



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2021 – 12:21 PM EDT

PDB ID : 7LJU  
Title : Porcine Dihydropyrimidine Dehydrogenase (DPD) crosslinked with 5-Ethynyluracil (5EU)  
Authors : Butrin, A.; Forouzesh, D.; Beaupre, B.; Wawrzak, Z.; Liu, D.; Moran, G.  
Deposited on : 2021-01-30  
Resolution : 1.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
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) : 2.18

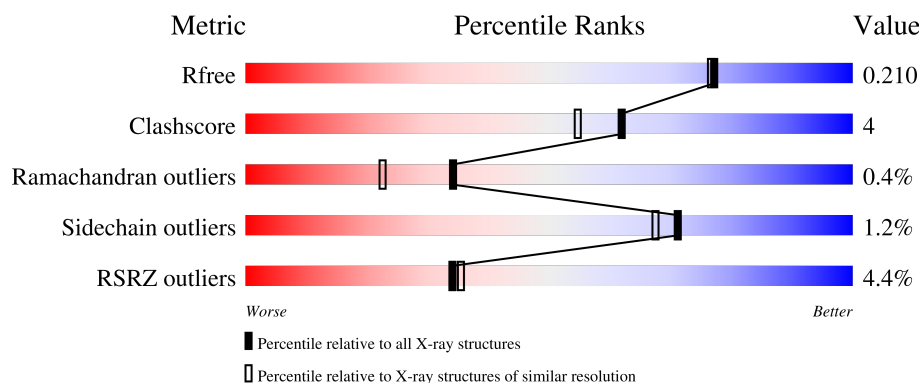
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1025	<div> <div>4%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	B	1025	<div> <div>5%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	C	1025	<div> <div>4%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	D	1025	<div> <div>4%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>

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
6	FNR	A	1108	X	-	-	-
6	FNR	B	1107	X	-	-	-
6	FNR	C	1107	X	-	-	-
6	FNR	D	1108	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34870 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.

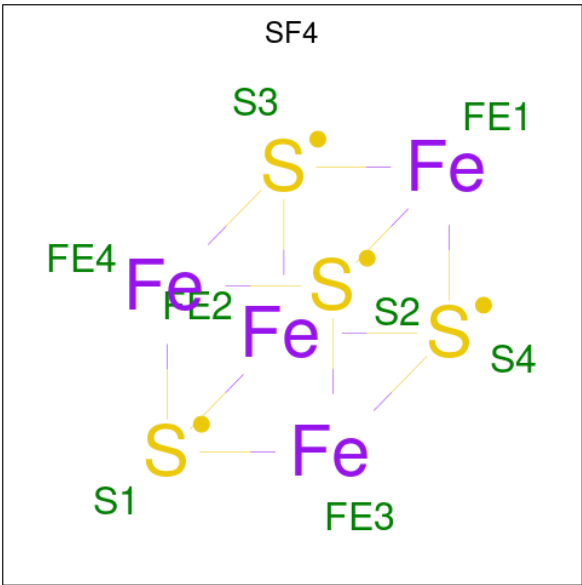
- Molecule 1 is a protein called Dihydropyrimidine dehydrogenase [NADP(+)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	66	0	0
			7727	4900	1306	1465	56			
1	C	1004	Total	C	N	O	S	0	0	0
			7656	4859	1295	1450	52			
1	D	1017	Total	C	N	O	S	43	0	0
			7746	4914	1314	1462	56			
1	B	1004	Total	C	N	O	S	0	0	0
			7656	4859	1295	1450	52			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



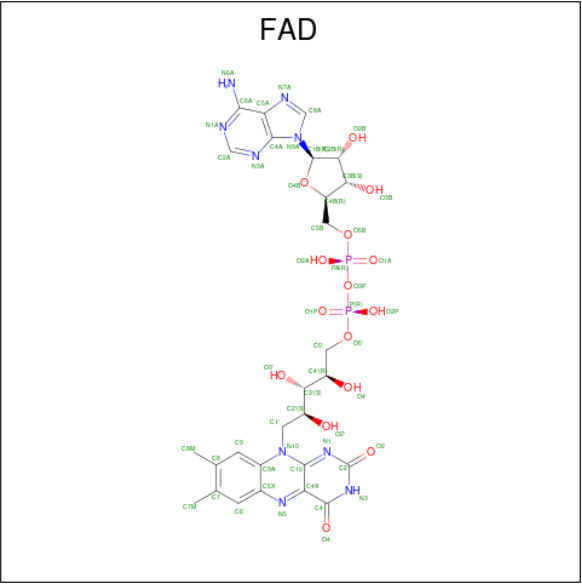
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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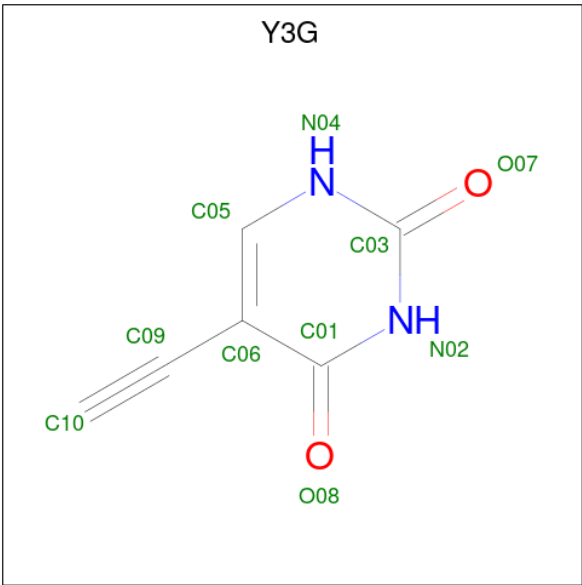
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



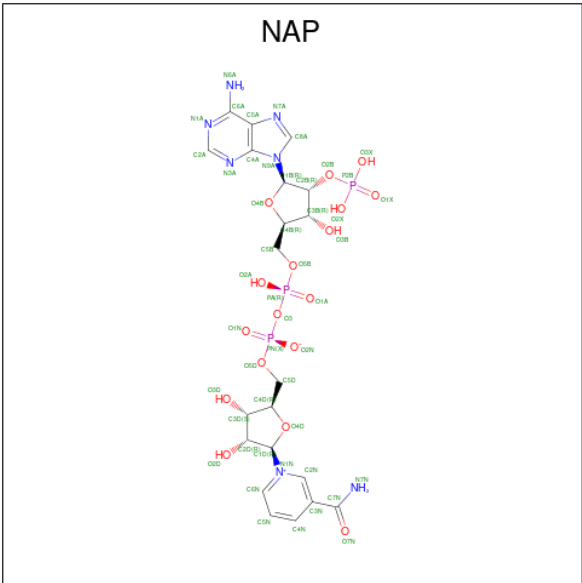
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 5-ethynylpyrimidine-2,4(1H,3H)-dione (three-letter code: Y3G) (formula:  $C_6H_4N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



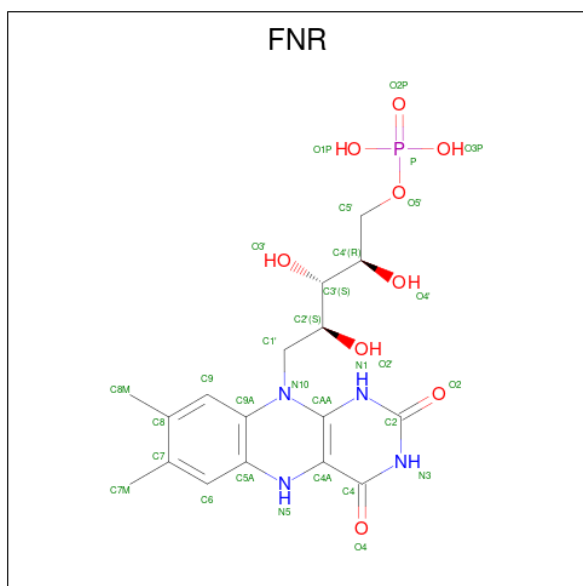
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	6	2	2		
4	C	1	Total	C	N	O	0	0
			10	6	2	2		
4	D	1	Total	C	N	O	0	0
			10	6	2	2		
4	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]P  
TERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (three-letter code: FNR)  
(formula: C<sub>17</sub>H<sub>23</sub>N<sub>4</sub>O<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
6	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
6	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
6	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	867	Total	O	0	0
			867	867		

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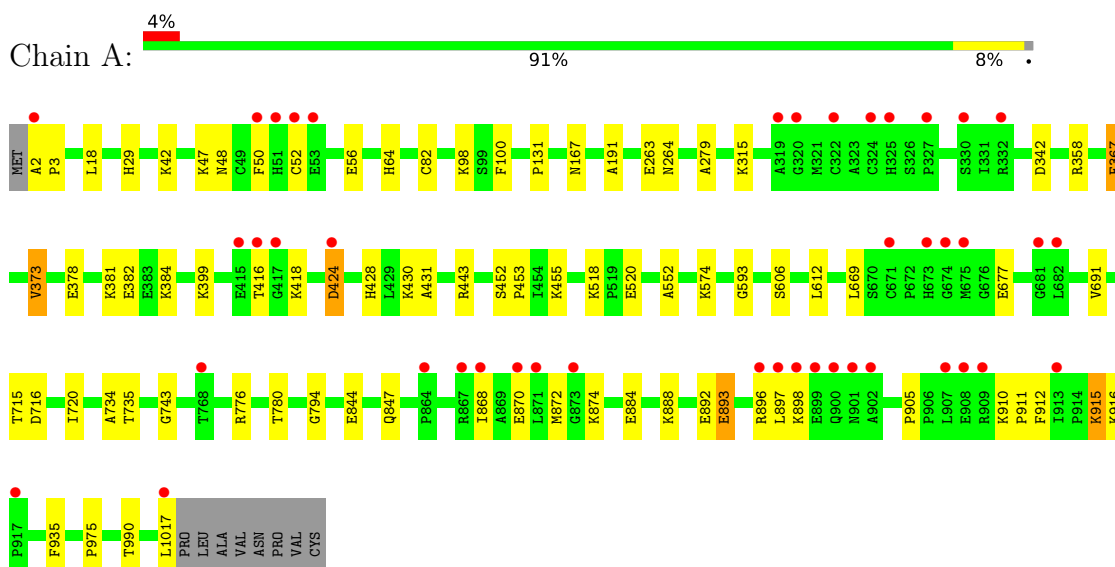
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	861	Total 861	O 861	0	0
7	D	891	Total 891	O 891	0	0
7	B	770	Total 770	O 770	0	0

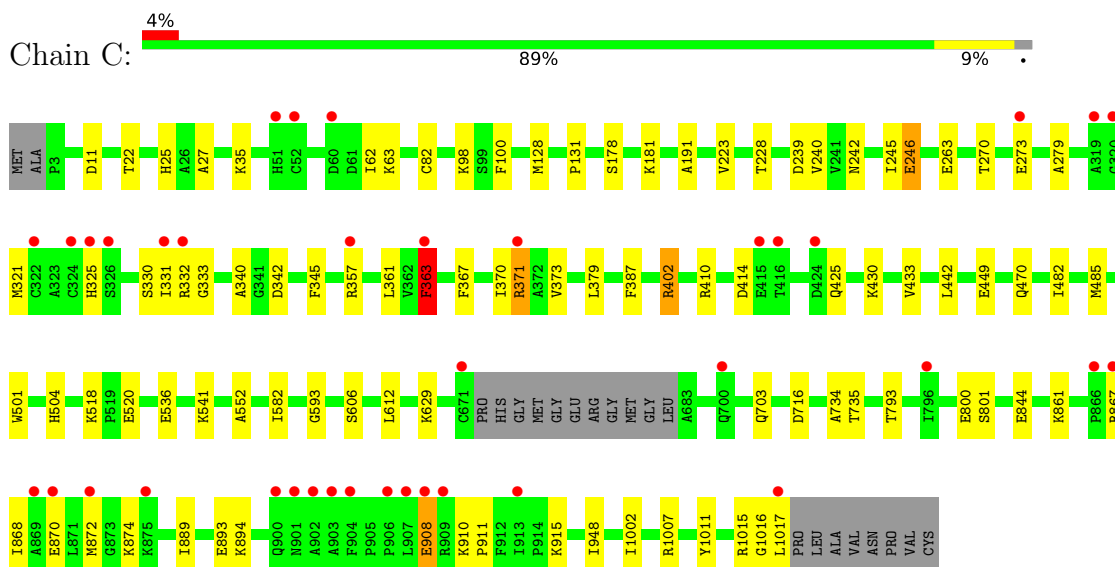
### 3 Residue-property plots [i](#)

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

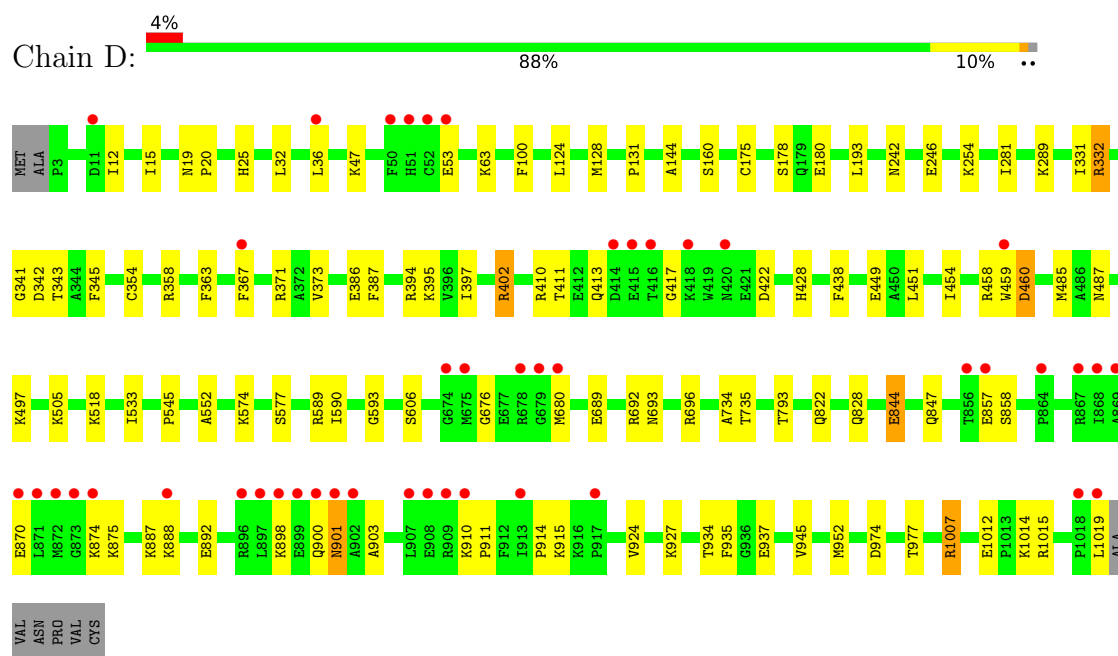
- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



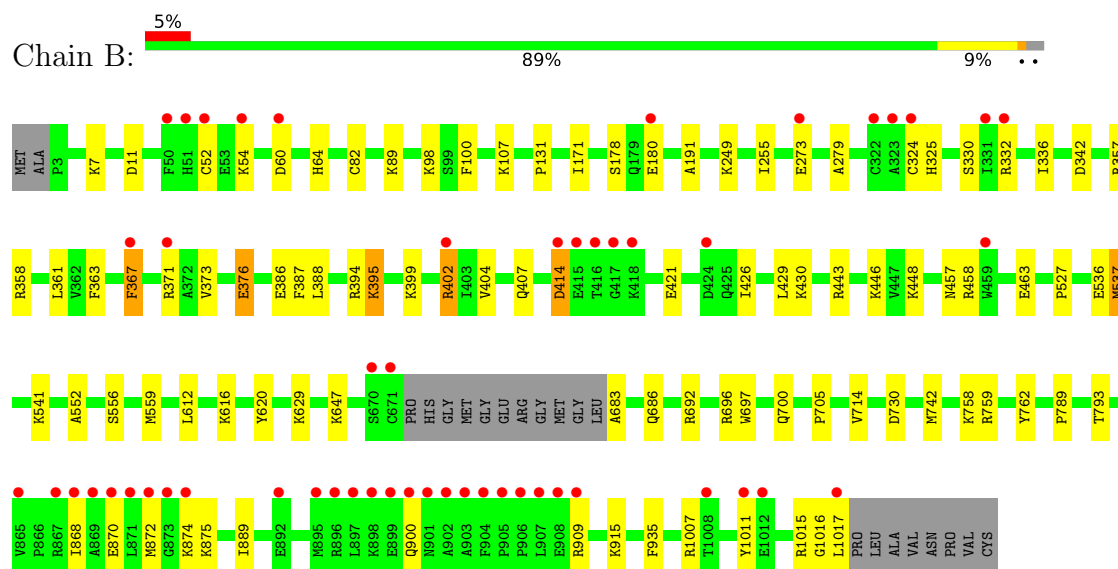
- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.06Å 158.94Å 163.21Å 90.00° 96.03° 90.00°	Depositor
Resolution (Å)	40.59 – 1.87 45.46 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.59-1.87) 98.3 (45.46-1.87)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.172 , 0.211 0.172 , 0.210	Depositor DCC
$R_{free}$ test set	16922 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	34870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FNR, FAD, Y3G, NAP

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	0.42	1/7887 (0.0%)	0.64	3/10691 (0.0%)
1	B	0.42	2/7813 (0.0%)	0.86	8/10590 (0.1%)
1	C	0.42	1/7813 (0.0%)	0.67	6/10590 (0.1%)
1	D	0.42	0/7908	0.75	4/10719 (0.0%)
All	All	0.42	4/31421 (0.0%)	0.73	21/42590 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	367	PHE	CB-CG	-7.49	1.38	1.51
1	A	367	PHE	CB-CG	-6.73	1.40	1.51
1	C	246	GLU	CB-CG	-6.26	1.40	1.52
1	B	395	LYS	CB-CG	-5.28	1.38	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	GLU	OE1-CD-OE2	-33.12	83.55	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	GLU	OE1-CD-OE2	-32.35	84.48	123.30
1	D	844	GLU	OE1-CD-OE2	-31.96	84.94	123.30
1	B	536	GLU	CG-CD-OE1	23.64	165.57	118.30
1	B	376	GLU	CG-CD-OE1	20.64	159.57	118.30
1	D	844	GLU	CG-CD-OE1	20.39	159.08	118.30
1	D	844	GLU	CG-CD-OE2	-16.94	84.41	118.30
1	B	376	GLU	CG-CD-OE2	-16.57	85.16	118.30
1	B	536	GLU	CG-CD-OE2	-16.56	85.18	118.30
1	C	363	PHE	CB-CG-CD2	-15.60	109.88	120.80
1	A	424	ASP	CB-CG-OD2	-10.41	108.94	118.30
1	C	363	PHE	CB-CG-CD1	9.15	127.20	120.80
1	C	363	PHE	CB-CA-C	8.52	127.44	110.40
1	A	424	ASP	CB-CG-OD1	8.44	125.90	118.30
1	B	361	LEU	CA-CB-CG	7.69	132.99	115.30
1	C	363	PHE	N-CA-CB	-6.00	99.81	110.60
1	C	363	PHE	CD1-CG-CD2	-5.85	110.69	118.30
1	A	443	ARG	CG-CD-NE	5.85	124.08	111.80
1	B	448	LYS	CD-CE-NZ	-5.83	98.28	111.70
1	C	908	GLU	CA-CB-CG	5.76	126.08	113.40
1	D	395	LYS	CD-CE-NZ	-5.62	98.78	111.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	ASP	Sidechain
1	A	50	PHE	Peptide
1	B	376	GLU	Sidechain
1	C	363	PHE	Sidechain
1	D	332	ARG	Sidechain
1	D	844	GLU	Sidechain

## 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	7727	0	7737	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7656	0	7677	69	0
1	C	7656	0	7677	77	0
1	D	7746	0	7769	80	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
3	A	53	0	30	2	0
3	B	53	0	30	2	0
3	C	53	0	30	2	0
3	D	53	0	31	3	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	48	0	25	6	0
5	B	48	0	25	7	0
5	C	48	0	25	5	0
5	D	48	0	25	7	0
6	A	31	0	21	3	0
6	B	31	0	21	1	0
6	C	31	0	21	1	0
6	D	31	0	21	3	0
7	A	867	0	0	15	3
7	B	770	0	0	19	3
7	C	861	0	0	14	2
7	D	891	0	0	22	1
All	All	34870	0	31165	275	5

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

All (275) 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:D:875:LYS:NZ	7:D:1201:HOH:O	1.84	1.06
1:C:340:ALA:HB2	1:C:363:PHE:HD2	1.17	1.02
1:D:332:ARG:NH1	7:D:1202:HOH:O	1.93	0.99
1:B:909:ARG:NH2	7:B:1201:HOH:O	1.99	0.96
1:C:340:ALA:HB2	1:C:363:PHE:CD2	2.04	0.92
1:D:689:GLU:OE1	1:D:692:ARG:NH1	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:SER:OG	1:B:180:GLU:OE2	1.91	0.88
1:D:175:CYS:SG	7:D:1251:HOH:O	2.37	0.83
1:C:470:GLN:NE2	7:C:1206:HOH:O	2.14	0.80
1:B:402:ARG:O	7:B:1202:HOH:O	2.00	0.79
1:C:703:GLN:OE1	7:C:1201:HOH:O	2.00	0.79
1:B:399:LYS:O	7:B:1202:HOH:O	2.00	0.78
1:D:693:ASN:OD1	1:D:696:ARG:NH2	2.17	0.78
1:A:896:ARG:NH2	7:A:1204:HOH:O	2.17	0.77
1:A:884:GLU:OE1	7:A:1201:HOH:O	2.02	0.77
1:A:263:GLU:OE1	7:A:1202:HOH:O	2.03	0.77
1:D:354:CYS:O	7:D:1202:HOH:O	2.01	0.76
1:D:331:ILE:N	7:D:1202:HOH:O	2.13	0.76
1:D:505:LYS:NZ	7:D:1207:HOH:O	2.18	0.75
1:C:716:ASP:OD1	7:C:1202:HOH:O	2.06	0.74
1:A:52:CYS:SG	7:A:1564:HOH:O	2.46	0.74
1:C:402:ARG:NH1	7:C:1205:HOH:O	2.08	0.74
1:C:246:GLU:OE2	1:C:908:GLU:HB2	1.86	0.74
1:C:908:GLU:OE2	7:C:1203:HOH:O	2.06	0.74
1:D:449:GLU:OE1	7:D:1204:HOH:O	2.07	0.73
1:D:696:ARG:NH1	7:D:1209:HOH:O	2.21	0.72
1:C:870:GLU:OE2	7:C:1204:HOH:O	2.07	0.71
1:A:342:ASP:HB3	5:A:1107:NAP:C4N	2.21	0.70
1:B:342:ASP:HB3	5:B:1106:NAP:C4N	2.22	0.70
1:D:870:GLU:HA	1:D:874:LYS:HE2	1.75	0.68
1:B:54:LYS:NZ	7:B:1210:HOH:O	2.26	0.68
1:D:413:GLN:O	7:D:1205:HOH:O	2.10	0.68
1:A:1017:LEU:O	7:A:1203:HOH:O	2.13	0.67
1:C:363:PHE:CE2	1:C:370:ILE:HD11	2.30	0.67
1:C:1015:ARG:O	1:C:1017:LEU:N	2.28	0.67
5:D:1107:NAP:O1A	7:D:1206:HOH:O	2.13	0.66
1:D:927:LYS:NZ	7:D:1203:HOH:O	1.97	0.66
1:A:52:CYS:HB3	1:A:384:LYS:HB2	1.76	0.66
1:B:60:ASP:OD2	7:B:1203:HOH:O	2.15	0.65
1:D:131:PRO:HB2	1:D:373:VAL:HG11	1.78	0.64
1:D:178:SER:OG	1:D:180:GLU:OE1	2.14	0.64
5:D:1107:NAP:O5D	5:D:1107:NAP:H6N	2.00	0.61
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.65	0.61
1:A:910:LYS:HD3	1:A:911:PRO:HD2	1.82	0.61
1:C:485:MET:HE3	7:C:1701:HOH:O	2.00	0.61
1:A:715:THR:HG23	1:B:686:GLN:HG2	1.81	0.60
1:B:407:GLN:NE2	1:B:426:ILE:HB	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:GLU:OE1	1:C:541:LYS:HE2	2.03	0.59
1:C:552:ALA:HB2	6:C:1107:FNR:H7M3	1.85	0.59
1:D:910:LYS:HE2	1:D:911:PRO:HD2	1.82	0.59
1:D:552:ALA:HB2	6:D:1108:FNR:H7M3	1.84	0.58
1:B:404:VAL:HG13	7:B:1202:HOH:O	2.01	0.58
1:C:518:LYS:O	1:C:520:GLU:HG3	2.03	0.58
1:C:371:ARG:HH12	5:C:1106:NAP:H3B	1.68	0.58
1:B:52:CYS:SG	7:B:1702:HOH:O	2.35	0.57
1:B:900:GLN:OE1	7:B:1205:HOH:O	2.17	0.57
1:A:131:PRO:HB2	1:A:373:VAL:HG11	1.86	0.57
1:A:264:ASN:ND2	7:A:1208:HOH:O	2.23	0.57
1:C:242:ASN:O	1:C:246:GLU:HG2	2.04	0.57
1:D:32:LEU:O	1:D:36:LEU:HD13	2.04	0.57
1:D:574:LYS:NZ	6:D:1108:FNR:H5	2.02	0.57
1:A:780:THR:HG22	1:B:762:TYR:CZ	2.40	0.57
1:D:397:ILE:HD13	1:D:428:HIS:CE1	2.39	0.57
1:B:357:ARG:NH2	7:B:1204:HOH:O	2.16	0.57
1:B:430:LYS:NZ	7:B:1229:HOH:O	2.38	0.57
1:B:541:LYS:NZ	7:B:1228:HOH:O	2.36	0.56
1:A:56:GLU:OE2	1:A:898:LYS:NZ	2.38	0.56
1:A:915:LYS:HD3	7:A:1236:HOH:O	2.04	0.56
1:B:692:ARG:O	1:B:696:ARG:HG3	2.05	0.56
3:B:1105:FAD:C5X	5:B:1106:NAP:C5N	2.84	0.56
1:B:131:PRO:HB2	1:B:373:VAL:HG11	1.88	0.55
1:C:270:THR:HA	1:C:273:GLU:HG2	1.87	0.55
1:C:1015:ARG:C	1:C:1017:LEU:H	2.09	0.55
1:C:342:ASP:HB2	5:C:1106:NAP:C5N	2.37	0.55
1:C:520:GLU:HB3	1:D:25:HIS:CD2	2.42	0.55
1:C:333:GLY:H	1:C:357:ARG:HG2	1.72	0.54
1:C:915:LYS:HG3	7:C:1311:HOH:O	2.07	0.54
1:A:399:LYS:HD3	7:A:1395:HOH:O	2.06	0.54
1:A:574:LYS:NZ	6:A:1108:FNR:H5	2.05	0.54
1:B:915:LYS:HG2	7:B:1351:HOH:O	2.06	0.54
1:A:669:LEU:HD13	1:A:691:VAL:HG22	1.89	0.54
1:C:263:GLU:OE1	1:C:449:GLU:HG2	2.07	0.54
1:A:776:ARG:O	1:A:780:THR:HG23	2.08	0.54
1:C:800:GLU:HG3	1:C:801:SER:N	2.21	0.54
1:C:582:ILE:HD11	1:D:1015:ARG:CZ	2.38	0.54
3:D:1105:FAD:N5	5:D:1107:NAP:H4N	2.22	0.54
1:B:556:SER:O	1:B:559:MET:HB2	2.06	0.54
3:B:1105:FAD:N5	5:B:1106:NAP:C4N	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:915:LYS:HA	1:D:915:LYS:HE2	1.90	0.53
1:C:246:GLU:OE2	1:C:908:GLU:CB	2.54	0.53
1:C:363:PHE:CZ	1:C:370:ILE:HD11	2.43	0.53
1:D:289:LYS:HE3	1:D:438:PHE:HB3	1.91	0.53
1:D:63:LYS:HE3	1:D:128:MET:HG2	1.91	0.53
1:A:518:LYS:O	1:A:520:GLU:HG2	2.08	0.53
1:A:367:PHE:CE1	1:B:367:PHE:CZ	2.97	0.53
1:B:394:ARG:NH2	1:B:421:GLU:OE1	2.34	0.53
1:D:358:ARG:NH1	7:D:1228:HOH:O	2.41	0.53
1:D:888:LYS:HE3	1:D:892:GLU:OE2	2.08	0.52
1:B:457:ASN:HB3	1:B:463:GLU:HG2	1.90	0.52
1:D:900:GLN:CD	1:D:901:ASN:H	2.13	0.52
1:B:759:ARG:HG2	1:B:759:ARG:HH11	1.74	0.52
1:A:378:GLU:O	1:A:382:GLU:HG2	2.10	0.52
1:C:178:SER:H	1:C:181:LYS:HE3	1.74	0.52
1:D:977:THR:OG1	7:D:1201:HOH:O	2.10	0.52
1:A:552:ALA:HB2	6:A:1108:FNR:H7M3	1.92	0.51
1:D:341:GLY:HA2	1:D:371:ARG:HB2	1.91	0.51
1:D:934:THR:OG1	1:D:937:GLU:HG3	2.10	0.51
1:A:42:LYS:HB2	7:A:1220:HOH:O	2.10	0.51
3:C:1105:FAD:C5X	5:C:1106:NAP:C5N	2.88	0.51
1:B:446:LYS:NZ	7:B:1237:HOH:O	2.43	0.51
1:A:612:LEU:HD11	1:B:935:PHE:CE1	2.46	0.51
1:B:1015:ARG:O	1:B:1017:LEU:N	2.44	0.51
1:A:868:ILE:O	1:A:872:MET:HG2	2.11	0.51
1:A:18:LEU:HD11	1:A:975:PRO:HA	1.93	0.50
1:C:442:LEU:O	7:C:1207:HOH:O	2.20	0.50
1:D:371:ARG:NH2	7:D:1206:HOH:O	2.16	0.50
3:A:1105:FAD:C5X	5:A:1107:NAP:C4N	2.90	0.49
1:C:910:LYS:NZ	7:C:1232:HOH:O	2.45	0.49
1:C:82:CYS:O	1:C:98:LYS:HD2	2.11	0.49
1:D:574:LYS:HZ2	6:D:1108:FNR:H5	1.59	0.49
1:C:363:PHE:HE2	1:C:370:ILE:HD11	1.77	0.49
1:D:12:ILE:O	1:D:15:ILE:HG22	2.12	0.49
1:B:89:LYS:NZ	7:B:1244:HOH:O	2.45	0.49
1:C:582:ILE:HD12	1:D:1019:LEU:HD11	1.95	0.48
1:B:870:GLU:HG3	1:B:889:ILE:HD13	1.95	0.48
1:A:367:PHE:HB2	1:B:386:GLU:OE2	2.13	0.48
1:B:552:ALA:HB2	6:B:1107:FNR:H7M3	1.95	0.48
1:A:743:GLY:O	7:A:1205:HOH:O	2.20	0.48
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:LEU:O	1:D:454:ILE:HG12	2.14	0.48
1:B:171:ILE:HG23	1:B:527:PRO:HD3	1.95	0.48
1:A:935:PHE:CE1	1:B:612:LEU:HD11	2.48	0.48
1:B:1007:ARG:HD3	1:B:1011:TYR:HB2	1.95	0.48
3:C:1105:FAD:N5	5:C:1106:NAP:C4N	2.77	0.48
1:C:868:ILE:HD11	1:C:893:GLU:HG2	1.96	0.48
1:D:124:LEU:HD13	1:D:160:SER:HB2	1.96	0.47
1:D:927:LYS:HB2	1:D:927:LYS:HE2	1.64	0.47
1:C:861:LYS:HG3	1:D:144:ALA:O	2.14	0.47
1:B:191:ALA:O	1:B:279:ALA:HA	2.15	0.47
1:A:342:ASP:CB	5:A:1107:NAP:C4N	2.91	0.47
1:C:342:ASP:HB3	5:C:1106:NAP:C4N	2.45	0.47
1:D:410:ARG:HD3	1:D:422:ASP:OD2	2.13	0.47
1:B:342:ASP:CB	5:B:1106:NAP:C5N	2.93	0.47
3:A:1105:FAD:N5	5:A:1107:NAP:C4N	2.78	0.47
1:B:874:LYS:HA	1:B:874:LYS:CE	2.45	0.46
1:C:35:LYS:HE3	1:D:485:MET:HG3	1.97	0.46
1:D:858:SER:HA	1:D:952:MET:HG2	1.98	0.46
1:C:331:ILE:HG22	1:C:331:ILE:O	2.16	0.46
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.97	0.46
1:B:683:ALA:HB3	1:B:686:GLN:OE1	2.15	0.46
1:A:367:PHE:CZ	1:B:367:PHE:CZ	3.04	0.46
1:A:428:HIS:O	7:A:1206:HOH:O	2.21	0.46
1:B:686:GLN:HG3	1:B:714:VAL:HG12	1.98	0.46
1:C:844:GLU:OE2	1:C:915:LYS:NZ	2.30	0.46
1:D:974:ASP:CG	7:D:1201:HOH:O	2.53	0.46
1:B:394:ARG:O	1:B:395:LYS:HG2	2.16	0.46
1:C:734:ALA:HA	1:C:735:THR:HA	1.74	0.46
1:B:443:ARG:O	1:B:443:ARG:HG2	2.16	0.46
1:C:228:THR:HG23	1:C:321:MET:HG3	1.97	0.45
1:C:593:GLY:HA3	1:C:606:SER:OG	2.16	0.45
1:C:582:ILE:HD11	1:D:1015:ARG:NE	2.31	0.45
1:B:900:GLN:NE2	7:B:1242:HOH:O	2.45	0.45
1:C:330:SER:O	1:C:331:ILE:HD13	2.16	0.45
1:B:759:ARG:HG2	1:B:759:ARG:NH1	2.31	0.45
1:C:63:LYS:HE3	1:C:128:MET:HB3	1.98	0.45
1:A:381:LYS:HG2	7:A:1264:HOH:O	2.16	0.45
1:A:892:GLU:O	1:A:896:ARG:HG2	2.17	0.45
1:D:898:LYS:NZ	7:D:1239:HOH:O	2.43	0.45
1:B:342:ASP:HB2	5:B:1106:NAP:C5N	2.46	0.45
1:C:191:ALA:O	1:C:279:ALA:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:LEU:HD11	1:D:935:PHE:CE1	2.52	0.45
1:A:574:LYS:HZ2	6:A:1108:FNR:H5	1.64	0.45
1:C:62:ILE:HD12	1:C:379:LEU:HD22	1.98	0.45
1:B:457:ASN:HB3	1:B:463:GLU:CG	2.47	0.45
1:C:363:PHE:HE2	1:C:370:ILE:CD1	2.30	0.45
1:A:716:ASP:OD1	7:A:1207:HOH:O	2.21	0.45
1:D:914:PRO:O	1:D:915:LYS:HE2	2.17	0.45
1:A:430:LYS:HG2	1:A:431:ALA:N	2.32	0.44
1:C:367:PHE:CZ	1:D:367:PHE:CE2	3.05	0.44
1:B:399:LYS:O	1:B:402:ARG:HD3	2.18	0.44
1:A:82:CYS:O	1:A:98:LYS:HD2	2.16	0.44
1:D:487:ASN:HB3	5:D:1107:NAP:O2D	2.17	0.44
1:D:53:GLU:HG2	1:D:887:LYS:HB3	1.98	0.44
1:C:872:MET:HE1	7:C:1745:HOH:O	2.17	0.44
1:D:402:ARG:NH2	7:D:1264:HOH:O	2.51	0.44
1:A:2:ALA:N	7:A:1252:HOH:O	2.50	0.44
1:A:191:ALA:O	1:A:279:ALA:HA	2.17	0.44
1:B:537:MET:HG3	1:B:789:PRO:HB3	1.99	0.44
1:D:577:SER:HB3	7:D:1651:HOH:O	2.16	0.44
1:D:343:THR:HA	3:D:1105:FAD:HM73	2.00	0.43
1:D:410:ARG:HG2	1:D:411:THR:N	2.32	0.43
1:D:459:TRP:O	1:D:460:ASP:HB2	2.17	0.43
1:A:734:ALA:HA	1:A:735:THR:HA	1.72	0.43
1:C:25:HIS:HB2	7:C:1903:HOH:O	2.17	0.43
1:C:331:ILE:HD12	1:C:433:VAL:HG21	2.00	0.43
1:D:19:ASN:OD1	1:D:20:PRO:HD2	2.18	0.43
1:D:193:LEU:HD23	1:D:281:ILE:HD13	2.00	0.43
1:D:857:GLU:OE2	1:D:857:GLU:HA	2.18	0.43
1:C:867:ARG:HD2	1:C:872:MET:CE	2.48	0.43
1:B:342:ASP:CB	5:B:1106:NAP:C4N	2.95	0.43
1:B:371:ARG:HG2	7:B:1221:HOH:O	2.19	0.43
1:B:705:PRO:HA	1:B:730:ASP:OD2	2.19	0.43
1:A:870:GLU:O	1:A:874:LYS:HG3	2.18	0.43
1:D:734:ALA:HA	1:D:735:THR:HA	1.74	0.43
1:C:1007:ARG:HD3	1:C:1011:TYR:HB2	2.01	0.43
1:A:29:HIS:HB2	7:B:1239:HOH:O	2.19	0.43
1:D:593:GLY:HA3	1:D:606:SER:OG	2.19	0.43
3:D:1105:FAD:C5X	5:D:1107:NAP:C4N	2.97	0.43
1:B:414:ASP:OD2	7:B:1206:HOH:O	2.21	0.43
1:B:868:ILE:H	1:B:872:MET:HE3	1.84	0.43
1:B:249:LYS:HE3	1:B:255:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:PHE:HE1	1:D:387:PHE:HE2	1.67	0.42
1:D:589:ARG:HG3	1:D:590:ILE:HG13	2.02	0.42
1:C:178:SER:N	1:C:181:LYS:HE3	2.35	0.42
1:D:857:GLU:CD	1:D:858:SER:H	2.22	0.42
1:C:340:ALA:CB	1:C:363:PHE:CD2	2.91	0.42
1:A:367:PHE:CZ	1:B:367:PHE:CE1	3.07	0.42
1:B:342:ASP:HB2	5:B:1106:NAP:C6N	2.50	0.42
1:D:342:ASP:CB	5:D:1107:NAP:C4N	2.98	0.42
1:C:131:PRO:HB2	1:C:373:VAL:HG11	2.01	0.42
1:C:178:SER:H	1:C:181:LYS:CE	2.32	0.42
1:B:647:LYS:HA	1:B:697:TRP:CE3	2.55	0.42
1:A:416:THR:HG23	1:A:418:LYS:H	1.85	0.42
1:B:446:LYS:HE2	1:B:446:LYS:HB2	1.73	0.42
1:D:924:VAL:HA	1:D:927:LYS:HD3	2.02	0.41
1:C:223:VAL:HG23	1:C:245:ILE:HD13	2.02	0.41
1:C:501:TRP:O	1:C:504:HIS:HB3	2.20	0.41
1:A:315:LYS:NZ	7:A:1265:HOH:O	2.53	0.41
1:D:485:MET:HE3	7:D:1554:HOH:O	2.21	0.41
1:D:533:ILE:O	1:D:545:PRO:HD3	2.21	0.41
1:B:875:LYS:HB3	1:B:875:LYS:HE3	1.77	0.41
1:A:888:LYS:O	1:A:892:GLU:HG3	2.21	0.41
1:D:394:ARG:HA	1:D:394:ARG:HD3	1.79	0.41
1:D:1014:LYS:HB3	7:D:1849:HOH:O	2.19	0.41
1:A:990:THR:HG22	1:A:990:THR:O	2.21	0.41
1:C:22:THR:HG23	1:D:828:GLN:HG3	2.02	0.41
1:C:629:LYS:HA	1:C:629:LYS:HD2	1.86	0.41
1:B:82:CYS:O	1:B:98:LYS:HD2	2.21	0.41
1:C:239:ASP:OD1	1:C:240:VAL:N	2.54	0.41
1:C:345:PHE:HE1	1:C:387:PHE:HE2	1.66	0.41
1:D:367:PHE:HZ	1:D:387:PHE:HB2	1.85	0.41
1:A:342:ASP:HB3	5:A:1107:NAP:C3N	2.50	0.41
1:A:342:ASP:HB2	5:A:1107:NAP:C5N	2.51	0.41
1:C:270:THR:HA	1:C:273:GLU:CG	2.51	0.41
1:A:47:LYS:NZ	1:A:48:ASN:OD1	2.50	0.41
1:A:452:SER:HA	1:A:453:PRO:HA	1.87	0.41
1:A:844:GLU:O	1:A:847:GLN:HG2	2.20	0.41
1:C:894:LYS:NZ	7:C:1250:HOH:O	2.51	0.41
1:D:367:PHE:HZ	1:D:387:PHE:CB	2.33	0.41
1:D:371:ARG:NH1	5:D:1107:NAP:O2X	2.54	0.41
1:D:458:ARG:HG3	7:D:1832:HOH:O	2.21	0.41
1:A:893:GLU:O	1:A:897:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:910:LYS:HG3	1:C:911:PRO:HD2	2.03	0.41
1:D:945:VAL:HG13	1:D:1007:ARG:HG2	2.03	0.41
1:C:410:ARG:HG3	1:C:425:GLN:HB3	2.02	0.41
1:B:696:ARG:O	1:B:700:GLN:HG3	2.21	0.41
1:C:870:GLU:HA	1:C:874:LYS:HE2	2.03	0.40
1:D:242:ASN:O	1:D:246:GLU:HG2	2.21	0.40
1:D:254:LYS:HB2	1:D:254:LYS:HE2	1.92	0.40
1:B:742:MET:O	1:B:742:MET:HG3	2.21	0.40
1:D:449:GLU:OE2	7:D:1210:HOH:O	2.22	0.40
1:B:107:LYS:HB3	7:B:1634:HOH:O	2.21	0.40
1:A:167:ASN:HB3	1:A:912:PHE:CD2	2.56	0.40
1:C:27:ALA:O	1:D:497:LYS:HE2	2.20	0.40
1:C:367:PHE:HB2	1:D:386:GLU:OE2	2.21	0.40
1:B:387:PHE:C	1:B:388:LEU:HD23	2.42	0.40
1:B:629:LYS:HD2	1:B:629:LYS:HA	1.90	0.40
1:B:874:LYS:HA	1:B:874:LYS:HE3	2.04	0.40
1:A:593:GLY:HA3	1:A:606:SER:OG	2.22	0.40
1:A:691:VAL:HG21	1:A:720:ILE:HG23	2.04	0.40
1:C:430:LYS:NZ	7:C:1217:HOH:O	2.35	0.40
1:C:870:GLU:HG3	1:C:889:ILE:HG23	2.04	0.40
1:B:336:ILE:HD11	1:B:429:LEU:HG	2.03	0.40
1:B:394:ARG:HA	1:B:394:ARG:HD3	1.72	0.40
1:B:616:LYS:HD3	1:B:620:TYR:CZ	2.57	0.40

All (5) 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)
7:A:1879:HOH:O	7:C:1910:HOH:O[1_556]	2.12	0.08
7:C:1752:HOH:O	7:B:1791:HOH:O[2_655]	2.13	0.07
7:A:1980:HOH:O	7:B:1963:HOH:O[1_455]	2.15	0.05
7:D:2031:HOH:O	7:B:1949:HOH:O[2_656]	2.18	0.02
7:A:1778:HOH:O	7:A:2028:HOH:O[1_455]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1014/1025 (99%)	974 (96%)	36 (4%)	4 (0%)	34	22
1	B	1000/1025 (98%)	964 (96%)	32 (3%)	4 (0%)	34	22
1	C	1000/1025 (98%)	967 (97%)	30 (3%)	3 (0%)	41	30
1	D	1015/1025 (99%)	973 (96%)	37 (4%)	5 (0%)	29	17
All	All	4029/4100 (98%)	3878 (96%)	135 (3%)	16 (0%)	34	22

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	905	PRO
1	C	325	HIS
1	B	414	ASP
1	C	1016	GLY
1	D	676	GLY
1	D	901	ASN
1	D	903	ALA
1	B	324	CYS
1	C	414	ASP
1	D	417	GLY
1	A	677	GLU
1	D	822	GLN
1	B	325	HIS
1	B	1016	GLY
1	A	794	GLY
1	A	3	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	841/854 (98%)	834 (99%)	7 (1%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	834/854 (98%)	820 (98%)	14 (2%)	60	54
1	C	834/854 (98%)	826 (99%)	8 (1%)	76	73
1	D	844/854 (99%)	833 (99%)	11 (1%)	69	64
All	All	3353/3416 (98%)	3313 (99%)	40 (1%)	71	67

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	100	PHE
1	A	373	VAL
1	A	455	LYS
1	A	893	GLU
1	A	915	LYS
1	A	916	LYS
1	C	11	ASP
1	C	100	PHE
1	C	332	ARG
1	C	361	LEU
1	C	363	PHE
1	C	371	ARG
1	C	402	ARG
1	C	793	THR
1	D	47	LYS
1	D	100	PHE
1	D	363	PHE
1	D	402	ARG
1	D	460	ASP
1	D	518	LYS
1	D	680	MET
1	D	793	THR
1	D	847	GLN
1	D	1007	ARG
1	D	1012	GLU
1	B	7	LYS
1	B	11	ASP
1	B	64	HIS
1	B	100	PHE
1	B	273	GLU
1	B	330	SER
1	B	332	ARG

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Mol	Chain	Res	Type
1	B	358	ARG
1	B	363	PHE
1	B	402	ARG
1	B	458	ARG
1	B	537	MET
1	B	758	LYS
1	B	793	THR

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

Mol	Chain	Res	Type
1	A	25	HIS
1	A	700	GLN
1	C	847	GLN
1	D	23	GLN
1	D	25	HIS
1	D	428	HIS
1	D	487	ASN
1	B	407	GLN
1	B	487	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

32 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
5	NAP	D	1107	-	45,52,52	2.31	12 (26%)	56,80,80	1.97	14 (25%)
2	SF4	B	1101	1	0,12,12	0.00	-	-		
3	FAD	A	1105	-	51,58,58	4.56	20 (39%)	60,89,89	2.35	13 (21%)
2	SF4	D	1101	1	0,12,12	0.00	-	-		
2	SF4	A	1104	1	0,12,12	0.00	-	-		
5	NAP	B	1106	-	45,52,52	2.64	16 (35%)	56,80,80	1.90	15 (26%)
4	Y3G	D	1106	-	9,10,10	2.30	5 (55%)	6,13,13	5.89	5 (83%)
6	FNR	C	1107	-	31,33,33	3.87	13 (41%)	40,50,50	2.54	12 (30%)
5	NAP	A	1107	-	45,52,52	2.69	11 (24%)	56,80,80	1.93	13 (23%)
2	SF4	A	1101	1	0,12,12	0.00	-	-		
4	Y3G	C	1108	1	9,10,10	2.61	4 (44%)	6,13,13	8.99	6 (100%)
6	FNR	A	1108	-	31,33,33	3.82	15 (48%)	40,50,50	2.36	11 (27%)
2	SF4	D	1102	1	0,12,12	0.00	-	-		
2	SF4	A	1102	1	0,12,12	0.00	-	-		
2	SF4	B	1104	1	0,12,12	0.00	-	-		
2	SF4	D	1103	1	0,12,12	0.00	-	-		
4	Y3G	B	1108	1	9,10,10	2.56	4 (44%)	6,13,13	8.72	5 (83%)
2	SF4	C	1102	1	0,12,12	0.00	-	-		
3	FAD	D	1105	-	51,58,58	4.50	22 (43%)	60,89,89	2.44	12 (20%)
4	Y3G	A	1106	-	9,10,10	2.11	2 (22%)	6,13,13	5.69	5 (83%)
2	SF4	D	1104	1	0,12,12	0.00	-	-		
5	NAP	C	1106	-	45,52,52	2.41	14 (31%)	56,80,80	1.88	14 (25%)
2	SF4	C	1103	1	0,12,12	0.00	-	-		
3	FAD	C	1105	-	51,58,58	4.56	21 (41%)	60,89,89	2.40	15 (25%)
2	SF4	C	1101	1	0,12,12	0.00	-	-		
6	FNR	B	1107	-	31,33,33	3.94	14 (45%)	40,50,50	2.02	9 (22%)
2	SF4	B	1102	1	0,12,12	0.00	-	-		
2	SF4	B	1103	1	0,12,12	0.00	-	-		
3	FAD	B	1105	-	51,58,58	4.62	20 (39%)	60,89,89	2.49	12 (20%)
2	SF4	C	1104	1	0,12,12	0.00	-	-		
6	FNR	D	1108	-	31,33,33	3.74	13 (41%)	40,50,50	2.22	9 (22%)
2	SF4	A	1103	1	0,12,12	0.00	-	-		

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
5	NAP	D	1107	-	-	6/31/67/67	0/5/5/5
3	FAD	A	1105	-	-	2/30/50/50	0/6/6/6
2	SF4	B	1101	1	-	-	0/6/5/5
2	SF4	D	1101	1	-	-	0/6/5/5
2	SF4	A	1104	1	-	-	0/6/5/5
5	NAP	B	1106	-	-	5/31/67/67	0/5/5/5
4	Y3G	D	1106	-	-	0/0/2/2	0/1/1/1
6	FNR	C	1107	-	1/1/4/4	7/18/18/18	0/3/3/3
5	NAP	A	1107	-	-	3/31/67/67	0/5/5/5
2	SF4	A	1101	1	-	-	0/6/5/5
4	Y3G	C	1108	1	-	0/0/2/2	0/1/1/1
6	FNR	A	1108	-	1/1/4/4	7/18/18/18	0/3/3/3
2	SF4	D	1102	1	-	-	0/6/5/5
2	SF4	A	1102	1	-	-	0/6/5/5
2	SF4	B	1104	1	-	-	0/6/5/5
2	SF4	D	1103	1	-	-	0/6/5/5
4	Y3G	B	1108	1	-	0/0/2/2	0/1/1/1
3	FAD	D	1105	-	-	2/30/50/50	0/6/6/6
2	SF4	C	1102	1	-	-	0/6/5/5
4	Y3G	A	1106	-	-	0/0/2/2	0/1/1/1
5	NAP	C	1106	-	-	1/31/67/67	0/5/5/5
2	SF4	D	1104	1	-	-	0/6/5/5
2	SF4	C	1103	1	-	-	0/6/5/5
3	FAD	C	1105	-	-	1/30/50/50	0/6/6/6
2	SF4	C	1101	1	-	-	0/6/5/5
6	FNR	B	1107	-	1/1/4/4	8/18/18/18	0/3/3/3
2	SF4	B	1102	1	-	-	0/6/5/5
2	SF4	B	1103	1	-	-	0/6/5/5
3	FAD	B	1105	-	-	1/30/50/50	0/6/6/6
2	SF4	C	1104	1	-	-	0/6/5/5
6	FNR	D	1108	-	1/1/4/4	7/18/18/18	0/3/3/3
2	SF4	A	1103	1	-	-	0/6/5/5

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1105	FAD	O4B-C1B	14.26	1.61	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1105	FAD	O4B-C1B	14.23	1.60	1.41
3	B	1105	FAD	C2B-C1B	-14.17	1.32	1.53
3	C	1105	FAD	O4B-C1B	14.08	1.60	1.41
3	D	1105	FAD	O4B-C1B	13.65	1.60	1.41
3	C	1105	FAD	C2B-C1B	-13.41	1.33	1.53
3	D	1105	FAD	C2B-C1B	-13.33	1.33	1.53
3	A	1105	FAD	C2B-C1B	-13.22	1.33	1.53
6	B	1107	FNR	CAA-N1	11.36	1.47	1.33
3	B	1105	FAD	C10-N1	11.25	1.47	1.33
5	B	1106	NAP	P2B-O2B	11.01	1.80	1.59
3	A	1105	FAD	C10-N1	10.92	1.47	1.33
6	C	1107	FNR	CAA-N1	10.88	1.47	1.33
6	A	1108	FNR	CAA-N1	10.54	1.46	1.33
3	D	1105	FAD	C10-N1	10.38	1.46	1.33
3	C	1105	FAD	C10-N1	10.18	1.46	1.33
5	D	1107	NAP	P2B-O2B	10.18	1.78	1.59
6	D	1108	FNR	CAA-N1	10.12	1.46	1.33
3	B	1105	FAD	C5X-N5	9.73	1.51	1.35
5	A	1107	NAP	P2B-O2B	9.48	1.77	1.59
3	C	1105	FAD	C5X-N5	9.45	1.51	1.35
3	D	1105	FAD	C4X-N5	9.30	1.46	1.33
3	C	1105	FAD	C4X-N5	9.28	1.46	1.33
3	B	1105	FAD	C4X-N5	9.19	1.46	1.33
3	D	1105	FAD	C5X-N5	9.16	1.50	1.35
5	C	1106	NAP	P2B-O2B	8.98	1.76	1.59
3	A	1105	FAD	C5X-N5	8.91	1.50	1.35
3	A	1105	FAD	C4X-N5	8.87	1.46	1.33
3	A	1105	FAD	C9A-N10	8.11	1.49	1.38
3	C	1105	FAD	C9A-N10	7.87	1.49	1.38
3	D	1105	FAD	C9A-N10	7.57	1.48	1.38
5	A	1107	NAP	C4N-C3N	7.55	1.52	1.39
3	B	1105	FAD	C9A-N10	7.39	1.48	1.38
3	D	1105	FAD	C4-N3	7.37	1.45	1.33
3	A	1105	FAD	C4-N3	7.29	1.45	1.33
3	A	1105	FAD	C4-C4X	7.28	1.53	1.41
3	C	1105	FAD	C4-C4X	7.16	1.53	1.41
3	C	1105	FAD	C4-N3	6.99	1.45	1.33
3	B	1105	FAD	C4-N3	6.94	1.45	1.33
3	D	1105	FAD	C4-C4X	6.88	1.53	1.41
3	B	1105	FAD	C4-C4X	6.65	1.52	1.41
3	C	1105	FAD	C2-N3	6.52	1.51	1.38
5	A	1107	NAP	C5N-C4N	6.51	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1107	FNR	C4A-N5	6.49	1.42	1.33
6	C	1107	FNR	C4-C4A	6.46	1.52	1.41
5	B	1106	NAP	C5N-C4N	6.44	1.52	1.38
6	B	1107	FNR	C4A-N5	6.43	1.42	1.33
6	D	1108	FNR	C9A-N10	6.38	1.47	1.38
6	B	1107	FNR	C4A-CAA	-6.31	1.32	1.38
3	D	1105	FAD	C2-N3	6.28	1.50	1.38
6	B	1107	FNR	C9A-N10	6.25	1.47	1.38
6	C	1107	FNR	C5A-N5	6.22	1.45	1.35
6	D	1108	FNR	C4A-N5	6.20	1.42	1.33
3	A	1105	FAD	C2-N3	6.19	1.50	1.38
6	A	1108	FNR	C9A-N10	6.16	1.46	1.38
3	C	1105	FAD	O4B-C4B	-6.15	1.31	1.45
6	D	1108	FNR	C4-C4A	6.11	1.51	1.41
6	A	1108	FNR	O4-C4	6.00	1.39	1.24
5	C	1106	NAP	C5N-C4N	6.00	1.51	1.38
6	B	1107	FNR	C9A-C5A	-5.97	1.30	1.42
6	C	1107	FNR	C9A-N10	5.97	1.46	1.38
6	A	1108	FNR	C9A-C5A	-5.96	1.30	1.42
6	D	1108	FNR	C4A-CAA	-5.92	1.32	1.38
3	B	1105	FAD	O4B-C4B	-5.91	1.31	1.45
6	A	1108	FNR	C4A-N5	5.90	1.41	1.33
5	B	1106	NAP	C4N-C3N	5.88	1.49	1.39
6	D	1108	FNR	O4-C4	5.87	1.39	1.24
6	B	1107	FNR	O4-C4	5.87	1.39	1.24
3	D	1105	FAD	O4B-C4B	-5.86	1.31	1.45
3	A	1105	FAD	O4B-C4B	-5.81	1.32	1.45
5	C	1106	NAP	C4N-C3N	5.79	1.49	1.39
6	A	1108	FNR	C4-C4A	5.75	1.51	1.41
3	B	1105	FAD	C4X-C10	5.74	1.44	1.38
6	A	1108	FNR	C4A-CAA	-5.69	1.33	1.38
3	B	1105	FAD	C2-N3	5.69	1.49	1.38
6	C	1107	FNR	O4-C4	5.60	1.38	1.24
6	B	1107	FNR	C4-C4A	5.57	1.51	1.41
6	A	1108	FNR	C5A-N5	5.56	1.44	1.35
5	A	1107	NAP	C2N-N1N	5.52	1.41	1.35
6	C	1107	FNR	C9A-C5A	-5.41	1.31	1.42
3	A	1105	FAD	C4X-C10	5.39	1.44	1.38
5	D	1107	NAP	C5N-C4N	5.38	1.50	1.38
6	B	1107	FNR	C5A-N5	5.34	1.44	1.35
6	D	1108	FNR	C9A-C5A	-5.27	1.32	1.42
6	D	1108	FNR	C5A-N5	5.24	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1108	FNR	C6-C5A	5.08	1.49	1.41
6	C	1107	FNR	C4A-CAA	-5.07	1.33	1.38
3	B	1105	FAD	C2-N1	5.05	1.48	1.38
4	C	1108	Y3G	C06-C09	4.99	1.52	1.43
3	C	1105	FAD	C4X-C10	4.98	1.43	1.38
4	D	1106	Y3G	C06-C09	4.97	1.52	1.43
3	C	1105	FAD	C2-N1	4.96	1.48	1.38
3	D	1105	FAD	C4X-C10	4.93	1.43	1.38
6	D	1108	FNR	C6-C5A	4.92	1.49	1.41
4	B	1108	Y3G	C06-C09	4.90	1.52	1.43
6	B	1107	FNR	C9-C9A	4.90	1.50	1.40
6	C	1107	FNR	C9-C9A	4.88	1.50	1.40
6	C	1107	FNR	C6-C5A	4.88	1.49	1.41
6	B	1107	FNR	C6-C5A	4.83	1.49	1.41
3	A	1105	FAD	C2-N1	4.75	1.47	1.38
4	A	1106	Y3G	C06-C09	4.70	1.52	1.43
6	D	1108	FNR	C9-C9A	4.70	1.50	1.40
3	D	1105	FAD	C2-N1	4.58	1.47	1.38
6	A	1108	FNR	C9-C9A	4.53	1.49	1.40
5	D	1107	NAP	C4N-C3N	4.41	1.46	1.39
5	A	1107	NAP	PN-O5D	4.35	1.76	1.59
5	A	1107	NAP	C7N-N7N	4.32	1.41	1.33
3	C	1105	FAD	C1'-N10	4.20	1.52	1.48
6	C	1107	FNR	C4-N3	4.14	1.40	1.33
6	A	1108	FNR	C4-N3	4.07	1.40	1.33
6	B	1107	FNR	C4-N3	4.02	1.40	1.33
4	C	1108	Y3G	C09-C10	3.95	1.31	1.17
4	B	1108	Y3G	C09-C10	3.82	1.31	1.17
5	D	1107	NAP	C7N-N7N	3.70	1.40	1.33
3	D	1105	FAD	C1'-N10	3.58	1.51	1.48
5	C	1106	NAP	PN-O5D	3.56	1.73	1.59
5	B	1106	NAP	PN-O5D	3.55	1.73	1.59
5	B	1106	NAP	C2N-N1N	3.52	1.39	1.35
6	D	1108	FNR	C4-N3	3.52	1.39	1.33
3	D	1105	FAD	C6A-N6A	3.51	1.46	1.34
3	A	1105	FAD	C2A-N3A	3.44	1.37	1.32
3	A	1105	FAD	C6A-N6A	3.41	1.46	1.34
5	B	1106	NAP	C7N-N7N	3.40	1.39	1.33
5	C	1106	NAP	O2B-C2B	-3.33	1.32	1.44
5	A	1107	NAP	O2B-C2B	-3.30	1.32	1.44
3	B	1105	FAD	C1'-N10	3.29	1.51	1.48
3	C	1105	FAD	C6A-N6A	3.27	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1107	NAP	O2B-C2B	-3.27	1.32	1.44
3	B	1105	FAD	C6A-N6A	3.26	1.45	1.34
6	C	1107	FNR	C2-N1	3.25	1.44	1.38
3	B	1105	FAD	C2A-N3A	3.15	1.37	1.32
3	D	1105	FAD	C2A-N3A	3.14	1.37	1.32
3	D	1105	FAD	C5A-C4A	-3.13	1.32	1.40
3	A	1105	FAD	C1'-N10	3.13	1.51	1.48
3	B	1105	FAD	C5'-C4'	3.11	1.56	1.51
5	B	1106	NAP	O2B-C2B	-3.06	1.33	1.44
3	C	1105	FAD	C8M-C8	3.05	1.57	1.51
3	D	1105	FAD	C8M-C8	2.99	1.57	1.51
3	C	1105	FAD	C2A-N3A	2.98	1.36	1.32
3	B	1105	FAD	C7M-C7	2.98	1.57	1.51
3	B	1105	FAD	C8M-C8	2.94	1.56	1.51
3	A	1105	FAD	C5A-C4A	-2.94	1.33	1.40
5	C	1106	NAP	C7N-N7N	2.93	1.38	1.33
3	A	1105	FAD	C8M-C8	2.90	1.56	1.51
3	C	1105	FAD	O3B-C3B	-2.89	1.36	1.43
3	A	1105	FAD	O3B-C3B	-2.88	1.36	1.43
4	B	1108	Y3G	C03-N02	-2.82	1.32	1.38
5	A	1107	NAP	C6N-N1N	2.82	1.42	1.35
3	C	1105	FAD	C5A-C4A	-2.81	1.33	1.40
3	C	1105	FAD	C7M-C7	2.76	1.56	1.51
6	B	1107	FNR	C2-N1	2.75	1.43	1.38
5	C	1106	NAP	C3N-C7N	-2.72	1.46	1.50
3	B	1105	FAD	C5A-C4A	-2.72	1.33	1.40
3	D	1105	FAD	C7M-C7	2.71	1.56	1.51
3	B	1105	FAD	O3B-C3B	-2.69	1.36	1.43
5	C	1106	NAP	C6N-N1N	2.66	1.41	1.35
3	D	1105	FAD	C5'-C4'	2.66	1.55	1.51
3	A	1105	FAD	C7M-C7	2.64	1.56	1.51
3	A	1105	FAD	O2B-C2B	2.62	1.49	1.43
5	D	1107	NAP	C2N-N1N	2.61	1.38	1.35
6	A	1108	FNR	C2-N1	2.61	1.43	1.38
3	C	1105	FAD	C5'-C4'	2.54	1.55	1.51
4	B	1108	Y3G	C03-N04	-2.54	1.33	1.38
3	D	1105	FAD	O3B-C3B	-2.52	1.37	1.43
5	C	1106	NAP	C2N-C3N	-2.51	1.35	1.39
5	B	1106	NAP	C2A-N3A	2.50	1.36	1.32
5	B	1106	NAP	C6N-N1N	2.50	1.41	1.35
4	C	1108	Y3G	C03-N04	-2.48	1.33	1.38
5	C	1106	NAP	C2N-N1N	2.46	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1107	NAP	C6N-C5N	-2.45	1.33	1.38
5	B	1106	NAP	C2A-N1A	2.43	1.38	1.33
4	D	1106	Y3G	C01-C06	-2.43	1.37	1.43
4	C	1108	Y3G	C03-N02	-2.41	1.33	1.38
5	B	1106	NAP	C2N-C3N	-2.36	1.35	1.39
6	B	1107	FNR	P-O1P	-2.35	1.45	1.54
5	A	1107	NAP	O4D-C1D	2.35	1.44	1.41
6	A	1108	FNR	P-O3P	-2.33	1.45	1.54
5	D	1107	NAP	PN-O5D	2.32	1.68	1.59
6	B	1107	FNR	P-O3P	-2.30	1.46	1.54
3	D	1105	FAD	O4-C4	-2.30	1.18	1.24
5	B	1106	NAP	O5D-C5D	-2.28	1.36	1.44
5	C	1106	NAP	O4D-C1D	2.27	1.44	1.41
5	A	1107	NAP	C4A-N3A	2.26	1.38	1.35
5	B	1106	NAP	C4A-N3A	2.22	1.38	1.35
4	D	1106	Y3G	C03-N04	-2.21	1.33	1.38
5	D	1107	NAP	O2D-C2D	-2.19	1.37	1.43
5	A	1107	NAP	C6N-C5N	-2.18	1.33	1.38
5	C	1106	NAP	O4B-C4B	-2.18	1.40	1.45
5	D	1107	NAP	C6N-N1N	2.17	1.40	1.35
6	D	1108	FNR	P-O1P	-2.17	1.46	1.54
5	D	1107	NAP	C3N-C7N	-2.16	1.47	1.50
5	B	1106	NAP	C3N-C7N	-2.15	1.47	1.50
5	D	1107	NAP	C2N-C3N	-2.15	1.35	1.39
5	C	1106	NAP	C2A-N1A	2.13	1.37	1.33
4	D	1106	Y3G	O08-C01	-2.12	1.19	1.24
4	A	1106	Y3G	O08-C01	-2.11	1.19	1.24
6	D	1108	FNR	C2-N1	2.11	1.42	1.38
5	B	1106	NAP	C6N-C5N	-2.09	1.34	1.38
6	A	1108	FNR	P-O1P	-2.09	1.46	1.54
6	C	1107	FNR	P-O1P	-2.06	1.46	1.54
4	D	1106	Y3G	C03-N02	-2.03	1.34	1.38
5	B	1106	NAP	O4B-C4B	-2.03	1.40	1.45
5	C	1106	NAP	C6N-C5N	-2.03	1.34	1.38
3	C	1105	FAD	C6-C7	2.03	1.42	1.37
3	D	1105	FAD	C4A-N3A	2.03	1.38	1.35
6	A	1108	FNR	O4'-C4'	-2.02	1.39	1.43

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1108	Y3G	C06-C09-C10	-16.31	123.85	176.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1108	Y3G	C06-C09-C10	-15.83	125.42	176.48
4	D	1106	Y3G	N04-C03-N02	-10.58	120.02	128.43
4	A	1106	Y3G	N04-C03-N02	-10.50	120.08	128.43
4	C	1108	Y3G	N04-C03-N02	-9.67	120.74	128.43
4	B	1108	Y3G	C06-C01-N02	-9.16	118.02	124.40
3	B	1105	FAD	C4-N3-C2	8.31	122.16	115.14
6	C	1107	FNR	C1'-N10-C9A	8.11	124.68	118.29
4	B	1108	Y3G	C01-N02-C03	7.91	121.82	115.14
3	C	1105	FAD	C5A-C6A-N6A	7.81	132.22	120.35
3	B	1105	FAD	C5A-C6A-N6A	7.56	131.84	120.35
4	C	1108	Y3G	C06-C01-N02	-7.44	119.21	124.40
4	C	1108	Y3G	C01-N02-C03	7.37	121.36	115.14
4	B	1108	Y3G	N04-C03-N02	-7.15	122.74	128.43
5	C	1106	NAP	C5N-C4N-C3N	-7.15	111.88	120.34
5	B	1106	NAP	C5N-C4N-C3N	-7.04	112.02	120.34
3	A	1105	FAD	C5A-C6A-N6A	6.95	130.91	120.35
3	D	1105	FAD	C5A-C6A-N6A	6.90	130.84	120.35
3	D	1105	FAD	C1'-N10-C9A	6.90	123.72	118.29
3	A	1105	FAD	C7M-C7-C8	6.60	134.26	120.74
4	D	1106	Y3G	C01-N02-C03	6.55	120.67	115.14
5	A	1107	NAP	C5N-C4N-C3N	-6.53	112.62	120.34
3	A	1105	FAD	C7M-C7-C6	-6.43	104.96	120.34
5	D	1107	NAP	C5N-C4N-C3N	-6.36	112.81	120.34
3	B	1105	FAD	C7M-C7-C8	6.31	133.66	120.74
3	D	1105	FAD	C4-N3-C2	6.28	120.44	115.14
3	B	1105	FAD	C7M-C7-C6	-6.25	105.39	120.34
3	D	1105	FAD	C7M-C7-C8	6.22	133.49	120.74
3	C	1105	FAD	C4-N3-C2	6.07	120.27	115.14
3	A	1105	FAD	C4-N3-C2	6.01	120.22	115.14
6	D	1108	FNR	C1'-N10-C9A	5.95	122.98	118.29
3	D	1105	FAD	C7M-C7-C6	-5.93	106.15	120.34
6	A	1108	FNR	C1'-N10-C9A	5.87	122.91	118.29
6	A	1108	FNR	C4-N3-C2	5.87	120.10	115.14
3	D	1105	FAD	N3A-C2A-N1A	-5.83	119.56	128.68
4	D	1106	Y3G	C06-C01-N02	-5.80	120.36	124.40
3	C	1105	FAD	N3A-C2A-N1A	-5.76	119.67	128.68
6	C	1107	FNR	O5'-C5'-C4'	-5.76	93.98	109.36
3	A	1105	FAD	N3A-C2A-N1A	-5.69	119.78	128.68
4	A	1106	Y3G	C01-N02-C03	5.68	119.94	115.14
3	B	1105	FAD	C1'-N10-C9A	5.58	122.69	118.29
3	C	1105	FAD	C1'-N10-C9A	5.51	122.63	118.29
3	C	1105	FAD	C7M-C7-C6	-5.44	107.33	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1107	FNR	O5'-C5'-C4'	-5.35	95.08	109.36
5	A	1107	NAP	O7N-C7N-C3N	5.29	125.97	119.63
4	A	1106	Y3G	C06-C01-N02	-5.26	120.73	124.40
3	C	1105	FAD	N6A-C6A-N1A	-5.18	107.82	118.57
6	D	1108	FNR	O5'-C5'-C4'	-5.04	95.89	109.36
3	C	1105	FAD	C7M-C7-C8	5.04	131.07	120.74
5	A	1107	NAP	PN-O3-PA	-5.04	115.53	132.83
5	B	1106	NAP	PN-O3-PA	-5.01	115.65	132.83
3	B	1105	FAD	N3A-C2A-N1A	-4.96	120.92	128.68
5	D	1107	NAP	PN-O3-PA	-4.96	115.82	132.83
6	A	1108	FNR	O5'-C5'-C4'	-4.95	96.15	109.36
3	B	1105	FAD	N6A-C6A-N1A	-4.95	108.31	118.57
5	C	1106	NAP	PN-O3-PA	-4.90	116.00	132.83
6	B	1107	FNR	C4-N3-C2	4.86	119.24	115.14
6	D	1108	FNR	C4-N3-C2	4.76	119.17	115.14
6	C	1107	FNR	C4-N3-C2	4.75	119.15	115.14
6	C	1107	FNR	O4'-C4'-C3'	4.66	120.42	109.10
3	D	1105	FAD	C5X-C9A-N10	4.62	121.06	117.72
3	D	1105	FAD	N6A-C6A-N1A	-4.50	109.23	118.57
3	A	1105	FAD	N6A-C6A-N1A	-4.45	109.33	118.57
6	D	1108	FNR	O1P-P-O5'	4.44	118.56	106.73
6	C	1107	FNR	O1P-P-O5'	4.42	118.49	106.73
6	A	1108	FNR	C5A-C9A-N10	4.33	120.86	117.72
6	A	1108	FNR	O4'-C4'-C3'	4.28	119.49	109.10
3	A	1105	FAD	C1'-N10-C9A	4.19	121.59	118.29
3	B	1105	FAD	C4X-C4-N3	-4.13	117.79	123.43
5	D	1107	NAP	O2B-P2B-O1X	-4.12	93.49	109.39
6	C	1107	FNR	C9A-N10-CAA	-4.11	116.53	121.91
6	A	1108	FNR	C9A-N10-CAA	-4.11	116.53	121.91
4	A	1106	Y3G	C05-N04-C03	4.02	122.00	115.36
6	B	1107	FNR	C5A-C9A-N10	4.00	120.61	117.72
6	D	1108	FNR	O4'-C4'-C3'	3.97	118.74	109.10
6	C	1107	FNR	C5A-C9A-N10	3.89	120.54	117.72
6	A	1108	FNR	O3'-C3'-C4'	3.89	118.21	108.81
6	B	1107	FNR	O4'-C4'-C3'	3.84	118.44	109.10
5	D	1107	NAP	O7N-C7N-C3N	3.74	124.11	119.63
6	D	1108	FNR	C9A-N10-CAA	-3.73	117.03	121.91
6	A	1108	FNR	O1P-P-O5'	3.67	116.50	106.73
6	B	1107	FNR	O1P-P-O5'	3.61	116.34	106.73
4	D	1106	Y3G	C05-N04-C03	3.57	121.25	115.36
3	C	1105	FAD	C4X-C4-N3	-3.54	118.59	123.43
6	A	1108	FNR	C4A-C4-N3	-3.50	118.65	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1106	NAP	C2N-C3N-C4N	3.48	122.20	118.26
5	B	1106	NAP	O7N-C7N-C3N	3.47	123.79	119.63
3	C	1105	FAD	C5X-C9A-N10	3.46	120.22	117.72
3	A	1105	FAD	C4X-C4-N3	-3.45	118.72	123.43
5	B	1106	NAP	C2N-C3N-C4N	3.41	122.13	118.26
3	C	1105	FAD	C8M-C8-C7	-3.39	113.80	120.74
6	B	1107	FNR	C9A-N10-CAA	-3.30	117.59	121.91
4	C	1108	Y3G	C05-N04-C03	3.29	120.79	115.36
5	D	1107	NAP	O5D-PN-O1N	-3.29	96.21	109.07
3	A	1105	FAD	C5X-C9A-N10	3.23	120.06	117.72
5	A	1107	NAP	C2N-C3N-C4N	3.16	121.84	118.26
5	D	1107	NAP	PN-O5D-C5D	-3.13	103.30	121.68
6	B	1107	FNR	O3'-C3'-C4'	3.12	116.36	108.81
3	D	1105	FAD	C4X-C4-N3	-3.11	119.17	123.43
6	C	1107	FNR	C4A-C4-N3	-3.11	119.17	123.43
3	A	1105	FAD	C4X-N5-C5X	3.08	119.84	116.77
6	D	1108	FNR	O3'-C3'-C4'	3.07	116.23	108.81
6	D	1108	FNR	C5A-C9A-N10	3.06	119.93	117.72
5	B	1106	NAP	O2B-P2B-O1X	-3.05	97.62	109.39
5	C	1106	NAP	O2B-P2B-O1X	-3.04	97.67	109.39
6	B	1107	FNR	C1'-N10-C9A	2.98	120.64	118.29
6	D	1108	FNR	C4A-C4-N3	-2.96	119.39	123.43
5	D	1107	NAP	O7N-C7N-N7N	-2.89	118.47	122.58
6	C	1107	FNR	O2'-C2'-C3'	-2.89	102.07	109.10
6	B	1107	FNR	C4A-C4-N3	-2.89	119.48	123.43
5	C	1106	NAP	O7N-C7N-C3N	2.84	123.03	119.63
5	A	1107	NAP	O7N-C7N-N7N	-2.83	118.55	122.58
3	B	1105	FAD	C8M-C8-C7	-2.81	114.99	120.74
3	D	1105	FAD	C5'-C4'-C3'	-2.76	106.88	112.20
3	C	1105	FAD	O4B-C1B-C2B	-2.75	102.91	106.93
3	B	1105	FAD	C5X-C9A-N10	2.74	119.70	117.72
6	C	1107	FNR	O3'-C3'-C4'	2.74	115.42	108.81
5	D	1107	NAP	O3X-P2B-O2X	2.73	118.08	107.64
5	D	1107	NAP	C2N-C3N-C4N	2.69	121.31	118.26
3	B	1105	FAD	C5'-C4'-C3'	-2.69	107.01	112.20
4	A	1106	Y3G	C06-C05-N04	-2.64	119.47	123.42
3	C	1105	FAD	C4X-N5-C5X	2.64	119.41	116.77
5	B	1106	NAP	O7N-C7N-N7N	-2.60	118.89	122.58
5	B	1106	NAP	PA-O5B-C5B	-2.59	106.52	121.68
3	C	1105	FAD	C7-C6-C5X	-2.58	117.56	121.22
5	A	1107	NAP	O2B-P2B-O1X	-2.53	99.62	109.39
5	C	1106	NAP	O3X-P2B-O2X	2.52	117.28	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1106	NAP	C3B-C2B-C1B	-2.52	98.14	102.89
5	D	1107	NAP	C3B-C2B-C1B	-2.51	98.16	102.89
3	C	1105	FAD	C5'-C4'-C3'	-2.50	107.37	112.20
6	A	1108	FNR	O2'-C2'-C3'	-2.49	103.04	109.10
5	B	1106	NAP	O3X-P2B-O2X	2.49	117.15	107.64
5	D	1107	NAP	PA-O5B-C5B	-2.49	107.11	121.68
4	D	1106	Y3G	C06-C05-N04	-2.47	119.73	123.42
5	A	1107	NAP	O3X-P2B-O2X	2.43	116.93	107.64
3	A	1105	FAD	C8M-C8-C7	-2.42	115.77	120.74
5	C	1106	NAP	C6N-C5N-C4N	2.41	122.94	119.44
3	D	1105	FAD	C9A-N10-C10	-2.40	118.77	121.91
5	C	1106	NAP	O7N-C7N-N7N	-2.39	119.18	122.58
3	A	1105	FAD	O4'-C4'-C5'	-2.38	104.56	109.92
5	D	1107	NAP	C2A-N1A-C6A	-2.37	114.69	118.75
5	A	1107	NAP	PA-O5B-C5B	-2.36	107.87	121.68
5	C	1106	NAP	O5D-PN-O1N	-2.35	99.90	109.07
3	A	1105	FAD	C7-C6-C5X	-2.28	117.99	121.22
5	D	1107	NAP	O4B-C4B-C3B	2.25	109.57	105.11
3	C	1105	FAD	C8M-C8-C9	2.25	125.72	120.34
5	A	1107	NAP	C3B-C2B-C1B	-2.24	98.67	102.89
5	B	1106	NAP	O5D-PN-O1N	-2.24	100.32	109.07
5	C	1106	NAP	PA-O5B-C5B	-2.24	108.56	121.68
3	B	1105	FAD	O4B-C1B-C2B	-2.23	103.67	106.93
5	B	1106	NAP	C2A-N1A-C6A	-2.21	114.98	118.75
5	B	1106	NAP	PN-O5D-C5D	-2.20	108.76	121.68
5	B	1106	NAP	O4B-C4B-C3B	2.18	109.43	105.11
3	D	1105	FAD	C3B-C2B-C1B	2.17	104.25	100.98
4	C	1108	Y3G	C06-C05-N04	-2.17	120.17	123.42
5	B	1106	NAP	C6N-C5N-C4N	2.16	122.58	119.44
5	C	1106	NAP	C6N-N1N-C2N	-2.15	120.01	121.97
5	C	1106	NAP	C2A-N1A-C6A	-2.12	115.13	118.75
5	A	1107	NAP	C2A-N1A-C6A	-2.12	115.13	118.75
5	A	1107	NAP	O4B-C4B-C3B	2.11	109.30	105.11
5	C	1106	NAP	C3B-C2B-C1B	-2.10	98.94	102.89
5	D	1107	NAP	C6N-N1N-C2N	-2.10	120.06	121.97
4	B	1108	Y3G	C06-C05-N04	-2.09	120.29	123.42
5	B	1106	NAP	O3X-P2B-O2B	-2.09	96.63	105.99
5	A	1107	NAP	O5D-PN-O1N	-2.08	100.96	109.07
6	C	1107	FNR	O3P-P-O5'	2.06	112.21	106.73
5	A	1107	NAP	PN-O5D-C5D	-2.05	109.64	121.68
6	A	1108	FNR	O5'-P-O2P	2.05	112.22	106.47
6	C	1107	FNR	C4A-CAA-N10	2.03	122.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1106	NAP	PN-O5D-C5D	-2.01	109.91	121.68

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1108	FNR	C4'
6	C	1107	FNR	C4'
6	D	1108	FNR	C4'
6	B	1107	FNR	C4'

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1107	NAP	C5D-O5D-PN-O3
5	B	1106	NAP	C5D-O5D-PN-O3
6	A	1108	FNR	C3'-C4'-C5'-O5'
6	A	1108	FNR	O4'-C4'-C5'-O5'
6	C	1107	FNR	O3'-C3'-C4'-O4'
6	C	1107	FNR	C3'-C4'-C5'-O5'
6	C	1107	FNR	O4'-C4'-C5'-O5'
6	D	1108	FNR	C3'-C4'-C5'-O5'
6	D	1108	FNR	O4'-C4'-C5'-O5'
6	B	1107	FNR	C1'-C2'-C3'-C4'
6	B	1107	FNR	O3'-C3'-C4'-O4'
6	B	1107	FNR	C3'-C4'-C5'-O5'
6	B	1107	FNR	O4'-C4'-C5'-O5'
6	A	1108	FNR	O3'-C3'-C4'-O4'
6	D	1108	FNR	O3'-C3'-C4'-O4'
6	C	1107	FNR	C2'-C3'-C4'-O4'
6	B	1107	FNR	C2'-C3'-C4'-O4'
5	D	1107	NAP	O4D-C4D-C5D-O5D
6	A	1108	FNR	C2'-C3'-C4'-O4'
6	D	1108	FNR	C2'-C3'-C4'-O4'
6	C	1107	FNR	O3'-C3'-C4'-C5'
6	D	1108	FNR	O2'-C2'-C3'-C4'
6	B	1107	FNR	O2'-C2'-C3'-C4'
6	A	1108	FNR	O2'-C2'-C3'-C4'
6	C	1107	FNR	C4'-C5'-O5'-P
6	D	1108	FNR	C4'-C5'-O5'-P
6	B	1107	FNR	C4'-C5'-O5'-P
6	A	1108	FNR	C4'-C5'-O5'-P
6	D	1108	FNR	O3'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
3	A	1105	FAD	PA-O3P-P-O5'
3	D	1105	FAD	PA-O3P-P-O5'
5	A	1107	NAP	C2B-O2B-P2B-O3X
5	D	1107	NAP	C2B-O2B-P2B-O2X
5	B	1106	NAP	C5D-O5D-PN-O2N
5	A	1107	NAP	O4B-C4B-C5B-O5B
5	B	1106	NAP	O4D-C4D-C5D-O5D
6	B	1107	FNR	O3'-C3'-C4'-C5'
3	C	1105	FAD	O4B-C4B-C5B-O5B
3	A	1105	FAD	O4B-C4B-C5B-O5B
5	D	1107	NAP	C3D-C4D-C5D-O5D
6	A	1108	FNR	O3'-C3'-C4'-C5'
3	B	1105	FAD	O4B-C4B-C5B-O5B
5	A	1107	NAP	C5D-O5D-PN-O3
6	C	1107	FNR	O2'-C2'-C3'-C4'
3	D	1105	FAD	O4B-C4B-C5B-O5B
5	B	1106	NAP	O4B-C4B-C5B-O5B
5	D	1107	NAP	C5D-O5D-PN-O1N
5	B	1106	NAP	C5D-O5D-PN-O1N
5	C	1106	NAP	O4B-C4B-C5B-O5B
5	D	1107	NAP	O4B-C4B-C5B-O5B

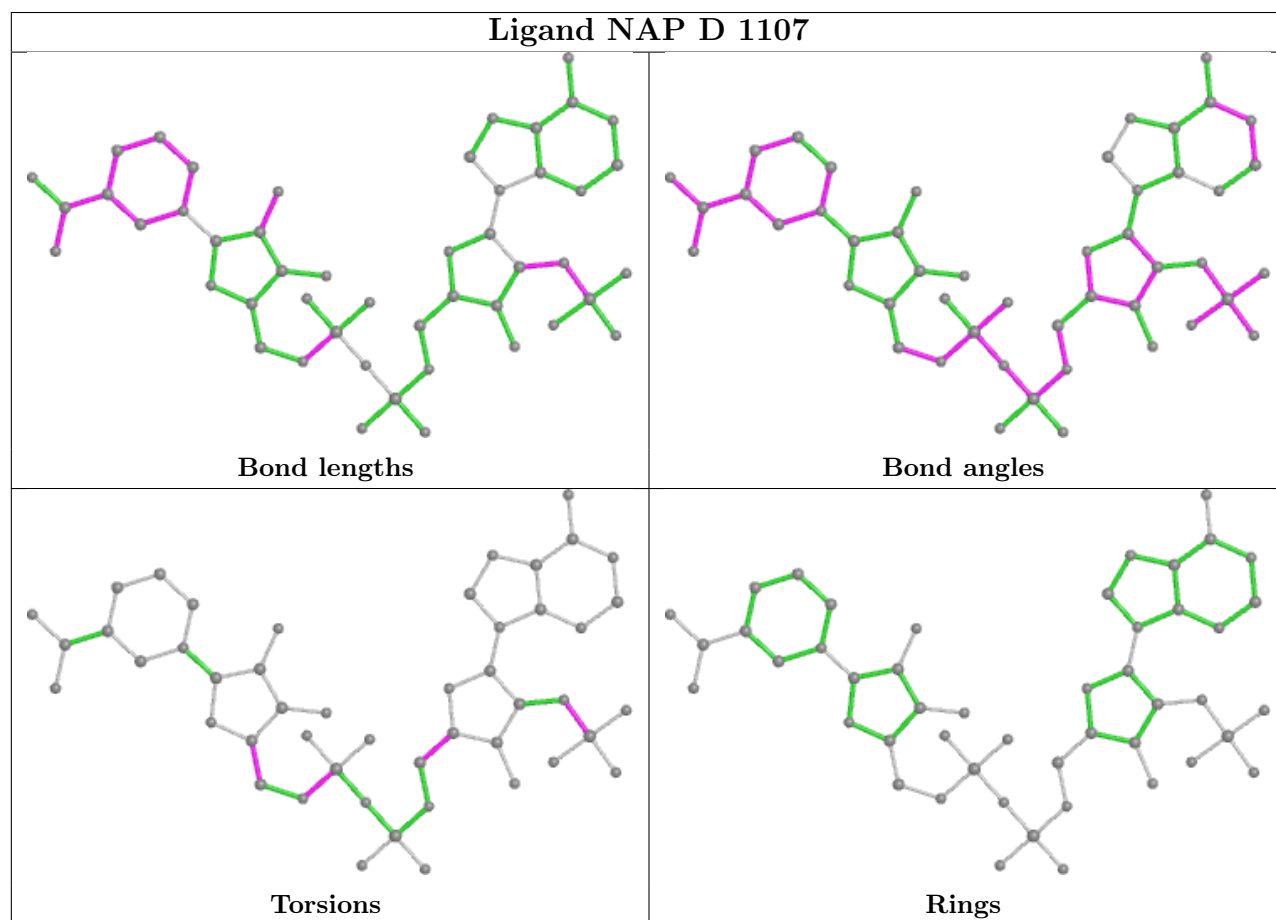
There are no ring outliers.

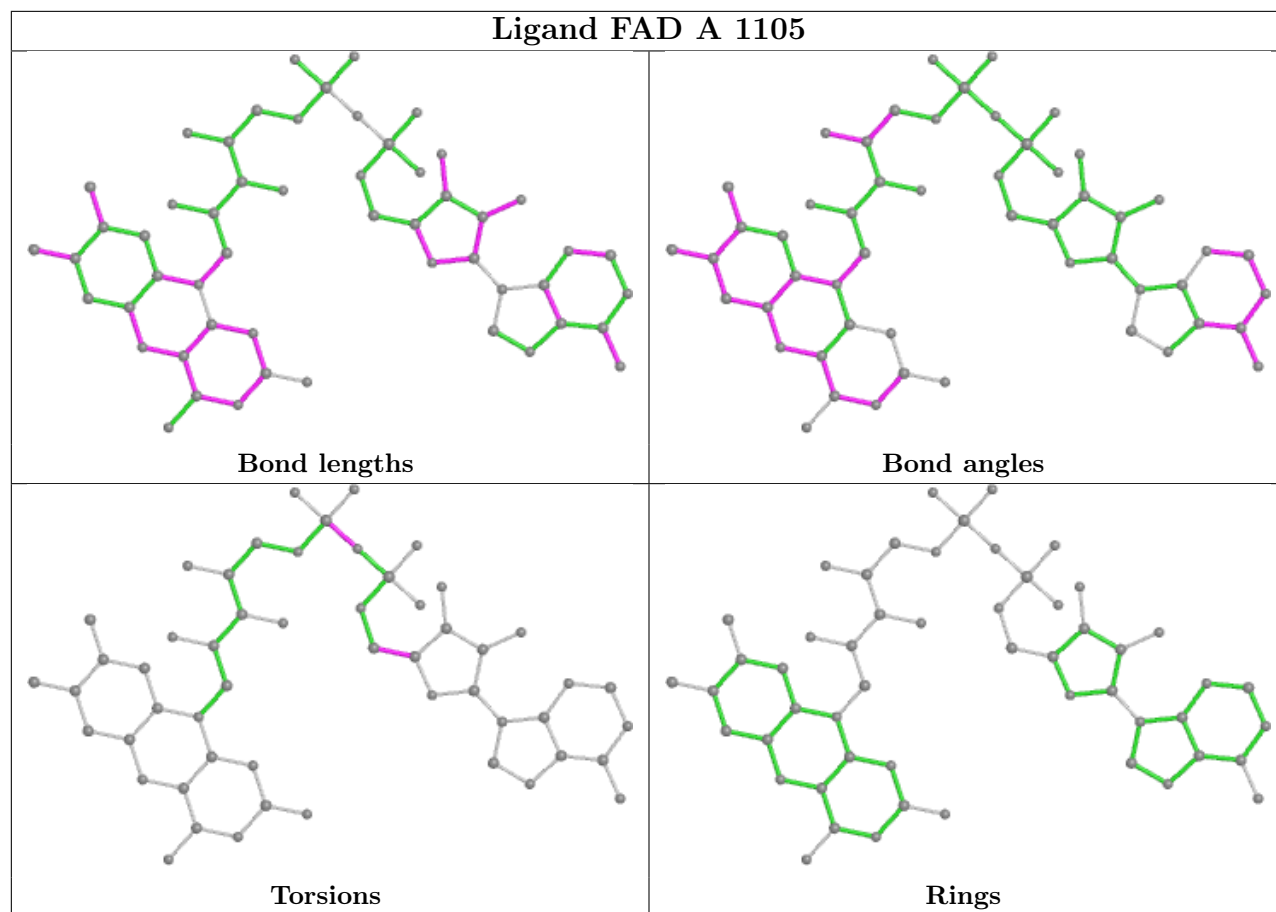
12 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1107	NAP	7	0
3	A	1105	FAD	2	0
5	B	1106	NAP	7	0
6	C	1107	FNR	1	0
5	A	1107	NAP	6	0
6	A	1108	FNR	3	0
3	D	1105	FAD	3	0
5	C	1106	NAP	5	0
3	C	1105	FAD	2	0
6	B	1107	FNR	1	0
3	B	1105	FAD	2	0
6	D	1108	FNR	3	0

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

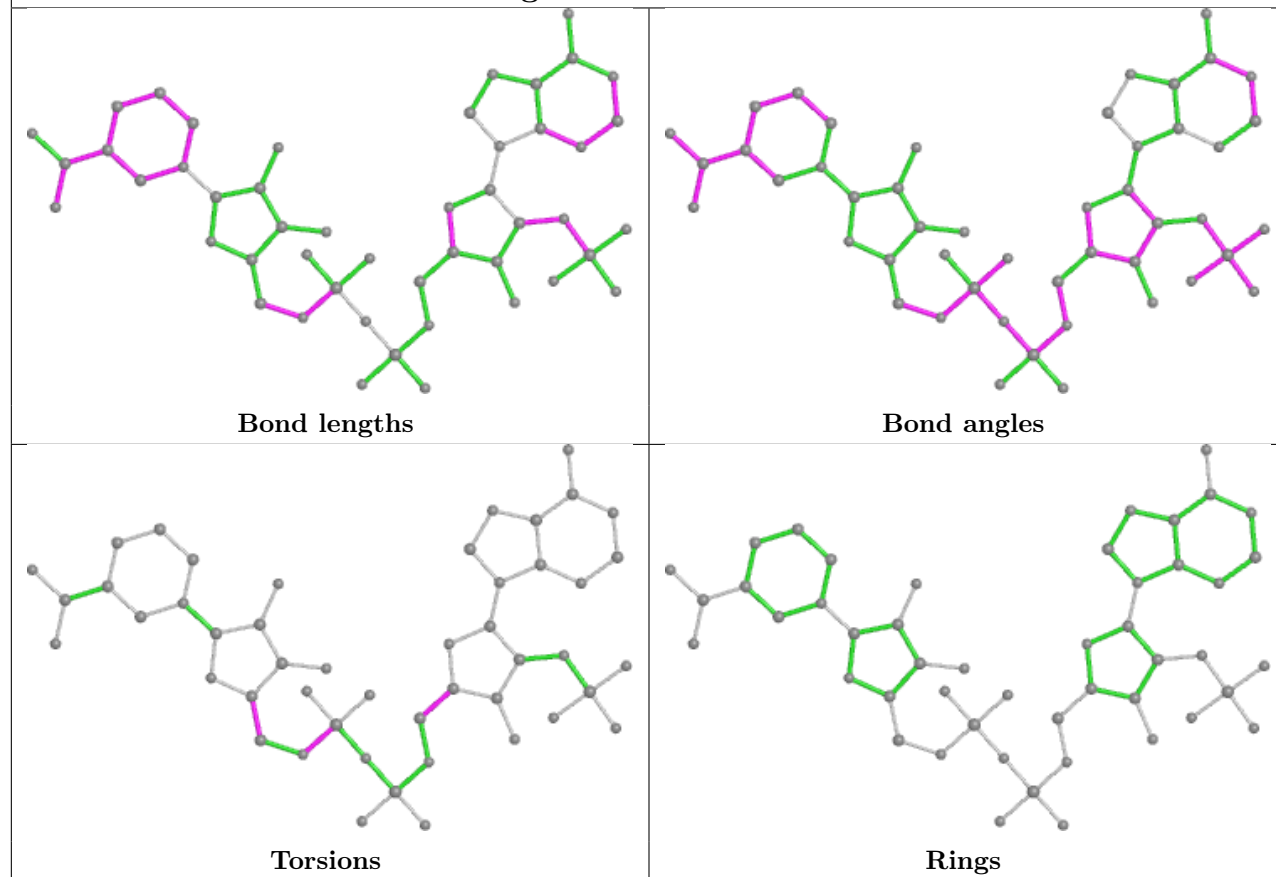
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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



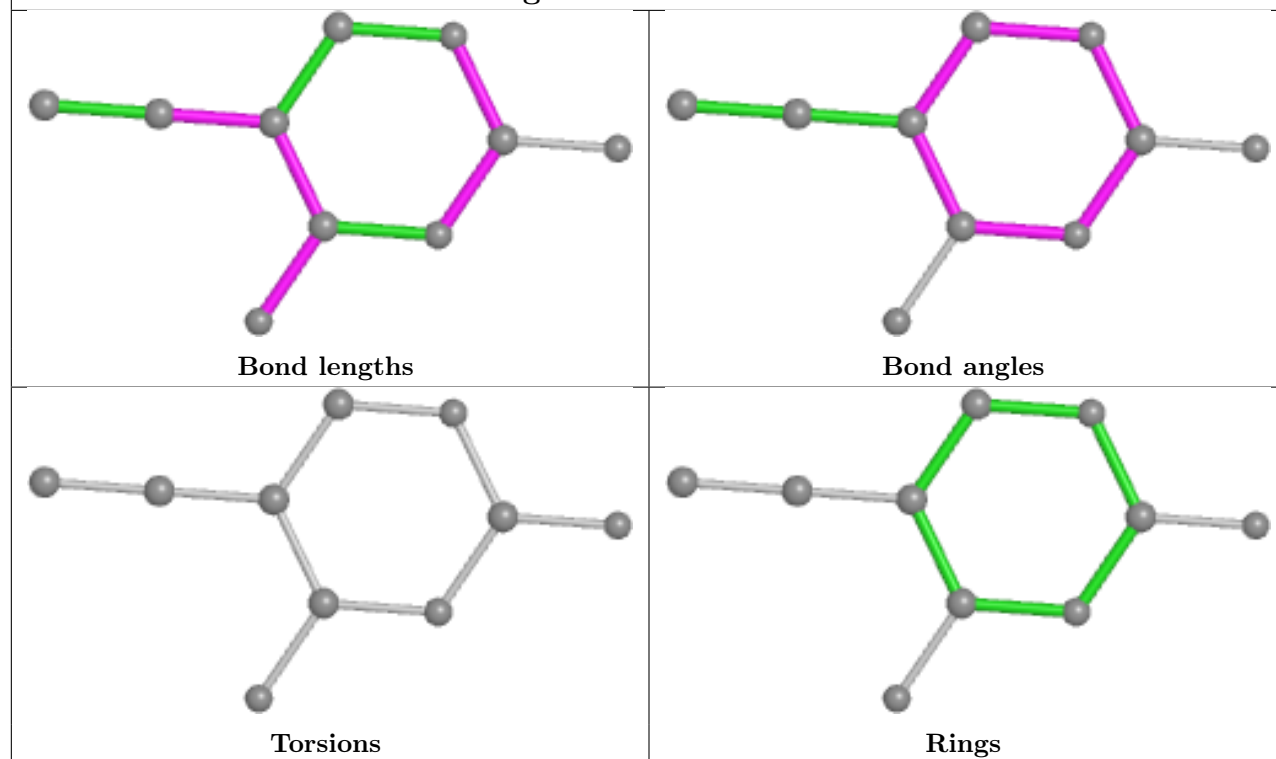




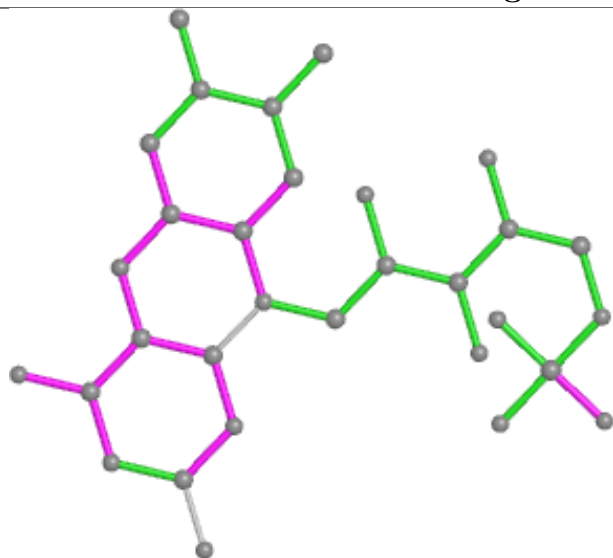
## Ligand NAP B 1106



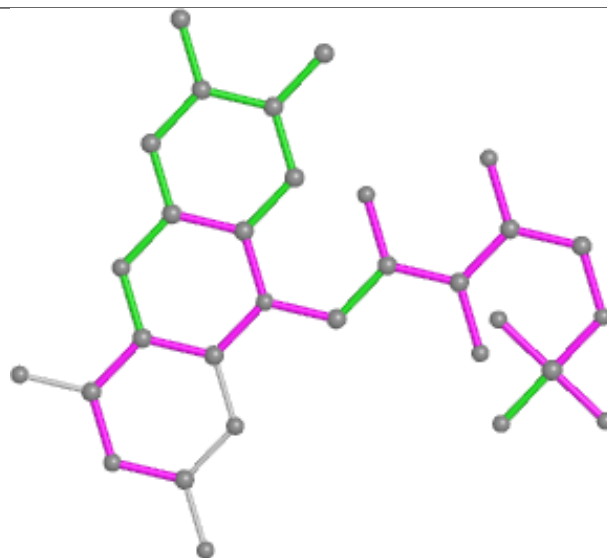
## Ligand Y3G D 1106



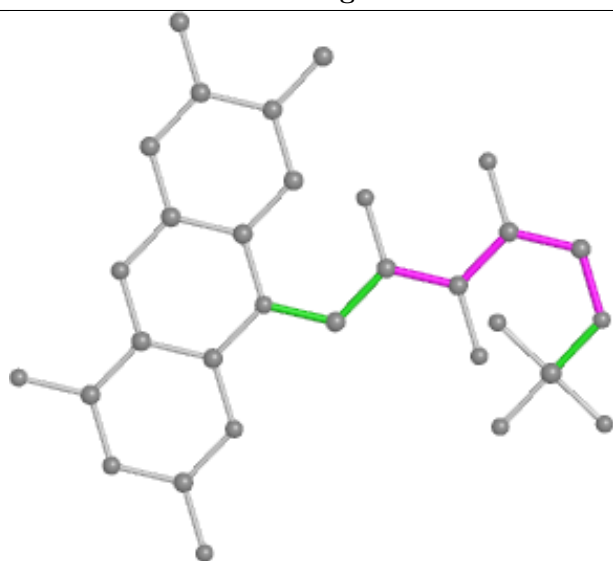
## Ligand FNR C 1107



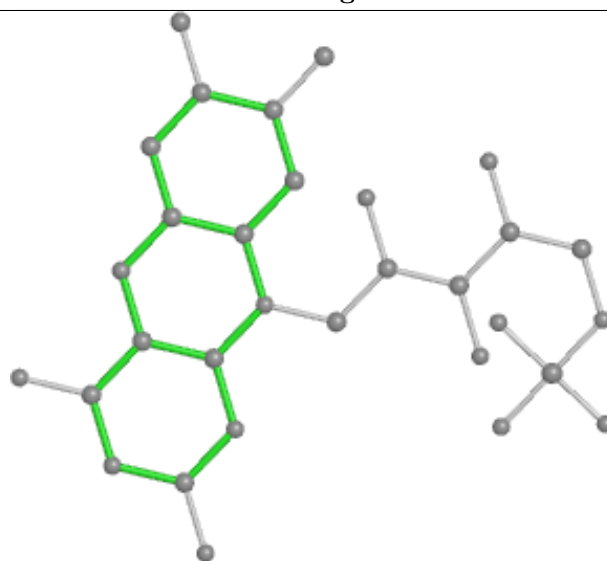
Bond lengths



Bond angles

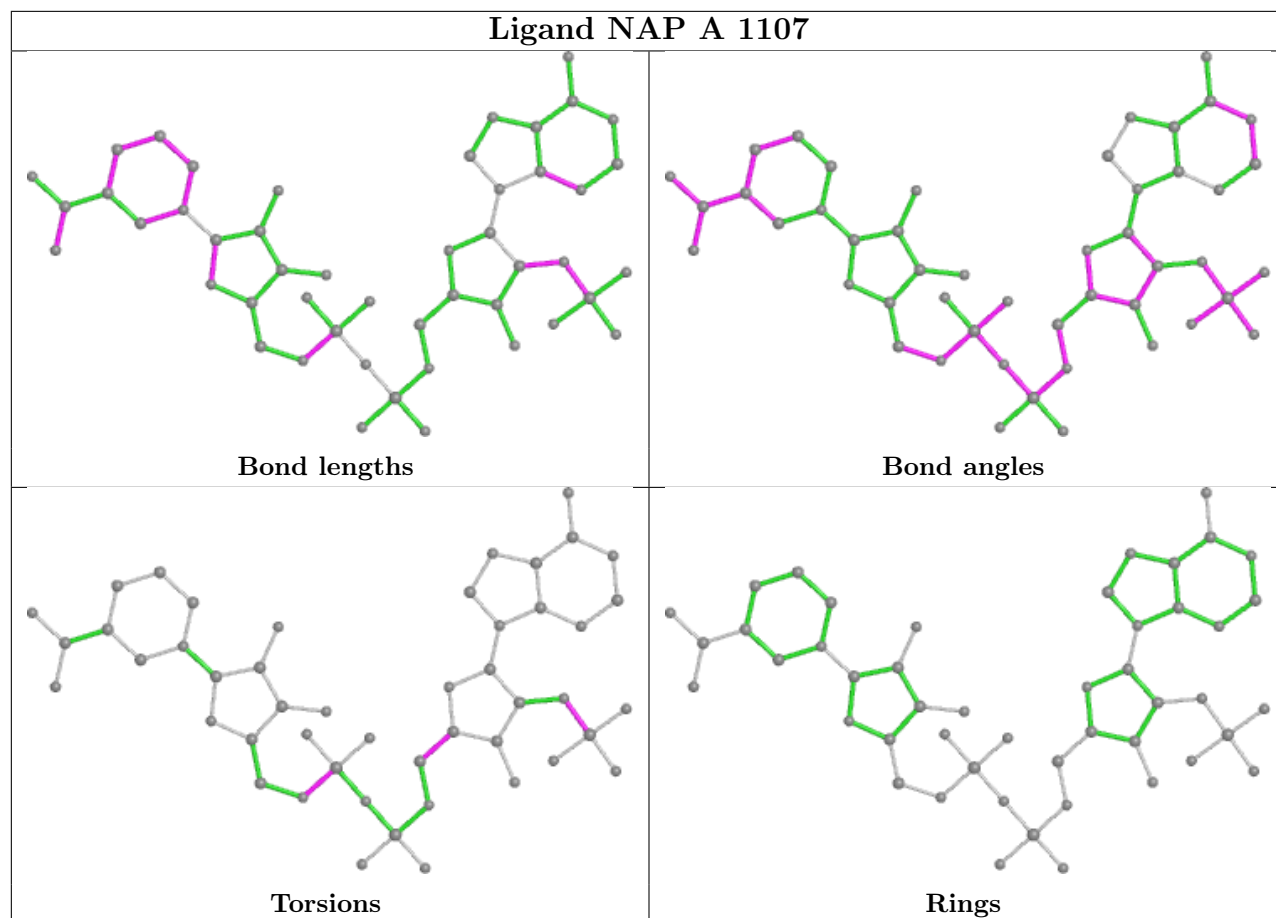


Torsions

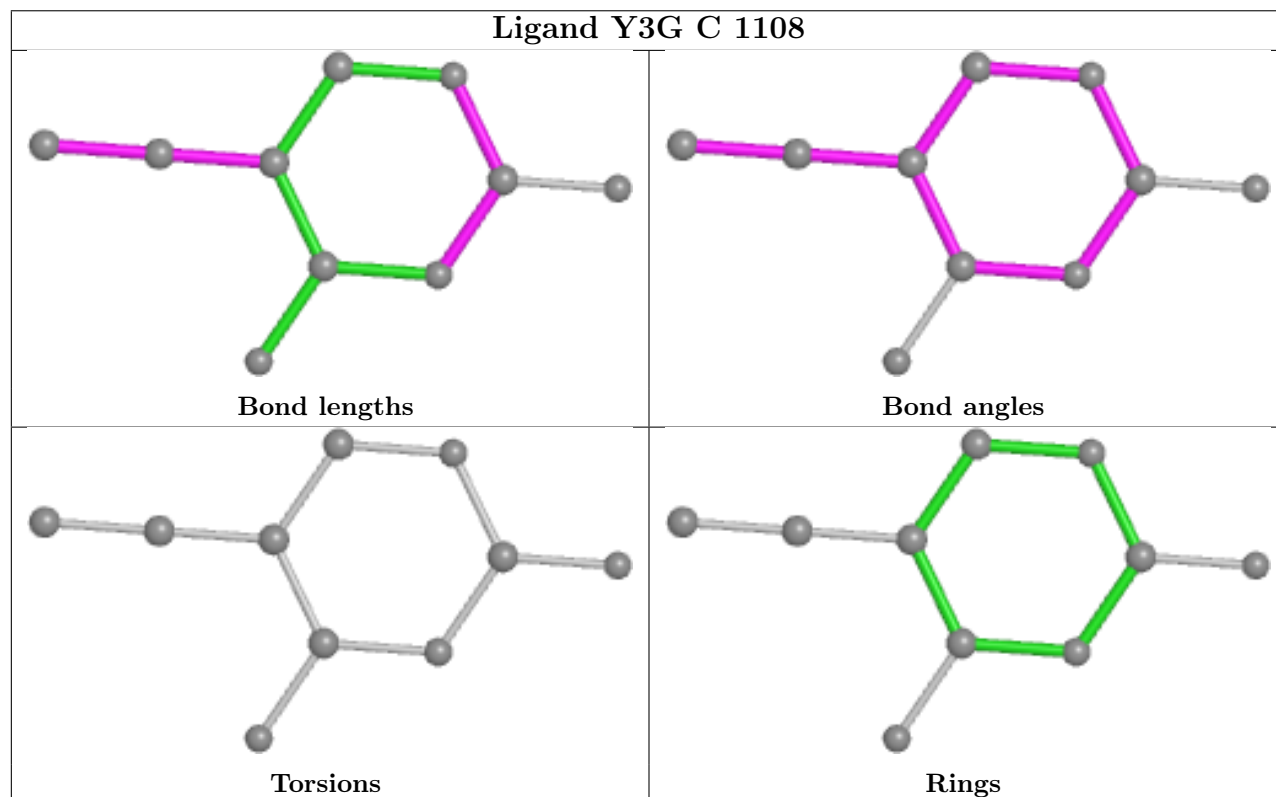


Rings

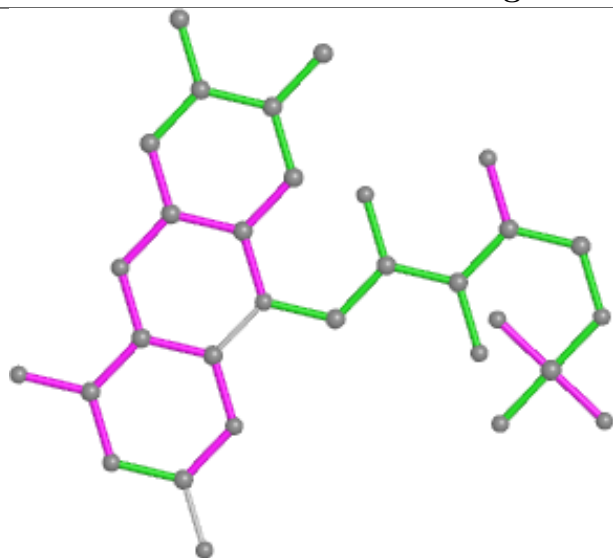
## Ligand NAP A 1107



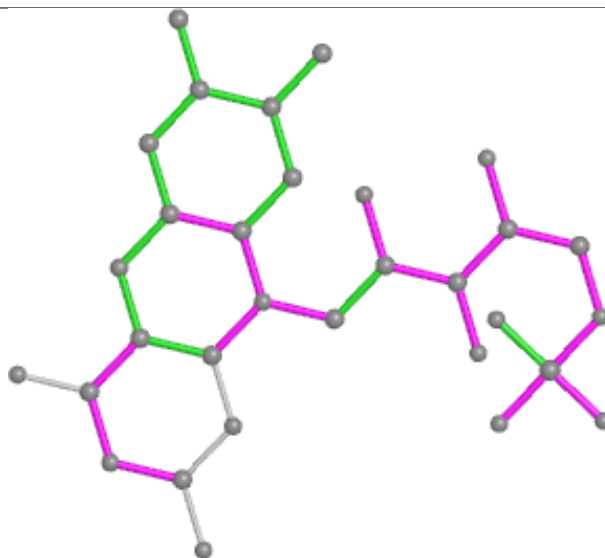
## Ligand Y3G C 1108



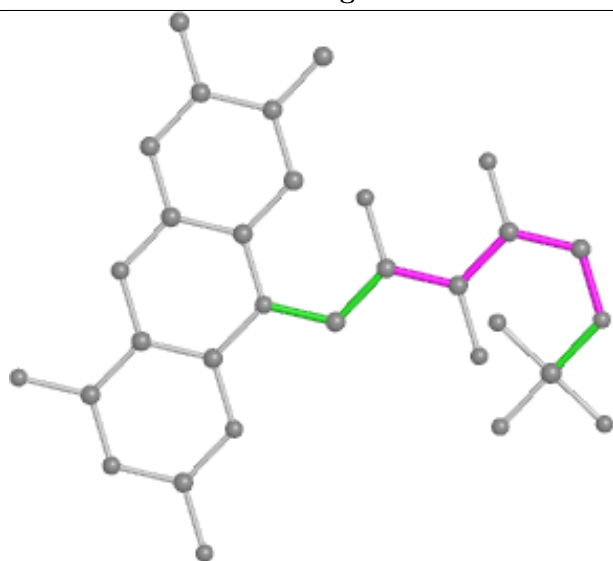
## Ligand FNR A 1108



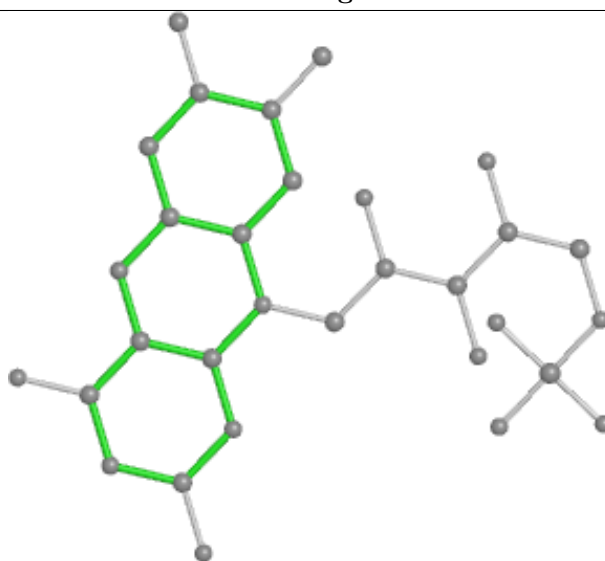
Bond lengths



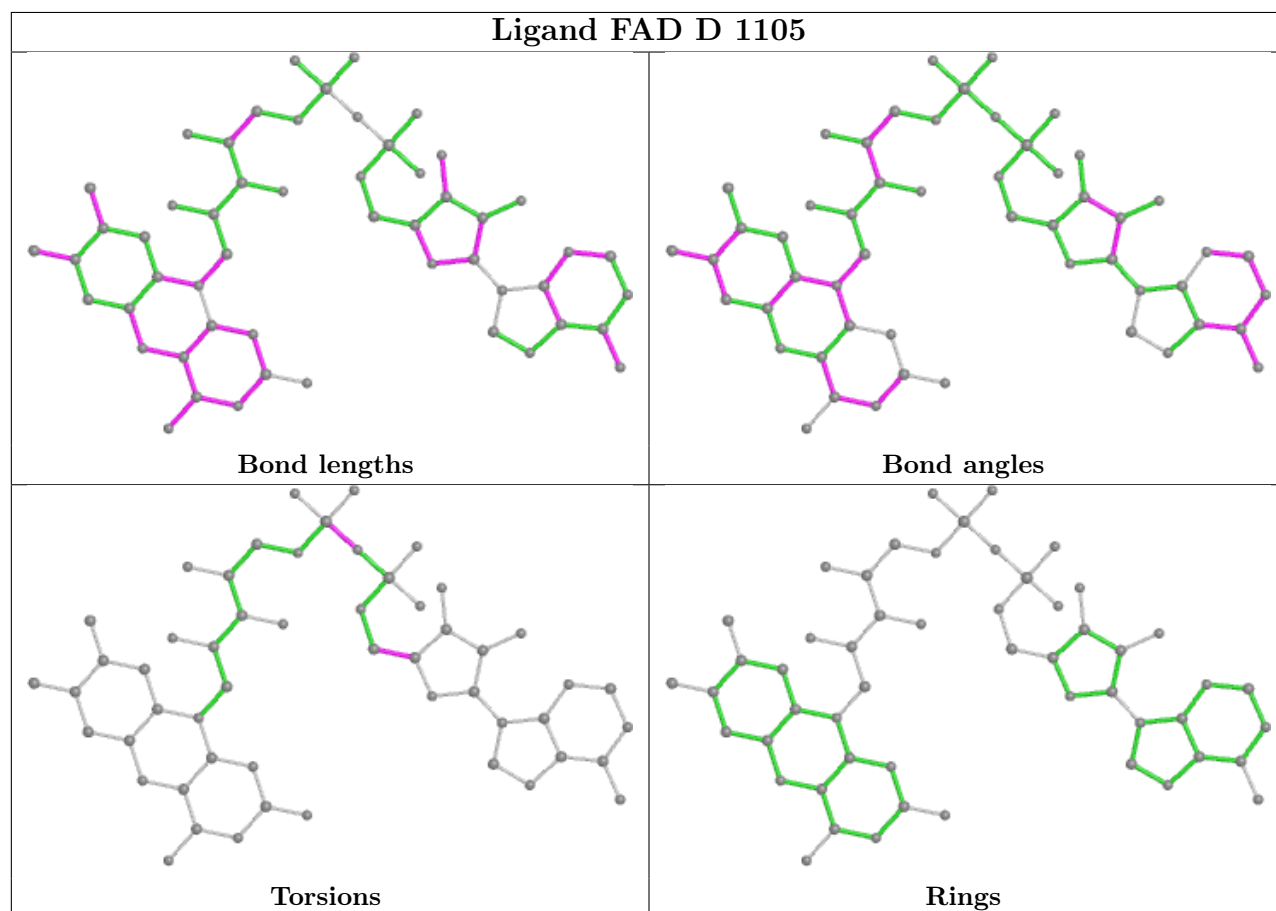
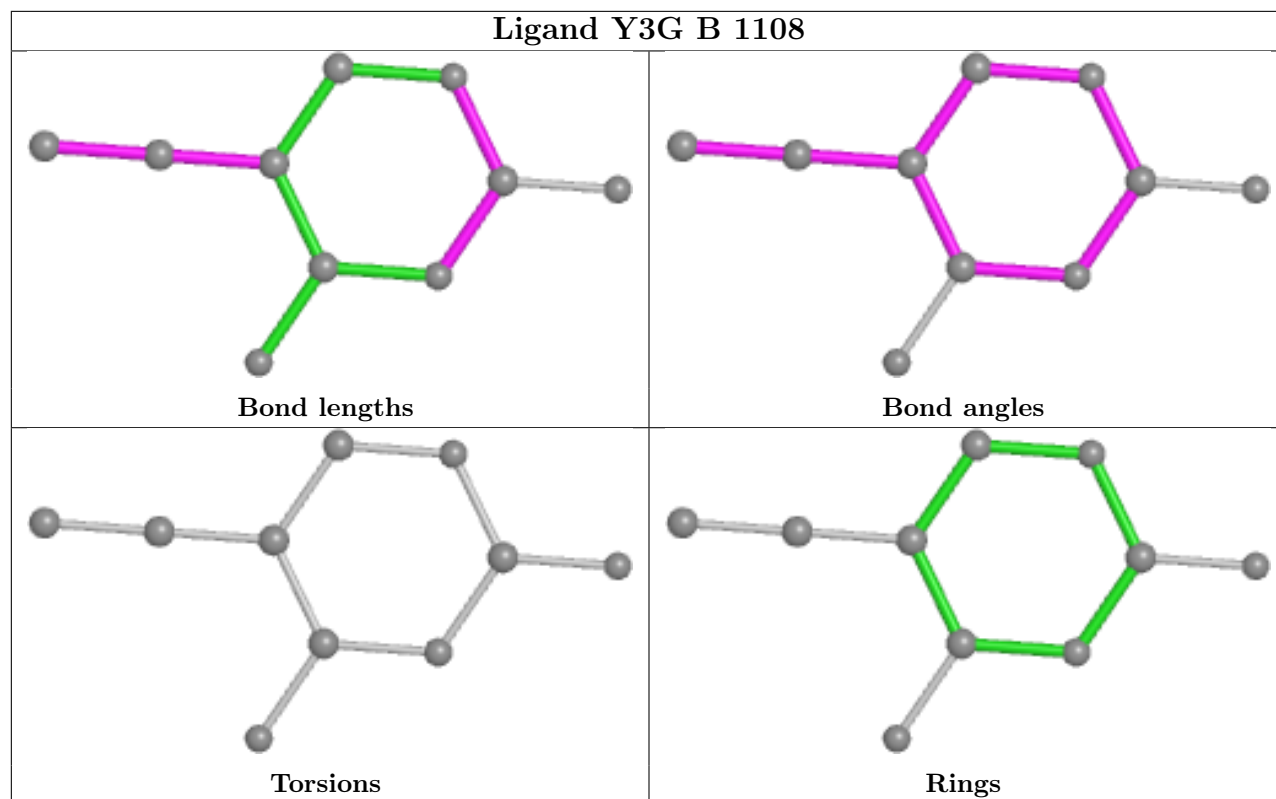
Bond angles

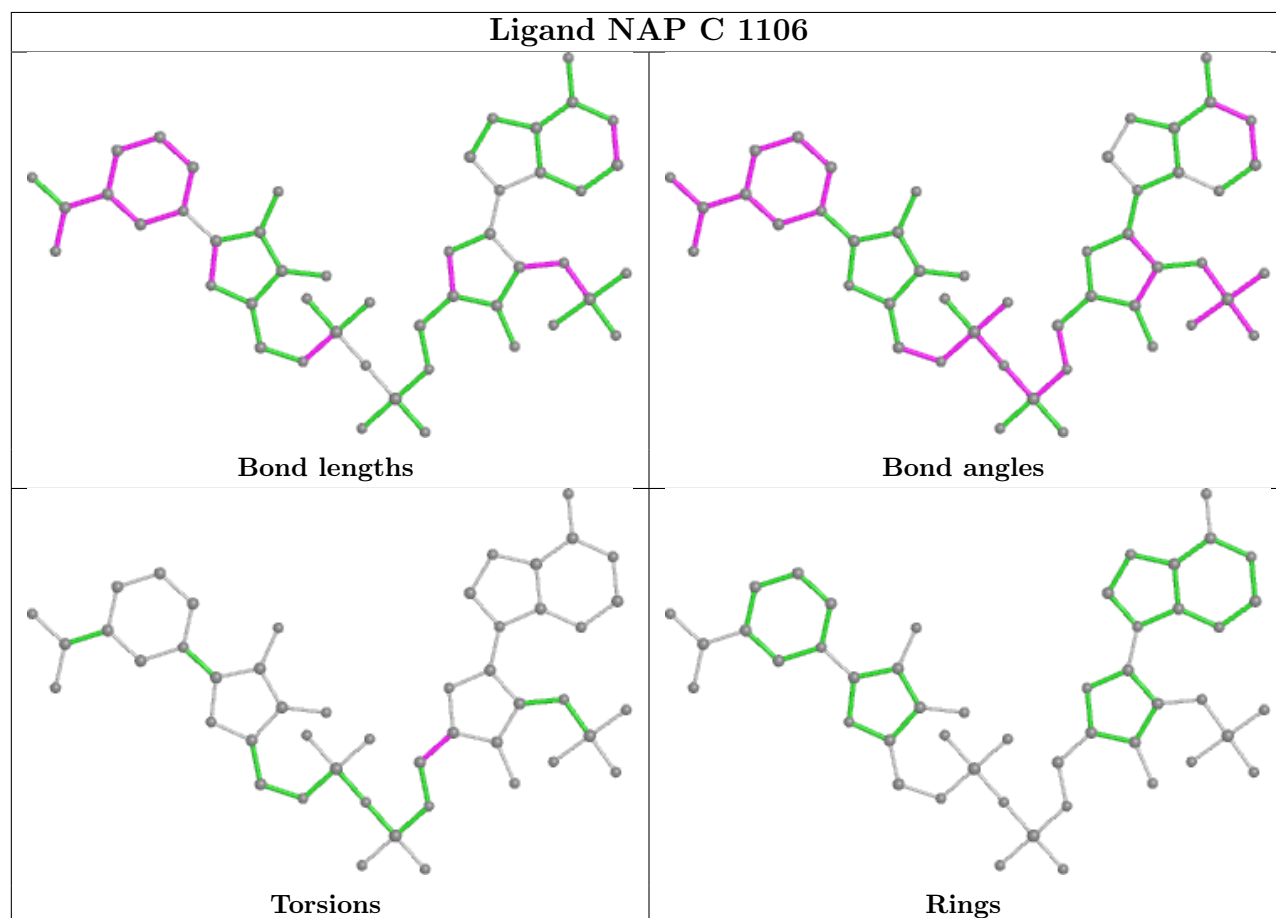
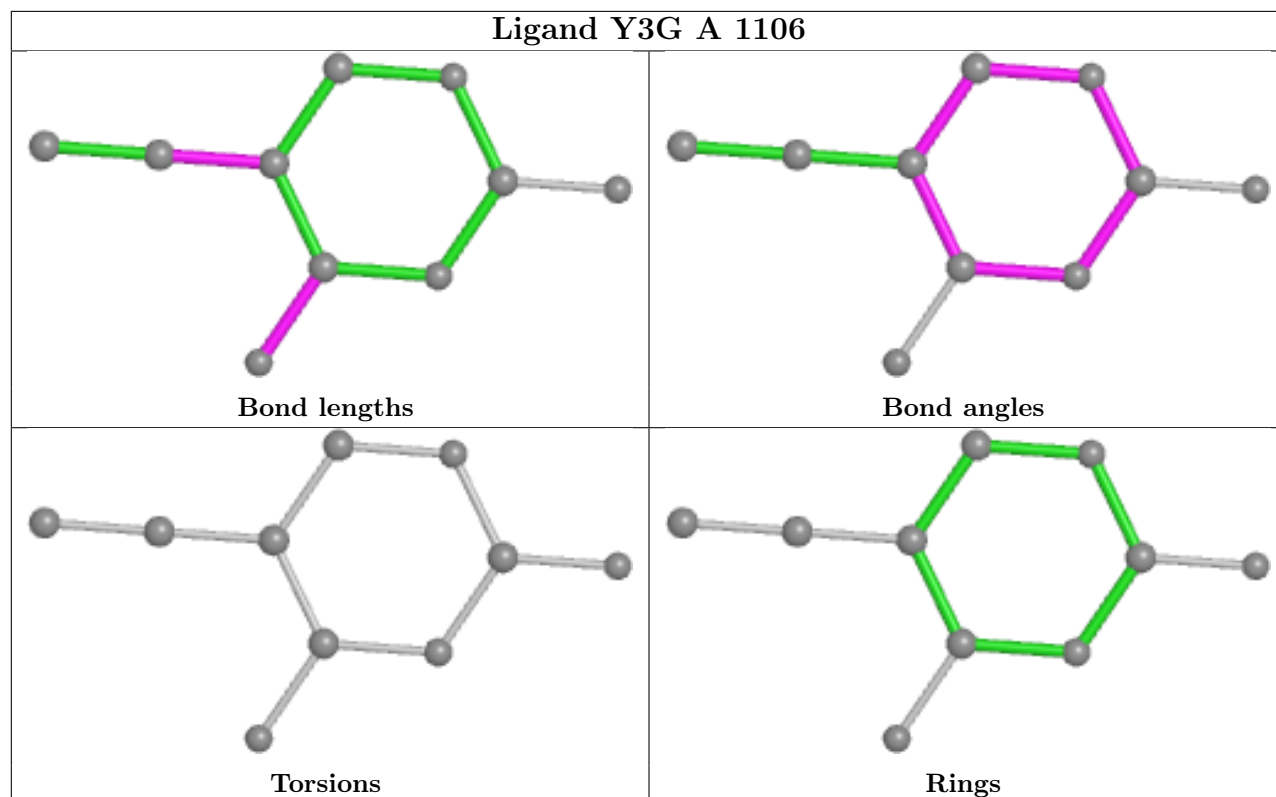


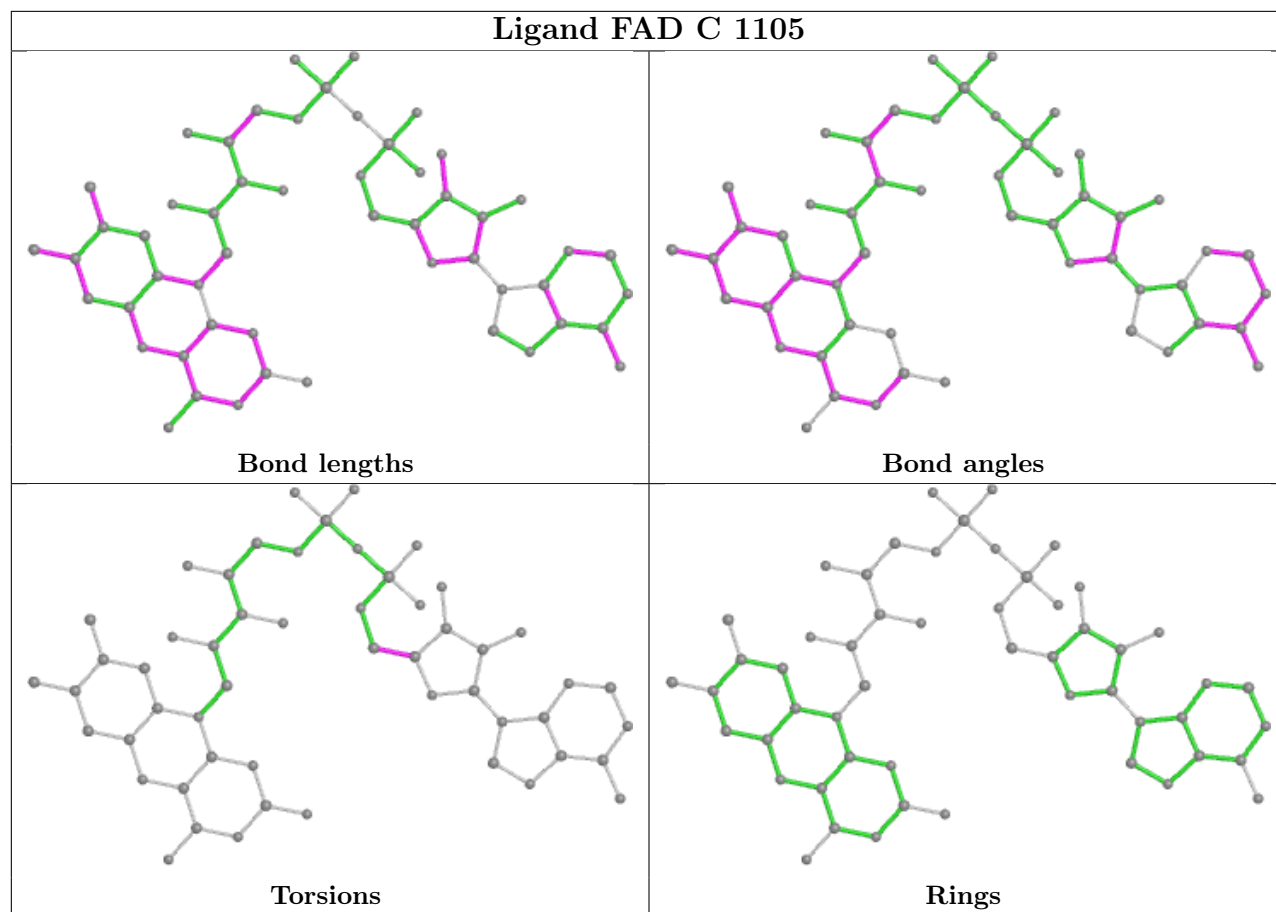
Torsions



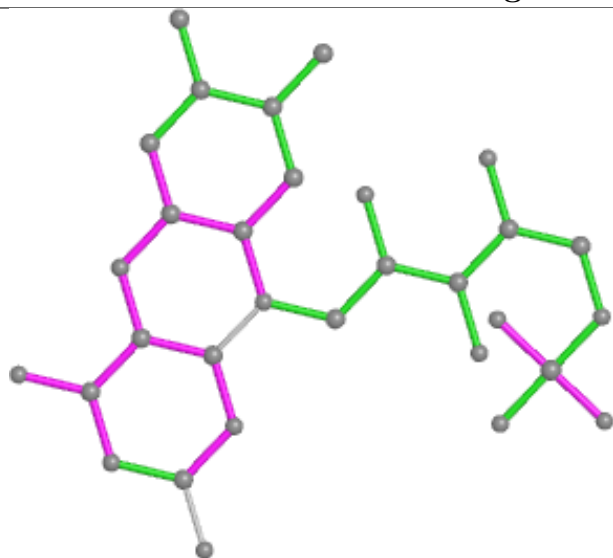
Rings



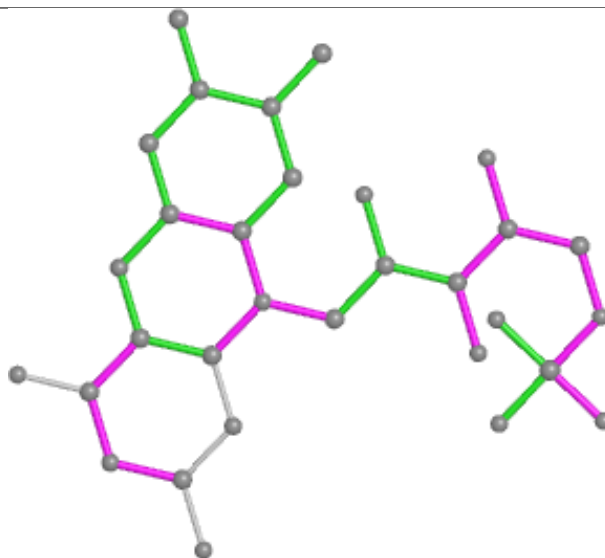




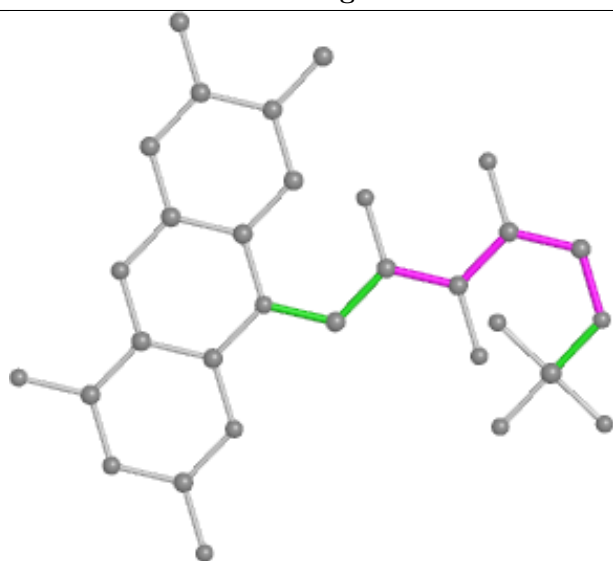
## Ligand FNR B 1107



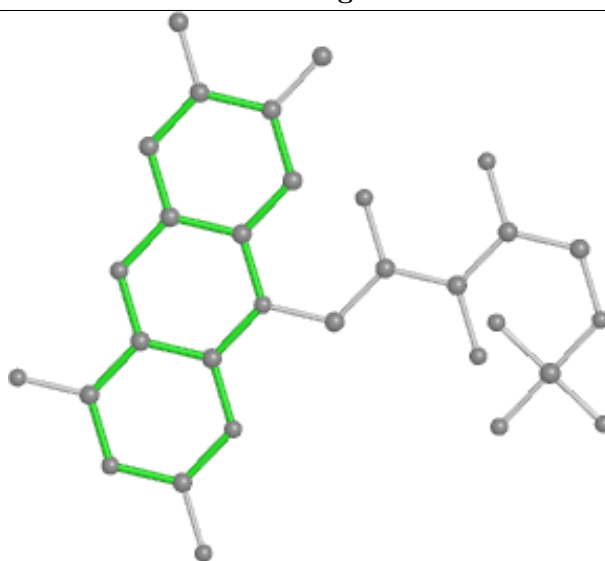
Bond lengths



Bond angles

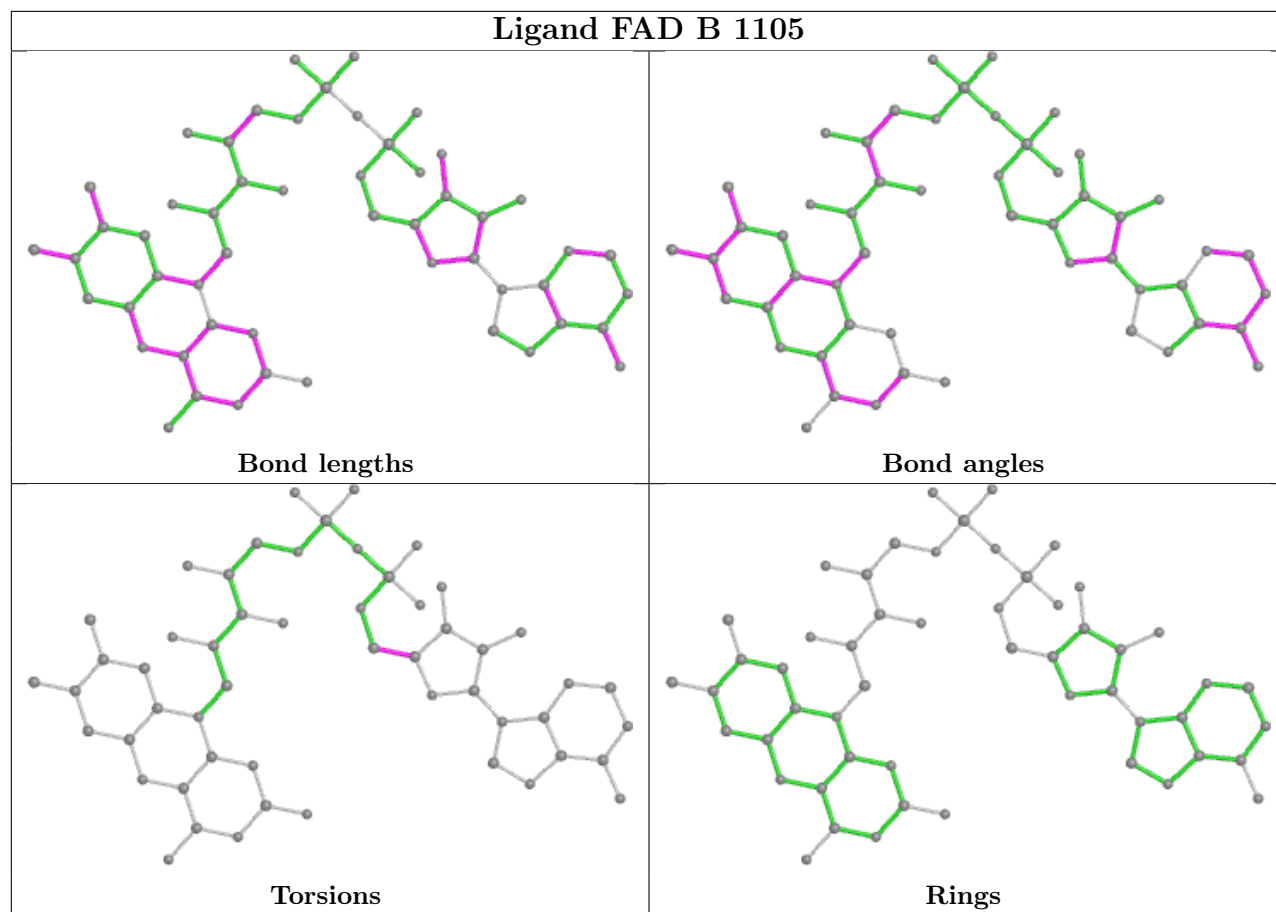


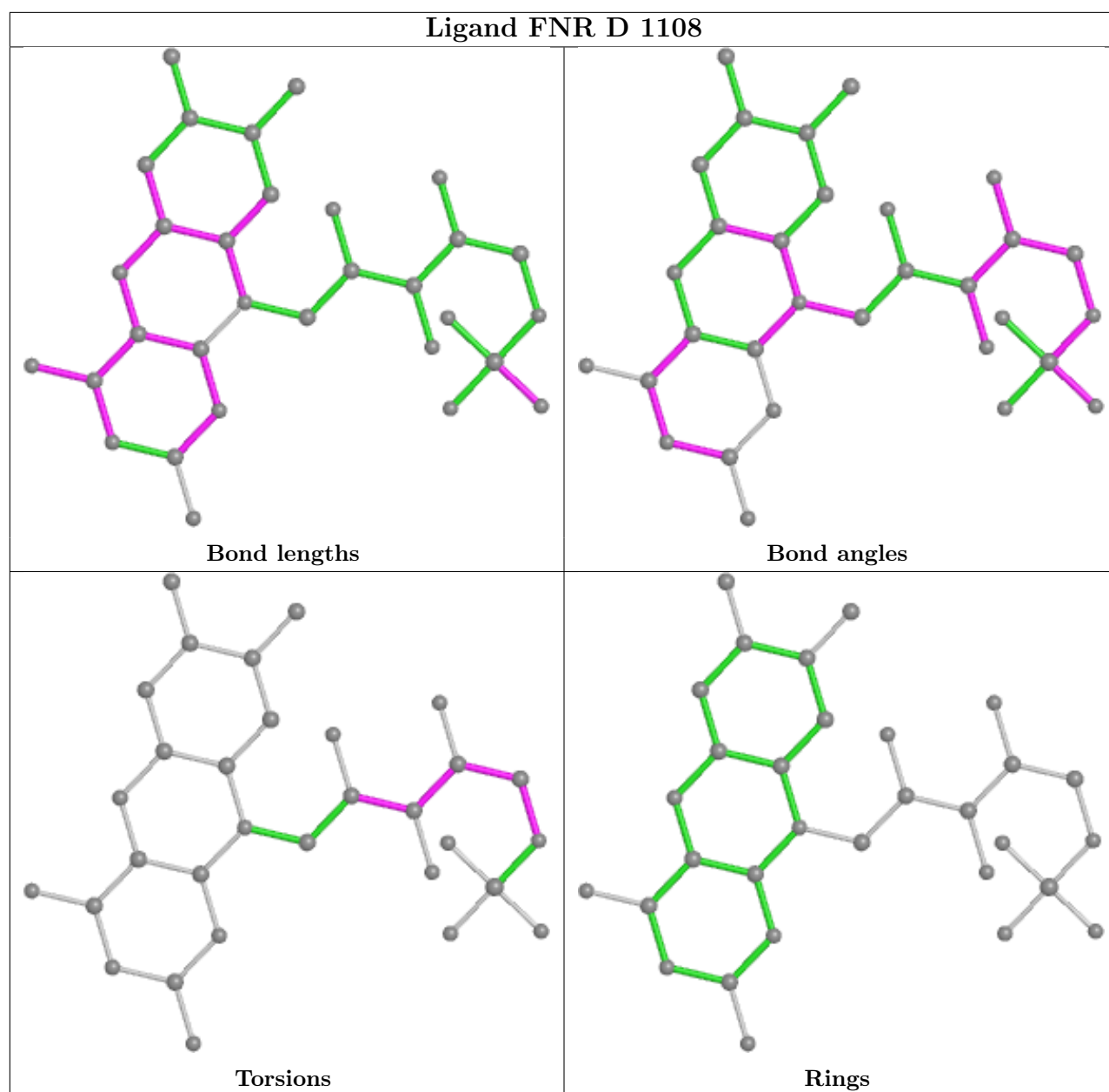
Torsions



Rings







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1007/1025 (98%)	0.15	43 (4%)	35	36	15, 23, 45, 91	0
1	B	1004/1025 (97%)	0.17	53 (5%)	26	28	15, 23, 47, 108	0
1	C	1004/1025 (97%)	0.06	38 (3%)	40	42	15, 22, 42, 74	0
1	D	1011/1025 (98%)	0.12	45 (4%)	33	34	15, 23, 45, 80	0
All	All	4026/4100 (98%)	0.12	179 (4%)	34	35	15, 23, 45, 108	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	907	LEU	13.6
1	B	907	LEU	12.7
1	B	901	ASN	11.5
1	B	902	ALA	11.3
1	A	2	ALA	11.2
1	B	904	PHE	9.9
1	B	1017	LEU	9.3
1	D	907	LEU	8.9
1	A	324	CYS	8.7
1	D	902	ALA	8.1
1	A	1017	LEU	8.0
1	B	416	THR	7.9
1	B	908	GLU	7.7
1	B	900	GLN	7.3
1	D	901	ASN	7.1
1	B	903	ALA	7.0
1	B	52	CYS	6.8
1	A	681	GLY	6.7
1	D	900	GLN	6.7
1	D	869	ALA	6.6
1	B	905	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
1	C	1017	LEU	6.3
1	A	901	ASN	6.1
1	B	906	PRO	6.0
1	A	899	GLU	5.8
1	B	324	CYS	5.7
1	D	52	CYS	5.7
1	A	675	MET	5.6
1	B	870	GLU	5.6
1	C	52	CYS	5.5
1	A	682	LEU	5.5
1	C	867	ARG	5.5
1	B	897	LEU	5.4
1	A	900	GLN	5.4
1	A	51	HIS	5.4
1	A	897	LEU	5.3
1	D	51	HIS	5.3
1	D	899	GLU	5.2
1	D	897	LEU	5.2
1	B	869	ALA	5.2
1	A	902	ALA	5.2
1	A	870	GLU	5.2
1	A	908	GLU	5.2
1	D	415	GLU	5.1
1	B	896	ARG	5.0
1	A	896	ARG	4.9
1	C	415	GLU	4.8
1	D	873	GLY	4.7
1	C	325	HIS	4.7
1	B	867	ARG	4.7
1	B	899	GLU	4.6
1	C	907	LEU	4.4
1	A	415	GLU	4.4
1	D	908	GLU	4.3
1	D	416	THR	4.3
1	C	416	THR	4.3
1	C	671	CYS	4.2
1	B	415	GLU	4.1
1	C	363	PHE	4.1
1	A	867	ARG	4.1
1	D	680	MET	4.0
1	A	52	CYS	4.0
1	C	901	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	418	LYS	4.0
1	D	674	GLY	3.9
1	B	414	ASP	3.9
1	B	909	ARG	3.9
1	B	332	ARG	3.9
1	C	908	GLU	3.8
1	B	871	LEU	3.8
1	C	872	MET	3.8
1	C	332	ARG	3.8
1	B	872	MET	3.8
1	A	416	THR	3.8
1	D	870	GLU	3.7
1	B	322	CYS	3.7
1	B	898	LYS	3.7
1	B	60	ASP	3.6
1	C	326	SER	3.6
1	C	322	CYS	3.6
1	B	54	LYS	3.6
1	D	871	LEU	3.6
1	A	673	HIS	3.5
1	C	319	ALA	3.5
1	D	909	ARG	3.4
1	D	874	LYS	3.4
1	C	331	ILE	3.4
1	A	50	PHE	3.4
1	A	909	ARG	3.4
1	B	868	ILE	3.3
1	C	902	ALA	3.3
1	D	896	ARG	3.3
1	B	892	GLU	3.3
1	B	865	VAL	3.2
1	A	864	PRO	3.2
1	B	874	LYS	3.2
1	D	675	MET	3.2
1	D	459	TRP	3.2
1	A	671	CYS	3.2
1	D	1018	PRO	3.2
1	B	671	CYS	3.1
1	C	900	GLN	3.1
1	B	873	GLY	3.1
1	A	917	PRO	3.1
1	C	320	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	414	ASP	3.1
1	C	869	ALA	3.0
1	C	913	ILE	3.0
1	B	367	PHE	3.0
1	D	913	ILE	2.9
1	C	870	GLU	2.9
1	A	322	CYS	2.9
1	B	418	LYS	2.8
1	B	323	ALA	2.8
1	B	371	ARG	2.8
1	B	459	TRP	2.8
1	B	51	HIS	2.7
1	D	867	ARG	2.7
1	C	324	CYS	2.7
1	A	424	ASP	2.7
1	D	11	ASP	2.7
1	B	424	ASP	2.7
1	D	678	ARG	2.7
1	D	872	MET	2.6
1	A	873	GLY	2.6
1	A	325	HIS	2.6
1	C	909	ARG	2.6
1	D	679	GLY	2.6
1	A	868	ILE	2.6
1	B	895	MET	2.6
1	A	332	ARG	2.6
1	D	36	LEU	2.5
1	A	327	PRO	2.5
1	A	320	GLY	2.5
1	A	913	ILE	2.5
1	C	357	ARG	2.5
1	C	273	GLU	2.5
1	C	903	ALA	2.5
1	C	906	PRO	2.5
1	D	888	LYS	2.5
1	D	910	LYS	2.5
1	D	1019	LEU	2.5
1	D	868	ILE	2.4
1	A	417	GLY	2.4
1	B	180	GLU	2.4
1	A	330	SER	2.4
1	A	871	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	904	PHE	2.3
1	B	50	PHE	2.3
1	A	319	ALA	2.3
1	B	417	GLY	2.3
1	D	857	GLU	2.3
1	D	917	PRO	2.3
1	D	50	PHE	2.3
1	D	367	PHE	2.3
1	A	674	GLY	2.3
1	C	866	PRO	2.3
1	B	1008	THR	2.3
1	B	402	ARG	2.3
1	A	898	LYS	2.2
1	D	420	ASN	2.2
1	B	331	ILE	2.2
1	C	700	GLN	2.2
1	C	60	ASP	2.2
1	B	273	GLU	2.2
1	A	768	THR	2.2
1	C	51	HIS	2.2
1	C	371	ARG	2.1
1	D	856	THR	2.1
1	D	898	LYS	2.1
1	C	796	ILE	2.1
1	D	53	GLU	2.1
1	B	1012	GLU	2.1
1	D	864	PRO	2.1
1	C	424	ASP	2.0
1	B	1011	TYR	2.0
1	B	670	SER	2.0
1	C	875	LYS	2.0
1	A	53	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

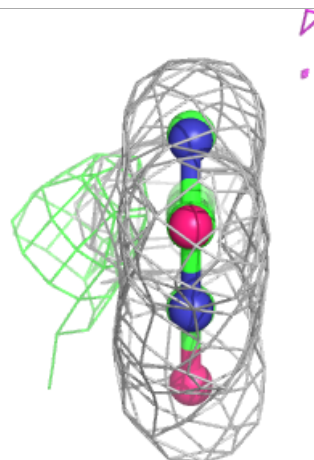
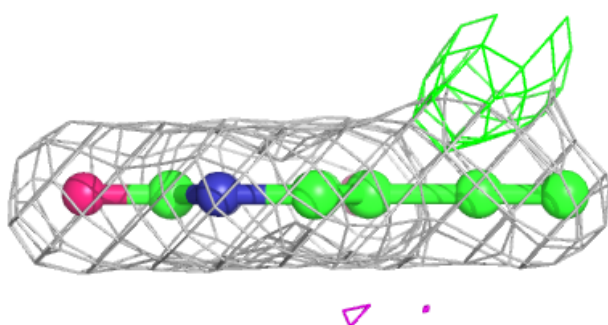
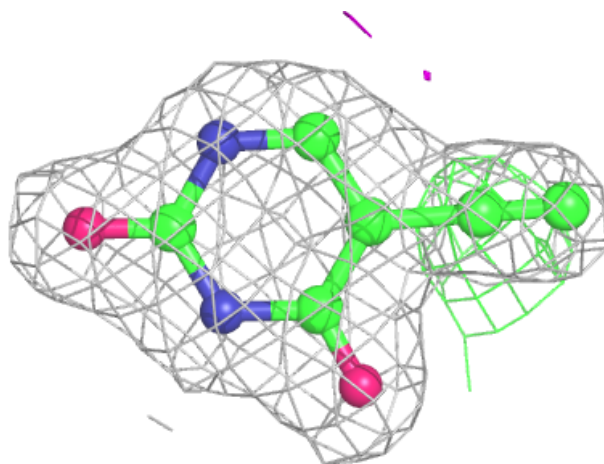
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	Y3G	A	1106	10/10	0.93	0.11	18,21,26,28	0
4	Y3G	B	1108	10/10	0.94	0.12	23,24,26,27	0
5	NAP	D	1107	48/48	0.95	0.15	22,27,40,46	0
5	NAP	B	1106	48/48	0.95	0.12	21,29,41,43	0
5	NAP	A	1107	48/48	0.96	0.12	19,26,35,36	0
4	Y3G	C	1108	10/10	0.96	0.09	18,20,24,25	0
3	FAD	B	1105	53/53	0.96	0.11	17,21,26,27	0
6	FNR	A	1108	31/31	0.96	0.14	16,19,21,23	0
6	FNR	C	1107	31/31	0.96	0.12	15,18,21,22	0
6	FNR	B	1107	31/31	0.96	0.10	15,20,24,27	0
3	FAD	C	1105	53/53	0.97	0.09	18,21,25,29	0
3	FAD	A	1105	53/53	0.97	0.10	15,19,25,27	0
5	NAP	C	1106	48/48	0.97	0.10	19,28,33,36	0
6	FNR	D	1108	31/31	0.97	0.13	16,18,21,24	0
4	Y3G	D	1106	10/10	0.97	0.09	17,20,26,26	0
3	FAD	D	1105	53/53	0.98	0.10	16,20,24,26	0
2	SF4	D	1104	8/8	0.98	0.07	16,17,18,18	0
2	SF4	A	1103	8/8	0.99	0.06	17,18,18,21	0
2	SF4	A	1104	8/8	0.99	0.06	18,20,20,21	0
2	SF4	C	1101	8/8	0.99	0.06	15,16,17,17	0
2	SF4	C	1102	8/8	0.99	0.06	15,17,18,18	0
2	SF4	C	1103	8/8	0.99	0.07	14,16,16,17	0
2	SF4	C	1104	8/8	0.99	0.07	17,18,18,18	0
2	SF4	D	1101	8/8	0.99	0.06	17,18,19,19	0
2	SF4	D	1102	8/8	0.99	0.06	17,18,18,18	0
2	SF4	D	1103	8/8	0.99	0.07	14,16,17,17	0
2	SF4	A	1101	8/8	0.99	0.06	17,18,20,21	0
2	SF4	B	1101	8/8	0.99	0.06	16,17,18,18	0
2	SF4	B	1102	8/8	0.99	0.06	16,18,19,19	0
2	SF4	B	1103	8/8	0.99	0.07	15,16,17,17	0
2	SF4	B	1104	8/8	0.99	0.07	16,17,18,19	0
2	SF4	A	1102	8/8	0.99	0.07	16,16,17,17	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.



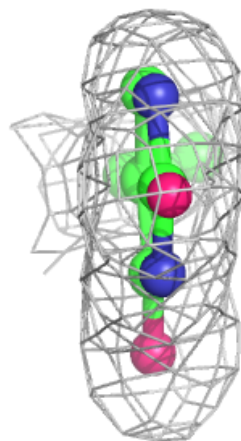
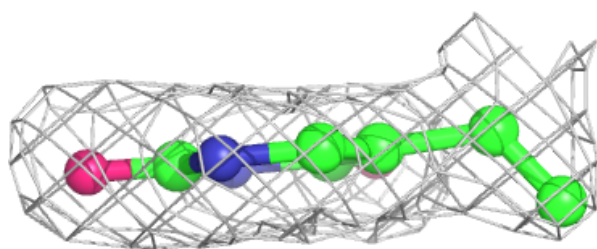
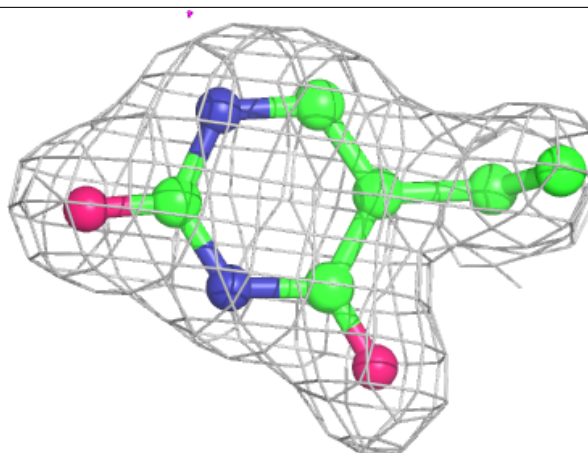
**Electron density around Y3G A 1106:**

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

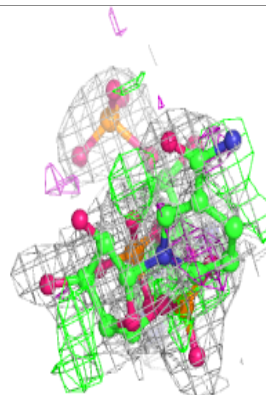
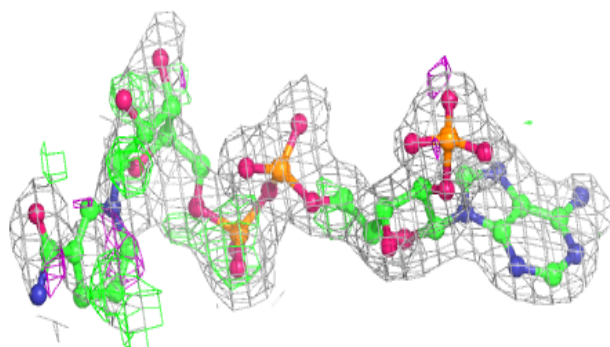
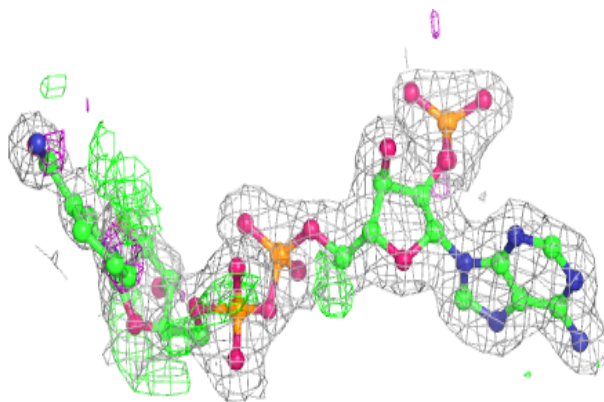


**Electron density around Y3G B 1108:**

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

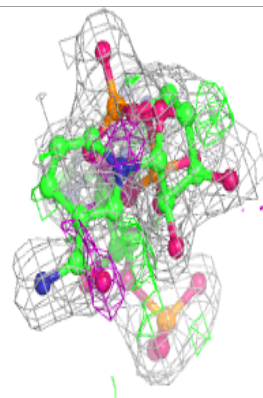
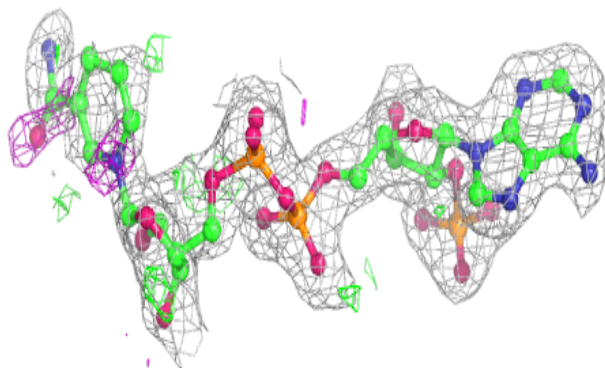
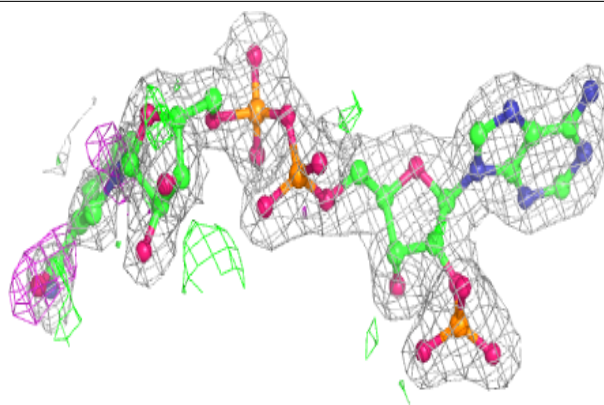
**Electron density around NAP D 1107:**

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

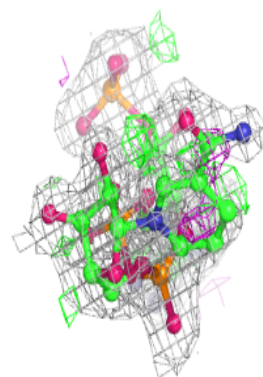
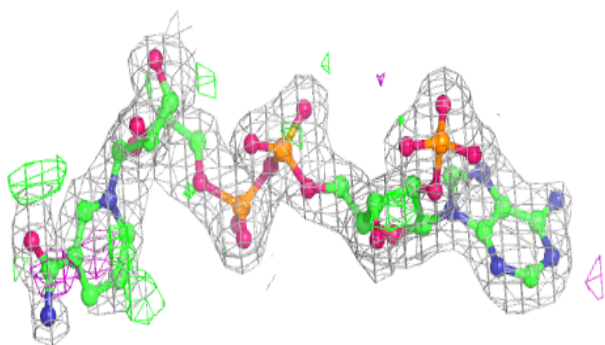
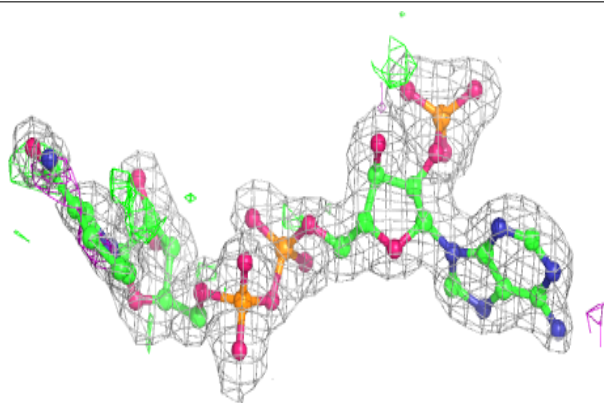


**Electron density around NAP B 1106:**

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

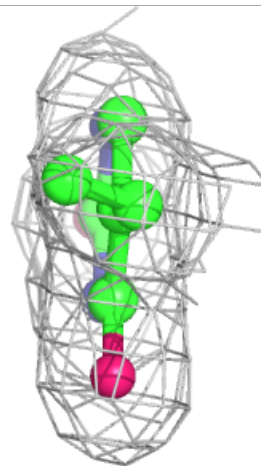
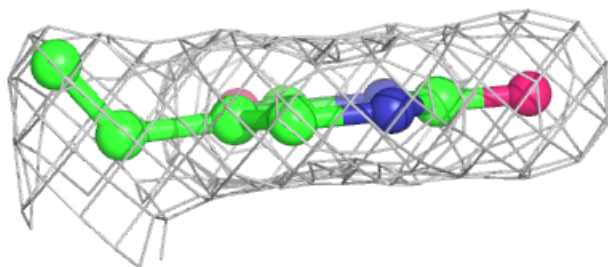
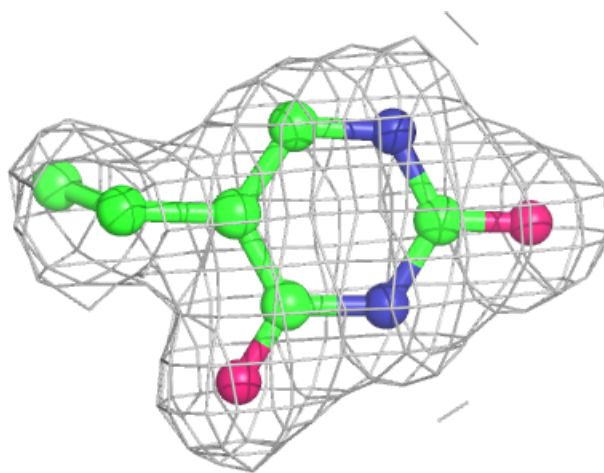
**Electron density around NAP A 1107:**

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



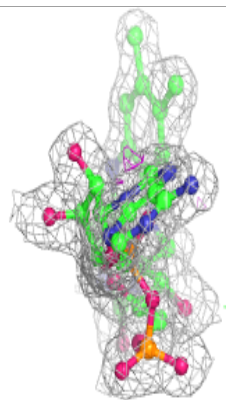
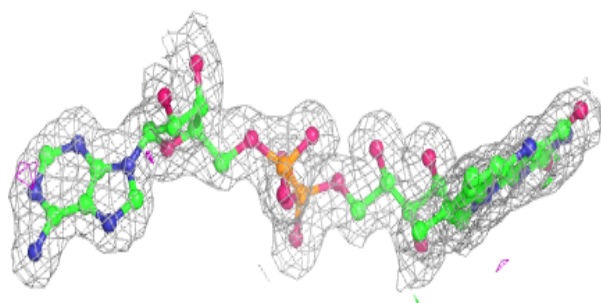
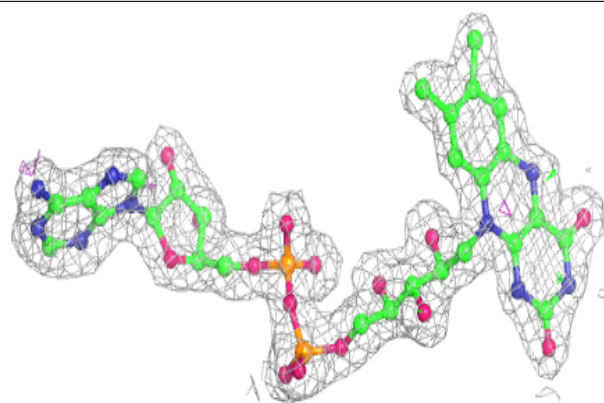
**Electron density around Y3G C 1108:**

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



**Electron density around FAD B 1105:**

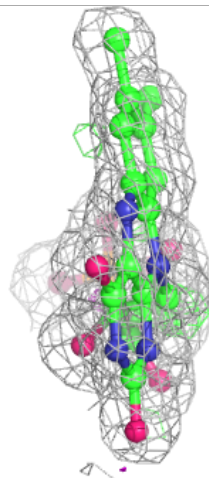
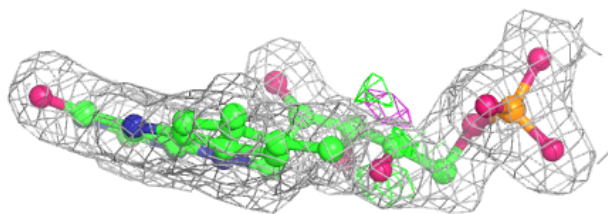
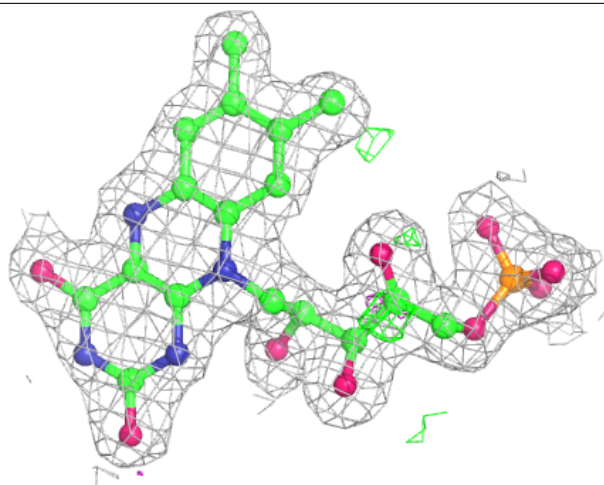
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





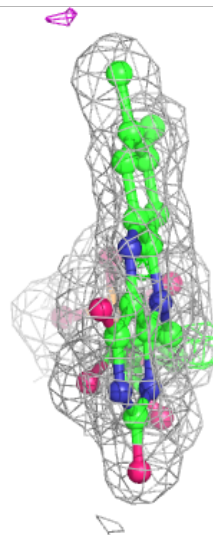
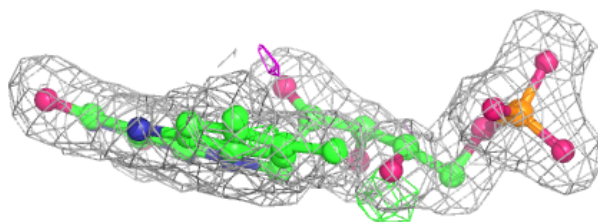
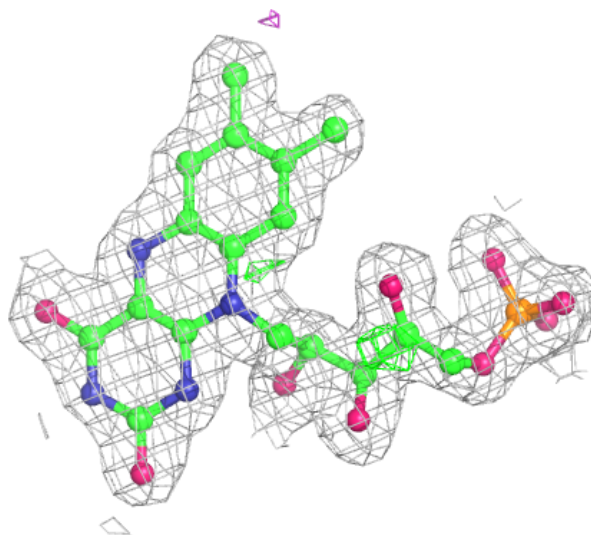
**Electron density around FNR A 1108:**

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



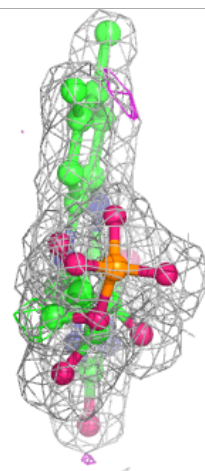
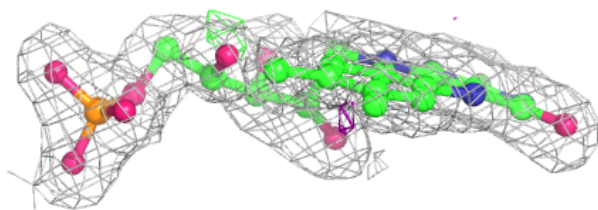
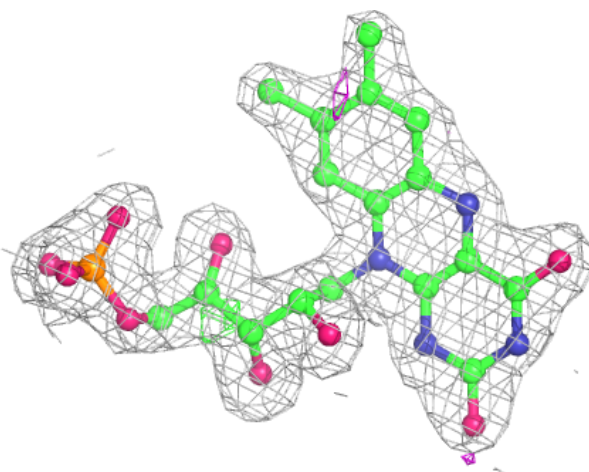
**Electron density around FNR C 1107:**

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



**Electron density around FNR B 1107:**

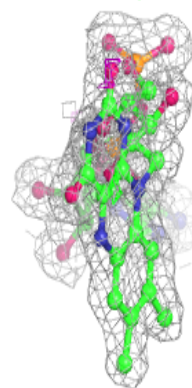
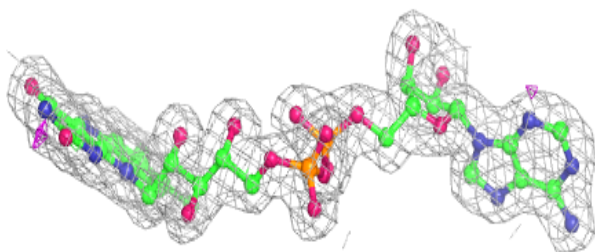
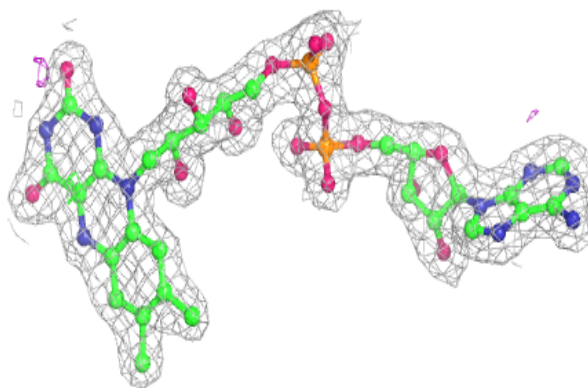
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



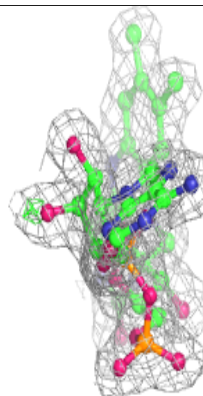
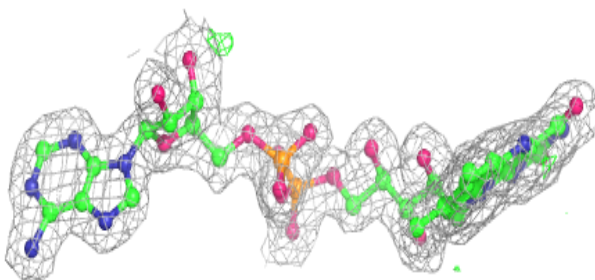
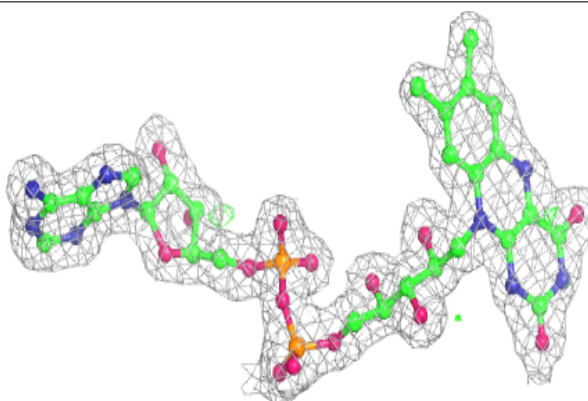


**Electron density around FAD C 1105:**

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

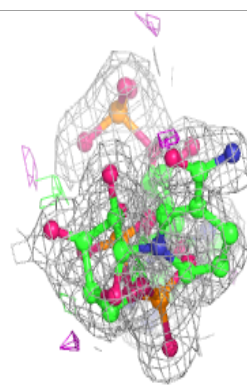
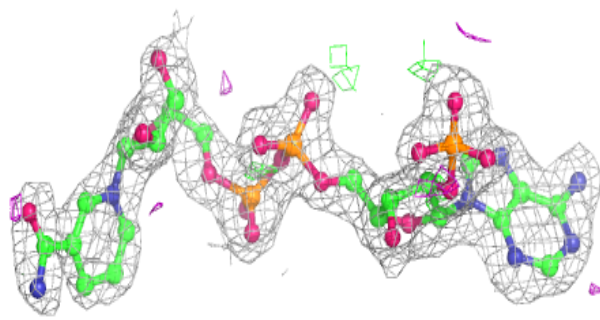
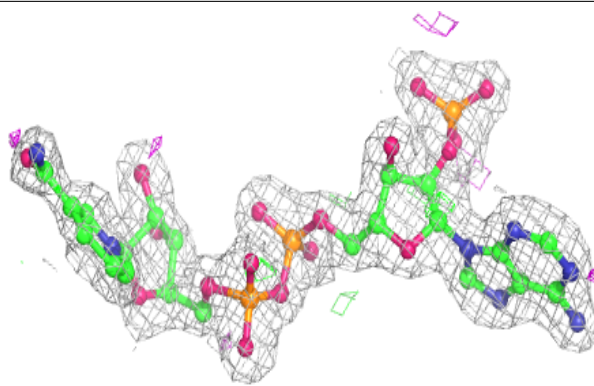
**Electron density around FAD A 1105:**

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

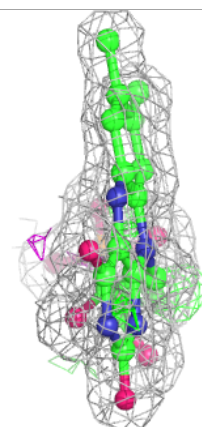
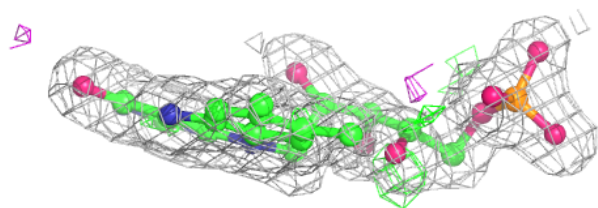
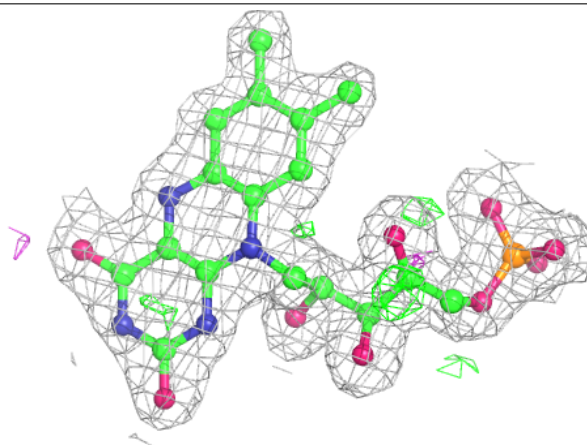


**Electron density around NAP C 1106:**

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

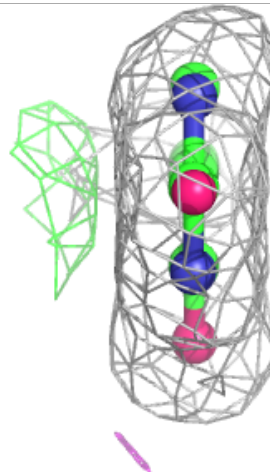
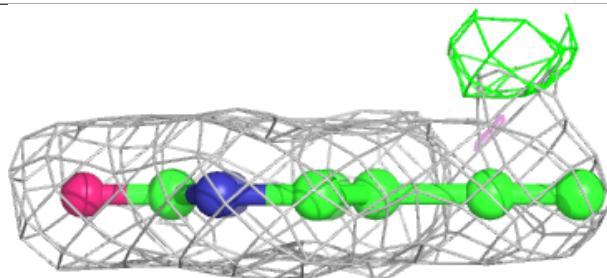
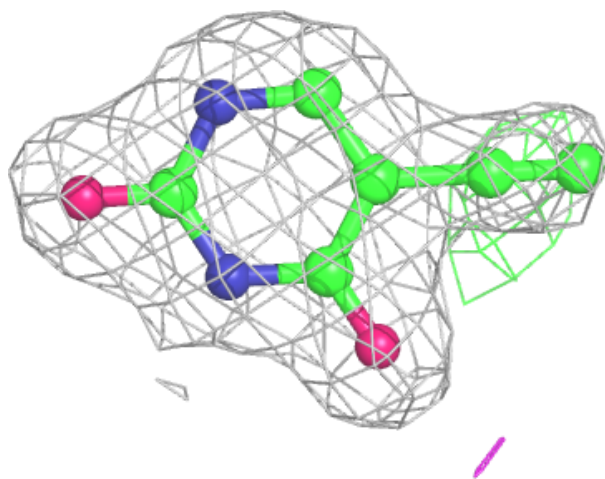
**Electron density around FNR D 1108:**

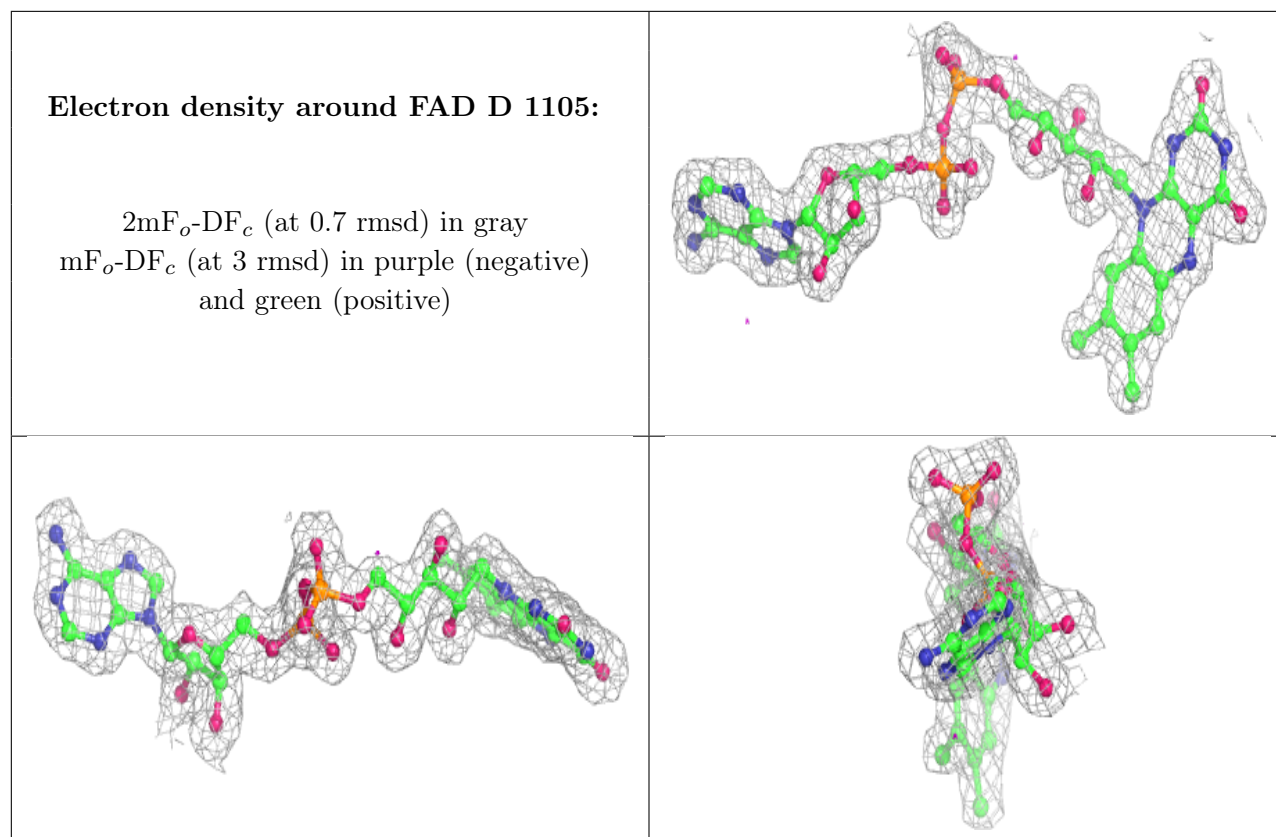
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Y3G D 1106:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.