



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:55 AM UTC

PDB ID : 1GT8 / pdb_00001gt8
Title : DIHYDROPYRIMIDINE DEHYDROGENASE (DPD) FROM PIG,
TERNARY COMPLEX WITH NADPH AND URACIL-4-ACETIC ACID
Authors : Dobritsch, D.; Ricagno, S.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on : 2002-01-14
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

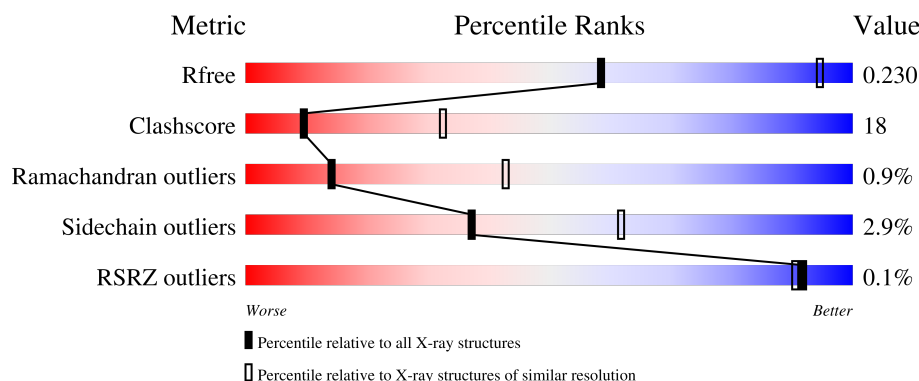
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1025	 67% 30% ..
1	B	1025	 65% 30% ..
1	C	1025	 63% 33% ..
1	D	1025	 60% 36% ..

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
2	SF4	A	1027	-	-	X	-
2	SF4	A	1028	-	-	X	-
2	SF4	B	1026	-	-	X	-
2	SF4	B	1027	-	-	X	-
2	SF4	B	1028	-	-	X	-
2	SF4	B	1029	-	-	X	-
2	SF4	C	1027	-	-	X	-
2	SF4	C	1028	-	-	X	-
2	SF4	D	1027	-	-	X	-
2	SF4	D	1028	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31588 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.

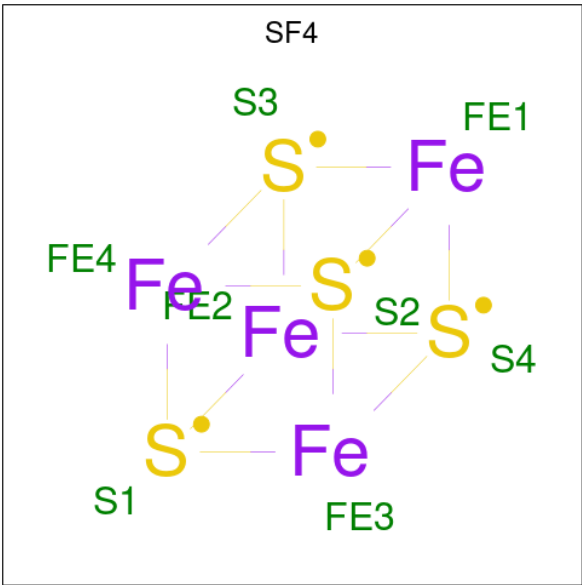
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1017	Total	C	N	O	S	0	0	0
			7755	4919	1312	1468	56			
1	B	1010	Total	C	N	O	S	0	0	0
			7703	4885	1304	1458	56			
1	C	1010	Total	C	N	O	S	0	0	0
			7708	4892	1303	1459	54			
1	D	1012	Total	C	N	O	S	0	0	0
			7718	4894	1307	1461	56			

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



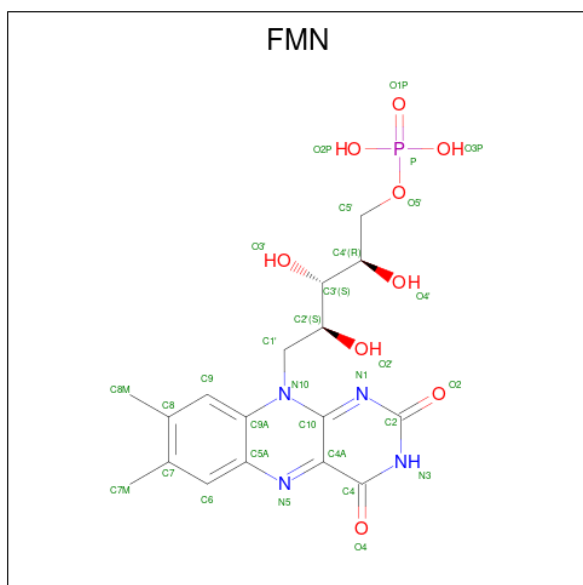
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S		
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S		
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S		
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S		
			8	4	4		
2	C	1	Total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

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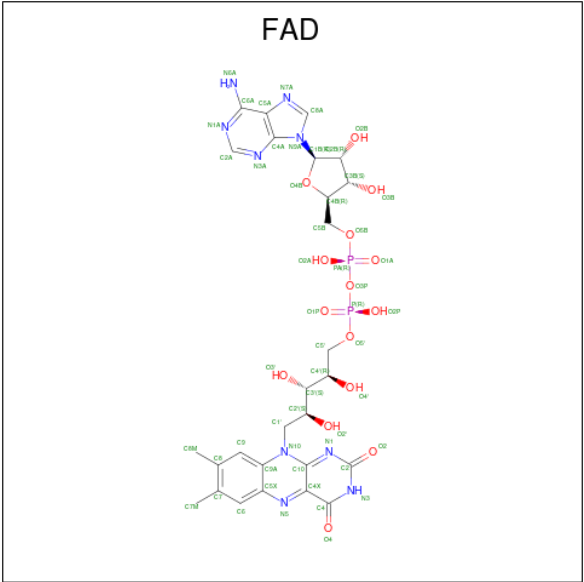
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



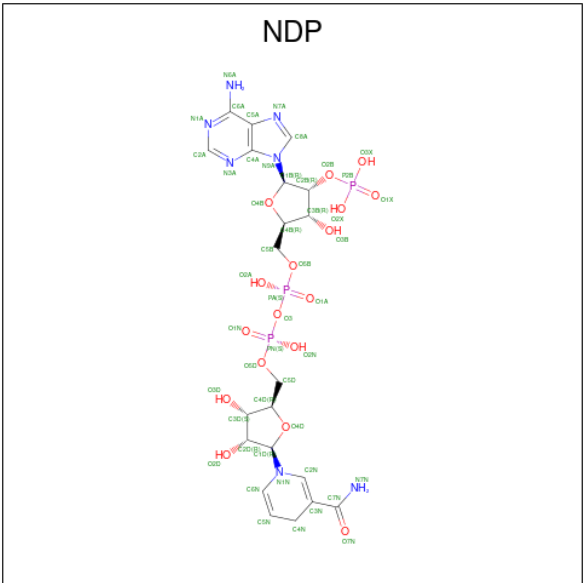
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



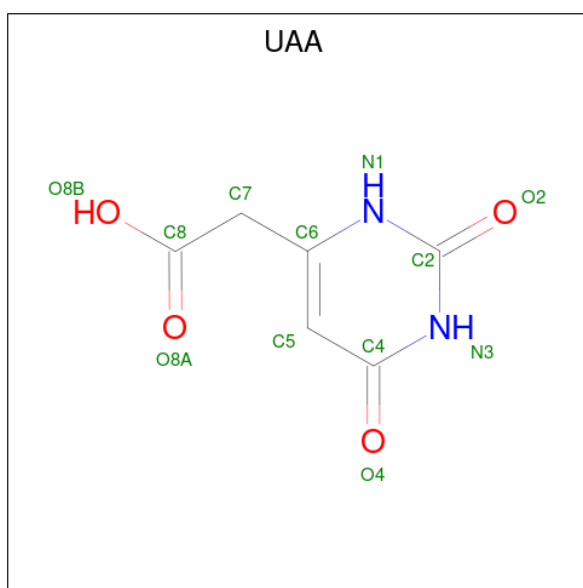
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	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		
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		

- Molecule 6 is URACIL-6-ACETIC ACID (CCD ID: UAA) (formula: $C_6H_6N_2O_4$).

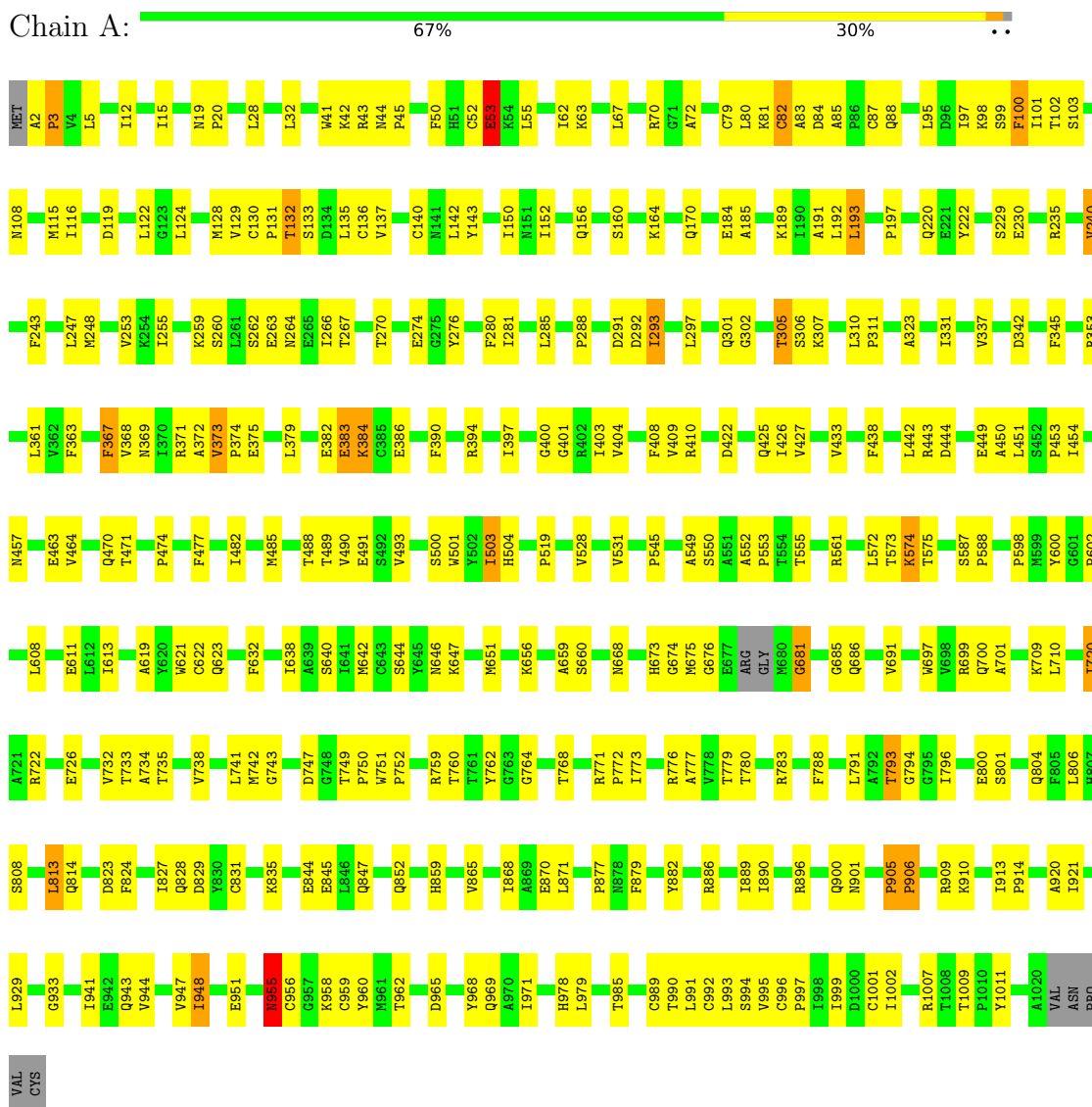


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	6	2	4		
6	B	1	Total	C	N	O	0	0
			12	6	2	4		
6	C	1	Total	C	N	O	0	0
			12	6	2	4		
6	D	1	Total	C	N	O	0	0
			12	6	2	4		

3 Residue-property plots

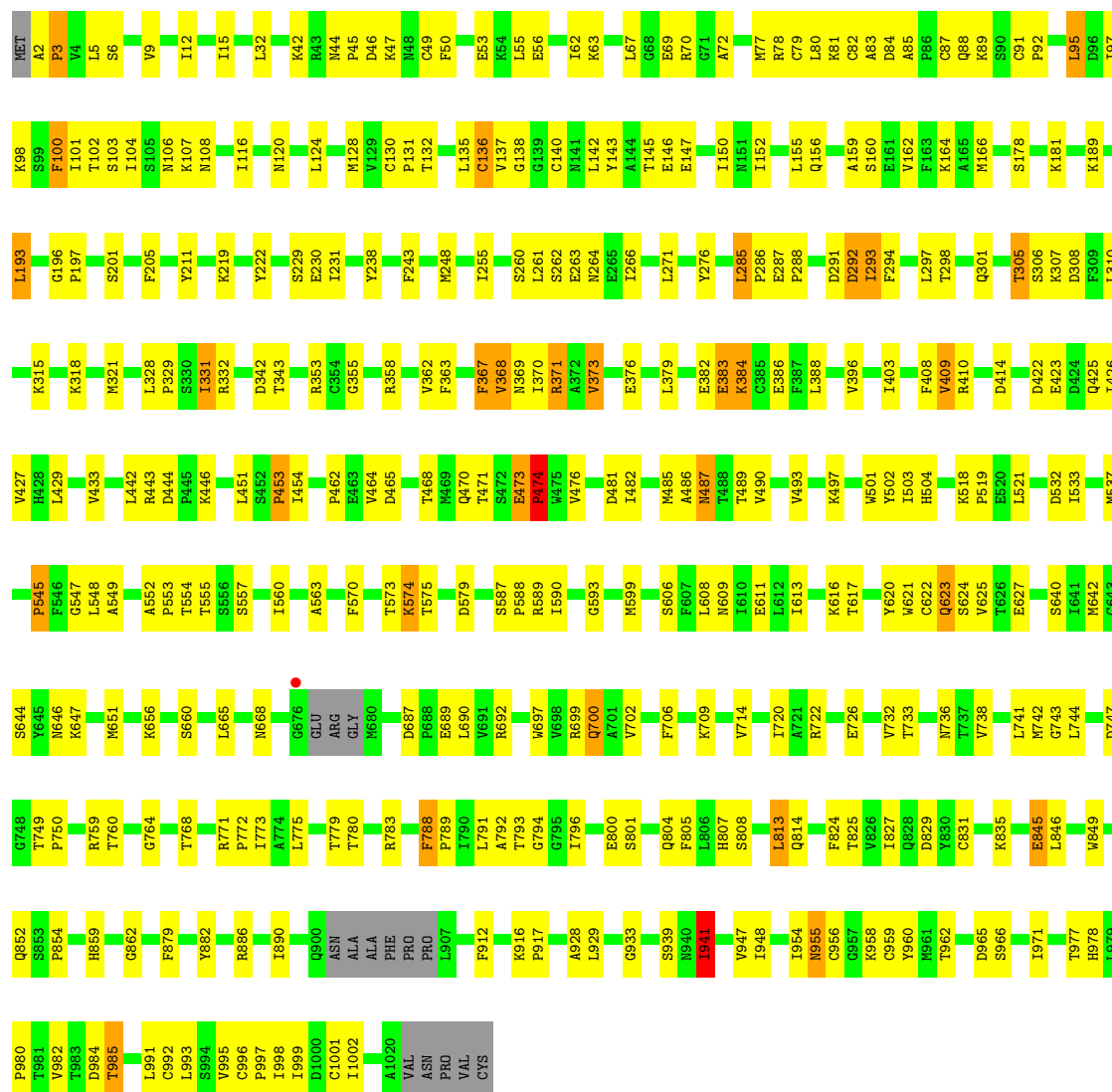
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DIHYDROPYRIMIDINE DEHYDROGENASE

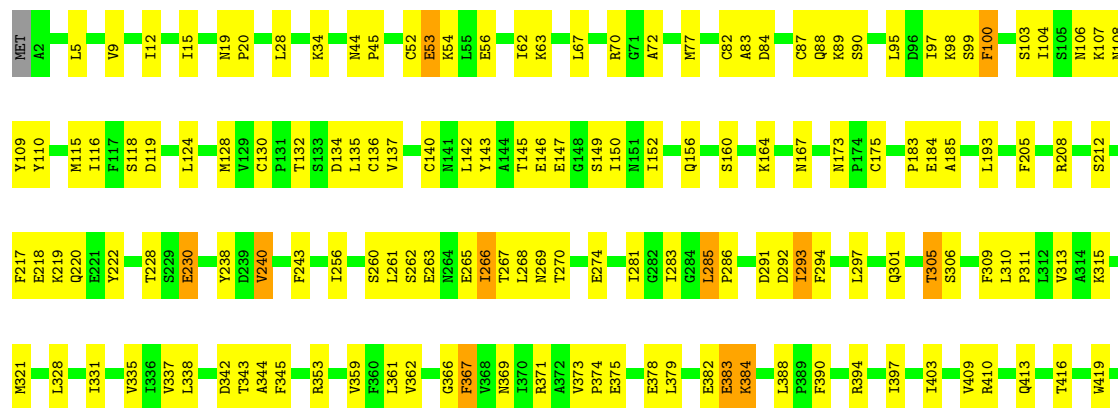


• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE





Chain C: 63% 33%



T962	C963	N964	G967	Y968	Q969	Q972	P975	H978	L979	P980	T981	V982	T985	C986	C989	T990	L991	C992	L993	S994	V995	C996	P997	I998	C1001	I1002	R1015	P1018	L1019	A1020	VAL	ASN	PRO	VAL	CYS												
T779	T780	I781	A782	R783	F788	A792	T793	G794	G795	I796	E800	S801	G802	L803	Q804	F805	L806	H807	S808	G809	A810	L813	Q814	V815	C816	I827	Q828	D829	Y830	Y839	L840	K841	S842	I843	E844	E845	W849	Q852	S853	P854	H859	Q860	K861	V865	A869	E870	L871
W872	G873	K874	L883	R886	K887	I890	E893	R896	L897	K898	N901	ALA	ALA	PHE	PRO	P906	R909	P914	K915	K916	P917	I918	P919	A920	I921	V924	L929	Q930	Y931	L932	F935	L938	I941	V945	A946	V947	I948	N955	C956	G957	K958	C959	Y960	M961			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.03Å 159.53Å 166.02Å 90.00° 97.16° 90.00°	Depositor
Resolution (Å)	29.75 – 3.30 29.75 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.75-3.30) 98.3 (29.75-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 3.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.269 (Not available) , 0.230	Depositor DCC
R_{free} test set	1247 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31588	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 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, FAD, SF4, NDP, UAA

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	0.58	0/7916	1.00	37/10729 (0.3%)
1	B	0.57	0/7860	1.00	37/10649 (0.3%)
1	C	0.52	0/7868	1.00	33/10667 (0.3%)
1	D	0.50	0/7876	0.98	28/10671 (0.3%)
All	All	0.54	0/31520	0.99	135/42716 (0.3%)

There are no bond length outliers.

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	LEU	CA-C-N	10.12	130.41	119.28
1	B	285	LEU	C-N-CA	10.12	130.41	119.28
1	A	285	LEU	CA-C-N	9.60	129.35	119.56
1	A	285	LEU	C-N-CA	9.60	129.35	119.56
1	C	904	PHE	CA-C-N	9.19	129.84	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7755	0	7781	279	0
1	B	7703	0	7735	286	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7708	0	7743	331	0
1	D	7718	0	7750	335	0
2	A	32	0	0	6	0
2	B	32	0	0	8	0
2	C	32	0	0	6	0
2	D	32	0	0	8	0
3	A	31	0	19	0	0
3	B	31	0	19	0	0
3	C	31	0	19	0	0
3	D	31	0	19	1	0
4	A	53	0	31	1	0
4	B	53	0	31	1	0
4	C	53	0	31	2	0
4	D	53	0	31	5	0
5	A	48	0	26	6	0
5	B	48	0	26	5	0
5	C	48	0	26	6	0
5	D	48	0	26	6	0
6	A	12	0	5	1	0
6	B	12	0	5	1	0
6	C	12	0	5	1	0
6	D	12	0	5	0	0
All	All	31588	0	31333	1120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 1120 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:C:136:CYS:SG	1:C:137:VAL:HG23	2.02	1.00
1:C:116:ILE:HD13	1:C:156:GLN:HG3	1.43	0.99
1:A:485:MET:HE1	1:B:32:LEU:HB2	1.46	0.97
1:C:410:ARG:NH1	1:D:427:VAL:HG13	1.84	0.92
1:A:32:LEU:HB2	1:B:485:MET:HE1	1.50	0.91

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1013/1025 (99%)	927 (92%)	72 (7%)	14 (1%)	9	33
1	B	1004/1025 (98%)	920 (92%)	77 (8%)	7 (1%)	18	49
1	C	1006/1025 (98%)	926 (92%)	74 (7%)	6 (1%)	21	52
1	D	1006/1025 (98%)	924 (92%)	73 (7%)	9 (1%)	14	43
All	All	4029/4100 (98%)	3697 (92%)	296 (7%)	36 (1%)	14	43

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	674	GLY
1	A	676	GLY
1	A	906	PRO
1	C	613	ILE
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	847/854 (99%)	828 (98%)	19 (2%)	45	66
1	B	842/854 (99%)	813 (97%)	29 (3%)	32	59
1	C	843/854 (99%)	824 (98%)	19 (2%)	44	66
1	D	844/854 (99%)	812 (96%)	32 (4%)	29	57
All	All	3376/3416 (99%)	3277 (97%)	99 (3%)	37	62

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	667	LEU
1	D	197	PRO
1	C	780	THR
1	C	941	ILE
1	D	367	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	173	ASN
1	C	878	ASN
1	D	822	GLN
1	C	470	GLN
1	C	693	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
2	SF4	B	1029	1	0,12,12	-	-	-		
5	NDP	C	1032	-	51,52,52	1.58	8 (15%)	71,80,80	1.61	14 (19%)
2	SF4	B	1026	1	0,12,12	-	-	-		
4	FAD	C	1031	-	58,58,58	2.48	23 (39%)	85,89,89	1.65	10 (11%)
6	UAA	B	1035	-	12,12,12	0.90	0	13,16,16	1.70	5 (38%)
3	FMN	A	1030	-	33,33,33	1.87	9 (27%)	48,50,50	1.77	11 (22%)
2	SF4	B	1028	1	0,12,12	-	-	-		
3	FMN	B	1030	-	33,33,33	1.94	8 (24%)	48,50,50	1.85	12 (25%)
2	SF4	D	1028	1	0,12,12	-	-	-		
2	SF4	C	1028	1	0,12,12	-	-	-		
3	FMN	C	1030	-	33,33,33	2.00	8 (24%)	48,50,50	1.79	10 (20%)
5	NDP	B	1032	-	51,52,52	1.67	7 (13%)	71,80,80	1.53	10 (14%)
2	SF4	A	1028	1	0,12,12	-	-	-		
2	SF4	C	1027	1	0,12,12	-	-	-		
2	SF4	A	1027	-	0,12,12	-	-	-		
2	SF4	D	1027	1	0,12,12	-	-	-		
2	SF4	D	1029	1	0,12,12	-	-	-		
2	SF4	C	1029	1	0,12,12	-	-	-		
4	FAD	B	1031	-	58,58,58	2.42	20 (34%)	85,89,89	1.66	7 (8%)
5	NDP	D	1032	-	51,52,52	1.83	11 (21%)	71,80,80	1.83	19 (26%)
2	SF4	A	1029	1	0,12,12	-	-	-		
6	UAA	D	1035	-	12,12,12	1.17	2 (16%)	13,16,16	1.66	4 (30%)
2	SF4	D	1026	1	0,12,12	-	-	-		
2	SF4	C	1026	1	0,12,12	-	-	-		
2	SF4	A	1026	-	0,12,12	-	-	-		
6	UAA	A	1035	-	12,12,12	1.01	0	13,16,16	1.58	3 (23%)
4	FAD	D	1031	-	58,58,58	2.51	20 (34%)	85,89,89	1.68	9 (10%)
2	SF4	B	1027	1	0,12,12	-	-	-		
4	FAD	A	1031	-	58,58,58	2.38	19 (32%)	85,89,89	1.66	7 (8%)
6	UAA	C	1035	-	12,12,12	0.89	0	13,16,16	1.74	4 (30%)
3	FMN	D	1030	-	33,33,33	1.89	9 (27%)	48,50,50	1.82	12 (25%)
5	NDP	A	1032	-	51,52,52	1.74	12 (23%)	71,80,80	1.89	15 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	1029	1	-	-	0/6/5/5
5	NDP	C	1032	-	-	5/34/77/77	0/5/5/5
4	FAD	C	1031	-	-	5/34/50/50	0/6/6/6
2	SF4	B	1026	1	-	-	0/6/5/5
6	UAA	B	1035	-	-	0/4/4/4	0/1/1/1
3	FMN	A	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	B	1028	1	-	-	0/6/5/5
5	NDP	B	1032	-	-	4/34/77/77	0/5/5/5
3	FMN	B	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	C	1028	1	-	-	0/6/5/5
3	FMN	C	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	D	1028	1	-	-	0/6/5/5
2	SF4	A	1028	1	-	-	0/6/5/5
2	SF4	C	1027	1	-	-	0/6/5/5
2	SF4	A	1027	-	-	-	0/6/5/5
4	FAD	B	1031	-	-	7/34/50/50	0/6/6/6
5	NDP	D	1032	-	-	4/34/77/77	0/5/5/5
2	SF4	C	1029	1	-	-	0/6/5/5
2	SF4	D	1027	1	-	-	0/6/5/5
2	SF4	D	1029	1	-	-	0/6/5/5
2	SF4	A	1029	1	-	-	0/6/5/5
6	UAA	D	1035	-	-	0/4/4/4	0/1/1/1
2	SF4	D	1026	1	-	-	0/6/5/5
2	SF4	C	1026	1	-	-	0/6/5/5
2	SF4	A	1026	-	-	-	0/6/5/5
6	UAA	A	1035	-	-	0/4/4/4	0/1/1/1
4	FAD	D	1031	-	-	4/34/50/50	0/6/6/6
2	SF4	B	1027	1	-	-	0/6/5/5
4	FAD	A	1031	-	-	5/34/50/50	0/6/6/6
6	UAA	C	1035	-	-	0/4/4/4	0/1/1/1
3	FMN	D	1030	-	-	1/18/18/18	0/3/3/3
5	NDP	A	1032	-	-	4/34/77/77	0/5/5/5

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1031	FAD	PA-O3P	10.51	1.70	1.59
4	C	1031	FAD	P-O3P	-10.23	1.48	1.59
4	D	1031	FAD	PA-O3P	10.20	1.70	1.59
4	A	1031	FAD	PA-O3P	9.29	1.69	1.59
4	A	1031	FAD	P-O3P	-8.20	1.50	1.59

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1031	FAD	O3P-PA-O1A	-8.90	83.92	110.70
4	A	1031	FAD	O3P-PA-O1A	-8.78	84.30	110.70
4	D	1031	FAD	O3P-PA-O1A	-8.66	84.66	110.70
4	C	1031	FAD	O3P-PA-O1A	-8.45	85.30	110.70
4	C	1031	FAD	O2A-PA-O3P	-7.54	86.89	107.27

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1031	FAD	C5B-O5B-PA-O3P
4	B	1031	FAD	C5B-O5B-PA-O3P
4	C	1031	FAD	C5B-O5B-PA-O3P
4	D	1031	FAD	C5B-O5B-PA-O3P
5	A	1032	NDP	O4D-C1D-N1N-C2N

There are no ring outliers.

28 monomers are involved in 64 short contacts:

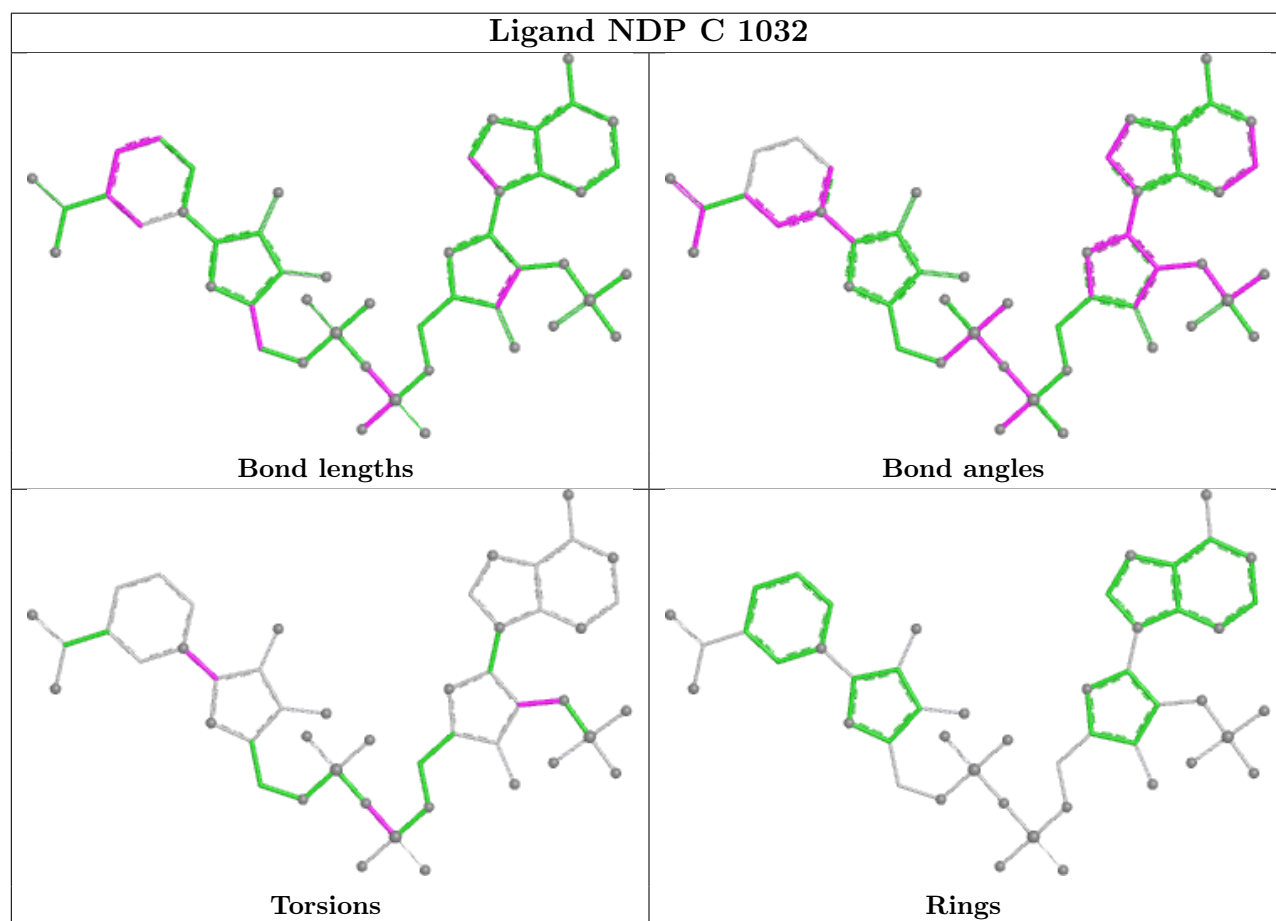
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1029	SF4	2	0
5	C	1032	NDP	6	0
2	B	1026	SF4	2	0
4	C	1031	FAD	2	0
6	B	1035	UAA	1	0
2	B	1028	SF4	2	0
2	D	1028	SF4	4	0
2	C	1028	SF4	2	0
5	B	1032	NDP	5	0
2	A	1028	SF4	2	0
2	C	1027	SF4	2	0
2	A	1027	SF4	2	0
2	D	1027	SF4	2	0
2	D	1029	SF4	1	0
2	C	1029	SF4	1	0
4	B	1031	FAD	1	0
5	D	1032	NDP	6	0
2	A	1029	SF4	1	0
2	D	1026	SF4	1	0
2	C	1026	SF4	1	0
2	A	1026	SF4	1	0

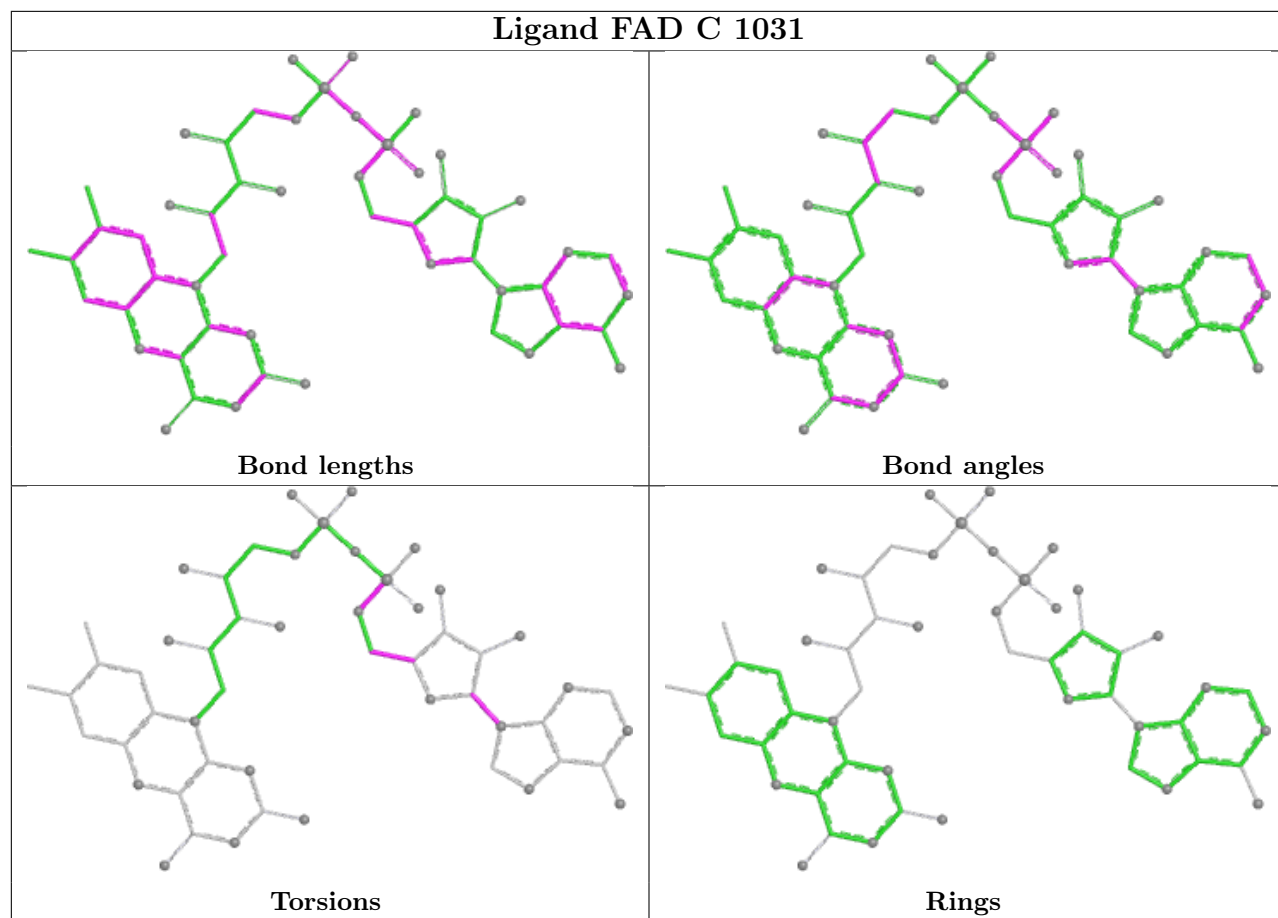
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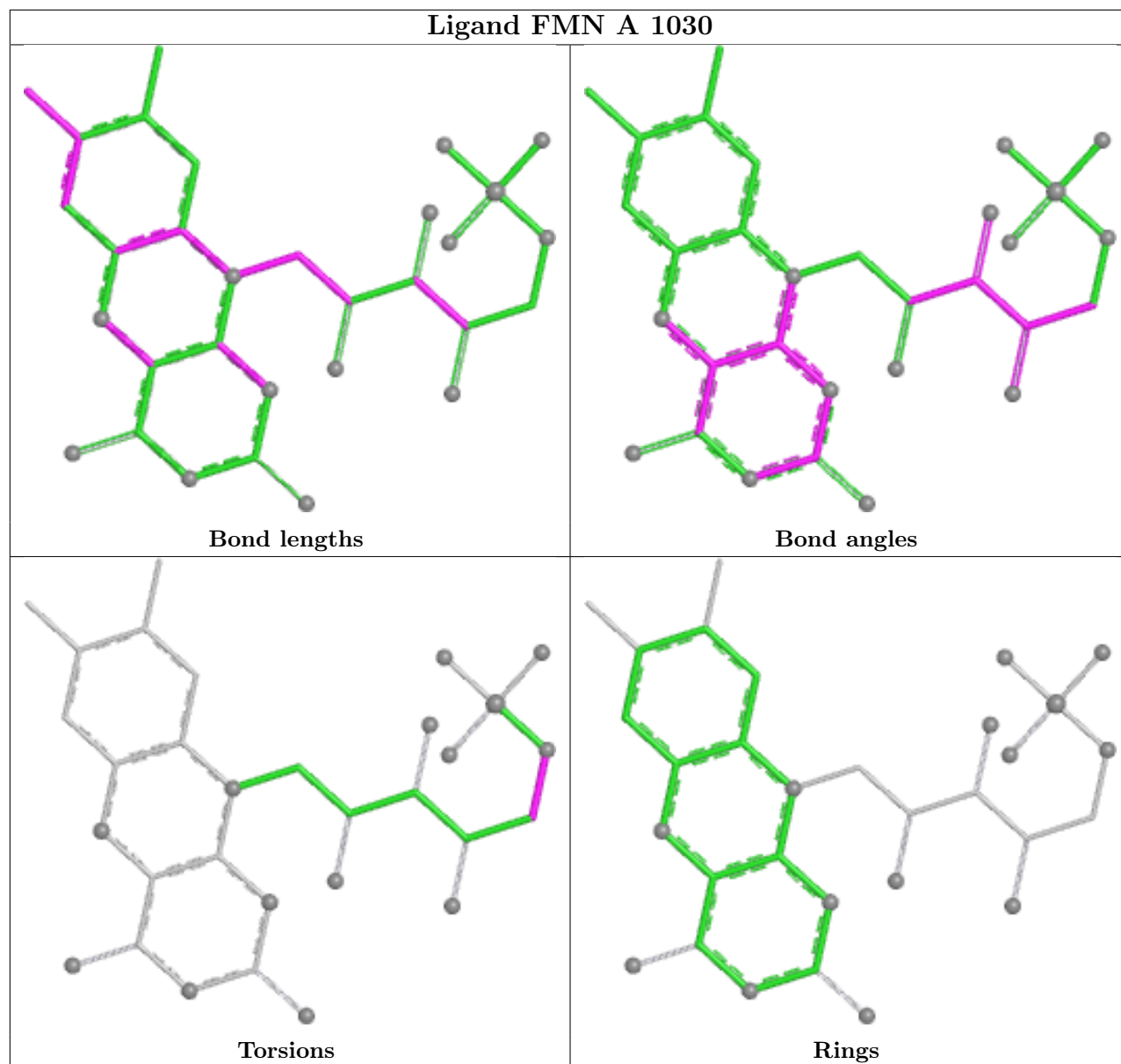
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1035	UAA	1	0
4	D	1031	FAD	5	0
2	B	1027	SF4	2	0
4	A	1031	FAD	1	0
6	C	1035	UAA	1	0
3	D	1030	FMN	1	0
5	A	1032	NDP	6	0

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.

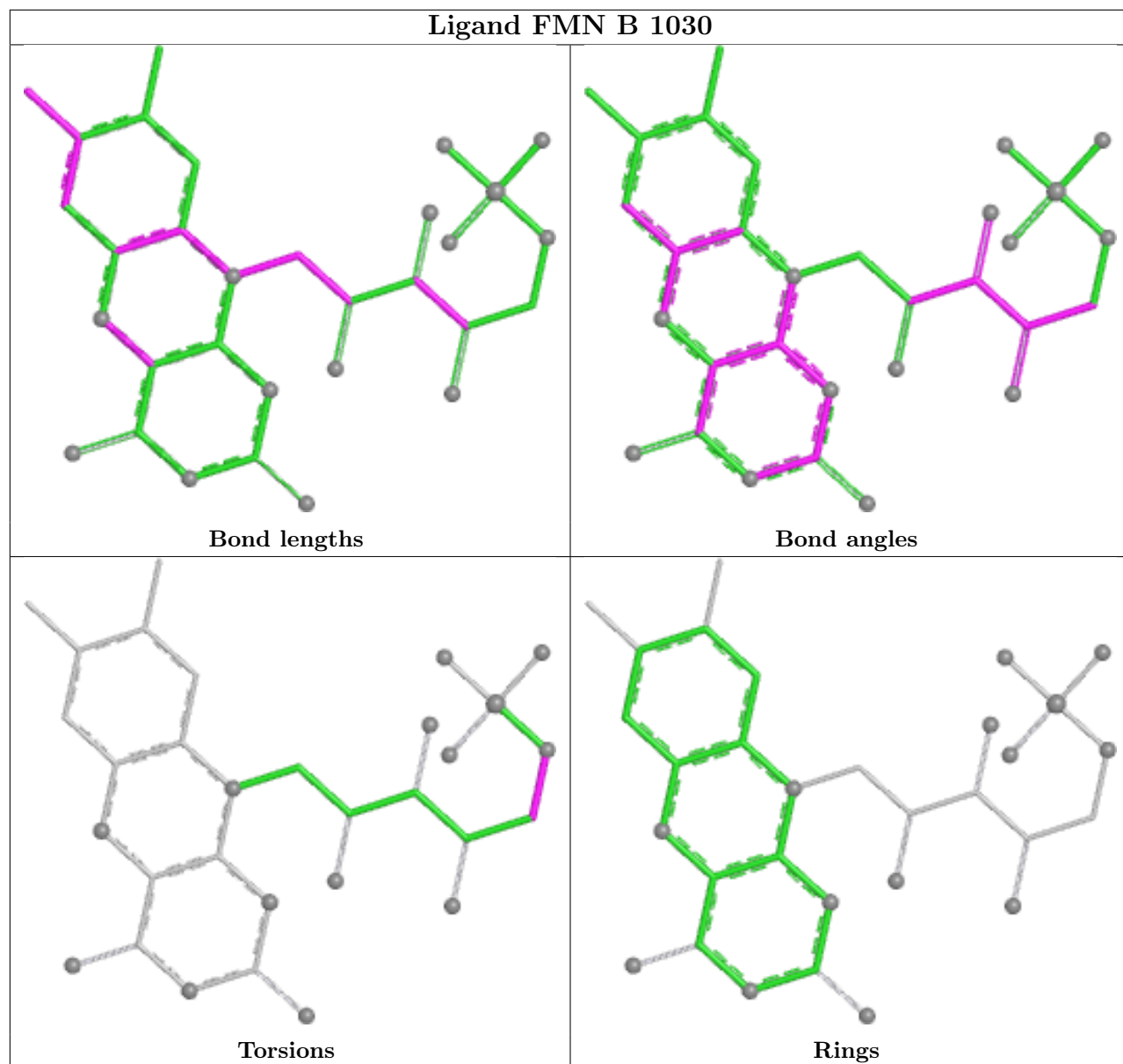




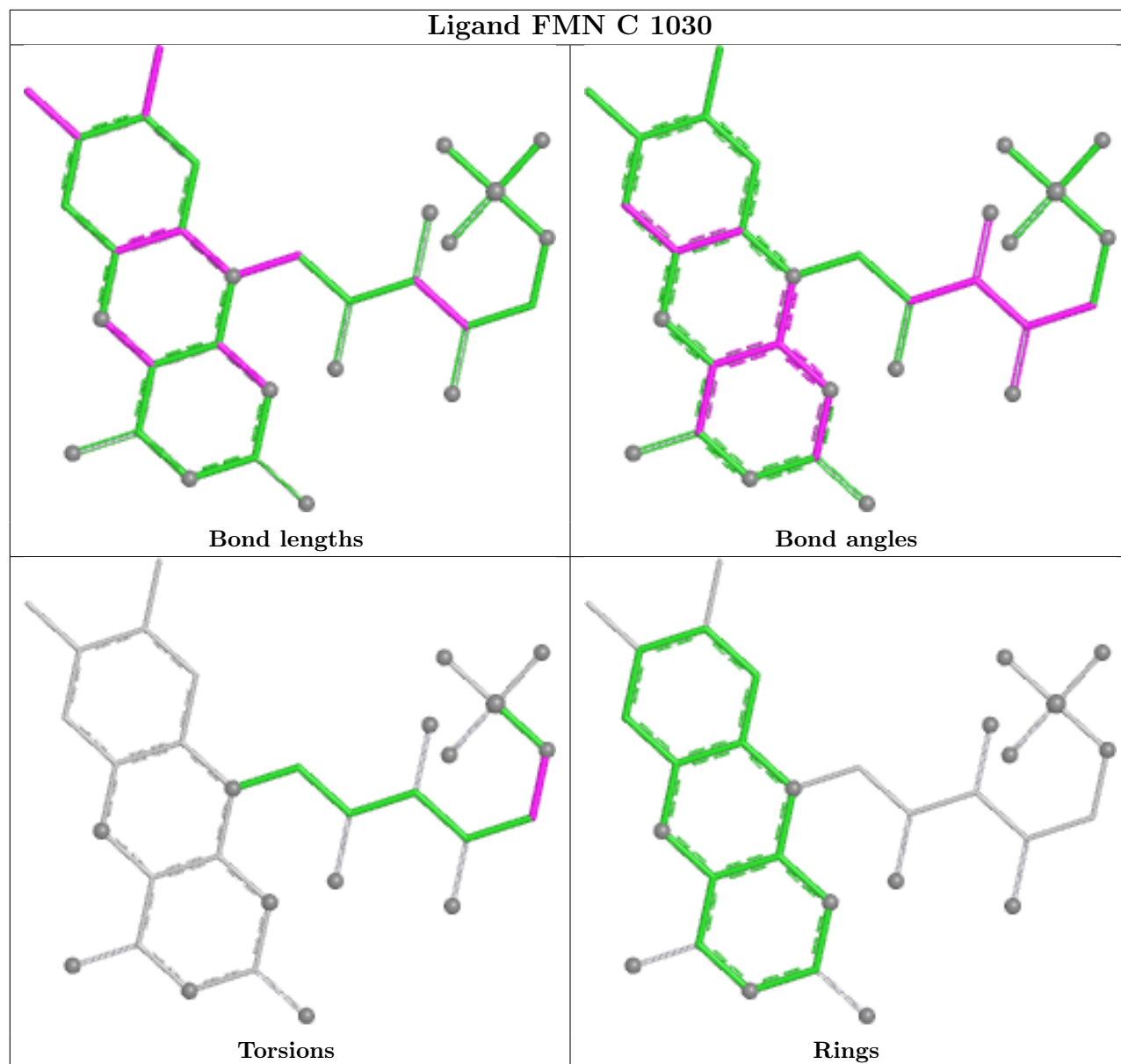
Ligand FMN A 1030

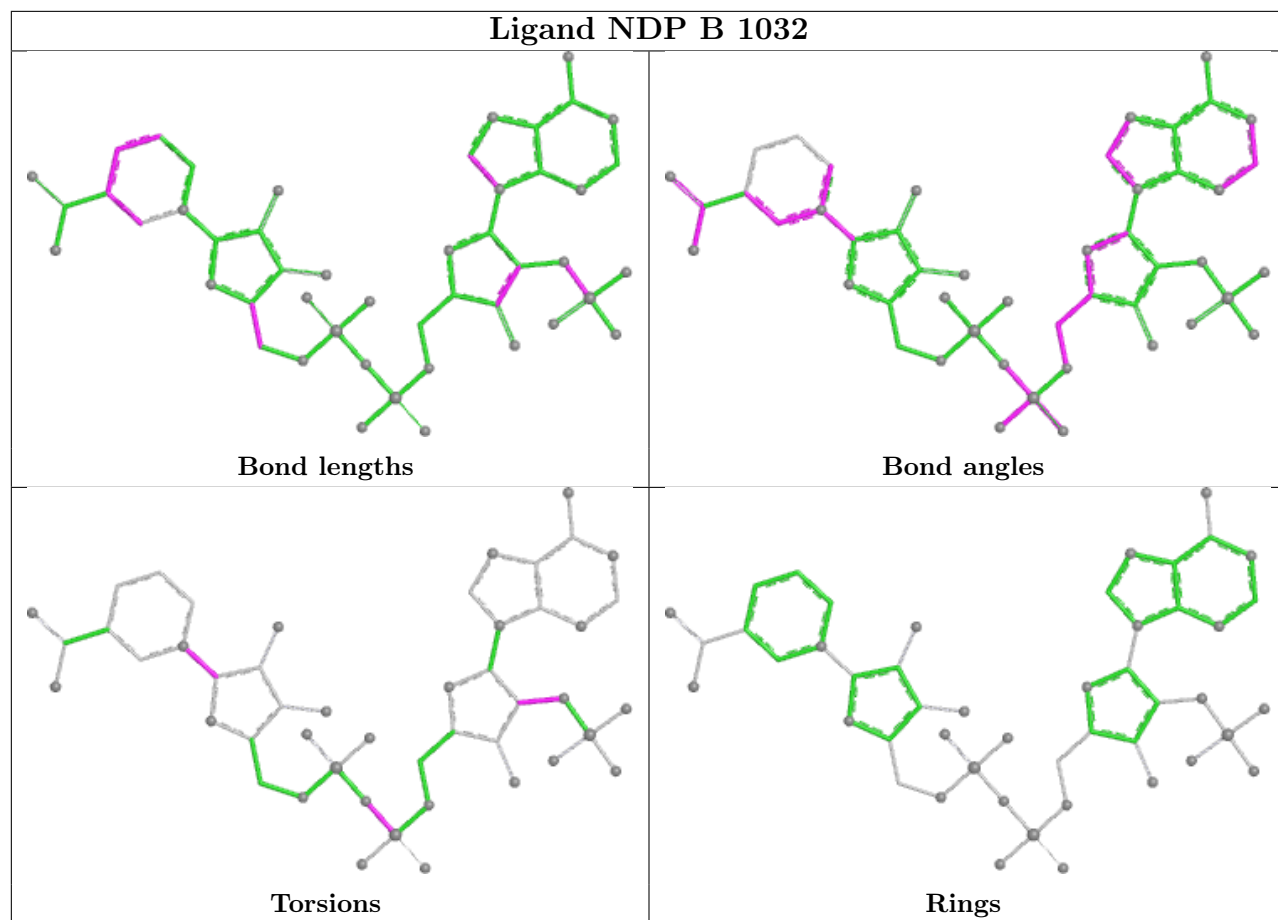


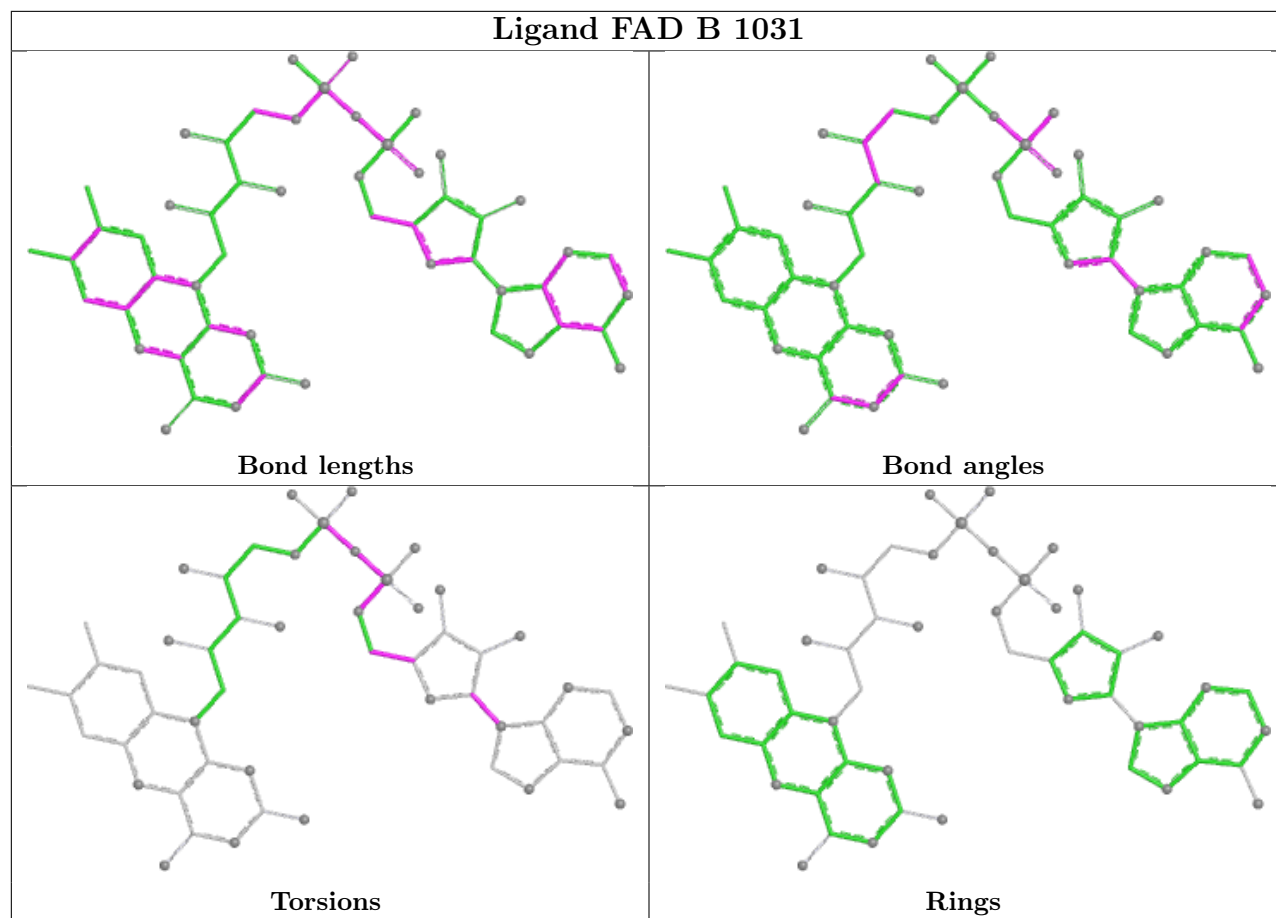
Ligand FMN B 1030

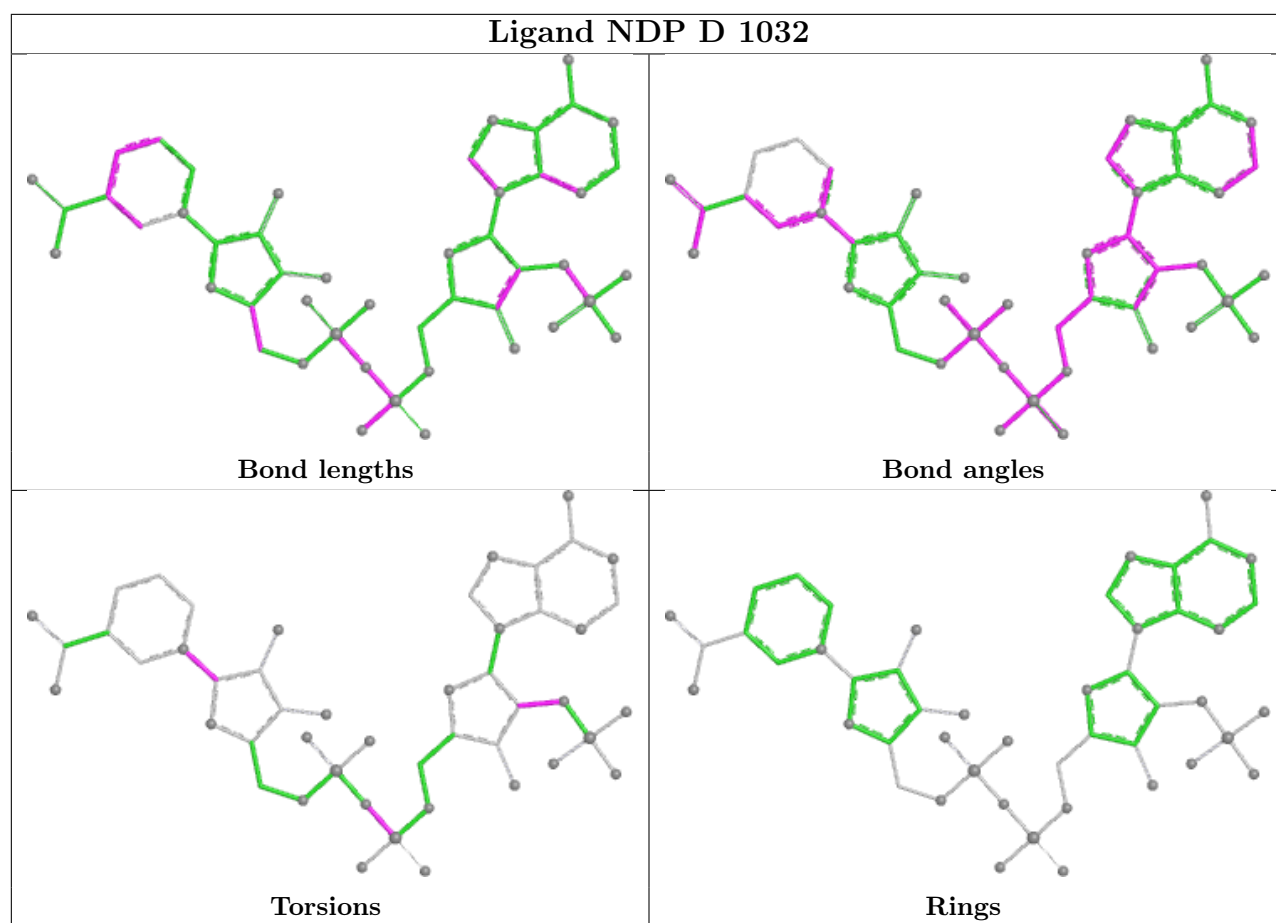


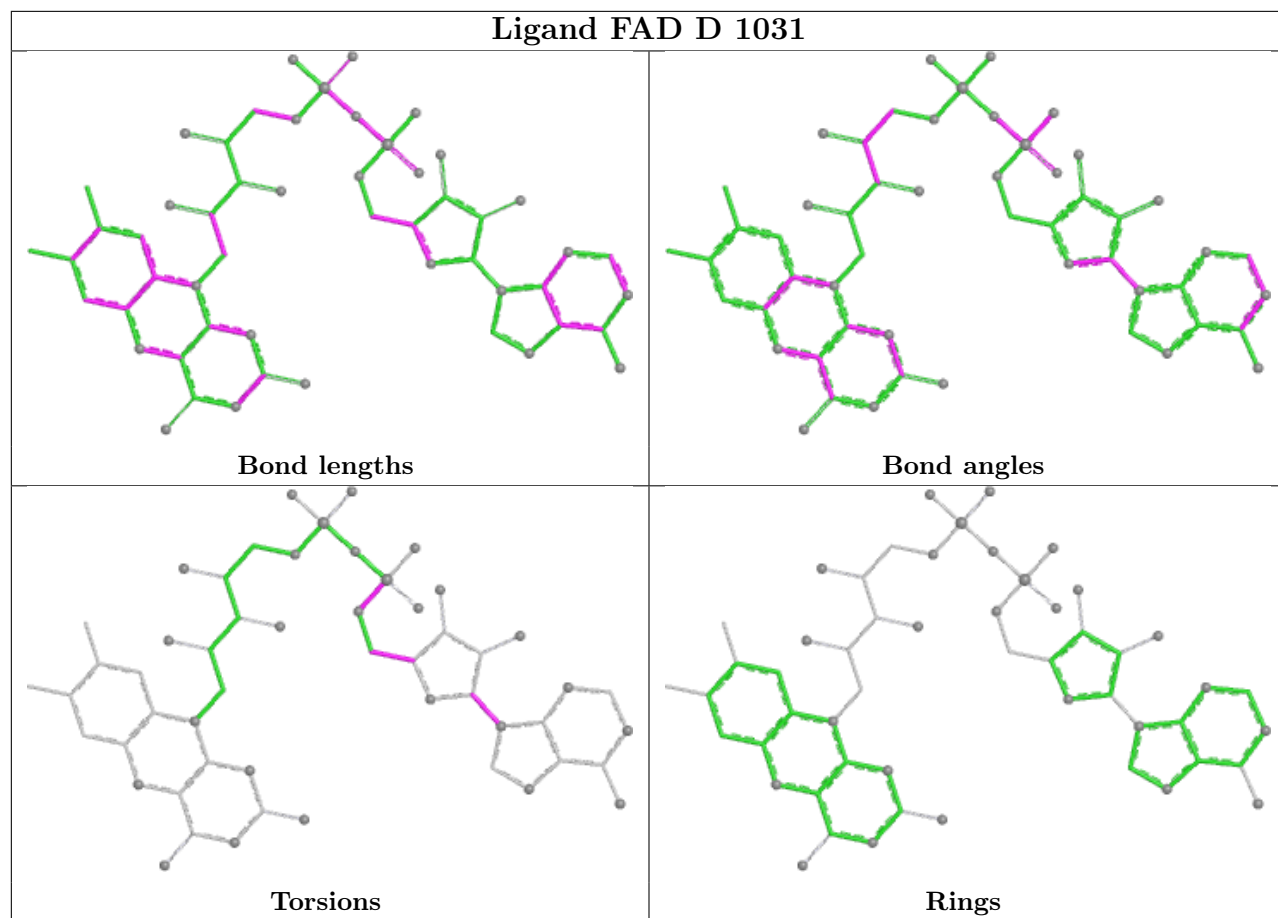
Ligand FMN C 1030

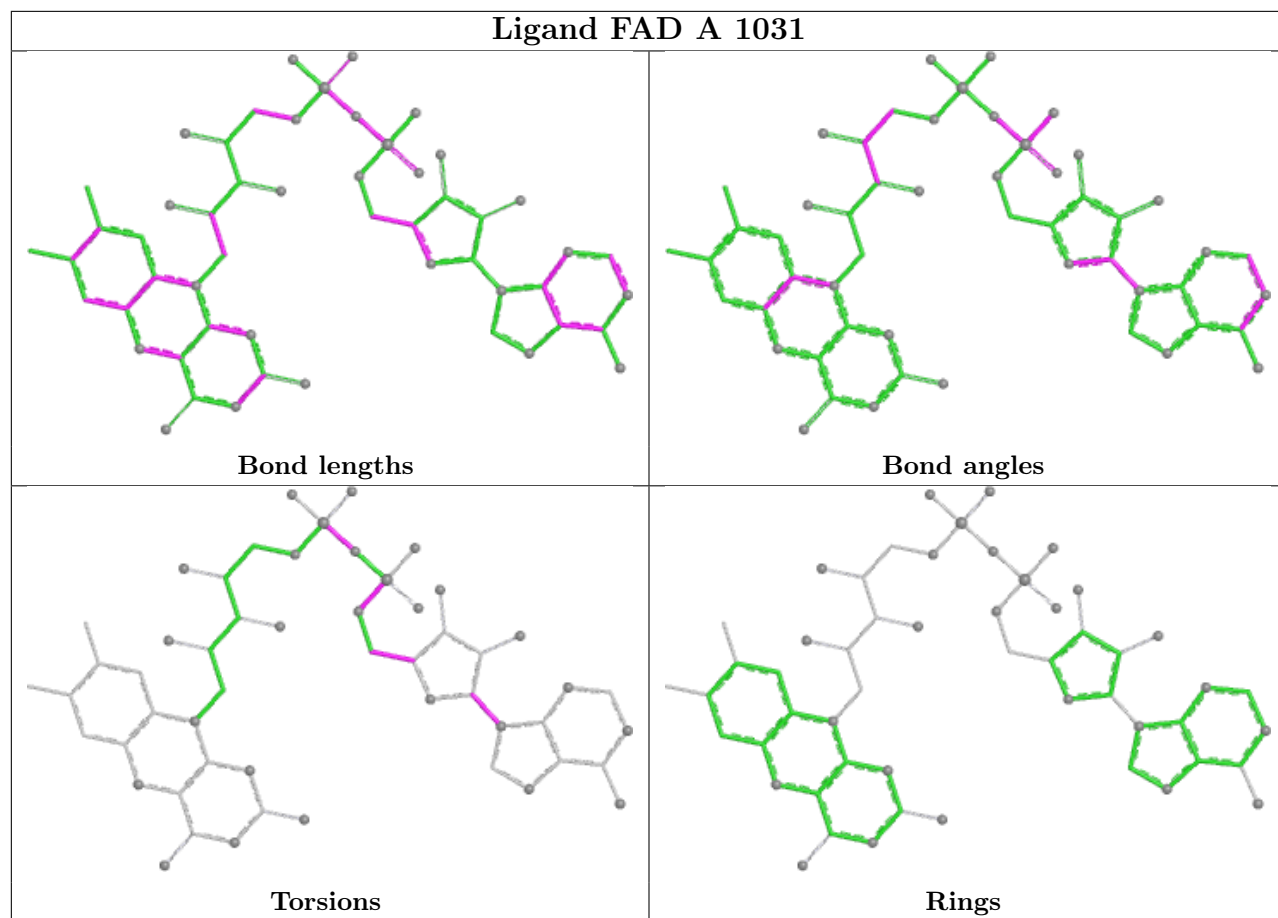




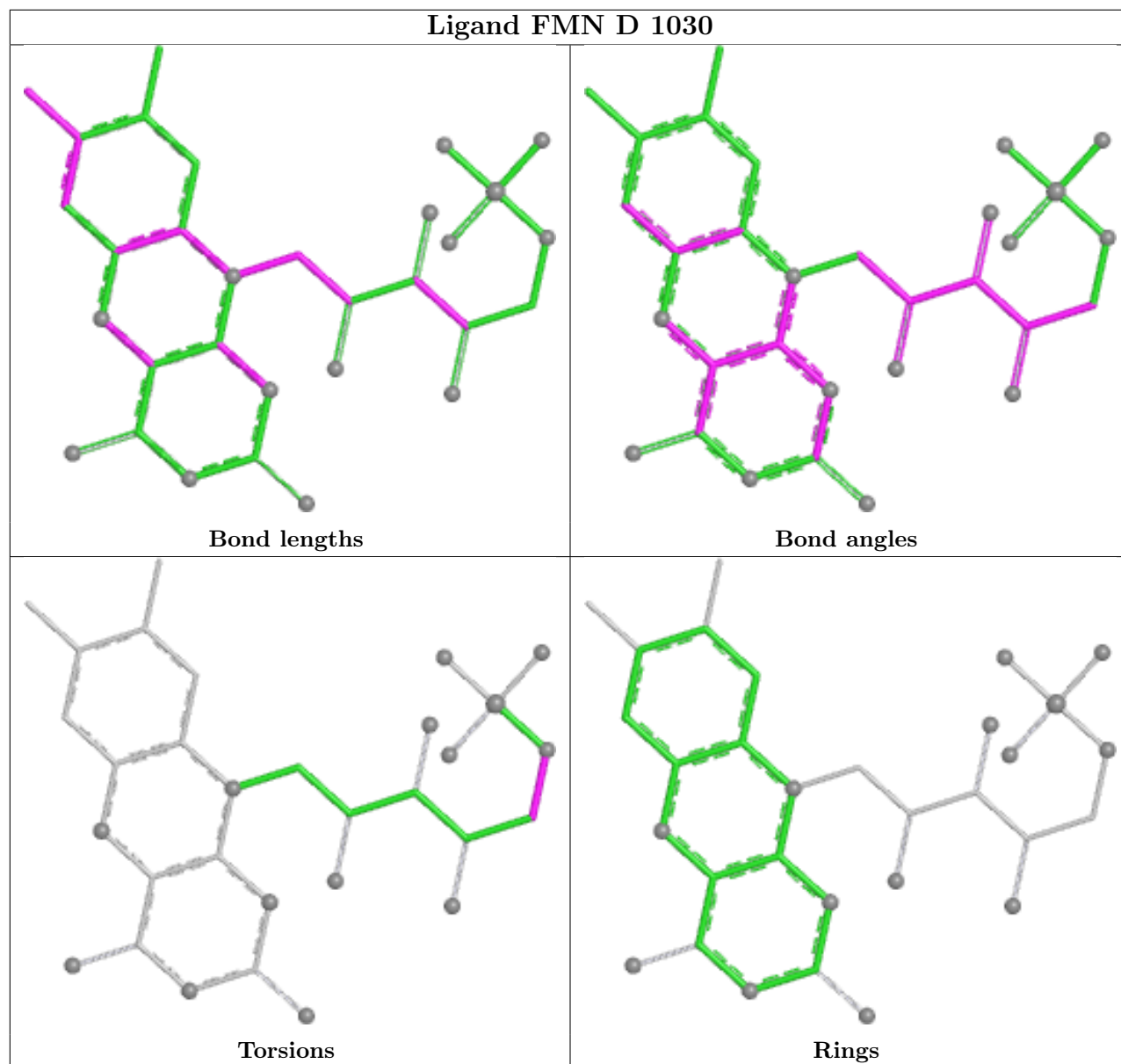


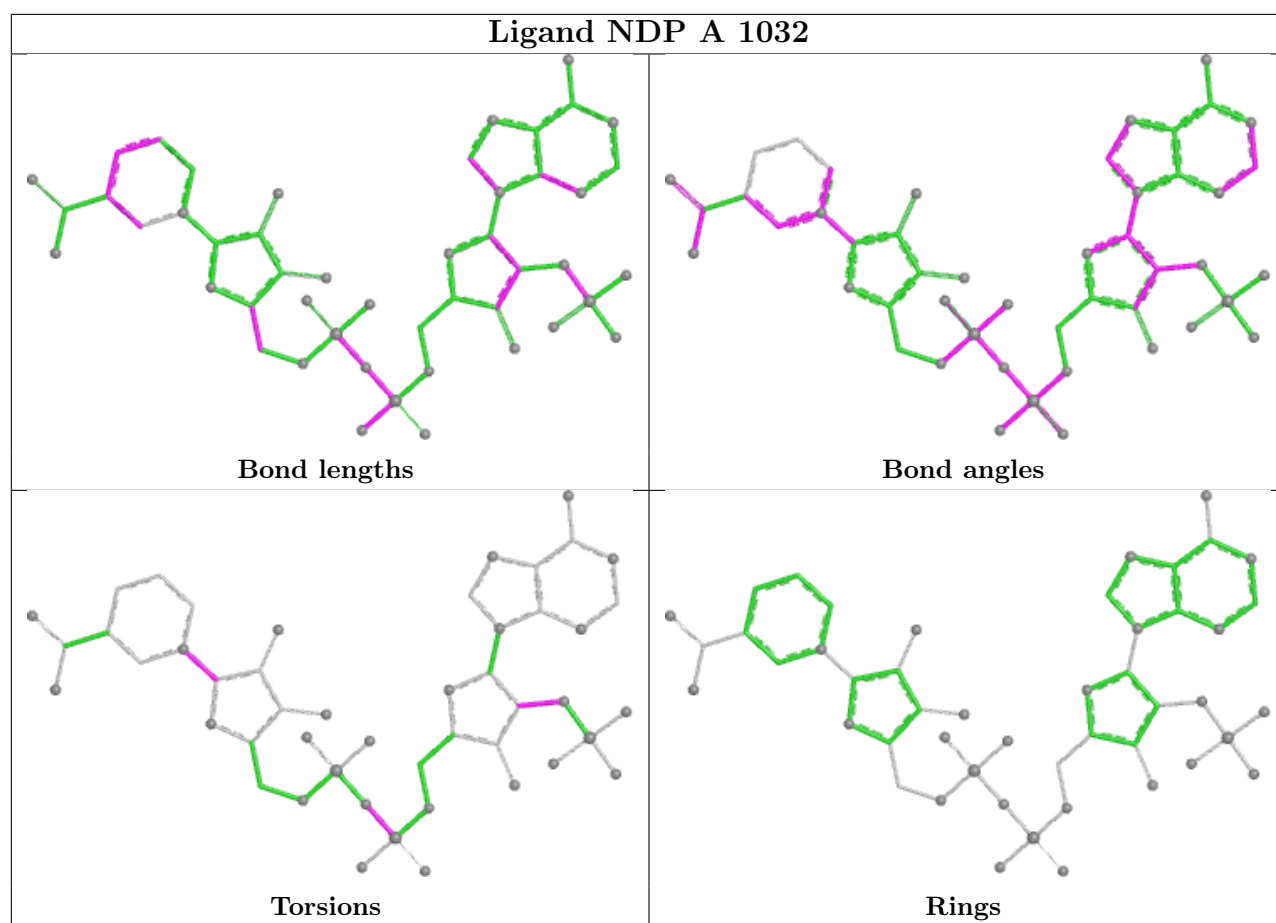






Ligand FMN D 1030





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1017/1025 (99%)	-0.64	0 100 100	7, 39, 93, 147	0
1	B	1010/1025 (98%)	-0.61	1 (0%) 92 90	7, 40, 96, 141	0
1	C	1010/1025 (98%)	-0.52	2 (0%) 91 86	14, 54, 106, 140	0
1	D	1012/1025 (98%)	-0.47	1 (0%) 92 90	14, 57, 107, 162	0
All	All	4049/4100 (98%)	-0.56	4 (0%) 92 90	7, 47, 102, 162	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	676	GLY	2.5
1	C	1014	LYS	2.4
1	C	657	ALA	2.4
1	D	17	ALA	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

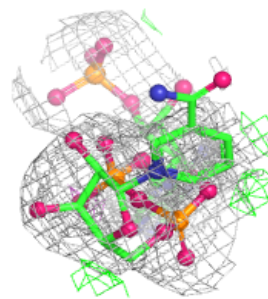
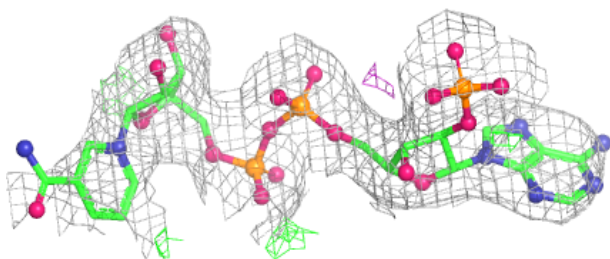
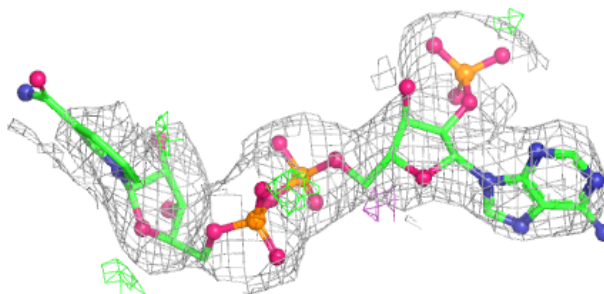
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	UAA	C	1035	12/12	0.70	0.11	138,140,144,144	0
6	UAA	D	1035	12/12	0.81	0.13	107,108,108,109	0
6	UAA	B	1035	12/12	0.85	0.16	146,147,148,148	0
6	UAA	A	1035	12/12	0.88	0.09	111,112,113,113	0
5	NDP	C	1032	48/48	0.92	0.09	53,57,86,88	0
5	NDP	D	1032	48/48	0.92	0.08	57,60,89,92	0
4	FAD	D	1031	53/53	0.92	0.07	40,46,60,60	0
3	FMN	D	1030	31/31	0.94	0.07	48,52,56,59	0
3	FMN	C	1030	31/31	0.94	0.07	45,48,52,55	0
5	NDP	B	1032	48/48	0.94	0.08	42,46,77,81	0
4	FAD	C	1031	53/53	0.95	0.07	29,36,49,50	0
3	FMN	A	1030	31/31	0.95	0.07	31,37,42,45	0
5	NDP	A	1032	48/48	0.95	0.07	42,47,76,78	0
4	FAD	A	1031	53/53	0.95	0.08	20,23,37,38	0
4	FAD	B	1031	53/53	0.95	0.07	19,25,35,37	0
3	FMN	B	1030	31/31	0.96	0.07	28,33,34,38	0
2	SF4	D	1029	8/8	0.98	0.06	39,40,41,42	0
2	SF4	A	1028	8/8	0.99	0.03	9,11,13,14	0
2	SF4	A	1029	8/8	0.99	0.05	18,21,23,24	0
2	SF4	B	1026	8/8	0.99	0.05	7,10,10,12	0
2	SF4	B	1027	8/8	0.99	0.05	4,4,4,4	0
2	SF4	B	1028	8/8	0.99	0.04	21,23,24,25	0
2	SF4	B	1029	8/8	0.99	0.03	13,15,16,18	0
2	SF4	C	1026	8/8	0.99	0.04	22,24,26,27	0
2	SF4	C	1027	8/8	0.99	0.04	25,26,27,28	0
2	SF4	C	1028	8/8	0.99	0.05	29,31,33,33	0
2	SF4	C	1029	8/8	0.99	0.07	34,35,37,37	0
2	SF4	D	1026	8/8	0.99	0.04	26,27,28,28	0
2	SF4	D	1027	8/8	0.99	0.05	28,30,32,32	0
2	SF4	D	1028	8/8	0.99	0.04	34,35,37,38	0
2	SF4	A	1026	8/8	0.99	0.05	18,21,24,24	0
2	SF4	A	1027	8/8	0.99	0.04	6,10,11,12	0

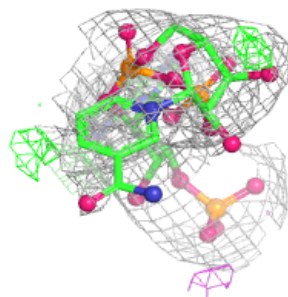
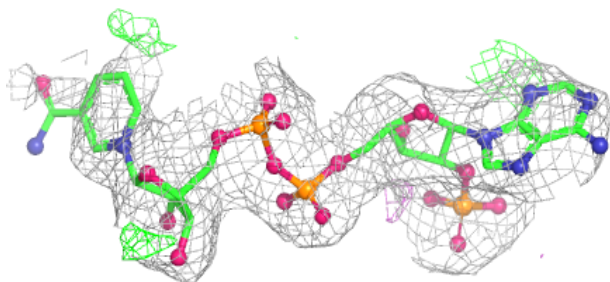
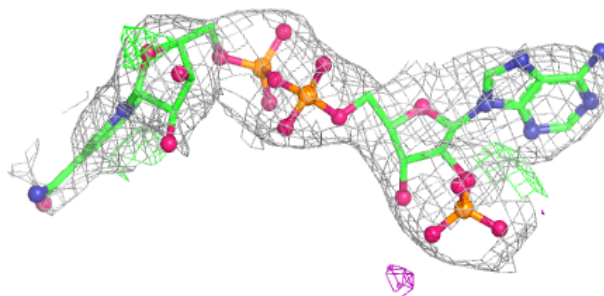
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP C 1032:

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

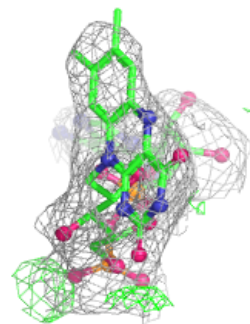
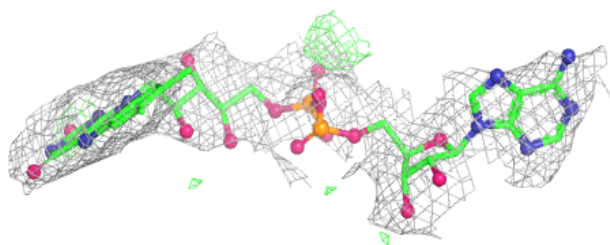
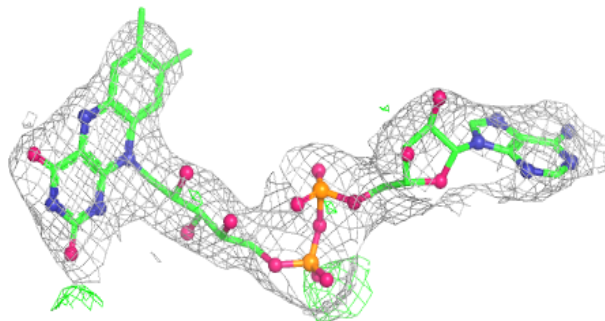
**Electron density around NDP D 1032:**

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



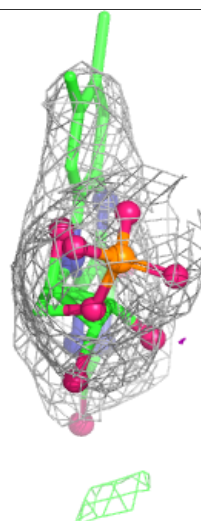
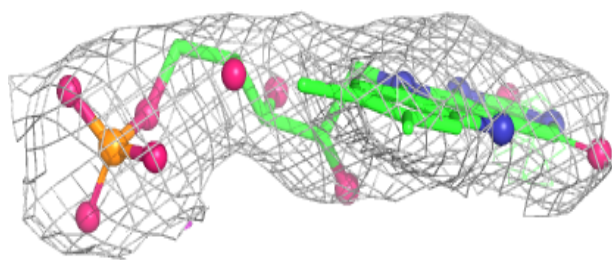
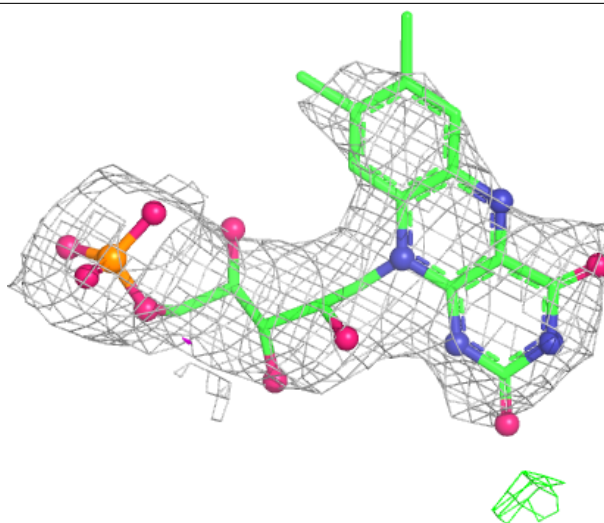
Electron density around FAD D 1031:

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



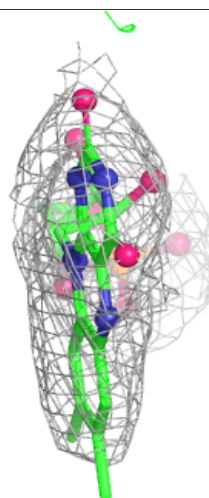
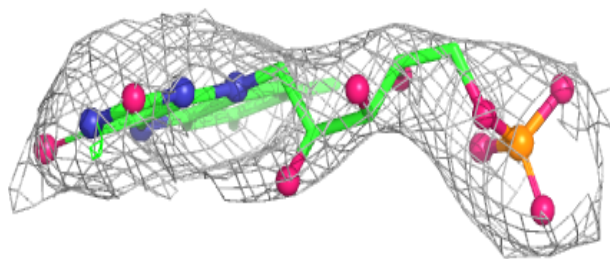
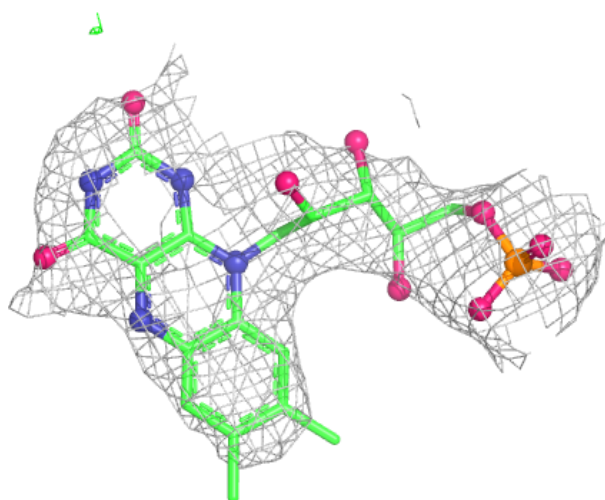
Electron density around FMN D 1030:

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and green (positive)



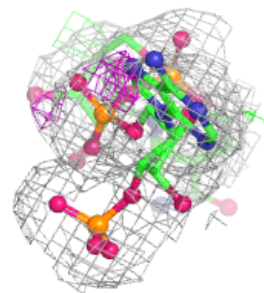
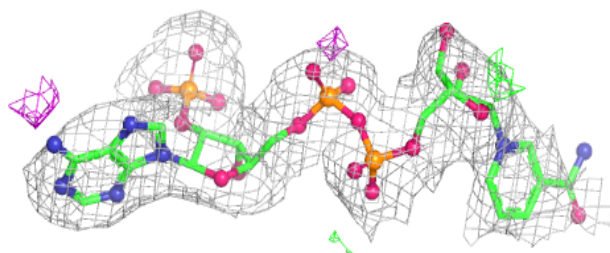
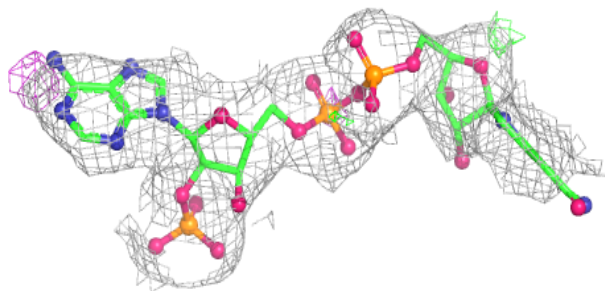
Electron density around FMN C 1030:

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and green (positive)

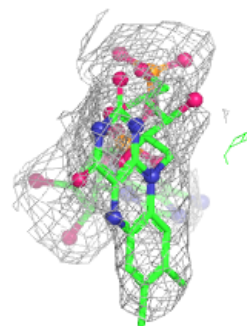
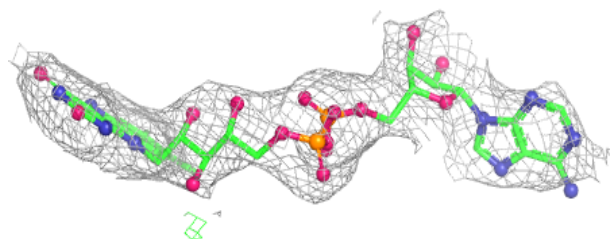
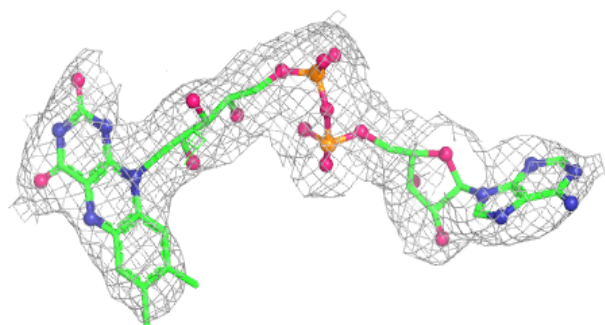


Electron density around NDP B 1032:

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and green (positive)

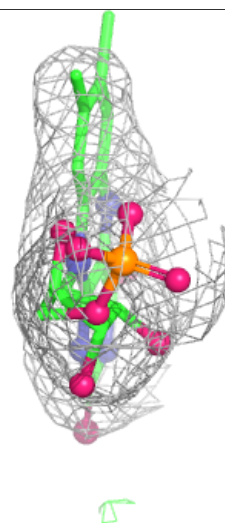
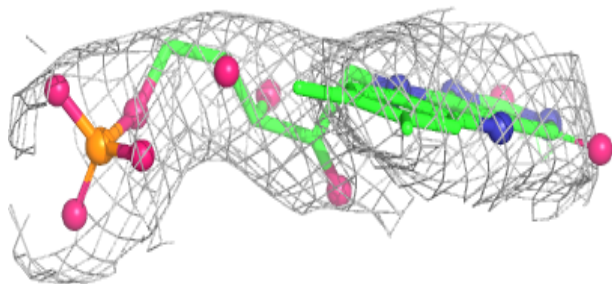
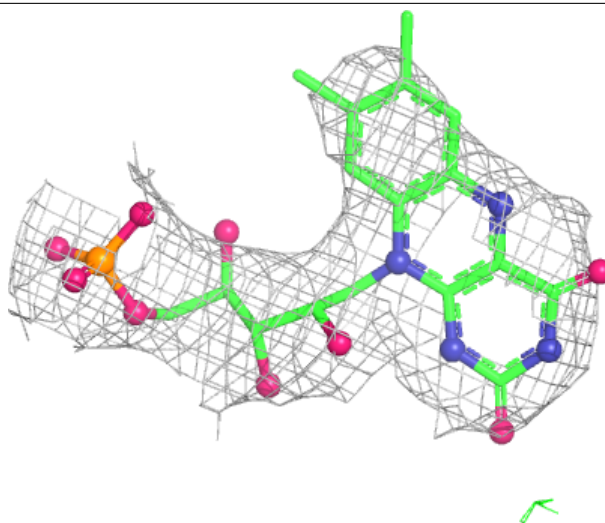
**Electron density around FAD C 1031:**

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and green (positive)



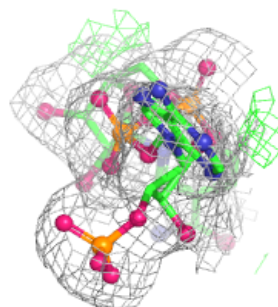
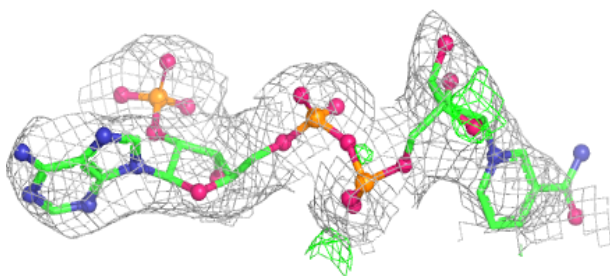
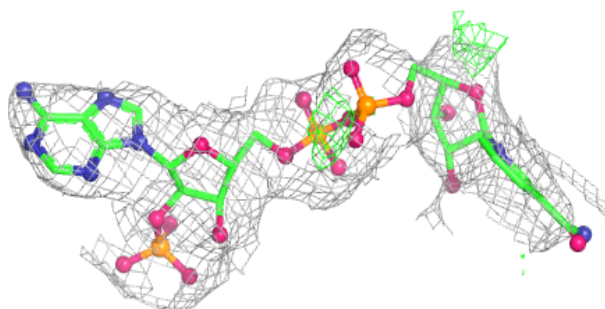
Electron density around FMN A 1030:

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

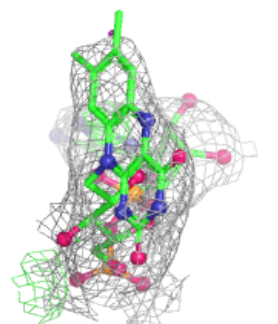
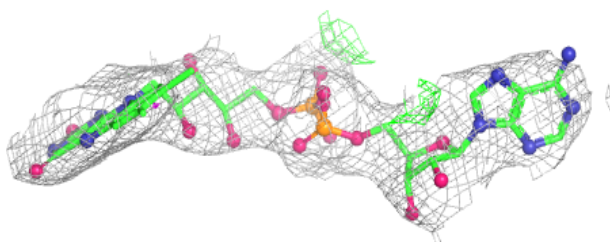
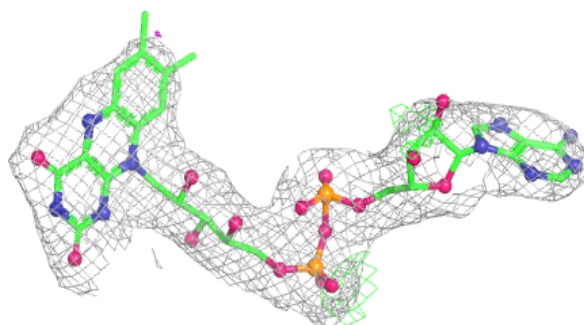


Electron density around NDP A 1032:

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

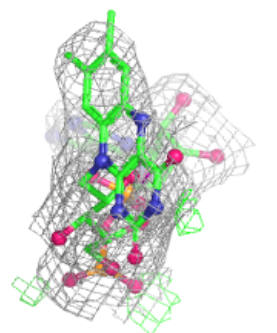
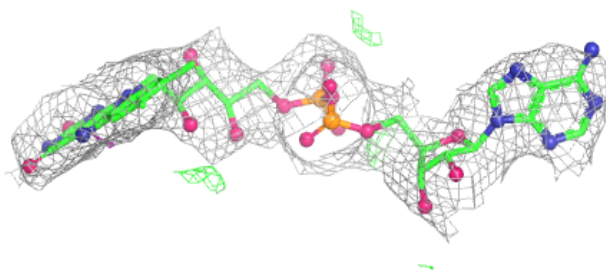
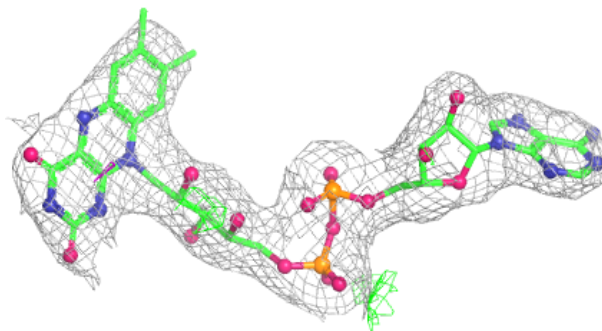
**Electron density around FAD A 1031:**

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



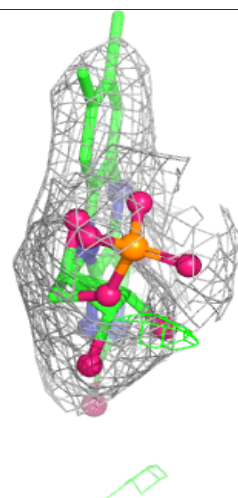
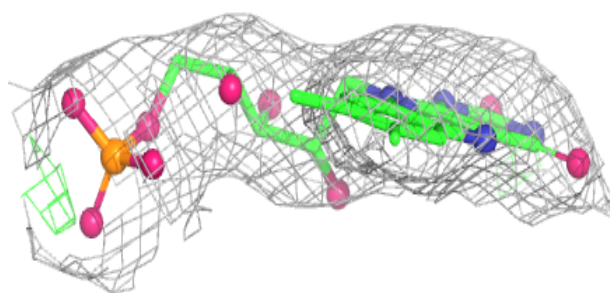
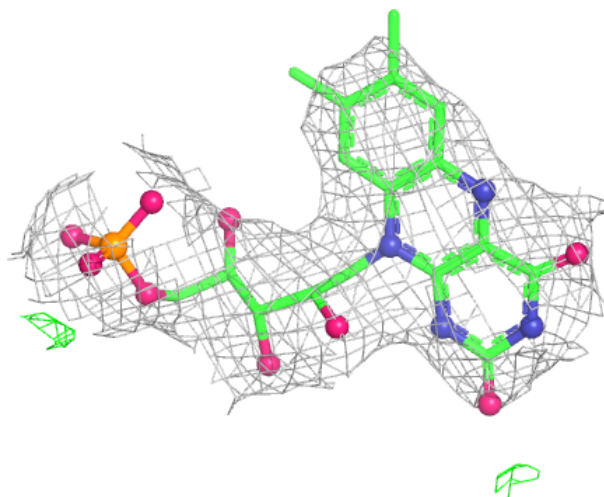
Electron density around FAD B 1031:

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



Electron density around FMN B 1030:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.