Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 05:36 PM EDT

PDB ID	:	4FZB
Title	:	Structure of thymidylate synthase ThyX complexed to a new inhibitor
Authors	:	Basta, T.; Boum, Y.; Briffotaux, J.; Becker, H.F.; Lamarre-Jouenne, I.; Lambry, J.C.; Skouloubris, S.; Liebl, U.; van Tilbeurgh, H.; Graille, M.; Myllylkallio, H.
Deposited on	:	2012-07-06
Resolution	:	2.59 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

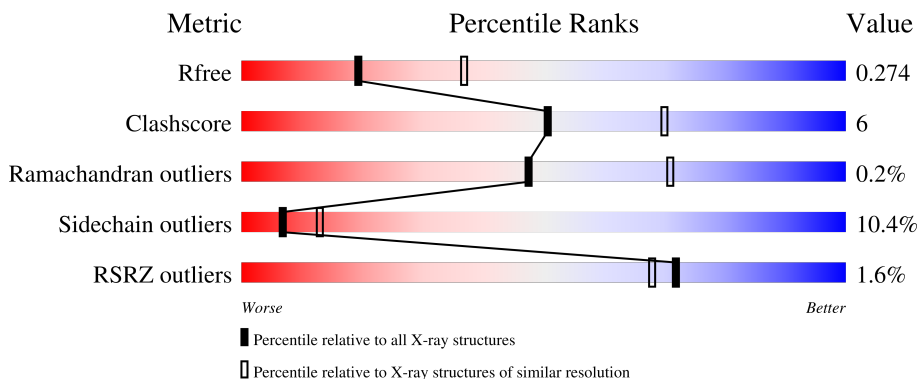|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.59 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	Percentile Ranks	Value
Rfree		0.274
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		10.4%
RSRZ outliers		1.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
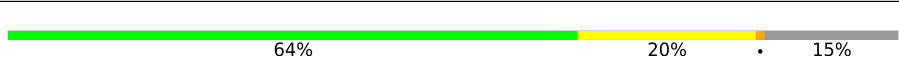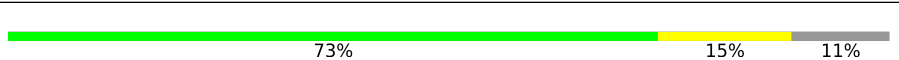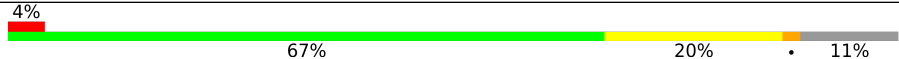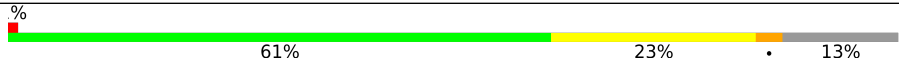
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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.

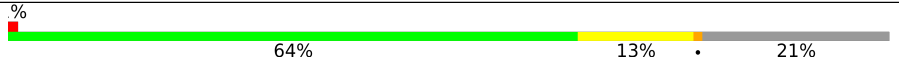| Mol	Chain	Length	Quality of chain
1	A	227	70% 12% • 16%
1	B	227	.% 62% 19% • 17%
1	C	227	.% 76% 13% • 9%
1	D	227	.% 68% 21% • 11%

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Mol	Chain	Length	Quality of chain
1	E	227	73% 15% 9%
1	F	227	70% 19% 9%
1	G	227	67% 14% 17%
1	H	227	65% 13% 21%
1	I	227	64% 20% 15%
1	J	227	64% 13% 21%
1	K	227	73% 15% 11%
1	L	227	67% 20% 11%
1	M	227	61% 23% 13%
1	N	227	59% 19% 22%
1	O	227	64% 22% 12%
1	P	227	69% 16% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	0VJ	B	303	-	X	-	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 26503 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 Probable thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1544	984	267	287	6			
1	B	188	Total	C	N	O	S	0	0	0
			1519	971	264	278	6			
1	C	207	Total	C	N	O	S	0	0	0
			1667	1060	291	308	8			
1	D	203	Total	C	N	O	S	0	0	0
			1642	1047	285	303	7			
1	E	206	Total	C	N	O	S	0	1	0
			1668	1060	293	307	8			
1	F	206	Total	C	N	O	S	0	0	0
			1666	1062	289	307	8			
1	G	188	Total	C	N	O	S	0	0	0
			1519	971	264	278	6			
1	H	179	Total	C	N	O	S	0	0	0
			1446	928	250	262	6			
1	I	193	Total	C	N	O	S	0	0	0
			1558	995	270	286	7			
1	J	179	Total	C	N	O	S	0	0	0
			1449	931	251	261	6			
1	K	201	Total	C	N	O	S	0	0	0
			1624	1034	283	300	7			
1	L	201	Total	C	N	O	S	0	0	0
			1624	1034	283	300	7			
1	M	197	Total	C	N	O	S	0	0	0
			1592	1019	275	291	7			
1	N	177	Total	C	N	O	S	0	0	0
			1432	921	247	258	6			
1	O	200	Total	C	N	O	S	0	0	0
			1617	1029	282	299	7			
1	P	197	Total	C	N	O	S	0	0	0
			1592	1015	276	294	7			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP O41156
A	-3	ALA	-	expression tag	UNP O41156
A	-2	SER	-	expression tag	UNP O41156
A	-1	MET	-	expression tag	UNP O41156
A	0	THR	-	expression tag	UNP O41156
A	1	GLY	-	expression tag	UNP O41156
A	217	HIS	-	expression tag	UNP O41156
A	218	HIS	-	expression tag	UNP O41156
A	219	HIS	-	expression tag	UNP O41156
A	220	HIS	-	expression tag	UNP O41156
A	221	HIS	-	expression tag	UNP O41156
A	222	HIS	-	expression tag	UNP O41156
B	-4	MET	-	expression tag	UNP O41156
B	-3	ALA	-	expression tag	UNP O41156
B	-2	SER	-	expression tag	UNP O41156
B	-1	MET	-	expression tag	UNP O41156
B	0	THR	-	expression tag	UNP O41156
B	1	GLY	-	expression tag	UNP O41156
B	217	HIS	-	expression tag	UNP O41156
B	218	HIS	-	expression tag	UNP O41156
B	219	HIS	-	expression tag	UNP O41156
B	220	HIS	-	expression tag	UNP O41156
B	221	HIS	-	expression tag	UNP O41156
B	222	HIS	-	expression tag	UNP O41156
C	-4	MET	-	expression tag	UNP O41156
C	-3	ALA	-	expression tag	UNP O41156
C	-2	SER	-	expression tag	UNP O41156
C	-1	MET	-	expression tag	UNP O41156
C	0	THR	-	expression tag	UNP O41156
C	1	GLY	-	expression tag	UNP O41156
C	217	HIS	-	expression tag	UNP O41156
C	218	HIS	-	expression tag	UNP O41156
C	219	HIS	-	expression tag	UNP O41156
C	220	HIS	-	expression tag	UNP O41156
C	221	HIS	-	expression tag	UNP O41156
C	222	HIS	-	expression tag	UNP O41156
D	-4	MET	-	expression tag	UNP O41156
D	-3	ALA	-	expression tag	UNP O41156
D	-2	SER	-	expression tag	UNP O41156
D	-1	MET	-	expression tag	UNP O41156
D	0	THR	-	expression tag	UNP O41156
D	1	GLY	-	expression tag	UNP O41156

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Chain	Residue	Modelled	Actual	Comment	Reference
D	217	HIS	-	expression tag	UNP O41156
D	218	HIS	-	expression tag	UNP O41156
D	219	HIS	-	expression tag	UNP O41156
D	220	HIS	-	expression tag	UNP O41156
D	221	HIS	-	expression tag	UNP O41156
D	222	HIS	-	expression tag	UNP O41156
E	-4	MET	-	expression tag	UNP O41156
E	-3	ALA	-	expression tag	UNP O41156
E	-2	SER	-	expression tag	UNP O41156
E	-1	MET	-	expression tag	UNP O41156
E	0	THR	-	expression tag	UNP O41156
E	1	GLY	-	expression tag	UNP O41156
E	217	HIS	-	expression tag	UNP O41156
E	218	HIS	-	expression tag	UNP O41156
E	219	HIS	-	expression tag	UNP O41156
E	220	HIS	-	expression tag	UNP O41156
E	221	HIS	-	expression tag	UNP O41156
E	222	HIS	-	expression tag	UNP O41156
F	-4	MET	-	expression tag	UNP O41156
F	-3	ALA	-	expression tag	UNP O41156
F	-2	SER	-	expression tag	UNP O41156
F	-1	MET	-	expression tag	UNP O41156
F	0	THR	-	expression tag	UNP O41156
F	1	GLY	-	expression tag	UNP O41156
F	217	HIS	-	expression tag	UNP O41156
F	218	HIS	-	expression tag	UNP O41156
F	219	HIS	-	expression tag	UNP O41156
F	220	HIS	-	expression tag	UNP O41156
F	221	HIS	-	expression tag	UNP O41156
F	222	HIS	-	expression tag	UNP O41156
G	-4	MET	-	expression tag	UNP O41156
G	-3	ALA	-	expression tag	UNP O41156
G	-2	SER	-	expression tag	UNP O41156
G	-1	MET	-	expression tag	UNP O41156
G	0	THR	-	expression tag	UNP O41156
G	1	GLY	-	expression tag	UNP O41156
G	217	HIS	-	expression tag	UNP O41156
G	218	HIS	-	expression tag	UNP O41156
G	219	HIS	-	expression tag	UNP O41156
G	220	HIS	-	expression tag	UNP O41156
G	221	HIS	-	expression tag	UNP O41156
G	222	HIS	-	expression tag	UNP O41156

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	MET	-	expression tag	UNP O41156
H	-3	ALA	-	expression tag	UNP O41156
H	-2	SER	-	expression tag	UNP O41156
H	-1	MET	-	expression tag	UNP O41156
H	0	THR	-	expression tag	UNP O41156
H	1	GLY	-	expression tag	UNP O41156
H	217	HIS	-	expression tag	UNP O41156
H	218	HIS	-	expression tag	UNP O41156
H	219	HIS	-	expression tag	UNP O41156
H	220	HIS	-	expression tag	UNP O41156
H	221	HIS	-	expression tag	UNP O41156
H	222	HIS	-	expression tag	UNP O41156
I	-4	MET	-	expression tag	UNP O41156
I	-3	ALA	-	expression tag	UNP O41156
I	-2	SER	-	expression tag	UNP O41156
I	-1	MET	-	expression tag	UNP O41156
I	0	THR	-	expression tag	UNP O41156
I	1	GLY	-	expression tag	UNP O41156
I	217	HIS	-	expression tag	UNP O41156
I	218	HIS	-	expression tag	UNP O41156
I	219	HIS	-	expression tag	UNP O41156
I	220	HIS	-	expression tag	UNP O41156
I	221	HIS	-	expression tag	UNP O41156
I	222	HIS	-	expression tag	UNP O41156
J	-4	MET	-	expression tag	UNP O41156
J	-3	ALA	-	expression tag	UNP O41156
J	-2	SER	-	expression tag	UNP O41156
J	-1	MET	-	expression tag	UNP O41156
J	0	THR	-	expression tag	UNP O41156
J	1	GLY	-	expression tag	UNP O41156
J	217	HIS	-	expression tag	UNP O41156
J	218	HIS	-	expression tag	UNP O41156
J	219	HIS	-	expression tag	UNP O41156
J	220	HIS	-	expression tag	UNP O41156
J	221	HIS	-	expression tag	UNP O41156
J	222	HIS	-	expression tag	UNP O41156
K	-4	MET	-	expression tag	UNP O41156
K	-3	ALA	-	expression tag	UNP O41156
K	-2	SER	-	expression tag	UNP O41156
K	-1	MET	-	expression tag	UNP O41156
K	0	THR	-	expression tag	UNP O41156
K	1	GLY	-	expression tag	UNP O41156

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Chain	Residue	Modelled	Actual	Comment	Reference
K	217	HIS	-	expression tag	UNP O41156
K	218	HIS	-	expression tag	UNP O41156
K	219	HIS	-	expression tag	UNP O41156
K	220	HIS	-	expression tag	UNP O41156
K	221	HIS	-	expression tag	UNP O41156
K	222	HIS	-	expression tag	UNP O41156
L	-4	MET	-	expression tag	UNP O41156
L	-3	ALA	-	expression tag	UNP O41156
L	-2	SER	-	expression tag	UNP O41156
L	-1	MET	-	expression tag	UNP O41156
L	0	THR	-	expression tag	UNP O41156
L	1	GLY	-	expression tag	UNP O41156
L	217	HIS	-	expression tag	UNP O41156
L	218	HIS	-	expression tag	UNP O41156
L	219	HIS	-	expression tag	UNP O41156
L	220	HIS	-	expression tag	UNP O41156
L	221	HIS	-	expression tag	UNP O41156
L	222	HIS	-	expression tag	UNP O41156
M	-4	MET	-	expression tag	UNP O41156
M	-3	ALA	-	expression tag	UNP O41156
M	-2	SER	-	expression tag	UNP O41156
M	-1	MET	-	expression tag	UNP O41156
M	0	THR	-	expression tag	UNP O41156
M	1	GLY	-	expression tag	UNP O41156
M	217	HIS	-	expression tag	UNP O41156
M	218	HIS	-	expression tag	UNP O41156
M	219	HIS	-	expression tag	UNP O41156
M	220	HIS	-	expression tag	UNP O41156
M	221	HIS	-	expression tag	UNP O41156
M	222	HIS	-	expression tag	UNP O41156
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N	-3	ALA	-	expression tag	UNP O41156
N	-2	SER	-	expression tag	UNP O41156
N	-1	MET	-	expression tag	UNP O41156
N	0	THR	-	expression tag	UNP O41156
N	1	GLY	-	expression tag	UNP O41156
N	217	HIS	-	expression tag	UNP O41156
N	218	HIS	-	expression tag	UNP O41156
N	219	HIS	-	expression tag	UNP O41156
N	220	HIS	-	expression tag	UNP O41156
N	221	HIS	-	expression tag	UNP O41156
N	222	HIS	-	expression tag	UNP O41156

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-4	MET	-	expression tag	UNP O41156
O	-3	ALA	-	expression tag	UNP O41156
O	-2	SER	-	expression tag	UNP O41156
O	-1	MET	-	expression tag	UNP O41156
O	0	THR	-	expression tag	UNP O41156
O	1	GLY	-	expression tag	UNP O41156
O	217	HIS	-	expression tag	UNP O41156
O	218	HIS	-	expression tag	UNP O41156
O	219	HIS	-	expression tag	UNP O41156
O	220	HIS	-	expression tag	UNP O41156
O	221	HIS	-	expression tag	UNP O41156
O	222	HIS	-	expression tag	UNP O41156
P	-4	MET	-	expression tag	UNP O41156
P	-3	ALA	-	expression tag	UNP O41156
P	-2	SER	-	expression tag	UNP O41156
P	-1	MET	-	expression tag	UNP O41156
P	0	THR	-	expression tag	UNP O41156
P	1	GLY	-	expression tag	UNP O41156
P	217	HIS	-	expression tag	UNP O41156
P	218	HIS	-	expression tag	UNP O41156
P	219	HIS	-	expression tag	UNP O41156
P	220	HIS	-	expression tag	UNP O41156
P	221	HIS	-	expression tag	UNP O41156
P	222	HIS	-	expression tag	UNP O41156

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

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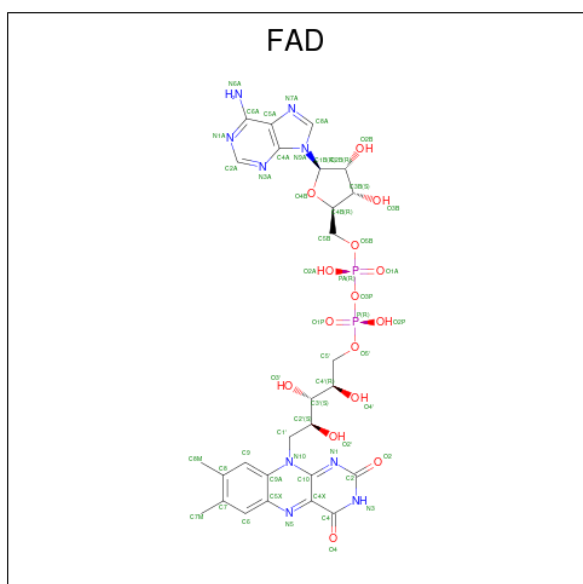
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F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

- Molecule 3 is 2-hydroxy-3-(4-methoxybenzyl)naphthalene-1,4-dione (three-letter code: 0VJ) (formula: $C_{18}H_{14}O_4$).
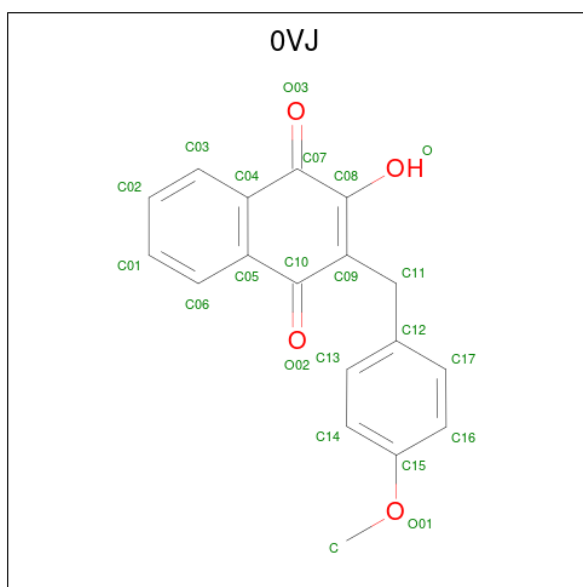
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 22	C 18	O 4	0	0
3	A	1	Total 22	C 18	O 4	0	0
3	B	1	Total 22	C 18	O 4	0	0
3	D	1	Total 22	C 18	O 4	0	0
3	E	1	Total 22	C 18	O 4	0	0
3	F	1	Total 22	C 18	O 4	0	0
3	G	1	Total 22	C 18	O 4	0	0
3	H	1	Total 22	C 18	O 4	0	0
3	I	1	Total 22	C 18	O 4	0	0
3	J	1	Total 22	C 18	O 4	0	0
3	K	1	Total 22	C 18	O 4	0	0
3	L	1	Total 22	C 18	O 4	0	0
3	M	1	Total 22	C 18	O 4	0	0
3	N	1	Total 22	C 18	O 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total 22	C 18	O 4	0	0
3	P	1	Total 22	C 18	O 4	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).
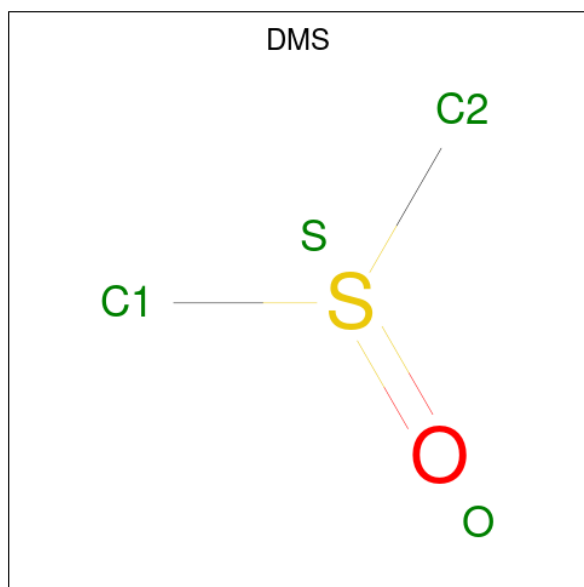
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	E	1	Total 4	C 2	O 1	S 1	0	0
4	F	1	Total 4	C 2	O 1	S 1	0	0
4	G	1	Total 4	C 2	O 1	S 1	0	0
4	H	1	Total 4	C 2	O 1	S 1	0	0
4	I	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	K	1	Total 4	C 2	O 1	S 1	0	0
4	M	1	Total 4	C 2	O 1	S 1	0	0
4	O	1	Total 4	C 2	O 1	S 1	0	0
4	P	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total 11	O 11	0	0
5	B	7	Total 7	O 7	0	0
5	C	2	Total 2	O 2	0	0
5	D	7	Total 7	O 7	0	0
5	E	8	Total 8	O 8	0	0
5	F	13	Total 13	O 13	0	0
5	G	13	Total 13	O 13	0	0
5	H	5	Total 5	O 5	0	0
5	I	3	Total 3	O 3	0	0
5	J	5	Total 5	O 5	0	0
5	K	2	Total 2	O 2	0	0
5	L	6	Total 6	O 6	0	0
5	M	3	Total 3	O 3	0	0
5	N	5	Total 5	O 5	0	0
5	O	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Probable thymidylate synthase

Chain A:
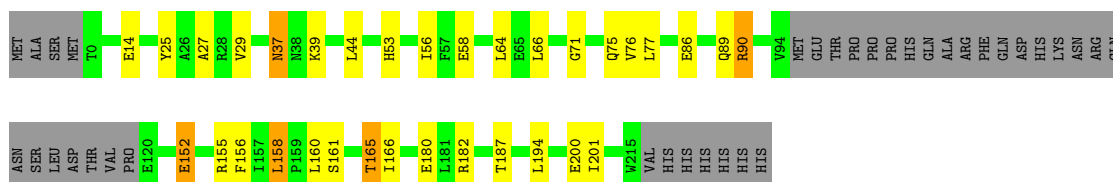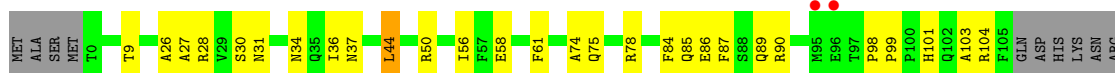
• Molecule 1: Probable thymidylate synthase

Chain B:
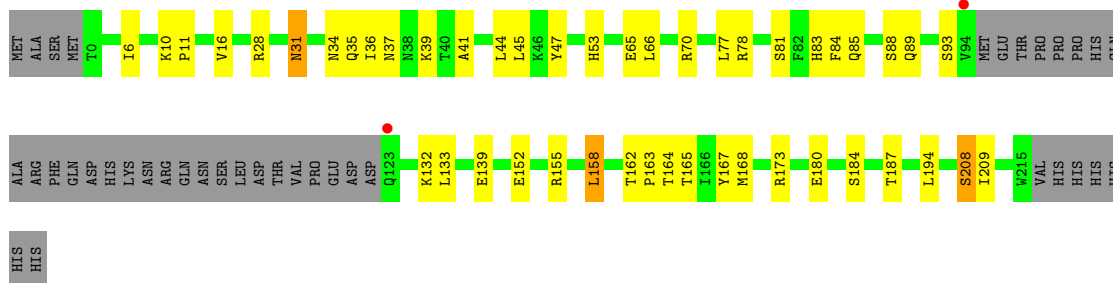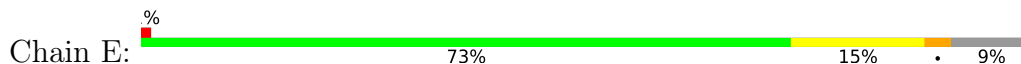
• Molecule 1: Probable thymidylate synthase
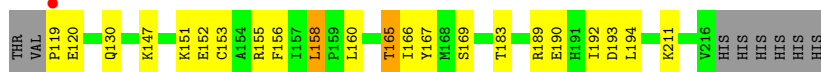
Chain C:

• Molecule 1: Probable thymidylate synthase

Chain D:

• Molecule 1: Probable thymidylate synthase

Chain E:
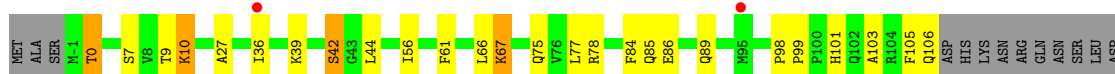

• Molecule 1: Probable thymidylate synthase

• Molecule 1: Probable thymidylate synthase

Chain F:

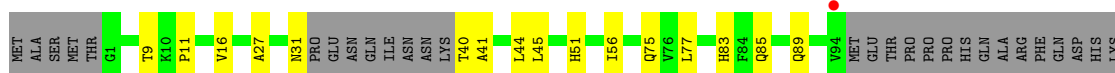• Molecule 1: Probable thymidylate synthase

• Molecule 1: Probable thymidylate synthase

Chain G:

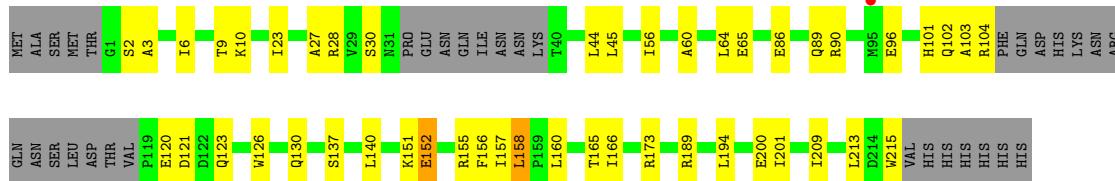• Molecule 1: Probable thymidylate synthase

• Molecule 1: Probable thymidylate synthase

Chain H:

• Molecule 1: Probable thymidylate synthase

• Molecule 1: Probable thymidylate synthase

Chain I:

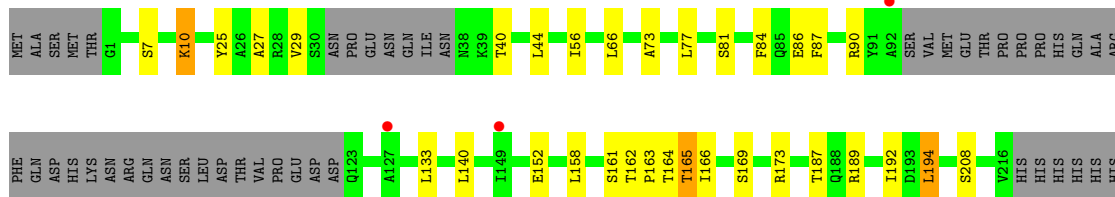• Molecule 1: Probable thymidylate synthase
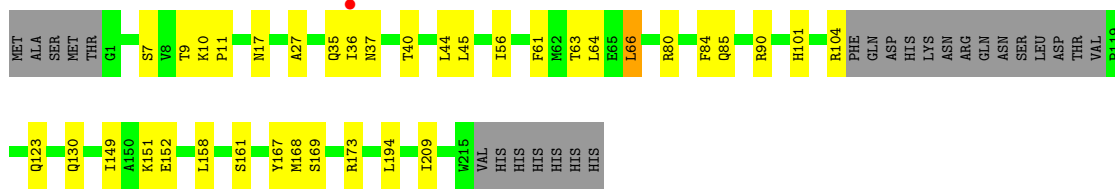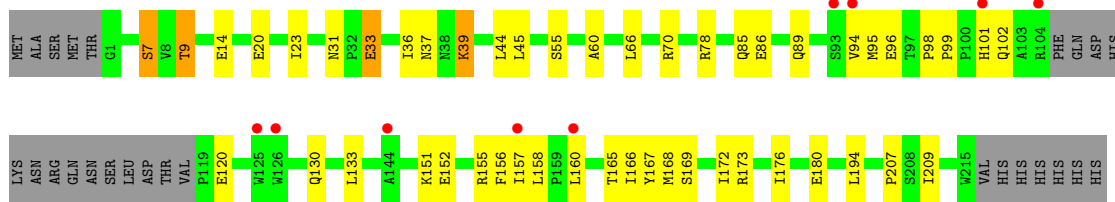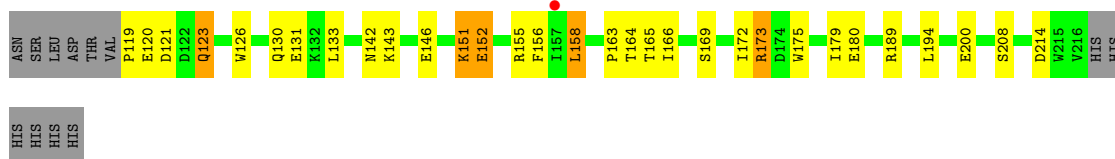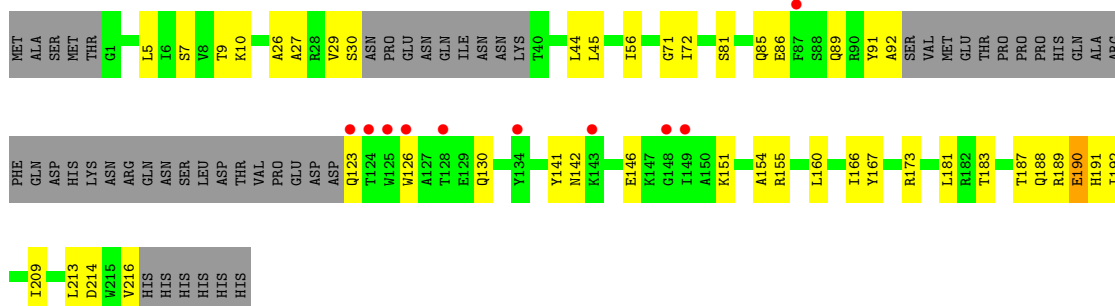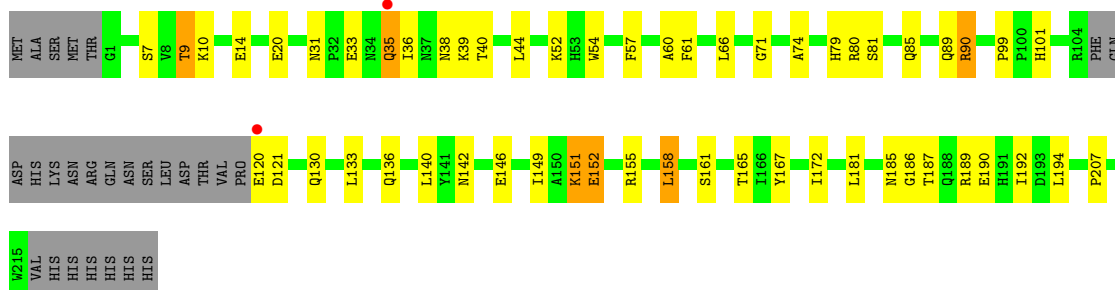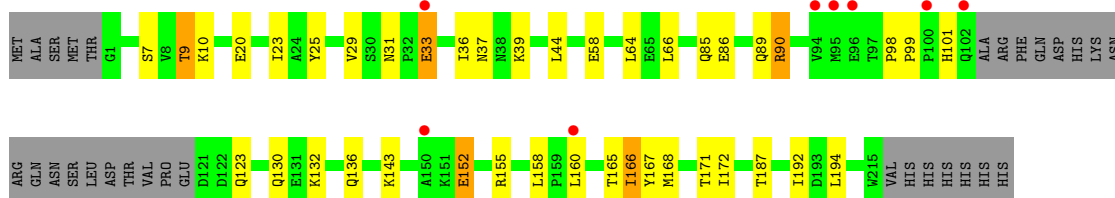
Chain J:

• Molecule 1: Probable thymidylate synthase

Chain K:

• Molecule 1: Probable thymidylate synthase

Chain L:

• Molecule 1: Probable thymidylate synthase

Chain M:

ASN SER LEU ASP THR VAL P119 E120 D121 D122 Q123 W126 Q130 E131 K132 L133 N142 K143 E146 K151 E152 R155 F156 I157 L158 P163 T164 T165 I166 S169 I172 R173 D174 W175 I179 E180 R189 L194 E200 S208 D214 W215 V216 HIS HIS

HIS HIS HIS HIS

● **Molecule 1: Probable thymidylate synthase**

Chain N:

4%

59%   19%   22%

MET ALA SER MET THR G1 L5 I6 S7 V8 T9 K10 A26 A27 R28 V29 S30 ASN PRO GLU ASN GLN ILE ASN ASN LYS T40 L44 L45 I56 G71 I72 S81 Q85 E86 F87 S88 Q89 R90 Y91 A92 SER VAL MET GLU THR PRO PRO PRO HIS GLN ALA ARG

PHE GLN ASP HIS LYS ASN ARG GLN ASN SER LEU ASP THR VAL PRO GLU ASP Q123 T124 W125 W126 A127 T128 E129 Q130 Y134 Y141 N142 K143 E146 K147 G148 I149 A150 K151 A154 R155 L160 I166 Y167 R173 L181 R182 T183 T187 Q188 R189 E190 H191 I192

I209 L213 D214 W215 V216 HIS HIS HIS HIS HIS

● **Molecule 1: Probable thymidylate synthase**

Chain O:

%

64%   22%   •   12%

MET ALA SER MET THR G1 S7 V8 T9 K10 E14 E20 N31 P32 E33 N34 Q35 I36 N37 N38 K39 T40 L44 K52 H53 W54 F57 A60 F61 L66 G71 A74 H79 R80 S81 Q85 Q89 R90 P99 P100 H101 R104 PHE GLN

ASP HIS LYS ASN ARG GLN ASN SER LEU ASP THR VAL PRO E120 D121 Q130 L133 Q136 L140 Y141 N142 E146 I149 A150 K151 E152 R155 L158 S161 T165 I166 Y167 I172 L181 N185 G186 T187 Q188 R189 E190 H191 I192 D193 L194 P207

W215 VAL HIS HIS HIS HIS HIS

● **Molecule 1: Probable thymidylate synthase**

Chain P:

4%

69%   16%   •   13%

MET ALA SER MET THR G1 S7 V8 T9 K10 E20 I23 A24 Y25 V29 S30 N31 P32 E33 I36 N37 N38 K39 L44 E58 L64 E65 L66 Q85 E86 Q89 R90 V94 M95 E96 T97 P98 P99 P100 H101 Q102 ALA ARG PHE GLN ASP HIS LYS ASN

ARG GLN ASN SER LEU ASP THR VAL PRO GLU D121 D122 Q123 Q130 E131 K132 Q136 K143 A150 K151 E152 R155 L158 P159 L160 T165 I166 Y167 M168 T171 I172 T187 I192 D193 L194 W215 VAL HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.97Å 120.58Å 128.25Å 111.65° 91.13° 90.18°	Depositor
Resolution (Å)	34.21 – 2.59 34.21 – 2.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.21-2.59) 92.8 (34.21-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.211 , 0.261 0.222 , 0.274	Depositor DCC
R_{free} test set	5633 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.146 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	26503	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, DMS, 0VJ

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	0.51	0/1578	0.72	0/2134
1	B	0.51	0/1553	0.72	0/2100
1	C	0.50	0/1707	0.72	0/2311
1	D	0.50	0/1681	0.74	0/2276
1	E	0.51	0/1710	0.73	0/2314
1	F	0.53	0/1706	0.73	0/2309
1	G	0.51	0/1553	0.72	0/2100
1	H	0.51	0/1478	0.72	0/1996
1	I	0.47	0/1595	0.71	0/2157
1	J	0.47	0/1481	0.71	0/1999
1	K	0.52	0/1663	0.70	0/2251
1	L	0.48	0/1663	0.70	0/2251
1	M	0.51	0/1630	0.73	0/2204
1	N	0.48	0/1464	0.71	0/1977
1	O	0.53	0/1655	0.72	0/2240
1	P	0.49	0/1630	0.72	0/2207
All	All	0.50	0/25747	0.72	0/34826

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1544	0	1533	13	0
1	B	1519	0	1519	22	0
1	C	1667	0	1652	19	0
1	D	1642	0	1627	25	0
1	E	1668	0	1657	20	0
1	F	1666	0	1652	28	0
1	G	1519	0	1519	21	0
1	H	1446	0	1448	12	0
1	I	1558	0	1546	22	0
1	J	1449	0	1456	15	0
1	K	1624	0	1610	13	0
1	L	1624	0	1610	23	0
1	M	1592	0	1584	30	1
1	N	1432	0	1437	23	0
1	O	1617	0	1602	26	1
1	P	1592	0	1578	16	0
2	A	106	0	62	0	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	E	53	0	31	1	0
2	F	106	0	62	3	0
2	H	53	0	31	1	0
2	I	106	0	62	2	0
2	J	53	0	31	3	0
2	K	53	0	31	0	0
2	M	53	0	31	1	0
2	N	53	0	31	2	0
2	O	53	0	31	1	0
2	P	53	0	31	2	0
3	A	44	0	28	0	0
3	B	22	0	14	2	0
3	D	22	0	14	1	0
3	E	22	0	14	0	0
3	F	22	0	14	0	0
3	G	22	0	14	0	0
3	H	22	0	14	0	0
3	I	22	0	14	2	0
3	J	22	0	14	1	0
3	K	22	0	14	0	0
3	L	22	0	14	0	0
3	M	22	0	14	4	0
3	N	22	0	14	4	0
3	O	22	0	14	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	22	0	14	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	1	0
4	E	4	0	6	2	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
4	H	4	0	6	0	0
4	I	4	0	6	0	0
4	K	4	0	6	1	0
4	M	4	0	6	3	0
4	O	4	0	6	0	0
4	P	4	0	6	0	0
5	A	11	0	0	0	0
5	B	7	0	0	0	0
5	C	2	0	0	0	0
5	D	7	0	0	0	0
5	E	8	0	0	0	0
5	F	13	0	0	0	0
5	G	13	0	0	0	0
5	H	5	0	0	0	0
5	I	3	0	0	0	0
5	J	5	0	0	0	0
5	K	2	0	0	0	0
5	L	6	0	0	0	0
5	M	3	0	0	0	0
5	N	5	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
All	All	26503	0	25828	296	1

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 6.

All (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:0:THR:HG21	1:F:190:GLU:HA	1.36	1.03
1:C:101:HIS:H	1:C:130:GLN:HE22	1.04	0.98
1:C:155:ARG:HA	1:C:158:LEU:HD22	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:HIS:H	1:C:130:GLN:NE2	1.83	0.76
1:J:87:PHE:HE1	1:J:165:THR:HG23	1.48	0.76
1:D:89:GLN:HB2	3:D:301:0VJ:H10	1.69	0.74
1:I:103:ALA:HB2	1:I:126:TRP:CD1	2.23	0.74
1:O:90:ARG:HG2	1:O:152:GLU:HG2	1.70	0.71
1:J:86:GLU:HG2	1:J:166:ILE:HG22	1.73	0.70
1:N:86:GLU:HG2	1:N:166:ILE:HG22	1.74	0.70
1:C:90:ARG:HH11	1:C:90:ARG:CG	2.05	0.70
1:M:101:HIS:H	1:M:130:GLN:HE22	1.39	0.70
1:J:81:SER:HB3	2:J:301:FAD:H52A	1.75	0.69
1:M:89:GLN:HE21	3:M:303:0VJ:H10	1.57	0.68
1:N:91:TYR:HB3	1:N:92:ALA:HA	1.75	0.67
1:L:45:LEU:HD13	1:L:209:ILE:HG13	1.78	0.66
1:I:89:GLN:HE21	3:I:304:0VJ:H10	1.60	0.65
1:M:85:GLN:HG3	4:M:302:DMS:C2	2.27	0.65
1:B:84:PHE:O	1:D:78:ARG:NH2	2.30	0.64
1:J:27:ALA:HB2	1:J:56:ILE:HD13	1.80	0.62
1:C:101:HIS:N	1:C:130:GLN:HE22	1.87	0.62
1:G:135:ALA:O	1:G:139:GLU:HG2	2.00	0.61
1:B:31:ASN:HB3	1:B:34:ASN:HB2	1.82	0.61
1:E:103:ALA:H	1:E:123:GLN:HE22	1.48	0.61
1:M:85:GLN:HG3	4:M:302:DMS:H22	1.82	0.61
1:N:81:SER:HB3	2:N:301:FAD:H52A	1.84	0.60
1:B:184:SER:O	1:B:187:THR:HG22	2.01	0.60
1:I:86:GLU:HB2	3:I:304:0VJ:H1	1.83	0.60
1:B:89:GLN:HE22	1:D:75:GLN:HG3	1.67	0.59
1:M:105:PHE:CZ	1:M:119:PRO:HG3	2.37	0.59
1:P:85:GLN:HB3	1:P:167:TYR:HB2	1.85	0.59
1:G:36:ILE:HG22	1:G:44:LEU:HD23	1.85	0.58
1:F:101:HIS:H	1:F:130:GLN:HE22	1.50	0.58
1:M:103:ALA:HB2	1:M:126:TRP:CD1	2.38	0.58
1:B:81:SER:HB3	2:B:301:FAD:H52A	1.85	0.58
1:I:101:HIS:H	1:I:130:GLN:HE22	1.52	0.58
1:D:86:GLU:HG2	1:D:166:ILE:HG22	1.86	0.57
1:K:85:GLN:HB3	1:K:167:TYR:HB2	1.85	0.57
1:F:89:GLN:HE22	1:H:75:GLN:HE21	1.52	0.57
1:M:30:SER:HB3	2:P:301:FAD:O4	2.05	0.57
1:A:64:LEU:HD11	1:A:201:ILE:HG21	1.87	0.56
1:D:26:ALA:O	1:D:30:SER:HB2	2.05	0.56
1:E:75:GLN:NE2	1:G:89:GLN:HE22	2.04	0.56
1:J:66:LEU:HB3	1:J:194:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:LYS:HB2	1:F:10:LYS:HB2	1.88	0.56
1:E:89:GLN:HE22	1:G:75:GLN:HE21	1.54	0.55
1:J:161:SER:HB3	1:L:156:PHE:HB3	1.88	0.55
1:M:12:VAL:HG21	1:N:5:LEU:HG	1.88	0.55
1:M:142:ASN:O	1:M:146:GLU:HG2	2.06	0.55
1:M:99:PRO:HD3	1:M:163:PRO:HG3	1.89	0.55
1:M:120:GLU:HA	1:M:123:GLN:HB2	1.88	0.55
1:F:85:GLN:HB3	1:F:167:TYR:HB2	1.88	0.55
1:N:72:ILE:HD12	1:N:191:HIS:HB2	1.89	0.55
1:H:27:ALA:HB2	1:H:56:ILE:HD13	1.89	0.54
1:I:3:ALA:HA	1:I:65:GLU:O	2.08	0.54
1:I:86:GLU:HG2	1:I:166:ILE:HG22	1.89	0.54
1:M:27:ALA:HB1	1:M:44:LEU:HD22	1.88	0.54
1:A:161:SER:HB3	1:C:156:PHE:HB3	1.88	0.54
1:E:89:GLN:NE2	1:G:75:GLN:HE21	2.06	0.54
1:F:0:THR:CG2	1:F:190:GLU:HA	2.24	0.54
1:D:103:ALA:H	1:D:123:GLN:HE22	1.56	0.53
1:L:66:LEU:HD11	1:L:168:MET:HB2	1.90	0.53
1:P:20:GLU:HA	1:P:23:ILE:HD12	1.90	0.53
1:P:86:GLU:HG2	1:P:166:ILE:HG22	1.90	0.53
1:C:29:VAL:HG23	4:D:302:DMS:H21	1.90	0.53
1:P:155:ARG:O	1:P:158:LEU:HB2	2.08	0.53
1:D:34:ASN:OD1	1:D:36:ILE:HB	2.08	0.53
1:O:9:THR:HG21	1:O:60:ALA:HA	1.90	0.53
1:C:66:LEU:O	1:C:165:THR:HA	2.09	0.53
1:K:61:PHE:CE1	1:K:169:SER:HB3	2.44	0.53
1:E:0:THR:N	1:E:1:GLY:HA3	2.24	0.53
1:L:155:ARG:O	1:L:158:LEU:HB2	2.08	0.53
1:F:155:ARG:HA	1:F:158:LEU:HD22	1.91	0.53
1:O:85:GLN:HB3	1:O:167:TYR:HB2	1.91	0.52
1:M:87:PHE:HE1	1:M:165:THR:HG23	1.75	0.52
1:I:102:GLN:HE21	1:I:104:ARG:HH21	1.57	0.52
1:D:87:PHE:HE1	1:D:165:THR:HG23	1.75	0.51
1:O:101:HIS:H	1:O:130:GLN:HE22	1.58	0.51
1:N:142:ASN:O	1:N:146:GLU:HG2	2.09	0.51
1:M:156:PHE:HB3	1:O:161:SER:HB3	1.92	0.51
1:M:166:ILE:HA	4:M:302:DMS:H13	1.93	0.51
1:F:0:THR:HG21	1:F:190:GLU:CA	2.25	0.51
1:N:209:ILE:HG22	1:N:213:LEU:HD12	1.93	0.51
1:O:9:THR:HA	1:P:9:THR:HA	1.92	0.51
1:P:25:TYR:O	1:P:29:VAL:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:7:SER:HB3	1:K:63:THR:HB	1.92	0.50
1:C:84:PHE:CE2	1:C:168:MET:HG3	2.45	0.50
1:K:66:LEU:HD11	1:K:168:MET:SD	2.52	0.50
1:F:183:THR:HA	1:F:192:ILE:HG23	1.93	0.50
1:I:10:LYS:HD3	1:J:10:LYS:HD3	1.94	0.50
1:A:155:ARG:HA	1:A:158:LEU:HD22	1.94	0.50
1:P:187:THR:HB	1:P:192:ILE:HG12	1.92	0.50
1:A:58:GLU:HB3	1:B:83:HIS:HB3	1.93	0.49
1:M:89:GLN:HB2	3:M:303:0VJ:H10	1.94	0.49
1:O:90:ARG:HH21	3:O:301:0VJ:H13	1.75	0.49
1:B:66:LEU:HD11	1:B:168:MET:SD	2.51	0.49
2:F:301:FAD:P	1:G:173:ARG:HH22	2.36	0.49
1:K:84:PHE:O	1:L:55:SER:HB2	2.13	0.49
1:C:90:ARG:HH11	1:C:90:ARG:HG3	1.75	0.49
1:N:188:GLN:HG3	3:N:302:0VJ:H9	1.94	0.49
1:F:75:GLN:NE2	1:H:89:GLN:HE22	2.11	0.49
1:I:90:ARG:HG2	1:I:152:GLU:HG2	1.95	0.49
1:J:140:LEU:HD23	1:L:133:LEU:HD22	1.95	0.49
1:F:36:ILE:O	1:F:39:LYS:HG2	2.12	0.48
1:K:101:HIS:H	1:K:130:GLN:HE22	1.61	0.48
1:F:66:LEU:O	1:F:165:THR:HA	2.13	0.48
1:O:89:GLN:HE21	3:O:301:0VJ:H10	1.78	0.48
1:O:71:GLY:O	1:O:74:ALA:HB3	2.13	0.48
1:K:27:ALA:HB2	1:K:56:ILE:HD13	1.95	0.48
1:N:183:THR:HA	1:N:192:ILE:HG23	1.95	0.48
1:M:155:ARG:O	1:M:158:LEU:HB2	2.14	0.48
1:O:142:ASN:O	1:O:146:GLU:HG2	2.13	0.48
1:O:187:THR:HB	1:O:192:ILE:HG12	1.96	0.48
1:D:85:GLN:HB3	1:D:167:TYR:HB2	1.96	0.48
1:D:101:HIS:H	1:D:130:GLN:HE22	1.61	0.48
1:E:85:GLN:HB3	1:E:167:TYR:HB2	1.96	0.48
1:J:187:THR:HB	1:J:192:ILE:HG12	1.95	0.48
1:D:101:HIS:H	1:D:130:GLN:NE2	2.12	0.47
1:I:155:ARG:O	1:I:158:LEU:HB2	2.15	0.47
1:O:81:SER:OG	2:O:302:FAD:O1A	2.30	0.47
1:A:71:GLY:HA2	1:A:160:LEU:HD12	1.95	0.47
1:C:86:GLU:HG2	1:C:166:ILE:HG22	1.96	0.47
1:O:155:ARG:O	1:O:158:LEU:HB2	2.14	0.47
1:C:90:ARG:HH11	1:C:90:ARG:HG2	1.80	0.47
1:H:11:PRO:HG2	1:H:16:VAL:HG12	1.95	0.47
1:D:27:ALA:HB2	1:D:56:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:9:THR:HG21	1:L:60:ALA:HA	1.96	0.47
1:M:8:VAL:HG23	1:M:62:MET:HB2	1.96	0.47
1:A:37:ASN:N	1:A:37:ASN:HD22	2.12	0.47
1:B:85:GLN:HB3	1:B:167:TYR:HB2	1.97	0.47
1:H:27:ALA:O	1:H:31:ASN:ND2	2.47	0.47
1:J:25:TYR:O	1:J:29:VAL:HG23	2.14	0.47
1:P:66:LEU:HD11	1:P:168:MET:SD	2.55	0.47
1:B:45:LEU:HD13	1:B:209:ILE:HG13	1.97	0.47
1:B:70:ARG:HH12	1:D:74:ALA:HB1	1.80	0.47
1:G:28:ARG:NH1	1:G:37:ASN:O	2.44	0.47
1:O:152:GLU:H	1:O:152:GLU:HG3	1.35	0.47
1:F:89:GLN:NE2	1:H:75:GLN:HE21	2.12	0.46
1:N:86:GLU:HG2	1:N:166:ILE:CG2	2.42	0.46
3:N:302:0VJ:H2	1:P:86:GLU:OE1	2.15	0.46
1:J:73:ALA:O	1:J:77:LEU:HB2	2.15	0.46
1:K:85:GLN:HG3	4:K:303:DMS:H13	1.97	0.46
1:N:151:LYS:O	1:N:155:ARG:HG3	2.15	0.46
1:P:90:ARG:HA	1:P:152:GLU:HG2	1.96	0.46
1:E:165:THR:O	4:E:303:DMS:H23	2.15	0.46
1:L:101:HIS:H	1:L:130:GLN:HE22	1.63	0.46
1:B:31:ASN:HB3	1:B:34:ASN:CB	2.46	0.46
1:F:86:GLU:HG2	1:F:166:ILE:HG22	1.98	0.46
1:F:101:HIS:H	1:F:130:GLN:NE2	2.13	0.46
1:N:188:GLN:HG3	3:N:302:0VJ:C16	2.46	0.46
1:F:0:THR:HB	1:F:193:ASP:OD2	2.16	0.46
1:P:98:PRO:HA	1:P:99:PRO:HD3	1.88	0.46
2:M:301:FAD:C6A	2:P:301:FAD:C6A	2.93	0.46
1:F:103:ALA:HB1	1:H:149:ILE:HG12	1.98	0.46
1:F:105:PHE:CE1	1:F:119:PRO:HG3	2.50	0.46
1:M:133:LEU:HD22	1:O:140:LEU:HD23	1.97	0.46
1:N:26:ALA:O	1:N:29:VAL:O	2.34	0.46
1:N:181:LEU:HD21	2:N:301:FAD:HM81	1.97	0.46
1:A:25:TYR:O	1:A:29:VAL:HG22	2.16	0.46
1:P:101:HIS:H	1:P:130:GLN:HE22	1.63	0.46
2:J:301:FAD:H2'	2:J:301:FAD:C9	2.46	0.45
1:L:20:GLU:HA	1:L:23:ILE:HD12	1.98	0.45
1:E:20:GLU:HA	1:E:23:ILE:HD12	1.98	0.45
1:D:90:ARG:HA	1:D:152:GLU:HG3	1.99	0.45
1:F:42:SER:OG	1:F:211:LYS:HD3	2.17	0.45
1:J:187:THR:O	1:J:192:ILE:HD11	2.17	0.45
1:N:85:GLN:HB3	1:N:167:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:PRO:HB3	1:G:22:LEU:HD22	1.98	0.45
1:L:36:ILE:HG23	1:L:39:LYS:HE2	1.98	0.45
1:B:155:ARG:O	1:B:158:LEU:HB2	2.17	0.45
1:G:58:GLU:HB3	1:H:83:HIS:HB3	1.99	0.45
1:G:140:LEU:HA	1:G:143:LYS:HB2	1.99	0.45
1:I:27:ALA:HB2	1:I:56:ILE:HD13	1.98	0.45
1:M:90:ARG:O	1:M:151:LYS:HG3	2.17	0.45
1:C:62:MET:HG2	1:C:64:LEU:HD12	1.99	0.45
1:E:152:GLU:H	1:E:152:GLU:HG3	1.42	0.45
1:F:67:LYS:HD3	1:F:165:THR:HB	1.99	0.45
1:I:213:LEU:HD13	1:I:215:TRP:CZ2	2.51	0.45
1:M:54:TRP:HB3	1:M:173:ARG:HG3	1.98	0.45
1:N:71:GLY:HA2	1:N:160:LEU:HD12	1.99	0.45
1:F:84:PHE:HA	1:F:167:TYR:O	2.17	0.45
1:H:41:ALA:O	1:H:45:LEU:HG	2.17	0.45
2:I:301:FAD:C6A	2:I:302:FAD:C6A	2.95	0.44
1:A:27:ALA:HB2	1:A:56:ILE:HD13	1.99	0.44
1:C:90:ARG:CG	1:C:90:ARG:NH1	2.75	0.44
1:C:120:GLU:O	1:C:124:THR:OG1	2.32	0.44
1:J:86:GLU:HG2	1:J:166:ILE:CG2	2.45	0.44
1:E:-3:ALA:HB1	1:E:189:ARG:HH12	1.83	0.44
1:M:90:ARG:HG2	1:M:152:GLU:HG2	2.00	0.44
1:I:64:LEU:HD11	1:I:201:ILE:HG21	1.99	0.44
1:I:103:ALA:HB1	1:K:149:ILE:HG12	2.00	0.44
1:O:90:ARG:NH2	3:O:301:0VJ:H13	2.32	0.44
1:D:183:THR:HA	1:D:192:ILE:HG23	1.99	0.44
1:B:11:PRO:HG2	1:B:16:VAL:HG12	1.99	0.44
3:B:303:0VJ:H14	1:D:188:GLN:HA	1.99	0.44
1:E:36:ILE:HG13	1:E:39:LYS:HE2	2.00	0.44
1:P:152:GLU:H	1:P:152:GLU:HG3	1.42	0.44
1:I:152:GLU:H	1:I:152:GLU:HG3	1.32	0.44
1:F:156:PHE:HB3	1:H:161:SER:HB3	2.00	0.43
1:L:70:ARG:HD2	1:L:70:ARG:HA	1.87	0.43
1:N:141:TYR:CD2	1:N:154:ALA:HB1	2.53	0.43
1:I:140:LEU:HG	1:I:157:ILE:HD13	1.99	0.43
1:L:86:GLU:HG2	1:L:166:ILE:CG2	2.47	0.43
1:F:75:GLN:O	1:F:78:ARG:HB2	2.18	0.43
1:M:86:GLU:HG2	1:M:166:ILE:HG22	2.00	0.43
1:D:191:HIS:HD2	1:D:191:HIS:O	2.01	0.43
1:E:2:SER:HB3	1:E:67:LYS:HB2	1.99	0.43
2:F:302:FAD:H52A	1:G:81:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:TYR:CZ	1:G:29:VAL:HG11	2.53	0.43
1:L:98:PRO:HA	1:L:99:PRO:HD3	1.91	0.43
1:O:36:ILE:HG22	1:O:39:LYS:HE2	1.99	0.43
1:E:200:GLU:HG2	1:E:217:HIS:NE2	2.33	0.43
1:M:88:SER:N	1:N:30:SER:HB2	2.34	0.43
1:B:88:SER:HA	3:B:303:0VJ:H4	2.00	0.43
1:J:84:PHE:O	1:L:78:ARG:NH2	2.51	0.43
1:K:11:PRO:HA	1:L:7:SER:HB2	2.00	0.43
1:M:100:PRO:HG3	1:M:131:GLU:HG3	2.00	0.43
3:M:303:0VJ:H14	1:O:186:GLY:O	2.19	0.43
2:J:301:FAD:H2'	2:J:301:FAD:H9	1.99	0.43
3:N:302:0VJ:H10	1:P:89:GLN:HB2	2.00	0.43
1:O:151:LYS:HZ1	1:P:33:GLU:HG2	1.84	0.43
1:E:87:PHE:N	4:E:303:DMS:H21	2.33	0.43
1:D:61:PHE:CE1	1:D:169:SER:HB3	2.54	0.43
1:F:66:LEU:HD12	1:F:166:ILE:HD11	2.01	0.43
1:G:206:PHE:HB3	1:G:209:ILE:HD12	2.01	0.43
1:M:103:ALA:HB1	1:O:149:ILE:HG12	2.00	0.43
1:H:85:GLN:HB3	1:H:167:TYR:HB2	2.01	0.43
1:H:152:GLU:H	1:H:152:GLU:HG3	1.53	0.43
1:K:151:LYS:NZ	1:L:33:GLU:OE1	2.52	0.43
1:M:86:GLU:HG2	1:M:166:ILE:CG2	2.49	0.43
1:N:86:GLU:HB2	3:P:302:0VJ:H1	2.00	0.43
1:O:20:GLU:OE1	1:O:207:PRO:HD2	2.19	0.43
1:O:66:LEU:O	1:O:165:THR:HA	2.19	0.43
1:A:182:ARG:O	1:A:187:THR:HG21	2.19	0.42
1:I:156:PHE:HB3	1:K:161:SER:HB3	2.01	0.42
1:M:98:PRO:HA	1:M:99:PRO:HD3	1.79	0.42
1:N:72:ILE:HD11	1:N:190:GLU:HG2	2.00	0.42
1:B:31:ASN:HB2	1:B:34:ASN:HB3	2.02	0.42
1:D:28:ARG:HG3	1:D:44:LEU:HD11	1.99	0.42
1:C:194:LEU:HD23	1:C:194:LEU:HA	1.90	0.42
1:J:162:THR:HA	1:J:163:PRO:HD3	1.95	0.42
1:A:66:LEU:O	1:A:165:THR:HA	2.19	0.42
1:A:75:GLN:HE21	1:C:89:GLN:HE22	1.67	0.42
1:E:161:SER:HB3	1:G:156:PHE:HB3	2.02	0.42
1:I:155:ARG:HA	1:I:158:LEU:HD22	2.01	0.42
1:B:6:ILE:HD11	1:B:65:GLU:HB2	2.00	0.42
3:J:302:0VJ:H10	1:L:89:GLN:HE21	1.85	0.42
1:G:187:THR:HB	1:G:192:ILE:HG13	2.02	0.42
1:F:98:PRO:HA	1:F:99:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:THR:HA	1:B:163:PRO:HD3	1.95	0.41
1:D:103:ALA:HB2	1:D:126:TRP:CD1	2.55	0.41
1:I:45:LEU:HD13	1:I:209:ILE:HG13	2.01	0.41
1:N:126:TRP:O	1:N:130:GLN:HB2	2.19	0.41
1:A:86:GLU:HG2	1:A:166:ILE:HG22	2.02	0.41
1:C:90:ARG:HB3	1:C:152:GLU:CG	2.50	0.41
1:B:41:ALA:O	1:B:45:LEU:HG	2.21	0.41
1:B:78:ARG:NH2	1:D:84:PHE:O	2.54	0.41
1:I:30:SER:HB2	2:I:302:FAD:O4	2.20	0.41
1:L:20:GLU:OE1	1:L:207:PRO:HD2	2.20	0.41
1:A:90:ARG:HA	1:A:152:GLU:HG3	2.03	0.41
1:B:45:LEU:HD12	1:B:208:SER:OG	2.20	0.41
2:C:301:FAD:H2'	2:C:301:FAD:H9	2.03	0.41
1:C:83:HIS:HB3	1:D:58:GLU:HB3	2.03	0.41
1:L:66:LEU:HD12	1:L:166:ILE:HG13	2.01	0.41
1:L:85:GLN:HB3	1:L:167:TYR:HB2	2.02	0.41
1:L:173:ARG:O	1:L:176:ILE:HB	2.21	0.41
1:M:86:GLU:HB2	3:M:303:0VJ:H1	2.02	0.41
1:N:27:ALA:HB2	1:N:56:ILE:HD13	2.02	0.41
1:P:58:GLU:HA	1:P:171:THR:HB	2.02	0.41
1:B:133:LEU:HD22	1:D:140:LEU:HD23	2.03	0.41
1:E:27:ALA:HB2	1:E:56:ILE:HD13	2.01	0.41
1:F:27:ALA:HB2	1:F:56:ILE:HD13	2.02	0.41
1:G:36:ILE:HG23	1:G:39:LYS:HE3	2.03	0.41
1:E:136:GLN:HE22	1:G:136:GLN:HE22	1.68	0.41
1:G:151:LYS:O	1:G:155:ARG:HG3	2.21	0.41
1:O:57:PHE:HB3	1:O:172:ILE:HG22	2.02	0.41
1:D:98:PRO:HA	1:D:99:PRO:HD3	1.93	0.40
1:E:61:PHE:CD1	1:F:61:PHE:HB2	2.56	0.40
1:G:54:TRP:HB3	1:G:173:ARG:HD2	2.03	0.40
1:I:23:ILE:HD11	1:I:60:ALA:HB3	2.03	0.40
1:D:187:THR:O	1:D:192:ILE:HD11	2.21	0.40
1:E:155:ARG:HA	1:E:158:LEU:HD22	2.04	0.40
2:E:301:FAD:C6A	2:H:302:FAD:C6A	2.99	0.40
2:F:302:FAD:N3A	1:G:173:ARG:NH1	2.60	0.40
1:M:175:TRP:O	1:M:179:ILE:HD12	2.21	0.40
1:F:151:LYS:O	1:F:155:ARG:HG3	2.22	0.40
1:N:45:LEU:HD13	1:N:209:ILE:HG12	2.03	0.40
1:O:9:THR:HB	1:O:61:PHE:H	1.86	0.40
1:O:79:HIS:HE1	1:O:181:LEU:HD23	1.86	0.40
1:B:36:ILE:HG21	1:B:47:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:LEU:HD12	1:G:158:LEU:HA	1.93	0.40
1:I:6:ILE:HD11	1:I:65:GLU:HB2	2.04	0.40
1:L:94:VAL:HG21	1:L:158:LEU:HD21	2.02	0.40
1:O:52:LYS:HB3	1:O:54:TRP:NE1	2.36	0.40
1:K:45:LEU:HD13	1:K:209:ILE:HG13	2.03	0.40
1:L:66:LEU:O	1:L:165:THR:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:0:THR:CG2	1:O:35:GLN:OE1[1_655]	2.11	0.09

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	187/227 (82%)	178 (95%)	7 (4%)	2 (1%)	14	30
1	B	184/227 (81%)	177 (96%)	7 (4%)	0	100	100
1	C	203/227 (89%)	194 (96%)	9 (4%)	0	100	100
1	D	199/227 (88%)	195 (98%)	4 (2%)	0	100	100
1	E	203/227 (89%)	193 (95%)	10 (5%)	0	100	100
1	F	202/227 (89%)	197 (98%)	5 (2%)	0	100	100
1	G	184/227 (81%)	179 (97%)	5 (3%)	0	100	100
1	H	173/227 (76%)	166 (96%)	7 (4%)	0	100	100
1	I	187/227 (82%)	181 (97%)	5 (3%)	1 (0%)	29	52
1	J	173/227 (76%)	170 (98%)	3 (2%)	0	100	100
1	K	197/227 (87%)	191 (97%)	5 (2%)	1 (0%)	29	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	197/227 (87%)	190 (96%)	7 (4%)	0	100	100
1	M	191/227 (84%)	186 (97%)	5 (3%)	0	100	100
1	N	171/227 (75%)	166 (97%)	4 (2%)	1 (1%)	25	47
1	O	196/227 (86%)	190 (97%)	4 (2%)	2 (1%)	15	32
1	P	193/227 (85%)	186 (96%)	7 (4%)	0	100	100
All	All	3040/3632 (84%)	2939 (97%)	94 (3%)	7 (0%)	47	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PHE
1	N	214	ASP
1	O	80	ARG
1	K	80	ARG
1	O	38	ASN
1	I	120	GLU
1	A	76	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/199 (83%)	151 (92%)	14 (8%)	10	21
1	B	162/199 (81%)	142 (88%)	20 (12%)	4	9
1	C	179/199 (90%)	161 (90%)	18 (10%)	7	14
1	D	176/199 (88%)	162 (92%)	14 (8%)	12	24
1	E	179/199 (90%)	160 (89%)	19 (11%)	6	12
1	F	179/199 (90%)	160 (89%)	19 (11%)	6	12
1	G	162/199 (81%)	150 (93%)	12 (7%)	13	28
1	H	153/199 (77%)	136 (89%)	17 (11%)	6	11
1	I	166/199 (83%)	149 (90%)	17 (10%)	7	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	153/199 (77%)	138 (90%)	15 (10%)	8	15
1	K	174/199 (87%)	157 (90%)	17 (10%)	8	15
1	L	174/199 (87%)	154 (88%)	20 (12%)	5	10
1	M	170/199 (85%)	146 (86%)	24 (14%)	3	6
1	N	151/199 (76%)	140 (93%)	11 (7%)	14	28
1	O	173/199 (87%)	151 (87%)	22 (13%)	4	8
1	P	171/199 (86%)	150 (88%)	21 (12%)	4	9
All	All	2687/3184 (84%)	2407 (90%)	280 (10%)	7	13

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	37	ASN
1	A	39	LYS
1	A	44	LEU
1	A	53	HIS
1	A	77	LEU
1	A	89	GLN
1	A	90	ARG
1	A	152	GLU
1	A	158	LEU
1	A	165	THR
1	A	180	GLU
1	A	194	LEU
1	A	200	GLU
1	B	10	LYS
1	B	28	ARG
1	B	31	ASN
1	B	35	GLN
1	B	37	ASN
1	B	39	LYS
1	B	44	LEU
1	B	53	HIS
1	B	77	LEU
1	B	93	SER
1	B	132	LYS
1	B	139	GLU
1	B	152	GLU
1	B	158	LEU

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Mol	Chain	Res	Type
1	B	164	THR
1	B	165	THR
1	B	173	ARG
1	B	180	GLU
1	B	194	LEU
1	B	208	SER
1	C	9	THR
1	C	14	GLU
1	C	33	GLU
1	C	36	ILE
1	C	44	LEU
1	C	90	ARG
1	C	124	THR
1	C	132	LYS
1	C	139	GLU
1	C	143	LYS
1	C	158	LEU
1	C	160	LEU
1	C	165	THR
1	C	180	GLU
1	C	187	THR
1	C	189	ARG
1	C	194	LEU
1	C	208	SER
1	D	9	THR
1	D	31	ASN
1	D	37	ASN
1	D	44	LEU
1	D	50	ARG
1	D	104	ARG
1	D	120	GLU
1	D	158	LEU
1	D	160	LEU
1	D	165	THR
1	D	180	GLU
1	D	189	ARG
1	D	194	LEU
1	D	216	VAL
1	E	4	LYS
1	E	9	THR
1	E	10	LYS
1	E	31	ASN

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Mol	Chain	Res	Type
1	E	36	ILE
1	E	44	LEU
1	E	50	ARG
1	E	120	GLU
1	E	121	ASP
1	E	132	LYS
1	E	139	GLU
1	E	152	GLU
1	E	158	LEU
1	E	165	THR
1	E	172	ILE
1	E	180	GLU
1	E	189	ARG
1	E	194	LEU
1	E	217	HIS
1	F	0	THR
1	F	7	SER
1	F	9	THR
1	F	10	LYS
1	F	42	SER
1	F	44	LEU
1	F	67	LYS
1	F	77	LEU
1	F	106	GLN
1	F	120	GLU
1	F	147	LYS
1	F	152	GLU
1	F	153	CYS
1	F	158	LEU
1	F	160	LEU
1	F	165	THR
1	F	169	SER
1	F	189	ARG
1	F	194	LEU
1	G	9	THR
1	G	10	LYS
1	G	44	LEU
1	G	77	LEU
1	G	139	GLU
1	G	151	LYS
1	G	152	GLU
1	G	158	LEU

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Mol	Chain	Res	Type
1	G	165	THR
1	G	189	ARG
1	G	194	LEU
1	G	200	GLU
1	H	9	THR
1	H	40	THR
1	H	44	LEU
1	H	51	HIS
1	H	77	LEU
1	H	124	THR
1	H	131	GLU
1	H	136	GLN
1	H	151	LYS
1	H	152	GLU
1	H	158	LEU
1	H	160	LEU
1	H	165	THR
1	H	169	SER
1	H	189	ARG
1	H	194	LEU
1	H	200	GLU
1	I	2	SER
1	I	9	THR
1	I	28	ARG
1	I	44	LEU
1	I	96	GLU
1	I	121	ASP
1	I	123	GLN
1	I	137	SER
1	I	151	LYS
1	I	152	GLU
1	I	158	LEU
1	I	160	LEU
1	I	165	THR
1	I	173	ARG
1	I	189	ARG
1	I	194	LEU
1	I	200	GLU
1	J	7	SER
1	J	10	LYS
1	J	40	THR
1	J	44	LEU

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Mol	Chain	Res	Type
1	J	90	ARG
1	J	133	LEU
1	J	152	GLU
1	J	158	LEU
1	J	164	THR
1	J	165	THR
1	J	169	SER
1	J	173	ARG
1	J	189	ARG
1	J	194	LEU
1	J	208	SER
1	K	9	THR
1	K	10	LYS
1	K	17	ASN
1	K	35	GLN
1	K	36	ILE
1	K	37	ASN
1	K	40	THR
1	K	44	LEU
1	K	64	LEU
1	K	66	LEU
1	K	90	ARG
1	K	104	ARG
1	K	123	GLN
1	K	152	GLU
1	K	158	LEU
1	K	173	ARG
1	K	194	LEU
1	L	7	SER
1	L	9	THR
1	L	14	GLU
1	L	31	ASN
1	L	33	GLU
1	L	37	ASN
1	L	39	LYS
1	L	44	LEU
1	L	95	MET
1	L	96	GLU
1	L	102	GLN
1	L	120	GLU
1	L	151	LYS
1	L	152	GLU

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Mol	Chain	Res	Type
1	L	157	ILE
1	L	160	LEU
1	L	169	SER
1	L	172	ILE
1	L	180	GLU
1	L	194	LEU
1	M	2	SER
1	M	9	THR
1	M	39	LYS
1	M	42	SER
1	M	44	LEU
1	M	77	LEU
1	M	102	GLN
1	M	104	ARG
1	M	121	ASP
1	M	123	GLN
1	M	143	LYS
1	M	151	LYS
1	M	152	GLU
1	M	158	LEU
1	M	164	THR
1	M	169	SER
1	M	172	ILE
1	M	173	ARG
1	M	180	GLU
1	M	189	ARG
1	M	194	LEU
1	M	200	GLU
1	M	208	SER
1	M	214	ASP
1	N	7	SER
1	N	9	THR
1	N	10	LYS
1	N	44	LEU
1	N	89	GLN
1	N	123	GLN
1	N	173	ARG
1	N	187	THR
1	N	189	ARG
1	N	190	GLU
1	N	216	VAL
1	O	7	SER

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Mol	Chain	Res	Type
1	O	9	THR
1	O	10	LYS
1	O	14	GLU
1	O	31	ASN
1	O	33	GLU
1	O	35	GLN
1	O	40	THR
1	O	44	LEU
1	O	90	ARG
1	O	99	PRO
1	O	120	GLU
1	O	121	ASP
1	O	133	LEU
1	O	136	GLN
1	O	151	LYS
1	O	152	GLU
1	O	158	LEU
1	O	185	ASN
1	O	189	ARG
1	O	190	GLU
1	O	194	LEU
1	P	7	SER
1	P	9	THR
1	P	10	LYS
1	P	31	ASN
1	P	33	GLU
1	P	36	ILE
1	P	37	ASN
1	P	39	LYS
1	P	44	LEU
1	P	64	LEU
1	P	90	ARG
1	P	123	GLN
1	P	132	LYS
1	P	136	GLN
1	P	143	LYS
1	P	152	GLU
1	P	160	LEU
1	P	165	THR
1	P	166	ILE
1	P	172	ILE
1	P	194	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	51	HIS
1	A	53	HIS
1	A	85	GLN
1	A	89	GLN
1	A	136	GLN
1	B	31	ASN
1	B	37	ASN
1	B	53	HIS
1	B	85	GLN
1	B	89	GLN
1	C	31	ASN
1	C	85	GLN
1	C	89	GLN
1	C	130	GLN
1	D	31	ASN
1	D	37	ASN
1	D	85	GLN
1	D	89	GLN
1	D	123	GLN
1	D	130	GLN
1	E	31	ASN
1	E	37	ASN
1	E	75	GLN
1	E	85	GLN
1	E	89	GLN
1	E	123	GLN
1	E	136	GLN
1	F	35	GLN
1	F	37	ASN
1	F	85	GLN
1	F	89	GLN
1	F	130	GLN
1	G	31	ASN
1	G	35	GLN
1	G	37	ASN
1	G	85	GLN
1	G	136	GLN
1	H	85	GLN
1	H	89	GLN
1	I	31	ASN

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type
1	I	85	GLN
1	I	89	GLN
1	I	102	GLN
1	I	130	GLN
1	J	75	GLN
1	J	85	GLN
1	K	37	ASN
1	K	85	GLN
1	K	130	GLN
1	L	31	ASN
1	L	37	ASN
1	L	85	GLN
1	L	89	GLN
1	L	196	ASN
1	M	17	ASN
1	M	85	GLN
1	M	89	GLN
1	M	130	GLN
1	N	85	GLN
1	N	136	GLN
1	O	37	ASN
1	O	85	GLN
1	O	89	GLN
1	O	123	GLN
1	O	130	GLN
1	O	177	HIS
1	P	31	ASN
1	P	34	ASN
1	P	85	GLN
1	P	89	GLN
1	P	130	GLN
1	P	136	GLN
1	P	177	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

45 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	0VJ	A	303	-	24,24,24	4.29	16 (66%)	31,34,34	3.54	12 (38%)
3	0VJ	B	303	-	24,24,24	5.12	16 (66%)	31,34,34	3.93	20 (64%)
4	DMS	B	302	-	3,3,3	0.96	0	3,3,3	1.31	0
3	0VJ	N	302	-	24,24,24	4.83	18 (75%)	31,34,34	3.44	12 (38%)
3	0VJ	K	301	-	24,24,24	4.79	18 (75%)	31,34,34	3.60	13 (41%)
4	DMS	O	303	-	3,3,3	0.69	0	3,3,3	0.18	0
3	0VJ	H	301	-	24,24,24	4.55	18 (75%)	31,34,34	2.99	12 (38%)
3	0VJ	I	304	-	24,24,24	4.41	16 (66%)	31,34,34	3.52	13 (41%)
4	DMS	A	304	-	3,3,3	1.04	0	3,3,3	1.06	0
2	FAD	H	302	-	53,58,58	1.43	8 (15%)	68,89,89	1.33	10 (14%)
2	FAD	I	302	-	53,58,58	1.72	13 (24%)	68,89,89	1.62	12 (17%)
3	0VJ	G	301	-	24,24,24	4.70	16 (66%)	31,34,34	3.29	10 (32%)
2	FAD	E	301	-	53,58,58	1.71	14 (26%)	68,89,89	1.62	12 (17%)
2	FAD	F	301	-	53,58,58	1.90	16 (30%)	68,89,89	1.61	21 (30%)
4	DMS	E	303	-	3,3,3	0.67	0	3,3,3	1.34	0
2	FAD	F	302	-	53,58,58	1.72	13 (24%)	68,89,89	1.62	12 (17%)
3	0VJ	M	303	-	24,24,24	4.67	18 (75%)	31,34,34	3.36	13 (41%)
3	0VJ	A	305	-	24,24,24	4.53	16 (66%)	31,34,34	3.37	14 (45%)
3	0VJ	F	304	-	24,24,24	4.47	16 (66%)	31,34,34	3.43	13 (41%)
2	FAD	P	301	-	53,58,58	1.72	13 (24%)	68,89,89	1.62	12 (17%)
4	DMS	D	302	-	3,3,3	0.96	0	3,3,3	1.08	0
2	FAD	A	302	-	53,58,58	1.72	14 (26%)	68,89,89	1.62	12 (17%)
4	DMS	C	302	-	3,3,3	0.79	0	3,3,3	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	DMS	F	303	-	3,3,3	0.78	0	3,3,3	0.94	0
4	DMS	H	303	-	3,3,3	1.07	0	3,3,3	0.92	0
3	0VJ	E	302	-	24,24,24	4.76	18 (75%)	31,34,34	2.94	12 (38%)
4	DMS	I	303	-	3,3,3	0.85	0	3,3,3	0.78	0
3	0VJ	D	301	-	24,24,24	4.55	16 (66%)	31,34,34	3.40	12 (38%)
4	DMS	M	302	-	3,3,3	0.72	0	3,3,3	0.46	0
2	FAD	K	302	-	53,58,58	1.45	12 (22%)	68,89,89	1.31	7 (10%)
2	FAD	J	301	-	53,58,58	1.84	13 (24%)	68,89,89	1.69	13 (19%)
3	0VJ	O	301	-	24,24,24	4.74	16 (66%)	31,34,34	3.78	14 (45%)
2	FAD	N	301	-	53,58,58	1.70	15 (28%)	68,89,89	1.75	16 (23%)
2	FAD	O	302	-	53,58,58	1.43	8 (15%)	68,89,89	1.54	16 (23%)
2	FAD	M	301	-	53,58,58	1.71	13 (24%)	68,89,89	1.62	12 (17%)
4	DMS	P	303	-	3,3,3	0.89	0	3,3,3	0.54	0
4	DMS	G	302	-	3,3,3	1.07	0	3,3,3	0.83	0
2	FAD	C	301	-	53,58,58	1.68	13 (24%)	68,89,89	1.52	12 (17%)
2	FAD	I	301	-	53,58,58	1.72	13 (24%)	68,89,89	1.63	12 (17%)
3	0VJ	L	301	-	24,24,24	4.88	18 (75%)	31,34,34	3.13	14 (45%)
3	0VJ	J	302	-	24,24,24	4.95	18 (75%)	31,34,34	3.62	9 (29%)
4	DMS	K	303	-	3,3,3	0.80	0	3,3,3	0.89	0
2	FAD	A	301	-	53,58,58	1.71	13 (24%)	68,89,89	1.62	12 (17%)
2	FAD	B	301	-	53,58,58	1.65	10 (18%)	68,89,89	1.51	12 (17%)
3	0VJ	P	302	-	24,24,24	4.51	17 (70%)	31,34,34	3.22	10 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0VJ	A	303	-	-	0/6/26/26	0/3/3/3
3	0VJ	B	303	-	-	2/6/26/26	0/3/3/3
3	0VJ	N	302	-	-	2/6/26/26	0/3/3/3
3	0VJ	K	301	-	-	0/6/26/26	0/3/3/3
3	0VJ	H	301	-	-	0/6/26/26	0/3/3/3
3	0VJ	I	304	-	-	0/6/26/26	0/3/3/3
2	FAD	H	302	-	-	6/30/50/50	0/6/6/6
2	FAD	I	302	-	-	3/30/50/50	0/6/6/6
3	0VJ	G	301	-	-	0/6/26/26	0/3/3/3

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W O R L D W I D E
PDB
PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	E	301	-	-	3/30/50/50	0/6/6/6
2	FAD	F	301	-	-	7/30/50/50	0/6/6/6
2	FAD	F	302	-	-	3/30/50/50	0/6/6/6
3	0VJ	M	303	-	-	0/6/26/26	0/3/3/3
3	0VJ	A	305	-	-	2/6/26/26	0/3/3/3
3	0VJ	F	304	-	-	0/6/26/26	0/3/3/3
2	FAD	P	301	-	-	3/30/50/50	0/6/6/6
2	FAD	A	302	-	-	3/30/50/50	0/6/6/6
3	0VJ	E	302	-	-	0/6/26/26	0/3/3/3
3	0VJ	D	301	-	-	2/6/26/26	0/3/3/3
2	FAD	K	302	-	-	5/30/50/50	0/6/6/6
2	FAD	J	301	-	-	9/30/50/50	0/6/6/6
3	0VJ	O	301	-	-	0/6/26/26	0/3/3/3
2	FAD	N	301	-	-	7/30/50/50	0/6/6/6
2	FAD	O	302	-	-	8/30/50/50	0/6/6/6
2	FAD	M	301	-	-	3/30/50/50	0/6/6/6
2	FAD	C	301	-	-	5/30/50/50	0/6/6/6
2	FAD	I	301	-	-	3/30/50/50	0/6/6/6
3	0VJ	L	301	-	-	0/6/26/26	0/3/3/3
3	0VJ	J	302	-	-	0/6/26/26	0/3/3/3
2	FAD	A	301	-	-	3/30/50/50	0/6/6/6
2	FAD	B	301	-	-	8/30/50/50	0/6/6/6
3	0VJ	P	302	-	-	0/6/26/26	0/3/3/3

All (472) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	0VJ	C03-C04	9.87	1.55	1.39
3	O	301	0VJ	C02-C01	9.82	1.64	1.38
3	E	302	0VJ	C02-C01	9.73	1.63	1.38
3	B	303	0VJ	C17-C12	9.73	1.59	1.38
3	O	301	0VJ	C17-C12	9.69	1.59	1.38
3	L	301	0VJ	C02-C01	9.63	1.63	1.38
3	N	302	0VJ	C17-C12	9.59	1.59	1.38
3	P	302	0VJ	C02-C01	9.51	1.63	1.38
3	J	302	0VJ	C02-C01	9.32	1.62	1.38
3	J	302	0VJ	C17-C12	9.32	1.58	1.38
3	K	301	0VJ	C02-C01	9.24	1.62	1.38
3	K	301	0VJ	O01-C15	9.22	1.56	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	303	0VJ	C02-C01	9.21	1.62	1.38
3	E	302	0VJ	C06-C05	9.21	1.54	1.39
3	L	301	0VJ	C17-C12	9.01	1.58	1.38
3	G	301	0VJ	C03-C04	8.96	1.54	1.39
3	N	302	0VJ	C02-C01	8.95	1.61	1.38
3	I	304	0VJ	C02-C01	8.86	1.61	1.38
3	G	301	0VJ	C02-C01	8.78	1.61	1.38
3	A	305	0VJ	C17-C12	8.77	1.57	1.38
3	A	305	0VJ	C02-C01	8.73	1.61	1.38
3	J	302	0VJ	C03-C04	8.69	1.53	1.39
3	H	301	0VJ	C02-C01	8.67	1.61	1.38
3	E	302	0VJ	C03-C04	8.67	1.53	1.39
3	B	303	0VJ	C02-C01	8.66	1.61	1.38
3	F	304	0VJ	C17-C12	8.53	1.57	1.38
3	O	301	0VJ	C03-C04	8.51	1.53	1.39
3	A	303	0VJ	C17-C12	8.49	1.57	1.38
3	M	303	0VJ	C03-C04	8.44	1.53	1.39
3	J	302	0VJ	O01-C15	8.42	1.55	1.37
3	B	303	0VJ	O01-C15	8.36	1.55	1.37
3	L	301	0VJ	C03-C04	8.34	1.53	1.39
3	E	302	0VJ	C17-C12	8.28	1.56	1.38
3	H	301	0VJ	C17-C12	8.28	1.56	1.38
3	M	303	0VJ	C17-C12	8.21	1.56	1.38
3	N	302	0VJ	C03-C04	8.21	1.53	1.39
3	J	302	0VJ	C06-C05	8.20	1.53	1.39
3	F	304	0VJ	C02-C01	8.13	1.59	1.38
3	I	304	0VJ	C17-C12	8.13	1.56	1.38
3	A	305	0VJ	C03-C04	8.09	1.52	1.39
3	D	301	0VJ	C03-C04	8.08	1.52	1.39
3	D	301	0VJ	C02-C01	8.00	1.59	1.38
3	P	302	0VJ	C17-C12	7.96	1.56	1.38
3	I	304	0VJ	O01-C15	7.90	1.54	1.37
3	K	301	0VJ	C03-C04	7.87	1.52	1.39
3	G	301	0VJ	O01-C15	7.84	1.53	1.37
3	A	303	0VJ	C02-C01	7.83	1.58	1.38
3	H	301	0VJ	C03-C04	7.74	1.52	1.39
3	B	303	0VJ	C11-C12	-7.66	1.39	1.51
3	K	301	0VJ	C11-C12	-7.64	1.39	1.51
3	P	302	0VJ	C03-C04	7.61	1.52	1.39
3	I	304	0VJ	C03-C04	7.55	1.51	1.39
3	L	301	0VJ	O01-C15	7.54	1.53	1.37
3	O	301	0VJ	O01-C15	7.54	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	304	0VJ	C03-C04	7.54	1.51	1.39
3	G	301	0VJ	C17-C12	7.53	1.55	1.38
3	D	301	0VJ	C17-C12	7.52	1.55	1.38
3	K	301	0VJ	C17-C12	7.44	1.54	1.38
3	N	302	0VJ	O01-C15	7.37	1.52	1.37
3	A	303	0VJ	C03-C04	7.37	1.51	1.39
3	D	301	0VJ	C06-C05	7.24	1.51	1.39
3	N	302	0VJ	C06-C05	7.13	1.51	1.39
3	A	303	0VJ	O01-C15	7.07	1.52	1.37
3	B	303	0VJ	C06-C05	7.07	1.51	1.39
3	B	303	0VJ	C04-C07	7.03	1.61	1.48
3	M	303	0VJ	C06-C05	6.99	1.51	1.39
3	F	304	0VJ	C06-C05	6.87	1.50	1.39
3	D	301	0VJ	O01-C15	6.87	1.51	1.37
3	H	301	0VJ	C06-C05	6.82	1.50	1.39
3	M	303	0VJ	O01-C15	6.70	1.51	1.37
3	L	301	0VJ	C06-C05	6.56	1.50	1.39
3	G	301	0VJ	C06-C05	6.56	1.50	1.39
3	J	302	0VJ	C17-C16	6.54	1.50	1.38
2	B	301	FAD	O4B-C1B	6.51	1.50	1.41
3	P	302	0VJ	O01-C15	6.43	1.51	1.37
3	G	301	0VJ	C04-C07	6.41	1.60	1.48
3	K	301	0VJ	C06-C05	6.39	1.50	1.39
3	A	305	0VJ	C11-C12	-6.36	1.41	1.51
3	D	301	0VJ	C17-C16	6.34	1.50	1.38
3	I	304	0VJ	C11-C12	-6.27	1.41	1.51
3	L	301	0VJ	C14-C13	6.22	1.50	1.38
3	O	301	0VJ	C06-C05	6.19	1.49	1.39
3	H	301	0VJ	C11-C12	-6.12	1.41	1.51
3	F	304	0VJ	O01-C15	6.10	1.50	1.37
3	N	302	0VJ	C17-C16	6.07	1.49	1.38
3	H	301	0VJ	O01-C15	6.06	1.50	1.37
3	A	303	0VJ	C04-C07	6.04	1.59	1.48
3	P	302	0VJ	C11-C09	5.95	1.59	1.51
3	A	305	0VJ	O01-C15	5.90	1.49	1.37
3	D	301	0VJ	C11-C12	-5.90	1.42	1.51
3	A	305	0VJ	C04-C07	5.89	1.59	1.48
3	I	304	0VJ	C06-C05	5.89	1.49	1.39
3	A	305	0VJ	C06-C05	5.84	1.49	1.39
3	L	301	0VJ	C17-C16	5.81	1.49	1.38
3	E	302	0VJ	O01-C15	5.66	1.49	1.37
3	M	303	0VJ	C11-C12	-5.62	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	302	0VJ	C06-C05	5.62	1.48	1.39
3	G	301	0VJ	C11-C12	-5.57	1.42	1.51
3	B	303	0VJ	C08-C07	5.52	1.60	1.46
3	H	301	0VJ	C14-C13	5.45	1.48	1.38
3	M	303	0VJ	C04-C07	5.38	1.58	1.48
3	A	305	0VJ	C17-C16	5.37	1.48	1.38
3	K	301	0VJ	C04-C07	5.37	1.58	1.48
3	A	303	0VJ	C17-C16	5.34	1.48	1.38
3	H	301	0VJ	C04-C07	5.29	1.58	1.48
3	P	302	0VJ	C17-C16	5.26	1.48	1.38
3	M	303	0VJ	C17-C16	5.25	1.48	1.38
3	L	301	0VJ	C04-C07	5.24	1.58	1.48
3	F	304	0VJ	C11-C12	-5.23	1.43	1.51
3	F	304	0VJ	C17-C16	5.20	1.48	1.38
3	A	303	0VJ	C11-C12	-5.17	1.43	1.51
3	O	301	0VJ	C11-C12	-5.16	1.43	1.51
3	B	303	0VJ	C14-C13	5.16	1.48	1.38
3	P	302	0VJ	C14-C13	5.11	1.48	1.38
3	G	301	0VJ	C17-C16	5.08	1.48	1.38
3	E	302	0VJ	C11-C09	5.08	1.58	1.51
3	E	302	0VJ	C04-C07	5.00	1.57	1.48
3	P	302	0VJ	C11-C12	-5.00	1.43	1.51
3	F	304	0VJ	C08-C07	4.97	1.58	1.46
3	F	304	0VJ	C04-C07	4.96	1.57	1.48
3	A	303	0VJ	C06-C05	4.92	1.47	1.39
2	F	301	FAD	C5'-C4'	4.88	1.58	1.51
3	O	301	0VJ	C14-C13	4.84	1.47	1.38
2	I	302	FAD	C1'-C2'	4.83	1.59	1.52
3	K	301	0VJ	C11-C09	4.81	1.58	1.51
2	I	301	FAD	C1'-C2'	4.80	1.59	1.52
2	F	302	FAD	C1'-C2'	4.79	1.59	1.52
2	A	302	FAD	C1'-C2'	4.78	1.59	1.52
2	A	301	FAD	C1'-C2'	4.78	1.59	1.52
2	P	301	FAD	C1'-C2'	4.77	1.59	1.52
2	M	301	FAD	C1'-C2'	4.76	1.59	1.52
3	L	301	0VJ	C14-C15	4.76	1.48	1.38
2	E	301	FAD	C1'-C2'	4.75	1.59	1.52
3	L	301	0VJ	C11-C12	-4.74	1.43	1.51
3	B	303	0VJ	C16-C15	4.67	1.48	1.38
3	E	302	0VJ	C14-C13	4.64	1.47	1.38
3	L	301	0VJ	C11-C09	4.63	1.57	1.51
3	K	301	0VJ	C17-C16	4.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	302	0VJ	C04-C07	4.60	1.56	1.48
3	G	301	0VJ	C14-C13	4.59	1.47	1.38
3	M	303	0VJ	C11-C09	4.57	1.57	1.51
2	J	301	FAD	O4'-C4'	4.55	1.53	1.43
3	K	301	0VJ	C14-C13	4.51	1.47	1.38
3	N	302	0VJ	C08-C07	4.49	1.57	1.46
3	N	302	0VJ	C04-C07	4.49	1.56	1.48
3	I	304	0VJ	O03-C07	-4.48	1.13	1.23
3	A	305	0VJ	O-C08	4.46	1.48	1.33
3	J	302	0VJ	C16-C15	4.45	1.47	1.38
3	I	304	0VJ	C17-C16	4.44	1.46	1.38
3	D	301	0VJ	C16-C15	4.41	1.47	1.38
3	G	301	0VJ	C11-C09	4.40	1.57	1.51
3	I	304	0VJ	C04-C07	4.40	1.56	1.48
3	N	302	0VJ	O03-C07	-4.39	1.14	1.23
2	J	301	FAD	C5'-C4'	4.39	1.58	1.51
3	F	304	0VJ	C14-C13	4.38	1.46	1.38
3	E	302	0VJ	C17-C16	4.37	1.46	1.38
3	N	302	0VJ	C11-C09	4.31	1.57	1.51
3	N	302	0VJ	O-C08	4.31	1.48	1.33
3	A	305	0VJ	O03-C07	-4.30	1.14	1.23
3	H	301	0VJ	C17-C16	4.29	1.46	1.38
3	O	301	0VJ	C16-C15	4.28	1.47	1.38
3	A	303	0VJ	O-C08	4.27	1.48	1.33
3	N	302	0VJ	C14-C13	4.24	1.46	1.38
3	O	301	0VJ	C04-C07	4.23	1.56	1.48
2	B	301	FAD	C4X-C10	4.20	1.56	1.44
3	F	304	0VJ	O-C08	4.19	1.47	1.33
2	O	302	FAD	O4B-C1B	4.19	1.46	1.41
3	O	301	0VJ	C17-C16	4.18	1.46	1.38
3	E	302	0VJ	C08-C07	4.17	1.56	1.46
2	N	301	FAD	C2A-N3A	4.17	1.38	1.32
3	P	302	0VJ	C04-C07	4.16	1.56	1.48
3	E	302	0VJ	C11-C12	-4.14	1.44	1.51
3	N	302	0VJ	C16-C15	4.13	1.46	1.38
2	N	301	FAD	O4B-C1B	4.13	1.46	1.41
2	F	301	FAD	C2A-N3A	4.10	1.38	1.32
2	C	301	FAD	C4X-C10	4.08	1.56	1.44
3	D	301	0VJ	C11-C09	4.08	1.56	1.51
3	D	301	0VJ	O-C08	4.08	1.47	1.33
3	M	303	0VJ	C14-C13	4.08	1.46	1.38
3	P	302	0VJ	C14-C15	4.06	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	0VJ	C04-C07	4.02	1.55	1.48
2	F	301	FAD	C4'-C3'	3.99	1.61	1.53
3	K	301	0VJ	O03-C07	-3.99	1.14	1.23
2	N	301	FAD	C6-C7	3.98	1.45	1.39
2	I	301	FAD	C9A-C5X	3.98	1.47	1.41
3	D	301	0VJ	C14-C13	3.98	1.46	1.38
3	M	303	0VJ	C08-C07	3.97	1.56	1.46
3	J	302	0VJ	C14-C15	3.97	1.46	1.38
3	D	301	0VJ	O03-C07	-3.96	1.14	1.23
2	E	301	FAD	C9A-C5X	3.96	1.47	1.41
2	P	301	FAD	C9A-C5X	3.95	1.47	1.41
2	A	301	FAD	C9A-C5X	3.94	1.47	1.41
2	I	302	FAD	C9A-C5X	3.94	1.47	1.41
3	G	301	0VJ	O02-C10	3.93	1.31	1.23
3	A	303	0VJ	O03-C07	-3.92	1.15	1.23
2	F	302	FAD	C9A-C5X	3.92	1.47	1.41
2	A	302	FAD	C9A-C5X	3.91	1.47	1.41
2	M	301	FAD	C9A-C5X	3.91	1.47	1.41
3	J	302	0VJ	C14-C13	3.90	1.45	1.38
3	O	301	0VJ	C11-C09	3.89	1.56	1.51
2	J	301	FAD	C2A-N3A	3.87	1.38	1.32
3	O	301	0VJ	O03-C07	-3.84	1.15	1.23
3	M	303	0VJ	O-C08	3.83	1.46	1.33
3	I	304	0VJ	C16-C15	3.82	1.46	1.38
3	O	301	0VJ	C08-C07	3.81	1.55	1.46
3	A	305	0VJ	C14-C15	3.79	1.46	1.38
3	I	304	0VJ	C14-C15	3.79	1.46	1.38
3	J	302	0VJ	O-C08	3.79	1.46	1.33
3	F	304	0VJ	C11-C09	3.76	1.56	1.51
3	H	301	0VJ	C08-C07	3.75	1.55	1.46
2	H	302	FAD	O4B-C1B	3.75	1.46	1.41
3	H	301	0VJ	C11-C09	3.70	1.56	1.51
2	C	301	FAD	C9A-C5X	3.69	1.47	1.41
2	J	301	FAD	C6-C7	3.63	1.44	1.39
3	G	301	0VJ	O-C08	3.62	1.45	1.33
2	C	301	FAD	C8A-N7A	-3.62	1.28	1.34
3	F	304	0VJ	C16-C15	3.61	1.45	1.38
3	J	302	0VJ	O03-C07	-3.61	1.15	1.23
2	F	301	FAD	O2'-C2'	3.61	1.51	1.43
2	K	302	FAD	C4X-C10	3.57	1.54	1.44
3	O	301	0VJ	O-C08	3.56	1.45	1.33
3	D	301	0VJ	C08-C07	3.55	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	302	FAD	C5'-C4'	3.51	1.56	1.51
2	F	301	FAD	C1'-C2'	3.51	1.57	1.52
3	N	302	0VJ	C14-C15	3.51	1.45	1.38
2	M	301	FAD	C5'-C4'	3.49	1.56	1.51
2	A	302	FAD	C5'-C4'	3.48	1.56	1.51
3	N	302	0VJ	C11-C12	-3.48	1.45	1.51
2	I	301	FAD	C5'-C4'	3.48	1.56	1.51
2	A	301	FAD	C5'-C4'	3.48	1.56	1.51
2	K	302	FAD	O4B-C1B	3.46	1.45	1.41
3	H	301	0VJ	C16-C15	3.46	1.45	1.38
2	F	302	FAD	O4B-C1B	3.45	1.45	1.41
3	L	301	0VJ	C16-C15	3.45	1.45	1.38
2	P	301	FAD	C5'-C4'	3.44	1.56	1.51
2	A	302	FAD	O4B-C1B	3.43	1.45	1.41
2	I	301	FAD	O4B-C1B	3.43	1.45	1.41
2	I	302	FAD	O4B-C1B	3.43	1.45	1.41
2	P	301	FAD	O4B-C1B	3.43	1.45	1.41
2	I	302	FAD	C5'-C4'	3.42	1.56	1.51
2	E	301	FAD	C5'-C4'	3.42	1.56	1.51
3	G	301	0VJ	C08-C07	3.41	1.54	1.46
2	A	301	FAD	O4B-C1B	3.41	1.45	1.41
2	E	301	FAD	O4B-C1B	3.38	1.45	1.41
3	E	302	0VJ	C05-C10	3.37	1.54	1.48
2	M	301	FAD	O4B-C1B	3.37	1.45	1.41
3	M	303	0VJ	C14-C15	3.37	1.45	1.38
3	J	302	0VJ	C11-C12	-3.36	1.46	1.51
2	C	301	FAD	C2A-N1A	3.36	1.40	1.33
3	K	301	0VJ	O-C08	3.36	1.45	1.33
3	H	301	0VJ	O02-C10	3.33	1.30	1.23
2	H	302	FAD	C4X-C10	3.31	1.54	1.44
2	B	301	FAD	C10-N10	3.31	1.44	1.37
3	A	303	0VJ	O02-C10	3.31	1.30	1.23
3	B	303	0VJ	C17-C16	3.30	1.44	1.38
2	F	301	FAD	O4B-C1B	3.30	1.45	1.41
3	H	301	0VJ	C14-C15	3.30	1.45	1.38
3	P	302	0VJ	C08-C07	3.30	1.54	1.46
3	E	302	0VJ	O03-C07	-3.30	1.16	1.23
3	J	302	0VJ	C11-C09	3.28	1.55	1.51
2	J	301	FAD	C9-C9A	3.24	1.44	1.39
2	C	301	FAD	C2A-N3A	3.24	1.37	1.32
3	B	303	0VJ	C14-C15	3.23	1.45	1.38
2	E	301	FAD	C10-N10	3.22	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	301	FAD	C10-N10	3.21	1.44	1.37
3	I	304	0VJ	C14-C13	3.20	1.44	1.38
2	I	301	FAD	C10-N10	3.20	1.44	1.37
3	K	301	0VJ	C08-C07	3.20	1.54	1.46
2	A	301	FAD	C10-N10	3.19	1.44	1.37
2	M	301	FAD	C10-N10	3.18	1.44	1.37
2	F	302	FAD	C10-N10	3.18	1.44	1.37
2	O	302	FAD	C4'-C3'	3.18	1.59	1.53
2	I	302	FAD	C10-N10	3.17	1.44	1.37
2	A	302	FAD	C10-N10	3.16	1.44	1.37
3	L	301	0VJ	O-C08	3.15	1.44	1.33
2	H	302	FAD	C6-C7	3.12	1.44	1.39
2	F	301	FAD	C8A-N7A	-3.10	1.29	1.34
3	J	302	0VJ	C05-C10	3.10	1.54	1.48
3	P	302	0VJ	O-C08	3.09	1.44	1.33
3	A	305	0VJ	C05-C10	3.09	1.54	1.48
2	C	301	FAD	C9-C9A	3.07	1.44	1.39
3	B	303	0VJ	C11-C09	3.03	1.55	1.51
3	A	305	0VJ	C16-C15	3.00	1.44	1.38
2	C	301	FAD	O4B-C1B	3.00	1.45	1.41
3	M	303	0VJ	O03-C07	-3.00	1.16	1.23
3	F	304	0VJ	C14-C15	2.93	1.44	1.38
2	J	301	FAD	C4X-C10	2.92	1.52	1.44
2	C	301	FAD	C4X-C4	2.91	1.55	1.44
2	O	302	FAD	C2'-C3'	2.87	1.58	1.53
2	F	301	FAD	C5A-C4A	-2.87	1.33	1.40
2	J	301	FAD	C8-C7	2.85	1.48	1.40
2	J	301	FAD	C1'-C2'	2.85	1.56	1.52
3	G	301	0VJ	O03-C07	-2.85	1.17	1.23
3	L	301	0VJ	C05-C04	2.84	1.45	1.40
3	A	305	0VJ	C14-C13	2.83	1.43	1.38
3	E	302	0VJ	C14-C15	2.83	1.44	1.38
2	E	301	FAD	C7M-C7	2.82	1.56	1.51
2	I	301	FAD	C7M-C7	2.82	1.56	1.51
2	A	302	FAD	C7M-C7	2.81	1.56	1.51
2	A	301	FAD	C7M-C7	2.80	1.56	1.51
2	F	301	FAD	C2'-C3'	2.80	1.58	1.53
3	L	301	0VJ	O02-C10	2.80	1.29	1.23
3	H	301	0VJ	O-C08	2.79	1.43	1.33
2	P	301	FAD	C7M-C7	2.79	1.56	1.51
2	F	302	FAD	C7M-C7	2.78	1.56	1.51
2	I	302	FAD	C7M-C7	2.78	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	301	FAD	O4'-C4'	2.78	1.49	1.43
2	H	302	FAD	C1'-C2'	2.77	1.56	1.52
2	M	301	FAD	C7M-C7	2.76	1.56	1.51
3	G	301	0VJ	C09-C10	2.76	1.54	1.47
2	K	302	FAD	C2A-N3A	2.75	1.36	1.32
2	J	301	FAD	C4X-C4	2.74	1.54	1.44
2	O	302	FAD	O3'-C3'	2.73	1.49	1.43
2	N	301	FAD	C4X-C4	2.73	1.54	1.44
2	N	301	FAD	O4B-C4B	2.73	1.51	1.45
3	A	303	0VJ	C09-C10	2.73	1.54	1.47
3	A	305	0VJ	C08-C07	2.71	1.53	1.46
3	F	304	0VJ	O02-C10	2.70	1.29	1.23
3	H	301	0VJ	C05-C10	2.69	1.53	1.48
2	I	302	FAD	C6-C7	2.69	1.43	1.39
2	N	301	FAD	C9-C9A	2.69	1.44	1.39
2	F	302	FAD	C6-C7	2.69	1.43	1.39
2	P	301	FAD	C6-C7	2.68	1.43	1.39
3	A	303	0VJ	C14-C13	2.67	1.43	1.38
2	A	302	FAD	C6-C7	2.67	1.43	1.39
2	I	302	FAD	O4-C4	2.66	1.28	1.23
3	J	302	0VJ	O02-C10	2.66	1.28	1.23
2	A	301	FAD	C6-C7	2.66	1.43	1.39
2	N	301	FAD	C5X-N5	2.66	1.44	1.39
2	N	301	FAD	C4X-C10	2.66	1.52	1.44
2	N	301	FAD	O4-C4	2.66	1.28	1.23
2	P	301	FAD	O4-C4	2.64	1.28	1.23
3	B	303	0VJ	O-C08	2.64	1.42	1.33
2	I	301	FAD	C6-C7	2.64	1.43	1.39
2	A	301	FAD	O4-C4	2.63	1.28	1.23
3	A	303	0VJ	C08-C07	2.63	1.52	1.46
2	E	301	FAD	C6-C7	2.63	1.43	1.39
2	A	302	FAD	O4-C4	2.62	1.28	1.23
2	M	301	FAD	C6-C7	2.62	1.43	1.39
2	B	301	FAD	C6-C7	2.62	1.43	1.39
2	F	302	FAD	O4-C4	2.61	1.28	1.23
3	J	302	0VJ	C05-C04	2.61	1.45	1.40
3	M	303	0VJ	C16-C15	2.61	1.43	1.38
2	E	301	FAD	O4-C4	2.61	1.28	1.23
2	M	301	FAD	O4-C4	2.61	1.28	1.23
3	L	301	0VJ	C05-C10	2.61	1.53	1.48
2	I	301	FAD	O4-C4	2.60	1.28	1.23
2	O	302	FAD	C2A-N3A	2.60	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	302	FAD	C4X-C10	2.60	1.51	1.44
3	K	301	0VJ	C14-C15	2.59	1.43	1.38
3	E	302	0VJ	C05-C04	2.59	1.45	1.40
2	P	301	FAD	C4X-C10	2.59	1.51	1.44
3	P	302	0VJ	C16-C15	2.58	1.43	1.38
2	I	301	FAD	C4X-C10	2.58	1.51	1.44
2	A	302	FAD	C4X-C10	2.58	1.51	1.44
2	J	301	FAD	C9-C8	2.58	1.43	1.39
3	H	301	0VJ	O03-C07	-2.58	1.17	1.23
2	E	301	FAD	O2'-C2'	2.58	1.48	1.43
2	A	302	FAD	O2'-C2'	2.58	1.48	1.43
2	M	301	FAD	O2'-C2'	2.57	1.48	1.43
2	A	301	FAD	C4X-C10	2.57	1.51	1.44
2	E	301	FAD	C4X-C10	2.57	1.51	1.44
3	E	302	0VJ	O-C08	2.57	1.42	1.33
2	I	302	FAD	C4X-C10	2.56	1.51	1.44
2	K	302	FAD	C1'-C2'	2.56	1.56	1.52
3	I	304	0VJ	C08-C07	2.56	1.52	1.46
2	A	301	FAD	O2'-C2'	2.55	1.48	1.43
2	H	302	FAD	C2A-N1A	2.55	1.38	1.33
2	M	301	FAD	C4X-C10	2.55	1.51	1.44
2	I	301	FAD	O2'-C2'	2.55	1.48	1.43
3	L	301	0VJ	C08-C07	2.55	1.52	1.46
2	P	301	FAD	O2'-C2'	2.55	1.48	1.43
2	M	301	FAD	C4X-C4	2.55	1.53	1.44
2	I	301	FAD	C4X-C4	2.54	1.53	1.44
2	P	301	FAD	C4X-C4	2.54	1.53	1.44
2	F	302	FAD	O2'-C2'	2.54	1.48	1.43
2	E	301	FAD	C4X-C4	2.54	1.53	1.44
2	A	301	FAD	C4X-C4	2.54	1.53	1.44
2	A	302	FAD	C4X-C4	2.54	1.53	1.44
2	I	302	FAD	C4X-C4	2.54	1.53	1.44
2	I	302	FAD	O2'-C2'	2.53	1.48	1.43
3	I	304	0VJ	O-C08	2.52	1.42	1.33
2	F	302	FAD	C4X-C4	2.52	1.53	1.44
3	K	301	0VJ	O02-C10	2.51	1.28	1.23
2	K	302	FAD	C4-N3	2.50	1.43	1.38
2	C	301	FAD	C6-C7	2.49	1.43	1.39
2	F	301	FAD	C4-N3	-2.49	1.34	1.38
3	M	303	0VJ	C05-C10	2.48	1.52	1.48
3	A	303	0VJ	C11-C09	2.48	1.54	1.51
3	A	303	0VJ	C16-C15	2.47	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	301	0VJ	C08-C09	2.47	1.40	1.36
3	O	301	0VJ	C14-C15	2.46	1.43	1.38
3	J	302	0VJ	C08-C07	2.43	1.52	1.46
2	F	301	FAD	C5X-N5	2.43	1.44	1.39
2	F	301	FAD	C4X-C10	2.42	1.51	1.44
3	N	302	0VJ	C09-C10	2.41	1.53	1.47
3	K	301	0VJ	C05-C10	2.40	1.52	1.48
3	N	302	0VJ	C05-C10	2.39	1.52	1.48
3	A	305	0VJ	C11-C09	2.38	1.54	1.51
2	O	302	FAD	C4X-C10	2.36	1.51	1.44
2	N	301	FAD	O3B-C3B	2.35	1.48	1.43
2	C	301	FAD	C2B-C1B	-2.34	1.50	1.53
3	F	304	0VJ	O03-C07	-2.34	1.18	1.23
2	B	301	FAD	O4'-C4'	2.33	1.48	1.43
3	O	301	0VJ	C05-C04	2.33	1.44	1.40
3	K	301	0VJ	C13-C12	-2.33	1.33	1.38
2	C	301	FAD	C4A-N3A	2.32	1.38	1.35
2	H	302	FAD	C8A-N7A	-2.29	1.30	1.34
2	N	301	FAD	C6-C5X	2.29	1.43	1.40
2	O	302	FAD	C10-N10	2.27	1.42	1.37
2	H	302	FAD	C5X-N5	-2.27	1.35	1.39
3	E	302	0VJ	C16-C15	2.26	1.43	1.38
3	M	303	0VJ	O02-C10	2.25	1.28	1.23
3	P	302	0VJ	O03-C07	-2.24	1.18	1.23
3	N	302	0VJ	C08-C09	2.23	1.40	1.36
2	F	301	FAD	C10-N1	-2.23	1.28	1.33
2	F	301	FAD	C4X-C4	2.22	1.52	1.44
2	C	301	FAD	C5X-N5	2.21	1.43	1.39
2	H	302	FAD	C10-N10	2.21	1.42	1.37
2	F	301	FAD	PA-O2A	-2.21	1.44	1.55
3	P	302	0VJ	C08-C09	2.20	1.40	1.36
2	F	301	FAD	C6A-N6A	2.19	1.42	1.34
2	B	301	FAD	C4X-C4	2.18	1.52	1.44
2	K	302	FAD	O3'-C3'	2.17	1.48	1.43
2	K	302	FAD	C4'-C3'	2.16	1.57	1.53
3	B	303	0VJ	O02-C10	2.15	1.27	1.23
2	B	301	FAD	C5X-N5	2.13	1.43	1.39
3	D	301	0VJ	C13-C12	-2.13	1.34	1.38
3	I	304	0VJ	C11-C09	2.12	1.54	1.51
3	H	301	0VJ	C08-C09	2.12	1.39	1.36
2	J	301	FAD	C4'-C3'	2.10	1.57	1.53
3	E	302	0VJ	O02-C10	2.10	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	FAD	C8-C7	2.10	1.46	1.40
2	M	301	FAD	C8-C7	2.10	1.46	1.40
3	M	303	0VJ	C05-C04	2.10	1.44	1.40
2	J	301	FAD	O3'-C3'	2.09	1.47	1.43
3	P	302	0VJ	C05-C04	2.09	1.44	1.40
2	K	302	FAD	C4X-C4	2.09	1.52	1.44
2	K	302	FAD	O2-C2	-2.09	1.20	1.24
3	K	301	0VJ	C16-C15	2.08	1.42	1.38
2	A	302	FAD	C8-C7	2.08	1.46	1.40
2	I	301	FAD	C8-C7	2.08	1.46	1.40
2	N	301	FAD	C8-C7	2.08	1.46	1.40
2	A	301	FAD	C8-C7	2.08	1.46	1.40
2	P	301	FAD	C8-C7	2.08	1.46	1.40
2	F	302	FAD	C5X-N5	2.07	1.43	1.39
2	F	302	FAD	C8-C7	2.07	1.46	1.40
2	I	302	FAD	C8-C7	2.07	1.46	1.40
3	B	303	0VJ	C05-C04	2.06	1.44	1.40
2	O	302	FAD	C2A-N1A	2.06	1.37	1.33
2	B	301	FAD	C4A-N3A	2.06	1.38	1.35
2	I	302	FAD	C5X-N5	2.06	1.43	1.39
2	K	302	FAD	C9A-N10	2.05	1.44	1.41
3	D	301	0VJ	C08-C09	2.05	1.39	1.36
2	M	301	FAD	C5X-N5	2.05	1.43	1.39
2	N	301	FAD	C8A-N7A	-2.04	1.31	1.34
2	I	301	FAD	C5X-N5	2.04	1.43	1.39
2	B	301	FAD	C2A-N1A	2.04	1.37	1.33
2	K	302	FAD	O4-C4	2.04	1.27	1.23
2	A	301	FAD	C5X-N5	2.04	1.43	1.39
2	K	302	FAD	C2'-C3'	2.04	1.57	1.53
2	A	302	FAD	C5X-N5	2.04	1.43	1.39
2	N	301	FAD	C9A-C5X	2.04	1.44	1.41
2	P	301	FAD	C5X-N5	2.03	1.43	1.39
3	G	301	0VJ	C14-C15	2.03	1.42	1.38
2	B	301	FAD	C8A-N7A	-2.02	1.31	1.34
3	I	304	0VJ	C08-C09	2.02	1.39	1.36
2	C	301	FAD	C5'-C4'	2.02	1.54	1.51
2	A	302	FAD	C4-N3	2.01	1.42	1.38
2	E	301	FAD	C4-N3	2.01	1.42	1.38
2	E	301	FAD	C5X-N5	2.01	1.43	1.39
2	J	301	FAD	C5X-N5	2.00	1.43	1.39

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	301	0VJ	C11-C12-C13	-12.77	102.61	120.89
3	I	304	0VJ	C11-C12-C13	-12.71	102.69	120.89
3	J	302	0VJ	C11-C12-C13	-12.49	103.02	120.89
3	B	303	0VJ	C11-C12-C13	-12.45	103.07	120.89
3	A	303	0VJ	C11-C12-C13	-12.18	103.46	120.89
3	D	301	0VJ	C11-C12-C13	-11.90	103.86	120.89
3	A	305	0VJ	C11-C12-C13	-11.86	103.92	120.89
3	K	301	0VJ	C11-C12-C13	-11.81	103.99	120.89
3	M	303	0VJ	C11-C12-C13	-11.61	104.27	120.89
3	F	304	0VJ	C11-C12-C13	-11.45	104.50	120.89
3	N	302	0VJ	C11-C12-C13	-11.43	104.54	120.89
3	J	302	0VJ	C11-C12-C17	11.23	136.97	120.89
3	O	301	0VJ	C11-C12-C17	11.04	136.69	120.89
3	G	301	0VJ	C11-C12-C13	-10.69	105.58	120.89
3	P	302	0VJ	C11-C12-C13	-10.41	105.99	120.89
3	D	301	0VJ	C11-C12-C17	10.41	135.79	120.89
3	A	303	0VJ	C11-C12-C17	10.36	135.72	120.89
3	I	304	0VJ	C11-C12-C17	10.15	135.43	120.89
3	N	302	0VJ	C11-C12-C17	10.06	135.29	120.89
3	B	303	0VJ	C11-C12-C17	10.05	135.27	120.89
3	K	301	0VJ	C11-C12-C17	10.02	135.23	120.89
3	G	301	0VJ	C11-C12-C17	9.99	135.20	120.89
3	H	301	0VJ	C11-C12-C13	-9.93	106.68	120.89
3	L	301	0VJ	C11-C12-C13	-9.68	107.04	120.89
3	M	303	0VJ	C11-C12-C17	9.55	134.56	120.89
3	F	304	0VJ	C11-C12-C17	9.53	134.53	120.89
3	P	302	0VJ	C11-C12-C17	9.50	134.49	120.89
3	E	302	0VJ	C11-C12-C13	-9.14	107.81	120.89
3	L	301	0VJ	C11-C12-C17	9.11	133.93	120.89
3	H	301	0VJ	C11-C12-C17	8.56	133.14	120.89
3	A	305	0VJ	C11-C12-C17	8.26	132.72	120.89
3	E	302	0VJ	C11-C12-C17	7.65	131.84	120.89
2	E	301	FAD	O2'-C2'-C1'	6.93	126.56	109.80
2	I	301	FAD	O2'-C2'-C1'	6.93	126.56	109.80
2	A	301	FAD	O2'-C2'-C1'	6.93	126.55	109.80
2	M	301	FAD	O2'-C2'-C1'	6.93	126.55	109.80
2	I	302	FAD	O2'-C2'-C1'	6.92	126.52	109.80
2	P	301	FAD	O2'-C2'-C1'	6.91	126.51	109.80
2	A	302	FAD	O2'-C2'-C1'	6.91	126.50	109.80
2	F	302	FAD	O2'-C2'-C1'	6.90	126.49	109.80
3	B	303	0VJ	C12-C11-C09	-6.38	102.38	114.32
2	N	301	FAD	O4B-C1B-C2B	-6.25	97.80	106.93
3	F	304	0VJ	C12-C11-C09	-5.90	103.27	114.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	301	0VJ	C03-C04-C05	5.82	125.74	119.26
3	P	302	0VJ	C03-C04-C05	5.60	125.49	119.26
3	A	303	0VJ	C12-C11-C09	-5.50	104.02	114.32
3	B	303	0VJ	O-C08-C07	5.23	126.42	116.87
3	L	301	0VJ	C03-C04-C05	5.17	125.01	119.26
3	O	301	0VJ	C03-C04-C05	5.16	125.00	119.26
3	G	301	0VJ	C12-C11-C09	-5.03	104.89	114.32
2	J	301	FAD	C3B-C2B-C1B	4.98	108.47	100.98
2	O	302	FAD	O2'-C2'-C3'	4.77	120.70	109.10
3	A	303	0VJ	C13-C14-C15	4.77	125.57	119.73
2	C	301	FAD	C10-N1-C2	4.74	126.38	116.90
3	J	302	0VJ	C13-C14-C15	4.68	125.45	119.73
3	J	302	0VJ	C03-C04-C05	4.60	124.38	119.26
3	E	302	0VJ	C03-C04-C05	4.57	124.35	119.26
3	N	302	0VJ	C-O01-C15	4.55	127.38	117.51
3	K	301	0VJ	C05-C04-C07	-4.53	115.78	120.68
3	O	301	0VJ	C05-C04-C07	-4.44	115.87	120.68
2	J	301	FAD	C5'-C4'-C3'	-4.41	103.69	112.20
3	A	305	0VJ	C05-C04-C07	-4.35	115.98	120.68
3	M	303	0VJ	C03-C04-C05	4.34	124.08	119.26
3	E	302	0VJ	C05-C04-C07	-4.33	116.00	120.68
3	F	304	0VJ	O-C08-C07	4.29	124.70	116.87
3	D	301	0VJ	C12-C11-C09	-4.26	106.33	114.32
2	K	302	FAD	O4-C4-N3	4.23	128.23	120.12
3	L	301	0VJ	C-O01-C15	4.17	126.55	117.51
3	A	305	0VJ	C12-C11-C09	-4.09	106.66	114.32
3	H	301	0VJ	C12-C11-C09	-4.07	106.69	114.32
3	J	302	0VJ	C-O01-C15	4.06	126.33	117.51
3	N	302	0VJ	C03-C04-C05	4.05	123.76	119.26
3	N	302	0VJ	O-C08-C07	4.04	124.26	116.87
3	E	302	0VJ	O-C08-C07	4.04	124.25	116.87
3	G	301	0VJ	C-O01-C15	4.01	126.21	117.51
3	A	305	0VJ	C03-C04-C05	4.00	123.71	119.26
3	G	301	0VJ	C13-C14-C15	3.94	124.55	119.73
3	N	302	0VJ	C13-C14-C15	3.88	124.48	119.73
2	N	301	FAD	C10-N1-C2	3.88	124.67	116.90
3	M	303	0VJ	O-C08-C07	3.88	123.95	116.87
3	O	301	0VJ	C13-C14-C15	3.85	124.45	119.73
3	I	304	0VJ	C03-C04-C05	3.83	123.52	119.26
2	C	301	FAD	C4-C4X-N5	3.79	123.62	118.23
2	B	301	FAD	O2B-C2B-C3B	3.71	123.83	111.82
3	E	302	0VJ	C12-C11-C09	-3.71	107.37	114.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	304	0VJ	C-O01-C15	3.69	125.52	117.51
2	M	301	FAD	C10-N1-C2	3.66	124.23	116.90
2	P	301	FAD	C10-N1-C2	3.66	124.21	116.90
2	F	302	FAD	C10-N1-C2	3.65	124.21	116.90
2	I	301	FAD	C10-N1-C2	3.65	124.21	116.90
2	A	301	FAD	C10-N1-C2	3.65	124.20	116.90
2	A	302	FAD	C10-N1-C2	3.65	124.19	116.90
3	K	301	0VJ	O02-C10-C05	3.63	127.45	121.56
2	E	301	FAD	C10-N1-C2	3.63	124.15	116.90
2	I	302	FAD	C10-N1-C2	3.62	124.15	116.90
3	K	301	0VJ	O02-C10-C09	-3.61	114.76	120.56
3	H	301	0VJ	C03-C04-C05	3.60	123.27	119.26
3	B	303	0VJ	O-C08-C09	-3.60	114.65	120.96
3	O	301	0VJ	O-C08-C07	3.60	123.44	116.87
3	N	302	0VJ	O03-C07-C04	-3.59	115.75	121.56
3	B	303	0VJ	C03-C04-C05	3.56	123.22	119.26
3	K	301	0VJ	C13-C14-C15	3.56	124.08	119.73
3	A	305	0VJ	C13-C14-C15	3.55	124.08	119.73
3	D	301	0VJ	C05-C04-C07	-3.55	116.84	120.68
3	J	302	0VJ	C05-C04-C07	-3.55	116.84	120.68
3	G	301	0VJ	C03-C04-C05	3.54	123.20	119.26
3	I	304	0VJ	C06-C05-C10	-3.51	114.96	120.10
3	M	303	0VJ	C13-C14-C15	3.48	123.99	119.73
3	L	301	0VJ	C04-C05-C10	3.47	124.43	120.68
2	J	301	FAD	C10-N1-C2	3.47	123.84	116.90
2	H	302	FAD	C6-C5X-C9A	3.45	123.82	118.94
3	B	303	0VJ	C06-C05-C10	-3.45	115.04	120.10
2	P	301	FAD	O4-C4-N3	3.45	126.73	120.12
2	I	302	FAD	O4-C4-N3	3.45	126.72	120.12
2	I	301	FAD	O4-C4-N3	3.44	126.72	120.12
2	E	301	FAD	O4-C4-N3	3.44	126.72	120.12
3	K	301	0VJ	C12-C11-C09	-3.44	107.89	114.32
2	A	301	FAD	O4-C4-N3	3.43	126.69	120.12
2	M	301	FAD	O4-C4-N3	3.43	126.69	120.12
2	A	302	FAD	O4-C4-N3	3.42	126.67	120.12
2	F	302	FAD	O4-C4-N3	3.42	126.67	120.12
3	P	302	0VJ	C17-C16-C15	-3.41	115.56	119.73
3	O	301	0VJ	C12-C11-C09	-3.39	107.97	114.32
3	B	303	0VJ	O03-C07-C08	3.36	127.02	119.59
3	K	301	0VJ	O-C08-C07	3.34	122.98	116.87
3	H	301	0VJ	C04-C05-C10	3.34	124.29	120.68
2	B	301	FAD	C4A-C5A-N7A	3.33	112.87	109.40

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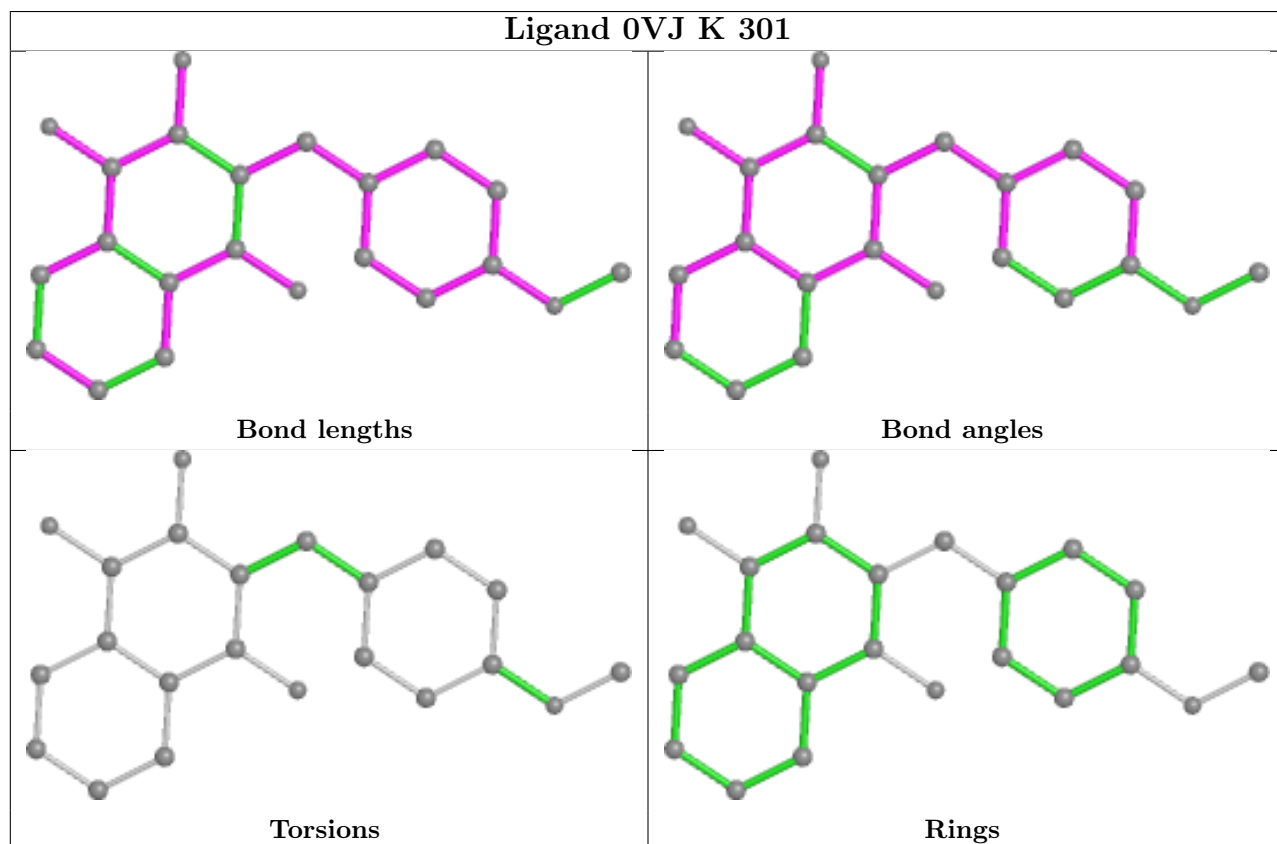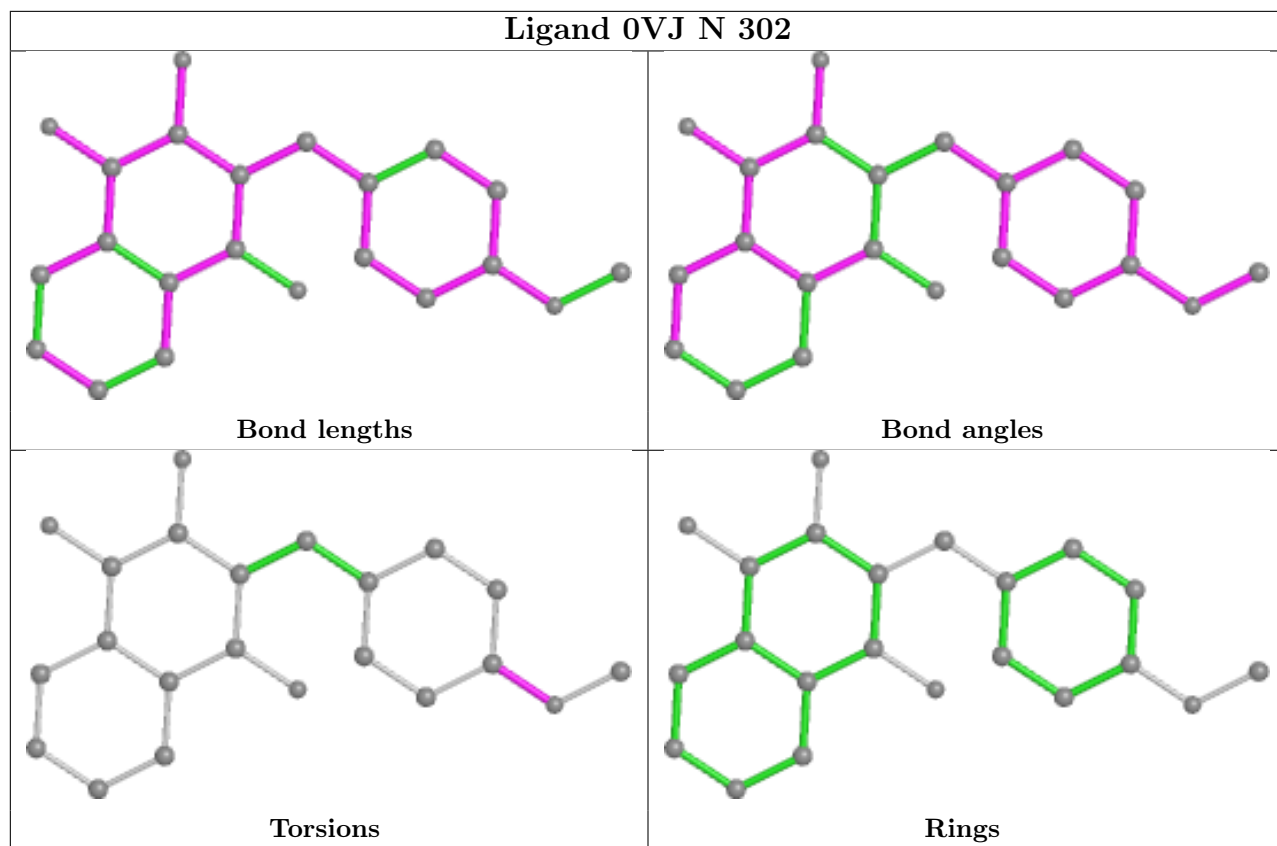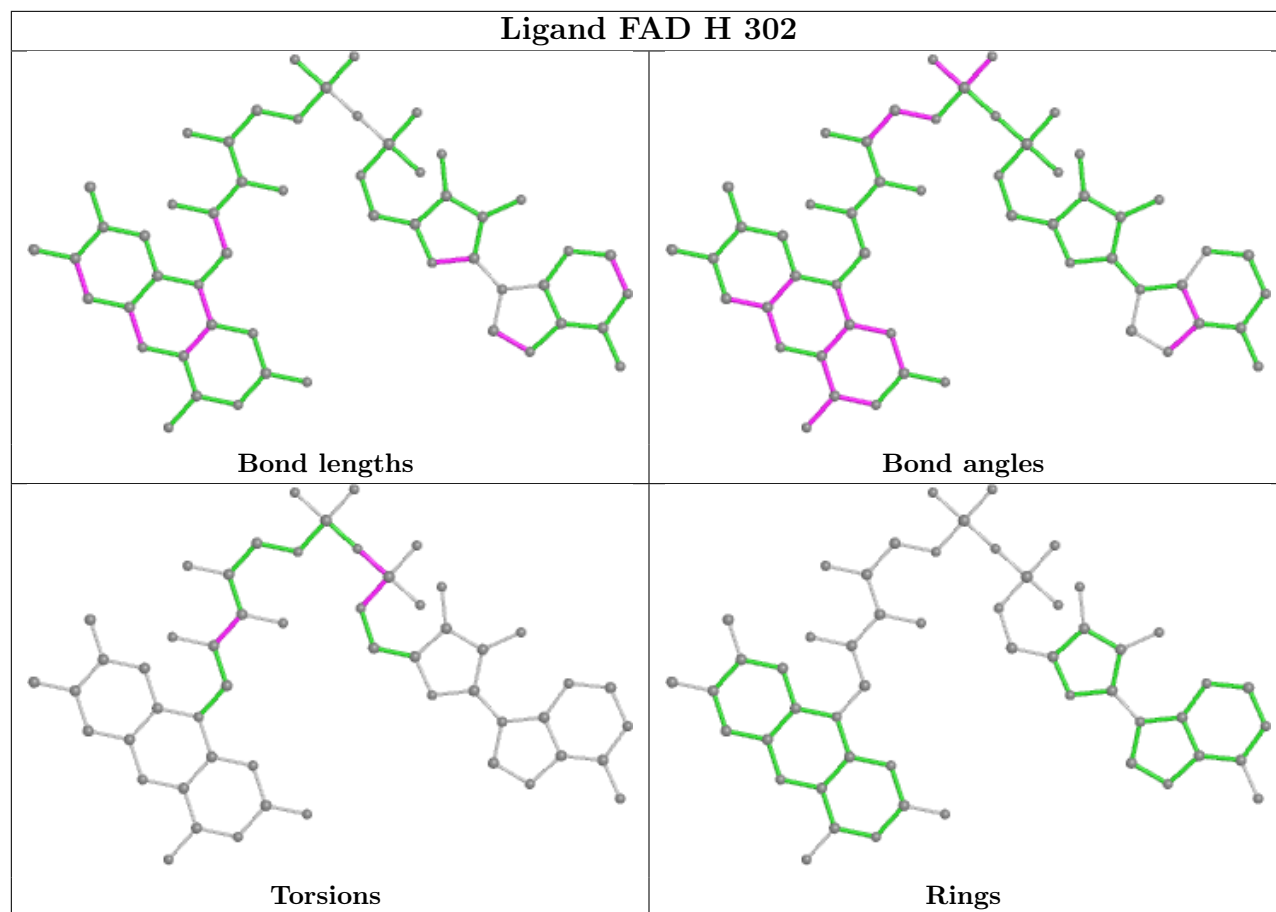| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	FAD	C3B-C2B-C1B	-3.32	95.97	100.98
3	P	302	0VJ	C05-C04-C07	-3.32	117.09	120.68
3	P	302	0VJ	C04-C05-C10	3.31	124.26	120.68
3	A	305	0VJ	C17-C12-C13	3.31	123.36	118.17
3	B	303	0VJ	C05-C04-C07	-3.30	117.11	120.68
3	L	301	0VJ	C02-C03-C04	-3.29	113.59	119.81
3	M	303	0VJ	C05-C04-C07	-3.29	117.12	120.68
3	I	304	0VJ	C-O01-C15	3.27	124.60	117.51
2	B	301	FAD	O2P-P-O5'	-3.24	92.69	107.75
3	D	301	0VJ	C13-C14-C15	3.24	123.69	119.73
3	D	301	0VJ	C03-C04-C05	3.24	122.86	119.26
2	F	301	FAD	C4X-C10-N1	-3.23	117.24	124.73
3	A	305	0VJ	C14-C13-C12	-3.22	116.60	121.03
3	I	304	0VJ	C16-C17-C12	-3.21	116.61	121.03
2	C	301	FAD	N3A-C2A-N1A	-3.20	123.67	128.68
3	O	301	0VJ	O03-C07-C04	-3.20	116.38	121.56
3	B	303	0VJ	C11-C09-C10	-3.19	112.13	117.12
2	J	301	FAD	O4B-C1B-C2B	-3.19	102.27	106.93
3	P	302	0VJ	C06-C05-C10	-3.17	115.45	120.10
3	B	303	0VJ	C-O01-C15	3.16	124.36	117.51
2	C	301	FAD	O2-C2-N3	3.14	124.74	118.65
2	H	302	FAD	O4-C4-N3	3.13	126.13	120.12
2	K	302	FAD	O4-C4-C4X	-3.12	118.31	126.60
2	N	301	FAD	C5'-C4'-C3'	-3.12	106.18	112.20
3	I	304	0VJ	C12-C11-C09	-3.12	108.49	114.32
3	L	301	0VJ	O02-C10-C05	3.11	126.61	121.56
3	O	301	0VJ	C02-C03-C04	-3.10	113.96	119.81
3	B	303	0VJ	C02-C03-C04	-3.09	113.97	119.81
3	B	303	0VJ	C13-C14-C15	3.07	123.48	119.73
3	B	303	0VJ	O03-C07-C04	-3.06	116.61	121.56
2	C	301	FAD	O2-C2-N1	-3.06	116.76	121.83
3	F	304	0VJ	C04-C05-C10	3.05	123.98	120.68
3	M	303	0VJ	C-O01-C15	3.04	124.10	117.51
2	O	302	FAD	C9-C9A-N10	3.03	125.94	121.84
3	J	302	0VJ	O02-C10-C05	3.03	126.46	121.56
3	M	303	0VJ	C02-C03-C04	-3.02	114.10	119.81
2	B	301	FAD	O3B-C3B-C4B	-3.02	102.32	111.05
3	P	302	0VJ	C02-C03-C04	-3.02	114.11	119.81
3	N	302	0VJ	C05-C04-C07	-3.02	117.42	120.68
3	G	301	0VJ	C05-C04-C07	-3.01	117.42	120.68
3	M	303	0VJ	O03-C07-C04	-3.01	116.69	121.56
2	O	302	FAD	O4-C4-N3	3.00	125.87	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	301	FAD	C4-C4X-N5	2.99	122.48	118.23
2	F	301	FAD	C10-N1-C2	2.99	122.87	116.90
2	F	301	FAD	C8M-C8-C9	-2.98	113.97	119.49
3	A	303	0VJ	C03-C04-C05	2.97	122.56	119.26
2	F	302	FAD	C5'-C4'-C3'	-2.96	106.49	112.20
2	N	301	FAD	C4'-C3'-C2'	-2.95	107.22	113.36
2	A	302	FAD	C5'-C4'-C3'	-2.95	106.51	112.20
2	M	301	FAD	C5'-C4'-C3'	-2.94	106.52	112.20
3	H	301	0VJ	C-O01-C15	2.94	123.90	117.51
2	I	301	FAD	C5'-C4'-C3'	-2.94	106.52	112.20
2	I	302	FAD	C5'-C4'-C3'	-2.94	106.52	112.20
2	A	301	FAD	C5'-C4'-C3'	-2.94	106.53	112.20
3	L	301	0VJ	C06-C05-C10	-2.93	115.80	120.10
2	P	301	FAD	C5'-C4'-C3'	-2.93	106.54	112.20
2	E	301	FAD	C5'-C4'-C3'	-2.93	106.54	112.20
3	B	303	0VJ	C04-C05-C10	2.92	123.84	120.68
2	N	301	FAD	O4'-C4'-C5'	2.92	116.48	109.92
2	H	302	FAD	C6-C5X-N5	-2.90	113.46	118.51
2	B	301	FAD	C10-N1-C2	2.88	122.66	116.90
2	B	301	FAD	C4X-C10-N1	-2.87	118.07	124.73
3	G	301	0VJ	C04-C05-C10	2.87	123.78	120.68
3	F	304	0VJ	C06-C05-C10	-2.87	115.90	120.10
3	A	305	0VJ	C04-C07-C08	2.86	121.53	117.06
2	J	301	FAD	C8M-C8-C7	2.86	126.59	120.74
2	O	302	FAD	O4B-C1B-C2B	-2.85	102.76	106.93
3	I	304	0VJ	C02-C03-C04	-2.83	114.47	119.81
3	E	302	0VJ	O-C08-C09	-2.82	116.02	120.96
3	F	304	0VJ	O03-C07-C04	-2.80	117.02	121.56
2	A	302	FAD	N3A-C2A-N1A	-2.80	124.31	128.68
2	I	301	FAD	N3A-C2A-N1A	-2.79	124.32	128.68
2	P	301	FAD	O4-C4-C4X	-2.78	119.23	126.60
2	J	301	FAD	O2'-C2'-C3'	2.77	115.85	109.10
3	I	304	0VJ	C04-C05-C10	2.77	123.68	120.68
2	I	302	FAD	O4-C4-C4X	-2.77	119.25	126.60
2	K	302	FAD	O2'-C2'-C3'	2.77	115.83	109.10
2	E	301	FAD	O4-C4-C4X	-2.76	119.27	126.60
2	F	302	FAD	N3A-C2A-N1A	-2.76	124.36	128.68
2	A	301	FAD	O4-C4-C4X	-2.76	119.27	126.60
2	I	301	FAD	O4-C4-C4X	-2.76	119.27	126.60
2	M	301	FAD	O4-C4-C4X	-2.76	119.28	126.60
2	A	302	FAD	O4-C4-C4X	-2.76	119.29	126.60
2	F	302	FAD	O4-C4-C4X	-2.76	119.29	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	302	FAD	N3A-C2A-N1A	-2.76	124.37	128.68
3	A	303	0VJ	O-C08-C07	2.75	121.90	116.87
2	O	302	FAD	O4'-C4'-C3'	2.75	115.79	109.10
2	A	301	FAD	N3A-C2A-N1A	-2.75	124.38	128.68
2	P	301	FAD	N3A-C2A-N1A	-2.75	124.38	128.68
2	C	301	FAD	O4'-C4'-C3'	-2.75	102.42	109.10
2	E	301	FAD	N3A-C2A-N1A	-2.74	124.40	128.68
2	N	301	FAD	C2B-C3B-C4B	-2.73	97.33	102.64
2	M	301	FAD	N3A-C2A-N1A	-2.73	124.41	128.68
3	G	301	0VJ	O-C08-C07	2.73	121.86	116.87
3	D	301	0VJ	C04-C07-C08	2.73	121.33	117.06
3	H	301	0VJ	C06-C05-C10	-2.71	116.12	120.10
3	L	301	0VJ	C12-C11-C09	-2.71	109.25	114.32
2	O	302	FAD	C10-N1-C2	2.70	122.30	116.90
3	F	304	0VJ	C13-C14-C15	2.68	123.01	119.73
2	H	302	FAD	N10-C10-N1	2.66	125.99	118.35
2	N	301	FAD	C2A-N1A-C6A	-2.65	114.22	118.75
3	A	305	0VJ	O-C08-C07	2.65	121.72	116.87
3	A	305	0VJ	C17-C16-C15	-2.65	116.49	119.73
3	D	301	0VJ	O03-C07-C04	-2.64	117.30	121.56
2	N	301	FAD	C4-C4X-N5	2.63	121.98	118.23
3	A	303	0VJ	C-O01-C15	2.62	123.20	117.51
3	O	301	0VJ	C-O01-C15	2.62	123.20	117.51
2	C	301	FAD	C4X-C10-N10	2.62	120.31	116.48
2	O	302	FAD	O2A-PA-O1A	2.62	125.19	112.24
2	H	302	FAD	O4-C4-C4X	-2.62	119.66	126.60
3	O	301	0VJ	C06-C05-C10	-2.62	116.27	120.10
2	F	301	FAD	C8M-C8-C7	2.61	126.08	120.74
2	F	301	FAD	C9A-C5X-N5	-2.59	119.61	122.43
3	K	301	0VJ	O03-C07-C04	-2.59	117.37	121.56
3	F	304	0VJ	C03-C04-C05	2.58	122.13	119.26
2	O	302	FAD	C6-C5X-C9A	2.57	122.58	118.94
2	C	301	FAD	C4X-C10-N1	-2.57	118.77	124.73
3	D	301	0VJ	C-O01-C15	2.56	123.07	117.51
2	H	302	FAD	C10-N1-C2	2.56	122.02	116.90
3	N	302	0VJ	C04-C07-C08	2.56	121.06	117.06
2	O	302	FAD	C4X-C10-N1	-2.55	118.81	124.73
2	A	302	FAD	C4A-C5A-N7A	2.55	112.06	109.40
2	F	301	FAD	C6-C5X-C9A	2.55	122.55	118.94
2	M	301	FAD	C4A-C5A-N7A	2.54	112.05	109.40
2	I	302	FAD	C4A-C5A-N7A	2.54	112.05	109.40
2	F	302	FAD	C4A-C5A-N7A	2.54	112.04	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	304	0VJ	C05-C04-C07	-2.54	117.94	120.68
2	P	301	FAD	C4A-C5A-N7A	2.53	112.03	109.40
2	I	301	FAD	C4A-C5A-N7A	2.52	112.03	109.40
2	N	301	FAD	P-O3P-PA	2.52	141.48	132.83
3	D	301	0VJ	C04-C05-C10	2.52	123.41	120.68
2	A	301	FAD	C4A-C5A-N7A	2.52	112.02	109.40
3	N	302	0VJ	C02-C03-C04	-2.52	115.05	119.81
2	F	302	FAD	C4X-C10-N1	-2.52	118.89	124.73
2	I	301	FAD	C4X-C10-N1	-2.52	118.89	124.73
2	F	301	FAD	C5A-C6A-N6A	2.52	124.18	120.35
3	H	301	0VJ	C02-C03-C04	-2.51	115.06	119.81
2	I	302	FAD	C4X-C10-N1	-2.51	118.90	124.73
3	J	302	0VJ	C02-C03-C04	-2.51	115.07	119.81
2	M	301	FAD	C4X-C10-N1	-2.51	118.91	124.73
2	A	302	FAD	C4X-C10-N1	-2.51	118.92	124.73
2	B	301	FAD	C9A-C9-C8	2.51	124.34	119.30
2	A	301	FAD	C4X-C10-N1	-2.50	118.92	124.73
3	D	301	0VJ	O-C08-C07	2.50	121.44	116.87
2	H	302	FAD	C4X-C10-N1	-2.50	118.93	124.73
3	A	303	0VJ	C05-C04-C07	-2.50	117.98	120.68
2	E	301	FAD	C4A-C5A-N7A	2.50	112.00	109.40
3	H	301	0VJ	C05-C04-C07	-2.50	117.98	120.68
2	P	301	FAD	C4X-C10-N1	-2.49	118.94	124.73
2	E	301	FAD	C4X-C10-N1	-2.49	118.95	124.73
3	P	302	0VJ	C13-C14-C15	2.49	122.78	119.73
2	O	302	FAD	O5'-P-O1P	2.49	118.80	109.07
3	K	301	0VJ	C02-C03-C04	-2.48	115.13	119.81
2	B	301	FAD	O5'-P-O1P	2.47	118.70	109.07
3	E	302	0VJ	O03-C07-C04	-2.46	117.57	121.56
2	J	301	FAD	O2P-P-O1P	2.46	124.38	112.24
2	N	301	FAD	O2A-PA-O5B	-2.44	96.40	107.75
3	A	303	0VJ	C04-C05-C10	2.44	123.31	120.68
3	B	303	0VJ	C14-C13-C12	-2.43	117.69	121.03
2	N	301	FAD	C1B-N9A-C4A	2.42	130.90	126.64
2	F	301	FAD	O2P-P-O1P	2.42	124.22	112.24
3	B	303	0VJ	O02-C10-C09	-2.42	116.67	120.56
3	B	303	0VJ	C01-C02-C03	2.42	123.87	120.19
3	O	301	0VJ	C04-C07-C08	2.42	120.84	117.06
3	L	301	0VJ	C05-C10-C09	-2.40	114.03	118.42
2	N	301	FAD	O2A-PA-O1A	2.40	124.09	112.24
2	O	302	FAD	N10-C10-N1	2.39	125.22	118.35
2	J	301	FAD	C2A-N1A-C6A	-2.38	114.68	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	304	0VJ	C05-C04-C07	-2.37	118.12	120.68
3	I	304	0VJ	C17-C12-C13	2.36	121.88	118.17
3	K	301	0VJ	C04-C05-C10	2.35	123.22	120.68
2	F	301	FAD	C4A-C5A-N7A	-2.35	106.95	109.40
2	K	302	FAD	C5A-C6A-N6A	2.34	123.91	120.35
2	K	302	FAD	O4'-C4'-C3'	2.34	114.78	109.10
2	H	302	FAD	O5'-C5'-C4'	-2.34	103.12	109.36
3	L	301	0VJ	C01-C02-C03	2.33	123.74	120.19
2	F	301	FAD	N3A-C2A-N1A	-2.32	125.05	128.68
3	I	304	0VJ	O-C08-C07	2.32	121.11	116.87
3	A	303	0VJ	C06-C05-C10	-2.32	116.69	120.10
3	A	305	0VJ	C16-C17-C12	-2.32	117.83	121.03
2	B	301	FAD	N10-C10-N1	2.31	125.00	118.35
3	G	301	0VJ	C06-C05-C10	-2.30	116.72	120.10
3	B	303	0VJ	O02-C10-C05	2.30	125.28	121.56
3	L	301	0VJ	C05-C04-C07	-2.30	118.19	120.68
3	A	305	0VJ	O02-C10-C05	2.29	125.28	121.56
2	N	301	FAD	O4-C4-N3	2.29	124.51	120.12
3	E	302	0VJ	C04-C05-C10	2.29	123.16	120.68
3	E	302	0VJ	C11-C09-C10	2.29	120.69	117.12
3	A	303	0VJ	C16-C17-C12	-2.28	117.89	121.03
2	O	302	FAD	C5'-C4'-C3'	2.27	116.59	112.20
2	I	301	FAD	N10-C10-N1	2.26	124.84	118.35
2	N	301	FAD	O4'-C4'-C3'	2.26	114.58	109.10
3	L	301	0VJ	C03-C04-C07	-2.25	116.80	120.10
2	F	302	FAD	N10-C10-N1	2.25	124.83	118.35
2	P	301	FAD	N10-C10-N1	2.25	124.82	118.35
3	F	304	0VJ	C17-C16-C15	-2.25	116.98	119.73
2	A	301	FAD	N10-C10-N1	2.25	124.81	118.35
2	A	302	FAD	N10-C10-N1	2.25	124.81	118.35
2	M	301	FAD	N10-C10-N1	2.24	124.80	118.35
2	O	302	FAD	C5A-C6A-N6A	2.24	123.76	120.35
2	K	302	FAD	C10-N1-C2	2.24	121.38	116.90
2	E	301	FAD	N10-C10-N1	2.24	124.79	118.35
2	I	302	FAD	N10-C10-N1	2.24	124.78	118.35
2	O	302	FAD	O4-C4-C4X	-2.23	120.67	126.60
3	H	301	0VJ	C16-C17-C12	-2.23	117.95	121.03
3	B	303	0VJ	C17-C12-C13	2.22	121.65	118.17
2	N	301	FAD	O2'-C2'-C1'	2.21	115.15	109.80
3	K	301	0VJ	C04-C07-C08	2.21	120.51	117.06
3	O	301	0VJ	C14-C13-C12	-2.21	117.99	121.03
2	B	301	FAD	N6A-C6A-N1A	2.20	123.15	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	FAD	N10-C10-N1	2.19	124.65	118.35
2	P	301	FAD	C8M-C8-C9	-2.18	115.45	119.49
3	M	303	0VJ	C06-C05-C10	-2.18	116.90	120.10
2	J	301	FAD	O5'-C5'-C4'	-2.17	103.56	109.36
2	F	301	FAD	P-O3P-PA	2.17	140.28	132.83
2	J	301	FAD	O3'-C3'-C4'	2.17	114.06	108.81
3	P	302	0VJ	C-O01-C15	2.17	122.22	117.51
2	J	301	FAD	C9-C8-C7	-2.17	116.56	119.67
2	A	301	FAD	C8M-C8-C9	-2.17	115.48	119.49
2	F	302	FAD	C8M-C8-C9	-2.16	115.49	119.49
2	I	301	FAD	C8M-C8-C9	-2.16	115.50	119.49
2	C	301	FAD	O2P-P-O1P	2.16	122.91	112.24
2	M	301	FAD	C8M-C8-C9	-2.16	115.50	119.49
2	E	301	FAD	C8M-C8-C9	-2.16	115.50	119.49
2	A	302	FAD	C8M-C8-C9	-2.16	115.50	119.49
2	I	302	FAD	C8M-C8-C9	-2.16	115.50	119.49
2	F	301	FAD	O5'-C5'-C4'	-2.15	103.61	109.36
3	M	303	0VJ	C14-C13-C12	-2.15	118.07	121.03
2	N	301	FAD	O2P-P-O1P	2.14	122.83	112.24
2	H	302	FAD	C4A-C5A-N7A	2.14	111.63	109.40
3	H	301	0VJ	C01-C02-C03	2.13	123.43	120.19
3	A	303	0VJ	C14-C13-C12	-2.12	118.11	121.03
3	I	304	0VJ	C01-C02-C03	2.12	123.42	120.19
2	I	301	FAD	O4B-C4B-C3B	2.12	109.30	105.11
2	E	301	FAD	O4B-C4B-C3B	2.12	109.30	105.11
3	E	302	0VJ	C13-C14-C15	2.12	122.32	119.73
2	F	301	FAD	C1'-N10-C9A	-2.11	116.99	120.51
2	I	302	FAD	O4B-C4B-C3B	2.11	109.29	105.11
2	K	302	FAD	O2A-PA-O1A	2.11	122.68	112.24
3	J	302	0VJ	C04-C05-C10	2.11	122.96	120.68
3	F	304	0VJ	O03-C07-C08	2.10	124.24	119.59
2	F	302	FAD	O4B-C4B-C3B	2.10	109.27	105.11
2	P	301	FAD	O4B-C4B-C3B	2.10	109.27	105.11
2	A	301	FAD	O4B-C4B-C3B	2.10	109.26	105.11
3	N	302	0VJ	C17-C16-C15	-2.10	117.17	119.73
2	A	302	FAD	O4B-C4B-C3B	2.10	109.26	105.11
2	M	301	FAD	O4B-C4B-C3B	2.10	109.26	105.11
3	L	301	0VJ	C13-C14-C15	2.09	122.29	119.73
2	F	301	FAD	O4'-C4'-C3'	2.08	114.16	109.10
2	F	301	FAD	O4B-C4B-C5B	-2.08	102.53	109.37
2	C	301	FAD	O3B-C3B-C2B	2.07	118.53	111.82
3	M	303	0VJ	C04-C07-C08	2.06	120.28	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	301	0VJ	O03-C07-C08	2.06	124.15	119.59
2	O	302	FAD	C2B-C3B-C4B	2.06	106.65	102.64
2	F	301	FAD	C9-C9A-C5X	-2.06	116.22	120.11
2	A	302	FAD	O2B-C2B-C3B	2.05	118.45	111.82
2	F	302	FAD	O2B-C2B-C3B	2.05	118.45	111.82
2	I	302	FAD	O2B-C2B-C3B	2.05	118.45	111.82
2	M	301	FAD	O2B-C2B-C3B	2.05	118.45	111.82
2	B	301	FAD	O4-C4-N3	2.05	124.04	120.12
2	P	301	FAD	O2B-C2B-C3B	2.05	118.44	111.82
2	F	301	FAD	O2A-PA-O1A	2.05	122.36	112.24
3	A	305	0VJ	C02-C03-C04	-2.05	115.94	119.81
3	D	301	0VJ	C06-C05-C10	-2.05	117.10	120.10
2	A	301	FAD	O2B-C2B-C3B	2.05	118.44	111.82
2	I	301	FAD	O2B-C2B-C3B	2.05	118.44	111.82
2	O	302	FAD	C5X-N5-C4X	2.04	121.46	118.07
2	E	301	FAD	O2B-C2B-C3B	2.04	118.41	111.82
3	O	301	0VJ	C04-C05-C10	2.04	122.88	120.68
2	C	301	FAD	C1'-C2'-C3'	2.03	115.47	109.79
3	M	303	0VJ	C01-C02-C03	2.03	123.28	120.19
2	F	301	FAD	C5X-N5-C4X	2.03	121.44	118.07
3	E	302	0VJ	C14-C13-C12	-2.02	118.25	121.03
2	J	301	FAD	C10-C4X-N5	-2.02	120.57	124.86
2	H	302	FAD	O2P-P-O1P	2.01	122.20	112.24
2	F	301	FAD	C9A-C9-C8	2.01	123.35	119.30
2	C	301	FAD	C4'-C3'-C2'	2.01	117.54	113.36
3	N	302	0VJ	C04-C05-C10	2.00	122.84	120.68
2	B	301	FAD	O4'-C4'-C3'	2.00	113.96	109.10

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	FAD	C5B-O5B-PA-O1A
2	C	301	FAD	C1'-C2'-C3'-C4'
2	H	302	FAD	P-O3P-PA-O5B
2	H	302	FAD	C1'-C2'-C3'-C4'
2	J	301	FAD	C5B-O5B-PA-O1A
2	J	301	FAD	C3'-C4'-C5'-O5'
2	J	301	FAD	O4'-C4'-C5'-O5'
2	K	302	FAD	P-O3P-PA-O5B
2	N	301	FAD	C3'-C4'-C5'-O5'
2	N	301	FAD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	N	301	FAD	C5'-O5'-P-O1P
3	D	301	0VJ	C16-C15-O01-C
3	A	305	0VJ	C16-C15-O01-C
3	A	305	0VJ	C14-C15-O01-C
3	D	301	0VJ	C14-C15-O01-C
2	K	302	FAD	O3'-C3'-C4'-O4'
2	O	302	FAD	O3'-C3'-C4'-O4'
2	O	302	FAD	C2'-C3'-C4'-O4'
2	K	302	FAD	C2'-C3'-C4'-O4'
2	F	301	FAD	O3'-C3'-C4'-O4'
2	J	301	FAD	O2'-C2'-C3'-C4'
3	N	302	0VJ	C16-C15-O01-C
2	F	301	FAD	C2'-C3'-C4'-O4'
3	N	302	0VJ	C14-C15-O01-C
2	J	301	FAD	P-O3P-PA-O1A
2	O	302	FAD	P-O3P-PA-O1A
2	O	302	FAD	C2'-C3'-C4'-C5'
2	B	301	FAD	O3'-C3'-C4'-O4'
2	A	301	FAD	P-O3P-PA-O5B
2	A	302	FAD	P-O3P-PA-O5B
2	B	301	FAD	P-O3P-PA-O5B
2	C	301	FAD	P-O3P-PA-O5B
2	E	301	FAD	P-O3P-PA-O5B
2	F	301	FAD	P-O3P-PA-O5B
2	F	302	FAD	P-O3P-PA-O5B
2	I	301	FAD	P-O3P-PA-O5B
2	I	302	FAD	P-O3P-PA-O5B
2	M	301	FAD	P-O3P-PA-O5B
2	O	302	FAD	P-O3P-PA-O5B
2	P	301	FAD	P-O3P-PA-O5B
3	B	303	0VJ	C16-C15-O01-C
2	B	301	FAD	C5B-O5B-PA-O3P
2	N	301	FAD	C5'-O5'-P-O3P
2	A	301	FAD	PA-O3P-P-O2P
2	A	302	FAD	PA-O3P-P-O2P
2	E	301	FAD	PA-O3P-P-O2P
2	F	301	FAD	PA-O3P-P-O2P
2	F	302	FAD	PA-O3P-P-O2P
2	I	301	FAD	PA-O3P-P-O2P
2	I	302	FAD	PA-O3P-P-O2P
2	M	301	FAD	PA-O3P-P-O2P
2	P	301	FAD	PA-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	B	301	FAD	C5B-O5B-PA-O2A
2	J	301	FAD	C5B-O5B-PA-O2A
2	N	301	FAD	C5'-O5'-P-O2P
2	C	301	FAD	C1'-C2'-C3'-O3'
2	H	302	FAD	C1'-C2'-C3'-O3'
2	B	301	FAD	C2'-C3'-C4'-O4'
3	B	303	0VJ	C14-C15-O01-C
2	F	301	FAD	PA-O3P-P-O1P
2	N	301	FAD	C4'-C5'-O5'-P
2	J	301	FAD	O2'-C2'-C3'-O3'
2	F	301	FAD	O3'-C3'-C4'-C5'
2	K	302	FAD	O3'-C3'-C4'-C5'
2	O	302	FAD	O3'-C3'-C4'-C5'
2	F	301	FAD	P-O3P-PA-O1A
2	J	301	FAD	P-O3P-PA-O5B
2	H	302	FAD	C5B-O5B-PA-O3P
2	J	301	FAD	C5B-O5B-PA-O3P
2	A	301	FAD	PA-O3P-P-O1P
2	A	302	FAD	PA-O3P-P-O1P
2	B	301	FAD	P-O3P-PA-O1A
2	B	301	FAD	PA-O3P-P-O1P
2	C	301	FAD	P-O3P-PA-O1A
2	C	301	FAD	PA-O3P-P-O2P
2	E	301	FAD	PA-O3P-P-O1P
2	F	302	FAD	PA-O3P-P-O1P
2	H	302	FAD	P-O3P-PA-O1A
2	I	301	FAD	PA-O3P-P-O1P
2	I	302	FAD	PA-O3P-P-O1P
2	K	302	FAD	P-O3P-PA-O1A
2	M	301	FAD	PA-O3P-P-O1P
2	N	301	FAD	PA-O3P-P-O2P
2	O	302	FAD	PA-O3P-P-O1P
2	P	301	FAD	PA-O3P-P-O1P
2	H	302	FAD	C5B-O5B-PA-O1A
2	O	302	FAD	C5'-O5'-P-O1P

There are no ring outliers.

25 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	0VJ	2	0
3	N	302	0VJ	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	304	0VJ	2	0
2	H	302	FAD	1	0
2	I	302	FAD	2	0
2	E	301	FAD	1	0
2	F	301	FAD	1	0
4	E	303	DMS	2	0
2	F	302	FAD	2	0
3	M	303	0VJ	4	0
2	P	301	FAD	2	0
4	D	302	DMS	1	0
3	D	301	0VJ	1	0
4	M	302	DMS	3	0
2	J	301	FAD	3	0
3	O	301	0VJ	3	0
2	N	301	FAD	2	0
2	O	302	FAD	1	0
2	M	301	FAD	1	0
2	C	301	FAD	1	0
2	I	301	FAD	1	0
3	J	302	0VJ	1	0
4	K	303	DMS	1	0
2	B	301	FAD	1	0
3	P	302	0VJ	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 0VJ A 303

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ B 303

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ N 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ K 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ H 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ I 304

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD H 302

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD I 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ G 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD E 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD F 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD F 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ M 303

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ A 305

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ F 304

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD P 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ E 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD K 302

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD J 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ O 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD N 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD O 302

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD M 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD I 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ L 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ J 302

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 0VJ P 302

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	191/227 (84%)	-0.08	0	100	100	27, 46, 77, 94	0
1	B	188/227 (82%)	0.02	2 (1%)	80	78	28, 50, 89, 119	0
1	C	207/227 (91%)	0.02	3 (1%)	75	71	27, 51, 91, 104	0
1	D	203/227 (89%)	-0.09	2 (0%)	82	80	28, 45, 71, 90	0
1	E	206/227 (90%)	-0.08	2 (0%)	82	80	26, 49, 86, 107	0
1	F	206/227 (90%)	-0.05	3 (1%)	73	70	24, 44, 74, 111	0
1	G	188/227 (82%)	-0.12	0	100	100	27, 46, 71, 99	0
1	H	179/227 (78%)	-0.03	3 (1%)	70	66	30, 48, 72, 108	0
1	I	193/227 (85%)	-0.13	1 (0%)	91	89	23, 49, 74, 91	0
1	J	179/227 (78%)	0.18	3 (1%)	70	66	32, 57, 91, 101	0
1	K	201/227 (88%)	-0.04	1 (0%)	91	89	32, 51, 90, 110	0
1	L	201/227 (88%)	0.17	9 (4%)	33	26	31, 54, 99, 130	0
1	M	197/227 (86%)	-0.07	2 (1%)	82	80	29, 51, 78, 92	0
1	N	177/227 (77%)	0.24	10 (5%)	24	19	29, 58, 102, 138	0
1	O	200/227 (88%)	0.02	2 (1%)	82	80	34, 53, 93, 119	0
1	P	197/227 (86%)	0.22	8 (4%)	37	30	29, 60, 101, 120	0
All	All	3113/3632 (85%)	0.01	51 (1%)	72	68	23, 51, 89, 138	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	104	ARG	5.6
1	F	95	MET	5.4
1	N	125	TRP	4.6
1	J	149	ILE	3.9
1	N	126	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLN	3.6
1	F	119	PRO	3.5
1	O	35	GLN	3.4
1	N	149	ILE	3.4
1	C	104	ARG	3.2
1	N	143	LYS	3.2
1	P	96	GLU	3.1
1	I	95	MET	3.1
1	P	94	VAL	3.0
1	P	100	PRO	3.0
1	B	94	VAL	3.0
1	P	95	MET	3.0
1	N	123	GLN	3.0
1	C	36	ILE	2.9
1	M	95	MET	2.8
1	L	94	VAL	2.8
1	N	128	THR	2.8
1	P	102	GLN	2.7
1	O	120	GLU	2.7
1	E	36	ILE	2.7
1	H	124	THR	2.6
1	L	93	SER	2.6
1	P	150	ALA	2.6
1	L	125	TRP	2.5
1	P	33	GLU	2.5
1	F	36	ILE	2.5
1	L	157	ILE	2.5
1	K	36	ILE	2.4
1	L	160	LEU	2.3
1	N	124	THR	2.3
1	E	95	MET	2.3
1	D	96	GLU	2.3
1	N	87	PHE	2.3
1	H	134	TYR	2.3
1	M	157	ILE	2.2
1	N	134	TYR	2.2
1	L	144	ALA	2.2
1	C	203	ILE	2.1
1	N	148	GLY	2.1
1	L	126	TRP	2.1
1	L	101	HIS	2.1
1	D	95	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	92	ALA	2.1
1	J	127	ALA	2.0
1	H	94	VAL	2.0
1	P	160	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathrm{\AA}^2$)	Q<0.9
4	DMS	P	303	4/4	0.90	0.17	78,87,87,91	0
4	DMS	G	302	4/4	0.93	0.25	70,70,71,76	0
3	0VJ	N	302	22/22	0.93	0.17	59,65,70,71	0
3	0VJ	I	304	22/22	0.94	0.18	38,44,48,49	0
3	0VJ	J	302	22/22	0.94	0.16	51,55,59,60	0
2	FAD	I	302	53/53	0.94	0.15	33,34,35,37	0
3	0VJ	P	302	22/22	0.94	0.18	44,47,53,57	0
4	DMS	A	304	4/4	0.94	0.40	63,70,74,74	0
3	0VJ	A	305	22/22	0.94	0.18	35,40,44,48	0
3	0VJ	F	304	22/22	0.94	0.19	52,58,61,62	0
3	0VJ	L	301	22/22	0.95	0.17	39,42,48,51	0
2	FAD	P	301	53/53	0.95	0.14	33,34,35,37	0
2	FAD	I	301	53/53	0.95	0.15	33,34,35,37	0
2	FAD	E	301	53/53	0.95	0.15	33,34,35,37	0
2	FAD	M	301	53/53	0.95	0.17	33,34,35,37	0
2	FAD	N	301	53/53	0.95	0.13	44,45,47,48	0
3	0VJ	H	301	22/22	0.96	0.14	27,33,39,39	0
2	FAD	F	302	53/53	0.96	0.16	33,34,35,37	0
3	0VJ	A	303	22/22	0.96	0.18	34,39,43,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	0VJ	K	301	22/22	0.96	0.15	21,26,34,35	0
2	FAD	J	301	53/53	0.96	0.13	42,44,46,48	0
3	0VJ	M	303	22/22	0.96	0.17	33,43,52,53	0
3	0VJ	B	303	22/22	0.96	0.14	24,27,36,40	0
3	0VJ	D	301	22/22	0.96	0.14	45,50,56,56	0
3	0VJ	E	302	22/22	0.96	0.15	32,39,43,44	0
2	FAD	O	302	53/53	0.96	0.14	40,41,43,44	0
4	DMS	H	303	4/4	0.96	0.20	60,62,63,69	0
3	0VJ	G	301	22/22	0.96	0.17	30,39,47,47	0
2	FAD	H	302	53/53	0.97	0.15	45,46,47,49	0
2	FAD	K	302	53/53	0.97	0.14	37,38,40,40	0
4	DMS	C	302	4/4	0.97	0.23	63,64,65,65	0
4	DMS	D	302	4/4	0.97	0.13	63,63,67,74	0
4	DMS	E	303	4/4	0.97	0.18	57,64,68,70	0
4	DMS	F	303	4/4	0.97	0.12	60,63,67,74	0
2	FAD	A	302	53/53	0.97	0.16	33,34,35,37	0
2	FAD	B	301	53/53	0.97	0.13	40,41,43,44	0
4	DMS	M	302	4/4	0.97	0.21	80,87,87,88	0
3	0VJ	O	301	22/22	0.97	0.15	18,27,33,36	0
2	FAD	C	301	53/53	0.98	0.13	33,34,36,38	0
2	FAD	A	301	53/53	0.98	0.14	33,34,35,37	0
4	DMS	I	303	4/4	0.98	0.20	81,84,87,89	0
4	DMS	K	303	4/4	0.98	0.19	54,54,60,61	0
2	FAD	F	301	53/53	0.98	0.14	28,29,30,32	0
4	DMS	O	303	4/4	0.98	0.16	53,56,60,63	0
4	DMS	B	302	4/4	0.98	0.25	44,46,55,55	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 0VJ N 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
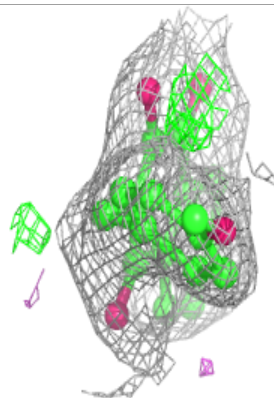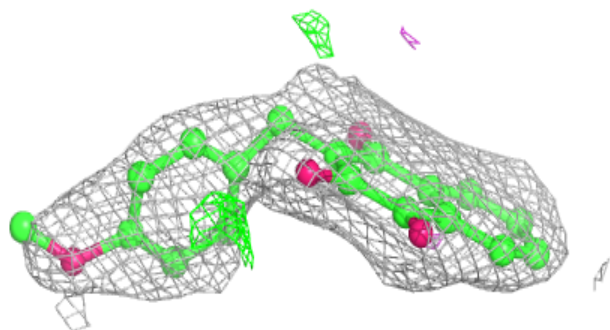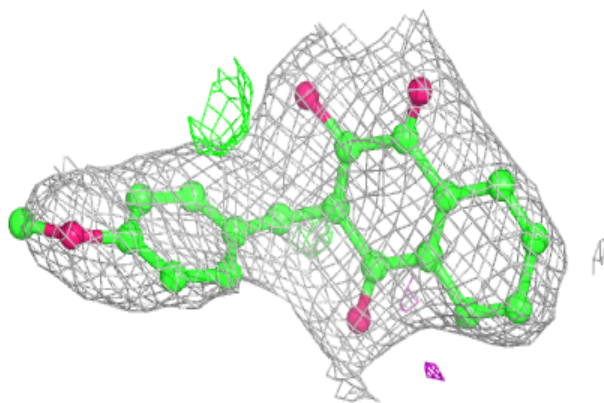
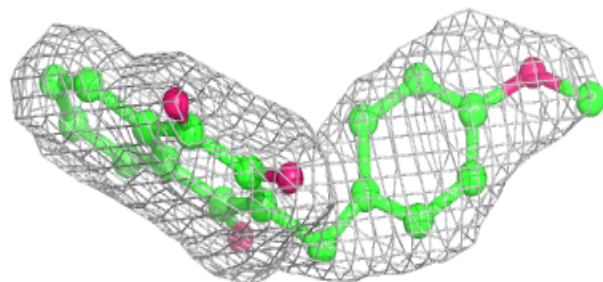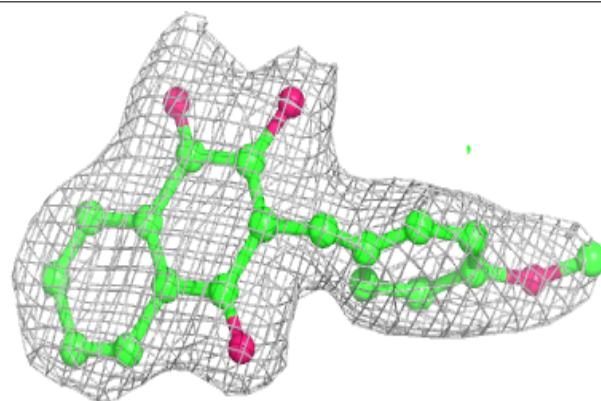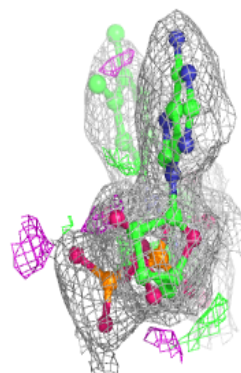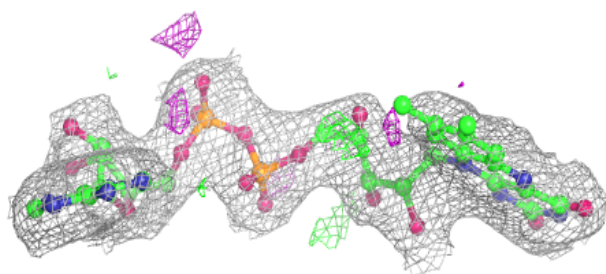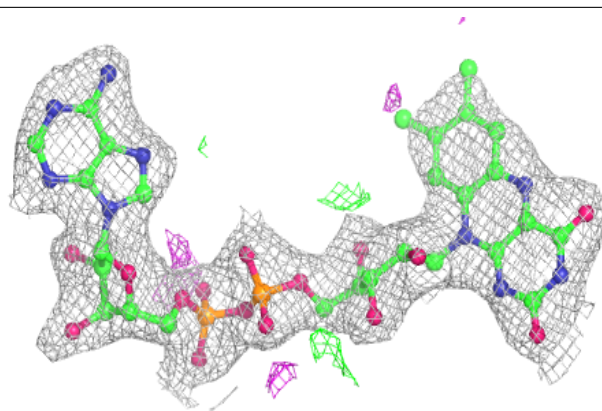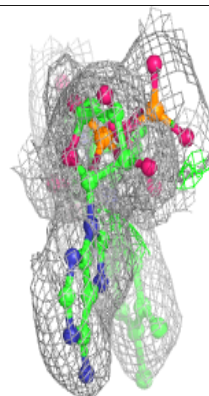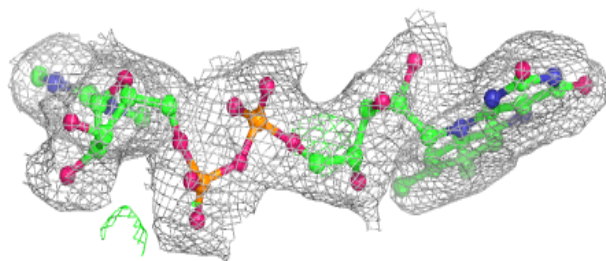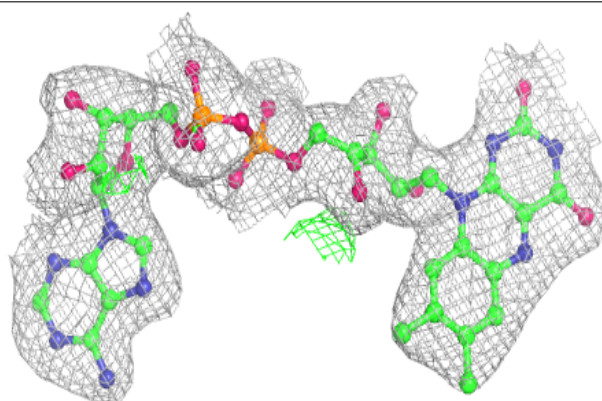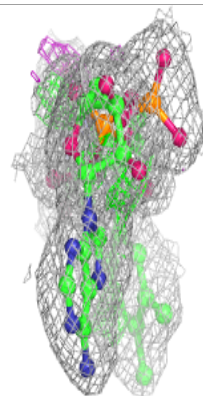**Electron density around 0VJ I 304:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
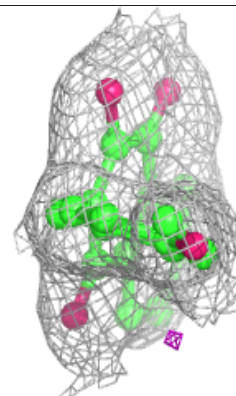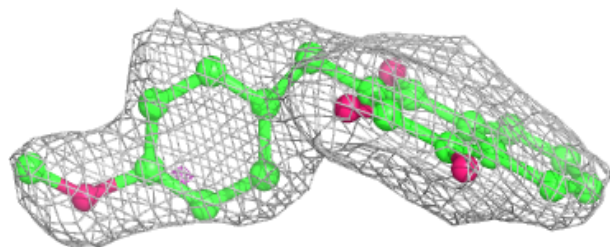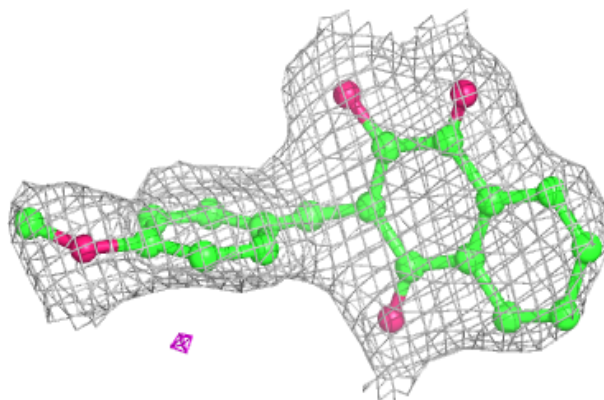
Electron density around 0VJ J 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
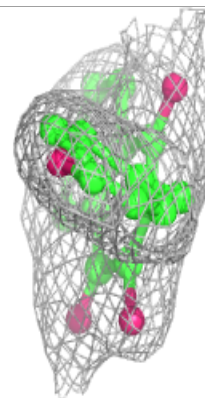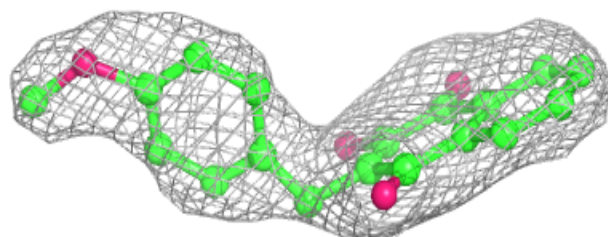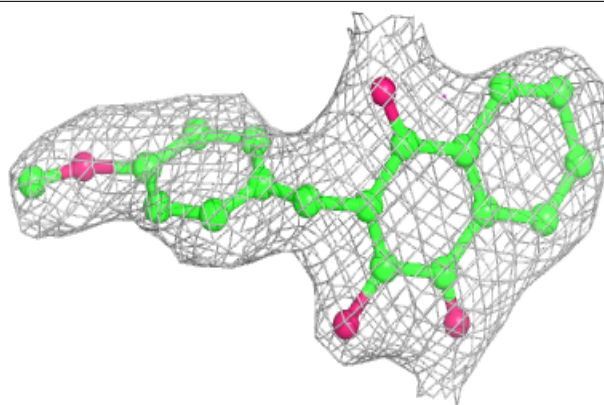
Electron density around FAD I 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
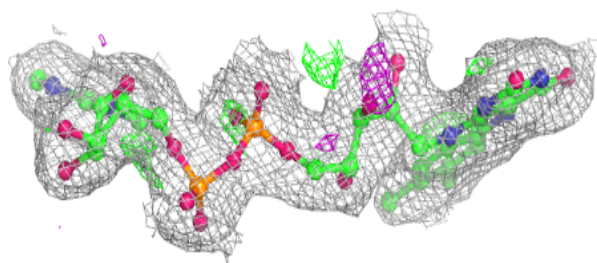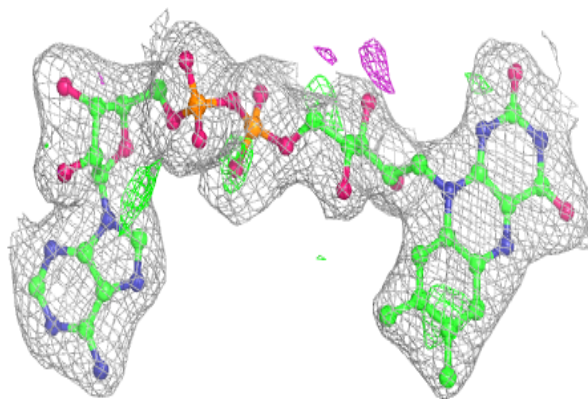$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
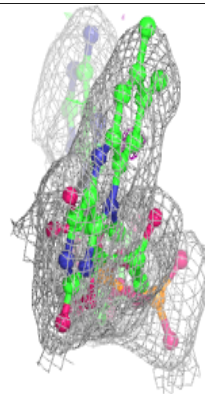and green (positive)
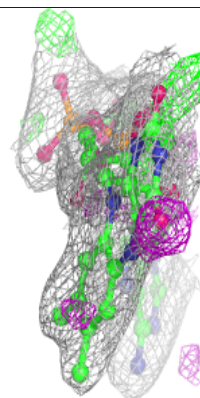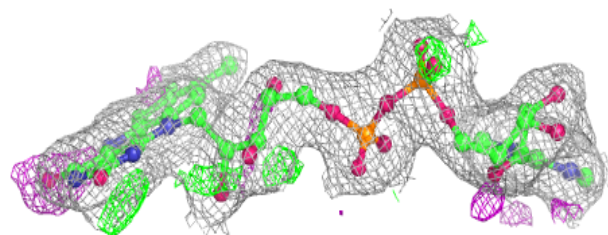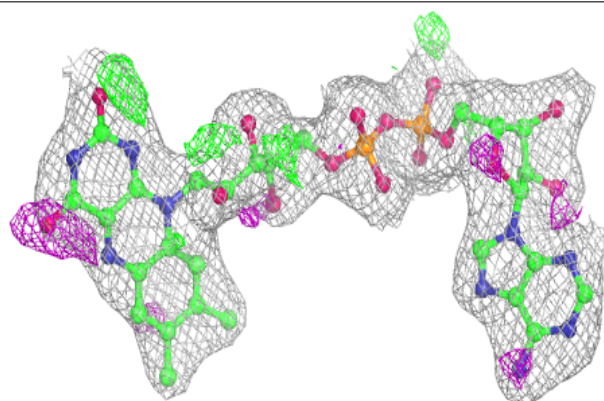
Electron density around 0VJ P 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
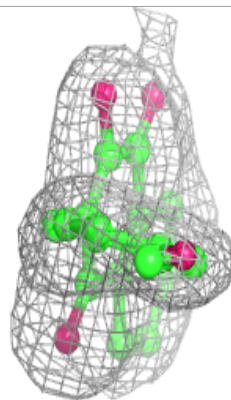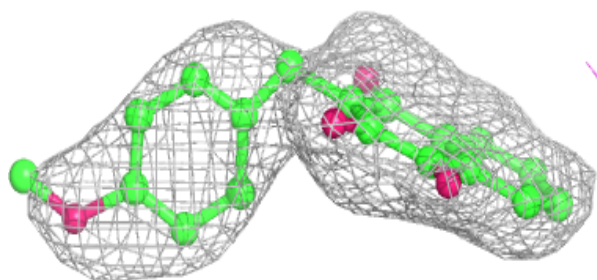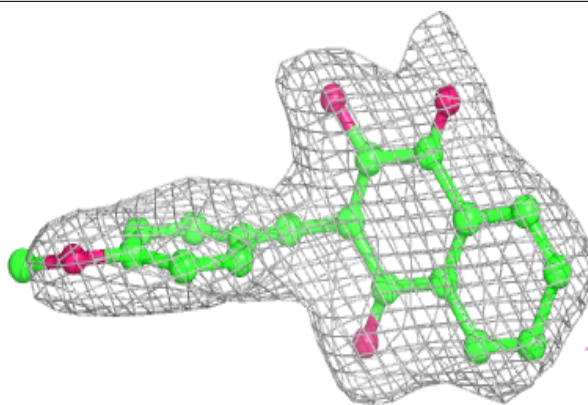
Electron density around 0VJ A 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
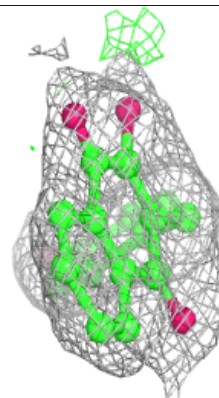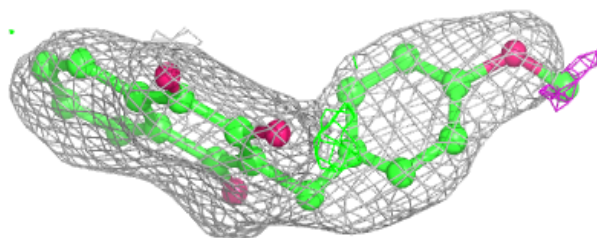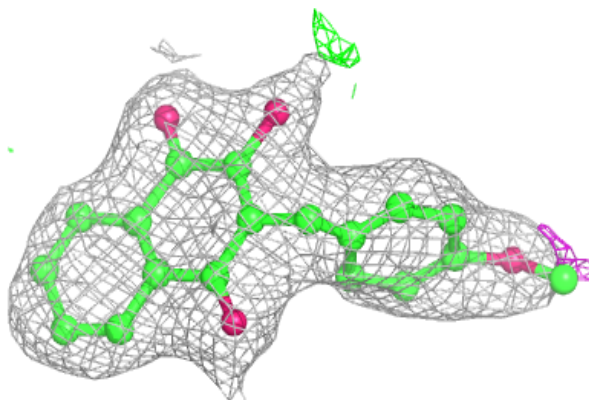
Electron density around 0VJ F 304:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
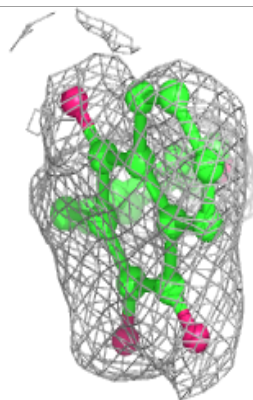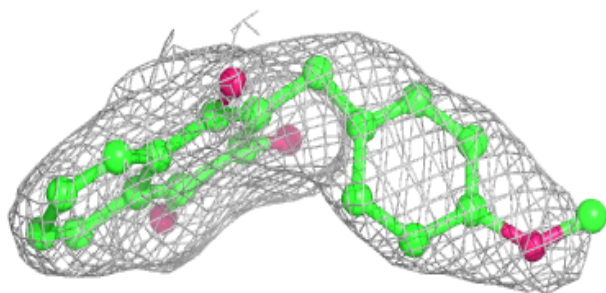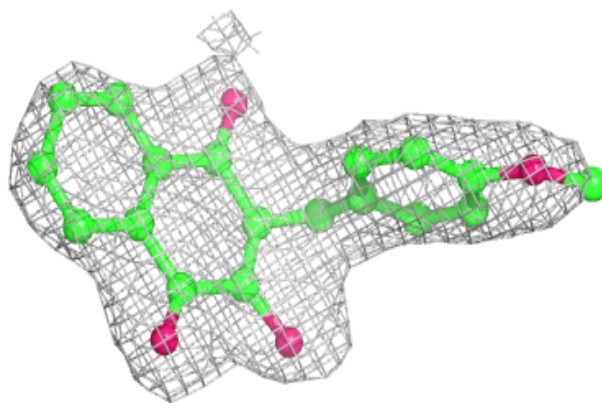
Electron density around 0VJ L 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
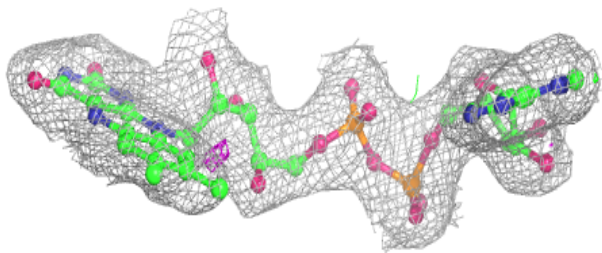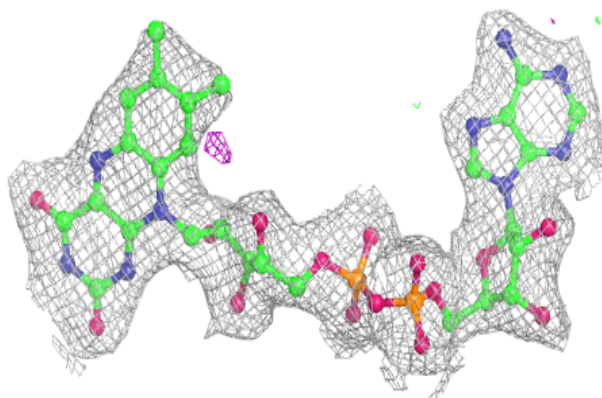and green (positive)
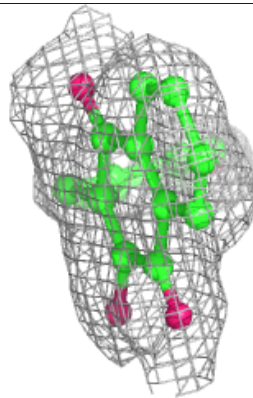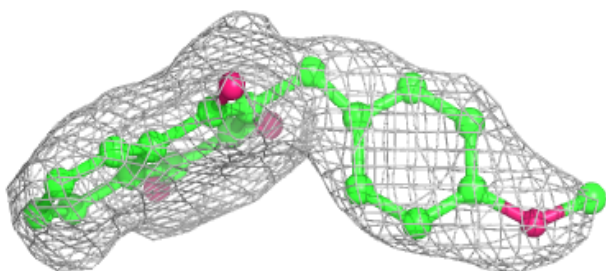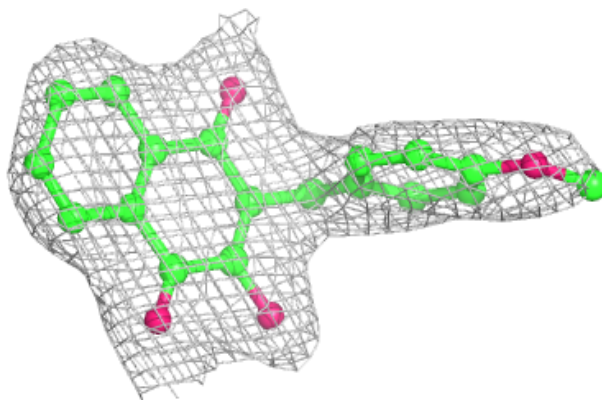
Electron density around FAD P 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
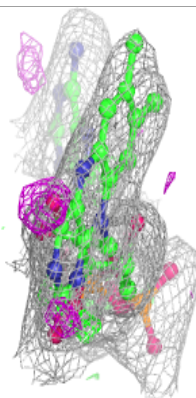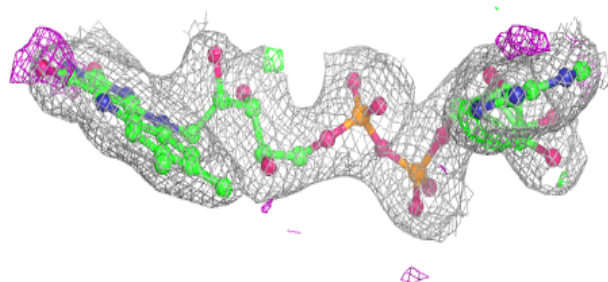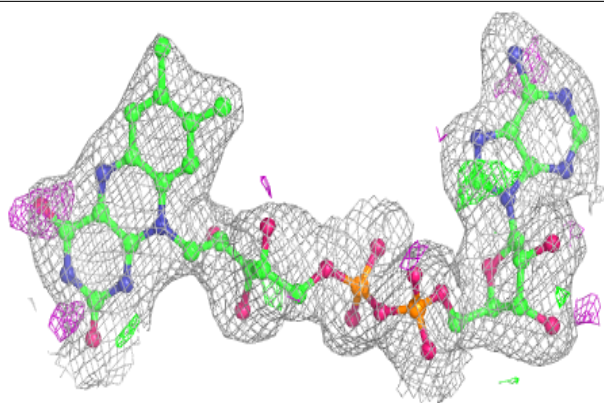
Electron density around FAD I 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
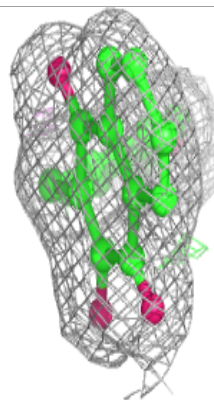and green (positive)
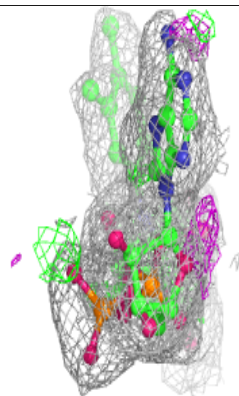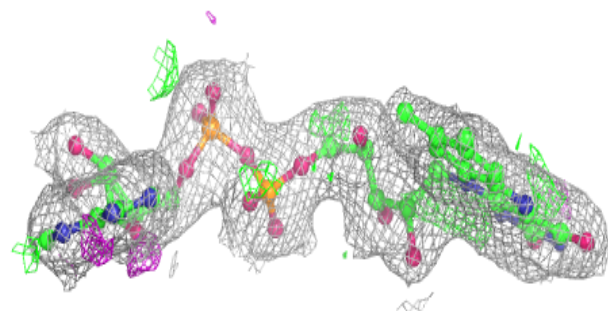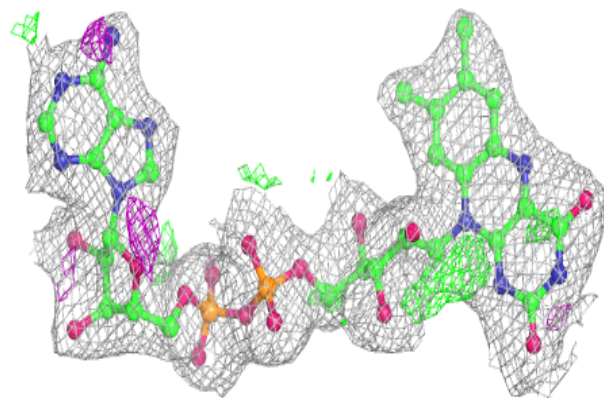
Electron density around FAD E 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
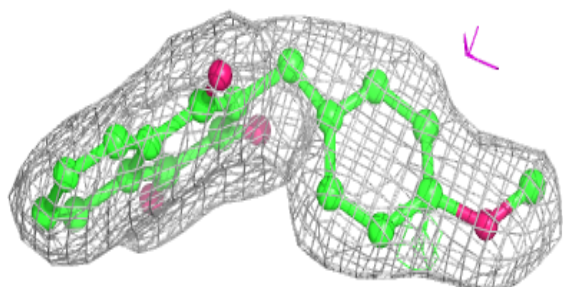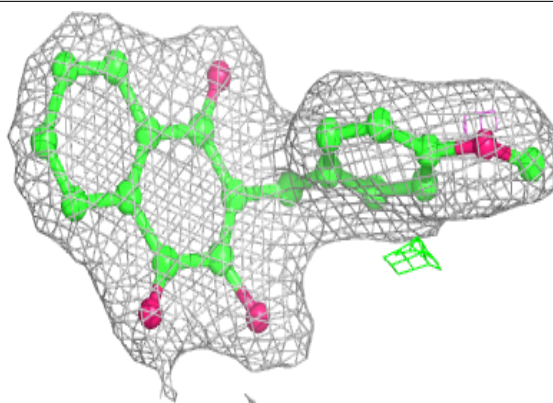and green (positive)
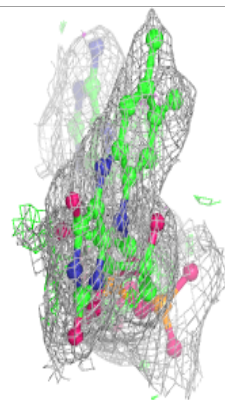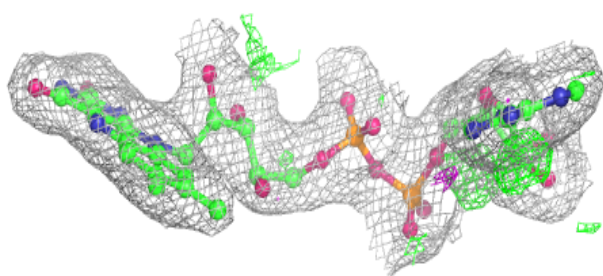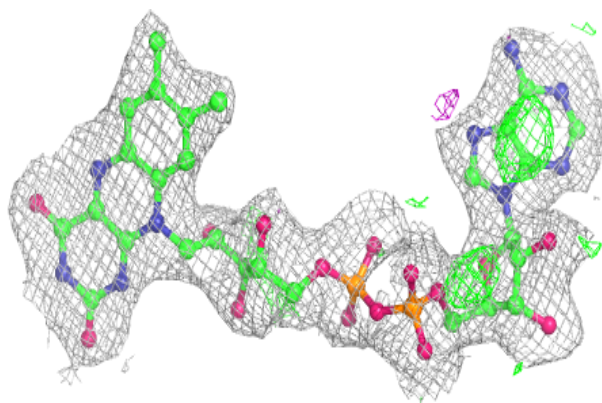
Electron density around FAD M 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
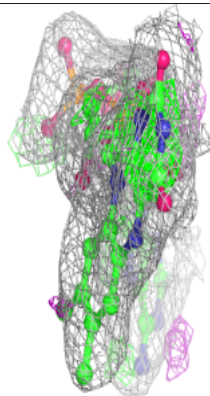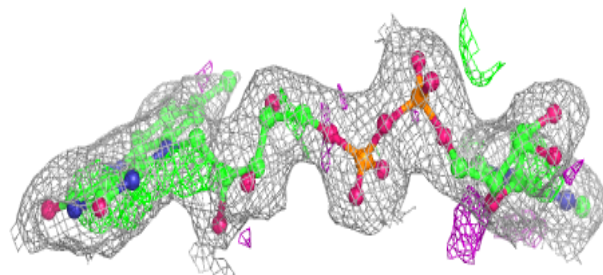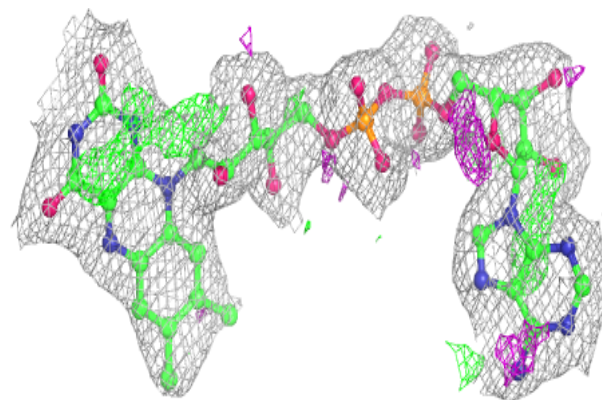
Electron density around FAD N 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
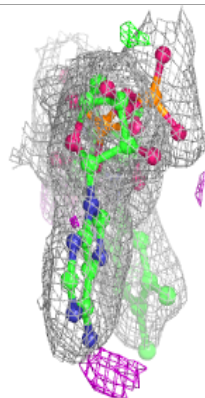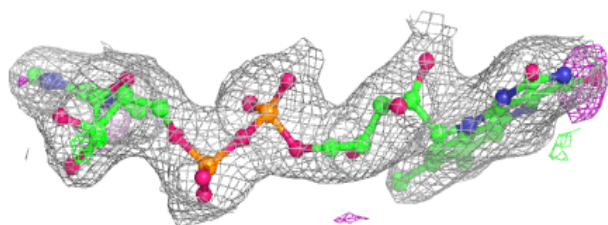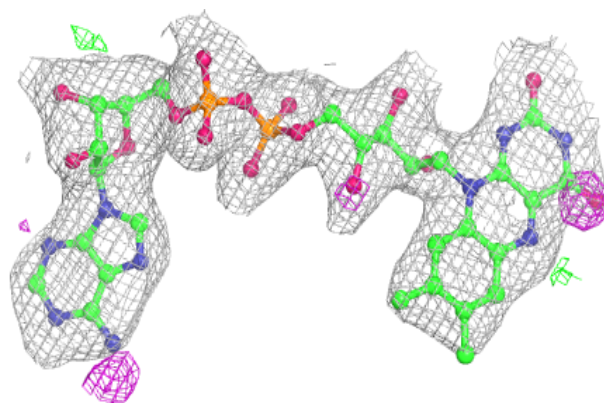
Electron density around 0VJ H 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
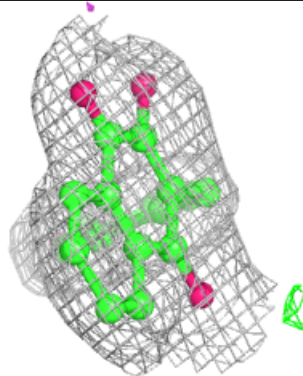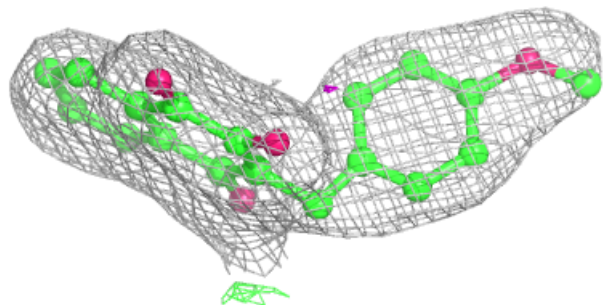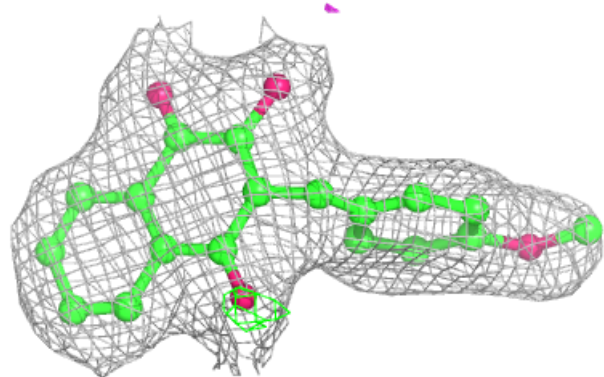
Electron density around FAD F 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
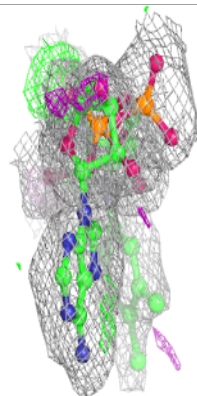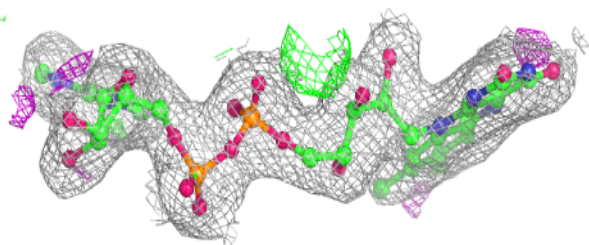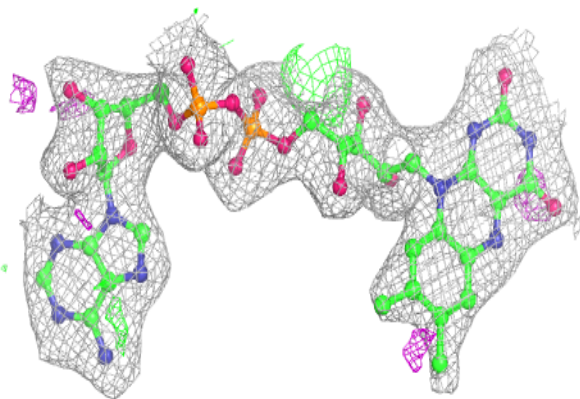
Electron density around 0VJ A 303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
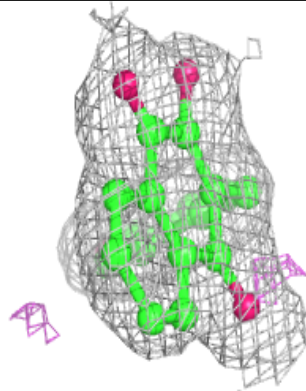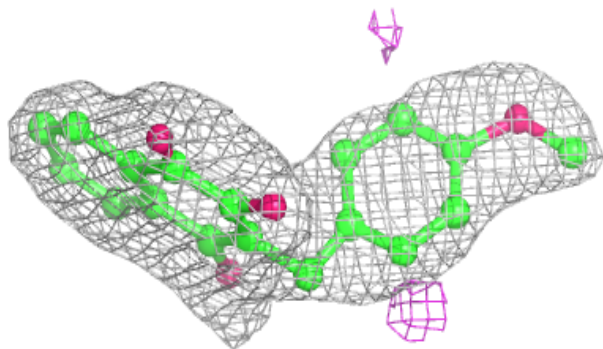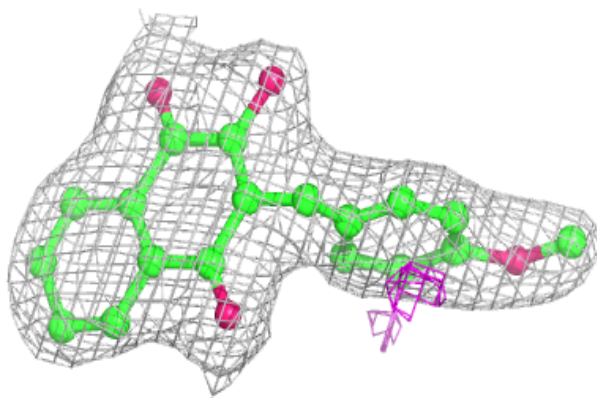
Electron density around 0VJ K 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
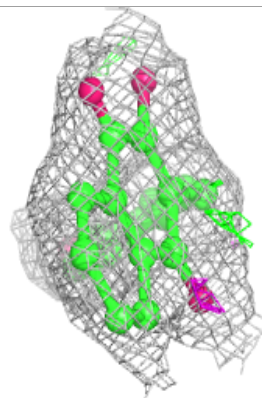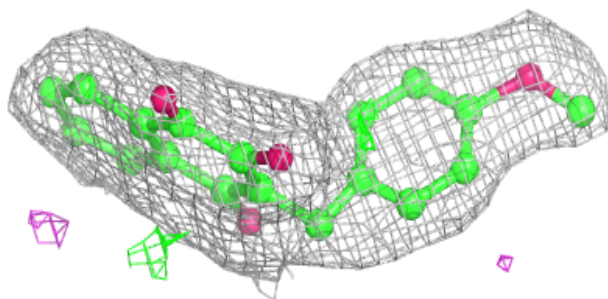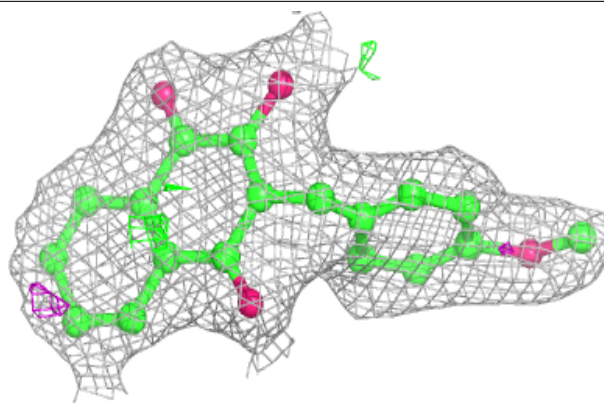
Electron density around FAD J 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
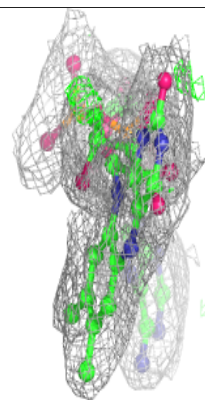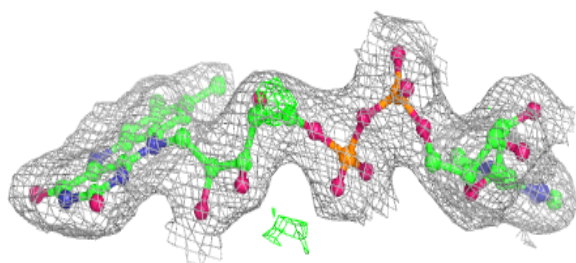and green (positive)
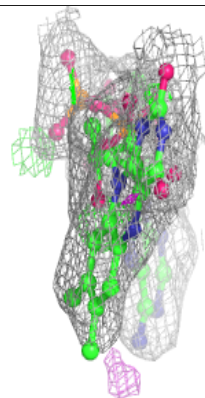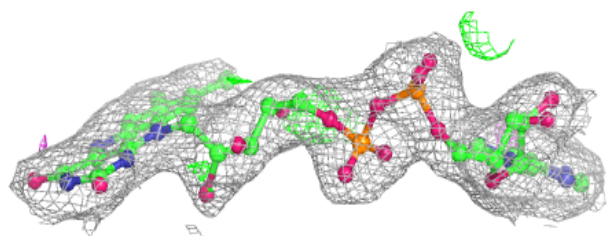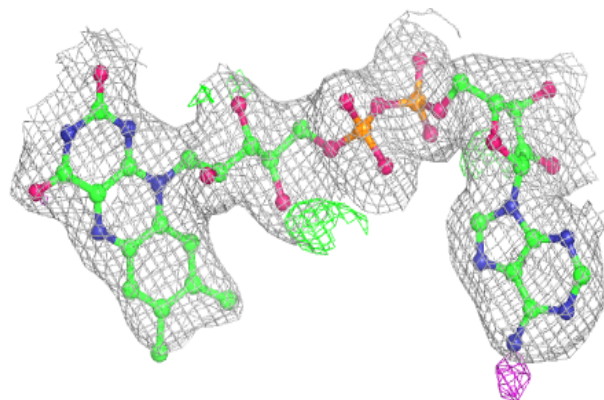
Electron density around 0VJ M 303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
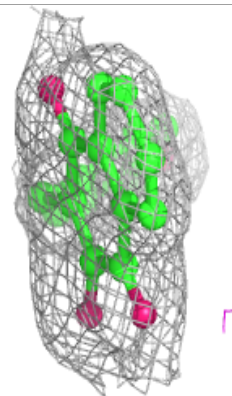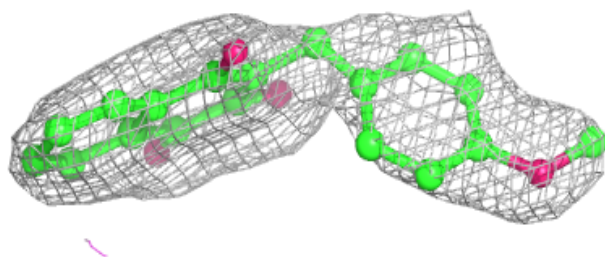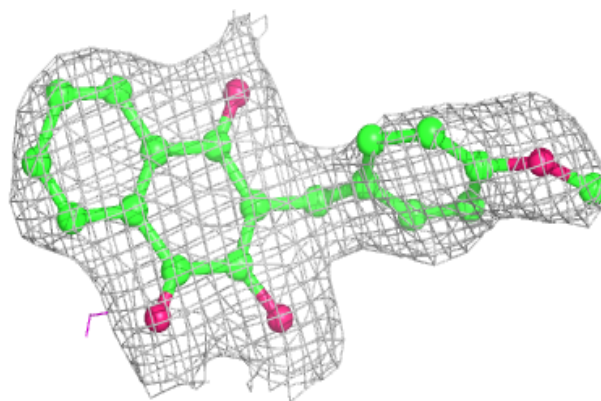
Electron density around 0VJ B 303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
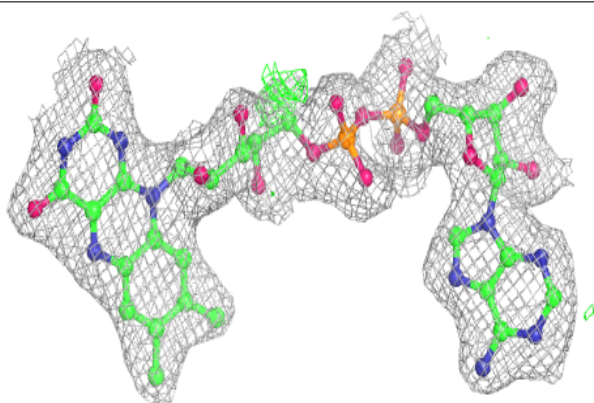$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
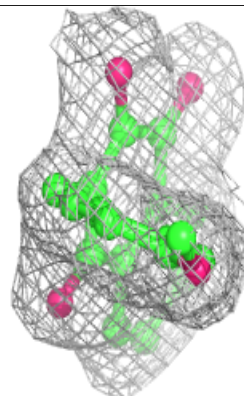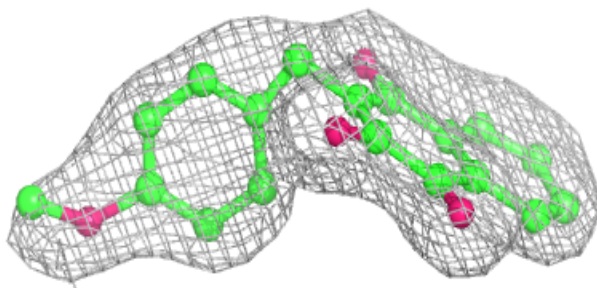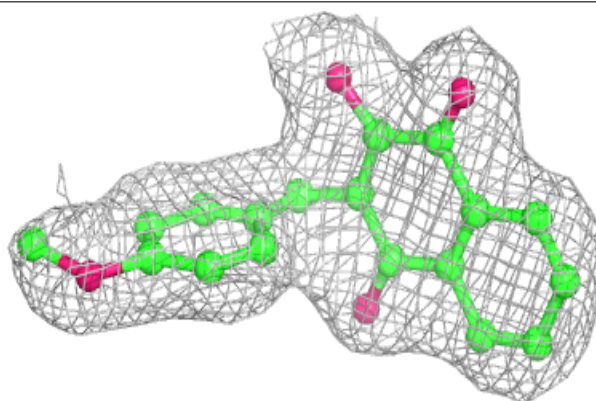
Electron density around 0VJ D 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
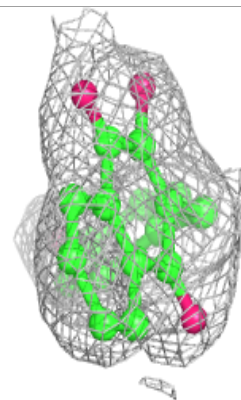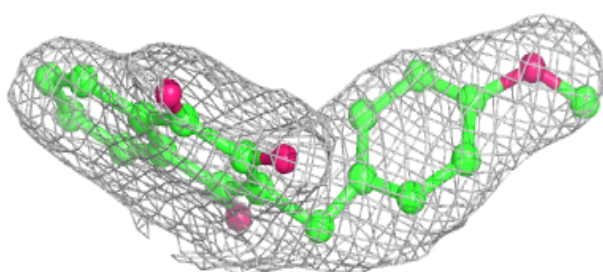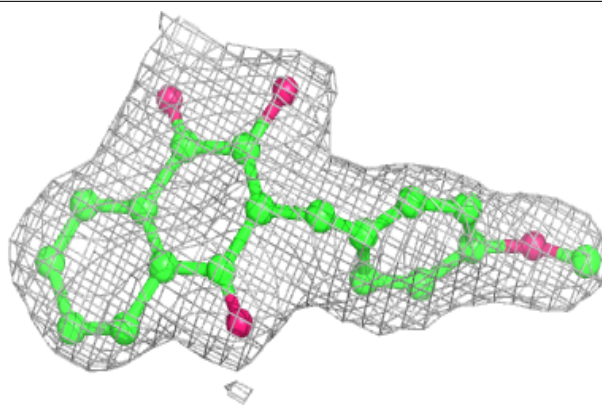
Electron density around 0VJ E 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
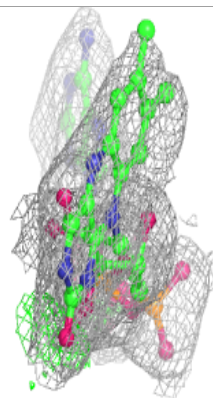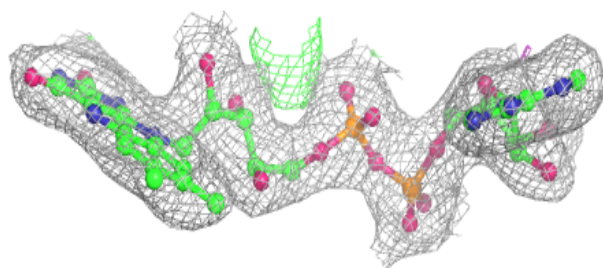and green (positive)
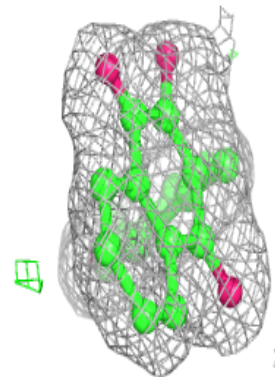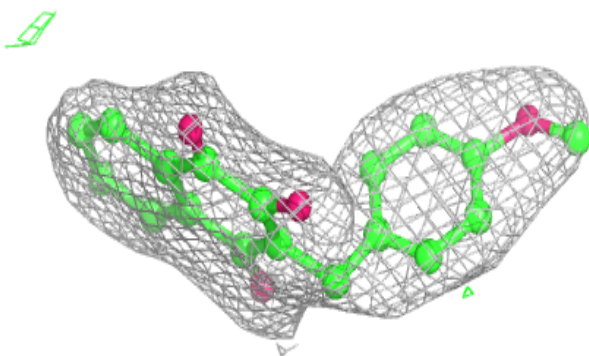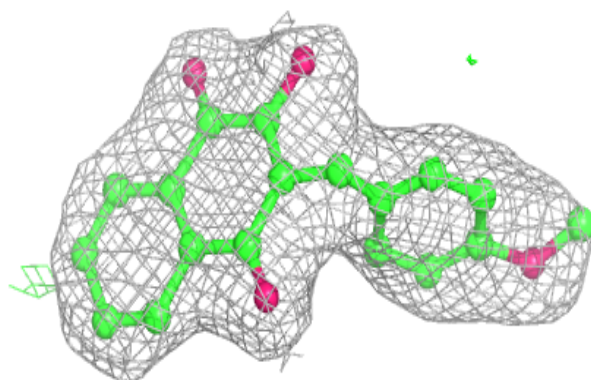
Electron density around FAD O 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
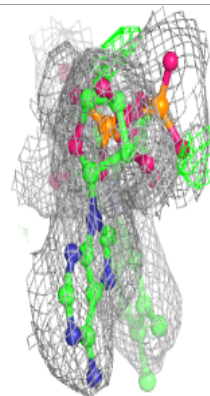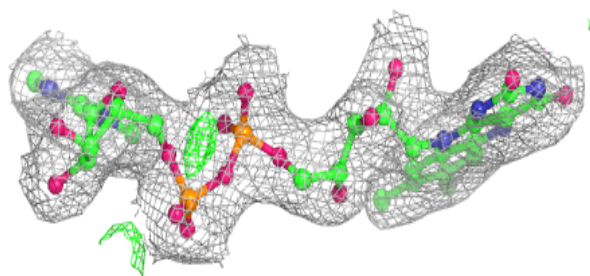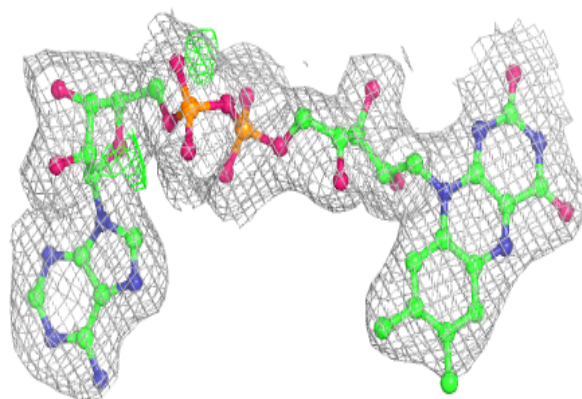
Electron density around 0VJ G 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
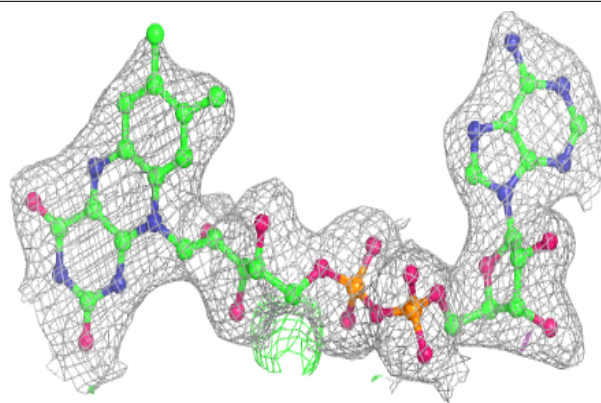mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
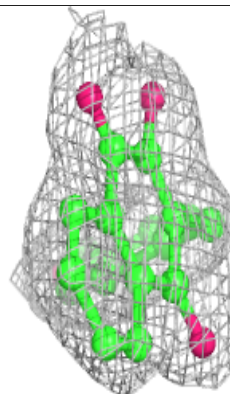
Electron density around FAD H 302:

$2mF_o$-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 302:

$2mF_o$-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 302:

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 301:

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 0VJ O 301:

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

Electron density around FAD C 301:

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

Electron density around FAD A 301:

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

Electron density around FAD F 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
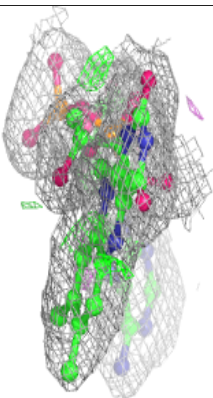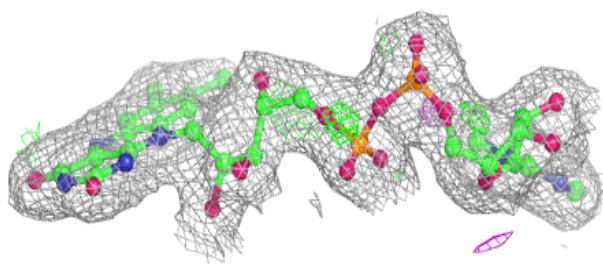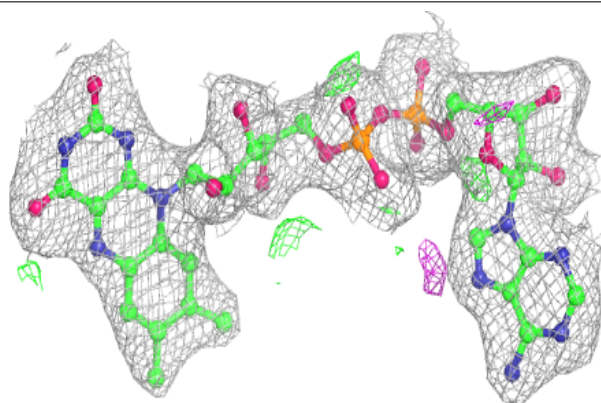
6.5 Other polymers (i)

There are no such residues in this entry.