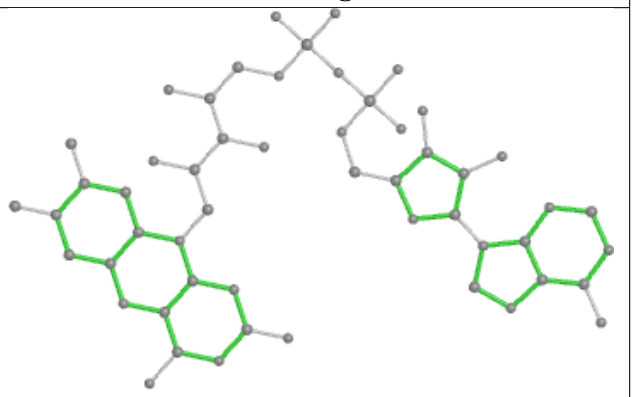

Rings

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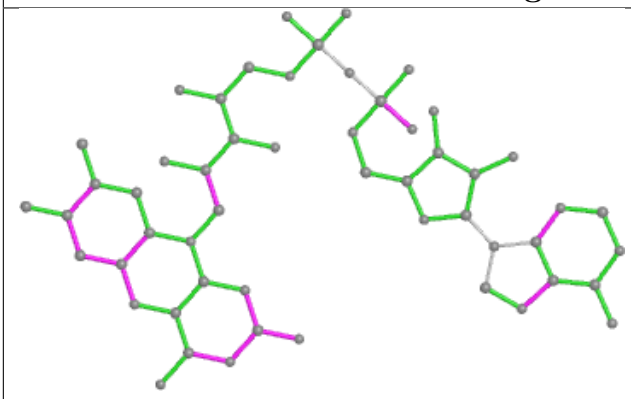

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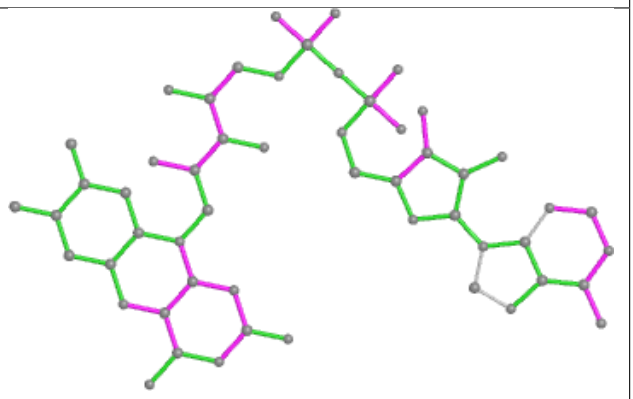
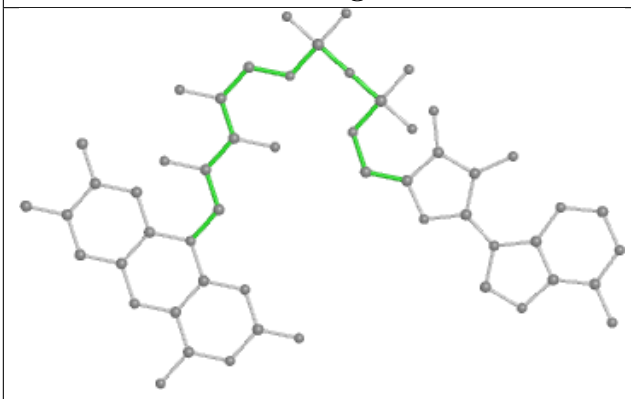


Bond angles



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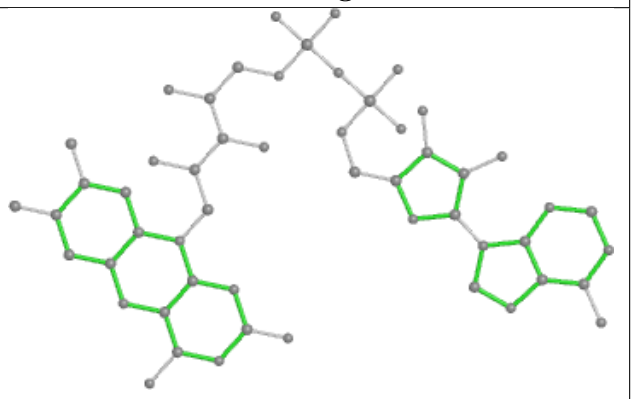
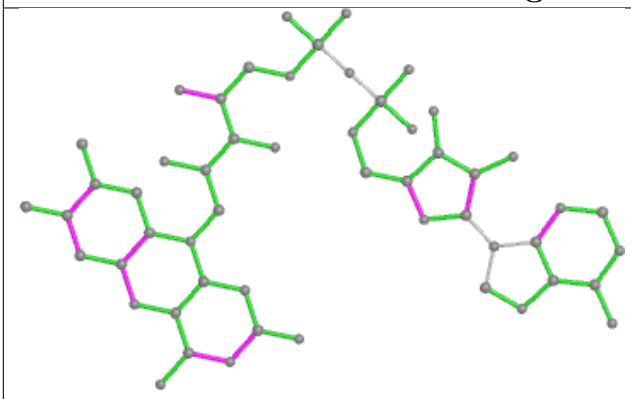


Rings

Ligand FAD P 601



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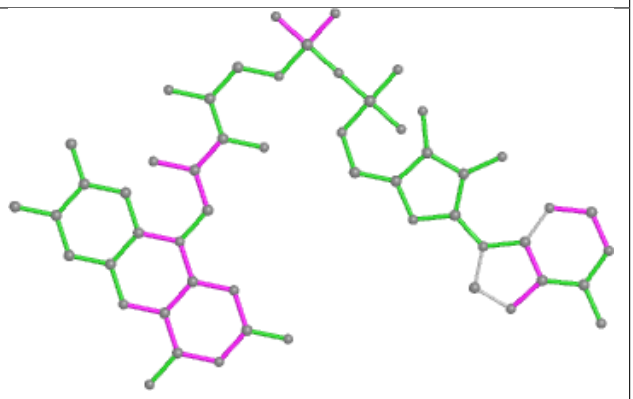
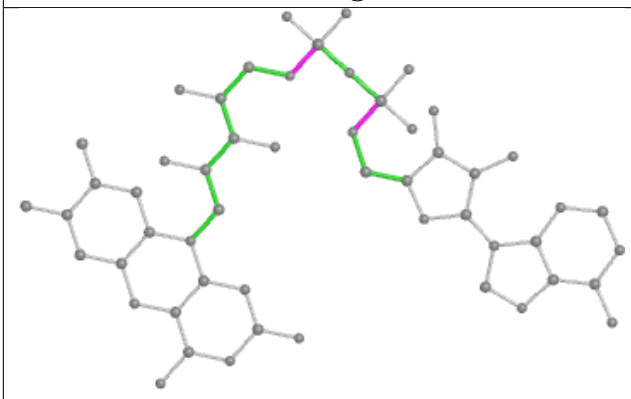
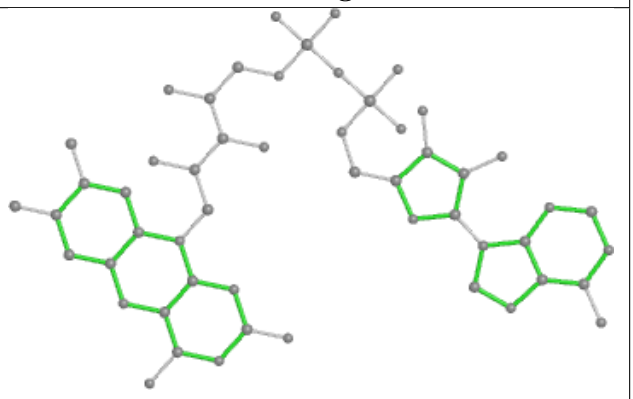


Bond angles

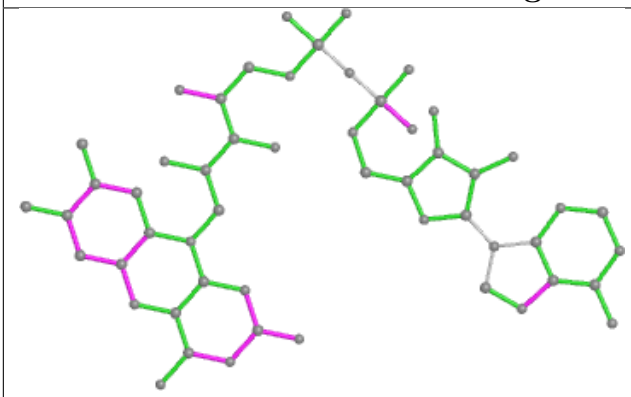


Torsions

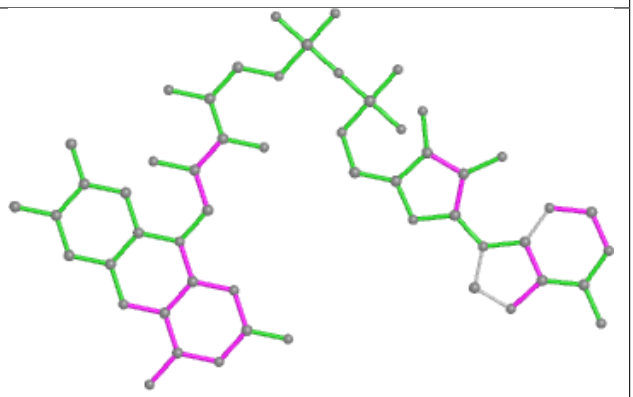


Rings

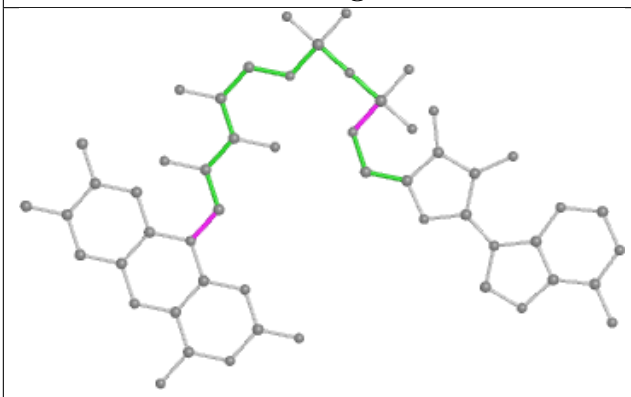
Ligand FAD H 601



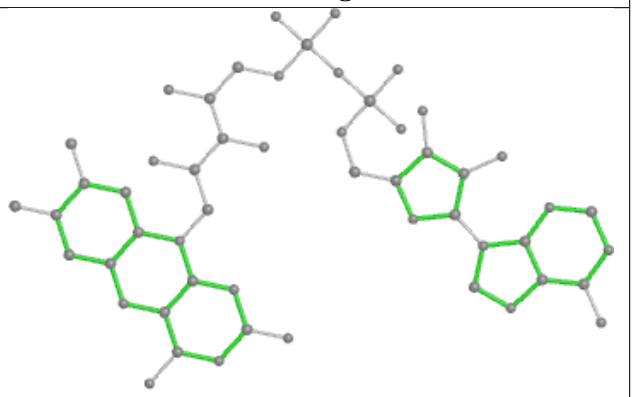
Bond lengths



Bond angles

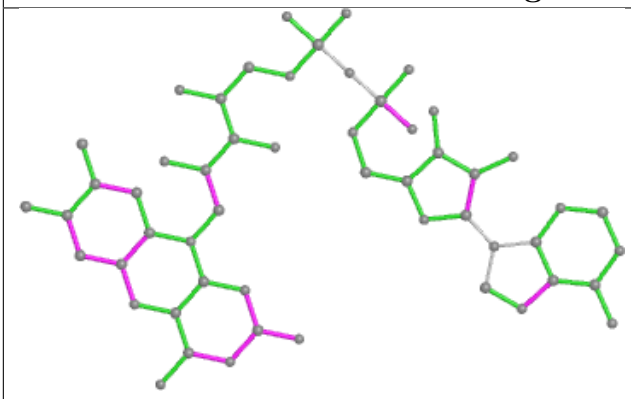


Torsions

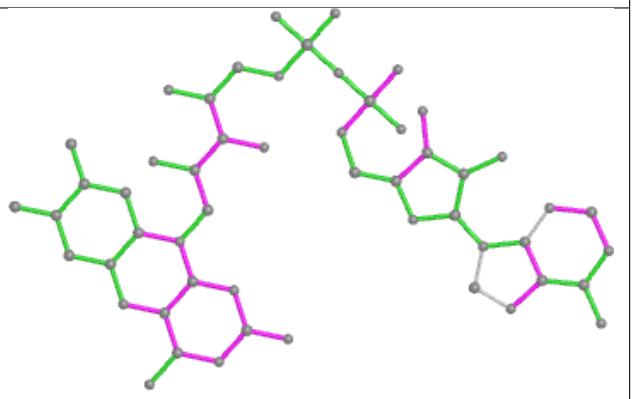


Rings

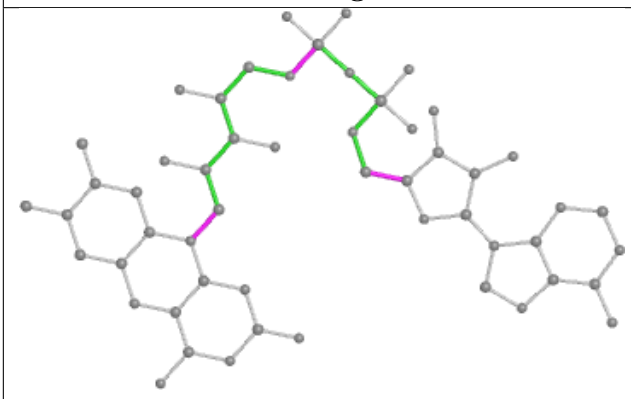
Ligand FAD O 601



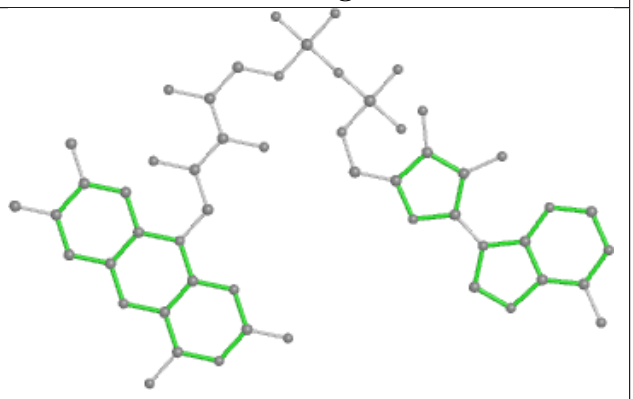
Bond lengths



Bond angles

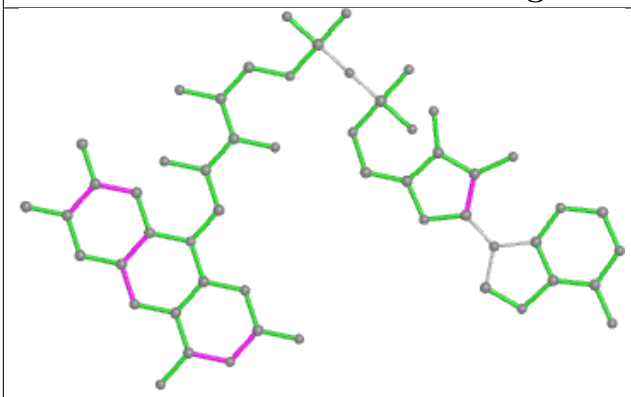


Torsions

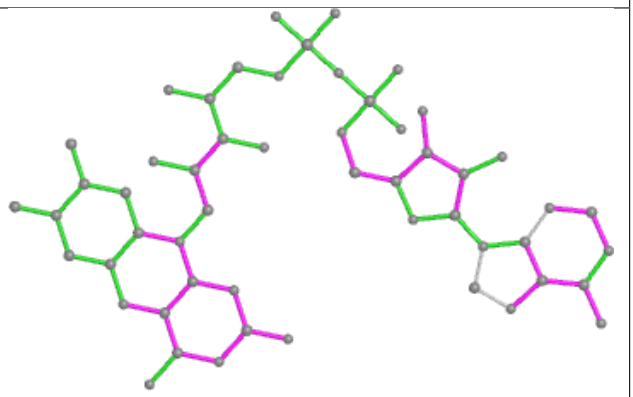


Rings

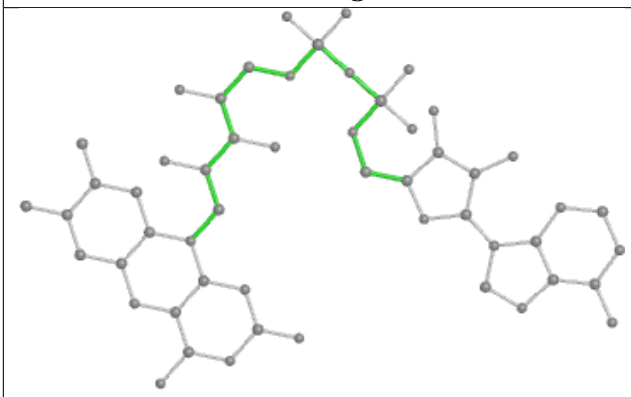
Ligand FAD F 601



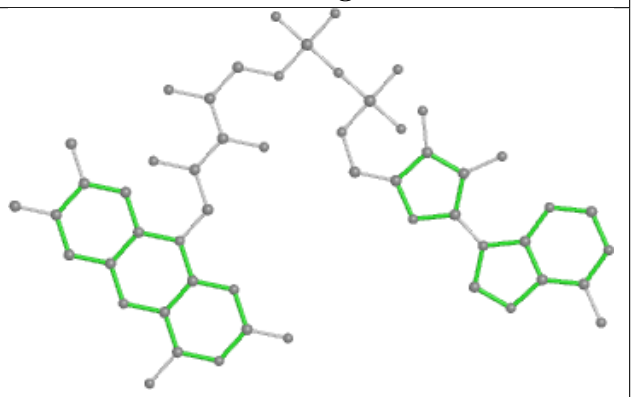
Bond lengths



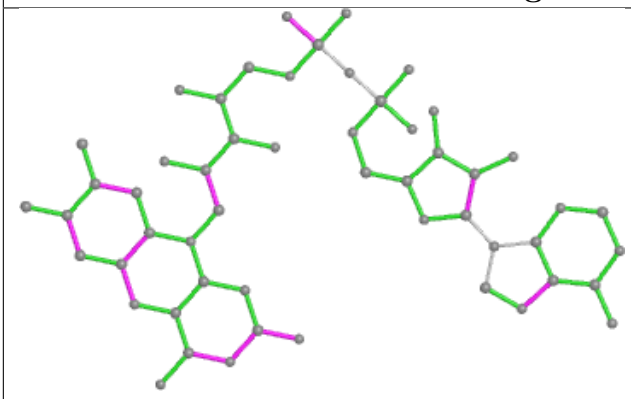
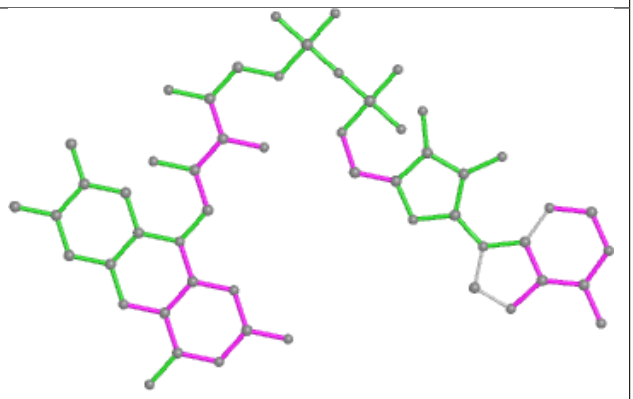
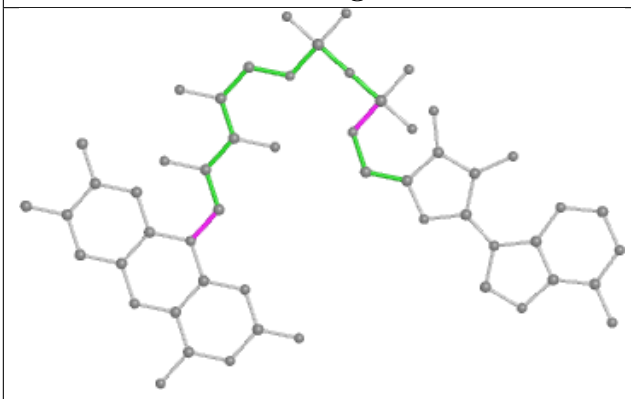
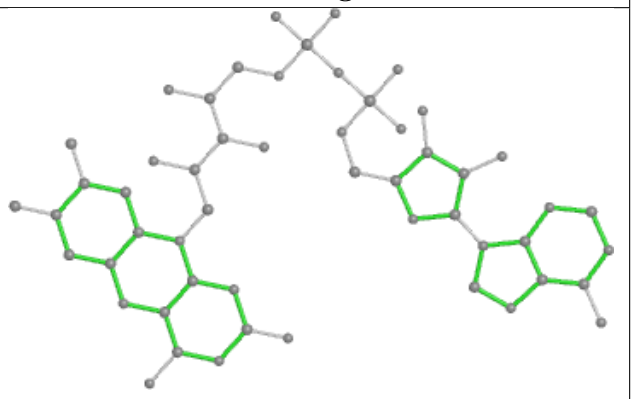
Bond angles



Torsions



Rings

Ligand FAD R 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	396/413 (95%)	-0.71	4 (1%)	82	80	20, 35, 64, 107	0
1	B	396/413 (95%)	-0.70	4 (1%)	82	80	20, 34, 61, 106	0
1	C	396/413 (95%)	-0.68	4 (1%)	82	80	21, 33, 64, 104	0
1	D	396/413 (95%)	-0.69	5 (1%)	77	75	21, 36, 65, 109	0
1	E	396/413 (95%)	-0.67	3 (0%)	86	84	20, 33, 63, 106	0
1	F	396/413 (95%)	-0.72	4 (1%)	82	80	20, 36, 64, 112	0
1	G	396/413 (95%)	-0.68	3 (0%)	86	84	22, 36, 66, 105	0
1	H	396/413 (95%)	-0.67	3 (0%)	86	84	21, 34, 62, 103	0
1	I	396/413 (95%)	-0.71	4 (1%)	82	80	21, 36, 63, 113	0
1	J	396/413 (95%)	-0.64	3 (0%)	86	84	22, 36, 64, 104	0
1	K	396/413 (95%)	-0.68	4 (1%)	82	80	22, 36, 65, 105	0
1	L	396/413 (95%)	-0.69	4 (1%)	82	80	23, 35, 63, 107	0
1	M	396/413 (95%)	-0.73	3 (0%)	86	84	22, 37, 64, 108	0
1	N	396/413 (95%)	-0.68	4 (1%)	82	80	21, 35, 62, 108	0
1	O	396/413 (95%)	-0.67	3 (0%)	86	84	21, 33, 62, 106	0
1	P	396/413 (95%)	-0.67	4 (1%)	82	80	23, 37, 66, 109	0
1	Q	396/413 (95%)	-0.67	3 (0%)	86	84	21, 34, 62, 109	0
1	R	396/413 (95%)	-0.66	5 (1%)	77	75	21, 37, 64, 112	0
1	S	396/413 (95%)	-0.67	3 (0%)	86	84	24, 37, 64, 107	0
1	T	396/413 (95%)	-0.69	4 (1%)	82	80	21, 36, 63, 108	0
1	U	396/413 (95%)	-0.69	3 (0%)	86	84	23, 36, 63, 108	0
1	V	396/413 (95%)	-0.67	4 (1%)	82	80	23, 35, 64, 107	0
1	W	396/413 (95%)	-0.67	3 (0%)	86	84	24, 37, 63, 110	0
1	X	396/413 (95%)	-0.66	5 (1%)	77	75	23, 37, 63, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	9504/9912 (95%)	-0.68	89 (0%)	84	82	20, 36, 64, 113	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	2	THR	7.5
1	Q	2	THR	7.4
1	F	2	THR	7.3
1	I	2	THR	7.3
1	J	2	THR	7.2
1	C	2	THR	7.1
1	K	2	THR	7.0
1	E	2	THR	6.9
1	A	2	THR	6.7
1	L	2	THR	6.5
1	P	3	ASP	6.5
1	G	2	THR	6.4
1	S	2	THR	6.4
1	P	2	THR	6.4
1	N	2	THR	6.3
1	R	2	THR	6.3
1	W	2	THR	6.2
1	W	3	ASP	6.2
1	I	3	ASP	6.2
1	V	2	THR	6.2
1	T	2	THR	6.1
1	M	2	THR	6.1
1	X	2	THR	6.1
1	U	2	THR	6.1
1	B	3	ASP	6.1
1	O	3	ASP	6.0
1	E	3	ASP	5.9
1	F	3	ASP	5.9
1	C	3	ASP	5.9
1	H	2	THR	5.7
1	D	2	THR	5.6
1	J	3	ASP	5.5
1	N	3	ASP	5.4
1	H	3	ASP	5.4
1	X	3	ASP	5.3
1	B	2	THR	5.3
1	T	3	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
1	R	3	ASP	5.2
1	D	3	ASP	5.0
1	S	3	ASP	5.0
1	Q	3	ASP	4.9
1	K	3	ASP	4.8
1	L	3	ASP	4.6
1	U	3	ASP	4.6
1	V	3	ASP	4.5
1	G	3	ASP	4.2
1	A	3	ASP	4.2
1	M	3	ASP	4.1
1	P	5	ARG	4.0
1	Q	5	ARG	4.0
1	U	5	ARG	3.9
1	I	5	ARG	3.7
1	R	5	ARG	3.7
1	E	5	ARG	3.5
1	B	4	ILE	3.4
1	F	5	ARG	3.2
1	N	5	ARG	3.2
1	G	5	ARG	3.2
1	X	6	SER	3.1
1	T	4	ILE	3.1
1	W	5	ARG	3.0
1	X	5	ARG	2.9
1	K	5	ARG	2.9
1	C	5	ARG	2.8
1	D	5	ARG	2.8
1	L	5	ARG	2.8
1	H	4	ILE	2.7
1	N	4	ILE	2.6
1	V	4	ILE	2.5
1	P	6	SER	2.5
1	D	4	ILE	2.4
1	F	4	ILE	2.4
1	M	5	ARG	2.4
1	C	4	ILE	2.4
1	X	4	ILE	2.4
1	S	5	ARG	2.3
1	T	5	ARG	2.3
1	R	4	ILE	2.2
1	A	4	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	4	ILE	2.2
1	J	5	ARG	2.2
1	O	5	ARG	2.1
1	B	5	ARG	2.1
1	V	163	ALA	2.1
1	A	5	ARG	2.1
1	R	6	SER	2.1
1	K	4	ILE	2.1
1	I	4	ILE	2.1
1	D	312	TYR	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
3	GOL	Q	602	6/6	0.86	0.16	47,59,63,63	0
3	GOL	T	602	6/6	0.87	0.17	50,60,62,63	0
3	GOL	I	602	6/6	0.90	0.12	52,58,66,66	0
3	GOL	K	602	6/6	0.91	0.19	48,56,64,74	0
3	GOL	M	602	6/6	0.91	0.10	49,55,60,60	0
3	GOL	L	602	6/6	0.92	0.17	48,53,61,66	0
3	GOL	F	602	6/6	0.93	0.09	49,57,61,68	0
3	GOL	U	602	6/6	0.93	0.19	51,60,66,73	0
3	GOL	V	602	6/6	0.93	0.23	51,57,63,65	0
3	GOL	A	602	6/6	0.94	0.13	44,51,61,66	0
3	GOL	J	602	6/6	0.94	0.17	50,58,65,69	0
3	GOL	S	602	6/6	0.94	0.17	56,60,63,68	0
3	GOL	W	602	6/6	0.94	0.15	56,61,69,70	0

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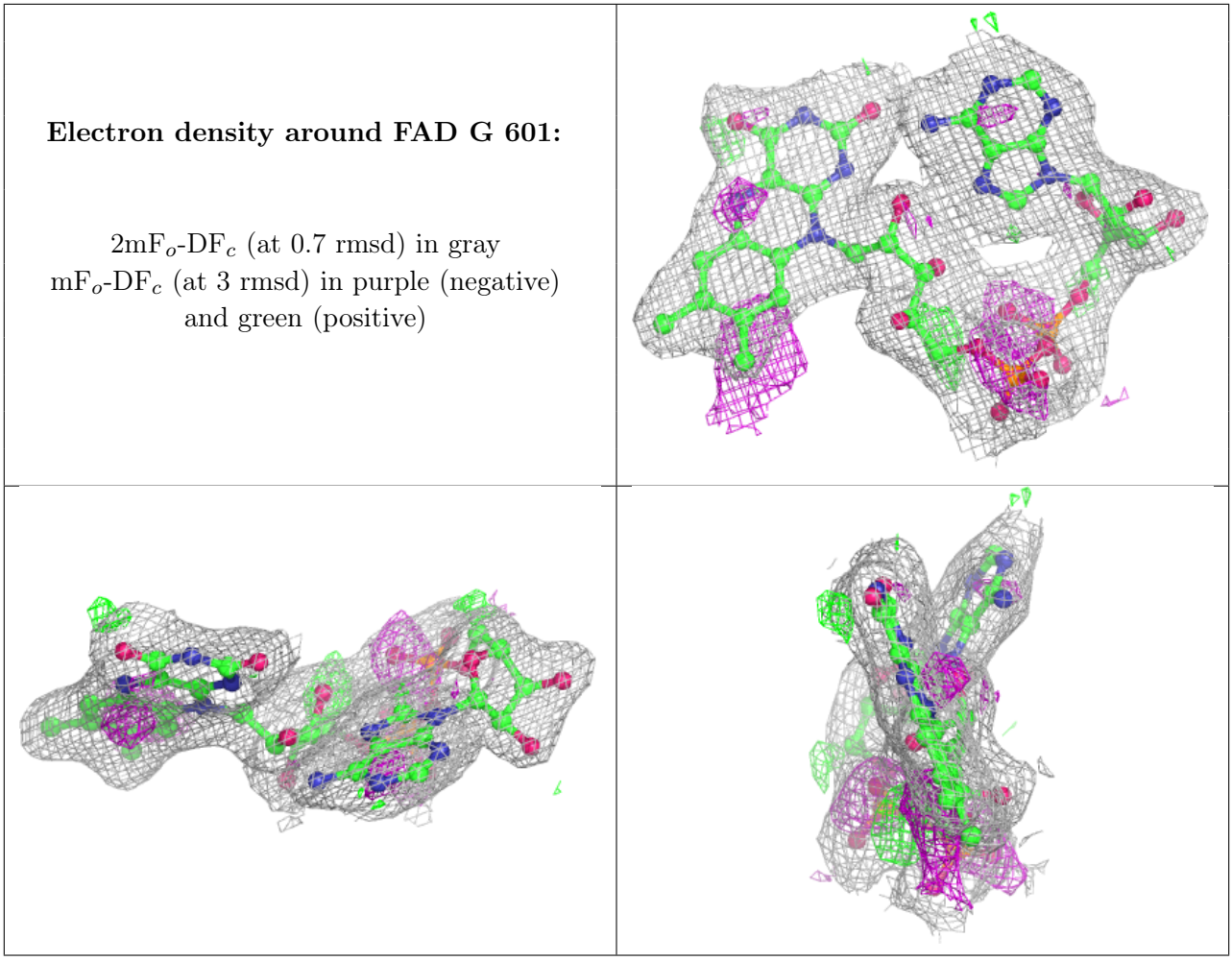
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	R	602	6/6	0.95	0.17	56,60,63,63	0
3	GOL	G	602	6/6	0.95	0.12	47,54,60,62	0
3	GOL	X	602	6/6	0.95	0.22	51,62,67,76	0
2	FAD	G	601	53/53	0.96	0.11	30,41,60,70	0
2	FAD	H	601	53/53	0.96	0.10	25,35,59,63	0
2	FAD	I	601	53/53	0.96	0.10	22,38,61,66	0
2	FAD	K	601	53/53	0.96	0.10	28,40,61,69	0
2	FAD	Q	601	53/53	0.96	0.10	26,36,55,67	0
2	FAD	R	601	53/53	0.96	0.12	30,39,62,73	0
3	GOL	N	602	6/6	0.96	0.12	49,54,61,71	0
3	GOL	O	602	6/6	0.96	0.17	44,54,60,72	0
2	FAD	S	601	53/53	0.96	0.10	30,38,58,71	0
2	FAD	U	601	53/53	0.96	0.11	29,39,60,65	0
2	FAD	V	601	53/53	0.96	0.11	26,39,60,71	0
2	FAD	B	601	53/53	0.96	0.10	25,35,59,60	0
3	GOL	B	602	6/6	0.96	0.11	39,53,61,64	0
3	GOL	C	602	6/6	0.96	0.14	44,56,60,61	0
3	GOL	D	602	6/6	0.96	0.15	49,56,62,67	0
2	FAD	C	601	53/53	0.96	0.10	28,36,56,71	0
2	FAD	D	601	53/53	0.97	0.11	26,39,58,66	0
2	FAD	E	601	53/53	0.97	0.09	25,34,57,68	0
2	FAD	T	601	53/53	0.97	0.11	28,38,61,65	0
2	FAD	J	601	53/53	0.97	0.09	26,37,57,69	0
2	FAD	F	601	53/53	0.97	0.10	27,37,59,61	0
2	FAD	W	601	53/53	0.97	0.11	30,38,60,73	0
2	FAD	X	601	53/53	0.97	0.11	28,37,59,65	0
3	GOL	P	602	6/6	0.97	0.11	51,56,59,63	0
2	FAD	L	601	53/53	0.97	0.10	28,40,61,72	0
2	FAD	M	601	53/53	0.97	0.09	23,37,59,66	0
2	FAD	N	601	53/53	0.97	0.10	26,37,58,72	0
2	FAD	O	601	53/53	0.97	0.12	24,35,58,68	0
3	GOL	E	602	6/6	0.97	0.12	45,56,58,62	0
2	FAD	P	601	53/53	0.97	0.10	30,40,62,74	0
2	FAD	A	601	53/53	0.97	0.09	27,38,59,63	0
3	GOL	H	602	6/6	0.97	0.16	45,56,62,69	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.

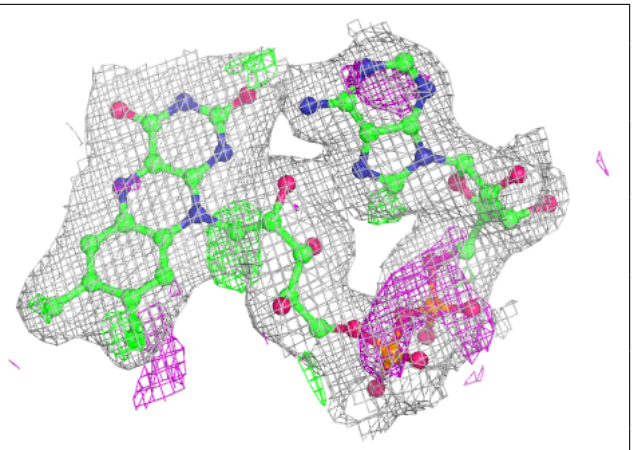
Electron density around FAD G 601:

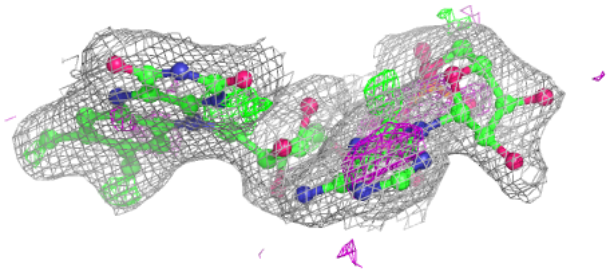
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

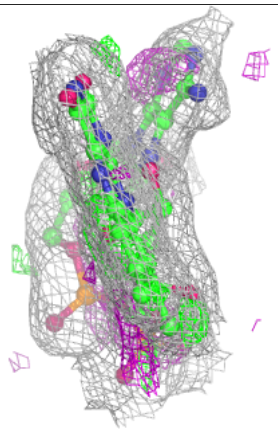


Electron density around FAD H 601:

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

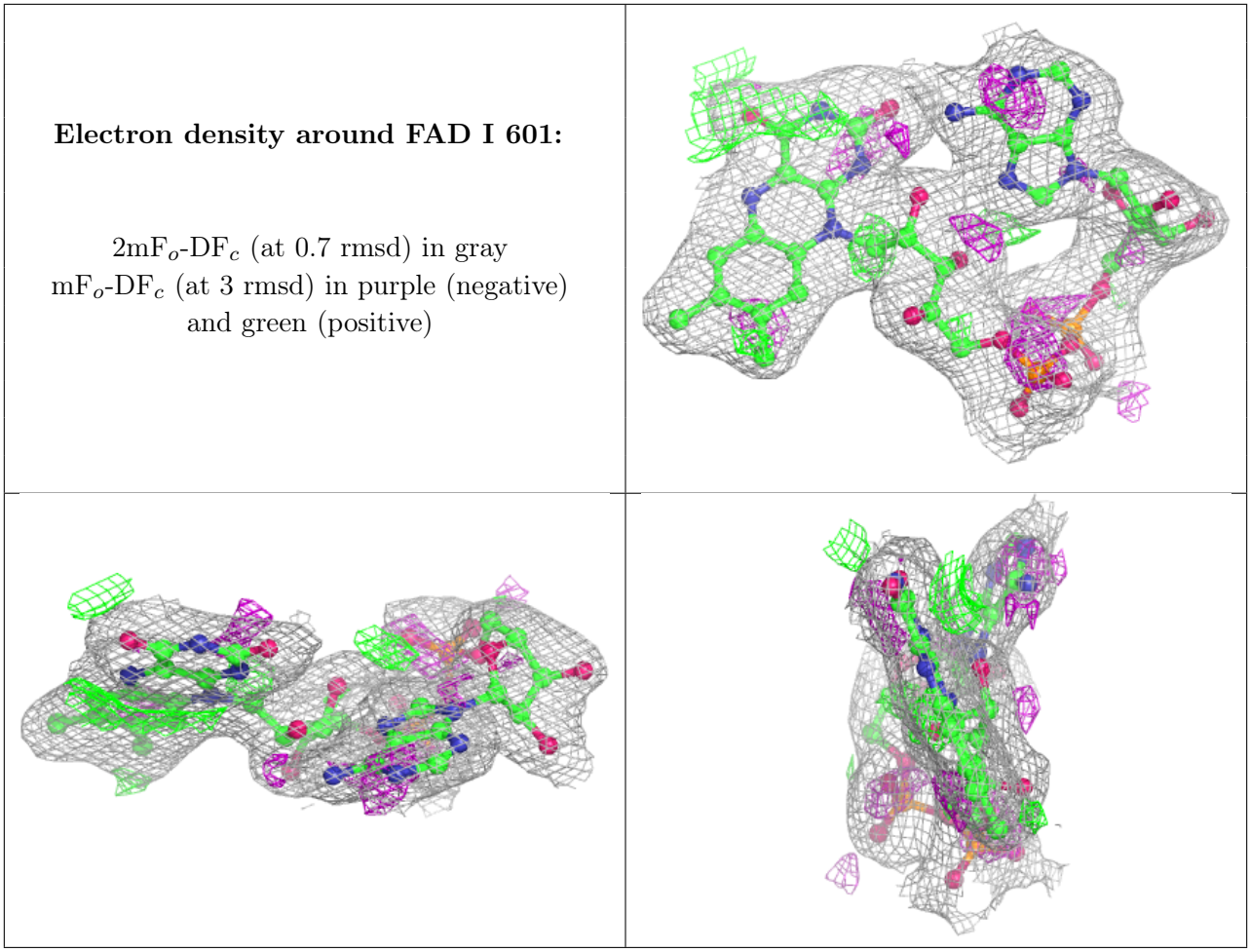






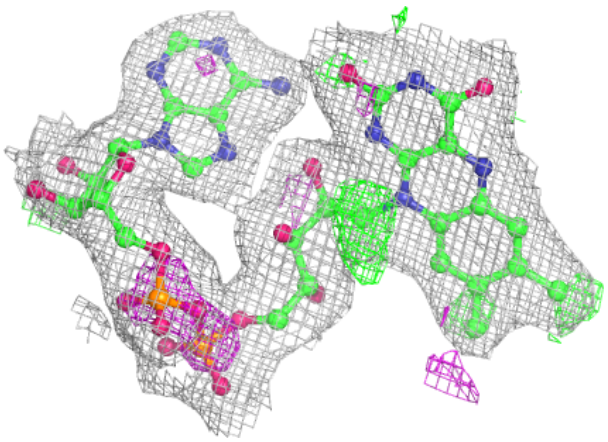
Electron density around FAD I 601:

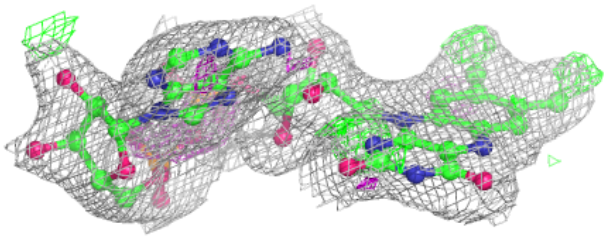
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

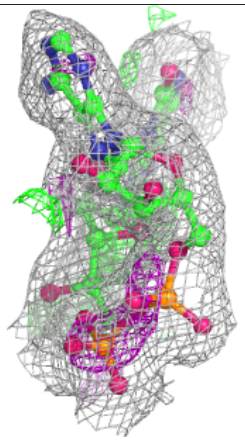


Electron density around FAD K 601:

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

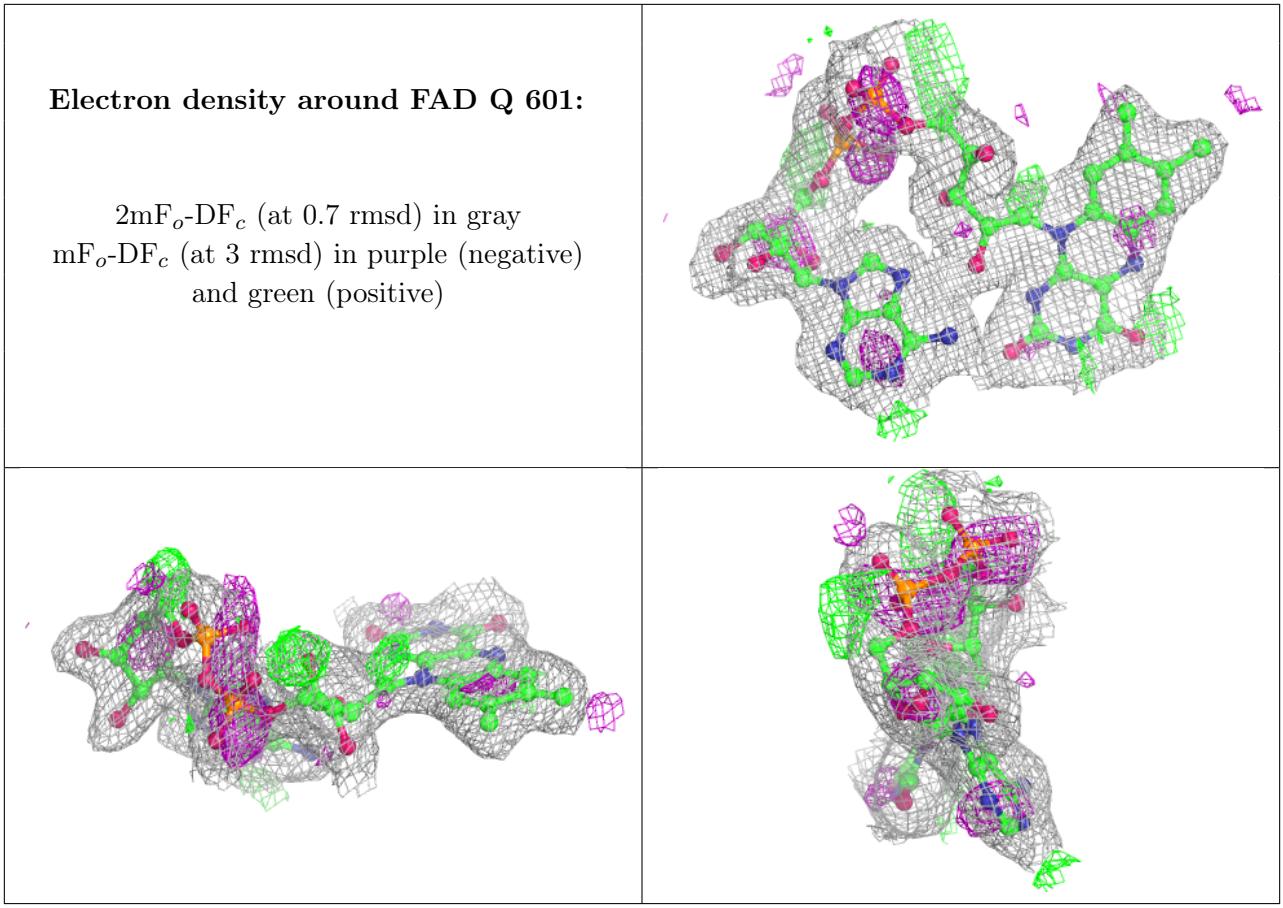






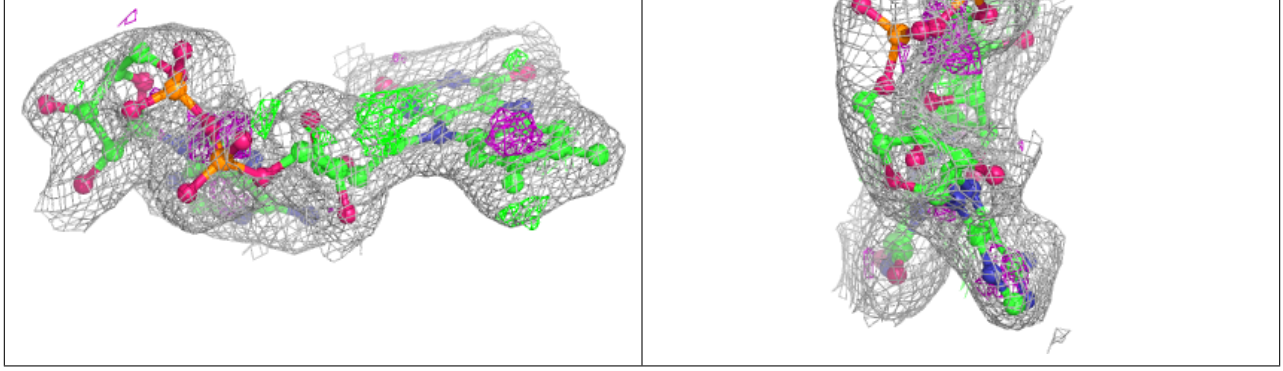
Electron density around FAD Q 601:

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



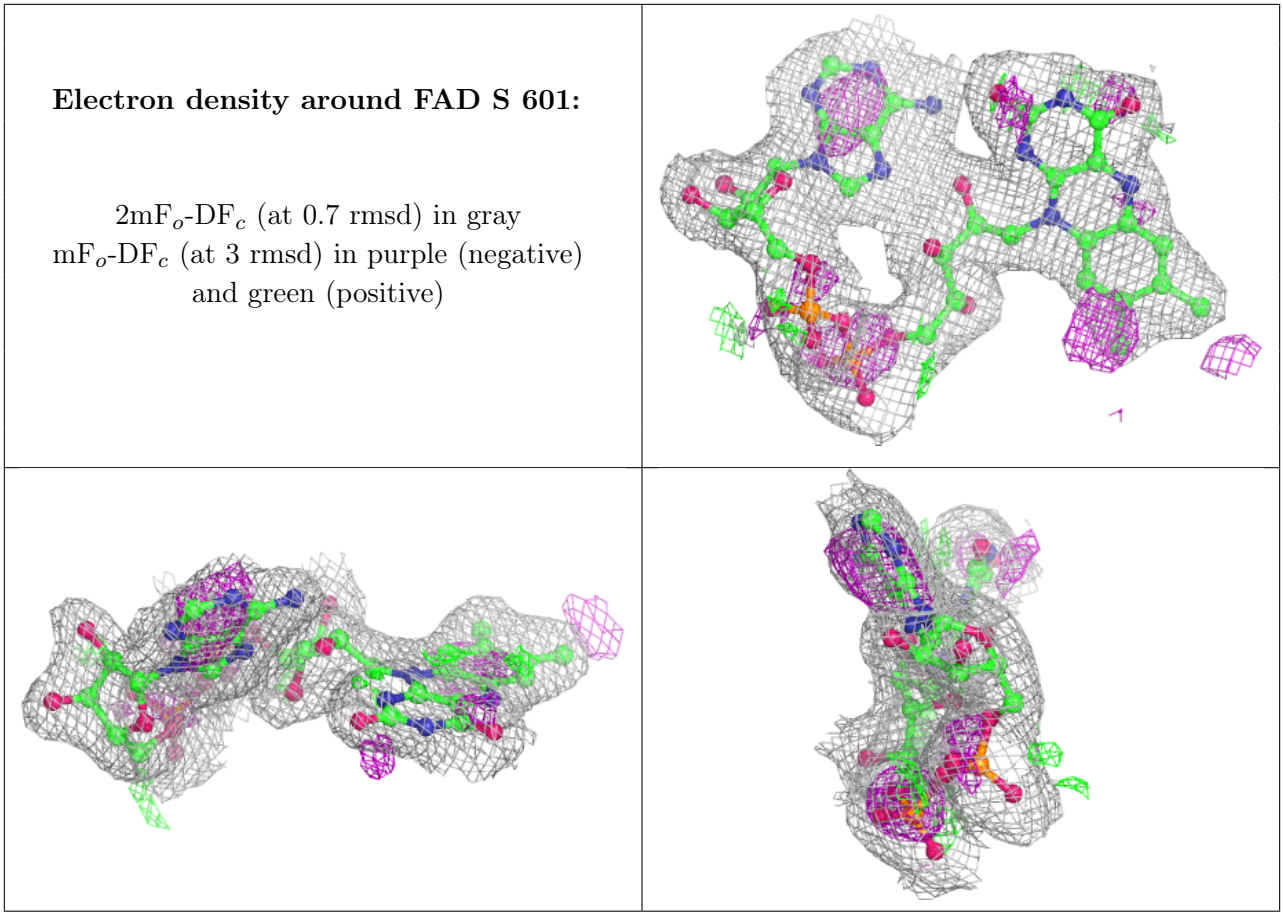
Electron density around FAD R 601:

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



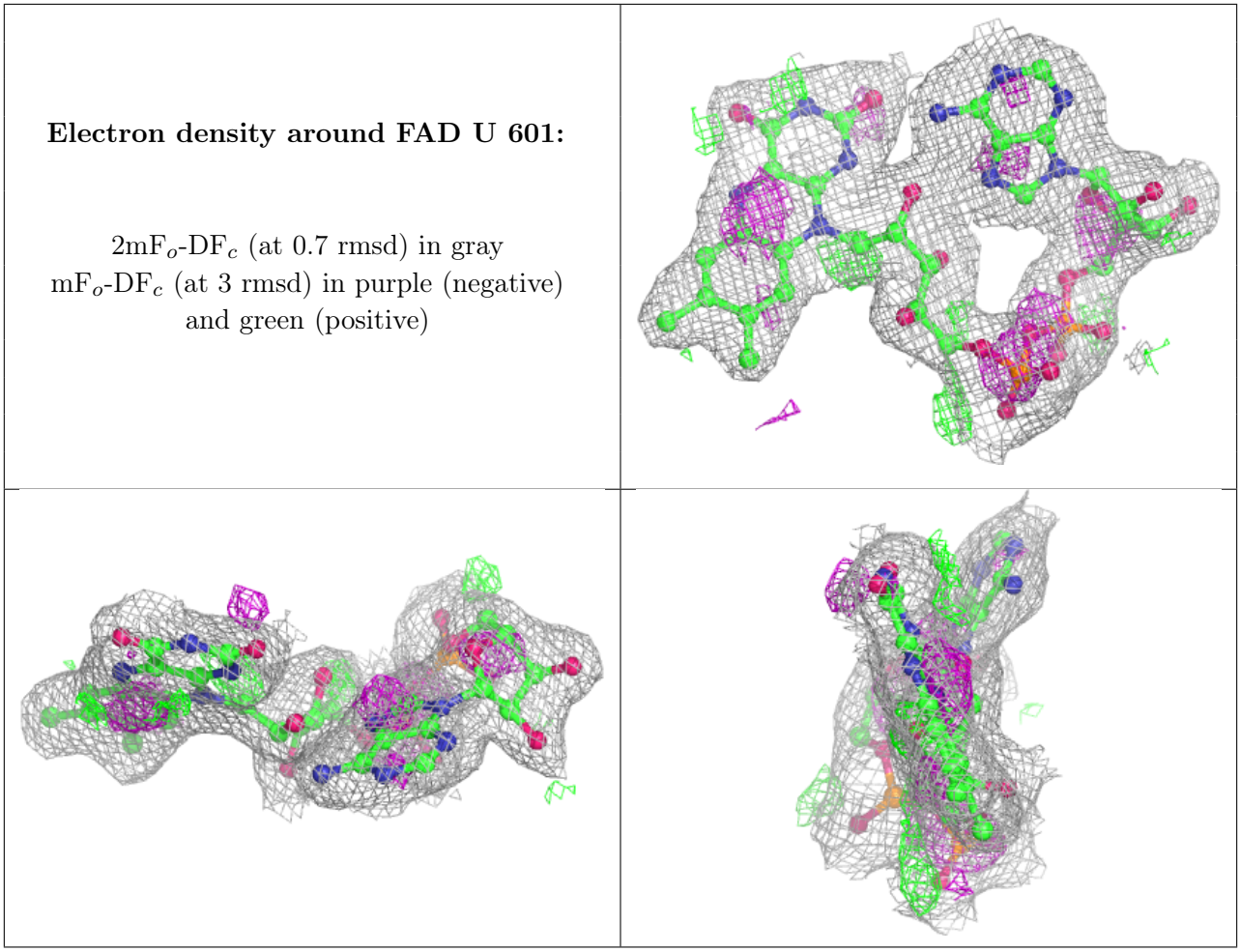
Electron density around FAD S 601:

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



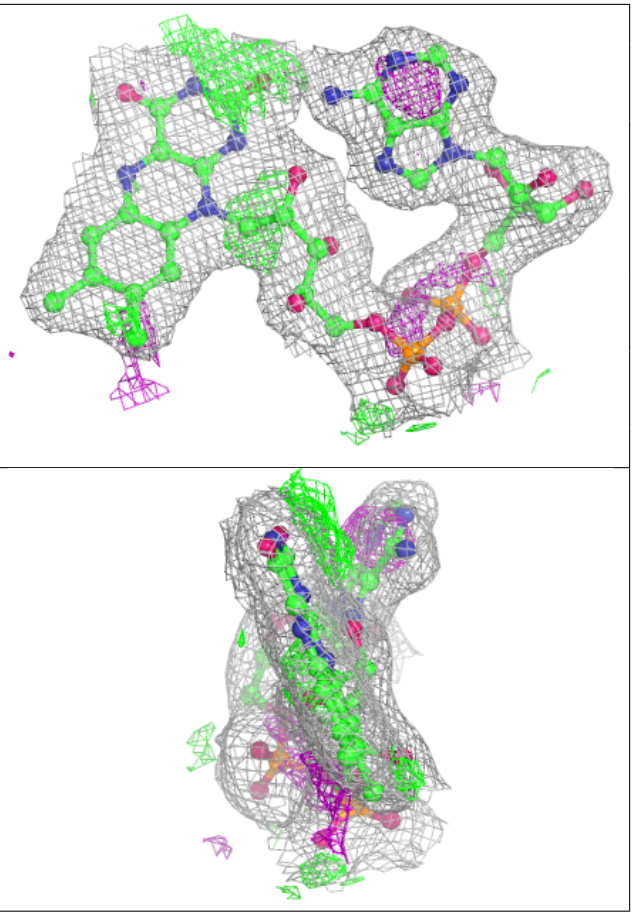
Electron density around FAD U 601:

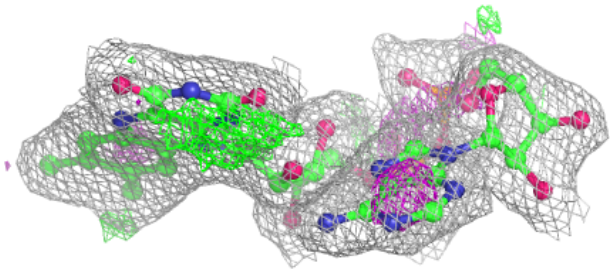
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD V 601:

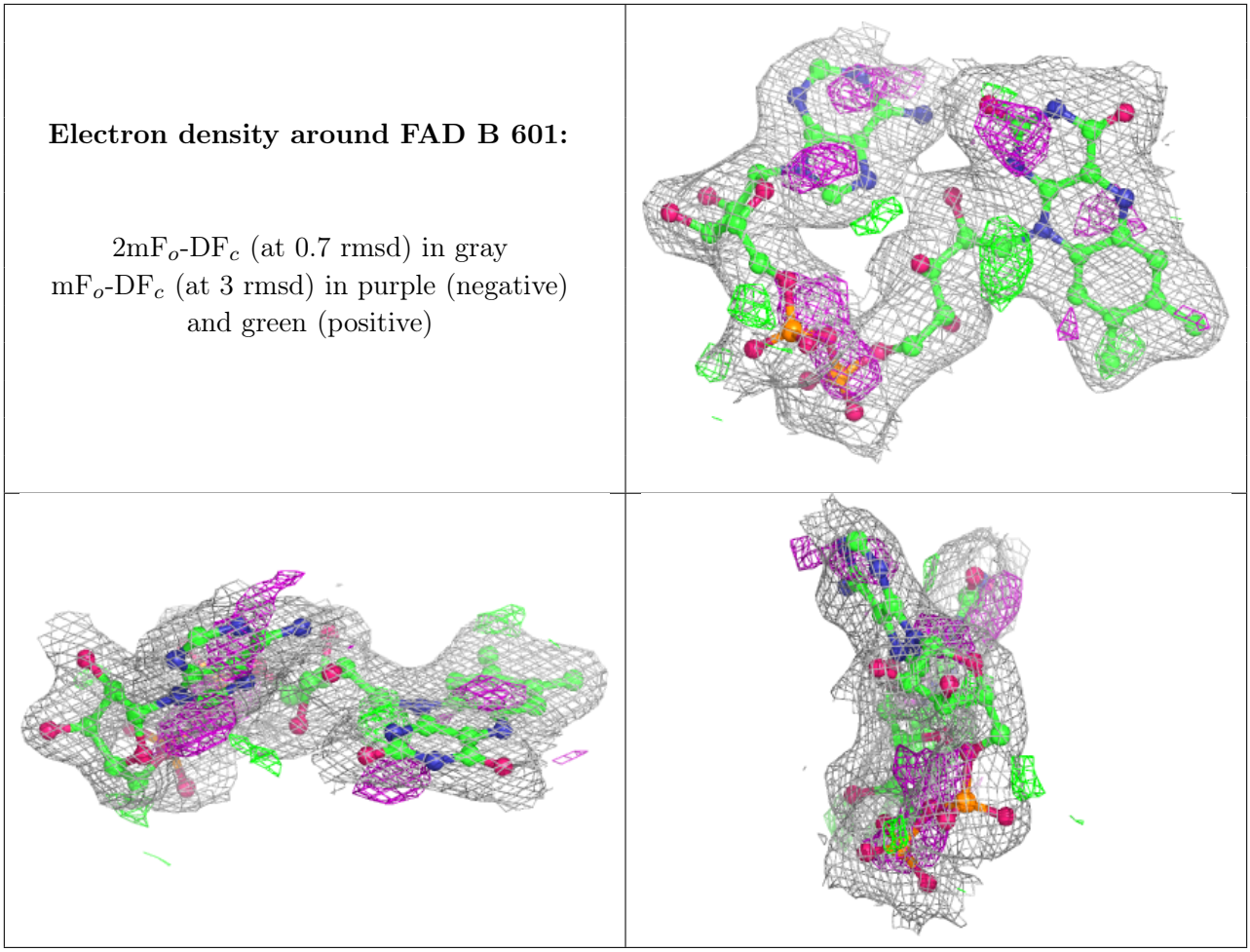
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





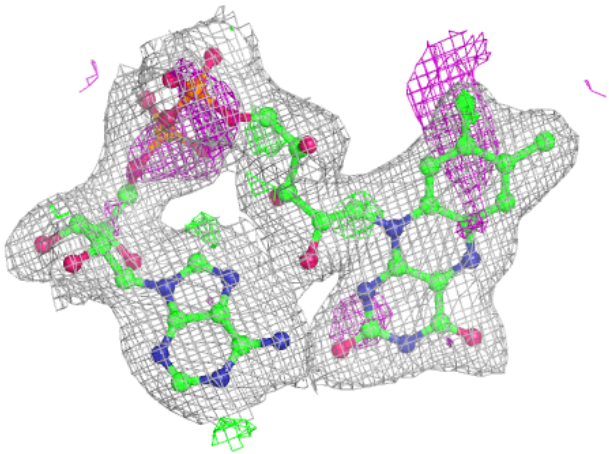
Electron density around FAD B 601:

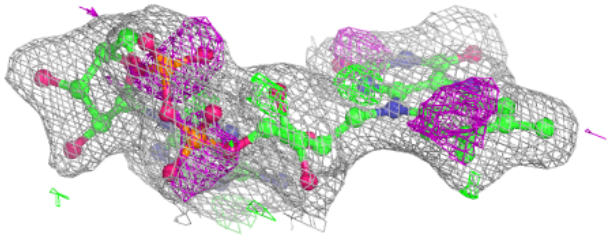
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

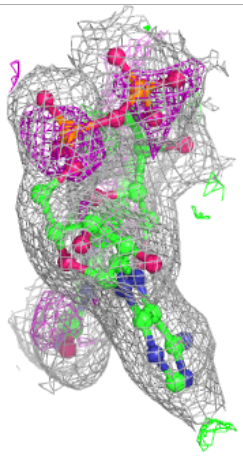


Electron density around FAD C 601:

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

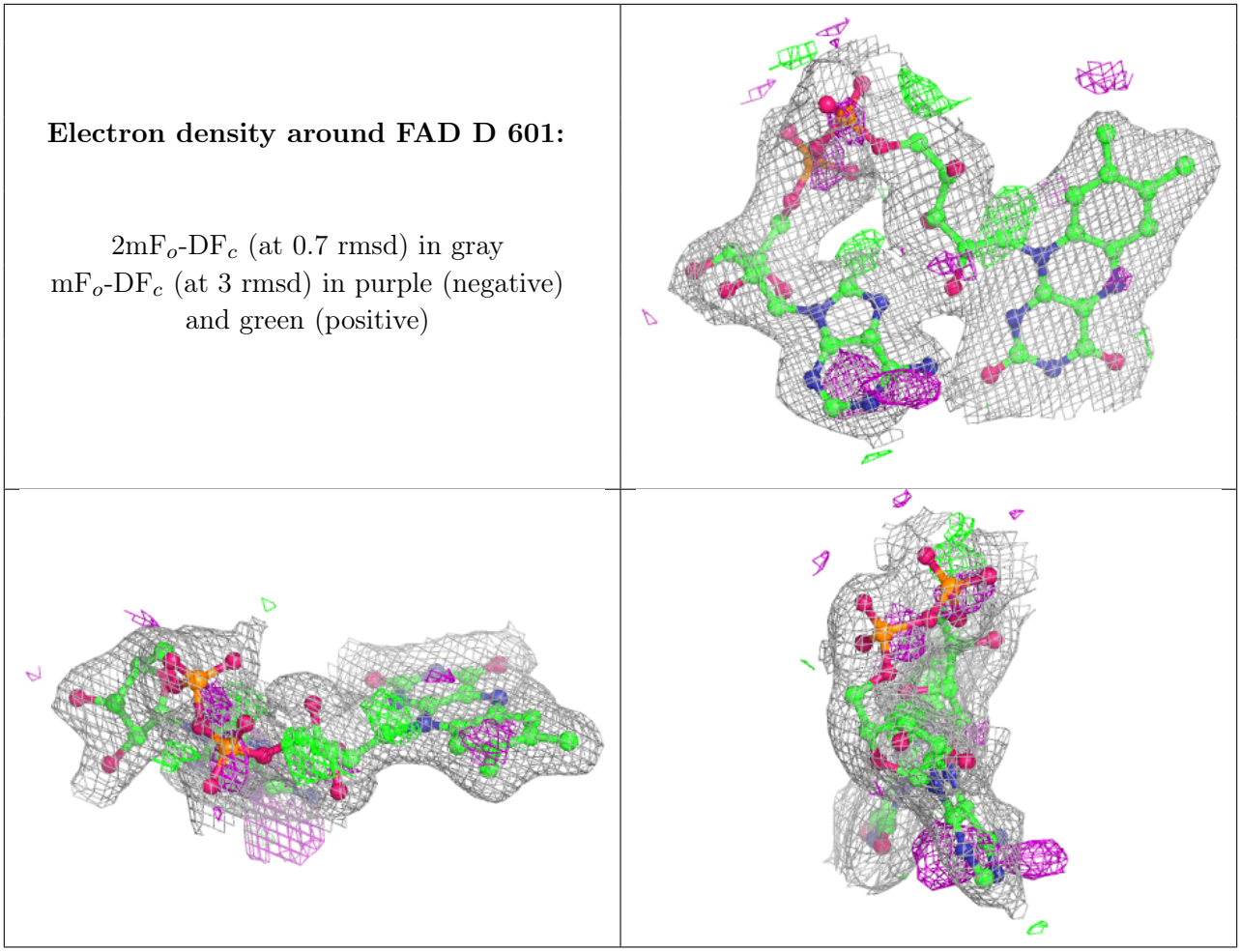






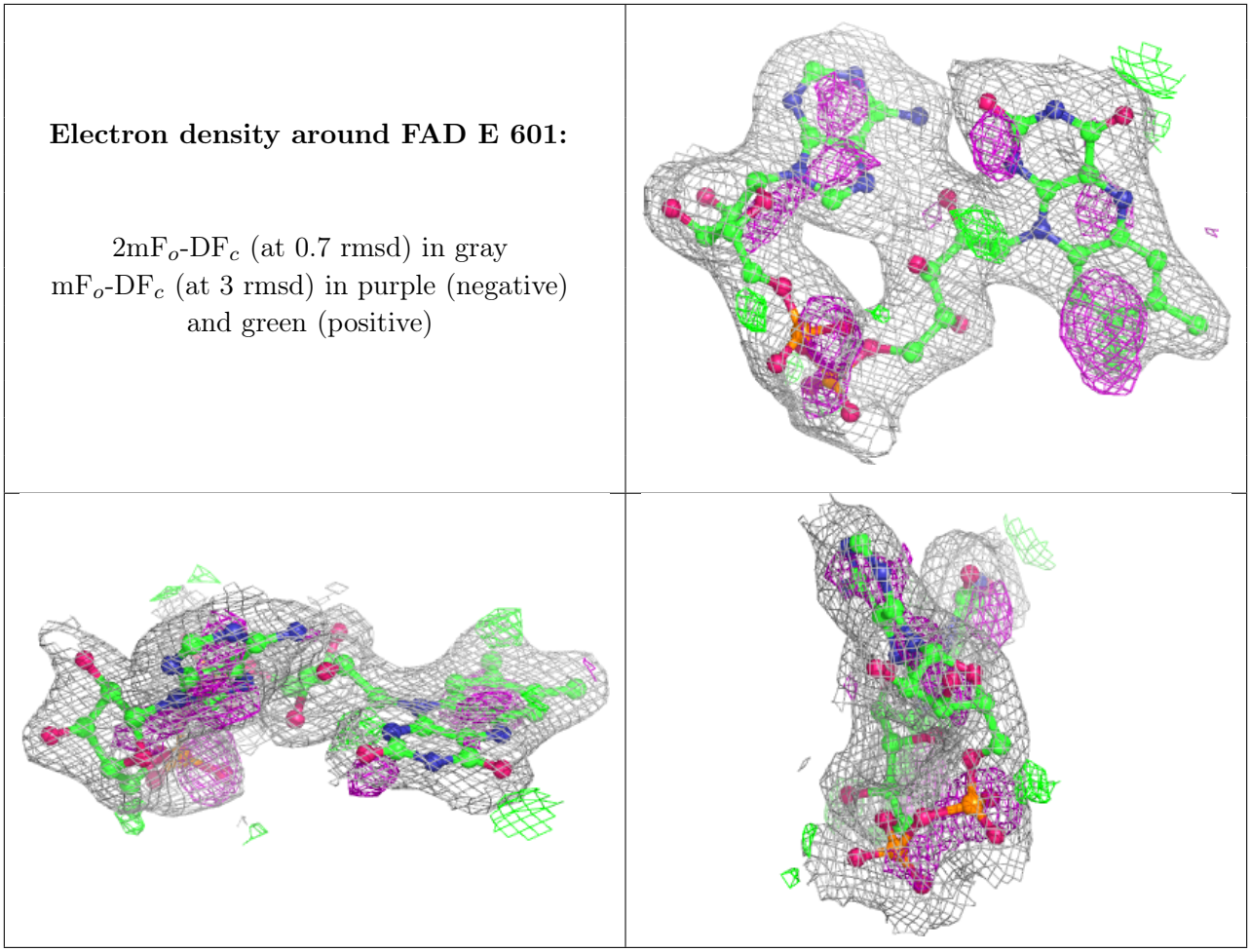
Electron density around FAD D 601:

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



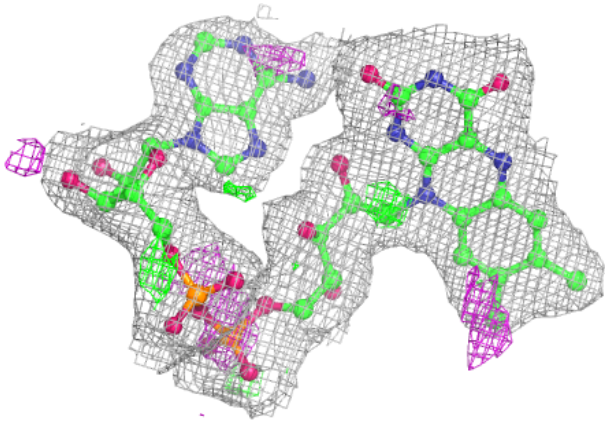
Electron density around FAD E 601:

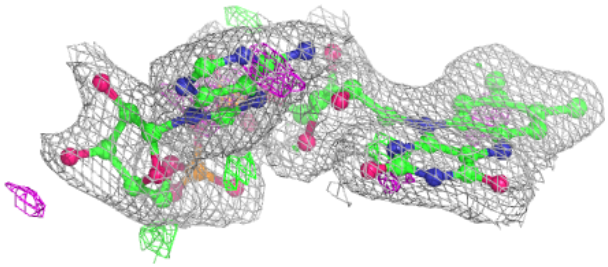
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

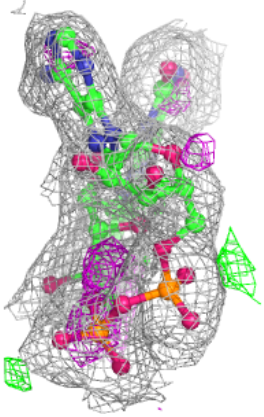


Electron density around FAD T 601:

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

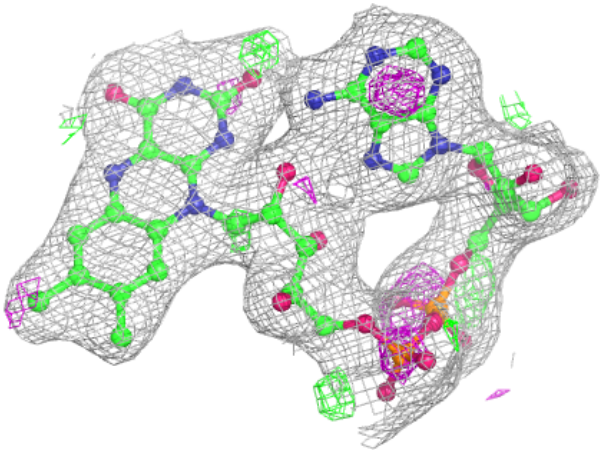


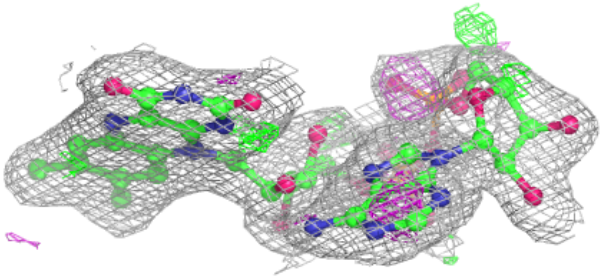


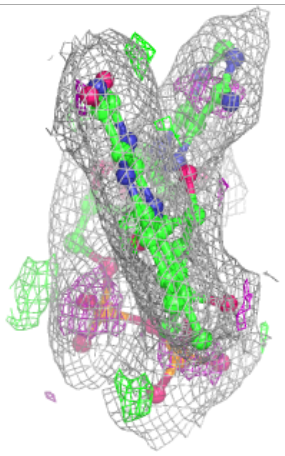


Electron density around FAD J 601:

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

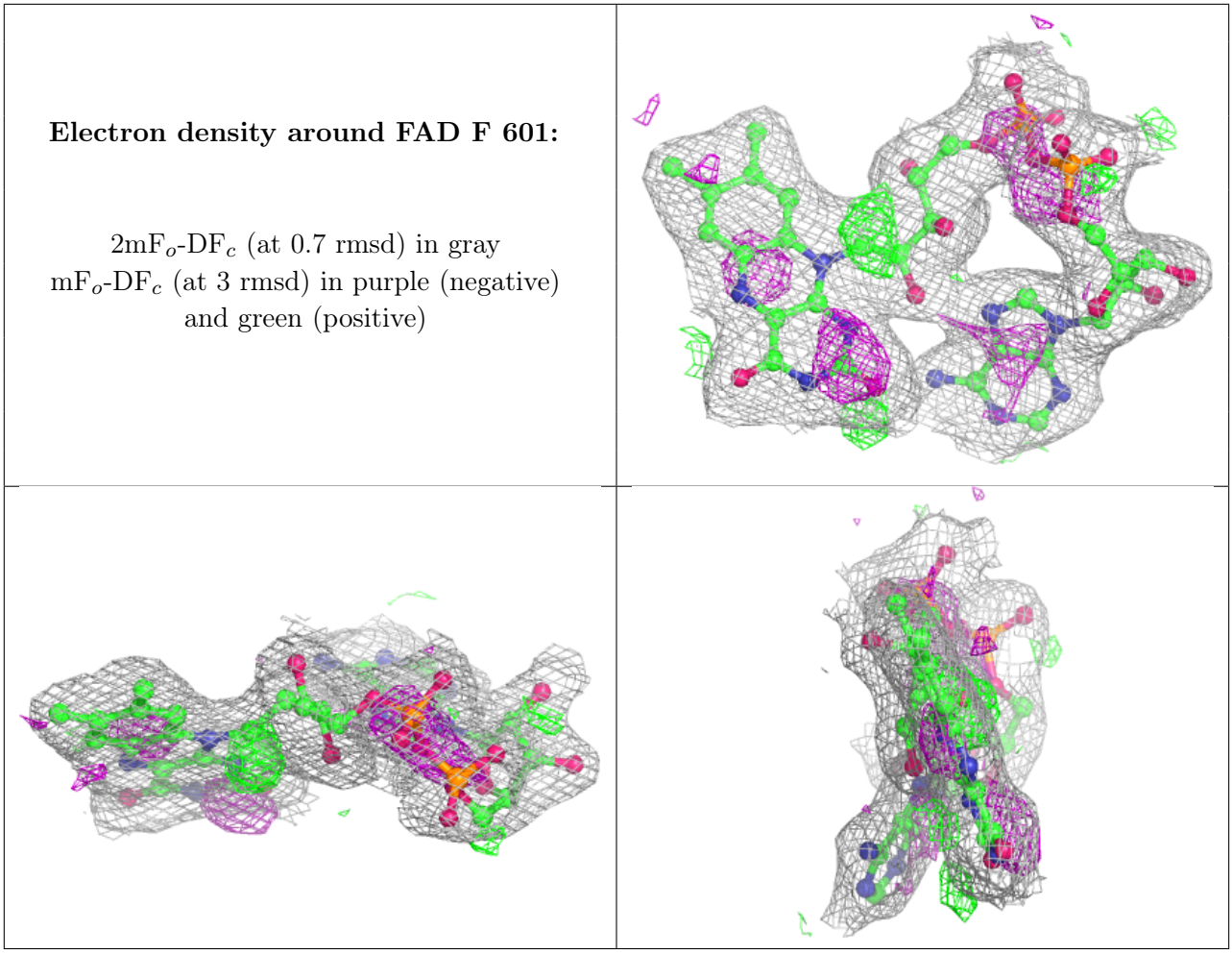






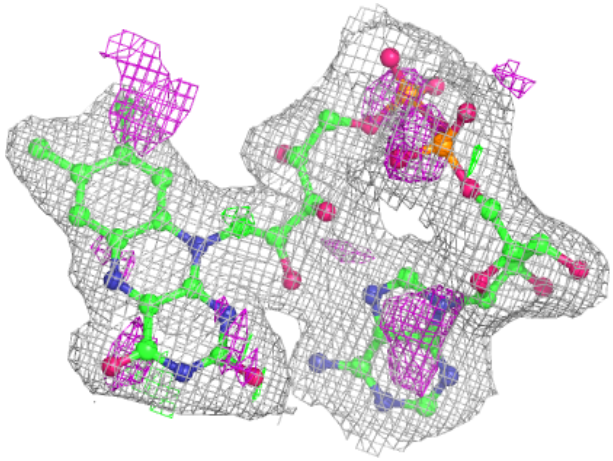
Electron density around FAD F 601:

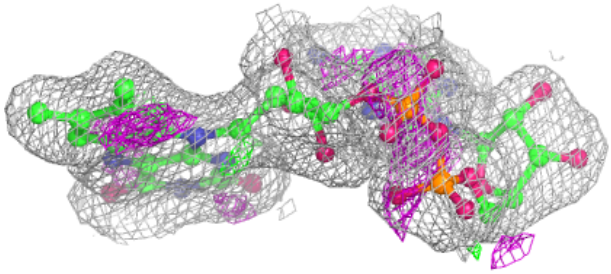
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

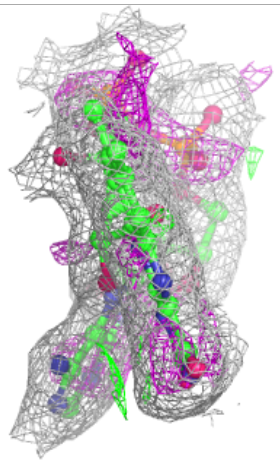


Electron density around FAD W 601:

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

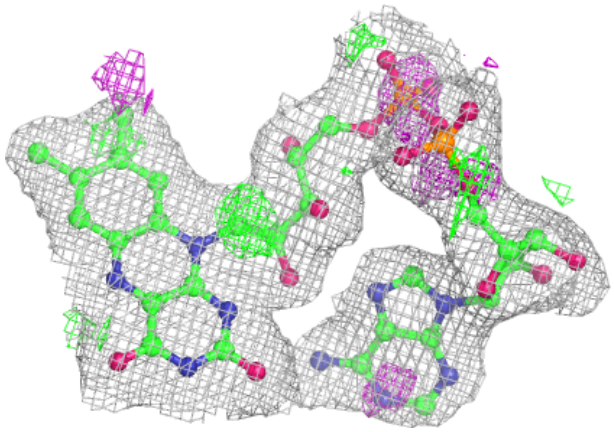


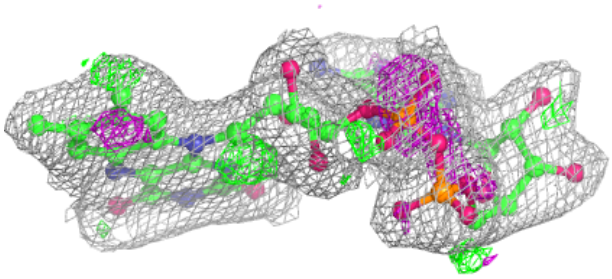


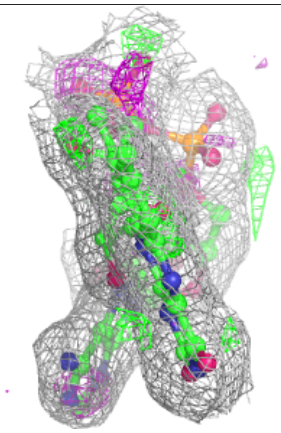


Electron density around FAD X 601:

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

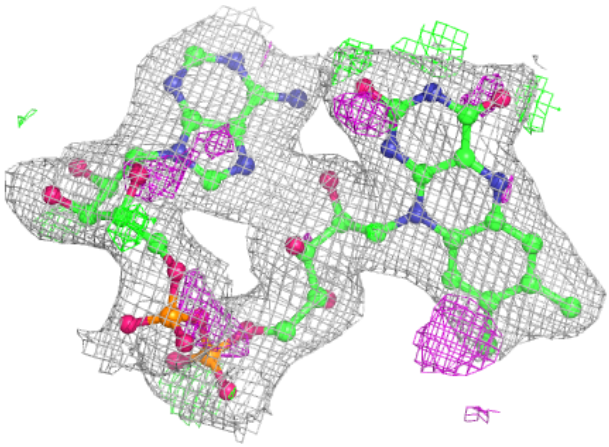


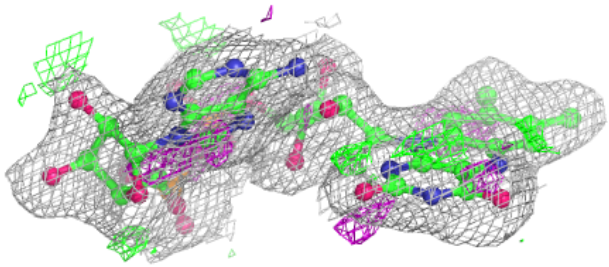


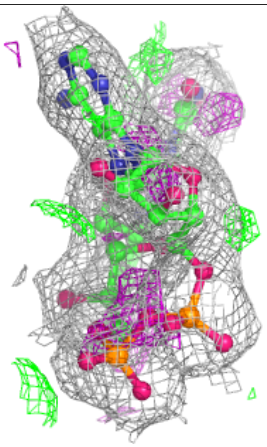


Electron density around FAD L 601:

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

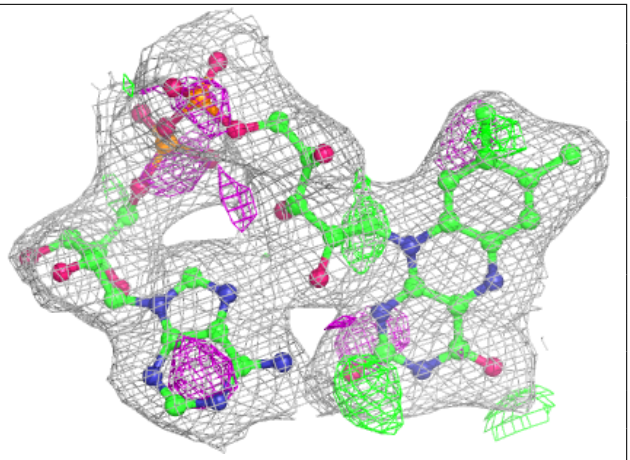


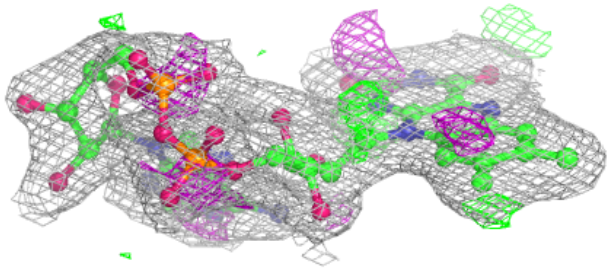


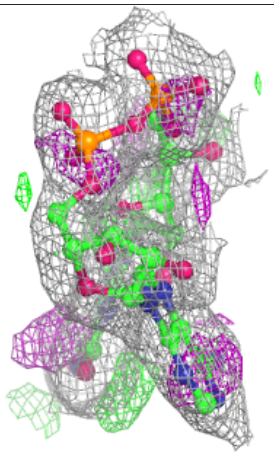


Electron density around FAD M 601:

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

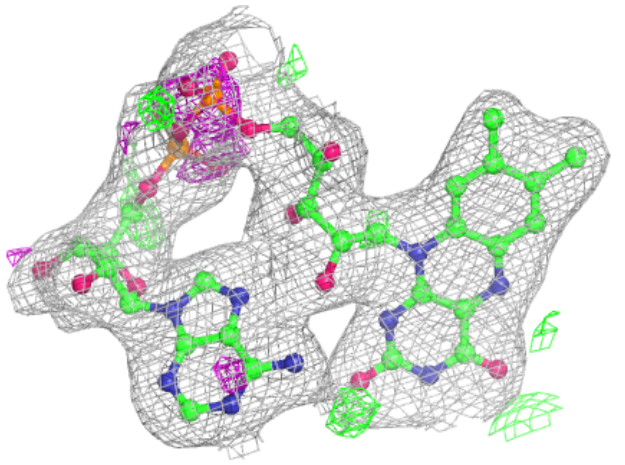


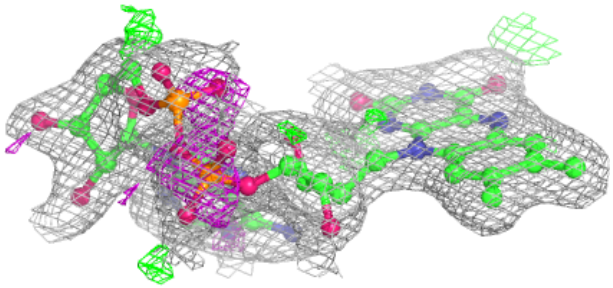


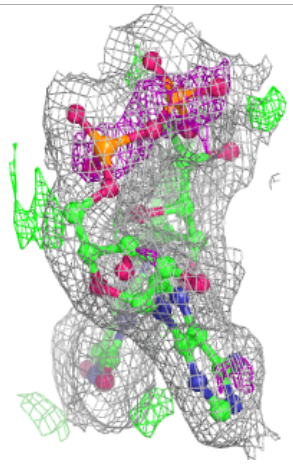


Electron density around FAD N 601:

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

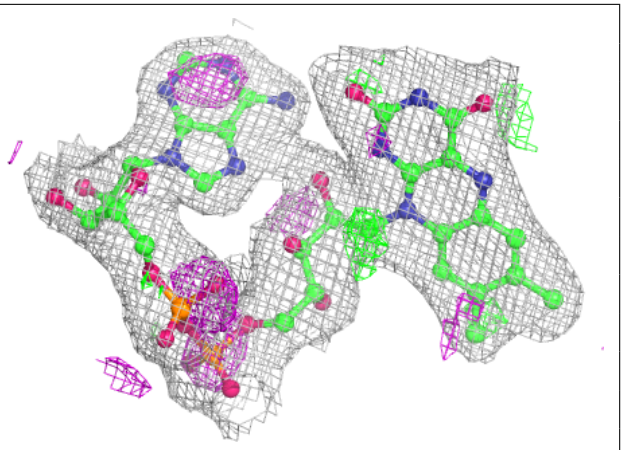


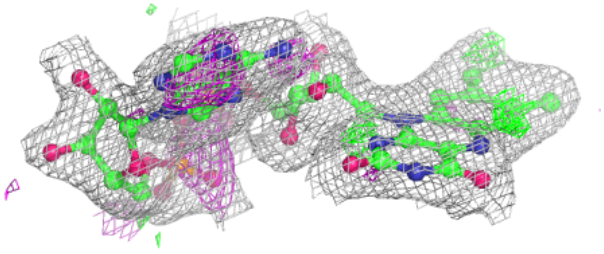


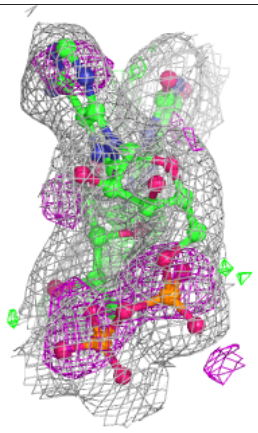


Electron density around FAD O 601:

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

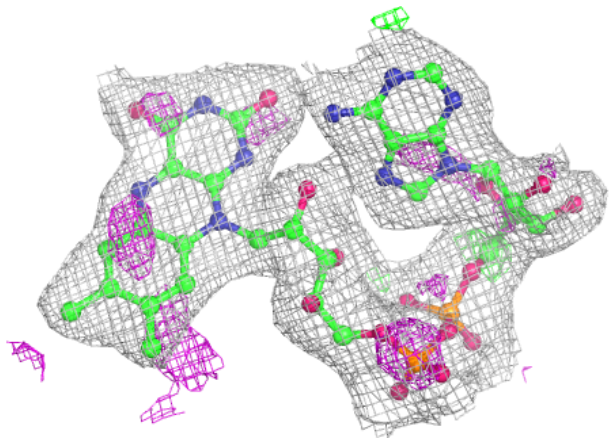


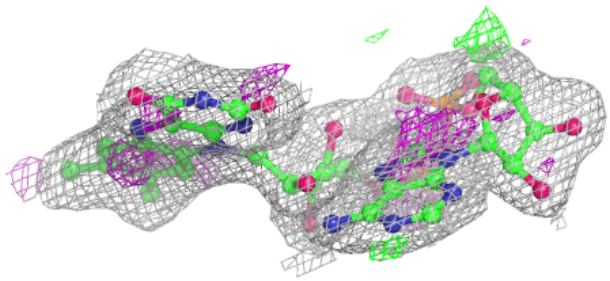


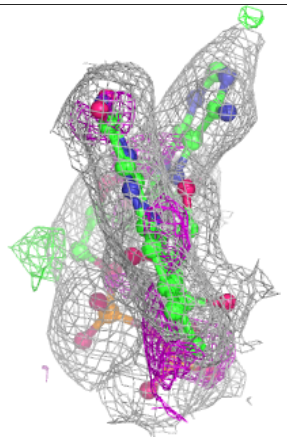


Electron density around FAD P 601:

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

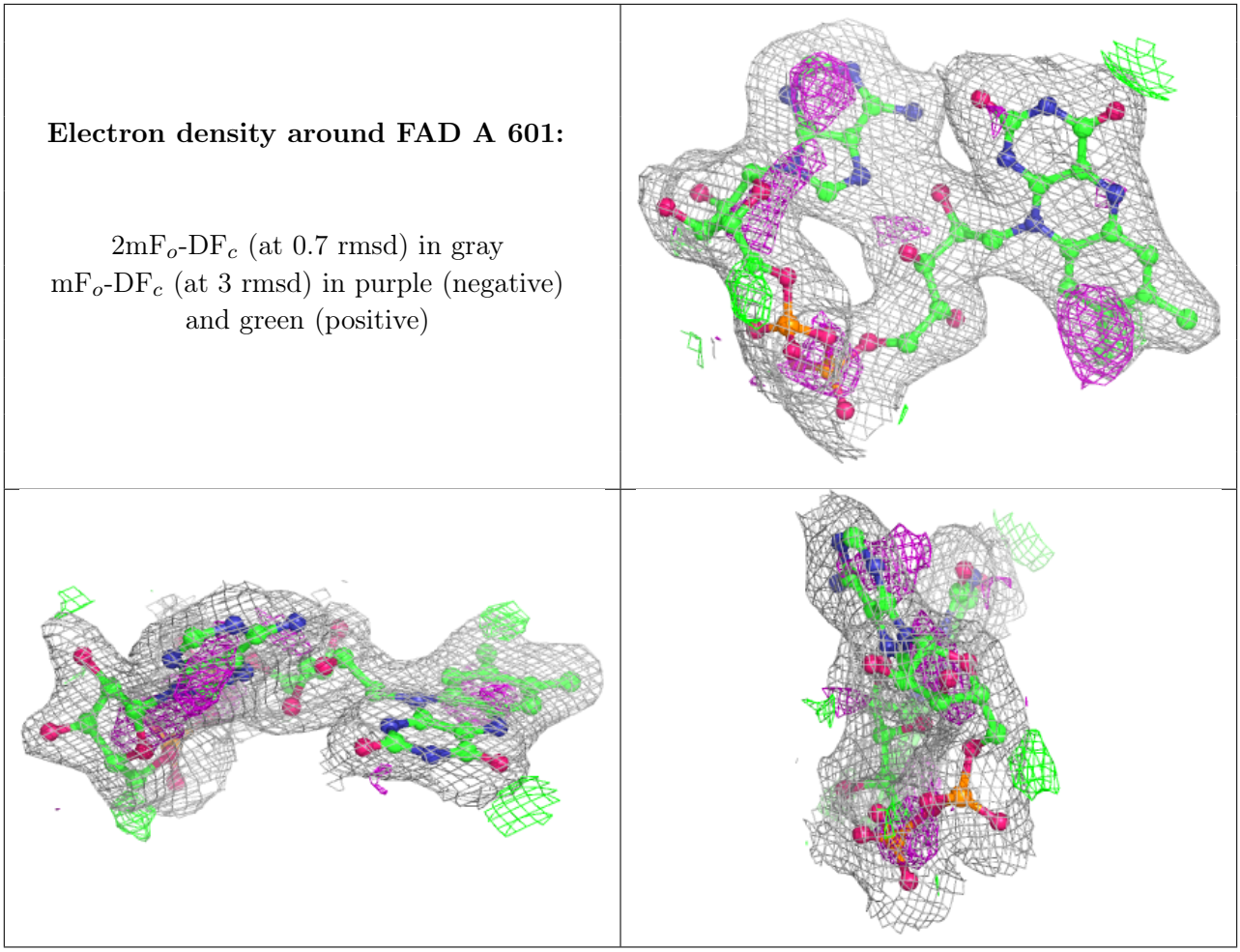






Electron density around FAD A 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.